

N, N'- BIS(2-HYDROXYCYCLOHEXYL) ETHYLENEDIAMINE.

The ethylenediamine (1.0 g , 1.66×10^{-2} mol) was dissolved in 60 ml of anhydrous ethanol and to this was added cyclohexene oxide (6.5 g , 6.66×10^{-2} mol) . The solution was allowed to reflux for approximately 6 Hours with a CaCl_2 drying tube forming a precipitate in the reaction vessel. The precipitate was collected and allowed to air dry. The solution was refluxed for a further 24 Hours. Evaporation of the solvent resulted in a clear oil that solidified on drying. The solid residue was dissolved in 50 ml acetone and precipitated on evaporation to give a white solid.

Mw $\text{C}_{12}\text{H}_{22}\text{N}_2\text{O}_2 = 268.39 \text{ g mol}^{-1}$

Mass collected = 3.4 g

Yield = 80 %

ANALYSIS	EXPECTED	OBSERVED
% C	65.59	65.58
% H	11.01	11.23
% N	10.93	10.93

N, N'- Bis(2-HYDROXYCYCLOHEXYL) PROPYLENEDIAMINE.

Dissolved the propylene diamine (1.0 g , 1.35×10^{-2} mol) together with the cyclohexene oxide (5.3 g , 5.40×10^{-2} mol) in 60 ml of anhydrous ethanol and allowed to reflux at 80 ° C for 24 Hours with a CaCl_2 drying tube. A pale yellow oil remained after removal of the solvent which solidified when placed under reduced pressure to dry. The solid was dissolved in 35 ml of acetone and left to evaporate at room temperature to render a white solid product.

$$\text{M.v } \text{C}_{15} \text{H}_{30} \text{N}_2 \text{O}_2 = 270.41 \text{ g mol}^{-1}$$

Mass collected = 2.9 g

Yield = 79.5 %

ANALYSIS	EXPECTED	OBSERVED
% C	66.63	66.61
% H	11.18	11.71
% N	10.35	10.31

(2-HYDROXYCYCLOHEXYL)-12-ANE N₄

The macrocycle 12 ane N₄ (2.3 g, 8.51×10^{-3} mol) was dissolved in 100ml of anhydrous ethanol by stirring. To this was added cyclohexene oxide (1.1 g, 1.12×10^{-2} mol) and refluxed for 48 hours at 80 ° C with a CaCl₂ drying tube. On removing the solvent a pale yellow oil was obtained. This was placed under reduced pressure to dry and solidified in the process. Taking up this residue in acetone and cooling to 0 ° C in a refrigerator for 24 Hours afforded a white crystalline solid.

Mw C₁₄ H₃₀ N₄ O = 270.42 g mol⁻¹

Mass collected = 3.0 g

Yield = 83 %

ANALYSIS	EXPECTED	OBSERVED
% C	62.18	52.59
% H	11.18	11.91
% N	20.72	19.94

Cu(II)(2-HYDROXYCYCLOHEXYL)-12-ANE N₃ PERCHLORATE

Copper perchlorate (0.8 g , 2.16×10^{-3} mol) was added to 15 ml of deionised water. A 10 ml aqueous solution of KOH (0.3 g , 5.35×10^{-3} mol) was added dropwise with constant stirring in an ice-bath. The macrocycle (0.5 g , 1.85×10^{-3} mol) was dissolved in 10 ml of deionised water and added forming a purple precipitate with stirring. the solution was warmed gently to 60 ° C and the pH adjusted in a dropwise fashion with perchloric acid (12 M). the solution became clear and was allowed to cool down to room temperature. Solvent evaporated down to dryness and the solid residues were dissolved in acetone filtering off the excess KOH. An additional 0.8 g of the metal salt was added to aid crystallisation and this was dissolved in 25 ml of deionised water. Slow evaporation yielded crystals of the copper complex.



Mass collected = 0.71 g

Yield = 72 %

ANALYSIS	EXPECTED	OBSERVED
% C	31.56	31.25
% H	5.67	5.46
% N	10.51	10.04

**Ni(II)-N,N'-Bis(2-HYDROXYCYCLOHEXYL)-TRANS-1,2-DIAMINOCYCLOHEXANE
PERCHLORATE**

Dissolved the ligand (0.8 g , 2.58×10^{-3} mol) in 80 ml of absolute alcohol by refluxing until the solution became clear. Nickel perchlorate (1.0 g , 2.73×10^{-3} mol i.e 10 % excess) in 15 ml of absolute alcohol was added dropwise with stirring. A reddish solution was obtained initially but turned a pale blue on complete complex formation. Allowed to reflux for at 100 ° C (oil bath) for 15 minutes. Evaporation of the solvent resulted in the nickel complex that was taken up in water and recrystallised.

Mw $C_{12}H_{34}N_2O_{10}Cl_2Ni = 568.08 \text{ g mol}^{-1}$

Mass collected = 1.3 g

Yield = 89. %

ANALYSIS	EXPECTED	OBSERVED
% C	38.06	37.96
% H	6.03	5.91
% N	4.93	4.67

Cu(II) 1,7-Bis(2-HYDROXYCYCLOHEXYL) DIETHYLENE**TRIAMINE PERCHLORATE.**

Copper perchlorate (0.7 g, 1.89×10^{-3} mol) was dissolved in 15 ml of deionised water. An aqueous solution of KOH (0.2 g, 3.56×10^{-3} mol) was added with continuous stirring in an ice-bath for 35 minutes. The aqueous ligand (0.6 g, 2.00×10^{-3} mol) was then added at 70 ° C. metal complex and any hydroxide was forced back into solution by adjusting the pH with 1.5 ml of perchloric acid (12 M). The solution was cooled down and on slow evaporation purple crystals of the complex were obtained.

$$\text{Mw } C_{16} H_{33} N_3 O_{10} Cl_2 Cu = 561.90 \text{ g mol}^{-1}$$

$$\text{Mass collected} = 0.73 \text{ g}$$

$$\text{Yield} = 64.9 \%$$

ANALYSIS	EXPECTED	OBSERVED
% C	34.20	33.95
% H	5.92	5.75
% N	7.48	7.16

Cu(II) 1,4 BIS(2-HDROXYCYCLOHEXYL) PROPYLENEDIAMINE**PERCHLORATE.**

Copper perchlorate (0.5 g, 1.35×10^{-3} mol) was dissolved in 20 ml of deionised water. A 10 ml KOH aqueous solution (0.15 g, 2.70×10^{-3} mol) was added with continuous stirring in an ice-bath. The ligand (0.4 g, 1.48×10^{-3} mol) was dissolved in 10 ml of deionised water and added dropwise to the above solution. After gentle warming (i.e. 60-65° C) for 20 minutes the solution was allowed to cool down. Slow evaporation gave dark blue crystals of the complex.

$$\text{MW } C_{15} H_{30} N_2 O_{10} Cl_2 Cu = 532.86 \text{ g mol}^{-1}$$

Mass collected = 0.82 g

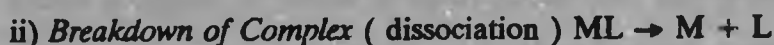
Yield = 57.7 %

ANALYSIS	EXPECTED	OBSERVED
% C	33.81	33.38
% H	5.67	5.71
% N	5.26	5.46

POTENTIOMETRY

POTENTIOMETRIC DETERMINATION OF STABILITY CONSTANTS

Stability constants can be determined considering two possible equilibria:



The choice of equilibrium to be studied is dependent on the kinetics of each. Studying complex formation is chosen when the kinetics of dissociation is very slow. ie. association kinetics is fast

Conversely when the dissociation kinetics is fast then stability constants are best determined by breaking the complex. In the first instance the formation constants are determined by titrating a metal and a protonated ligand in solution, with a base to form the complexing species (Lehn & Montavon 1978). The latter involves the titration of the metal complex in solution with acid, to break down the complex and demetallate the ligand.

The formation constants in this presentation, that were determined potentiometrically, were generally determined by forming the metal complex rather relying on a fast dissociation rate.

The nature of certain ligands, usually macrocycles and their derivatives, is such that neither the dissociation or association equilibria are sufficiently fast to allow for accurate determination of formation constants by conventional titration techniques. In such systems the metal complexes reach equilibrium

very slowly and stability constants based on conventional potentiometry will be inaccurate. Sufficient time is necessary to reach equilibrium (Clarke & Martell 1991). The "batch method" or "out-of-cell" titration (Zompa 1978) is an alternative for formation constant determination when faced with slow kinetics. Solutions of metal complexes are prepared in separate sealed containers each having equivalent amounts of metal ion and ligand, but differing amounts of titrant. The titration increments are arranged so as to fall within a region of partial complex formation. The potential or pH of the solutions are then determined until values become constant indicating that equilibrium has been reached. The time required to reach equilibrium may vary from days to weeks depending on the slow proton equilibrium between species.

INSTRUMENTATION

Potential (mv) data for solutions were recorded using a Radiometer PHM84 research pH meter equipped with a combined glass/reference electrode (Type GK 2402B or GK 2401C) or a Beckman 4341 pH meter equipped with a Beckman Refillable Combination electrode (Model no. 39536 (saturated KCL) or Model no. 39539 (4M KCL saturated with AgCl)).

Titration were carried out at constant temperature in a water -jacketed cell connected to a Haake G thermostated water circulating bath. The solutions were constantly stirred by a Kartell (2228 (MDO.TKO 220V 50 Hz)) stirrer and a 10 ml microburette was used to deliver the titrant.

The potentiometric data was analysed using the ESTA program (May et al

1985, Murray et al 1984), that analyses potentiometric data via a number of optimisation procedures, on a 486PC microcomputer.

STANDARDISATION AND CALIBRATION

The potentiometric cell was calibrated for the combination glass electrode before each titration. A solution consisting of 0.05M HNO₃ in 0.05M NaNO₃ (5ml) and 0.10M NaNO₃ (15ml) was titrated with 0.05M NaOH in 0.05M NaNO₃, to determine the standard electrode potential and the electrode calibration slope that has a value approximating the Nernstian slope ($2.3026 \times RT/F$). In practice the value for the slope is usually lower. The expression for the EMF of the cell at constant ionicity is expressed as (Rossotti & Rossotti 1961, 1961, 1978, May et al 1982) :

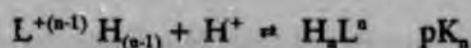
$$E_{cell} = E'_{cell} + E_j + k \log[H^+]$$

E_j - Σ liquid junction potentials (constant) May et al (1982)

E_j causes a deviation from linearity of the E_{cell} versus $\log[H^+]$ plot as one approaches the two extremes of the pH scale. The calibration constants E'_{cell} and k can be calculated from the linear E_{cell} versus $\log[H^+]$ plots using a least squares fit on the data. Points were taken in the regions $2.3 < \text{pH} < 3$ and $10.8 < \text{pH} < 11.8$, where $\text{pH} = -\log[H^+]$. These regions of pH have adequate concentration buffering and the cell EMF values obtained will be reliable. Calibrations were carried out at the beginning and end of each titration.

Potentiometric titrations were done at $25 \pm 0.1^\circ\text{C}$ in aqueous solution at ionic strength, $I = 0.1\text{M}$. Sodium nitrate was chosen to be the background electrolyte. Metal solutions were prepared from analytical reagent grade metal nitrate salts and standardised against EDTA (Vogel 1961). Standard solutions of HNO_3 (0.05M & 0.01M) and NaOH (0.05M & 0.01M) were prepared with the latter being standardised against Potassium Hydrogen Fththalate (0.01M). The acid solutions were standardised against the already standardised base solution while ligand solutions were standardised from their pK_a determination titrations.

METHOD OF DETERMINING THE STABILITY CONSTANTS



The protonation constants of the ligands were calculated by titrating a solution of the ligand ($5 \times 10^{-3}\text{M}$, 10ml) in 0.1M NaNO_3 (10ml) with base 0.01M NaOH in 0.09M NaNO_3 .

The stability constants for the metal ions were determined by titrating solutions containing a fixed amount of ligand ($5 \times 10^{-3}\text{M}$, 5ml), an equivalent amount of acid, so as to completely protonate the ligand, and different amounts of the metal ion (0.0333M) to be complexed. Varying the metal to ligand ratio checks the reliability of the analytical method and the reproducibility of the results. The metal-ligand ratios were varied between 1:1 and 1:2.5 and were largely done in triplicate. In certain cases a duplicate

analysis reproduced results extremely accurately and a triplicate analysis was then not carried out. An adequate volume (10 ml) of 0.1M NaNO_3 was added to the cell for each titration to attain the required starting volume.

Potentiometric data was analysed by submitting a model suggesting species that exist in solution. This model is then adjusted in terms of the standard deviations determined for each species, and the feasibility of the species considering the system being studied. There is an inherent danger of generating "computer designated species" that would almost certainly not be present in solution. It is therefore necessary to assess the validity of the model submitted.

For the macrocyclic ligand the kinetics of complexation are too slow for a direct determination of stability constants and the out-of-cell technique was used.

Stock solutions were prepared and used to prepare independent solutions with equivalent amounts of ligand and metal, and an appropriate amount of acid to fully protonate the ligand. To each solution was then added an increment of sodium hydroxide to generate solutions with different $\bar{n}$ values (different degrees of complex formation). The ionic strength was retained at 0.1M using sodium nitrate. Solutions were sealed with microfilm tape, to prevent any changes in volume, and immersed in a water bath thermostated at 25°C and allowed to stand for periods ranging from one to eight weeks. The solutions were examined potentiometrically at regular intervals until it became evident that a satisfactory equilibrium was reached.

SPECTROSCOPY

SPECTROSCOPIC STUDIES OF METAL COMPLEXES

The visible spectra of metal complexes are used to determine the stability constants for metal ions where the properties of ligands render potentiometric studies inaccurate or impossible. Complexes themselves are used as probes to determine the stability constants of other metal ions. Studies of other metal complexes are carried out by using a metal complex probe that permits metal to metal competition. Changes, such as a decrease in the intensity of a band in the spectrum, occurs as the metal in the complex is replaced by its competitor.

INSTRUMENTATION

The spectra were recorded using a Cary 2300 UV/VIS spectrophotometer which was thermostated at 25°C by a circulatory Haake G water bath. Quartz cuvettes (1.000 ± 0.001 cm) were used that were cleaned carefully with acetone and dried. Solutions of the metal complexes were prepared by having approximately equimolar ratios of metal and ligand (1:1:1) in 0.1M sodium perchlorate. It was necessary to have the ligand in a very slight excess to ensure that all of the metal was complexed. Where the complex was successfully crystallised, the crystalline compound was used. The baseline correction was recorded with 0.1M NaClO₄ as the background electrolyte and the complexes were obtained by scanning the wavelength limits from 850nm to 350nm at a scan rate of 1.0 nm s⁻¹.

X-RAY ANALYSIS OF CRYSTALS

CRYSTAL PREPARATION

Complexes were synthesized by reacting free ligand with the metal salt at high pH in aqueous solution. To optimise conditions for the desired species the pH was adjusted by adding perchloric acid. Alternatively the complexes were synthesized by refluxing equivalent amounts of metal and ligand in methanol. The calculated densities were verified by floatation in mixtures of 1,2-dibromoethane and chloroform.

Suitable crystals for X-ray diffraction (Stout & Jensen 1968) were selected after examination under a polarising microscope. The criterion for judging a crystal to be suitable was the periodic extinction of light on rotation in any direction. Single crystals are necessary, and the problems of twinning and adhering microcrystallites cannot be present to obtain an accurate data set. Crystal quality was verified by, the oscillation, zero and first layer Weissenberg photographs taken using Cu-K α radiation and a Huber Weissenberg camera. Cell constants and the space group can be concluded from systematic examination of the photographs.

The crystal may begin drying out and subsequently decompose. Sealing the crystal from the atmosphere in a Linderman tube or enveloping the crystal in an alternative medium (coating crystal with medicinal parafilm) is a solution. A data collection may also be carried out keeping the crystal surrounded by a thin film of the mother liquor.

DATA COLLECTION AND REDUCTION

Intensity data was collected on an Enraf-Nonius CAD-4 diffractometer (were indicated) at room temperature using an incident beam graphite monochromated Mo-K α radiation. Cell dimensions were calculated from a full-matrix least squares refinement of 25 reflections. Intensity data was corrected for Lorentz polarisation and absorption.

SOLUTION AND REFINEMENT OF STRUCTURE

Structures of metal complexes were solved by Patterson methods using the SHELXS86 program (Sheldrick 1985). This primarily places the heavy atoms in the structure which must be then refined by full-matrix least squares using the SHELX76 program (Sheldrick 1978). Structures obtained in the USA (Texas A & M university) with Prof. Riebenspiess used SHELX93.

Successive difference Fourier maps locates all the non-hydrogen atoms of the cation and anion which are refined anisotropically to accommodate all of their electron density. The positions of hydrogen atoms are then geometrically calculated with ideal bond lengths of 1.08Å .

The perchlorate counter ions were refined with anisotropic thermal parameters; but when disorder was encountered, each component of the disorder was refined as a rigid body. The rigid bodies were defined by Cl-O and O-O distances of 1.44Å and 2.35Å respectively. In the event of disorder manifesting itself in the cation, the data can be collected at a lower temperature to "freeze" out the structure. This has the effect of reducing the

disorder of the cation and the anion simultaneously.

The atomic scattering factors for the heavy metal atoms were obtained from the International tables of Crystallography (Ibers & Hamilton 1974).

REFERENCES

- ADAMSON, A. W., 1954, *J. Am. Chem. Soc.*, 76, 1578
- ALCOCK, N. W., BALAKRISHNAN, K. P., MOORE, P., 1986, *J. Chem. Soc., Dalton Trans.*, 1743
- ALCOCK, N. W., OMAR, H. A., MOORE, P., PIERPOINT, C., 1985, *J. Chem. Soc., Dalton Trans.*, 219
- ALFHEIM, T., BUØEN, S., DALE, J., KRAUTWURST, K. D., 1986, *Acta. Chem. Scand.*, B 40, 40
- ANDEREGG, G., 1975, *Helv. Chim. Acta*, 58, 1218
- ANICHINI, A., FABBRIZZI, I., PAOLETTI, P., 1977, *Inorg. Chim. Acta.*, 22, L25
- ANICHINI, A., FABBRIZZI, L., PAOLETTI, P., CLAY, R. M., 1978, *J. Chem. Soc., Dalton Trans.*, 577
- ANNIE-BLIGH, S. W., CHOI, N., EVAGOROU, E. G., MCPARTLIN, M., CUMMINS, W. J., KELLY, J. D., 1992, *Polyhedron*, v11, 19, 2571
- ARNAUD-NEU, F., SCHWING-WEILL, M. J., JUILLARD, J., LOUIS, R., WEISS, R., 1978, *Inorg. Nucl. Chem. Lett.*, 14, 367
- ARNAUD-NEU, F., SANCHEZ, M., SCHWING-WEILL, M., LEHN, J. M., 1985, *Helv. Chim. Acta*, 68, 456
- ASATO, E., TOFTLUND, H., KIDA, S., MIKURIYA, N., MURRAY, K. S., 1989,

Inorg. Chim. Acta., 165, 207

BERTRAND, J. A., ELLER, P. G., 1975, *Prog. Inorg. Chem.*, 21, 29

BHAVAN, R., HANCOCK, R. D., WADE, P. W., BOEYENS, J. C. A., DOBSON, S. M., 1990, *Inorg. Chim. Acta*, 171, 235

BIGOLI, F., BRAIBAUTI, S., TIRIPICCHIO, A., TIRIPICCHIO-CAMELLINI, M., 1971, *Acta Crystallogr., Sect. B*, 27, 1427

BJERRUM, J., "Metal amine formation in Aqueous solution," P. Haase & Son, 1941 Copenhagen

BRECHBIEL, M. W., GANSOW, O. A., ATCHER, R. W., SCHOLM, J., ESTERAN, J., SIMPSON, L. E., COLCHER, D., 1986, *Inorg. Chem.*, 25, 2772

BRECHBIEL, M. W., GANSOW, O. A., 1992, *J. Chem. Soc. Perkin Trans.*, 1, 1173

BRAUMAN, J. I., BLAIR, L. K., 1968, *J. Am. Chem. Soc.*, 90, 6561

BRAUMAN, J. I., BLAIR, L. K., 1969, *J. Am. Chem. Soc.*, 91, 2126

BRAUMAN, J. I., RIVEROS, J. M., BLAIR, L. K., *J. Am. Chem. Soc.*, 93, 3914

BULLMAN, R. A., 1987, *Struct. Bonding*, 67, 91

BUØEN, S., DALE, J., GROTH, P., KRAUS, J., 1982, *J. Chem. Soc., Chem. Commun.*, 1172

BUSCH, D. H., 1978, *Acc. Chem. Res.*, 11, 393

BUSCH, D. H., CAIRNS, C. J., 1978, *Prog. Macrocyclic Chem.*, 3, 1

BUSCH, D. H., 1990, *Coord. Chem. Rev.*, 100, 119

BUSCH, D. H., 1993, *Chem. Rev.*, 93, 847

BUSCHMANN, H. J., 1985, *Inorg. Chim. Acta*, 102, 95

CABBINESS, D. K., MARGERUM, D. W., 1969, *J. Am. Chem. Soc.*, 91, 6540

CARLSON, G. A., MCREYNOLDS, J. P., VERHOEK, F. H., 1945, *J. Am. Chem. Soc.*, 67, 1334

CHEN, L. H., CHUNG, C. S., 1988, *Inorg. Chem.*, 27, 1880

CHRISTENSEN, J. J., EATOUGH, D. J., IZATT, R. M., 1974, *Chem. Rev.*, 74, 351

CLARKE, E. T., MARTELL, A. E., 1991, *Inorg. Chim. Acta*, 190, 37

COMBA, P., CURTIS, N. F., LAWRENCE, G. A., SARGESSON, A. M., SKELTON, B. W., WHITE, A. H., 1986, *Inorg. Chem.*, 25, 4260

COTTON, F. A., WILKINSON, G., 1980, "Advanced Inorganic Chemistry. A Comprehensive Text." 4TH ed. John Wiley & Sons

COX, J. P. L., MORPHY, J. R., JANKOWSKI, K. J., PARKER, D., 1989, *Pure Appl. Chem.*, 61, 1637

CLARK, H., CRAMER, R. D., VANOPDENBOSCH, N., 1989, *J. Comp. Chem.*, 10, 982

CRAM, D. J., 1983, *Science*, 219, 1177

CRAM, D. J., KANEHISA, T., HELGESON, R. C., BROWN, S. B., KNOBLER, C. B., MAVERICK, F., TRUEBLOOD, K. N., 1985, *J. Am. Chem. Soc.*, 107, 3645

DAMU, K., HANCOCK, R. D., WADE, P. W., BOEYENS, J. C. A., BILLING, D. G., DOBSON, S. M., 1991, *J. Chem. Soc., Dalton Trans.*, 293

DAMU, K., MAUMELA, H., HANCOCK, R. D., BOEYENS, J. C. A., DOBSON, S. M., 1991, *J. Chem. Soc., Dalton Trans.*, 2717

DAVIDSON, W. R., KEBARLE, P., 1976, *J. Am. Chem. Soc.*, 98, 6132

DEI, A., GORI, R., 1975, *J. Chem. Soc., Chem. Commun.*, 19, 807

DE SOUSA HEALY, M., REST, A. J., 1978, *Inorg. Chem. Radiochem.*, 21, 1

DE SOUSA, A. S., CROFT, G. J. B., WAGNER, C. A., MICHAEL, J. P., HANCOCK, R. D., 1991, *Inorg. Chem.*, 30, 3525

DE SOUSA, A. S., HANCOCK, R. D., 1994, *J. Chem. Soc., Chem. Commun.*, in the press

DESHPANDE, S. V., DE NARDO, S. J., MEARES, C. F., MCCALL, M. J., ADAMS, G. P., MOI, M. K., DE NARDO, G. L., 1988, *J. Nucl. Med.*, 29, 217

DEUTSCH, E., LIBSON, K., JURISSON, S., LINDOY, L. F., 1983, *Prog. Inorg. Chem.*, 30, 75

DIETRICH, B., LEHN, J. M., SAUVAGE, J. P., 1973, *Tetrahedron*, 29, 1629

FABBRIZZI, L., PAOLETTI, P., LEVER, A. B. P., 1976, *Inorg. Chem.*, 17, 1042

FRAUSTO DA SILVA, J. J. R., 1983, *J. Chem. Educ.*, 60, 390

GANDOUR, R. D., FRONCZEK, F. R., GATTO, V. J., MINGANTI, C., SCHULTZ, R. A., WHITE, B. D., ARNOLD, K. A., MAZZOTTI, A. D., MILLER, S. R., GOKEL, G. W., 1986, *J. Am. Chem. Soc.*, 108, 4078

GANS, P., VACCA, A., SABATINI, A., 1976, *Inorg. Chim. Acta*, 18, 273

GATTO, V. J., GOKEL, G. W., 1984, *J. Org. Chem.*, 106, 8240

GOKEL, G. W., WHITE, B. D., MALLIN, J., ARNOLD, K. A., FRONCZEK, F. R., GANDOUR, R. D., GEHRIG, L. M. B., 1989, *J. Org. Chem.*, 54, 937

GOKEL, G. W., DISHONG, D. M., DIAMOND, C. J., 1980, *J. Chem. Soc., Chem. Commun.*, 1053

GOKEL, G. W., KORZENIOWSKI, S. H., 1982, "Macrocyclic Polyether Synthesis", Eds; HAFNER, K., REES, W. C., TOST, B. M., LEIN, J. M., SCHLEYER, PVR., ZAHNRADNIK, R., Springer-Verlag, New York, p12

GREEN, B. R., HANCOCK, R. D., 1982, *J. S. Afr. Inst. Min. Metall.*, 82, 303

HALL, J. L., DEAN, W. E., 1960, *J. Am. Chem. Soc.*, 82, 3300

HALL, J. L., DEAN, W. E., PACOFKY, E. A., 1960, *J. Am. Chem. Soc.*, 82, 3303

HANCOCK, R. D., 1980, *J. Chem. Soc., Dalton Trans.*, 416

HANCOCK, R. D., 1986, *Pure Appl. Chem.*, 58, 1445

HANCOCK, R. D., 1989, *Prog. Inorg. Chem.*, 37, 187

HANCOCK, R. D., 1990, *Acc. Chem. Res.*, 23, 253

HANCOCK, R. D., 1992, *J. Chem. Edu.*, 69, 615

HANCOCK, R. D., 1993, *Pure & Appl. Chem.*, 65, 5, 941

HANCOCK, R. D., 1995, to be published

HANCOCK, R. D., BHAVAN, R., SHAIKJEE, M. S., WADE, P. W., KEARN, A., 1986, *Inorg. Chim. Acta.*, 112, L23

HANCOCK, R. D., BHAVAN, R., WADE, P. W., BOEYENS, J. C. A., DOBSON, S. M., 1989, *Inorg. Chem.*, 28, 187

HANCOCK, R. D., BHAVAN, R., WADE, P. W., BOEYENS, J. C. A., DOBSON, S. M., 1989, *Inorg. Chem.*, 28, 2788

HANCOCK, R. D., DE SOUSA, A. S., 1995, *J. Chem. Soc., Chem. Commun.*, in the Press

HANCOCK, R. D., DOBSON, S. M., EVERS, A., WADE, P. W., NGWENYA, M. P., BOEYENS, J. C. A., WAINWRIGHT, K. P., 1988, *J. Am. Chem. Soc.*, 110, 2788

HANCOCK, R. D., EVERS, A., NGWENYA, M. P., WADE, P. W., 1987, *J. Chem. Soc., Chem. Commun.*, 1129

- HANCOCK, R. D., MARTELL, A. E., 1988, *Comments Inorg. Chem.*, 6, 237
- HANCOCK, R. D., MARTELL, A. E., 1989, *Chem. Rev.*, 89, 1875
- HANCOCK, R. D., MARTELL, A. E., 1995, *Adv. Inorg. Chem.*, in the press
- HANCOCK, R. D., MARSICANO, F., 1976, *J. Chem. Soc., Dalton Trans.*, 1096
- HANCOCK, R. D., MCDOUGALL, G. J., 1980, *J. Am. Chem. Soc.*, 102, 6551
- HANCOCK, R. D., MCDOUGALL, G. J., MARSICANO, F., 1979, *Inorg. Chem.*, 18, 2847
- HANCOCK, R. D., NAKANI, B. S., 1984, *J. Coord. Chem.*, 13, 299
- HANCOCK, R. D., NAKANI, B. S., MARSICANO, F., 1983, *Inorg. Chem.*, 22, 2531
- HANCOCK, R. D., SHAIKJEE, M. S., DOBSON, S. M., BOEYENS, J. C. A., 1988^b, *Inorg. Chim. Acta*, 154, 229
- HANCOCK, R. D., WADE, P. W., 1987, *Inorg. Chim. Acta.*, 130, 251
- HANCOCK, R. D., WADE, P. W., NGWENYA, M. P., DE SOUSA, A. S., DAMU, K. V., 1990, *Inorg. Chem.*, 29, 1968
- HARRISON, A., WALKER, C. A., PEREIRA, K. A., PARKER, D., ROYLE, L., PULUKKODY, K., NORMAN, T. J., 1993, *Magnetic Resonance Imaging*, 11, 761
- HAY, R. W., PUJARI, M. P., THOMAS-MOODIE, W., CRAIG, S., RICHENS, D. T., FEROTI, A., UNGARETTI, L., 1987, *J. Chem. Soc. Dalton Trans.* 2605

HAY, R. W., PUJARI, M. P., KORYBUT-DASZKIEWICZ, B., FERGUSON, G., RUHL, B. L., 1980, *J. Chem. Soc. Dalton Trans.*, 85

HENDERSON, W. A., SPERATI, C. A., 1960, *J. Am. Chem. Soc.*, 82, 5791

HEDINGER, M., KADEN, T. A., 1983, *Helv. Chim. Acta.*, 66, 861

HERTLI, L., KADEN, T. A., 1975, *Chimia*, 29, 304

HINZ, F. P., MARGERUM, D. W., 1974, *Inorg. Chem.*, 13, 2941

HINZ, F. P., MARGERUM, D. W., 1974, *J. Am. Chem. Soc.*, 96, 4993

IBERS, J. A., HAMILTON, W. C., 1974, "International tables for X-ray Crystallography", Vol. IV, Kynoch Press, Birmingham, England.

JONES, F. M., ARNETT, E. M., 1974, *Prog. Phys. Org. Chem.*, 11, 263

JONES, R. W., STALEY, R. H., 1976, *J. Am. Chem. Soc.*, 98, 3998

JONES, T. E., ZIMMER, L. L., DIADDARIO, L. L., RORABACHER, D. B., 1975, *J. Am. Chem. Soc.*, 97, 7163

JURISSON, S., BERNING, D., JIA, W., MA, D., 1993, *Chem. Rev.*, 93, 1137

KADEN, T. A., 1984, *Topics Curr. Chem.*, 121, 157

KAPPES, H. M., STALEY, R. H., 1982, *J. Am. Chem. Soc.*, 104, 1813

KAPPES, H. M., STALEY, R. H., 1982, *J. Am. Chem. Soc.*, 104, 1819

- KAUFFMAN, E., LEHN, J. M., SAUVAGE, J. P., 1976, *Helv. Chim. Acta*, 59, 1099
- KIMURA, E., YAMAOKA, M., MORIOKA, M., KOIKE, T., 1986, *Inorg. Chem.*, 25, 3883
- KIMURA, E., UENISHI, K., KOIKE, T., IITAKA, Y., 1986, *Chem. Lett.*, 1137
- KODAMA, M., KIMURA, E., 1975, *J. Chem. Soc., Chem. Commun.*, 9, 326
- KODAMA, M., KIMURA, E., 1975, *J. Chem. Soc., Chem. Commun.*, 21, 891
- KODAMA, M., KIMURA, E., 1976, *Bull. Chem. Soc. Jpn.*, 49, 2465
- KODAMA, M., KIMURA, E., 1976, *J. Chem. Soc., Dalton Trans.*, 116
- KOGAMA, H., YOSHINO, H., 1972, *Bull. Chem. Soc. Jpn.*, 45, 481
- KULSTAD, S., MALMSTEN, L. A., 1980, *J. Inorg. Nucl. Chem.*, 42, 573
- LAUFFER, R. B., 1987, *Chem. Rev.*, 87, 901
- LEHN, J. M., 1973, *Struct. Bond.*, 16, 1
- LEHN, J. M., SAUVAGE, J. P., 1975, *J. Am. Chem. Soc.*, 97, 6700
- LEHN, J. M., 1978, *Acc. Chem. Res.*, 11, 49
- LEHN, J. M., MONTAVON, 1978, *Helv. Chim. Acta.*, 61, 67
- LEHN, J. M., 1988, *J. Inclusion Phenom.*, 6, 397
- LINDOY, I. F., 1975, *Chem. Soc. Rev.*, 4, 421

LINDOY, L. F., ADAM, K. R., LEONG, A. J., LIP, H. C., SKELTON, B. W., WHITE, A. H., 1982, *J. Am. Chem. Soc.*, 105, 4645

LINDOY, L. F., ADAM, K. R., BRIGDEN, L. G., HENRICK, K., MCPARTLIN, M., MIMAGH, B., TASKER, P., 1985, *J. Chem. Soc., Chem. Commun.*, 710

LINDOY, L. F., ANDEREGG, G., EKSTROM, A., SMITH, R. J., 1980, *J. Am. Chem. Soc.*, 102, 2670

LINDOY, L. F., BUSCH, D. H., 1971, *Prep. Inorg. React.*, 6, 1

LOTZ, T. J., KADEN, T. A., 1977, *J. Chem. Soc., Chem. Commun.*, 15

LOTZ, T. J., KADEN, T. A., 1978, *Helv. Chim. Acta.*, 61, 1376

MARTELL, A. E., 1956, *Recl. Trav. Chim.*, 75, 6

MARTELL, A. E., 1964, *Essays in Coordination Chemistry*, eds. SCHNEIDER, W., ANDEREGG, G., GUT, R., (Berkhauser Verlag, Basel), 52

MARTELL, A. E., 1966, *Adv. Chem. Ser.*, 62, 272

MARTELL, A. E., SMITH, R. M., 1974-1989, *Critical Stability Constants*, Plenum, New York, Vols. 1-6

MARTELL, A. E., MOTEKAITIS, R. J., 1990, *The Environmental Chemistry and Toxicology of Aluminium*; Lewis, T. E., ed.; Lewis Publishers: Chelsea, MI

MARTELL, A. E., HANCOCK, R. D., MOTEKAITIS, R. J., 1994, *Coord. Chem. Rev.*, 133, 39

MARTIN, L. Y., DE HAYES, L. J., ZOMPA, L. J., BUSCH, D. H., 1974, *J. Am. Chem. Soc.*, 96, 4047

MAY, P. M., BULLMAN, R. A., 1983, *Prog. Med. Chem.*, 20, 226

MAY, P. M., MURRAY, K., WILLIAMS, D. R., 1985, *Talanta*, 32, 483

MAY, P. M., WILLIAMS, D. R., LINDER, P. W., TORRINGTON, R. G., 1982, *Talanta*, 29, 249

MCDUGALL, G. J., HANCOCK, R. D., BOEYENS, J. C. A., 1978, *J. Chem. Soc., Dalton Trans.*, 1438

MCDUGALL, G. J., HANCOCK, R. D., 1980, *J. Chem. Soc., Dalton Trans.*, 654

MEARS, C. F., WENSEL, T. G., 1984, *Acc. Chem. Res.*, 17, 202

MINACHEVA, L. K., ANTYSYSHKINA, A. S., PORAI-KOSHITS, M. A., 1974, *Zh. Struct. Khim.*, 15, 478

MORPHY, J. R., PARKER, D., ALEXANDER, R., BAINS, A., EATON, M. A. W., HARRISON, A., MILLICAN, A., TITMAS, R., WEATHERBY, D., 1988, *J. Chem. Soc., Chem. Commun.*, 156

MUNRO, D., 1977, *Chem. Br.*, 13, 100

MUNSON, M. S. B., 1965, *J. Am. Chem. Soc.*, 87, 2332

MURRAY, K., MAY, P. M., 1984, *ESTA User's Manual*, (UWIST, Cardiff)

MYERS, T. A., 1978, *Inorg. Chem.*, 17, 952

ORAMA, M., SAARINEN, H., KAILA, I., 1979, *Finn. Chem. Lett.*, 182

ORAMA, O., ORAMA, M., 1979, *Finn. Chem. Lett.*, 136

PALLAVICINI, P. S., PEROTTI, A., PCGGI, A., SEGHI, B., FABBRIZZI, L., 1987 *J. Am. Chem. Soc.*, 109, 5139

PAOLETTI, P., FABBRIZZI, L., BARBUCCI, R., 1973, *Inorg. Chem.*, 12, 1961

PARKER, D., PULUKKODY, K. P., NORMAN, T. J., ROYLE, L., BROAN, C. J., 1993, *J. Chem. Soc., Perkin Trans. II*, 605

PARKER, D., 1990, *Chem. Soc. Rev.*, 19, 271

PARKER, D., 1983, *Adv. Inorg. Chem. Radiochim.*, 26, 1

PATRICK, G., HANCOCK, R. D., 1991, *Inorg. Chem.*, 30, 1419

PEARSON, R. G., 1963, *J. Am. Chem. Soc.*, 85, 3533

PENDERSON, C. J., 1967, *J. Am. Chem. Soc.*, 89, 7017

PILICHOWSKI, J. F., LEHN, J. M., SAUVAGE, J. P., GRAMAIN, J. C., 1985, *Tetrahedron*, 41, 1959

RAMASUBBU, A., WAINWRIGHT, K. P., 1982, *J. Chem. Soc., Chem. Commun.*, 277

RASMUSSEN, S. E., 1956, *Acta. Chem. Scand.*, 10, 1279

- RAYMOND, K. N., MULLER, G., MATZANYE, F., 1984, *Top. Curr. Chem.*, 123, 49
- RICHMAN, J. E., ATKINS, T. J., 1974, *J. Am. Chem. Soc.*, 96, 2268
- RIESEN, A., ZEHNDER, M., KADEN, T. A., 1986, *Helv. Chim. Acta.*, 69, 2067
- RIESEN, A., ZEHNDER, M., KADEN, T. A., 1986, *Helv. Chim. Acta.*, 69, 2074
- ROSSA, L., VOGTLE, F., 1983, *Top. Curr. Chem.*, 113, 1
- ROSSOTTI, F. J. C., ROSSOTTI, H., 1965, *J. Chem. Ed.*, 42, 375
- ROSSOTTI, F. J. C., ROSSOTTI, H., 1961, *The Determination of Stability Constants*, (McGraw-Hill, London), p145
- ROSSOTTI, H., 1978, *The Study of ionic Equilibria. An Introduction*, (Longmans, London), p83
- SARGESON, A. M., 1984, *Pure Appl. Chem.*, 56, 1603
- SARGESON, A. M., 1979, *Chem. Br.*, 15, 23
- SCHWARZENBACH, G., 1952, *Helv. Chim. Acta.*, 35, 2344
- SCHWARZENBACH, G., GUT, R., ANDEREGG, G., 1954, *Helv. Chim. Acta.*, 37, 937
- SHANNON, R. D., 1976, *Acta. Crystallogr., Sect. A*, 32A, 751
- SHAIKJEE, M. S., 1987, Msc Thesis, University of the Witwatersrand, Johannesburg,

SHELDRICK, G. M., 1978, "Computing in Crystallography" eds; Schenk, H., Olthof-Hazelkamp, R., Van Koningsveld, H., Bassi, G. C., Delft University Press, Holland

SHELDRICK, G. M., 1985, "Crystallographic Computing" eds; KRUGER, G., GODDARD, R., Oxford University Press, London

SPIESS, B., ARNAUD-NEU, F., SCHWING-WEILL, M. J., 1980, *Helv. Chim. Acta.*, 63, 2287

STALEY, R. H., BEAUCHAMP, J. L., 1975, *J. Am. Chem. Soc.*, 97, 5920

STOUT, G. H., JENSEN, L. H., 1968, "X-Ray Structure Determination", Macmillan, London

STUDER, M., KADEN, T. A., 1986, *Helv. Chim. Acta.*, 69, 2081

STUDER, M., KADEN, T. A., MACKE, H. R., 1990, *Helv. Chim. Acta.*, 73, 149

SUH, M. P., SHIN, W., KIM, H., KOO, C. H., 1987, *Inorg. Chem.*, 26, 1846

TAAGEPERA, M., DE FREES, D., HEHRE, W. J., TAFT, R. W., 1980, *J. Am. Chem. Soc.*, 102, 424

TAFT, R. W., WOLF, J. F., BEAUCHAMP, J. L., G., SORRANO, G., ARNETT, E. M., 1978, *J. Am. Chem. Soc.*, 100, 1240

TAFT, R. W., WOLF, J. F., STALEY, R. H., KOPPEL, I., TAAGEPERA, M., MCIVER, R. T., BEAUCHAMP, J. L., 1977, *J. Am. Chem. Soc.*, 99, 5417

THOM, V. J., FOX, C. C., BOEYENS, J. C. A., HANCOCK, R. D., 1984, *J. Am. Chem. Soc.*, 106, 5947

THOM, V. J., HANCOCK, R. D., 1985, *J. Chem. Soc., Dalton Trans.*, 1877

THOM, V. J., HOSKEN, G. D., HANCOCK, R. D., 1985, *Inorg. Chem.*, 24, 3373

THOM, V. J., SHAIK'EE, M. S., HANCOCK, R. D., 1986, *Inorg. Chem.*, 25, 2992

TROTMAN-DICKENSON, A. F., 1949, *J. Chem. Soc.*, 1293

TSUKUBE, H., 1984, *J. Chem. Soc., Chem. Commun.*, 315

TSUKUBE, H., TAKAGI, K., HIGASHIYAMA, T., IWACHIDO, T., HAYAMA, N., 1986, *J. Chem. Soc., Perkins Trans. I*, 1033

TWEEDLE, H. F., DISCHINO, D. D., DELANEY, E. J., EMSWILER, J. E., PRASAD, J. S., SRIVASTAVA, S. K., 1991, *Inorg. Chem.*, 30, 1265

UPPAL, J. S., STALEY, R. H., 1982, *J. Am. Chem. Soc.*, 104, 1235

UPPAL, J. S., STALEY, R. H., 1982, *J. Am. Chem. Soc.*, 104, 1238

VOGEL, A. I., 1961, *A Textbook of Quantitative Inorganic Analysis, Including Elementary Instrumental Analysis*, 3rd. Edition (Longmans, London)

WADE, P. W., HANCOCK, R. D., BOEYENS, J. C. A., DOBSON, S. M., 1990, *J. Chem. Soc., Dalton Trans.*, 483

WADE, P. W., HANCOCK, R. D., 1987, *Inorg. Chim. Acta.*, 130, 251

WAINWRIGHT, K. P., 1980, *Inorg. Chem.*, 19, 1396

WAINWRIGHT, K. P., 1980, *J. Chem. Soc., Dalton Trans.*, 2117

WESTLEY, J. W., 1977, *Adv. Appl. Microbiol.*, 22, 177

WOODIN, R. L., BEAUCHAMP, J. L., 1975, *J. Am. Chem. Soc.*, 97, 5920

WOODIN, R. L., BEAUCHAMP, J. L., 1978, *J. Am. Chem. Soc.*, 100, 501

YAOUANG, J. J., LE BRIS, N., LE GALL, G., CLEMENT, J. C., HANDEL, H., DES
ABEAYES, H., 1991, *J. Chem. Soc., Chem. Commun.*, 206

YEH, S. M., SHERMAN, D. G., MEARES, C. F., 1979, *Anal. Biochem.*, 100, 152

ZOMPA, L. J., 1978, *Inorg. Chem.*, 17, 2531

PUBLICATIONS

- 1) R. D. Hancock, P. W. Wade, M. P. Ngwenya A. S. de Sousa, and K. V. Damu, *"Ligand Design for complexation in aqueous solution. 2. Chelate ring size as a Basis for control of size-based selectivity of metal ions."* *Inorg. Chem.*, Vol. 29, pp 1968-1974, (1990).
- 2) A. S. de Sousa, G. J. B. Croft, C. A. Wagner, J. P. Michael, and R. D. Hancock, *"The effect of cyclohexylene Bridges on the Metal Ion Size-based Selectivity of Ligands in Aqueous Solution"*, *Inorg. Chem.*, Vol. 30, pp 3525-3529 (1991).
- 3) N. V. Jarvis, A. S. de Sousa, and R. D. Hancock, *"The Affinity of the Uranyl Ion for Nitrogen Donor Ligands"*, *Radiochem. Acta*, Vol. 57, p 33 (1992).
- 4) N. V. Jarvis, A. S. de Sousa, and R. D. Hancock, *"Stability of some complexes of Plutonium(IV) with Nitrogen-donor Ligands"*, *Radiochem. Acta*, Vol. 64, p 15 (1994).
- 5) A. S. de Sousa, and R. D. Hancock, *"Convenient Syntheses, based on Cyclohexene Oxide, of Highly Preorganised Ligands that display Metal Ion Size-based Selectivity"*, *Chem. Comm.* in the press.

CONFERENCE PROCEEDINGS

- 1) Inorganic '90. Golden Gate (March 1990)
"Structurally reinforced Dihydroxamic acids based on the Norbornane ring."
- 2) Conference Metal ions in solution. Malelane (April 1993)
"The effect of cyclohexylene bridges on the metal ion size based selectivity of ligands in aqueous solution."
- 3) Royal Australian Chemical Institute Inorganic Division Conference. University of Western Australia (July 1994)
"Metal complexes of β -hydroxyamines reinforced with cyclohexylene bridges in aqueous solution."

APPENDIX

(The appendix merely contains the structure factors in the order in which they are presented in this thesis)

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CU-THIEN

H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC
2	0	0	205	166	0	4	0	376	-317	0	8	0	242	-239	6	1	1	545	-563	-1	3	1	30	-46
4	0	0	470	494	1	4	0	639	-655	1	8	0	109	111	7	1	1	202	224	0	3	1	256	244
6	0	0	253	258	2	4	0	79	81	2	8	0	134	-137	8	1	1	144	155	1	3	1	373	-373
8	0	0	547	524	3	4	0	825	-812	3	8	0	117	117	9	1	1	86	-91	2	3	1	505	494
10	0	0	83	75	4	4	0	163	-136	4	8	0	197	194	10	1	1	47	52	3	3	1	245	-239
12	0	0	205	-196	5	4	0	42	38	5	8	0	75	62	11	1	1	54	-55	4	3	1	207	-168
14	0	0	248	-261	6	4	0	154	160	6	8	0	54	-59	12	1	1	128	-135	5	3	1	95	94
1	1	0	1591	-1669	7	4	0	349	331	7	8	0	79	-70	13	1	1	76	-62	6	3	1	238	243
2	1	0	1239	1267	8	4	0	228	-219	8	8	0	84	87	14	1	1	199	-203	7	3	1	704	680
3	1	0	652	-657	9	4	0	65	-69	9	8	0	193	-194	15	1	1	121	112	8	3	1	95	108
4	1	0	37	31	10	4	0	57	-52	10	8	0	78	-84	-14	2	1	77	76	9	3	1	189	187
5	1	0	384	370	11	4	0	302	-295	11	8	0	95	-96	-13	2	1	153	152	10	3	1	73	74
6	1	0	413	-388	12	4	0	65	64	12	8	0	61	65	-12	2	1	207	-202	11	3	1	230	-224
7	1	0	244	-238	1	5	0	659	652	1	10	0	122	123	-11	2	1	162	-185	-14	4	1	67	74
8	1	0	175	189	2	5	0	411	427	2	10	0	110	111	-10	2	1	35	29	-12	4	1	88	-97
9	1	0	531	-545	3	5	0	29	-15	-15	0	1	43	26	-9	2	1	418	-433	-11	4	1	97	101
10	1	0	92	104	4	5	0	98	94	-13	0	1	180	169	-8	2	1	502	509	-10	4	1	140	-148
11	1	0	55	45	5	5	0	260	-269	-11	0	1	151	126	-7	2	1	194	-203	-9	4	1	287	289
12	1	0	154	164	6	5	0	436	-440	-9	0	1	744	-769	-6	2	1	969	1033	-8	4	1	207	205
13	1	0	284	288	7	5	0	232	222	-7	0	1	73	36	-5	2	1	421	433	-7	4	1	51	-53
15	1	0	73	69	8	5	0	199	-201	-5	0	1	625	628	-4	2	1	537	566	-6	4	1	588	624
0	2	0	413	-412	9	5	0	191	178	-3	0	1	246	-214	-3	2	1	284	321	-4	4	1	182	-201
1	2	0	85	-101	10	5	0	117	117	3	0	1	980	1013	-2	2	1	285	-250	-3	4	1	124	-100
2	2	0	780	770	12	5	0	39	40	5	0	1	856	895	-1	2	1	351	-350	-2	4	1	568	-560
3	2	0	626	-656	13	5	0	114	-119	7	0	1	382	362	0	2	1	833	798	-1	4	1	234	269
4	2	0	534	-521	0	6	0	579	-578	9	0	1	302	-315	1	2	1	490	482	0	4	1	166	161
5	2	0	222	167	1	6	0	49	-40	11	0	1	64	85	2	2	1	414	412	1	4	1	168	-183
6	2	0	76	-46	2	6	0	254	-261	13	0	1	286	291	3	2	1	163	-195	2	4	1	966	971
7	2	0	597	565	3	6	0	51	36	15	0	1	64	52	4	2	1	405	406	3	4	1	126	-137
8	2	0	349	346	4	6	0	364	372	-15	1	1	61	-56	5	2	1	397	392	4	4	1	113	127
9	2	0	166	-168	5	6	0	167	172	-14	1	1	153	-145	6	2	1	818	-790	5	4	1	100	-114
10	2	0	174	184	6	6	0	38	37	-11	1	1	169	157	7	2	1	72	52	6	4	1	411	-399
11	2	0	296	-315	7	6	0	201	216	-10	1	1	335	333	8	2	1	131	-137	7	4	1	179	-164
12	2	0	68	-69	8	6	0	250	-254	-9	1	1	84	-95	9	2	1	261	-271	8	4	1	325	-327
13	2	0	131	-136	9	6	0	70	71	-8	1	1	557	591	10	2	1	94	-77	10	4	1	116	119
14	2	0	132	-132	10	6	0	145	-149	-7	1	1	311	-343	12	2	1	184	178	12	4	1	89	84
1	3	0	345	-331	11	6	0	68	-59	-6	1	1	237	-228	13	2	1	208	216	13	4	1	74	-75
2	3	0	1091	1090	12	6	0	101	96	-5	1	1	335	-358	14	2	1	106	-117	-11	5	1	142	141
3	3	0	114	-110	1	7	0	346	355	-4	1	1	557	-603	-12	3	1	60	-71	-10	5	1	137	-144
4	3	0	185	212	2	7	0	41	-43	-3	1	1	224	-238	-11	3	1	224	230	-9	5	1	84	-89
5	3	0	128	118	3	7	0	140	-134	-2	1	1	299	-314	-9	3	1	108	-103	-8	5	1	295	-310
6	3	0	369	-335	4	7	0	117	-127	-1	1	1	459	463	-8	3	1	49	-34	-7	5	1	208	-220
7	3	0	91	-99	5	7	0	206	-198	0	1	1	1118	1099	-7	3	1	1011	-1051	-6	5	1	99	93
8	3	0	127	-122	6	7	0	52	48	1	1	1	1330	1337	-6	3	1	137	116	-5	5	1	383	-401
9	3	0	76	-49	7	7	0	49	51	2	1	1	663	-626	-5	3	1	242	-286	-4	5	1	306	303
10	3	0	294	288	8	7	0	56	-55	3	1	1	621	-644	-4	3	1	423	-449	-3	5	1	324	308
12	3	0	275	291	9	7	0	197	202	4	1	1	1041	-992	-3	3	1	289	320	-2	5	1	164	-169
13	3	0	48	47	10	7	0	46	-43	5	1	1	77	-58	-2	3	1	350	350	-1	5	1	282	285
0	5	1	389	-383	7	7	1	62	-59	-11	1	2	72	83	14	2	2	101	-102	11	4	2	273	-277
1	5	1	290	-285	8	7	1	142	-132	-10	1	2	119	-120	-14	3	2	162	165	-13	5	2	126	-136
2	5	1	109	117	9	7	1	97	-89	-9	1	2	424	-430	-13	3	2	36	42	-12	5	2	68	-66
3	5	1	414	-422	-9	8	1	118	120	-8	1	2	85	112	-12	3	2	154	-149	-10	5	2	128	-118
4	5	1	380	381	-8	8	1	114	-117	-5	1	2	489	539	-10	3	2	54	-56	-9	5	2	34	35
5	5	1	225	201	-6	8	1	111	-116	-4	1	2	290	-304	3	3	2	56	-59	-8	5	2	97	122
6	5	1	285	281	-5	8	1	120	-115	-3	1	2	585	581	-8	3	2	315	326	-7	5	2	40	-34
7	5	1	365	350	-3	8	1	63	-64	-2	1	2	1164	-1178	-7	3	2	294	-296	-6	5	2	286	297
8	5	1	52	-42	-2	8	1	98	104	-1	1	2	125	-72	-6	3	2	603	622	-5	5	2	503	-511
10	5	1	89	-85	-1	8	1	284	284	0	1	2	620	-634	-5	3	2	252	248	-4	5	2	54	65
11	5	1	157	-169	1	8	1	263	266	1	1	2	232	-199	-4	3	2	95	-101	-3	5	2	328	-323
12	5	1	88	94	2	8	1	157	-148	2	1	2	705	-702	-3	3	2	339	-323	-2	5	2	432	-421
-11	6	1	90	93	3	8	1	79	-88	3	1	2	170	192	-2	3	2	1053	-1049	-1	5	2	140	126
-10	6	1	75	-83	5	8	1	170	-167	4	1	2	435	410	-1	3	2	423	-419	0	5	2	225	-217
-9	6	1	226	231	7	8	1	51	45	5	1	2	1551	1046	0	3	2	461	-448	1	5	2	233	226
-8	6	1	186	197	8	8	1	76	67	6	1	2	835	-825	2	3	2	435	396	2	5	2	515	498
-7	6	1	201	214	9	8	1	63	63	7	1	2	82	85	3	3	2	50	-19	5	5	2	367	-352
-6	6	1	52	60	-7	9	1	157	149	8	1	2	152	-158	4	3	2	197	-181	6	5	2	358	-343
-5	6	1	353	-354	-4	9	1	77	72	9	1	2	485	-456	6	3	2	636	-650	7	5	2	81	89
-4	6	1	57	58	-3	9	1	107	-111	10	1	2	78	64	7	3	2	114	140	8	5	2	316	-313
-3	6	1	184	-188	-2	9	1	38	-27	11	1	2	115	-113	8	3	2	361	-348	9	5	2	298	300
-2	6	1	257	-265	-1	9	1	95	-98	12	1	2	120	133	9	3	2	80	-83	10	5	2		

-5	7	2	261	-274	-1	0	3	1588	-1518	2	2	3	623	613	1	4	3	499	511	1	6	3	547	564
-4	7	2	101	-98	1	0	3	847	-825	3	2	3	382	396	2	4	3	538	531	2	6	3	197	192
-3	7	2	194	-193	3	0	3	692	-744	4	2	3	722	726	3	4	3	216	-211	4	6	3	65	-75
-2	7	2	117	124	5	0	3	980	955	5	2	3	58	-31	4	4	3	52	43	5	6	3	438	-422
-1	7	2	238	232	7	0	3	144	-114	6	2	3	546	-532	5	4	3	163	145	6	6	3	101	-102
0	7	2	60	65	9	0	3	593	-618	7	2	3	141	138	4	4	3	403	-419	9	6	3	185	186
1	7	2	363	363	13	0	3	255	266	9	2	3	229	209	7	4	3	50	23	10	6	3	95	85
2	7	2	56	-48	-15	1	3	75	-72	9	2	3	136	-135	8	4	3	310	-340	-11	7	3	54	-50
3	7	2	127	-132	-14	1	3	194	-208	10	2	3	167	153	9	4	3	69	69	-10	7	3	127	-131
5	7	2	226	-223	-12	1	3	134	-128	12	2	3	271	276	10	4	3	214	203	-8	7	3	245	-244
8	7	2	101	96	-11	1	3	144	159	13	2	3	193	184	12	4	3	212	205	-7	7	3	46	-33
9	7	2	190	175	-10	1	3	206	207	-14	3	3	47	-25	-12	5	3	62	70	-6	7	3	82	77
-8	8	2	168	-168	-9	1	3	108	126	-13	3	3	43	53	-11	5	3	136	141	-5	7	3	69	-64
-7	8	2	159	154	-8	1	3	673	663	-11	3	3	416	425	-10	5	3	66	-65	-4	7	3	316	327
-6	8	2	61	61	-7	1	3	129	-125	-10	3	3	86	79	-9	5	3	43	48	-3	7	3	187	202
-4	8	2	181	187	-6	1	3	136	133	-9	3	3	245	250	-8	5	3	279	-283	-2	7	3	117	-115
-3	8	2	134	-136	-5	1	3	29	15	-8	3	3	78	-89	-7	5	3	248	-230	-1	7	3	153	-158
-2	8	2	211	-212	-4	1	3	211	-271	-7	3	3	365	-341	-5	5	3	181	-161	0	7	3	344	-344
-1	8	2	205	-207	-3	1	3	414	413	-6	3	3	40	-18	-4	5	3	165	194	1	7	3	168	17
0	8	2	171	-156	-2	1	3	480	483	-5	3	3	30	-27	-3	5	3	95	106	2	7	3	166	-167
2	8	2	110	-109	-1	1	3	537	504	-4	3	3	157	-137	-2	5	3	201	-187	3	7	3	143	154
3	8	2	48	36	0	1	3	1945	1969	-3	3	3	1214	1260	-1	5	3	560	558	4	7	3	266	254
4	8	2	191	190	1	1	3	199	188	-2	3	3	111	-110	0	5	3	700	-702	6	7	3	170	164
6	8	2	125	128	2	1	3	867	836	-1	3	3	819	875	1	5	3	231	-234	7	7	3	60	55
7	8	2	105	-109	3	1	3	354	-348	0	3	3	171	170	2	5	3	87	-81	8	7	3	152	-158
8	8	2	104	-99	4	1	3	816	-817	1	3	3	230	-216	3	5	3	358	-343	10	7	3	93	-98
-7	9	2	88	81	6	1	3	85	-84	2	3	3	52	42	4	5	3	104	102	-9	8	3	143	143
-6	9	2	160	-157	7	1	3	436	419	3	3	3	585	-574	5	5	3	156	170	-8	8	3	40	-48
-4	9	2	122	119	8	1	3	248	261	4	3	3	73	49	6	5	3	144	148	-7	8	3	127	131
-2	9	2	144	147	9	1	3	63	-49	5	3	3	31	37	7	5	3	282	284	-6	8	3	91	-107
-1	9	2	124	115	10	1	3	127	141	6	3	3	195	-185	8	5	3	136	-120	-5	8	3	197	-202
1	9	2	127	127	11	1	3	222	-236	7	3	3	322	351	9	5	3	81	91	-4	8	3	128	120
2	9	2	121	-122	12	1	3	138	-131	8	3	3	132	116	10	5	3	164	-167	-3	8	3	101	-99
3	9	2	103	-107	14	1	3	165	-168	9	3	3	140	-109	11	5	3	203	-189	-2	8	3	179	184
5	9	2	132	-127	-14	2	3	43	43	11	3	3	346	-333	12	5	3	66	75	-1	8	3	161	165
6	9	2	132	119	-13	2	3	148	154	13	3	3	150	-141	13	5	3	45	-40	0	8	3	64	62
-3	10	2	82	-74	-12	2	3	208	-231	-12	4	3	182	-187	-11	6	3	62	67	-1	8	3	92	88
-1	10	2	145	-134	-10	2	3	319	-329	-10	4	3	277	-297	-10	6	3	37	-25	2	8	3	152	-152
0	10	2	73	-65	-9	2	3	338	-340	-9	4	3	201	199	-9	6	3	230	239	-3	8	3	104	-102
1	10	2	114	118	-7	2	3	109	-110	-8	4	3	52	28	-8	6	3	163	157	5	8	3	231	-228
3	10	2	149	157	-6	2	3	253	233	-7	4	3	65	-78	-7	6	3	197	198	9	8	3	109	105
-15	0	3	124	130	-5	2	3	481	449	-6	4	3	376	361	-6	6	3	150	138	-7	9	3	124	120
-13	0	3	233	242	-4	2	3	147	-189	-5	4	3	102	-115	-5	6	3	75	-73	-5	9	3	64	67
-11	0	3	135	146	-3	2	3	374	321	-4	4	3	246	-235	-4	6	3	123	-141	-3	9	3	218	-208
-9	0	3	673	-661	-2	2	3	1669	-1732	-3	4	3	66	-73	-3	6	3	144	-157	-1	9	3	58	-48
-7	0	3	643	-658	-1	2	3	779	-776	-2	4	3	729	-756	-2	4	3	157	-147	0	9	3	98	-94
-5	0	3	192	185	0	2	3	47	45	-1	4	3	233	208	-1	6	3	431	430	-3	9	3	161	161
-4	9	3	160	155	13	1	4	232	236	-12	4	4	54	-50	-10	6	4	190	-192	-3	9	4	40	-33
-6	9	3	79	78	14	1	4	65	-49	-11	4	4	249	253	-9	6	4	136	138	-2	9	4	178	182
-3	10	3	112	-113	-12	2	4	62	-70	-8	4	4	361	-356	-8	6	4	244	-259	-1	9	4	44	53
-2	10	3	62	-54	-11	2	4	241	239	-7	4	4	543	-554	-7	6	4	79	-77	1	9	4	144	146
-2	10	3	106	103	-10	2	4	171	172	-6	4	4	198	220	-4	6	4	299	306	2	9	4	159	-158
0	10	3	50	48	-9	2	4	57	-59	-5	4	4	266	-259	-3	6	4	415	425	3	9	4	59	-43
1	10	3	56	50	-8	2	4	457	458	-4	4	4	84	85	-1	6	4	306	325	4	9	4	59	-59
2	10	3	184	-179	-7	2	4	320	-537	-3	4	4	36	41	0	6	4	414	-417	5	9	4	90	-83
-14	0	4	148	-148	-6	2	4	110	-104	-2	4	4	208	-205	1	6	4	43	58	6	9	4	79	81
-12	0	4	38	47	-5	2	4	487	-504	-1	4	4	687	671	3	6	4	128	-116	-1	10	4	118	-113
-10	0	4	491	471	-4	2	4	353	-385	0	4	4	268	259	4	6	4	362	359	0	10	4	56	-52
-8	0	4	748	745	-3	2	4	871	856	1	4	4	297	-306	6	6	4	318	308	1	10	4	73	68
-6	0	4	93	-81	-2	2	4	367	349	3	4	4	278	-289	7	6	4	48	26	-13	0	5	171	175
-4	0	4	633	-625	-1	2	4	185	-208	4	4	4	204	200	10	6	4	86	-85	-9	0	5	466	-474
-2	0	4	1046	-988	0	2	4	801	792	5	4	4	209	199	11	6	4	88	-92	-7	0	5	76	-77
0	0	4	152	105	1	2	4	181	-236	7	4	4	497	473	-9	7	4	209	212	-5	0	5	692	719
2	0	4	693	-758	2	2	4	383	373	8	4	4	213	194	-8	7	4	71	-75	-3	0	5	850	837
4	0	4	1219	-1231	3	2	4	715	-728	9	4	4	128	124	-7	7	4	130	128	-1	0	5	1211	1133
6	0	4	608	-608	4	2	4	666	-632	10	4	4	77	-67	-6	7	4	69	-76	1	0	5	611	-630
10	0	4	350	373	5	2	4	131	-139	11	4	4	230	-243	-5	7	4	254	-257	3	0	5	636	631
12	0	4	164	-180	6	2	4	241	-211	12	4	4	77	68	-4	7	4	75	-75	5	0	5	686	645
14	0	4	128	-128	7	2	4	413	408	13	4	4	75	-83	-3	7	4	219	-227	7	0	5	184	182
-14	1	4	43	38	9	2	4	79	37	-13	5	4	112	-103	-2	7	4	154	-157	9	0	5	657	-615
-13	1	4	111	109	10	2	4	71	-54	-12	5	4	97	-96	-1	7	4	224	219	11	0	5	201	-199
-12	1	4	71	-67	11	2	4	117	-133	-11	5	4												

-11	2	5	120	112	11	3	5	234	-233	12	5	5	44	-32	5	8	5	179	-182	6	1	6	111	-110
-10	2	5	158	-173	13	3	5	77	-88	-11	6	5	43	-30	6	8	5	63	66	8	1	6	69	-99
-9	2	5	162	-184	-13	4	5	96	-93	-10	6	5	78	-80	8	8	5	106	108	9	1	6	303	-313
-8	2	5	102	90	-12	4	5	79	-90	-9	6	5	217	225	-5	9	5	86	85	10	1	6	105	106
-7	2	5	212	218	-11	4	5	60	-61	-8	6	5	78	-67	-4	9	5	48	50	11	1	6	83	-110
-6	2	5	275	280	-10	4	5	235	-229	-6	6	5	106	118	-3	9	5	121	-124	12	1	6	108	111
-5	2	5	360	349	-8	4	5	230	258	-5	6	5	258	-252	-1	9	5	170	-166	13	1	6	158	164
-4	2	5	26	16	-7	4	5	184	-164	-4	6	5	188	-186	0	9	5	94	-92	-14	2	6	42	-49
-3	2	5	359	359	-6	4	5	405	429	-3	6	5	266	-262	1	9	5	85	86	-13	2	6	56	46
-2	2	5	1429	-1436	-5	4	5	291	-275	-2	6	5	111	-107	3	9	5	130	133	-12	2	6	192	-197
-1	2	5	1016	-985	-3	4	5	290	-271	-1	6	5	158	147	4	9	5	80	74	-11	2	6	443	438
0	2	5	315	249	-2	4	5	523	-514	0	6	5	63	-54	6	9	5	64	65	-10	2	6	92	86
1	2	5	431	-446	-1	4	5	58	-81	1	6	5	248	238	0	10	5	59	55	-9	2	6	286	272
2	2	5	78	41	0	4	5	643	-631	2	6	5	338	336	-14	0	6	217	-213	-8	2	6	293	289
3	2	5	223	189	1	4	5	417	368	3	6	5	28	24	-12	0	6	88	-78	-7	2	6	81	68
4	2	5	530	489	2	4	5	366	365	4	6	5	89	81	-10	0	6	187	202	-6	2	6	77	101
5	2	5	502	489	3	4	5	86	-99	5	6	5	388	-395	-8	0	6	686	673	-5	2	6	72	-65
6	2	5	438	-425	4	4	5	74	93	6	6	5	84	81	-6	0	6	290	-272	-4	2	6	497	-447
7	2	5	297	-307	5	4	5	141	-141	7	6	5	33	-37	-4	0	6	592	-569	-3	2	6	764	771
8	2	5	107	-81	6	4	5	507	-483	8	6	5	79	-76	-2	0	6	701	-621	-2	2	6	168	200
9	2	5	92	75	7	4	5	159	140	9	6	5	240	229	0	0	6	925	936	-1	2	6	833	827
10	2	5	108	-97	8	4	5	234	-213	10	6	5	72	90	2	0	6	692	696	0	2	6	382	399
11	2	5	170	171	9	4	5	121	106	-10	7	5	75	-82	4	0	6	720	-768	1	2	6	622	-608
12	2	5	80	90	10	4	5	114	126	-8	7	5	223	-231	6	0	6	181	142	2	2	6	182	184
13	3	5	68	-77	11	4	5	78	73	-7	7	5	52	32	8	0	6	84	70	3	2	6	563	-559
-12	3	5	74	0	12	4	5	188	191	-6	7	5	59	62	10	0	6	375	405	4	2	6	492	-475
-11	3	5	198	206	-12	5	5	121	118	-5	7	5	67	-73	12	0	6	131	-127	5	2	6	316	-305
-10	3	5	199	206	-11	5	5	168	175	-4	7	5	373	371	14	0	6	146	-150	6	2	6	495	-480
-9	3	5	133	139	-10	5	5	44	-44	-3	7	5	40	-33	-14	1	6	37	11	7	2	6	229	248
-8	3	5	88	79	-9	5	5	99	89	0	7	5	313	-322	-13	1	6	215	210	8	2	6	253	241
-7	3	5	536	-546	-8	5	5	96	-100	1	7	5	156	-163	-12	1	6	119	-125	9	2	6	124	-109
-6	3	5	90	63	-7	5	5	134	-146	4	7	5	219	219	-11	1	6	64	62	11	2	6	281	-277
-5	3	5	162	-155	-6	5	5	199	196	6	7	5	211	206	-10	1	6	238	-245	12	2	6	39	-27
-4	3	5	258	227	-5	5	5	136	-152	7	7	5	52	-50	-9	1	6	372	-374	13	2	6	125	-128
-3	3	5	469	475	-4	5	5	416	410	8	7	5	137	-129	-8	1	6	89	80	-14	3	6	46	54
-2	3	5	355	-332	-3	5	5	435	429	10	7	5	131	-124	-7	1	6	321	-332	-12	3	6	168	-170
-1	3	5	922	914	-2	5	5	308	321	-6	1	5	119	126	-6	1	6	127	112	-10	3	6	499	-491
0	3	5	42	43	-1	5	5	317	302	-7	8	5	150	148	-5	1	6	445	417	-9	3	6	106	-80
1	3	5	261	-209	0	5	5	208	-180	-6	8	5	122	-119	-4	1	6	158	136	-8	3	6	125	-105
2	3	5	26	-10	2	5	5	88	-75	-5	8	5	134	-133	-3	1	6	706	634	-7	3	6	133	-135
3	3	5	572	-546	3	5	5	310	-316	-4	8	5	61	54	-3	1	6	604	-666	-6	3	6	249	262
4	3	5	196	188	-1	5	6	259	257	7	7	6	81	-77	-3	1	7	219	-246	-3	3	7	394	392
5	3	5	241	-241	0	5	6	171	-164	9	7	6	180	181	-2	1	7	252	-241	-2	3	7	121	-154
6	3	5	209	218	1	5	6	343	364	-8	8	6	136	-139	-1	1	7	495	477	-1	3	7	313	280
7	3	5	1056	-1080	2	5	6	150	154	-7	8	6	70	75	0	1	7	216	190	0	3	7	55	-47
8	3	5	139	120	3	5	6	126	125	-4	8	6	253	257	1	1	7	594	-576	1	3	7	58	-93
9	3	5	341	-334	4	5	6	297	298	-3	8	6	64	-72	2	1	7	63	42	2	3	7	36	-42
10	3	5	151	149	5	5	6	372	-375	-2	8	6	123	126	3	1	7	101	-89	3	3	7	861	-860
11	3	5	921	997	6	5	6	116	-123	-1	8	6	80	-79	4	1	7	734	-762	6	3	7	156	-165
12	3	5	153	165	7	5	6	114	93	0	8	6	198	-196	5	1	7	157	-156	7	3	7	407	392
13	3	5	396	379	8	5	6	142	-145	1	8	6	84	76	6	1	7	520	-532	8	3	7	162	147
14	3	5	238	254	9	5	6	134	134	3	8	6	206	203	7	1	7	110	112	9	3	7	87	68
15	3	5	159	-193	10	5	6	128	111	4	8	6	170	173	9	1	7	103	100	11	3	7	164	-177
16	3	5	37	-66	12	5	6	131	127	6	8	6	149	156	10	1	7	189	188	-12	4	7	104	-110
17	3	5	230	210	-10	6	6	121	-124	7	8	6	84	-82	11	1	7	38	-51	-11	4	7	55	52
18	3	5	44	-32	-9	6	6	102	120	8	8	6	104	-97	12	1	7	74	-80	-10	4	7	172	-177
19	3	5	252	253	-8	6	6	248	-246	-6	9	6	143	-145	14	1	7	113	-107	-9	4	7	195	201
20	3	5	247	252	-7	6	6	71	-58	-5	9	6	90	-83	-14	2	7	82	83	-8	4	7	87	63
21	3	5	94	96	-5	6	6	56	-60	-3	9	6	78	-82	-13	2	7	78	84	-7	4	7	118	113
22	3	5	186	182	-4	6	6	263	282	-2	9	6	159	167	-12	2	7	93	-92	-6	4	7	648	647
23	3	5	257	-268	-3	6	6	109	98	0	9	6	68	66	-10	2	7	368	-358	-5	4	7	100	96
24	3	5	357	-353	-2	6	6	131	-126	1	9	6	67	67	-9	2	7	291	-264	-4	4	7	83	-85
25	3	5	74	-72	-1	6	6	163	135	2	9	6	218	-207	-8	2	7	308	307	-2	4	7	516	-520
26	3	5	219	-239	0	6	6	442	-448	4	9	6	52	-46	-7	2	7	254	-224	0	4	7	77	-76
27	3	5	140	153	1	6	6	154	-177	5	9	6	74	-74	-6	2	7	209	215	1	4	7	178	180
28	3	5	448	432	2	6	6	199	-200	-13	0	7	88	76	-5	2	7	50	31	2	4	7	371	389
29	3	5	252	-249	3	6	6	128	-144	-11	0	7	150	-128	-4	2	7	346	341	3	4	7	247	-224
30	3	5	625	623	4	6	6	137	137	-9	0	7	579	-529	-3	2	7	552	560	4	4	7	430	427
31	3	5	376	-390	6	6	6	146	149	-7	0	7	440	-403	-2	2	7	718	-687	5	4	7	344	-318
32	3	5	75	71	7	6	6	83	82	-5	0	7	935	907	-1	2	7	303	-295	6	4	7	153	-148
33	3	5	136	-151	8	6	6	82	-78	-3	0	7	648	629	0	2	7	196	239	7	4	7	121	-90
34	3	5	613	-591	9	6	6	85	80	-1	0	7	170	190	1									

-4	6	7	89	-107	-10	0	8	82	89	1	2	8	136	154	3	4	8	414	-418	-8	7	8	56	-49
-5	6	7	244	-229	-8	0	8	231	234	2	2	8	218	214	4	4	8	272	291	-7	7	8	95	99
-2	6	7	32	-43	-6	0	8	327	-325	3	2	8	381	-367	5	4	8	97	-99	-5	7	8	163	-168
-1	6	7	61	72	-4	0	8	1136	-1124	4	2	8	339	-298	7	4	8	197	173	-4	7	8	135	126
0	6	7	237	-264	0	0	8	363	362	5	2	8	178	129	9	4	8	116	104	-3	7	8	239	-240
1	6	7	159	170	2	0	8	528	547	6	2	8	239	-219	10	4	8	154	-144	-2	7	8	60	41
2	6	7	267	266	4	0	8	409	-369	7	2	8	52	517	11	4	8	172	-176	-1	7	8	40	38
5	6	7	354	-339	6	0	8	190	-158	8	2	8	242	251	-12	5	8	90	-106	0	7	8	103	92
6	6	7	94	-96	8	0	8	129	111	9	2	8	63	39	-10	5	8	193	-201	1	7	8	274	271
7	6	7	101	-85	10	0	8	329	355	10	2	8	246	252	-9	5	8	92	94	2	7	8	72	63
8	6	7	67	-82	12	0	8	40	34	11	2	8	120	-114	-7	5	8	52	51	3	7	8	82	-81
9	6	7	165	174	-14	1	8	39	41	-13	2	8	75	-82	-6	5	8	228	253	4	7	8	96	85
-10	7	7	77	-81	-13	1	8	206	191	-12	3	8	70	-66	-5	5	8	311	-293	5	7	8	225	-213
-9	7	7	81	81	-11	1	8	145	136	-11	3	8	46	-54	-4	5	8	222	-229	8	7	8	67	66
-8	7	7	228	-219	-10	1	8	238	-245	-10	3	8	239	-248	-3	5	8	360	-368	9	7	8	155	154
-7	7	7	34	91	-9	1	8	176	-197	-8	3	8	56	56	-2	5	8	222	-209	-7	8	8	84	84
-5	7	7	47	-46	-6	1	8	194	192	-7	3	8	253	-264	-1	5	8	70	58	-5	8	8	72	83
-4	7	7	275	292	-6	1	8	243	252	-6	3	8	320	338	0	5	8	200	-197	-4	8	8	142	149
-3	7	7	40	56	-5	1	8	487	501	-5	3	8	142	139	1	5	8	134	118	-3	8	8	46	-38
-2	7	7	141	133	-4	1	8	184	-146	-4	3	8	207	204	2	5	8	263	255	-2	8	8	126	118
0	7	7	263	-265	-3	1	8	761	793	-3	3	8	151	144	4	5	8	228	222	-1	8	8	78	-73
2	7	7	61	-61	-2	1	8	487	-477	-2	3	8	778	-793	5	5	8	203	-219	0	8	8	243	-247
4	7	7	270	263	-1	1	8	36	29	-1	3	8	269	-249	6	5	8	61	-53	2	8	8	60	-56
6	7	7	193	195	0	1	8	102	-128	0	3	8	265	-301	7	5	8	43	-56	3	8	8	111	111
8	7	7	75	-89	1	1	8	554	-578	1	3	8	41	-45	8	5	8	123	-117	4	8	8	78	79
9	7	7	53	-50	2	1	8	40	66	2	3	8	354	323	9	5	8	223	208	5	8	8	56	-51
-7	8	7	76	76	3	1	8	44	-10	3	3	8	184	171	10	5	8	69	71	6	8	8	156	149
-6	8	7	158	-168	5	1	8	528	504	4	3	8	315	298	11	5	8	53	61	7	8	8	117	-117
-5	8	7	110	-117	6	1	8	69	-63	5	3	8	92	-106	-11	6	8	60	74	-5	9	8	93	-100
-4	8	7	49	-49	7	1	8	99	-119	6	3	8	355	-335	-10	6	8	77	-75	-2	9	8	165	171
-3	8	7	272	-284	8	1	8	221	-211	7	3	8	139	123	-9	6	8	168	173	0	9	8	86	83
-1	8	7	99	96	9	1	8	328	-321	8	3	8	313	-305	-8	6	8	130	-126	1	9	8	72	76
2	8	7	198	196	10	1	8	34	15	9	3	8	45	-51	-7	6	8	89	-91	2	9	8	97	-105
3	8	7	203	-199	11	1	8	203	-202	10	3	8	56	65	-6	6	8	92	111	4	9	8	69	-68
5	8	7	70	-76	12	1	8	73	65	12	3	8	152	160	-5	6	8	74	-76	-13	0	9	232	222
-11	0	9	235	211	2	2	9	341	342	8	4	9	146	-152	6	7	9	176	172	8	1	10	91	-92
-9	0	9	318	-332	3	2	9	209	211	10	4	9	81	80	8	7	9	90	-84	9	1	10	138	-127
-7	0	9	274	-279	4	2	9	426	427	11	4	9	49	38	-6	8	9	94	-92	11	1	10	66	-66
-5	0	9	418	406	5	2	9	196	194	12	4	9	137	135	-5	8	9	88	-87	-12	2	10	92	-86
-3	0	9	411	359	7	2	9	48	-34	-11	5	9	122	131	-3	8	9	149	-155	-11	2	10	205	196
-1	0	9	805	-833	8	2	9	128	-131	-10	5	9	103	-99	-2	8	9	85	89	-10	2	10	100	87
1	0	9	903	-917	9	2	9	193	-208	-9	5	9	134	138	0	8	9	40	58	-8	2	10	210	182
3	0	9	300	-273	10	2	9	173	172	-8	5	9	166	-166	1	8	9	169	170	-7	2	10	323	-296
5	0	9	267	398	11	2	9	117	-114	-7	5	9	172	-164	2	8	9	119	-116	-5	2	10	635	-625
7	0	9	88	-81	12	2	9	144	161	-6	5	9	97	-90	4	8	9	40	-29	-4	2	10	440	-457
9	0	9	183	-177	13	2	9	43	47	-5	5	9	219	-212	5	8	9	162	-168	-2	2	10	305	-331
11	0	9	103	-122	-13	3	9	63	68	-4	5	9	230	246	-4	9	9	109	111	-1	2	10	159	179
13	0	9	64	73	-11	3	9	312	319	-3	5	9	179	178	-3	9	9	57	-58	1	2	10	259	-249
-12	1	9	249	-249	-10	3	9	67	65	-2	5	9	120	-107	-2	9	9	74	62	2	2	10	132	127
-11	1	9	266	266	-9	3	9	282	269	-1	5	9	222	223	-1	9	9	132	-137	3	2	10	484	-484
-10	1	9	66	76	-8	3	9	84	91	0	5	9	474	-482	2	9	9	42	-39	4	2	10	117	-133
-9	1	9	156	162	-7	3	9	69	-73	1	5	9	146	-139	2	9	9	120	120	5	2	10	91	-97
-8	1	9	364	366	-6	3	9	117	-106	2	5	9	237	-222	-12	0	10	253	-247	6	2	10	259	-264
-7	1	9	117	-111	-5	3	9	247	-264	3	5	9	314	-309	-10	0	10	154	123	7	2	10	243	241
-5	1	9	54	-24	-3	3	9	246	241	7	5	9	120	122	-8	0	10	532	491	8	2	10	114	103
-4	1	9	685	-648	-2	3	9	272	-253	9	5	9	46	46	-6	0	10	54	-40	9	2	10	104	95
-3	1	9	331	358	-1	3	9	582	578	-4	5	9	154	-148	-4	0	10	743	-699	10	2	10	137	145
-2	1	9	104	129	0	3	9	161	161	11	5	9	61	-56	-2	0	10	235	234	11	2	10	86	-86
-1	1	9	119	135	1	3	9	207	-227	-9	6	9	197	202	0	0	10	106	141	-12	3	10	95	-91
0	1	9	324	359	2	3	9	105	-108	-7	6	9	110	110	2	0	10	286	309	-11	3	10	74	82
1	1	9	122	-120	3	3	9	704	-688	-5	6	9	193	203	4	0	10	622	-640	-10	3	10	240	-247
2	1	9	567	569	5	3	9	201	-191	-4	6	9	168	-181	6	0	10	381	-408	-8	3	10	183	168
3	1	9	472	-465	6	3	9	107	-119	-3	6	9	63	66	8	0	10	121	-133	-6	3	10	498	474
4	1	9	234	-242	7	3	9	199	210	-1	6	9	241	-243	10	0	10	223	203	-5	3	10	109	121
5	1	9	43	-44	9	3	9	45	-20	-3	6	9	205	200	12	0	10	51	-44	-4	3	10	330	315
6	1	9	195	-209	10	3	9	82	75	0	6	9	92	-86	-13	1	10	129	125	-2	3	10	152	-163
7	1	9	81	-52	11	3	9	205	-212	-10	1	10	303	300	-10	1	10	228	-214	0	3	10	123	-134
8	1	9	203	202	-12	4	9	154	-161	2	6	9	68	86	-9	1	10	288	-253	1	3	10	280	-300
10	1	9	239	261	-10	4	9	296	-308	3	6	9	56	48	-8	1	10	54	64	2	3	10	608	619
11	1	9	113	-115	-8	4	9	81	-78	4	6	9	111	115	-7	1	10	298	-259	4	3	10	276	282
13	1	9	67	-70	-6	4	9	134	127	5	6	9	151	-156	-6	1	10	399	397	5	3	10	65	-52
-13	2	9	114	117	-4	4	9	295	298	-5	1	10	139	-130										

-2	5	10	256	-269	-11	0	11	159	160	3	2	11	76	-77	-6	5	11	101	99	-4	0	12	567	-533
-1	5	10	201	201	-9	0	11	76	70	4	2	11	48	-59	-5	5	11	257	-261	-2	0	12	279	287
2	5	10	193	188	-7	0	11	273	-305	5	2	11	64	55	-4	5	11	263	263	0	0	12	528	512
3	5	10	93	-70	-5	0	11	642	638	6	2	11	41	-56	-3	5	11	42	22	2	0	12	573	547
4	5	10	224	221	-3	0	11	451	486	8	2	11	338	-338	-2	5	11	173	164	4	0	12	141	-148
5	5	10	262	-243	-1	0	11	59	52	9	2	11	141	-142	-1	5	11	292	292	6	0	12	81	-87
6	5	10	144	-154	1	0	11	553	-574	11	2	11	89	-92	0	5	11	175	-179	8	0	12	101	92
7	5	10	109	-101	5	0	11	453	439	12	2	11	78	72	1	5	11	201	-214	10	0	12	231	250
8	5	10	103	-105	7	0	11	77	-96	-11	3	11	159	148	2	5	11	144	-148	-11	1	12	71	82
9	5	10	72	87	9	0	11	275	-289	-9	3	11	115	106	3	5	11	181	-182	-10	1	12	153	-161
-9	6	10	80	84	11	0	11	142	-146	-8	3	11	127	133	4	5	11	117	114	-9	1	12	183	-178
-3	6	10	222	-229	-13	1	11	63	-64	-7	3	11	264	-275	6	5	11	105	95	-8	1	12	172	-160
-7	6	10	70	-57	-12	1	11	286	-273	-6	3	11	151	-158	7	5	11	165	156	-7	1	12	278	-260
-6	6	10	50	41	-11	1	11	99	105	-5	3	11	241	-260	8	5	11	85	-77	-6	1	12	170	155
-5	6	10	164	-165	-8	1	11	127	145	-4	3	11	151	140	10	5	11	84	-95	-5	1	12	42	50
-4	6	10	316	309	-6	1	11	116	-93	-3	3	11	175	171	-9	6	11	134	133	-3	1	12	281	270
-3	6	10	105	109	-5	1	11	190	-218	-2	3	11	48	-64	-7	6	11	97	87	-2	1	12	255	-252
-2	6	10	275	260	-4	1	11	802	-810	-1	3	11	444	450	-6	6	11	127	131	-1	1	12	239	-237
-1	6	10	99	109	-3	1	11	271	260	0	3	11	224	191	-5	6	11	221	-224	0	1	12	178	-180
0	6	10	302	-323	-2	1	11	192	-218	1	3	11	182	188	-4	6	11	79	79	1	1	12	699	-679
1	6	10	58	56	-1	1	11	314	324	2	3	11	146	131	-3	6	11	296	-310	2	1	12	327	328
2	6	10	50	47	1	1	11	182	198	3	3	11	373	-372	-2	6	11	74	-72	3	1	12	129	-123
3	6	10	49	-45	1	1	11	65	53	4	3	11	88	92	1	6	11	250	248	4	1	12	53	52
4	6	10	193	187	2	1	11	288	293	5	3	11	59	62	3	6	11	55	-56	5	1	12	149	151
6	6	10	166	155	3	1	11	193	-194	6	3	11	79	-66	4	6	11	140	137	6	1	12	68	83
7	6	10	77	75	4	1	11	139	-135	7	3	11	301	305	5	6	11	153	-160	8	1	12	146	-133
-7	7	10	114	122	5	1	11	87	76	8	3	11	59	65	9	6	11	122	122	9	1	12	173	-182
-6	7	10	99	-100	6	1	11	169	-145	9	3	11	153	149	-8	7	11	147	-150	10	1	12	95	94
-5	7	10	155	-165	7	1	11	139	132	11	3	11	88	-82	-6	7	11	35	37	11	1	12	69	-71
-12	2	12	131	-133	3	4	12	365	-365	2	8	12	45	-52	10	2	13	48	-8	-3	6	13	212	-209
-11	2	12	234	232	4	4	12	63	-78	3	8	12	78	76	-11	3	13	138	141	-2	6	13	120	-129
-9	2	12	183	174	5	4	12	76	-73	-9	0	13	165	-143	-10	3	13	98	-93	-1	6	13	64	65
-8	2	12	282	272	7	4	12	219	217	-7	0	13	374	-360	-9	3	13	47	50	0	6	13	61	-58
-7	2	12	94	-110	8	4	12	41	-35	-3	0	13	560	555	-7	3	13	305	-290	1	6	13	124	121
-6	2	12	157	-159	-10	5	12	171	-176	1	0	13	409	-457	-5	3	13	447	-438	3	6	13	46	40
-5	2	12	158	-157	-9	5	12	103	97	-4	3	13	94	78	-4	3	13	89	-81	4	6	13	87	87
-4	2	12	136	-132	-7	5	12	128	109	5	0	13	371	380	-1	3	13	61	78	5	6	13	214	-218
-3	2	12	126	117	-6	5	12	248	242	7	0	13	72	73	0	3	13	112	142	7	6	13	85	-79
-1	2	12	472	441	-4	5	12	200	188	9	0	13	137	-140	1	3	13	77	-62	-5	7	13	69	65
0	2	12	274	270	-3	5	12	84	-100	-12	1	13	172	-167	2	3	13	60	84	-4	7	13	155	161
1	2	12	123	-123	-2	5	12	170	-187	-10	1	13	95	84	3	3	13	356	-354	-2	7	13	103	104
2	2	12	266	261	-1	5	12	187	184	-8	1	13	356	332	5	3	13	136	-145	0	7	13	128	-135
3	2	12	400	-398	1	5	12	337	327	-7	1	13	101	-97	7	3	13	248	235	2	7	13	146	-140
4	2	12	119	119	2	5	12	152	138	-6	1	13	92	75	9	3	13	88	94	3	7	13	54	57
5	2	12	102	-107	3	5	12	119	124	-5	1	13	236	-238	-10	4	13	157	-150	4	7	13	79	78
6	2	12	185	-186	4	5	12	195	198	-4	1	13	345	-353	-9	4	13	58	52	-2	8	13	84	83
7	2	12	68	63	5	5	12	99	-93	-3	1	13	245	-258	-7	4	13	70	70	1	8	13	148	147
8	2	12	60	62	6	5	12	107	-116	-2	1	13	63	-78	-6	4	13	380	375	-8	0	14	148	159
10	2	12	112	105	8	5	12	96	-99	-1	1	13	277	293	-5	4	13	106	-100	-6	0	14	78	-58
11	2	12	97	-107	9	5	12	95	98	0	1	13	241	245	-4	4	13	278	288	-4	0	14	486	-489
-12	3	12	132	-134	-8	6	12	213	-216	1	1	13	194	-188	-2	4	13	197	-208	-2	0	14	451	-466
-11	3	12	63	63	-7	6	12	48	-88	2	1	13	169	203	0	4	13	38	-50	0	0	14	243	262
-10	3	12	290	-299	-5	6	12	125	-122	3	1	13	290	-318	1	4	13	69	63	2	0	14	183	181
-8	3	12	48	-44	-4	6	12	168	173	4	1	13	118	-113	2	4	13	160	158	4	0	14	59	-62
-6	3	12	308	320	-2	6	12	59	64	5	1	13	72	77	3	4	13	43	-53	6	0	14	166	-152
-4	3	12	48	-49	-1	6	12	42	47	6	1	13	289	-296	4	4	13	218	219	8	0	14	126	128
-3	3	12	103	104	0	6	12	289	-282	9	1	13	108	92	5	4	13	65	-72	10	0	14	152	157
-2	3	12	261	-241	2	6	12	202	-195	10	1	13	116	114	6	4	13	135	-145	-11	1	14	119	122
0	3	12	216	-191	3	6	12	88	-90	-11	2	13	81	69	7	4	13	77	-80	-10	1	14	49	-50
1	3	12	21	-87	4	6	12	99	98	-10	2	13	173	-172	8	4	13	169	-164	-9	1	14	69	-76
2	3	12	300	292	5	6	12	34	-36	-9	2	13	134	-122	-9	5	13	97	85	-7	1	14	70	-86
3	3	12	61	-57	6	6	12	98	102	-8	2	13	130	122	-8	5	13	128	-132	-6	1	14	255	258
4	3	12	316	319	8	6	12	52	-49	-7	2	13	96	-85	-7	5	13	121	-140	-5	1	14	206	187
5	3	12	109	117	-7	7	12	100	105	-6	2	13	475	462	-6	5	13	57	-66	-3	1	14	381	382
8	3	12	156	-164	-5	7	12	106	-102	-5	2	13	139	139	-5	5	13	229	-214	-1	1	14	56	41
-11	4	12	200	206	-4	7	12	42	64	-4	2	13	132	129	-4	5	13	184	183	0	1	14	307	-316
-10	4	12	42	-44	-3	7	12	171	-171	-3	2	13	80	84	-2	5	13	110	121	1	1	14	357	-371
-9	4	12	173	177	-1	7	12	63	68	-2	2	13	76	67	-1	5	13	187	187	2	1	14	111	124
-7	4	12	102	-88	0	7	12	34	17	0	2	13	93	-105	0	5	13	122	-116	3	1	14	82	-81
-5	4	12	296	-291	1	7	12	206	205	1	2	13	289	-309	2	5	13	43	-43	5	1	14	187	178
-4	4	12	69	96																				

8	3	14	226	-214	5	0	15	201	193	-7	4	15	66	65	4	1	16	142	152	3	5	16	35	-43
-9	4	14	60	63	7	0	15	42	33	-6	4	15	276	279	5	1	16	219	219	4	5	16	103	95
-7	4	14	133	-145	9	0	15	126	-125	-4	4	15	96	84	7	1	16	117	115	5	5	16	90	-86
-6	4	14	57	52	-11	1	15	67	71	-3	4	15	62	-62	8	1	16	114	-109	-5	6	16	53	-48
-5	4	14	318	-325	-9	1	15	105	96	-2	4	15	218	-215	-9	2	16	112	105	-4	6	16	59	50
-4	4	14	213	211	-8	1	15	270	263	-1	4	15	150	153	-8	2	16	181	185	-2	6	16	124	137
-3	4	14	105	96	-6	1	15	135	134	0	4	15	163	-155	-7	2	16	175	-170	0	6	16	90	-93
-1	4	14	323	318	-5	1	15	108	-101	1	4	15	83	77	-6	2	16	101	105	2	6	16	141	-140
0	4	14	76	39	-4	1	15	139	-122	2	4	15	63	51	-5	2	16	225	-222	-7	0	17	117	-115
1	4	14	104	101	-3	1	15	52	42	4	4	15	147	143	1	2	16	92	-91	-5	0	17	86	89
3	4	14	122	-136	-1	1	15	148	142	5	4	15	49	-36	-3	2	16	86	-110	-3	0	17	328	321
5	4	14	54	44	0	1	15	371	377	8	4	15	107	-118	-2	2	16	79	-82	1	0	17	127	-127
6	4	14	63	63	1	1	15	74	85	-8	5	15	122	-120	0	2	16	172	183	3	0	17	159	-165
7	4	14	181	174	2	1	15	270	264	-6	5	15	63	-55	-1	2	16	182	189	5	0	17	196	197
8	4	14	52	-46	3	1	15	139	-132	-5	5	15	174	-166	3	2	16	208	-221	7	0	17	98	100
9	4	14	105	98	6	1	15	174	-176	-4	5	15	86	94	4	2	16	102	-86	-8	1	17	157	157
-7	5	14	84	83	7	1	15	107	97	-1	5	15	174	184	6	2	16	103	-95	-7	1	17	54	-47
-6	5	14	172	173	10	1	15	75	77	0	5	15	147	-144	7	2	16	127	122	-5	1	17	99	-89
-5	5	14	122	-131	-10	2	15	233	-230	2	5	15	119	-122	8	2	16	42	-31	-4	1	17	205	-212
-4	5	14	118	127	-9	2	15	89	-90	3	5	15	141	-139	-7	3	16	40	-44	-2	1	17	167	-164
-3	5	14	226	-220	-8	2	15	92	-82	5	5	15	45	-48	-6	3	16	332	336	-1	1	17	156	165
-2	5	14	174	-177	-7	2	15	128	-134	6	5	15	76	76	-4	3	16	112	128	0	1	17	150	158
0	5	14	84	-71	-6	2	15	146	140	7	5	15	100	102	-2	3	16	96	-100	2	1	17	127	120
4	1	17	47	-33	-3	4	17	13																

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	1-25	315	325	13		7	3-21	398	418	11		1	5-19	104	59	36		7	3-17	213	199	12		5	7-16	246	247	15	
5	1-25	316	301	12		9	3-21	217	214	15		3	5-19	125	113	27		9	3-17	105	95	29		7	7-16	109	90	35	
0	0-24	293	322	14		11	3-21	116	56	33		5	5-19	246	250	14		11	3-17	223	218	14		9	7-16	42	48	41	
2	0-24	373	389	11		0	4-21	502	477	9		7	5-19	167	169	20		13	3-17	250	242	14		0	8-16	354	363	12	
4	0-24	320	335	13		2	4-21	390	401	10		9	5-19	41	75	40		15	3-17	179	183	20		2	8-16	266	269	14	
6	0-24	246	254	16		4	4-21	230	212	14		11	5-19	90	26	56		0	4-17	306	310	10		4	8-16	303	302	13	
8	0-24	305	323	13		6	4-21	211	183	16		0	6-19	202	215	19		2	4-17	427	435	9		1	1-15	511	521	7	
1	1-24	139	183	20		8	4-21	238	246	15		2	6-19	99	147	43		4	4-17	619	621	8		3	1-15	476	470	7	
3	1-24	93	125	51		10	4-21	419	402	11		4	6-19	134	167	29		6	4-17	701	732	8		5	1-15	195	207	11	
5	1-24	139	111	27		1	5-21	94	72	48		6	6-19	301	291	12		8	4-17	324	323	10		7	1-15	410	402	7	
7	1-24	258	218	14		3	5-21	68	71	67		8	6-19	304	311	13		10	4-17	220	221	15		9	1-15	672	692	8	
9	1-24	148	141	26		5	5-21	150	109	25		0	0-18	328	317	9		12	4-17	467	467	10		11	1-15	645	636	8	
0	2-24	234	229	17		7	5-21	107	89	40		2	0-18	647	659	8		14	4-17	380	375	11		13	1-15	394	362	8	
2	2-24	218	219	17		9	5-21	67	37	67		4	0-18	940	918	8		1	5-17	144	161	21		15	1-15	177	181	18	
4	2-24	141	138	28		0	0-20	486	477	8		6	0-18	479	474	8		3	5-17	127	149	24		17	1-15	169	192	22	
6	2-24	171	176	23		2	0-20	463	488	8		8	0-18	607	657	8		5	5-17	142	163	22		0	2-15	196	188	11	
8	2-24	287	262	13		4	0-20	676	695	8		10	0-18	402	405	9		7	5-17	246	239	14		2	2-15	221	219	10	
3	3-24	359	359	12		6	0-20	98	77	34		12	0-18	111	38	29		9	5-17	294	263	12		4	2-15	259	252	9	
5	3-24	346	347	12		8	0-20	97	91	35		14	0-18	351	339	11		11	5-17	90	105	47		6	2-15	498	501	7	
1	1-23	337	314	11		10	0-20	534	557	9		16	0-18	413	396	10		13	5-17	101	140	44		8	2-15	354	345	8	
3	1-23	314	306	12		12	0-20	446	441	10		1	1-18	101	99	27		0	6-17	319	304	11		10	2-15	251	265	11	
5	1-23	301	320	12		14	0-20	322	321	12		3	1-18	734	714	7		2	6-17	281	297	13		12	2-15	242	244	12	
7	1-23	316	307	12		1	1-20	77	49	56		5	1-18	610	619	8		4	6-17	317	314	12		14	2-15	247	231	13	
9	1-23	213	229	17		3	1-20	205	205	15		7	1-18	35	48	35		6	6-17	253	262	14		16	2-15	257	252	13	
11	1-23	166	222	24		5	1-20	336	346	10		9	1-18	115	120	26		8	6-17	230	228	15		1	3-15	599	595	7	
0	2-23	249	224	15		7	1-20	196	192	15		11	1-18	103	58	31		10	6-17	214	205	17		3	3-15	318	316	8	
2	2-23	256	264	15		9	1-20	92	139	44		13	1-18	80	52	57		1	7-17	294	308	13		5	3-15	453	463	8	
4	2-23	187	171	18		11	1-20	39	9	39		15	1-18	136	160	27		3	7-17	251	233	14		7	3-15	278	262	10	
6	2-23	149	130	24		13	1-20	72	80	48		0	2-18	36	104	36		5	7-17	237	239	15		9	3-15	55	17	55	
8	2-23	218	205	16		0	2-20	201	191	15		2	2-18	104	392	8		7	7-17	315	338	12		11	3-15	175	186	16	
10	2-23	212	212	19		2	2-20	356	354	10		4	2-18	585	563	7		9	7-17	311	325	13		13	3-15	256	260	12	
1	3-23	95	19	47		4	2-20	357	363	10		6	2-18	588	579	7		0	0-16	115	101	20		15	3-15	158	180	22	
3	3-23	191	177	20		6	2-20	293	314	11		8	2-18	150	163	19		2	0-16	187	208	12		17	3-15	42	94	41	
5	3-23	282	285	13		8	2-20	101	139	35		10	2-18	81	64	49		4	0-16	920	914	8		0	4-15	513	503	8	
7	3-23	99	164	46		10	2-20	145	158	23		12	2-18	287	264	11		6	0-16	831	820	8		2	4-15	290	292	9	
9	3-23	42	85	42		12	2-20	241	256	15		14	2-18	225	224	16		8	0-16	612	582	7		4	4-15	484	476	7	
2	4-23	424	436	11		14	2-20	142	178	28		16	2-18	180	194	21		10	0-16	419	399	8		6	4-15	718	752	8	
4	4-23	219	218	17		1	3-20	309	296	11		1	3-18	453	451	8		12	0-16	390	394	9		8	4-15	478	474	8	
6	4-23	202	181	19		3	3-20	73	84	73		3	3-18	448	441	8		14	0-16	531	522	9		10	4-15	428	418	8	
0	0-22	602	605	9		5	3-20	245	254	13		5	3-18	546	535	8		16	0-16	364	358	11		12	1-15	415	421	9	
2	0-22	565	543	8		7	3-20	512	493	9		7	3-18	453	471	9		1	1-16	373	366	8		14	4-15	294	295	12	
4	0-22	207	214	15		9	3-20	323	336	11		9	3-18	386	376	9		3	1-16	507	508	7		16	4-15	280	288	14	
6	0-22	68	89	67		11	3-20	135	135	26		11	3-18	255	246	13		5	1-16	91	124	28		1	5-15	469	460	8	
8	0-22	197	199	17		13	3-20	127	147	31		13	3-18	86	107	55		7	1-16	69	70	51		3	5-15	193	189	14	
10	0-22	383	376	11		0	4-20	40	81	39		15	3-18	227	231	17		9	1-16	554	549	7		5	5-15	131	139	21	
12	0-22	525	521	10		2	4-20	131	124	26		0	4-18	38	87	37		11	1-16	206	209	13		7	5-15	89	98	37	
1	1-22	39	83	39		4	4-20	143	146	23		2	4-18	247	234	12		13	1-16	37	30	37		9	5-15	145	140	21	
3	1-22	95	52	39		6	4-20	243	229	14		4	4-18	213	199	13		15	1-16	164	144	20		11	5-15	293	320	12	
5	1-22	131	132	25		8	4-20	246	273	14		6	4-18	88	48	41		17	1-16	134	143	29		13	5-15	98	117	43	
7	1-22	155	134	22		10	4-20	41	79	41		8	4-18	38	58	38		0	2-16	644	635	7		15	5-15	42	77	42	
9	1-22	167	164	20		12	4-20	120	154	35		10	4-18	39	55	39		2	2-16	626	632	7		0	6-15	481	487	9	
11	1-22	175	140	20		1	5-20	216	224	16		12	4-18	63	122	63		4	2-16	325	323	7		2	6-15	805	816	8	
0	2-22	298	294	12		3	5-20	221	212	16		14	4-18	126	69	31		6	2-16	474	444	7		4	6-15	539	536	8	
2	2-22	332	318	10		5	5-20	221	242	16		1	5-18	329	305	10		8	2-16	269	263	10		6	6-15	37	82	37	
4	2-22	232	210	14		7	5-20	248	259	14		3	5-18	86	100	48		10	2-16	223	233	12		8	6-15	192	184	16	
6	2-22	219	218	16		9	5-20	306	293	12		5	5-18	208	193	15		12	2-16	309	293	10		10	6-15	284	283	12	
8	2-22	214	202	15		0	6-20	279	277	14		7	5-18	414	430	10		14	2-16	188	203	18		12	6-15	257	280	14	
10	2-22	185	211	20		2	6-20	189	195	19		9	5-18	357	351	11		16	2-16	269	265	14							

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
8	2-14	254	268	10	5	5-13	60	44	60	14	6-12	152	133	24	4	0-10	924	850	7	2	2-9	1062	1112	8	2	2-9	1062	1112	8
10	2-14	331	341	9	7	5-13	99	81	28	1	7-12	191	190	16	6	0-10	931	884	7	4	2-9	166	158	9	4	2-9	166	158	9
12	2-14	320	320	10	9	5-13	36	51	35	3	7-12	137	146	23	8	0-10	1416	1405	9	6	2-9	605	587	6	6	2-9	605	587	6
14	2-14	259	245	12	11	5-13	285	295	11	5	7-12	38	86	37	10	0-10	751	775	7	8	2-9	633	655	6	8	2-9	633	655	6
16	2-14	323	306	11	13	5-13	198	207	16	7	7-12	286	274	11	12	0-10	134	127	17	10	2-9	629	618	7	10	2-9	629	618	7
18	2-14	126	165	32	15	5-13	88	77	55	9	7-12	332	328	11	14	0-10	571	581	8	12	2-9	369	370	6	12	2-9	369	370	6
1	3-14	601	617	7	0	6-13	587	586	8	11	7-12	117	140	32	16	0-10	614	632	8	14	2-9	519	515	8	14	2-9	519	515	8
3	3-14	308	308	8	2	6-13	367	372	9	13	7-12	112	100	38	18	0-10	380	363	10	16	2-9	202	214	15	16	2-9	202	214	15
5	3-14	321	300	8	4	6-13	276	265	11	0	8-12	197	206	17	1	1-10	361	361	6	18	2-9	102	125	39	18	2-9	102	125	39
7	3-14	369	319	-8	6	6-13	365	356	9	2	8-12	242	242	14	3	1-10	658	631	6	1	3-9	845	844	7	1	3-9	845	844	7
9	3-14	489	511	8	8	6-13	368	371	9	4	8-12	357	375	11	5	1-10	376	359	6	3	3-9	737	751	7	3	3-9	737	751	7
11	3-14	782	770	8	10	6-13	211	219	15	6	8-12	489	488	9	7	1-10	173	164	9	5	3-9	343	328	6	5	3-9	343	328	6
13	3-14	377	392	10	12	6-13	211	230	16	8	8-12	428	409	10	9	1-10	66	74	36	7	3-9	56	65	56	7	3-9	56	65	56
15	3-14	105	91	36	14	6-13	337	325	12	10	8-12	172	189	23	11	1-10	295	301	8	9	3-9	327	327	7	9	3-9	327	327	7
17	3-14	241	232	15	1	7-13	413	433	9	1	9-12	42	5	41	13	1-10	684	687	8	11	3-9	682	693	8	11	3-9	682	693	8
0	4-14	34	88	33	3	7-13	406	407	9	3	9-12	84	96	84	15	1-10	422	433	9	13	3-9	144	168	18	13	3-9	144	168	18
2	4-14	390	398	8	5	7-13	358	341	10	5	9-12	122	97	32	17	1-10	152	154	21	15	3-9	121	86	25	15	3-9	121	86	25
4	4-14	253	226	10	7	7-13	206	198	16	1	1-11	948	971	7	19	1-10	41	69	41	17	3-9	196	225	17	17	3-9	196	225	17
6	4-14	184	175	14	9	7-13	298	286	12	3	1-11	1346	1307	8	0	2-10	103	78	15	0	4-9	599	595	6	0	4-9	599	595	6
8	4-14	220	212	12	11	7-13	377	389	11	5	1-11	416	423	6	2	2-10	452	455	5	2	4-9	750	761	7	2	4-9	750	761	7
10	4-14	68	61	67	0	8-13	59	110	58	7	1-11	482	497	6	4	2-10	669	672	6	4	4-9	966	931	8	4	4-9	966	931	8
12	4-14	104	108	30	2	8-13	227	193	14	9	1-11	716	720	7	6	2-10	1039	1041	8	6	4-9	1145	1115	9	6	4-9	1145	1115	9
14	4-14	77	65	77	4	8-13	78	13	77	11	1-11	337	347	8	8	2-10	437	423	6	8	4-9	615	645	7	8	4-9	615	645	7
16	4-14	147	119	25	6	8-13	174	152	20	13	1-11	339	355	9	10	2-10	53	85	53	10	4-9	409	363	-8	10	4-9	409	363	-8
1	5-14	709	727	8	8	8-13	41	24	41	15	1-11	410	409	9	12	2-10	525	520	7	12	4-9	555	543	8	12	4-9	555	543	8
3	5-14	244	250	11	1	9-13	43	90	43	17	1-11	219	223	15	14	2-10	376	377	8	14	4-9	411	404	9	14	4-9	411	404	9
5	5-14	189	184	14	3	9-13	315	284	12	19	1-11	174	193	22	16	2-10	159	175	19	16	4-9	377	366	10	16	4-9	377	366	10
7	5-14	464	443	8	0	0-12	600	631	6	0	2-11	933	900	7	18	2-10	206	198	16	18	4-9	269	303	15	18	4-9	269	303	15
9	5-14	430	438	9	2	0-12	421	441	6	2	2-11	899	868	7	1	3-10	1301	1284	9	1	5-9	510	498	7	1	5-9	510	498	7
11	5-14	306	293	10	4	0-12	1037	1031	8	4	2-11	369	372	6	3	3-10	1218	1207	9	3	5-9	178	168	11	3	5-9	178	168	11
13	5-14	237	244	15	6	0-12	1358	1349	9	6	2-11	208	208	9	5	3-10	91	88	20	5	5-9	253	267	9	5	5-9	253	267	9
15	5-14	206	198	17	8	0-12	1145	1156	9	8	2-11	359	341	7	7	3-10	758	745	7	7	5-9	309	305	9	7	5-9	309	305	9
0	6-14	234	238	12	10	0-12	561	563	7	10	2-11	234	231	10	9	3-10	603	583	7	9	5-9	58	79	57	9	5-9	58	79	57
2	6-14	84	61	42	12	0-12	227	239	11	12	2-11	332	331	9	11	3-10	306	313	9	11	5-9	55	83	55	11	5-9	55	83	55
4	6-14	316	293	10	14	0-12	276	270	11	14	2-11	427	421	8	13	3-10	679	668	8	13	5-9	440	431	9	13	5-9	440	431	9
6	6-14	362	356	9	16	0-12	256	239	12	16	2-11	93	75	40	15	3-10	453	445	9	15	5-9	163	150	21	15	5-9	163	150	21
8	6-14	38	33	38	18	0-12	390	384	11	18	2-11	126	45	29	17	3-10	183	186	18	17	5-9	41	80	41	17	5-9	41	80	41
10	6-14	59	64	58	1	1-12	1140	1083	9	1	3-11	410	428	6	0	4-10	273	274	8	0	6-9	591	573	7	0	6-9	591	573	7
12	6-14	196	190	18	3	1-12	665	698	6	3	3-11	311	311	7	2	4-10	801	801	7	2	6-9	223	228	11	2	6-9	223	228	11
14	6-14	241	228	16	5	1-12	85	106	21	5	3-11	592	579	7	4	4-10	97	95	21	4	6-9	839	838	8	4	6-9	839	838	8
1	7-14	198	196	16	7	1-12	97	114	20	7	3-11	355	353	7	6	4-10	457	462	7	6	6-9	633	636	8	6	6-9	633	636	8
3	7-14	365	363	10	9	1-12	370	362	7	9	3-11	106	112	22	8	4-10	106	99	21	8	6-9	192	188	13	8	6-9	192	188	13
5	7-14	280	300	12	11	1-12	310	302	8	11	3-11	430	436	6	10	4-10	34	67	33	10	6-9	432	422	8	10	6-9	432	422	8
7	7-14	159	149	20	13	1-12	251	258	11	13	3-11	355	359	9	12	4-10	35	53	35	12	6-9	273	258	12	12	6-9	273	258	12
9	7-14	112	143	34	15	1-12	245	227	13	15	3-11	119	139	27	14	4-10	177	169	17	14	6-9	191	194	17	14	6-9	191	194	17
11	7-14	138	93	26	17	1-12	39	51	39	17	3-11	211	188	16	16	4-10	91	55	45	16	7-9	512	504	8	16	7-9	512	504	8
0	8-14	249	207	14	19	1-12	42	35	42	0	4-11	465	461	6	1	5-10	465	465	7	3	7-9	453	458	8	3	7-9	453	458	8
2	8-14	370	359	11	0	2-12	285	230	-7	2	4-11	802	844	8	3	5-10	800	814	8	5	7-9	572	594	8	5	7-9	572	594	8
4	8-14	395	386	10	2	2-12	568	577	6	4	4-11	789	789	7	5	5-10	975	968	8	7	7-9	282	280	11	7	7-9	282	280	11
6	8-14	274	276	14	4	2-12	578	580	6	6	4-11	1032	1027	8	7	5-10	402	390	7	9	7-9	406	406	9	9	7-9	406	406	9
8	8-14	335	344	12	6	2-12	604	601	7	8	4-11	901	922	8	9	5-10	336	309	8	11	7-9	448	461	10	11	7-9	448	461	10
1	1-13	923	923	7	8	2-12	485	509	7	10	4-11	503	492	8	11	5-10	458	447	9	13	7-9	231	217	15	13	7-9	231	217	15
3	1-13	110	90	16	10	2-12	268	274	9	12	4-11	320	312	9	13	5-10	151	178	20	0	8-9	113	50	29	0	8-9			

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
14	2	-0	303	298	9	19	3	-7	42	76	42	19	3	-6	275	268	14	18	4	-5	390	387	11	18	4	-4	42	25	41
16	2	-8	194	185	16	0	4	-7	795	790	7	0	4	-6	239	220	7	1	5	-5	405	411	6	1	5	-4	750	784	7
16	2	-8	260	263	14	2	4	-7	819	827	7	2	4	-6	98	78	14	3	5	-5	459	459	6	3	5	-4	937	931	8
3	3	-8	1736	1783	8	4	4	-7	860	828	7	4	4	-6	54	68	53	5	5	-5	77	71	27	5	5	-4	889	900	8
3	3	-8	787	767	7	6	4	-7	1053	1031	6	6	4	-6	613	575	6	7	5	-5	256	262	9	7	5	-4	612	583	6
5	3	-8	241	240	7	8	4	-7	675	577	7	8	4	-6	302	301	7	9	5	-5	484	480	7	9	5	-4	274	243	9
7	3	-8	858	868	7	10	4	-7	449	460	7	10	4	-6	292	285	8	11	5	-5	219	213	12	11	5	-4	280	281	10
9	3	-8	399	411	7	12	4	-7	603	583	7	12	4	-6	287	286	10	13	5	-5	154	147	18	13	5	-4	367	386	10
11	3	-8	447	442	7	14	4	-7	415	415	9	14	4	-6	105	110	29	15	5	-5	39	9	38	15	5	-4	362	362	10
13	3	-8	676	701	8	16	4	-7	410	407	10	16	4	-6	68	71	67	17	5	-5	145	153	26	17	5	-4	290	288	13
15	3	-8	410	377	9	18	4	-7	370	370	11	18	4	-6	72	58	72	0	6	-5	849	874	8	0	6	-4	102	101	20
17	3	-8	336	343	11	1	5	-7	766	772	7	1	5	-6	478	460	6	2	6	-5	564	548	7	2	6	-4	115	86	17
0	4	-8	458	457	6	3	5	-7	371	363	7	3	5	-6	662	657	6	4	6	-5	32	48	31	4	6	-4	438	443	7
2	4	-8	556	526	6	5	5	-7	93	67	21	5	5	-6	438	445	7	6	6	-5	238	218	10	6	6	-4	443	430	7
4	4	-8	50	48	50	7	5	-7	96	82	22	7	5	-6	262	270	9	8	6	-5	827	802	8	8	6	-4	476	459	7
6	4	-8	236	225	9	9	5	-7	67	84	57	9	5	-6	640	627	7	10	6	-5	668	667	8	10	6	-4	460	457	8
8	4	-8	64	109	48	11	5	-7	385	392	8	11	5	-6	595	502	8	12	6	-5	279	282	11	12	6	-4	114	112	27
10	4	-8	475	481	7	13	5	-7	176	172	16	13	5	-6	342	331	10	14	6	-5	240	250	14	14	6	-4	39	22	39
12	4	-8	35	31	34	15	5	-7	78	40	74	15	5	-6	316	320	12	16	6	-5	245	238	15	16	6	-4	156	164	25
14	4	-8	316	317	10	17	5	-7	178	179	21	17	5	-6	268	274	14	1	7	-5	314	292	8	1	7	-4	118	96	20
16	4	-8	83	27	56	0	6	-7	764	771	7	0	6	-6	344	338	7	3	7	-5	834	842	8	3	7	-4	167	138	14
18	4	-8	42	7	41	2	6	-7	404	412	7	2	6	-6	203	187	10	5	7	-5	826	823	8	5	7	-4	570	566	8
1	5	-8	494	487	6	4	6	-7	423	420	7	4	6	-6	165	138	13	7	7	-5	348	347	9	7	7	-4	428	435	8
3	5	-8	575	560	7	6	6	-7	120	131	19	6	6	-6	505	454	7	9	7	-5	370	346	9	9	7	-4	158	186	18
5	5	-8	886	870	8	8	6	-7	328	316	9	8	6	-6	353	354	8	11	7	-5	420	422	9	11	7	-4	126	151	25
7	5	-8	216	202	10	10	6	-7	909	908	9	10	6	-6	308	317	11	13	7	-5	400	394	10	13	7	-4	158	148	22
9	5	-8	208	196	12	12	6	-7	492	502	9	12	6	-6	267	245	11	0	8	-5	55	19	54	0	8	-4	827	826	8
11	5	-8	534	535	7	14	6	-7	158	172	21	14	6	-6	115	157	32	2	8	-5	36	44	35	2	8	-4	709	703	8
13	5	-8	347	377	10	16	6	-7	103	119	44	16	6	-6	140	125	28	4	8	-5	217	191	13	4	8	-4	451	441	9
15	5	-8	319	296	11	1	7	-7	356	342	9	1	7	-6	335	318	9	6	8	-5	38	56	37	6	8	-4	370	356	9
17	5	-8	213	206	17	3	7	-7	304	299	9	3	7	-6	146	138	17	8	8	-5	70	87	70	8	8	-4	338	339	10
0	6	-8	274	268	9	5	7	-7	574	559	8	5	7	-6	35	92	34	10	8	-5	39	15	39	10	8	-4	339	347	11
2	6	-8	354	355	6	7	7	-7	338	319	9	7	7	-6	413	413	8	12	8	-5	41	58	41	12	8	-4	324	299	12
4	6	-8	280	287	9	9	7	-7	400	421	9	9	7	-6	331	338	10	1	9	-5	453	453	9	1	9	-4	67	54	67
6	6	-8	87	71	31	11	7	-7	401	408	10	11	7	-6	313	300	11	3	9	-5	381	367	10	3	9	-4	98	134	38
8	6	-8	87	116	35	13	7	-7	332	305	11	13	7	-6	344	338	11	5	9	-5	386	378	10	5	9	-4	125	165	27
10	6	-8	443	443	9	0	8	-7	167	157	17	0	8	-6	477	461	8	7	9	-5	327	325	12	7	9	-4	87	50	51
12	6	-8	298	273	11	2	8	-7	36	58	36	2	8	-6	381	364	9	9	9	-5	84	89	69	9	9	-4	83	69	54
14	6	-8	110	73	73	4	8	-7	172	169	17	4	8	-6	396	382	9	0	10	-5	262	284	14	0	10	-4	398	397	10
16	6	-8	165	165	23	6	8	-7	112	113	20	6	8	-6	390	380	9	2	10	-5	41	87	41	2	10	-4	290	308	13
1	7	-8	522	513	7	8	8	-7	100	145	37	8	8	-6	435	420	9	4	10	-5	41	58	41	4	10	-4	113	129	36
3	7	-8	517	507	3	10	8	-7	40	22	40	10	8	-6	405	418	10	0	0	-4	782	819	5	6	10	-4	307	318	14
5	7	-8	59	71	59	12	8	-7	82	68	82	12	8	-6	304	315	13	2	0	-4	1197	1176	5	1	1	-3	924	867	5
7	7	-8	36	44	35	1	9	-7	500	493	9	1	9	-6	94	15	40	4	0	-4	2424	2464	5	3	1	-3	1066	1055	5
9	7	-8	379	384	10	3	9	-7	449	425	9	3	9	-6	89	89	44	6	0	-4	2463	2525	6	5	1	-3	1160	1132	6
11	7	-8	399	397	10	5	9	-7	221	222	15	5	9	-6	89	73	46	8	0	-4	1545	1469	8	7	1	-3	895	892	7
13	7	-8	195	204	18	7	9	-7	332	322	11	7	9	-6	111	101	34	10	0	-4	568	580	6	9	1	-3	403	415	5
15	7	-8	406	425	9	9	9	-7	290	290	13	9	9	-6	41	75	41	12	0	-4	281	284	8	11	1	-3	576	595	6
2	8	-8	229	217	13	0	10	-7	169	166	22	0	10	-6	299	321	13	14	0	-4	604	640	7	13	1	-3	763	783	8
4	8	-8	493	493	9	2	10	-7	42	108	42	2	10	-6	376	372	12	16	0	-4	513	540	8	15	1	-3	527	525	8
6	8	-8	563	528	8	4	10	-7	88	47	62	4	10	-6	141	171	28	18	0	-4	367	372	10	17	1	-3	317	305	10
8	8	-8	403	404	10	0	0	-6	1071	1142	6	1	1	-5	1002	958	6	1	1	-4	799	736	5	19	1	-3	233	234	15
10	8	-8	355	343	11	2	0	-6	2382	2438	6	3	1	-5	1090	1095	6	3	1	-4	318	311	4	0	2	-3	370	358	4
12	8	-8	202	198	18	4	0	-6	2781	2960	6	5	1	-5	605	604	5	5	1	-4	311	314	5	2	2	-3	1258	1229	6
1	9	-8	40	49	39	6	0	-6	1133	1115	7	7	1	-5	1095	1037	8	7	1	-4	629	601	5	4	2	-3	704	711	6
3	9	-8	95	76	40	8	0	-6	836	739	7	9	1	-5	1207	1176	9	9	1	-4	1288	1238	8	6	2	-3	633	627	6
5	9	-8	100	65	39	10	0	-6	618	608	6	11	1	-5	264	277	8	11	1	-4	424	416	6	8	2	-3	1404	1444	8
7	9	-8	128	87	28	12	0	-6	229	227	9	13	1	-5	124	132	18	13	1	-4	88	51	27	10	2	-3	916	935	8
9	9	-8	42	8	41</																								

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
17	5	-3	42	44	41	17	5	-2	351	338	12	3	7	-1	675	675	7	7	7	0	278	273	10	5	9	1	108	139	35
0	6	-3	650	641	6	0	6	-2	448	443	7	5	7	-1	656	668	7	9	7	0	559	562	8	7	9	1	323	312	12
2	6	-3	442	447	7	2	6	-2	243	251	8	7	7	-1	329	326	9	11	7	0	332	309	10	9	9	1	374	356	11
4	6	-3	941	928	8	4	6	-2	64	67	50	9	7	-1	412	427	9	13	7	0	117	101	33	0	10	1	42	40	41
6	6	-3	976	970	8	6	6	-2	300	295	8	1	7	-1	406	413	9	0	8	0	319	305	9	2	10	1	196	183	19
8	6	-3	296	298	9	8	6	-2	529	538	7	13	7	-1	203	220	17	2	8	0	497	517	8	4	10	1	216	189	16
10	6	-3	128	81	21	10	6	-2	263	260	11	0	8	-1	144	151	18	4	8	0	546	545	8	6	10	1	139	177	29
12	6	-3	225	219	14	12	6	-2	143	140	21	2	8	-1	92	135	35	6	8	0	326	321	10	2	0	2	534	448	-4
14	6	-3	388	383	10	14	6	-2	187	175	17	4	8	-1	311	295	10	8	8	0	435	416	9	4	0	2	1967	2067	6
16	6	-3	360	343	11	16	6	-2	184	165	20	6	8	-1	37	37	37	10	8	0	430	421	10	6	0	2	782	921	6
1	7	-3	821	797	8	1	7	-2	322	310	8	8	8	-1	38	29	38	12	8	0	264	286	15	8	0	2	136	135	10
3	7	-3	955	966	9	3	7	-2	441	440	8	10	8	-1	40	54	39	1	9	0	221	201	14	10	0	2	1270	1279	9
5	7	-3	667	652	7	5	7	-2	438	451	8	12	8	-1	97	51	44	3	9	0	140	154	23	12	0	2	1160	1169	9
7	7	-3	316	311	9	7	7	-2	402	394	8	1	9	-1	379	393	9	5	9	0	134	146	26	14	0	2	467	480	8
9	7	-3	348	337	9	9	7	-2	296	299	11	3	9	-1	451	462	9	7	9	0	40	97	40	16	0	2	414	404	9
11	7	-3	389	389	10	11	7	-2	88	71	45	5	9	-1	276	246	12	9	9	0	136	169	28	18	0	2	262	240	13
13	7	-3	269	256	13	13	7	-2	96	80	43	7	9	-1	305	311	12	0	10	0	261	248	14	1	1	2	970	1015	4
0	8	-3	36	11	35	0	8	-2	612	596	8	9	9	-1	371	371	11	2	10	0	338	350	12	3	1	2	463	470	4
2	8	-3	149	154	19	2	8	-2	690	674	8	0	10	-1	41	77	40	4	10	0	350	342	11	5	1	2	1578	1637	6
4	8	-3	52	57	51	4	8	-2	652	672	8	2	10	-1	192	207	19	6	10	0	293	293	14	7	1	2	979	982	7
6	8	-3	71	82	70	6	8	-2	316	303	10	4	10	-1	193	224	20	1	1	1	1100	1129	4	9	1	2	28	27	27
8	8	-3	38	52	37	8	8	-2	280	225	-11	6	10	-1	43	102	42	3	1	1	155	153	5	11	1	2	193	193	11
10	8	-3	78	64	78	10	8	-2	370	358	10	4	0	0	2757	2969	5	5	1	1	1424	1439	6	13	1	2	99	57	25
12	8	-3	120	42	32	12	8	-2	253	267	15	6	0	0	541	606	5	7	1	1	998	995	8	15	1	2	300	291	11
1	9	-3	391	377	9	1	9	-2	119	91	26	9	0	0	456	461	5	9	1	1	314	287	6	17	1	2	274	298	13
3	9	-3	485	470	9	3	9	-2	106	93	33	10	0	0	1172	1213	9	11	1	1	590	585	7	19	1	2	108	129	40
5	9	-3	468	467	9	5	9	-2	181	168	17	12	0	0	1206	1238	9	13	1	1	536	537	7	0	2	2	170	162	5
7	9	-3	286	278	12	7	9	-2	40	24	39	14	0	0	349	339	8	15	1	1	310	316	10	2	2	2	1589	1669	6
9	9	-3	183	168	19	9	9	-2	75	49	75	16	0	0	356	356	10	17	1	1	310	300	11	4	2	2	791	764	4
0	10	-3	203	174	17	0	10	-2	333	339	11	18	0	0	320	326	12	19	1	1	268	272	14	6	2	2	584	618	6
2	10	-3	83	111	72	2	10	-2	315	329	12	1	1	0	105	69	-5	2	2	1	608	601	5	8	2	2	1083	1091	8
4	10	-3	225	213	17	4	10	-2	352	388	11	3	1	0	952	992	5	4	2	1	385	399	4	10	2	2	440	442	7
6	10	-3	208	201	18	6	10	-2	387	385	11	5	1	0	2775	3038	-6	6	2	1	591	591	6	12	2	2	222	235	10
2	0	-2	2045	2207	4	1	1	-1	2091	2135	3	7	1	0	156	162	8	8	2	1	376	352	6	14	2	2	247	245	11
4	0	-2	179	181	5	3	1	-1	1608	1643	5	9	1	0	822	818	7	10	2	1	375	392	7	16	2	2	181	173	17
6	0	-2	972	976	7	5	1	-1	1699	1724	6	11	1	0	556	565	7	12	2	1	615	608	7	18	2	2	330	321	12
8	0	-2	1238	1295	8	7	1	-1	132	116	9	13	1	0	394	373	7	14	2	1	85	114	38	1	3	2	1373	1370	7
10	0	-2	1321	1306	9	9	1	-1	304	287	6	15	1	0	66	35	66	16	2	1	228	208	13	3	3	2	1009	1033	7
12	0	-2	1094	1084	9	11	1	-1	927	904	8	17	1	0	145	160	22	18	2	1	270	245	13	5	3	2	829	892	7
14	0	-2	555	572	7	13	1	-1	918	942	8	19	1	0	185	161	19	1	3	1	512	514	5	7	3	2	1073	1121	8
16	0	-2	437	447	8	15	1	-1	443	454	8	0	2	0	125	98	-7	3	3	1	1203	1197	7	9	3	2	561	550	7
18	0	-2	435	437	10	17	1	-1	235	243	14	2	2	0	1456	1502	5	5	3	1	502	472	5	11	3	2	397	386	7
1	1	-2	764	747	4	19	1	-1	129	138	30	4	2	0	930	992	6	7	3	1	997	972	8	13	3	2	644	617	7
3	1	-2	1546	1604	5	2	2	-1	123	128	7	6	2	0	101	101	11	9	3	1	1043	1038	8	15	3	2	347	344	10
5	1	-2	1254	1266	6	4	2	-1	1363	1345	6	8	2	0	496	525	5	11	3	1	164	151	13	17	3	2	329	310	11
7	1	-2	1313	1337	7	6	2	-1	974	967	7	10	2	0	666	655	6	13	3	1	136	120	19	0	4	2	93	94	14
9	1	-2	215	205	7	8	2	-1	703	681	6	12	2	0	632	652	7	15	3	1	179	188	17	2	4	2	319	291	5
11	1	-2	497	515	7	10	2	-1	462	462	6	14	2	0	350	352	9	17	3	1	174	166	19	4	4	2	82	42	19
13	1	-2	550	526	7	12	2	-1	608	616	7	16	2	0	37	40	37	0	4	1	1815	1837	8	6	4	2	205	193	8
15	1	-2	188	181	14	14	2	-1	35	78	34	18	2	0	274	238	13	2	4	1	1458	1416	8	8	4	2	126	117	17
17	1	-2	38	27	37	16	2	-1	60	24	59	1	1	0	1409	1437	6	4	4	1	518	550	5	10	4	2	166	181	14
19	1	-2	72	118	71	18	2	-1	314	312	12	3	3	0	1459	1466	7	6	4	1	301	316	7	12	4	2	188	167	13
0	2	-2	156	149	6	1	3	-1	635	602	5	5	3	0	856	861	6	8	4	1	878	886	8	14	4	2	93	91	39
2	2	-2	328	543	5	3	3	-1	1478	1479	7	7	3	0	741	795	6	10	4	1	890	876	8	16	4	2	74	75	73
4	2	-2	524	526	5	5	3	-1	774	733	6	9	3	0	348	343	7	12	4	1	703	715	8	1	5	2	162	120	10
6	2	-2	470	472	5	7	3	-1	481	459	6	11	3	0	382	393	7	14	4	1	468	460	8	3	5	2	462	464	6
8	2	-2	786	812	7	9	3	-1	781	762	7	13	3	0	609	632	8	16	4	1	229	266	16	5	5	2	715	754	7
10	2	-2	499	490	6	11	3	-1	87	128	27	15	3	0	424	413	9	1	5	1	236	248	7	7	5	2	690		

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	10	2	247	255	16	7	1	4	1029	999	8	1	3	5	715	730	6	17	3	6	292	301	14	6	6	7	330	323	9
4	10	2	172	182	22	9	1	4	547	581	6	3	3	5	1093	1048	8	0	4	6	223	219	8	8	6	7	350	367	10
1	1	3	400	421	4	11	1	4	134	122	15	5	3	5	631	587	6	2	4	6	28	84	27	10	6	7	267	275	12
3	1	3	504	494	4	13	1	4	101	100	26	7	3	5	179	189	10	4	4	6	299	313	7	12	6	7	410	405	10
5	1	3	1251	1243	7	15	1	4	266	254	11	9	3	5	195	190	11	6	4	6	91	107	24	14	6	7	408	402	11
7	1	3	1604	1655	8	17	1	4	289	271	13	11	3	5	226	237	11	8	4	6	196	204	12	1	7	7	912	922	9
9	1	3	791	849	7	0	2	4	8	107	10	13	3	5	246	254	12	10	4	6	35	32	34	3	7	7	528	535	8
11	1	3	383	391	7	2	2	4	1316	1288	6	15	3	5	312	308	11	12	4	6	68	52	68	5	7	7	207	211	14
13	1	3	338	332	9	4	2	4	799	778	6	17	3	5	265	250	14	14	4	6	215	192	15	7	7	7	504	490	9
15	1	3	464	455	8	6	2	4	810	815	7	0	4	5	795	820	7	16	4	6	124	105	31	9	7	7	420	440	10
17	1	3	452	449	9	8	2	4	729	722	7	2	4	5	1419	1417	9	1	5	6	766	782	7	11	7	7	250	297	14
0	2	3	365	385	4	10	2	4	186	183	11	4	4	5	788	794	7	3	5	6	728	716	7	0	8	7	161	159	18
2	2	3	1032	1090	6	12	2	4	253	253	10	6	4	5	547	537	6	5	5	6	270	259	9	2	8	7	58	100	57
4	2	3	1184	1184	7	14	2	4	316	348	10	8	4	5	566	573	7	7	5	6	377	363	8	4	8	7	39	54	38
6	2	3	689	632	6	16	2	4	297	326	12	10	4	5	577	575	7	9	5	6	598	610	7	6	8	7	181	156	18
8	2	3	209	227	7	18	2	4	342	333	12	12	4	5	692	678	8	11	5	6	540	519	8	8	8	7	41	62	40
10	2	3	302	299	7	1	3	4	197	203	6	14	4	5	495	499	9	13	5	6	424	421	10	10	8	7	92	107	56
12	2	3	477	487	7	3	3	4	737	760	6	16	4	5	240	280	16	15	5	6	317	322	12	1	9	7	241	231	14
14	2	3	463	463	8	5	3	4	1087	1029	8	1	5	5	29	61	28	0	6	6	329	342	8	3	9	7	279	272	14
16	2	3	200	207	16	7	3	4	1199	1185	9	3	5	5	54	87	54	2	6	6	746	746	7	5	9	7	303	300	13
18	2	3	133	141	29	9	3	4	648	651	7	5	5	5	246	261	9	4	6	6	488	504	7	7	9	7	265	265	15
1	3	3	928	919	7	11	3	4	374	372	8	7	5	5	489	508	7	6	6	6	252	256	11	0	10	7	187	169	21
3	3	3	935	932	7	13	3	4	488	489	8	9	5	5	154	156	16	8	6	6	171	151	15	2	10	7	284	284	14
5	3	3	422	417	5	15	3	4	335	342	10	11	5	5	133	145	22	10	6	6	123	113	25	0	0	8	2131	2155	7
7	3	3	615	612	6	17	3	4	334	333	12	13	5	5	103	88	36	12	6	6	173	176	20	2	0	8	587	609	5
9	3	3	409	412	7	0	4	4	144	142	10	15	5	5	205	176	17	14	6	6	307	290	13	4	0	8	346	337	6
11	3	3	155	156	15	2	4	4	585	566	6	0	6	5	837	855	8	1	7	6	482	479	8	6	0	8	635	599	6
13	3	3	149	149	18	4	4	4	132	120	12	2	6	5	626	605	7	3	7	6	497	491	8	8	0	8	1414	1451	10
15	3	3	143	123	21	6	4	4	103	115	18	4	6	5	533	538	7	5	7	6	399	406	9	10	0	8	1388	1394	10
17	3	3	225	192	16	8	4	4	159	169	13	6	6	5	448	457	8	7	7	6	80	63	51	12	0	8	366	373	9
0	4	3	879	864	7	10	4	4	193	202	13	8	6	5	368	371	9	9	7	6	39	86	39	14	0	8	38	37	38
2	4	3	1068	1119	8	12	4	4	112	101	25	10	6	5	325	314	10	11	7	6	239	244	15	16	0	8	442	431	10
4	4	3	695	716	6	14	4	4	179	151	17	12	6	5	250	241	13	0	8	6	436	448	9	1	1	8	169	167	8
6	4	3	535	528	6	16	4	4	41	77	41	14	6	5	365	392	12	2	8	6	474	489	8	3	1	8	543	542	5
8	4	3	868	891	8	1	5	4	529	521	6	1	7	5	373	370	8	4	8	6	405	421	10	5	1	8	1264	1235	9
10	4	3	645	673	7	3	5	4	464	436	6	3	7	5	657	667	8	6	8	6	349	343	11	7	1	8	76	71	28
12	4	3	598	608	8	5	5	4	428	430	7	5	7	5	373	388	9	8	8	6	315	324	12	9	1	8	265	270	9
14	4	3	531	525	9	7	5	4	573	562	7	7	7	5	242	258	12	10	8	6	286	382	11	11	1	8	576	585	7
16	4	3	278	265	13	9	5	4	621	636	7	9	7	5	498	504	9	1	9	6	129	111	27	13	1	8	412	402	9
1	5	3	126	119	13	11	5	4	341	337	9	11	7	5	415	413	10	3	9	6	82	77	69	15	1	8	75	77	75
3	5	3	591	593	7	13	5	4	205	204	16	13	7	5	262	264	16	5	9	6	137	44	27	17	1	8	137	87	29
5	5	3	388	396	7	15	5	4	387	399	11	0	8	5	79	32	47	7	9	6	119	129	35	0	2	8	575	572	5
7	5	3	497	476	7	0	6	4	78	46	31	2	8	5	51	116	60	0	10	6	321	327	12	2	2	8	923	955	8
9	5	3	239	261	11	2	6	4	784	782	7	4	8	5	264	257	12	2	10	6	294	287	14	4	2	8	1240	1226	9
11	5	3	36	48	35	4	6	4	714	719	7	6	8	5	39	35	38	1	1	7	911	921	7	6	2	8	189	232	-10
13	5	3	38	84	38	6	6	4	146	153	17	8	8	5	128	114	18	3	1	7	421	422	5	8	2	8	223	232	10
15	5	3	91	102	49	8	6	4	85	92	36	10	8	5	41	7	19	5	1	7	706	668	6	10	2	8	445	431	7
0	6	3	620	673	7	10	6	4	148	129	19	1	9	5	253	273	14	7	1	7	606	599	7	12	2	8	374	381	9
2	6	3	651	656	7	12	6	4	209	201	15	3	9	5	212	234	17	9	1	7	617	627	7	14	2	8	382	374	10
4	6	3	556	553	7	14	6	4	311	325	12	5	9	5	473	460	9	11	1	7	743	744	8	16	2	8	168	165	22
6	6	3	441	424	7	1	7	4	289	283	9	7	9	5	342	362	12	13	1	7	389	371	8	1	3	8	331	332	6
8	6	3	564	565	8	3	7	4	590	595	8	0	10	5	293	287	13	15	1	7	101	114	36	3	3	8	373	409	6
10	6	3	589	599	8	5	7	4	733	734	8	2	10	5	195	217	20	17	1	7	245	225	15	5	3	8	808	796	6
12	6	3	132	67	24	7	7	4	255	251	11	4	10	5	148	168	28	0	2	7	690	688	6	7	3	8	485	484	7
14	6	3	80	49	79	9	7	4	120	61	6	0	0	6	1119	1114	6	2	2	7	284	287	6	9	3	8	795	772	7
1	7	3	252	247	10	11	7	4	151	144	21	2	0	6	1220	1246	6	4	2	7	1066	1064	9	11	3	8	716	726	8
3	7	3	349	373	5	13	7	4	216	233	17	4	0	6	2052	2044	7	6	2	7	665	644	7	13	3	8	280	287	12
5	7	3	807	814	8	0	8	4	799	823	9	6	0	6	1196	1194	8	8	2	7	83	92	25	15	3	8	202	210	18

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
8	8	8	313	306	12	14	2	10	366	373	10	1	7	11	376	374	9	9	3	13	246	243	13	0	2	15	196	216	12
1	9	8	204	198	18	16	2	10	181	178	22	3	7	11	85	88	46	11	3	13	248	256	14	2	2	15	504	543	7
3	9	8	98	88	46	1	3	10	237	246	8	5	7	11	388	403	10	13	3	13	259	277	15	4	2	15	371	393	9
5	9	8	80	103	80	3	3	10	729	795	7	7	7	11	607	595	9	0	4	13	337	323	8	6	2	15	236	238	12
0	10	8	294	283	13	5	3	10	316	310	7	9	7	11	301	281	13	2	4	13	773	775	8	8	2	15	267	277	12
1	1	9	837	796	7	7	3	10	329	336	8	0	8	11	40	48	39	4	4	13	852	891	8	10	2	15	379	375	10
3	1	9	186	161	8	9	3	10	1043	1026	9	2	8	11	40	37	40	6	4	13	682	664	8	12	2	15	283	275	13
5	1	9	957	953	8	11	3	10	558	562	8	4	8	11	128	134	30	8	4	13	420	422	9	1	1	15	627	639	7
7	1	9	723	710	7	13	3	10	200	204	16	6	8	11	75	59	74	10	4	13	223	219	16	3	3	15	202	170	13
9	1	9	951	957	8	15	3	10	305	295	13	1	9	11	159	146	23	12	4	13	290	290	14	5	5	15	101	90	30
11	1	9	828	798	8	0	4	10	277	278	8	3	9	11	291	290	14	1	5	13	501	526	8	7	7	15	95	93	37
13	1	9	170	176	18	2	4	10	572	554	7	0	0	12	623	633	6	3	5	13	107	111	27	9	7	15	238	254	15
15	1	9	218	201	16	4	4	10	266	266	9	2	0	12	1274	1286	9	5	5	13	93	112	36	11	3	15	244	226	15
0	2	9	550	539	5	6	4	10	74	76	42	4	0	12	1657	1614	10	7	5	13	209	188	15	0	4	15	515	500	8
2	2	9	154	133	10	8	4	10	35	45	35	6	0	12	756	730	7	9	5	13	133	80	26	2	4	15	597	592	8
4	2	9	493	466	6	10	4	10	70	92	70	8	0	12	115	87	23	11	5	13	125	70	1	4	4	15	689	674	8
6	2	9	226	223	9	12	4	10	96	19	40	10	0	12	407	382	8	0	6	13	580	597	8	6	4	15	595	605	8
8	2	9	247	248	9	14	4	10	42	87	42	12	0	12	508	474	8	2	6	13	339	345	10	8	4	15	323	320	11
10	2	9	711	715	7	1	5	10	239	251	10	14	0	12	315	313	12	4	6	13	247	220	12	10	4	15	234	229	16
12	2	9	442	461	9	3	5	10	150	139	15	1	1	12	758	757	7	6	6	13	311	306	12	1	5	15	107	53	28
14	2	9	193	192	17	5	5	10	705	707	7	3	1	12	128	116	15	8	6	13	330	332	12	3	5	15	38	78	37
16	2	9	268	245	14	7	5	10	861	865	9	5	1	12	268	276	8	10	6	13	322	338	12	5	5	15	119	131	29
1	3	9	862	858	7	9	5	10	259	245	12	7	1	12	53	141	-53	1	7	13	367	355	10	7	5	15	193	177	17
3	3	9	584	584	7	11	5	10	193	158	17	9	1	12	88	14	35	3	7	13	317	309	11	9	5	15	229	209	15
5	3	9	167	168	12	12	5	10	271	289	14	11	1	12	213	230	14	5	7	13	429	438	10	0	6	15	468	482	9
7	3	9	402	415	7	0	6	10	560	568	7	13	1	12	116	96	32	7	7	13	337	329	12	2	6	15	162	168	20
9	3	9	222	170	-11	2	6	10	505	524	8	15	1	12	110	132	41	0	8	13	91	96	50	4	6	15	126	112	28
11	3	9	99	32	32	4	6	10	88	89	37	0	2	12	267	258	8	2	8	13	41	9	41	6	6	15	258	236	14
13	3	9	294	319	12	6	6	10	129	140	23	2	2	12	559	551	7	4	8	13	43	47	42	8	6	15	308	308	13
15	3	9	174	189	21	8	6	10	285	284	12	4	2	12	657	634	7	0	0	14	266	267	8	1	7	15	588	558	9
0	4	9	605	609	6	10	6	10	179	180	19	6	2	12	383	387	8	2	0	14	744	755	7	3	7	15	363	379	12
2	4	9	809	786	7	12	6	10	180	197	22	8	2	12	317	313	9	4	0	14	1203	1187	9	5	7	15	158	155	24
4	4	9	586	575	7	1	7	10	443	449	8	10	2	12	229	216	13	6	0	14	799	811	8	0	8	15	42	43	42
6	4	9	528	530	7	3	7	10	213	210	14	12	2	12	306	306	11	8	0	14	224	206	12	2	8	15	43	59	42
8	4	9	985	984	9	5	7	10	241	244	14	14	2	12	371	348	11	10	0	14	336	339	10	0	0	16	97	86	25
10	4	9	617	636	8	7	7	10	316	314	11	1	3	12	822	799	7	12	0	14	485	482	10	2	0	16	692	689	7
12	4	9	231	245	14	9	7	10	114	106	35	3	3	12	633	637	7	14	0	14	297	292	14	4	0	16	862	877	8
14	4	9	308	317	12	0	8	10	298	292	11	5	3	12	409	403	8	1	1	14	627	628	7	6	0	16	659	645	8
1	5	9	166	169	13	2	8	10	344	395	10	7	3	12	633	633	7	3	1	14	203	200	10	8	0	16	626	629	8
3	5	9	367	384	8	4	8	10	335	334	11	9	3	12	383	397	9	5	1	14	33	37	33	10	0	16	492	471	9
5	5	9	373	385	8	6	8	10	425	424	10	11	3	12	103	100	35	7	1	14	70	90	69	12	0	16	129	145	31
7	5	9	114	127	25	8	8	10	368	375	12	13	3	12	350	343	12	9	1	14	245	257	12	1	1	16	155	157	15
9	5	9	210	194	14	1	9	10	105	116	42	0	4	12	126	139	18	11	1	14	258	250	13	3	1	16	143	143	17
11	5	9	227	232	14	3	9	10	42	87	42	2	4	12	438	431	7	13	1	14	105	102	40	5	1	16	91	75	35
13	5	9	122	112	31	5	9	10	43	23	43	4	4	12	169	175	14	0	2	14	871	860	8	7	1	16	234	235	13
0	6	9	564	579	7	1	1	11	519	519	6	6	4	12	404	389	9	2	2	14	646	652	7	9	1	16	330	319	11
2	6	9	653	666	8	3	1	11	784	774	7	8	4	12	210	220	14	4	2	14	158	155	16	11	1	16	208	204	17
4	6	9	379	370	9	5	1	11	606	606	7	10	4	12	67	29	66	6	2	14	208	197	12	0	2	16	660	649	7
6	6	9	560	575	8	7	1	11	504	494	7	12	4	12	41	65	40	8	2	14	431	424	8	2	2	16	88	80	32
8	6	9	286	302	11	9	1	11	531	537	8	1	5	12	423	433	8	10	2	14	331	326	10	4	2	16	188	185	14
10	6	9	93	77	45	11	1	11	380	366	9	3	5	12	459	459	8	12	2	14	272	265	13	6	2	16	436	418	9
12	6	9	306	311	13	13	1	11	286	270	12	5	5	12	560	538	8	1	3	14	584	577	7	8	2	16	338	329	10
1	7	9	765	760	8	15	1	11	338	350	12	7	5	12	558	531	8	3	3	14	599	591	7	10	2	16	273	262	13
3	7	9	317	327	10	0	2	11	910	911	8	9	5	12	368	373	10	5	3	14	725	724	8	12	2	16	261	255	15
5	7	9	307	308	11	2	2	11	482	495	6	11	5	12	297	311	13	7	3	14	416	400	9	1	3	16	529	515	7
7	7	9	522	518	9	4	2	11	476	490	6	0	6	12	482	506	8	9	3	14	197	183	16	3	3	16	530	520	8
9	7	9	317	319	12	6	2	11	97	141	26	2	6	12	305	318	10	11	3	14	358	341	11	5	3	16	319	334	10
11	7	9	221	243	18																								

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
10	2	17	267	270	13	5	1	18	38	46	37	5	1	19	237	241	14	7	1	20	213	209	17	2	4	21	382	369	11
1	17	96	118	32		7	1	18	137	143	24	7	1	19	226	224	15	0	2	20	197	173	15	4	4	21	376	361	11
3	3	17	307	287	10	9	1	18	229	220	15	9	1	19	204	182	18	2	2	20	109	156	33	1	5	21	43	59	42
5	3	17	178	178	18	0	2	18	52	76	52	0	2	19	122	134	24	4	2	20	354	337	11	0	0	22	634	637	9
7	3	17	316	307	12	2	2	18	99	55	32	2	2	19	177	175	17	6	2	20	292	287	12	2	0	22	296	302	12
9	3	17	157	163	24	4	2	18	451	421	9	4	2	19	110	103	32	8	2	20	195	218	20	4	0	22	275	271	14
0	4	17	314	323	10	6	2	18	329	346	11	6	2	19	235	225	14	1	3	20	401	421	10	6	0	22	288	289	14
2	4	17	347	361	10	8	2	18	247	245	14	8	2	19	392	401	11	3	3	20	469	470	9	1	1	22	195	186	18
4	4	17	520	533	9	10	2	18	233	251	17	1	3	19	38	61	38	5	3	20	336	328	11	3	1	22	192	174	19
6	4	17	409	411	10	1	3	18	507	493	8	3	3	19	183	185	18	7	3	20	208	203	18	5	1	22	43	131	42
8	4	17	342	332	12	3	3	18	408	414	9	5	3	19	351	356	11	0	4	20	104	90	36	0	2	22	320	291	11
1	5	17	102	112	36	5	3	18	201	212	17	7	3	19	165	172	22	2	4	20	41	80	40	2	2	22	208	205	17
3	5	17	99	83	39	7	3	18	249	267	15	0	4	19	451	454	9	4	4	20	68	54	67	4	2	22	180	167	21
5	5	17	106	85	35	9	3	18	377	370	11	2	4	19	299	310	12	6	4	20	43	87	42	1	3	22	302	293	13
7	5	17	105	112	41	0	4	18	113	98	28	4	4	19	381	380	11	1	5	20	332	314	11	3	3	22	37	380	11
0	6	17	308	314	12	2	4	18	39	63	38	6	4	19	472	446	10	3	5	20	449	444	11	0	4	22	107	37	40
2	6	17	193	202	18	4	4	18	84	20	54	1	5	19	129	105	28	0	6	20	254	280	16	2	4	22	43	33	43
4	6	17	173	177	22	6	4	18	98	77	43	3	5	19	168	175	22	1	1	21	435	460	10	1	1	23	273	267	14
6	6	17	348	352	12	8	4	18	113	68	38	5	5	19	71	36	70	3	1	21	454	469	10	3	1	23	240	245	16
1	7	17	389	386	11	1	5	18	414	402	10	0	6	19	193	222	20	5	1	21	238	259	15	0	2	23	237	240	15
3	7	17	236	236	17	3	5	18	285	280	13	2	6	19	280	284	14	7	1	21	202	185	19	2	2	23	269	272	15
0	0	18	337	320	9	5	5	18	418	413	11	0	0	20	483	491	9	0	2	21	278	257	12	1	3	23	79	55	79
2	0	18	612	615	8	7	5	18	392	392	11	2	0	20	573	581	8	2	2	21	205	200	16	0	0	24	321	308	12
4	0	18	431	421	9	0	6	18	105	75	38	4	0	20	196	187	18	4	2	21	162	154	22	2	0	24	457	433	11
6	0	18	501	499	8	2	6	18	78	72	78	6	0	20	347	319	11	6	2	21	271	277	15	1	1	24	76	96	76
8	0	18	569	569	9	4	6	18	112	136	39	8	0	20	333	346	13	1	1	21	133	154	27	0	2	24	223	236	18
10	0	18	143	79	26	1	7	18	120	90	36	1	1	20	198	169	15	3	3	21	157	176	24						
1	1	18	191	184	13	1	1	19	666	679	8	3	1	20	145	127	22	5	3	21	173	203	23						
3	1	18	298	285	10	3	1	19	485	501	8	5	1	20	115	100	32	0	4	21	481	47	10						

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
2	0	0	1793.35	1606.26	59.58	5	7	0	75.06	50.03	28.84	3	15	0	47.63	27.94	51.04
4	0	0	822.69	794.50	50.17	6	7	0	541.38	490.02	43.32	4	15	0	51.82	71.43	29.02
6	0	0	507.64	536.82	42.75	7	7	0	70.35	-17.99	59.26	5	15	0	20.68	-60.08	51.26
8	0	0	120.89	113.81	34.24	0	8	0	627.08	509.73	13.96	6	15	0	26.05	73.18	32.91
1	1	0	182.54	255.75	15.70	1	8	0	1222.10	1024.79	47.35	0	16	0	5.45	-47.53	43.53
2	1	0	78.73	132.08	15.26	2	8	0	1018.05	1005.66	45.99	1	16	0	1513.65	1629.82	84.89
3	1	0	1191.01	1285.80	55.71	3	8	0	455.61	469.59	43.60	2	16	0	62.46	59.82	27.78
4	1	0	111.86	96.74	21.65	4	8	0	390.40	416.93	16.10	3	16	0	886.93	825.58	65.78
5	1	0	518.43	508.54	53.02	5	8	0	226.88	230.91	10.40	4	16	0	49.60	12.76	55.12
6	1	0	16.30	63.55	28.33	6	8	0	67.63	111.08	30.64	5	16	0	27.58	-30.51	52.86
7	1	0	68.42	84.41	29.71	7	8	0	33.64	83.72	32.40	6	16	0	22.77	36.71	44.01
8	1	0	15.05	31.67	42.00	1	9	0	321.94	370.33	27.43	1	17	0	431.07	1191.87	93.04
0	2	0	10731.04	10399.31	320.32	2	9	0	659.40	602.92	43.29	2	17	0	11.89	97.42	27.62
1	2	0	2568.69	2429.08	77.90	3	9	0	800.46	893.35	51.40	3	17	0	69.75	49.50	56.91
2	2	0	2041.67	1962.33	70.11	4	9	0	201.04	178.32	27.28	4	17	0	15.32	87.66	28.92
3	2	0	28.38	20.59	29.19	5	9	0	483.91	514.83	42.47	5	17	0	3.76	-42.19	57.01
4	2	0	887.48	880.20	52.77	6	9	0	174.81	203.36	31.85	0	18	0	489.23	589.75	53.78
5	2	0	808.04	807.15	59.91	7	9	0	8.97	29.46	57.84	1	18	0	445.27	561.32	47.34
6	2	0	162.87	167.69	29.47	0	10	0	14.96	-12.30	27.85	2	18	0	67.30	66.14	28.26
7	2	0	439.60	434.87	36.78	1	10	0	2818.71	2793.07	99.81	3	18	0	372.30	297.82	33.81
8	2	0	24.27	17.87	59.61	2	10	0	85.99	99.25	13.83	4	18	0	53.18	86.26	31.86
1	3	0	2197.71	2052.18	67.95	3	10	0	4.34	37.85	22.99	5	18	0	18.99	27.23	57.76
2	3	0	44.11	25.39	26.29	4	10	0	26.27	-67.97	46.99	1	19	0	27.52	130.73	34.59
3	3	0	106.87	54.33	18.10	5	10	0	452.09	446.29	40.57	2	19	0	21.04	-71.66	53.28
4	3	0	671.22	578.70	48.01	6	10	0	11.12	-39.67	52.25	3	19	0	0.45	78.61	31.09
5	3	0	2.16	55.41	26.43	7	10	0	0.11	22.50	57.27	4	19	0	0.16	16.24	55.57
6	3	0	23.73	-3.99	49.70	1	11	0	298.92	473.20	46.78	0	20	0	132.29	137.42	29.04
7	3	0	8.36	-79.53	52.89	2	11	0	107.06	108.39	22.92	1	20	0	3.40	1.77	53.00
0	4	0	912.44	932.98	35.33	3	11	0	6.90	59.78	23.59	2	20	0	89.65	155.18	30.58
1	4	0	6306.83	5798.18	180.30	4	11	0	68.17	75.00	27.61	3	20	0	20.62	35.71	51.52
2	4	0	1.93	10.85	25.88	5	11	0	14.62	75.20	27.96	4	20	0	68.96	85.79	73.37
3	4	0	761.70	768.38	44.43	6	11	0	12.11	23.17	53.65	1	21	0	9.31	-38.79	54.98
4	4	0	159.43	191.16	23.30	7	11	0	0.43	1.97	56.53	2	21	0	3.67	92.91	31.15
5	4	0	841.51	815.82	61.05	0	12	0	644.81	714.01	44.60	3	21	0	6.61	13.51	52.98
6	4	0	140.21	153.91	29.48	1	12	0	76.75	124.02	21.21	0	22	0	1.18	-41.65	51.89
7	4	0	123.99	112.77	32.34	2	12	0	1849.94	1768.11	76.84	1	22	0	41.23	29.23	38.76
1	5	0	0.18	9.05	13.07	3	12	0	255.04	297.89	28.22	2	22	0	22.82	6.24	55.44
2	5	0	45.45	55.45	16.32	4	12	0	298.72	280.59	30.82	3	22	0	53.00	95.07	33.11
3	5	0	87.79	93.68	18.27	5	12	0	119.43	35.43	52.64	1	23	0	6.63	-91.73	59.21
4	5	0	463.79	459.18	45.99	6	12	0	124.19	95.16	32.37	2	23	0	4.17	-42.97	59.62
5	5	0	12.54	21.66	45.36	1	13	0	2.49	17.70	39.60	0	24	0	0.01	32.34	54.69
6	5	0	35.54	26.06	50.27	2	13	0	13.19	71.33	27.25	-7	0	1	0.21	23.46	49.63
7	5	0	0.67	-74.11	54.72	3	13	0	85.91	100.10	26.14	-5	0	1	12.76	-29.29	41.65
0	6	0	8586.96	8204.88	253.58	4	13	0	6.34	-21.78	49.24	-3	0	1	973.07	2124.03	78.18
1	6	0	8.96	25.49	14.26	5	13	0	58.41	66.20	30.02	-1	0	1	489.34	802.84	245.19
2	6	0	69.42	-3.10	28.95	6	13	0	1.77	-46.16	55.53	1	0	1	13.23	39.48	10.10
3	6	0	549.33	514.54	41.31	0	14	0	47.34	120.04	23.05	3	0	1	944.11	949.91	48.20
4	6	0	287.48	255.33	26.41	1	14	0	111.16	102.99	24.37	5	0	1	23.86	-8.82	46.28
5	6	0	146.34	154.24	25.90	2	14	0	1421.30	1356.41	71.88	7	0	1	14	0.30	53.61
6	6	0	56.41	90.33	29.21	3	14	0	211.86	235.09	29.42	-8	1	1	21.43	282.07	35.90
7	6	0	0.55	29.16	52.85	4	14	0	357.70	381.32	33.90	-7	1	1	21.43	2.92	52.53
1	7	0	102.02	112.08	16.02	5	14	0	0.02	8.14	51.38	-6	1	1	20.33	218.51	30.51
2	7	0	6343.19	7090.04	225.03	6	14	0	26.02	51.05	56.25	-5	1	1	21.43	17.67	42.29
3	7	0	627.29	587.44	43.71	1	15	0	49.82	445.20	41.11	-4	1	1	185.17	289.36	17.78
4	7	0	7.60	-33.72	41.40	2	15	0	141.28	320.71	31.36	-3	1	1			

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-2	1	1	1574.68	1632.69	60.12	5	4	1	0.29	45.50	27.66	-2	0	1	363.11	626.68	10.86*
-1	1	1	4331.27	4588.34	142.30	6	4	1	77.15	88.37	29.35	-1	0	1	17.80	-38.13	27.42
0	1	1	114.24	137.08	11.05	7	4	1	64.14	-30.65	58.08	0	0	1	558.23	523.44	52.51
1	1	1	13642.70	14760.18	148.42	-8	5	1	19.20	19.04	59.56	1	0	1	401.11	394.47	33.18
2	1	1	4025.01	4233.57	137.70	-7	5	1	1.05	-37.12	52.99	2	0	1	2775.07	2989.21	106.68
3	1	1	5.99	-3.20	20.72	-6	5	1	278.17	273.12	32.01	3	0	1	863.25	898.23	55.61
4	1	1	1219.08	1874.19	61.77	-5	5	1	49.68	28.03	46.99	4	0	1	6.20	28.97	43.59
5	1	1	181.55	873.72	28.89	-4	5	1	208.23	211.57	23.85	5	0	1	5.20	-53.24	50.02
6	1	1	826.58	837.57	47.15	-3	5	1	1275.57	1319.94	58.43	6	0	1	63.84	63.39	31.94
7	1	1	1.97	-40.73	56.09	-2	5	1	175.70	160.30	17.27	7	0	1	0.80	-24.28	55.92
-8	2	1	23.88	191.56	16.32	-1	5	1	1311.00	1244.25	49.93	-7	9	1	55.39	23.56	57.96
-7	2	1	68.10	45.67	31.00	0	5	1	6359.85	5593.95	321.19	-6	9	1	398.75	328.19	13.91
-6	2	1	125.99	158.26	28.88	1	5	1	5610.35	5560.79	175.81	-5	9	1	1.43	45.86	28.23
-5	2	1	12.10	39.24	42.44	2	5	1	811.34	447.30	34.60	-4	9	1	500.48	450.06	38.21
-4	2	1	292.96	280.01	28.29	3	5	1	176.75	116.09	20.49	-3	9	1	52.04	-4.92	37.44
-3	2	1	835.15	850.52	44.87	4	5	1	499.68	470.81	36.03	-2	9	1	721.37	819.59	46.68
-2	2	1	4148.74	4091.55	131.53	5	5	1	205.70	201.92	29.62	-1	9	1	730.49	765.01	42.41
1	2	1	148.10	126.12	12.40	6	5	1	325.52	325.54	33.87	0	9	1	1098.04	1306.33	191.06
0	2	1	1167.57	992.86	42.93	7	5	1	27.01	4.73	57.59	1	9	1	154.96	108.24	17.71
1	2	1	4426.50	4273.05	134.92	-8	6	1	1.64	-160.68	60.66	2	9	1	1726.80	1833.21	75.09
2	2	1	551.52	542.03	15.13	-7	6	1	59.41	41.07	51.80	3	9	1	1268.09	1198.62	65.78
3	2	1	296.17	380.19	25.36	-6	6	1	351.61	295.16	32.87	4	9	1	37.42	11.67	44.60
4	2	1	2.15	10.41	39.35	-5	6	1	670.37	753.63	56.80	5	9	1	205.66	218.07	31.31
5	2	1	90.98	126.43	28.29	-4	6	1	22.72	36.58	37.38	6	9	1	9.26	52.20	52.85
6	2	1	175.64	185.59	30.80	-3	6	1	784.29	871.69	48.55	7	9	1	125.55	153.26	38.46
7	2	1	1.21	-104.83	56.77	-2	6	1	7099.08	1121.26	50.35	-7	10	1	0.10	32.58	53.01
-8	3	1	33.64	31.42	40.90	-1	6	1	4607.61	4617.13	148.28	-6	10	1	45.06	39.28	53.39
-7	3	1	1.48	51.85	29.08	0	6	1	29.78	62.37	42.33	-5	10	1	334.07	301.70	32.17
-6	3	1	45.17	91.52	27.99	1	6	1	14.44	25.93	14.84	-4	10	1	793.63	821.88	59.66
-5	3	1	222.29	198.52	27.15	2	6	1	344.08	378.54	33.52	-3	10	1	91.41	103.42	23.82
-4	3	1	198.94	187.80	22.47	3	6	1	28.38	34.61	20.17	-2	10	1	1799.48	1720.12	72.44
-3	3	1	240.28	194.85	18.33	4	6	1	1.15	-68.02	44.11	-1	10	1	75.86	122.85	18.39
-2	3	1	1323.46	1368.71	54.68	5	6	1	161.87	158.92	29.79	0	10	1	506.95	1590.08	1003.06
-1	3	1	7004.37	7143.50	220.09	6	6	1	116.64	127.36	31.66	1	10	1	22.03	197.09	20.40*
0	3	1	1858.30	1832.33	57.69	7	6	1	38.43	24.20	57.53	2	10	1	206.11	214.74	12.61
1	3	1	11375.50	11100.17	339.63	-7	7	1	23.87	-33.41	57.15	3	10	1	623.46	614.02	54.04
2	3	1	3034.81	2982.10	101.92	-6	7	1	80.75	135.56	29.71	4	10	1	3.68	32.80	45.98
3	3	1	619.25	547.60	40.56	-5	7	1	47.82	55.16	27.68	5	10	1	2.29	29.16	49.26
4	3	1	31.52	5.57	40.11	-4	7	1	186.92	155.18	25.14	6	10	1	45.33	-24.99	55.70
5	3	1	868.78	881.85	65.99	-3	7	1	1060.41	2228.61	86.01	7	10	1	18.33	17.48	62.07
6	3	1	50.38	63.73	29.67	-2	7	1	87.48	56.36	16.71	-7	11	1	48.72	94.99	32.73
7	3	1	106.26	144.59	32.92	-1	7	1	926.65	986.35	46.21	-6	11	1	37.72	95.15	30.30
-8	4	1	25.77	14.50	57.75	0	7	1	115.41	66.22	10.84	-5	11	1	36.72	-2.34	49.33
-7	4	1	10.51	-3.62	51.91	1	7	1	5.58	-18.34	26.60	-4	11	1	87.55	65.89	27.34
-6	4	1	301.17	305.87	32.21	2	7	1	2248.75	2258.50	84.56	-3	11	1	1314.99	1396.34	69.86
-5	4	1	118.54	111.11	26.08	3	7	1	555.20	1035.29	45.80	-2	11	1	125.01	141.58	22.10
-4	4	1	99.33	121.36	31.92	4	7	1	668.63	631.51	56.61	-1	11	1	10.29	28.71	18.41
-3	4	1	42.04	18.65	29.47	5	7	1	274.64	204.84	31.80	0	11	1	2999.33	2649.03	139.07
-2	4	1	2194.47	2117.65	75.80	6	7	1	502.54	654.94	60.57	1	11	1	313.99	295.82	26.72
-1	4	1	408.60	400.17	27.29	7	7	1	1.81	41.39	52.18	2	11	1	0.81	-33.05	37.27
0	4	1	41.44	74.92	22.40	-7	8	1	96.03	63.48	32.62	3	11	1	1876.11	1882.34	85.33
1	4	1	132.35	154.92	14.08	-6	8	1	61.52	-3.01	54.15	4	11	1	313.11	272.29	30.83
2	4	1	175.32	222.93	21.44	-5	8	1	200.76	182.48	29.44	5	11	1	25.02	25.42	50.59
3	4	1	29.79	62.15	18.47	-4	8	1	74.51	88.11	24.68	6	11	1	7.94	-24.53	54.64
4	4	1	7.78	9.34	39.80	-3	8	1	558.78	547.13	43.96	-7	12	1	23.64	-30.92	58.83

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-6	12	1	94.74	146.61	31.99	-2	16	1	7.23	40.07	48.02	2	21	1	52.43	88.11	30.99
-5	12	1	70.57	102.43	28.88	-1	16	1	47.99	88.70	29.69	3	21	1	1.83	-4.05	56.18
-4	12	1	148.10	172.80	28.91	0	16	1	971.30	668.16	447.60	-3	22	1	1.17	20.29	55.59
-3	12	1	199.91	232.65	27.92	1	16	1	0.32	-7.46	44.56	-2	22	1	16.72	141.06	32.35
-2	12	1	160.07	118.44	23.54	2	16	1	0.78	-13.34	48.70	-1	22	1	0.37	-34.32	53.95
-1	12	1	306.19	269.92	28.10	3	16	1	15.68	-21.46	52.96	0	22	1	84.41	8.37	41.00
0	12	1	71.43	1177.13	1005.92	4	16	1	1.40	60.67	38.54	1	22	1	14.85	34.34	53.22
1	12	1	2.20	88.54	23.24	5	16	1	6.95	42.29	55.12	2	22	1	35.27	121.49	31.94
2	12	1	39.17	41.89	25.16	-5	17	1	86.52	21.21	55.18	-2	23	1	64.08	71.96	33.95
3	12	1	4.27	-84.02	47.00	-4	17	1	0.34	3.88	52.09	-1	23	1	19.97	34.68	31.76
4	12	1	179.78	198.47	30.24	-3	17	1	48.10	80.28	28.97	0	23	1	10.83	-54.08	42.48
5	12	1	4.52	-44.18	51.44	-2	17	1	0.17	10.38	47.74	1	23	1	23.54	7.83	56.20
6	12	1	6.44	11.15	31.36	-1	17	1	40.93	57.64	27.69	2	23	1	10.30	36.74	55.18
-5	13	1	43.11	22.04	56.44	0	17	1	133.05	-129.71	158.51	-8	0	2	10.04	-46.07	55.60
-8	13	1	35.91	-28.96	50.77	1	17	1	5.55	-241.58	59.16*	-6	0	2	63.43	29.11	32.91
-4	13	1	496.42	522.77	42.86	2	17	1	1.52	31.02	27.68	-4	0	2	28.31	72.26	19.62
-3	13	1	175.42	189.78	27.47	3	17	1	535.54	651.77	62.70	-2	0	2	11224.15	11761.91	361.68
-2	13	1	446.06	409.86	35.01	4	17	1	3.41	28.32	36.43	0	0	2	19338.69	21996.62	484.38
-1	13	1	183.64	238.43	24.42	5	17	1	207.97	232.89	36.06	2	0	2	159.87	136.38	16.89
0	13	1	1023.73	912.09	41.18	-5	18	1	34.43	83.82	33.25	4	0	2	1275.56	1369.23	70.11
1	13	1	38.21	38.26	40.01	-4	18	1	46.18	127.24	29.50	6	0	2	255.99	195.82	32.67
2	13	1	1449.04	1457.58	72.92	-3	18	1	17.64	15.49	51.06	-8	1	2	40.23	-0.70	53.55
3	13	1	0.75	3.10	45.16	-2	18	1	5.95	-3.47	50.39	-7	1	2	216.32	346.73	32.77
4	13	1	491.45	488.48	43.11	-1	18	1	82.99	75.92	29.05	-6	1	2	13.49	0.08	45.64
5	13	1	45.53	-5.05	51.82	0	18	1	32.57	-115.90	38.65	-5	1	2	683.79	715.15	54.80
6	13	1	69.85	91.35	33.46	1	18	1	176.23	96.22	35.29*	-4	1	2	339.40	328.07	29.05
-5	14	1	2.40	18.61	55.54	2	20	1	96.64	184.12	32.33	-3	1	2	320.57	450.02	36.09
-5	14	1	170.50	151.33	32.13	3	18	1	23.54	-51.57	54.68	-2	1	2	245.64	313.50	30.20
-4	14	1	1.34	-6.60	50.73	4	18	1	21.59	28.61	53.04	-1	1	2	1323.28	1296.81	49.99
-3	14	1	131.82	174.11	28.48	5	18	1	6.74	50.61	57.18	0	1	2	3695.45	3826.39	87.23
-2	14	1	6.88	13.11	43.39	-5	19	1	2.53	41.90	56.94	1	1	2	13.43	3.63	26.32
-1	14	1	91.73	160.55	25.67	-4	19	1	10.88	-33.31	56.65	2	1	2	1.83	11.59	27.89
0	14	1	193.22	-340.89	72.42*	-3	19	1	115.89	46.91	51.57	3	1	2	204.43	207.85	22.18
1	14	1	52.07	56.95	25.06	2	19	1	334.46	376.93	32.61	4	1	2	25.38	38.94	43.20
2	14	1	45.56	224.37	29.85*	-1	19	1	65.82	18.53	51.52	5	1	2	41.17	69.22	28.27
3	14	1	10.72	-3.13	47.02	0	19	1	170.16	119.77	66.86	6	1	2	23.75	29.66	36.78
4	14	1	12.69	24.46	48.18	1	19	1	267.66	67.15	36.53*	7	1	2	10.00	50.61	54.75
5	14	1	29.96	26.49	51.45	2	19	1	362.67	406.43	34.44	-8	2	2	11.42	10.62	53.58
6	14	1	0.60	29.90	33.44	3	19	1	71.24	63.02	30.78	-7	2	2	603.66	603.82	61.49
-6	15	1	6.59	-36.79	54.61	4	19	1	74.36	69.54	32.89	-6	2	2	315.96	275.86	31.16
-5	15	1	37.46	76.88	30.28	-4	20	1	0.02	6.68	56.75	-5	2	2	0.13	-21.77	42.83
-4	15	1	304.49	236.69	32.11	-3	20	1	21.59	34.01	53.13	-4	2	2	145.46	154.28	21.69
-3	15	1	3.92	-65.81	48.25	-2	20	1	0.04	-3.03	57.71	-3	2	2	1041.43	1109.76	51.68
-2	15	1	260.11	269.64	29.11	-1	20	1	11.57	94.16	28.46	-2	2	2	861.52	884.40	43.44
-1	15	1	445.16	413.40	37.40	0	20	1	27.11	-181.70	41.45*	-1	2	2	4291.48	4048.35	130.16
0	15	1	1984.50	1653.08	65.99	1	20	1	12.42	-122.93	59.30	0	2	2	919.26	975.46	29.90
1	15	1	25.41	36.78	45.16	2	20	1	9.27	77.11	32.90	1	2	2	2840.99	2902.20	97.31
2	15	1	632.03	627.49	57.57	3	20	1	9.09	24.21	36.94	2	2	2	499.96	450.61	25.46
3	15	1	500.37	547.37	42.27	4	20	1	2.71	21.39	54.43	3	2	2	372.01	414.52	40.93
4	15	1	97.86	52.98	30.42	-4	21	1	21.81	26.17	58.62	4	2	2	574.32	556.76	52.82
5	15	1	205.34	155.00	34.20	-3	21	1	1.01	10.77	31.92	5	2	2	1305.86	1177.04	75.71
-6	16	1	14.45	26.15	58.70	-2	21	1	64.89	19.98	21.62	6	2	2	27.29	45.08	29.87
-5	16	1	9.91	42.83	53.12	-1	21	1	2.81	6.09	34.71	7	2	2	105.39	114.22	33.67
-4	16	1	82.09	89.84	29.94	0	21	1	76.30	-2.13	76.83	-8	3	2	0.14	-8.11	56.74
-3	16	1	36.97	-81.36	50.52	1	21	1	4.05	2.64	50.96	-7	3	2	16.17	69.45	29.66

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-6	3	2	59.67	59.74	28.26	1	6	2	18.31	17.70	25.19	-2	10	2	32.26	31.77	20.29
-5	3	2	109.42	143.38	26.18	2	6	2	31.03	16.41	30.31	-1	10	2	0.41	-5.59	32.83
-4	3	2	307.52	300.10	29.10	3	6	2	2365.55	2344.74	93.20	0	10	2	176.77	167.30	20.08
-3	3	2	98.01	117.92	17.90	4	6	2	190.61	172.44	29.16	1	10	2	538.82	528.98	41.64
-2	3	2	265.61	320.21	23.75	5	6	2	12.76	9.81	49.80	2	10	2	32.95	39.59	21.85
-1	3	2	244.94	295.60	28.96	6	6	2	118.87	181.90	31.25	3	10	2	46.27	85.87	25.26
0	3	2	3556.23	3427.23	149.96	7	6	2	76.01	94.67	34.44	4	10	2	17.99	-58.10	49.41
1	3	2	708.07	714.40	36.88	-8	7	2	0.07	47.20	57.00	5	16	2	309.70	338.01	33.16
2	3	2	1735.93	1860.09	71.65	-7	7	2	64.22	29.21	32.08	6	10	2	39.24	28.25	48.59
3	3	2	15.80	-25.74	37.80	-6	7	2	36.36	18.60	51.43	-7	11	2	1.58	44.09	56.17
4	3	2	31.44	32.23	44.84	-5	7	2	168.39	241.52	29.87	-4	11	2	162.65	150.92	32.97
5	3	2	109.31	117.69	30.18	-4	7	2	754.87	763.29	55.83	-5	11	2	0.03	-27.72	50.71
6	3	2	0.70	-9.61	37.54	-3	7	2	52.25	38.11	19.74	-4	11	2	63.23	76.75	27.30
7	3	2	17.27	23.07	41.92	-2	7	2	110.97	120.52	18.08	-3	11	2	323.71	301.69	27.51
-8	4	2	19.75	39.06	54.43	-1	7	2	370.43	348.57	32.48	-2	11	2	92.57	118.91	21.94
-7	4	2	225.81	213.72	32.45	0	7	2	234.84	283.18	22.29	-1	11	2	0.17	31.05	19.59
-6	4	2	0.63	-52.64	49.50	1	7	2	634.76	639.84	38.49	0	11	2	878.22	851.58	35.70
-5	4	2	1.49	30.08	25.59	2	7	2	159.14	133.62	19.77	1	11	2	270.18	251.11	23.97
-4	4	2	629.18	709.22	40.76	3	7	2	224.02	214.37	25.72	2	11	2	38.64	34.52	22.90
-3	4	2	8.45	17.99	16.95	4	7	2	35.52	36.78	47.32	3	11	2	98.74	107.69	26.53
-2	4	2	41.47	7.84	27.95	5	7	2	85.32	95.22	29.85	4	11	2	235.44	206.04	30.56
-1	4	2	2200.70	2096.94	75.11	6	7	2	65.80	127.92	31.77	5	11	2	0.00	2.98	49.29
0	4	2	24.45	26.96	13.49	-7	8	2	8.35	12.51	54.25	6	11	2	1.53	-4.18	57.64
1	4	2	113.76	112.41	14.39	-6	8	2	300.40	280.54	33.00	-7	12	2	17.10	46.67	56.24
2	4	2	82.93	101.37	17.79	-5	8	2	788.41	933.77	65.24	-6	12	2	20.49	68.10	30.20
3	4	2	1932.28	1813.41	77.73	-4	8	2	10.00	-7.04	41.86	-5	12	2	24.07	-32.17	51.56
4	4	2	85.90	-20.93	48.37	-3	8	2	31.05	33.56	34.97	-4	12	2	57.85	73.54	27.98
5	4	2	551.28	613.47	59.75	-2	8	2	644.38	738.24	45.59	-3	12	2	15.62	16.40	44.99
6	4	2	70.36	49.44	31.03	-1	8	2	353.19	322.44	33.11	-2	12	2	147.52	152.35	24.40
7	4	2	207.39	224.45	37.54	0	8	2	78.67	86.77	11.48	-1	12	2	56.21	79.87	21.78
-8	5	2	15.51	53.65	56.52	1	8	2	14.46	24.43	16.52	0	12	2	457.06	594.02	115.29
-7	5	2	20.12	44.72	50.75	2	8	2	17.02	-18.17	24.32	1	12	2	175.31	70.35	26.30
-6	5	2	0.13	-177.53	51.62*	3	8	2	2.13	41.41	23.31	2	12	2	542.36	489.29	50.61
-5	5	2	0.09	23.95	31.24	4	8	2	462.72	410.43	39.66	3	12	2	564.62	584.46	66.26
-4	5	2	427.08	479.46	32.45	5	8	2	358.34	312.76	33.82	4	12	2	604.89	598.71	59.19
-3	5	2	48.22	401.62	37.49	6	8	2	1.37	-3.96	53.80	5	12	2	0.03	-44.31	51.69
-2	5	2	496.72	479.79	35.71	-7	9	2	11.84	-0.75	56.15	6	12	2	172.09	185.50	35.11
-1	5	2	3.26	12.36	15.55	-6	9	2	204.85	190.61	31.56	-7	13	2	30.82	45.56	59.64
0	5	2	1521.81	1487.83	52.39	-5	9	2	1208.78	1416.77	78.86	-6	13	2	27.87	43.29	52.61
1	5	2	302.74	305.12	21.59	-4	9	2	99.19	111.60	26.70	-5	13	2	17.15	24.37	48.28
2	5	2	2.29	14.11	28.84	-3	9	2	15.96	-0.80	38.34	-4	13	2	0.08	0.61	48.67
3	5	2	1310.61	1298.64	64.51	-2	9	2	712.88	794.16	47.42	-3	13	2	360.95	377.00	37.08
4	5	2	244.38	195.04	29.14	-1	9	2	1258.50	1184.14	55.62	-2	13	2	44.11	27.04	24.47
5	5	2	13.96	15.08	48.30	0	9	2	127.52	68.53	37.53	-1	13	2	133.87	174.90	24.11
6	5	2	8.89	30.52	53.48	1	9	2	16.64	-25.79	29.70	0	13	2	71.66	177.24	82.04
7	5	2	6.04	-3.10	61.87	2	9	2	148.76	129.58	22.09	1	13	2	1081.11	1065.33	61.52
-8	6	2	8.78	-14.38	57.30	3	9	2	1064.83	921.27	60.47	2	13	2	49.44	87.01	26.49
-7	6	2	18.48	5.78	51.46	4	9	2	24.87	38.76	48.33	3	13	2	7.19	-32.05	46.95
-6	6	2	3.83	-13.90	49.37	5	9	2	60.03	84.02	28.60	4	13	2	47.60	42.24	50.97
-5	6	2	50.70	9.91	46.26	6	9	2	1.11	-96.60	59.12	5	13	2	2.96	17.74	52.56
-4	6	2	9.30	-6.83	39.21	-7	10	2	0.01	15.48	57.50	6	13	2	21.70	-47.11	63.45
-3	6	2	81.05	82.03	19.23	-6	10	2	39.22	41.39	52.24	-6	14	2	54.40	-52.77	58.54
-2	6	2	0.30	-38.58	28.08	-5	10	2	14.06	12.80	49.39	-5	14	2	55.91	45.39	29.75
-1	6	2	317.75	272.61	22.90	-4	10	2	64.50	91.62	54.16	-4	14	2	116.45	72.59	29.17
0	6	2	45.57	5.19	10.92	-3	10	2	141.78	112.70	24.23	-3	14	2	56.16	110.57	27.52

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-2	14	2	80.20	91.81	26.23	-2	19	2	5.98	30.06	37.26	-8	2	3	178.14	186.99	34.20
-1	14	2	0.05	-14.41	41.78	-1	19	2	69.77	170.43	31.66	-7	2	3	29.42	-21.01	49.83
0	14	2	17.19	-23.53	38.76	0	19	2	52.43	56.10	22.68	-6	2	3	387.07	403.37	38.72
1	14	2	1.05	-2.77	46.48	1	19	2	138.96	141.40	30.41	-5	2	3	7.85	-3.47	44.63
2	14	2	554.86	515.75	40.28	2	19	2	44.49	-6.98	51.27	-4	2	3	240.56	209.72	23.69
3	14	2	11.87	12.55	26.82	3	19	2	18.45	40.26	30.99	-3	2	3	791.03	796.65	47.23
4	14	2	229.84	303.58	32.22	4	19	2	4.01	0.54	56.52	-2	2	3	233.49	260.27	24.46
5	14	2	12.68	-37.63	51.89	-4	20	2	53.88	43.02	56.34	-1	2	3	6.38	10.28	27.97
-6	15	2	5.12	-0.30	54.76	-3	20	2	0.71	18.61	31.44	0	2	3	155.40	147.55	12.29
-5	15	2	64.59	79.70	30.98	-2	20	2	1.43	-48.33	51.88	1	2	3	1899.93	1942.11	74.72
-4	15	2	42.81	38.32	29.05	-1	20	2	32.58	-46.66	54.11	2	2	3	773.72	680.15	47.23
-3	15	2	166.34	182.61	30.20	0	20	2	123.49	179.30	21.49	3	2	3	14.84	58.85	23.98
-2	15	2	129.42	170.62	28.30	1	20	2	0.60	-70.42	54.95	4	2	3	73.31	106.27	27.82
-1	15	2	146.11	118.82	27.21	2	20	2	51.37	46.57	53.98	5	2	3	23.96	15.02	51.07
0	15	2	159.27	181.54	18.97	3	20	2	38.72	21.13	54.64	6	2	3	0.10	-69.28	54.90
1	15	2	92.44	-1246.67	87.43*	-4	21	2	21.32	-89.91	59.36	-8	3	3	1.30	44.25	55.00
2	15	2	80.93	49.60	49.91	-3	21	2	19.56	10.81	54.68	-7	3	3	12.17	40.42	50.33
3	15	2	3.30	-38.26	47.30	-2	21	2	1.39	-7.45	49.79	-6	3	3	46.54	-27.79	50.56
4	15	2	3.95	10.13	53.01	-1	21	2	106.29	118.71	31.57	-5	3	3	404.24	386.24	36.24
5	15	2	7.03	-8.48	57.98	0	21	2	4.15	54.06	27.87	-4	3	3	14.36	-13.40	37.85
-6	16	2	22.74	-23.02	60.87	1	21	2	38.33	30.91	31.83	-3	3	3	87.10	85.07	19.84
-5	16	2	79.42	42.78	57.17	2	21	2	20.72	-33.19	59.44	-2	3	3	1070.51	1129.02	51.76
-4	16	2	8.07	-8.96	51.65	3	21	2	14.03	3.06	54.45	-1	3	3	3342.80	3483.57	117.66
-3	16	2	742.95	683.92	64.29	-3	22	2	12.89	34.70	33.18	0	3	3	449.80	693.37	38.29
-2	16	2	68.84	72.42	28.13	-2	22	2	3.62	57.78	31.18	1	3	3	2.98	-29.68	28.08
-1	16	2	20.24	11.56	46.12	-1	22	2	2.60	66.79	33.26	2	3	3	1111.66	1300.42	60.17
0	16	2	24.28	96.90	44.08	0	22	2	7.22	28.82	22.81	3	3	3	204.74	253.37	26.00
1	16	2	2012.46	1833.45	90.03	1	22	2	56.62	30.34	31.64	4	3	3	150.99	210.94	29.26
2	16	2	123.91	120.08	29.06	2	22	2	77.97	-59.56	65.41	5	3	3	373.63	373.83	34.45
3	16	2	86.77	21.98	29.38	-2	23	2	3.18	52.64	55.68	6	3	3	0.67	-80.43	56.39
4	16	2	23.32	67.75	30.78	-1	23	2	6.94	-23.64	60.77	-8	4	3	131.64	104.43	34.26
5	16	2	7.47	61.90	31.50	0	23	2	4.89	3.90	36.66	-7	4	3	0.37	44.40	29.32
-5	17	2	0.00	-39.59	38.83	1	23	2	0.45	-39.33	57.33	-6	4	3	230.05	208.91	31.37
-4	17	2	2.32	-35.52	53.21	-7	0	3	99.80	83.82	30.36	-5	4	3	173.08	105.30	27.04
-3	17	2	0.44	32.22	29.57	-5	0	3	411.35	489.09	36.85	-4	4	3	165.49	264.83	25.53
-2	17	2	39.02	57.40	29.16	-3	0	3	4662.58	5032.10	165.91	-3	4	3	0.05	-16.73	33.78
-1	17	2	28.13	40.95	48.42	-1	0	3	1397.92	1658.09	64.89	-2	4	3	439.02	568.86	39.96
0	17	2	0.03	2.58	33.23	1	0	3	4619.61	5105.58	166.45	-1	4	3	13.93	-24.86	28.96
1	17	2	3.91	-191.05	59.68*	3	0	3	71.78	38.01	22.64	0	4	3	43.99	42.18	11.33
2	17	2	95.03	72.84	28.35	5	0	3	4.69	24.65	49.05	1	4	3	197.20	212.50	21.30
3	17	2	17.65	5.71	51.14	-8	1	3	1.41	-16.84	53.71	2	4	3	105.16	95.73	19.94
4	17	2	6.95	31.82	37.81	-7	1	3	0.09	0.19	51.34	3	4	3	73.35	20.86	31.58
-5	18	2	80.96	95.40	33.19	-6	1	3	299.83	293.31	31.27	4	4	3	173.10	183.03	29.80
-4	18	2	57.84	64.48	31.57	-5	1	3	0.09	-48.91	43.88	5	4	3	28.39	12.19	35.93
-3	18	2	85.27	21.84	51.72	-4	1	3	3.10	14.80	25.98	6	4	3	173.52	187.81	33.84
-2	18	2	358.03	302.71	32.60	-3	1	3	940.48	1021.95	52.22	-8	5	3	6.38	57.94	32.54
-1	18	2	258.83	290.65	31.40	-2	1	3	415.27	323.92	24.96	-7	5	3	15.89	-15.08	53.66
0	18	2	28.41	14.64	30.38	-1	1	3	1440.90	1437.27	59.30	-6	5	3	118.49	28.63	52.83
1	18	2	242.67	67.62	32.10*	0	1	3	2043.69	2019.15	52.96	-5	5	3	633.19	653.25	57.25
2	18	2	6.63	12.04	49.13	1	1	3	705.22	676.23	42.20	-4	5	3	25.56	21.42	40.17
3	18	2	121.78	102.52	30.25	2	1	3	3.24	19.43	31.70	-3	5	3	402.73	367.30	29.33
4	18	2	31.80	63.55	31.80	3	1	3	0.80	60.58	21.97	-2	5	3	521.46	451.73	37.87
-5	19	2	1.49	53.03	32.28	4	1	3	1100.19	1038.85	68.19	-1	5	3	330.01	136.01	17.79
-4	19	2	11.08	-45.44	53.50	5	1	3	41.83	31.67	28.09	0	5	3	43.12	43.35	14.01
-3	19	2	73.18	37.15	54.97	6	1	3	332.41	301.93	35.38	1	5	3	347.53	292.65	24.04

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
2	5	3	932.36	932.68	51.94	0	9	3	34.39	41.47	13.63	2	13	3	512.17	531.95	40.38
3	5	3	161.50	99.33	25.95	1	9	3	0.87	-4.93	33.99	3	13	3	80.31	68.96	27.44
4	5	3	239.41	253.49	29.31	2	9	3	475.40	479.68	48.41	4	13	3	54.55	28.68	51.76
5	5	3	254.88	229.23	39.48	3	9	3	475.36	415.24	38.92	5	13	3	2.97	-11.27	53.96
6	5	3	133.74	30.00	58.49	4	9	3	36.23	-16.11	50.55	-6	14	3	29.73	-13.74	56.54
-8	6	3	34.92	29.01	34.32	5	9	3	62.71	18.34	57.05	-5	14	3	166.05	173.98	31.77
-7	6	3	83.50	61.45	31.42	6	9	3	34.82	82.41	33.90	-4	14	3	11.57	23.92	35.18
-6	6	3	3.67	20.32	49.07	-7	10	3	15.21	34.99	37.31	-3	14	3	7.12	-60.28	47.75
-5	6	3	799.40	874.28	66.05	-6	10	3	7.81	-2.56	50.70	-2	14	3	63.73	98.96	27.20
-4	6	3	65.06	90.87	24.33	-5	10	3	89.59	47.37	29.25	-1	14	3	338.89	325.10	30.56
-3	6	3	632.21	586.26	45.40	-4	10	3	1832.44	1833.70	86.42	0	14	3	1.11	-20.86	61.85
-2	6	3	26.60	30.21	32.11	-3	10	3	13.48	-71.00	43.98	1	14	3	40.50	0.72	44.15
-1	6	3	57.80	54.25	17.50	-2	10	3	214.98	252.63	25.35	2	14	3	74.01	23.15	33.41
0	6	3	1.99	13.56	30.47	-1	10	3	0.68	25.52	34.67	3	14	3	24.72	25.68	33.94
1	6	3	456.76	435.38	37.07	0	10	3	75.44	90.39	14.67	4	14	3	13.56	47.50	50.74
2	6	3	0.16	-6.89	24.47	1	10	3	160.88	136.01	22.62	5	14	3	117.11	132.92	34.56
3	6	3	15.25	33.51	42.85	2	10	3	125.73	161.22	24.83	-6	15	3	19.46	24.58	55.82
4	6	3	41.40	-8.59	49.96	3	10	3	8.58	15.16	22.18	-5	15	3	3.31	50.25	51.81
5	6	3	13.81	-24.52	49.93	4	10	3	0.08	-46.68	47.25	-4	15	3	199.68	207.66	31.22
6	6	3	36.22	5.24	54.40	5	10	3	16.60	-26.22	54.05	-3	15	3	51.31	34.61	27.81
-7	7	3	109.54	123.32	32.40	6	10	3	13.12	16.95	33.59	-2	15	3	218.07	210.11	30.19
-6	7	3	84.65	72.07	30.00	-7	11	3	8.74	5.20	57.47	-1	15	3	55.46	94.06	28.14
-5	7	3	1749.53	1799.63	87.90	-6	11	3	43.44	1.16	53.19	0	15	3	574.31	507.76	32.56
-4	7	3	121.99	93.98	30.38	-5	11	3	480.41	501.38	43.45	1	15	3	84.41	36.13	47.66
-3	7	3	88.68	145.24	22.57	-4	11	3	236.08	228.90	31.93	2	15	3	353.96	343.16	31.70
-2	7	3	2.76	-22.95	33.46	-3	11	3	86.51	77.10	25.93	3	15	3	145.31	119.10	29.92
-1	7	3	168.13	197.15	20.58	-2	11	3	498.88	475.04	35.82	4	15	3	11.58	15.60	37.37
0	7	3	160.95	135.52	13.35	-1	11	3	0.06	-13.89	39.99	-6	16	3	13.34	36.50	55.14
1	7	3	630.69	619.34	41.78	0	12	3	4.23	45.08	20.14	-5	16	3	11.58	23.87	54.14
2	7	3	52.62	88.77	20.83	1	12	3	459.26	453.59	33.51	-4	16	3	83.38	97.33	30.27
3	7	3	349.02	392.11	35.87	2	12	3	11.52	41.26	42.84	-3	16	3	4.59	3.27	48.55
4	7	3	489.84	435.18	40.35	3	12	3	35.32	16.77	47.75	-2	16	3	139.41	171.54	30.15
5	7	3	0.15	28.81	35.04	4	12	3	7.34	40.14	28.88	-1	16	3	67.55	41.67	50.86
6	7	3	121.94	56.11	58.92	5	12	3	64.34	82.03	31.40	0	16	3	547.63	628.12	118.35
-7	8	3	34.34	100.80	31.44	-7	12	3	55.10	0.45	59.27	1	16	3	35.57	58.75	26.23
-6	8	3	41.76	67.45	29.52	-6	12	3	6.26	31.91	53.37	2	16	3	0.27	-53.94	47.86
-5	8	3	0.11	31.55	51.31	-5	12	3	120.34	166.52	30.24	3	16	3	0.17	-38.45	53.19
-4	8	3	62.62	96.15	25.90	-4	12	3	171.51	197.78	29.63	4	16	3	30.76	50.80	82.43
-3	8	3	306.91	302.81	26.27	-3	12	3	11.07	36.58	26.14	-5	17	3	22.62	-3.50	54.95
-2	8	3	85.19	32.84	36.62	-2	12	3	164.40	152.13	26.80	-4	17	3	6.00	-2.40	54.79
-1	8	3	107.08	25.58	34.31	-1	12	3	108.34	103.74	24.79	-3	17	3	18.49	20.70	50.76
0	8	3	105.36	101.23	22.22	0	12	3	138.36	135.45	17.31	-2	17	3	176.33	124.02	31.27
1	8	3	445.99	461.63	40.83	1	12	3	36.88	-21.63	42.53	-1	17	3	1.26	42.33	45.94
2	8	3	744.94	743.51	50.15	2	12	3	112.35	119.20	26.51	0	17	3	144.96	308.57	144.71
3	8	3	362.06	391.23	36.86	3	12	3	218.59	244.75	29.57	1	17	3	42.29	27.37	46.95
4	8	3	89.87	121.51	28.58	4	12	3	95.93	12.80	49.96	2	17	3	48.80	-14.73	50.59
5	8	3	24.93	-18.98	54.87	5	12	3	69.42	60.58	32.20	3	17	3	209.35	169.96	31.42
6	8	3	12.84	34.78	58.48	-6	13	3	52.88	36.60	32.19	4	17	3	8.14	1.92	55.53
-7	9	3	34.62	50.14	56.55	-5	13	3	28.34	-63.09	52.71	-5	18	3	2.49	-13.07	56.53
-6	9	3	118.59	72.44	30.93	-4	13	3	326.00	305.57	33.78	-4	18	3	8.12	-98.71	55.98
-5	9	3	2.22	46.07	28.37	-3	13	3	0.96	27.39	27.22	-3	18	3	38.61	9.22	53.55
-4	9	3	0.57	-10.66	45.24	-2	13	3	143.24	160.50	27.91	-2	18	3	217.47	230.80	33.55
-3	9	3	56.92	48.21	24.42	-1	13	3	18.28	103.91	45.79	-1	18	3	62.05	-46.40	53.83
-2	9	3	611.10	603.81	48.01	0	13	3	112.95	122.99	18.00	0	18	3	37.64	84.86	44.65
-1	9	3	290.21	370.54	29.44	1	13	3	36.03	16.53	43.05	1	18	3	2.11	-5.54	49.25

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
2	18	3	68.11	30.2E	55.31	-3	2	4	658.88	581.24	49.07	-6	6	4	0.89	36.91	28.59
3	18	3	17.88	-13.12	52.78	-2	2	4	20.08	34.26	34.90	-5	6	4	149.49	156.33	29.58
-4	19	3	7.79	-43.08	55.11	-1	2	4	317.20	312.30	27.92	-4	6	4	33.01	32.10	26.43
-3	19	3	86.73	100.89	31.67	0	2	4	491.53	431.18	29.40	-3	6	4	3.78	-21.28	41.81
-2	19	3	195.07	227.20	33.16	1	2	4	3.54	18.16	35.24	-2	6	4	652.37	712.39	50.74
-1	19	3	74.31	75.26	30.85	2	2	4	168.49	148.22	25.43	-1	6	4	0.38	22.99	34.53
0	19	3	1.00	-13.36	35.23	3	2	4	312.30	311.20	30.18	0	6	4	32.39	15.90	25.65
1	19	3	154.72	117.72	30.10	4	2	4	49.94	96.55	29.20	1	6	4	650.14	579.91	46.30
2	19	3	189.88	151.13	32.61	5	2	4	202.25	226.72	32.60	2	6	4	105.62	89.77	23.78
3	19	3	67.04	-3.42	58.62	6	2	4	58.16	25.81	42.58	3	6	4	647.02	633.73	56.83
-4	20	3	6.58	-24.74	54.86	-8	3	4	88.34	72.20	33.69	4	6	4	45.14	19.17	48.78
-3	20	3	12.55	14.80	56.71	-7	3	4	1.35	7.47	51.58	5	6	4	3.07	9.11	51.01
-2	20	3	0.93	30.03	55.40	-6	3	4	312.98	322.28	31.87	-7	7	4	232.02	247.62	34.98
-1	20	3	4.07	-38.61	53.48	-5	3	4	1.07	-82.90	46.59	-6	7	4	27.12	49.51	51.69
0	20	3	2.89	7.54	34.56	-4	3	4	783.03	857.00	57.12	-5	7	4	201.33	212.23	31.52
1	20	3	0.48	-26.50	51.06	-3	3	4	23.45	-23.15	38.63	-4	7	4	767.90	771.27	50.50
2	20	3	1.03	-45.27	55.91	-2	3	4	2583.78	2571.13	95.89	-3	7	4	446.09	448.63	49.37
-3	21	3	9.89	26.51	55.83	-1	3	4	9.66	25.14	32.80	-2	7	4	295.78	297.89	26.34
-2	21	3	12.18	34.11	53.56	0	3	4	246.98	246.73	15.71	-1	7	4	357.88	411.88	42.33
-1	21	3	11.29	3.48	54.09	1	3	4	71.17	101.47	20.60	0	7	4	28.18	38.17	15.16
0	21	3	5.10	-37.70	48.78	2	3	4	1246.54	1428.67	67.55	1	7	4	142.79	137.57	23.12
1	21	3	14.99	-0.55	50.43	3	3	4	82.01	114.22	27.35	2	7	4	7.55	-3.46	41.26
2	21	3	31.64	-99.45	58.70	4	3	4	43.42	37.44	29.12	3	7	4	411.51	381.64	37.90
-2	22	3	69.04	-47.83	61.61	5	3	4	4.53	-30.70	53.95	4	7	4	117.69	110.50	30.06
-1	22	3	0.07	-21.35	52.15	6	3	4	2.08	37.03	57.73	5	7	4	15.39	-31.46	56.48
0	22	3	92.62	92.47	22.87	-8	4	4	0.12	-47.63	56.84	-7	8	4	1.62	-43.01	57.37
1	22	3	8.94	-1.10	56.21	-7	4	4	4.12	-52.46	50.11	-6	8	4	2.64	-18.11	52.82
-8	0	4	34.71	-56.45	56.54	-6	4	4	2.74	-20.46	49.00	-5	8	4	608.95	673.77	61.80
-6	0	4	82.24	58.52	27.59	-5	4	4	13.82	-42.61	46.66	-4	8	4	734.75	807.83	68.94
-4	0	4	439.16	509.78	47.30	-4	4	4	476.83	474.22	37.12	-3	8	4	3.52	-73.00	44.61
-2	0	4	7153.68	7198.37	231.31	-3	4	4	133.83	997.27	58.68	-2	8	4	1.20	22.49	40.93
0	0	4	657.81	609.31	31.30	-2	4	4	51.35	663.15	46.64	-1	8	4	240.12	271.53	25.66
2	0	4	570.77	1022.02	58.16	-1	4	4	882.91	896.62	50.43	0	8	4	1.43	-9.60	27.48
4	0	4	302.70	322.87	30.64	0	4	4	7.16	-14.74	29.97	1	8	4	0.31	1.05	36.09
6	0	4	30.81	13.27	24.03	1	4	4	1057.33	1077.20	56.87	2	8	4	129.29	111.88	24.41
-8	1	4	13.93	62.98	30.95	2	4	4	0.89	25.82	37.72	3	8	4	2.46	-27.32	44.45
-7	1	4	674.59	733.35	64.14	3	4	4	474.10	411.37	38.12	4	8	4	0.71	7.64	49.70
-6	1	4	15.73	10.92	47.48	4	4	4	460.42	477.31	42.52	5	8	4	102.25	100.02	32.65
-5	1	4	649.88	605.16	56.46	5	4	4	107.82	79.89	32.20	-7	9	4	198.42	208.87	34.52
-4	1	4	420.18	495.42	49.22	6	4	4	58.96	52.64	60.69	-6	9	4	444.95	482.72	45.11
-3	1	4	52.17	78.96	21.06	-8	5	4	71.18	94.80	32.84	-5	9	4	2.89	-35.75	51.02
-2	1	4	288.47	307.99	27.54	-7	5	4	80.84	88.23	30.98	-4	9	4	339.14	357.67	42.25
-1	1	4	280.36	271.75	25.64	-6	5	4	156.55	115.54	30.92	-3	9	4	549.33	510.18	39.53
0	1	4	110.40	102.45	14.21	-5	5	4	598.26	628.35	58.68	-2	9	4	271.79	289.24	26.90
1	1	4	12.68	-1.44	36.88	-4	5	4	971.55	1013.00	63.75	-1	9	4	216.14	280.39	26.64
2	1	4	62.42	71.59	22.96	-3	5	4	174.80	187.81	24.77	0	9	4	312.26	267.74	18.61
3	1	4	242.41	259.72	28.21	-2	5	4	1169.99	1068.66	58.49	1	9	4	157.68	166.84	24.06
4	1	4	0.03	-15.26	46.92	-1	5	4	4.06	20.19	35.17	2	9	4	32.75	38.19	24.22
5	1	4	114.78	115.94	31.67	0	5	4	23.70	34.03	14.19	3	9	4	2.17	-44.58	44.98
6	1	4	15.30	47.18	54.34	1	5	4	608.65	531.42	45.07	4	9	4	90.30	78.66	30.36
-8	2	4	10.50	39.19	55.80	2	5	4	122.84	141.23	22.86	5	9	4	14.72	-29.69	57.58
-7	2	4	4.26	-49.93	52.41	3	5	4	103.97	150.55	27.03	-7	10	4	16.17	73.91	32.27
-6	2	4	16.61	30.15	48.59	4	5	4	5.48	-51.16	51.42	-6	10	4	0.01	42.78	33.02
-5	2	4	30.85	59.97	26.50	5	5	4	64.51	87.48	31.89	-5	10	4	1.96	5.24	48.02
-4	2	4	473.96	460.07	36.66	-7	6	4	0.72	18.59	51.34	-4	10	4	427.63	477.50	41.65

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-3	10	4	249.73	258.20	29.74	4	14	4	24.24	54.46	30.29	-1	0	5	1275.08	1146.27	63.89
-2	10	4	229.55	272.40	28.54	-6	15	4	65.84	102.17	33.78	1	0	5	2159.40	2384.28	100.20
-1	10	4	65.72	81.54	25.29	-5	15	4	29.12	33.69	38.86	3	0	5	24.06	17.32	43.37
0	10	4	130.78	106.15	22.70	-4	15	4	139.50	135.42	30.74	5	0	5	0.24	-19.84	53.27
1	10	4	174.09	214.88	25.43	-3	15	4	585.65	638.02	61.56	-7	1	5	0.57	3.12	52.16
2	10	4	0.24	11.25	42.81	-2	15	4	33.86	32.50	27.57	-6	1	5	3.83	-21.22	55.88
3	10	4	96.07	120.04	26.48	-1	15	4	64.15	80.45	29.09	-5	1	5	60.21	41.63	28.51
4	10	4	266.13	281.05	33.43	0	15	4	30.77	32.13	22.97	-4	1	5	258.29	209.23	29.10
5	10	4	41.83	10.06	57.35	1	15	4	123.33	87.50	29.01	-3	1	5	17.68	56.13	24.63
-7	11	4	4.85	10.41	56.30	2	15	4	3.00	-37.66	47.59	-2	1	5	1208.19	1315.21	66.46
-6	11	4	249.17	243.68	34.46	3	15	4	11.03	-21.65	35.27	-1	1	5	653.58	721.22	51.76
-5	11	4	267.48	285.86	33.07	4	15	4	69.65	52.61	32.87	0	1	5	137.87	165.37	18.22
-4	11	4	12.95	33.89	45.97	-5	16	4	35.16	28.29	58.52	1	1	5	6.08	-42.96	45.96
-3	11	4	343.22	328.42	31.87	-4	16	4	0.13	-12.12	52.34	2	1	5	435.97	394.78	33.16
-2	11	4	449.51	540.57	52.42	-3	16	4	65.92	77.27	30.85	3	1	5	100.84	134.08	25.12
-1	11	4	0.23	-23.30	43.81	-2	16	4	16.79	-46.98	50.74	4	1	5	392.07	401.20	41.75
0	11	4	377.64	403.02	45.67	-1	16	4	378.96	414.08	41.20	5	1	5	28.69	87.28	31.31
1	11	4	215.31	207.68	26.24	0	16	4	0.51	-1.60	34.05	-7	2	5	50.79	-31.95	55.71
2	11	4	7.97	-10.58	41.61	1	16	4	287.54	263.06	30.90	-6	2	5	719.56	674.74	61.77
3	11	4	37.49	4.77	47.25	2	16	4	39.40	38.60	28.51	-5	2	5	361.74	306.82	31.95
4	11	4	390.49	396.23	36.54	3	16	4	31.58	29.28	29.94	-4	2	5	586.23	551.22	56.11
5	11	4	20.59	6.28	58.49	-5	17	4	23.48	65.02	33.52	-3	2	5	450.54	339.66	35.44
-7	12	4	35.63	9.91	60.99	-4	17	4	32.73	133.04	30.94	-2	2	5	32.40	58.84	24.01
-6	12	4	0.51	26.74	38.12	-3	17	4	24.09	5.70	31.24	-1	2	5	1213.40	1163.49	65.16
-5	12	4	3.87	-88.87	53.70	-2	17	4	0.18	-23.03	52.91	0	2	5	1869.44	1767.02	57.25
-4	12	4	33.08	-28.05	50.40	-1	17	4	2.23	34.50	54.16	1	2	5	255.31	342.61	30.38
-3	12	4	11.09	-23.02	48.68	0	17	4	107.14	131.06	20.84	2	2	5	188.35	89.93	28.90
-2	12	4	396.41	442.78	39.66	1	17	4	55.17	81.58	28.49	3	2	5	18.31	9.76	43.94
-1	12	4	0.60	-37.45	46.67	2	17	4	11.13	-7.85	49.50	4	2	5	41.23	84.53	29.68
0	12	4	491.73	462.28	26.84	3	17	4	4.14	4.62	53.62	5	2	5	0.68	24.62	38.42
1	12	4	385.91	372.46	36.23	-4	18	4	13.03	46.62	56.37	-7	3	5	1.60	29.97	37.70
2	12	4	379.51	372.41	37.32	-2	18	4	4.29	19.48	52.64	-6	3	5	2.14	75.44	28.39
3	12	4	86.93	27.29	50.51	-2	18	4	226.33	200.55	32.65	-5	3	5	80.79	113.51	28.51
4	12	4	260.31	275.76	33.43	-1	18	4	118.90	125.30	32.00	-4	3	5	17.62	57.08	27.19
-6	13	4	62.91	42.73	57.02	0	18	4	81.04	45.67	26.03	-3	3	5	60.48	33.07	44.15
-5	13	4	110.62	162.25	31.05	1	18	4	84.02	84.54	28.65	-2	3	5	596.66	579.63	51.99
-4	13	4	0.01	9.86	50.51	2	18	4	3.76	-14.79	53.46	-1	3	5	574.09	460.57	53.18
-3	13	4	944.14	830.99	67.54	-4	19	4	1.71	30.98	39.62	0	3	5	214.35	287.50	33.42
-2	13	4	171.71	142.56	28.91	-3	19	4	88.03	24.38	33.77	1	3	5	3.47	7.97	43.83
-1	13	4	457.52	543.62	53.84	-2	19	4	3.04	31.85	56.65	2	3	5	317.12	332.09	30.93
0	13	4	0.60	14.76	31.63	-1	19	4	228.71	239.42	35.33	3	3	5	583.55	686.46	59.70
1	13	4	243.66	260.71	28.87	0	19	4	4.29	0.26	37.54	4	3	5	96.61	136.80	31.82
2	13	4	0.07	27.04	43.79	1	19	4	53.90	93.55	30.65	5	3	5	144.51	54.35	61.54
3	13	4	30.79	22.05	50.35	2	19	4	0.43	11.62	30.22	-7	4	5	6.77	-10.41	53.98
4	13	4	15.31	73.27	30.69	-3	20	4	18.53	96.31	32.65	-6	4	5	373.97	341.52	34.48
-6	14	4	28.57	-14.42	57.79	-2	20	4	38.02	-8.62	56.45	-5	4	5	34.46	0.95	48.86
-5	14	4	80.68	90.72	31.10	-1	20	4	30.09	-21.15	61.74	-4	4	5	319.00	296.14	31.02
-4	14	4	81.08	79.04	29.46	0	20	4	84.54	84.93	23.74	-3	4	5	5.87	29.23	44.99
-3	14	4	6.10	-18.50	51.54	1	20	4	2.07	31.81	51.35	-2	4	5	126.87	132.34	25.95
-2	14	4	31.32	8.52	47.33	-2	21	4	0.97	48.88	56.98	-1	4	5	439.51	466.65	47.35
-1	14	4	87.94	40.06	48.53	-1	21	4	173.11	246.84	37.24	0	4	5	1465.79	1390.99	61.41
0	14	4	310.60	335.55	23.31	0	21	4	17.54	44.61	25.66	1	4	5	249.43	250.27	27.74
1	14	4	99.36	111.04	24.34	-7	0	5	49.39	6.51	54.76	2	4	5	130.97	130.23	25.97
2	14	4	135.45	171.11	27.59	-5	0	5	1199.19	1163.18	72.00	3	4	5	67.83	81.88	26.38
3	14	4	37.27	12.92	49.01	-3	0	5	2149.18	1936.76	86.48	4	4	5	488.75	517.10	46.22

Structure Factors Table (continued) (*sum squared reffns.) for C(14) H(28) N(2) O(10) Cl(2)

Page 9

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
5	4	5	19.14	10.22	57.62	-3	9	5	1.58	19.48	28.76	-3	14	5	82.51	124.63	30.48
-7	5	5	2.97	31.62	54.69	-2	9	5	14.74	30.14	48.30	-2	14	5	137.12	-3.88	53.37
-6	5	5	45.48	42.55	21.07	-1	9	5	106.74	103.18	28.49	-1	14	5	283.77	301.87	32.39
-5	5	5	0.05	23.13	54.79	0	9	5	148.77	138.22	19.19	0	14	5	8.88	-62.99	38.20
-4	5	5	46.23	8.26	23.90	1	9	5	132.16	104.60	26.31	1	14	5	31.55	-3.16	48.47
-3	5	5	14.83	-9.70	44.85	2	9	5	2.87	29.17	43.58	2	14	5	48.59	65.60	28.49
-2	5	5	168.00	155.52	26.46	3	9	5	213.38	248.80	29.65	3	14	5	86.41	61.82	30.94
-1	5	5	0.46	30.82	21.59	4	9	5	38.82	20.79	53.85	-5	15	5	1.61	-23.07	56.48
0	5	5	106.39	84.99	17.88	-7	10	5	4.62	33.29	59.10	-4	15	5	12.84	-34.83	56.67
1	5	5	3.35	-24.74	43.46	-6	10	5	169.89	244.62	33.96	-3	15	5	46.15	87.37	29.52
2	5	5	61.45	67.03	24.59	-5	10	5	20.38	32.86	52.58	-2	15	5	66.63	117.43	30.78
3	5	5	47.25	41.69	42.70	-4	10	5	1226.60	987.28	72.07	-1	15	5	0.78	22.98	48.95
4	5	5	13.68	15.38	54.13	-3	10	5	6.66	-24.18	48.48	0	15	5	166.02	183.83	21.72
5	5	5	16.71	-15.49	59.24	-2	10	5	1020.67	1178.13	68.85	1	15	5	298.87	223.44	31.37
-7	6	5	162.14	221.85	33.52	-1	10	5	3.20	28.02	44.49	2	15	5	114.40	168.20	29.52
-6	6	5	22.35	45.80	53.09	0	10	5	303.19	315.18	21.15	3	15	5	9.28	46.92	52.61
-5	6	5	748.13	803.90	65.52	1	10	5	0.74	-20.57	43.21	-5	16	5	20.83	78.47	32.49
-4	6	5	11.15	-26.73	47.32	2	10	5	351.66	296.70	30.70	-4	16	5	212.97	208.15	34.93
-3	6	5	1285.67	1188.74	70.38	3	10	5	6.00	73.81	27.15	-3	16	5	0.99	0.51	52.20
-2	6	5	80.81	111.57	26.40	4	10	5	9.52	9.61	36.97	-2	16	5	1001.27	127.80	77.78
-1	6	5	1339.88	1333.58	69.99	-6	11	5	0.39	37.42	51.22	-1	16	5	111.75	117.56	30.68
0	6	5	116.88	121.88	18.72	-5	11	5	0.05	-25.44	52.83	0	16	5	70.53	97.55	21.42
1	6	5	535.51	607.65	52.60	-4	11	5	65.24	20.40	36.71	1	16	5	1.47	-24.38	52.21
2	6	5	6.01	-40.04	42.25	-3	11	5	13.94	13.31	49.00	2	16	5	109.47	116.16	30.40
3	6	5	31.61	27.52	46.42	-2	11	5	0.00	26.81	49.10	-4	17	5	14.44	-30.95	55.84
4	6	5	162.28	147.26	32.11	-1	11	5	42.58	95.50	28.21	-3	17	5	2.73	-3.02	55.51
5	6	5	34.96	39.63	56.86	0	11	5	0.06	9.82	33.39	-2	17	5	11.41	87.32	34.22
-7	7	5	26.14	47.37	55.86	1	11	5	119.19	93.26	27.17	-1	17	5	0.10	21.39	53.14
-6	7	5	9.47	63.74	29.55	2	11	5	10.64	-1.49	46.61	0	17	5	13.41	-2.80	36.50
-5	7	5	454.32	430.60	41.87	3	11	5	24.98	23.55	47.58	1	17	5	120.36	93.91	30.43
-4	7	5	63.68	34.25	50.63	4	11	5	5.09	-30.61	54.90	2	17	5	5.98	-33.47	53.73
-3	7	5	4.74	-16.43	48.43	-5	12	5	16.03	-31.05	56.06	-4	18	5	88.59	17.63	61.70
-2	7	5	5.31	59.38	26.05	-6	12	5	132.88	151.50	32.40	-3	18	5	50.34	-29.68	61.09
-1	7	5	36.41	53.40	26.82	-4	12	5	37.10	69.80	28.95	-2	18	5	155.63	322.70	36.34
0	7	5	146.51	186.04	22.31	-3	12	5	110.30	150.59	29.43	-1	18	5	17.48	-1.51	56.25
1	7	5	8.89	-8.15	43.35	-2	12	5	639.60	549.32	45.42	0	18	5	59.32	40.72	27.06
2	7	5	180.02	147.67	26.04	-1	12	5	166.38	149.32	30.04	1	18	5	17.43	-6.48	49.46
3	7	5	253.85	287.56	30.41	0	12	5	192.44	179.57	27.06	-3	19	5	6.50	-15.55	60.63
4	7	5	204.17	255.29	33.76	1	12	5	356.34	335.55	31.04	-2	19	5	12.00	26.47	59.65
-7	8	5	5.77	22.48	56.22	2	12	5	48.34	48.17	27.22	-1	19	5	170.84	193.58	34.81
-6	8	5	24.53	32.98	54.70	3	12	5	97.46	100.54	29.17	0	19	5	52.06	18.65	40.71
-5	8	5	698.73	746.78	64.48	4	12	5	55.13	93.76	31.58	-6	0	6	170.90	179.55	30.41
-4	8	5	185.77	181.86	30.44	-6	13	5	3.53	104.11	31.68	-4	0	6	3.32	-63.83	48.56
-3	8	5	235.22	246.85	30.53	-5	13	5	3.31	-2.20	53.56	-2	0	6	222.73	252.04	29.16
-2	8	5	341.66	307.02	30.77	-4	13	5	3.60	-14.49	52.55	0	0	6	43.72	47.13	25.11
-1	8	5	937.42	973.99	63.24	-3	13	5	0.83	22.12	48.82	2	0	6	120.15	138.15	29.41
0	8	5	361.41	399.12	30.71	-2	13	5	85.76	-4.17	52.30	4	0	6	109.94	138.27	29.95
1	8	5	353.58	375.40	35.97	-1	13	5	14.73	-1.78	35.45	-7	1	6	12.00	-12.91	53.92
2	8	5	354.23	353.24	29.33	0	13	5	325.98	288.53	22.47	-6	1	6	4.45	-22.61	52.15
3	8	5	78.74	84.58	27.00	1	13	5	160.91	156.52	27.93	-5	1	6	154.08	192.55	29.09
4	8	5	4.20	-56.64	53.32	2	13	5	43.28	38.88	27.22	-4	1	6	79.05	72.49	28.18
-7	9	5	16.72	38.82	56.72	1	13	5	1.21	-44.31	52.45	-3	1	6	94.92	19.63	50.81
-6	9	5	1.05	24.95	55.69	-6	14	5	33.33	28.92	42.03	-2	1	6	383.88	382.21	38.18
-5	9	5	67.11	76.73	30.05	-5	14	5	197.83	184.59	34.85	-1	1	6	274.16	301.21	30.75
-4	9	5	630.64	537.00	46.14	-4	14	5	24.99	70.18	30.13	0	1	6	190.00	184.43	21.40

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
1	1	6	1299.54	1147.35	73.21	4	6	6	575.02	567.19	43.18	-1	11	6	73.43	-25.69	52.29
2	1	6	162.52	79.65	31.35	-3	6	6	214.82	219.76	30.92	0	11	6	231.07	246.17	21.83
3	1	6	177.71	242.60	29.29	-2	6	6	125.43	150.55	28.50	1	11	6	13.21	55.30	26.67
4	1	6	21.89	47.26	48.17	-1	6	6	119.40	48.21	51.08	2	11	6	265.48	234.52	32.21
-5	2	6	43.45	-32.22	56.85	0	6	6	35.86	21.76	24.17	3	11	6	13.52	-185.35	54.04*
-6	2	6	39.21	38.30	53.31	1	6	6	229.87	216.42	29.19	-5	12	6	1.22	-13.16	54.82
-8	2	6	116.60	118.75	29.70	2	6	6	0.01	-63.57	47.06	-4	12	6	40.84	68.83	31.80
-4	2	6	6.30	81.49	27.29	3	6	6	1.06	-6.56	44.76	-3	12	6	228.97	203.64	33.75
-3	2	6	0.44	-102.59	47.51	4	6	6	53.29	-73.79	60.32	-2	12	6	66.70	19.86	54.13
-2	2	6	603.14	597.12	57.94	-7	7	6	8.20	-44.13	59.21	-1	12	6	2.57	-19.00	53.99
-1	2	6	166.29	143.51	29.33	-6	7	6	157.51	144.66	33.80	0	12	6	0.68	29.62	33.72
0	2	6	77.27	76.30	25.10	-5	7	6	69.81	87.76	30.15	1	12	6	149.07	134.36	30.35
1	2	6	3.83	44.60	47.21	-4	7	6	48.24	32.78	51.60	2	12	6	197.70	241.85	31.97
2	2	6	0.14	-48.21	52.43	-3	7	6	291.51	314.25	32.34	-5	13	6	82.72	85.05	33.89
3	2	6	112.32	148.29	29.11	-2	7	6	5.28	-60.60	50.35	-4	13	6	86.90	99.62	33.46
4	2	6	44.13	53.69	30.78	-1	7	6	658.47	738.23	61.84	-3	13	6	413.67	441.90	45.51
-7	3	6	21.67	20.12	39.61	0	7	6	394.92	360.28	22.88	-2	13	6	0.30	-101.47	55.16
-6	3	6	83.39	-52.66	56.61	1	7	6	905.56	858.19	65.41	-1	13	6	817.77	840.95	68.80
-5	3	6	0.38	15.75	48.88	2	7	6	3.08	-19.19	45.87	0	13	6	1.98	-62.85	49.12
-4	3	6	496.55	519.35	42.03	3	7	6	364.09	398.97	39.32	1	13	6	79.91	26.99	37.42
-3	3	6	0.50	30.24	46.72	-6	8	6	12.78	-35.06	55.68	2	13	6	1.43	-47.12	52.37
-2	3	6	1128.04	1060.91	68.06	-5	8	6	33.68	-28.94	53.75	-5	14	6	8.06	-14.49	58.67
-1	3	6	8.18	27.01	47.84	-4	8	6	2.69	12.61	51.42	-4	14	6	45.30	65.73	33.08
0	3	6	1591.82	1784.38	62.22	-3	8	6	1.52	-57.49	52.62	-3	14	6	38.10	99.21	31.95
1	3	6	49.19	41.78	48.61	-2	8	6	335.12	315.13	32.68	-2	14	6	26.44	65.70	31.00
2	3	6	488.84	548.24	43.92	-1	8	6	155.32	145.65	29.03	-1	14	6	100.16	127.21	32.41
3	3	6	35.32	35.60	56.42	0	8	6	6.71	-22.88	45.48	0	14	6	0.01	-50.17	52.76
4	3	6	22.35	0.18	59.06	1	8	6	7.89	16.85	46.21	1	14	6	10.63	46.60	51.23
-7	4	6	53.78	12.88	55.89	2	8	6	0.19	-20.58	46.69	2	14	6	0.74	49.49	53.14
-6	4	6	35.48	53.19	53.19	3	8	6	5.96	-65.02	47.43	-4	15	6	12.30	-4.83	56.12
-5	4	6	46.88	29.14	59.14	-6	9	6	106.44	90.37	34.01	-3	15	6	336.00	375.80	37.46
-4	4	6	121.88	89.10	59.10	-5	9	6	0.48	-117.01	55.86	-2	15	6	6.37	-43.13	57.87
-3	4	6	34.28	17.14	49.81	-4	9	6	106.80	98.93	30.80	-1	15	6	99.68	154.60	33.51
-2	4	6	17.62	16.29	47.73	-3	9	6	482.99	455.91	42.92	0	15	6	83.33	86.33	21.92
-1	4	6	103.16	147.61	29.02	-2	9	6	361.86	350.54	33.18	1	15	6	120.61	144.34	30.55
0	4	6	0.47	69.61	22.28	-1	9	6	53.71	-43.44	51.04	-4	16	6	4.26	-4.84	44.04
1	4	6	27.44	50.15	27.62	0	9	6	966.94	939.90	52.25	-3	16	6	60.97	8.70	62.48
2	4	6	23.08	5.18	50.61	1	9	6	15.77	42.14	44.00	-2	16	6	1.24	29.97	54.91
3	4	6	59.13	76.16	27.97	2	9	6	201.65	204.73	30.11	-1	16	6	16.61	-87.65	56.96
4	4	6	48.13	-74.91	63.87	3	9	6	156.10	180.06	30.24	0	16	6	4.49	13.04	37.97
-7	5	6	46.03	-63.22	58.66	-6	10	6	18.23	17.58	55.36	1	16	6	1.16	-29.51	53.05
-6	5	6	41.81	70.24	30.80	-5	10	6	18.63	-10.15	54.34	-3	17	6	3.08	-51.72	58.11
-5	5	6	167.02	163.83	31.52	-4	10	6	87.35	102.15	31.34	-2	17	6	38.67	-4.04	59.50
-4	5	6	933.19	795.00	66.00	-3	10	6	221.90	189.31	31.05	-1	17	6	65.14	55.03	55.44
-3	5	6	100.23	164.24	28.91	-2	10	6	74.61	73.51	29.72	0	17	6	152.88	189.61	35.76
-2	5	6	298.51	318.47	31.52	-1	10	6	83.11	99.23	29.44	-5	0	7	32.05	110.99	28.51
-1	5	6	95.11	58.72	29.59	0	10	6	7.61	-9.55	34.47	-3	0	7	89.82	88.48	29.36
0	5	6	123.58	148.80	27.93	1	10	6	13.37	26.19	46.75	-1	0	7	836.89	849.78	68.24
1	5	6	1053.07	1019.23	67.16	2	10	6	47.90	38.22	29.38	1	0	7	288.63	276.75	34.06
2	5	6	328.03	363.61	32.39	3	10	6	2.48	-58.33	51.70	3	0	7	100.99	124.40	32.38
3	5	6	56.48	73.88	26.51	-6	11	6	3.16	30.86	32.10	-6	1	7	32.41	35.34	53.54
4	5	6	3.68	46.19	53.66	-5	11	6	72.91	126.82	31.38	-5	1	7	49.77	69.67	29.16
-7	6	6	67.87	54.09	34.00	-4	11	6	296.06	245.59	34.73	-4	1	7	74.03	72.85	28.96
-6	6	6	71.91	12.41	55.13	-3	11	6	125.20	138.38	30.53	-3	1	7	2.05	8.23	47.05
-5	6	6	4.38	32.70	35.60	-2	11	6	234.61	260.16	32.39	-2	1	7	54.20	55.40	28.15

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-1	1	7	12.64	8.40	51.62	-4	7	7	28.78	35.74	50.64	-4	1	8	14.95	0.34	51.74
0	1	7	226.71	221.47	23.10	-3	7	7	64.03	32.02	52.79	-3	1	8	0.49	52.87	30.09
1	1	7	5.33	20.97	52.27	-2	7	7	181.91	151.75	31.65	-2	1	8	12.47	28.91	54.37
2	1	7	1.00	-2.91	52.60	-1	7	7	0.75	37.81	52.24	-1	1	8	191.93	191.10	34.62
3	1	7	3.42	32.74	55.98	0	7	7	44.17	0.88	39.04	0	1	8	63.75	53.00	70.17
-6	2	7	99.89	104.30	32.30	1	7	7	0.93	31.31	50.93	1	1	8	132.48	85.10	34.95
-5	2	7	7.09	27.50	51.74	2	7	7	0.12	-34.91	51.42	-5	2	8	1.45	-99.21	56.37
-4	2	7	2.87	13.55	48.50	-5	8	7	33.83	39.30	39.80	-4	2	8	89.22	133.74	32.28
-3	2	7	147.16	48.86	51.75	-4	8	7	54.40	46.69	54.46	-3	2	8	40.49	67.63	51.54
-2	2	7	40.02	69.80	28.31	-3	8	7	135.77	86.29	32.09	-2	2	8	70.82	110.17	31.83
-1	2	7	184.67	209.25	32.48	-2	8	7	8.99	38.81	52.43	-1	2	8	3.62	15.30	53.17
0	2	7	395.84	354.35	24.73	-1	8	7	120.18	93.75	31.52	0	2	8	29.31	9.17	29.27
1	2	7	18.28	47.35	53.28	0	8	7	70.84	85.70	25.68	1	2	8	134.52	103.28	36.27
2	2	7	191.02	202.34	23.87	1	8	7	83.84	84.72	30.30	-5	3	8	18.67	-1.99	58.23
3	2	7	66.96	120.45	33.21	2	8	7	106.14	31.92	54.22	-4	3	8	72.10	57.00	32.48
-6	3	7	0.24	-96.41	53.87	-5	9	7	57.36	14.83	57.87	-3	3	8	28.07	60.66	31.26
-5	3	7	250.47	219.09	32.56	-4	9	7	46.23	43.00	31.62	-2	3	8	44.78	17.40	57.06
-4	3	7	14.90	-22.97	51.60	-3	9	7	101.12	120.54	31.33	-1	3	8	70.25	-13.15	59.49
-3	3	7	126.20	129.36	30.09	-2	9	7	6.88	47.34	50.82	0	3	8	433.61	472.33	30.73
-2	3	7	28.68	8.32	50.24	-1	9	7	19.34	27.07	52.97	1	3	8	47.12	88.44	34.07
-1	3	7	715.38	730.12	64.92	0	9	7	0.07	-33.78	38.44	-5	4	8	5.95	-12.51	50.12
0	3	7	57.67	37.35	26.92	1	9	7	27.89	-4.61	53.31	-4	4	8	1.64	-27.33	56.16
1	3	7	16.44	34.05	52.70	2	9	7	2.64	-22.33	52.29	-3	4	8	1.05	-56.16	55.89
2	3	7	46.26	79.69	32.27	-5	10	7	7.72	-82.29	60.75	-2	4	8	24.09	-47.31	57.20
3	3	7	1.05	-6.11	58.25	-4	10	7	80.28	56.07	31.91	-1	4	8	25.88	-17.48	56.45
-6	4	7	19.23	55.93	31.66	-3	10	7	68.75	50.40	55.19	0	4	8	6.68	42.10	31.84
-5	4	7	17.71	-56.25	54.85	-2	10	7	238.69	246.34	34.11	1	4	8	197.57	208.75	36.53
-4	4	7	1.79	16.14	48.81	-1	10	7	36.49	41.48	55.52	-5	5	8	1.23	17.48	55.94
-3	4	7	95.97	95.65	30.39	0	10	7	162.15	117.00	23.04	-4	5	8	44.43	-14.69	60.01
-2	4	7	201.45	229.04	31.91	1	10	7	60.25	64.36	29.45	-3	5	8	8.40	18.31	54.76
-1	4	7	501.19	476.89	44.68	-5	11	7	52.02	63.56	34.41	-2	5	8	31.84	52.39	32.44
0	4	7	290.69	295.89	27.98	-4	11	7	31.39	83.56	31.92	-1	5	8	47.13	-18.91	57.68
1	4	7	166.51	167.42	32.51	-3	11	7	6.98	25.53	53.23	0	5	8	2.12	-20.96	59.78
2	4	7	481.20	511.59	45.71	-2	11	7	52.47	53.91	54.32	1	5	8	17.88	-77.22	59.17
3	4	7	1.24	-144.00	60.73	-1	12	7	0.11	14.36	55.23	-4	6	8	174.65	161.76	34.78
-6	5	7	9.82	14.22	56.62	0	11	7	34.87	48.67	37.65	-3	6	8	13.59	13.76	39.26
-5	5	7	67.20	63.39	32.44	1	11	7	115.57	127.43	32.26	-2	6	8	54.41	49.69	56.88
-4	5	7	1.35	37.89	50.75	-4	12	7	14.83	-6.71	57.66	-1	6	8	14.50	3.49	57.10
-3	5	7	55.17	29.68	30.15	-3	12	7	3.61	-6.91	58.42	0	6	8	139.72	142.90	24.24
-2	5	7	24.31	27.32	25.12	-2	12	7	269.12	295.37	36.50	-4	7	8	8.48	50.21	57.87
-1	5	7	395.35	448.85	42.33	-1	12	7	94.14	85.45	33.85	-3	7	8	17.05	5.06	56.53
0	5	7	271.94	276.13	23.52	0	12	7	113.32	76.20	47.45	-2	7	8	18.46	67.09	31.94
1	5	7	17.51	23.71	52.64	1	12	7	322.73	293.66	35.62	-1	7	8	189.18	165.78	36.20
2	5	7	11.23	-47.13	56.21	-4	13	7	37.14	37.54	59.59	0	7	8	157.85	182.98	25.42
-6	6	7	0.68	-43.78	57.62	-3	13	7	0.75	31.01	56.82	-4	8	8	111.70	40.00	62.12
-5	6	7	100.59	123.21	32.84	-2	13	7	361.16	305.49	38.30	-3	8	8	0.02	26.67	55.16
-4	6	7	19.33	31.82	50.95	-1	13	7	50.90	51.78	58.96	-2	8	8	34.23	-17.40	58.04
-3	6	7	159.10	135.56	31.07	0	13	7	0.04	3.12	38.90	-1	8	8	81.81	36.56	59.35
-2	6	7	89.09	-3.97	55.69	-3	14	7	66.73	43.50	57.80	0	8	8	23.20	-5.67	43.53
-1	6	7	408.32	510.80	43.43	-2	14	7	11.60	49.96	57.96	-3	9	8	17.39	29.16	34.30
0	6	7	133.84	148.85	22.73	-1	14	7	15.69	42.23	32.84	-2	9	8	63.25	95.96	34.04
1	6	7	212.21	225.85	32.41	-4	0	8	60.04	23.27	53.72	-1	9	8	37.91	66.97	34.15
2	6	7	17.49	-11.59	51.13	-2	0	8	150.37	204.88	32.04	-3	10	8	93.84	131.28	34.89
-6	7	7	63.70	133.86	33.28	0	0	8	28.08	11.09	38.82	-2	10	8	0.49	-28.50	60.23
-5	7	7	0.52	30.28	38.53	-5	1	8	112.11	73.84	33.07	-1	10	8	128.95	31.41	63.61

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TCA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	0	0	77	78	-5	1	1	78	-77	-3	7	1	118	104	-5	1	2	18	-16	3	9	2	18	-17
4	0	0	17	7	-3	1	1	17	-1	-1	7	1	41	38	-3	1	2	41	-41	-4	10	2	15	-19
8	0	0	66	66	-1	1	1	70	74	-1	1	1	22	17	-1	1	2	174	-176	-2	10	2	22	-21
1	1	0	11	-12	-1	1	1	186	191	5	7	1	43	42	-1	1	2	108	-105	-2	10	2	11	-2
3	1	0	15	15	3	1	1	40	-48	7	7	1	14	8	3	1	2	26	-26	6	10	2	20	22
7	1	0	18	15	5	1	1	9	-8	-6	8	1	24	19	7	1	2	15	-15	-3	11	2	25	30
9	1	0	12	-6	7	1	1	27	31	-4	8	1	22	16	-10	2	2	15	-20	1	11	2	34	-33
11	1	0	16	-6	9	1	1	24	29	0	8	1	13	-11	-6	2	2	27	22	-6	12	2	13	14
0	2	0	119	-126	-8	2	1	17	22	2	8	1	52	50	-4	2	2	18	-30	-2	12	2	12	-10
2	2	0	39	43	-6	2	1	41	37	4	8	1	14	17	-2	2	2	57	-59	3	13	2	20	24
4	2	0	41	46	-4	2	1	32	-47	-7	9	1	15	15	0	2	2	29	29	0	14	2	20	25
6	2	0	31	25	-2	2	1	83	84	-5	9	1	12	-12	2	2	2	22	-16	4	14	2	12	6
8	2	0	26	-25	0	2	1	32	37	-3	9	1	12	11	-9	3	2	34	37	-1	15	2	18	16
1	3	0	88	96	2	2	1	73	72	1	9	1	23	21	-5	3	2	14	4	1	15	2	23	30
3	3	0	40	46	4	2	1	9	-9	3	9	1	15	12	-3	3	2	38	-44	5	15	2	13	-2
5	3	0	18	4	8	2	1	21	-19	5	9	1	18	24	-1	3	2	126	126	-11	1	3	16	16
7	3	0	18	15	-9	3	1	18	-15	-6	10	1	11	-8	1	3	2	30	38	-7	1	3	42	-39
9	3	0	16	18	-7	3	1	21	-26	-4	10	1	25	25	3	3	2	14	18	-3	1	3	55	51
0	4	0	68	-67	-5	3	1	25	16	-2	10	1	12	14	5	3	2	25	-19	-1	1	3	29	26
2	4	0	9	-5	-3	3	1	18	16	0	10	1	10	13	7	3	2	12	10	1	1	3	49	-53
4	4	0	66	-63	-1	3	1	67	-70	2	10	1	23	-19	-10	4	2	12	8	3	1	3	29	-24
6	4	0	10	4	1	3	1	34	28	8	10	1	14	13	-8	4	2	30	-31	-6	2	3	47	44
1	5	0	29	27	3	3	1	28	27	-6	12	1	20	16	-6	4	2	32	-30	-4	2	3	23	24
3	5	0	70	73	5	3	1	14	10	0	12	1	16	15	-4	4	2	28	-25	0	2	3	79	-79
5	5	0	68	59	-12	4	1	15	6	2	12	1	42	42	0	4	2	96	-93	-2	2	3	13	-8
9	5	0	12	-11	-8	4	1	17	11	6	12	1	13	-8	2	4	2	21	-18	-9	3	3	19	-19
0	6	0	26	29	-6	4	1	39	-32	-9	13	1	13	4	-7	5	2	26	25	-5	3	3	17	13
2	6	0	22	18	-4	4	1	10	4	-1	13	1	36	38	-5	5	2	15	17	-3	3	3	11	-10
4	6	0	37	83	-2	4	1	36	28	7	13	1	18	14	-1	5	2	39	-41	-1	3	3	79	-81
6	6	0	17	-20	0	4	1	85	84	-6	14	1	12	-6	1	5	2	10	10	-8	4	3	10	8
1	7	0	10	10	2	4	1	76	-70	0	14	1	19	24	-10	6	2	18	16	-6	4	3	44	-36
3	7	0	25	-21	4	4	1	12	7	8	14	1	15	7	-8	6	2	38	43	-2	4	3	118	122
5	8	0	13	-18	-9	5	1	22	23	-5	15	1	13	12	-4	6	2	59	-55	0	4	3	57	54
2	8	0	13	20	-7	5	1	19	24	1	15	1	18	19	-2	6	2	29	-29	2	4	3	25	-26
6	8	0	10	14	-5	5	1	36	36	0	16	1	17	-17	0	6	2	26	28	6	4	3	20	22
3	9	0	41	-35	-3	5	1	92	-89	-5	17	1	14	7	4	6	2	51	-48	-11	5	3	11	5
5	9	0	22	-25	-1	5	1	14	13	-5	19	1	15	3	6	6	2	30	-30	-9	5	3	15	-9
4	10	0	16	-15	1	5	1	26	32	-1	19	1	14	3	5	7	2	34	-39	-7	5	3	16	-8
3	11	0	14	9	5	5	1	51	-50	-4	20	1	18	15	-3	7	2	38	-33	-5	5	3	22	22
0	12	0	27	27	-9	5	1	12	-4	-12	0	2	22	20	-1	7	2	15	16	-3	5	3	22	-13
0	14	0	25	-23	-2	6	1	37	35	-8	0	2	21	19	3	7	2	48	-44	-1	5	3	54	-53
2	14	0	16	-19	2	6	1	19	20	-6	0	2	17	22	-8	3	2	15	-16	1	5	3	14	-17
1	15	0	18	-19	4	6	1	37	32	-4	0	2	52	54	-4	8	2	82	73	-6	6	3	13	7
2	16	0	18	-18	6	6	1	21	22	-2	0	2	32	29	0	8	2	26	-27	-4	6	3	17	21
3	17	0	13	-6	8	6	1	15	-1	2	0	2	37	-39	2	8	2	11	-6	-2	6	3	59	-63
0	20	0	19	-11	-9	7	1	14	-15	4	0	2	29	3	4	8	2	48	53	0	6	3	13	-16
2	20	0	16	-3	-7	7	1	12	-21	-9	1	2	14	-18	-5	9	2	20	15	6	6	3	14	-20
-9	1	1	11	-15	-5	7	1	27	22	-7	1	2	18	-15	1	9	2	14	15	-9	7	3	34	39
-7	7	3	16	20	-8	2	4	14	-15	-1	1	5	26	27	-6	14	5	13	-9	1	7	7	16	15
-1	7	3	80	76	0	2	4	12	-18	1	1	5	21	18	-4	14	5	20	-23	-6	8	7	21	29
3	7	3	24	-25	-3	3	4	15	-22	3	1	5	16	-19	-6	0	6	28	27	-6	12	7	21	26
5	7	3	21	-23	-4	3	4	25	-19	-12	2	5	21	-19	-4	0	6	16	-4	-8	16	7	13	10
9	7	3	16	8	-8	4	4	11	-10	-10	2	5	17	-17	-2	0	6	32	-34	-4	16	7	16	-16
-4	8	3	55	-48	-2	4	4	27	25	-4	2	5	52	-49	0	0	6	11	-9	-2	16	7	13	3
-2	8	3	34	-31	-7	5	4	31	-31	2	2	5	27	29	6	0	6	23	-13	-12	0	8	26	-31
0	8	3	15	-18	-3	5	4	35	-27	4	2	5	14	10	-11	1	6	21	24	-4	0	8	77	-82
2	8	3	17	-13	-1	5	4	52	48	-5	3	5	15	16	-5	1	6	31	30	-2	0	8	23	-32
4	8	3	39	-44	1	5	4	15	-17	-3	3	5	45	-43	-3	1	6	71	70	-13	1	8	16	4
6	8	3	16	-14	7	5	4	20	25	-1	3	5	36	-37	1	1	6	10	-5	-3	1	8	11	12
-7	9	3	23	26	-6	6	4	22	-24	3	3	5	14	15	-2	2	6	39	34	-8	2	8	13	-8
-3	9	3	20	23	-2	6	4	15	-9	-10	4	5	20	22	-11	3	6	19	-17	-4	2	8	20	17
-1	9	3	22	-25	0	6	4	23	-18	-8	4	5	16	12	-3	3	6	61	-65	-3	3	8	20	-23
-8	10	3	14	-16	2	6	4	11	13	-4	4	5	11	5	3	3	6	12	6	-8	4	8	15	17
-4	10	3	18	20	6	6	4	12	-9	-2	4	5	57	57	-6	4	6	15	15	-2	4	8	15	16
-2	10	3	15	11	-9	7	4	29	-28	2	4	5	13	-8	-4	4	6	41	38	-9	5	8	17	-20
2	10	3	21	20	-3	7	4	35	27	-11	5	5	16	-13	2	4	6	17	17	-7	5	8	14	-13
-5	11	3	24	-22	-1	7	4	32	-28	-3	5	5	28	-30	4	4	6	16	17	3	5	8	18	-10
3	11	3	15	-15	1	7	4	11	13	-1	5	5	18	-20	-7	5	6	10	4	-8	6	8	20	-23
1	11	3	25	-25	5	7	4	21	20	-10	6	5	15	-19	-3	5	6	15	17	-4	6	8	11	-5
3	11	3	18	-18	-6	8	4	11	-7	-8	6	5	11	9	1	5	6	12	-9	-2	6	8	14	-11
-4	12	3	16	22	-4	8	4	15	14	-6	6	5	20	-19	-8	6	6	37	34	0	6	8	18	-22
-2	12	3	10	-10	-9	9	4	20	27	-2	6	5	40	-37	-4	6	6	14	-10	-2	8	8	15	8
0	12	3	19	15	-7	9	4	36	43	0	6	5	15	10	-7	7	6	36	37	2	8	8	13	-8
-5	13	3	14	19	-5	9	4	18	-19	-9	7	5	18											

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CU-TCA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	0	0	93	93	2	8	0	34	33	-3	1	1	208	-224	-5	5	1	27	27	3	9	1	44	-41
4	0	0	98	-92	4	8	0	14	-15	-1	1	1	92	-91	-3	5	1	82	80	5	9	1	15	-14
6	0	0	38	-27	6	8	0	69	67	-1	1	1	68	-67	-1	5	1	14	-14	7	9	1	42	42
8	0	0	36	38	8	8	0	57	54	3	1	1	124	-127	1	5	1	158	-153	9	9	1	76	78
10	0	0	14	11	10	8	0	12	12	5	1	1	51	-51	3	5	1	107	102	11	9	1	10	8
12	0	0	36	38	12	9	0	49	48	7	1	1	21	21	5	5	1	119	113	-10	10	1	32	-35
3	1	0	17	-21	3	9	0	69	69	9	1	1	18	17	7	5	1	38	-35	-8	10	1	7	1
5	1	0	14	-18	5	9	0	59	61	11	1	1	27	-30	9	5	1	49	-51	-6	10	1	31	31
7	1	0	44	42	7	9	0	71	73	-12	2	1	73	-72	-12	6	1	44	44	-4	10	1	38	-39
9	1	0	61	61	9	9	0	27	26	-10	2	1	64	-66	-10	6	1	47	47	0	10	1	60	57
11	1	0	62	62	11	9	0	11	3	-8	2	1	17	-18	-8	6	1	30	-31	2	10	1	15	-13
0	2	0	69	-58	0	10	0	13	-9	-6	2	1	115	-108	-6	6	1	62	51	4	10	1	46	-43
2	2	0	48	-48	2	10	0	126	125	-4	2	1	154	-157	-4	6	1	71	73	8	10	1	8	6
4	2	0	7	-13	4	10	0	130	130	-2	2	1	119	-120	-2	6	1	110	102	-9	11	1	51	-52
6	2	0	65	62	6	10	0	24	27	0	2	1	79	-71	0	6	1	140	-135	-7	11	1	70	-73
8	2	0	49	52	8	10	0	12	14	2	2	1	136	132	2	6	1	79	69	-3	11	1	55	-36
10	2	0	41	41	10	10	0	17	19	4	2	1	93	-91	4	6	1	128	125	-1	11	1	40	-39
12	2	0	20	17	12	10	0	27	26	6	2	1	102	-94	6	6	1	118	113	1	11	1	53	-58
1	3	0	132	-126	3	11	0	115	116	8	2	1	40	-47	8	6	1	13	-13	3	11	1	25	-25
3	3	0	80	79	5	11	0	71	73	10	2	1	12	-14	12	6	1	25	22	5	11	1	13	-15
5	3	0	62	-56	7	11	0	11	-12	12	2	1	84	-84	-9	7	1	34	34	7	11	1	23	-22
9	3	0	41	-43	2	12	0	11	10	-11	3	1	83	-83	-7	7	1	19	23	9	11	1	45	-44
0	4	0	257	-316	4	12	0	25	23	-9	3	1	40	-40	-5	7	1	172	168	-10	12	1	25	-24
2	4	0	42	-36	6	12	0	27	30	-7	3	1	1	-14	-3	7	1	152	145	-8	12	1	92	-95
4	4	0	72	67	8	12	0	20	-18	-5	3	1	151	-148	-1	7	1	86	73	-6	12	1	36	-35
6	4	0	134	-125	3	13	0	31	-31	-3	3	1	167	-168	1	7	1	30	29	-4	12	1	58	-61
8	4	0	70	-74	7	13	0	44	-48	-1	3	1	37	-37	3	7	1	81	79	-2	12	1	31	-31
10	4	0	29	-30	9	13	0	13	-12	1	3	1	36	-33	5	7	1	105	102	0	12	1	58	-72
12	4	0	9	-10	0	14	0	15	-14	3	3	1	106	-94	7	7	1	62	61	2	12	1	72	-73
1	5	0	95	-78	2	14	0	60	-58	5	3	1	59	-55	9	7	1	30	37	4	12	1	38	-41
3	5	0	26	-25	4	14	0	93	-93	7	3	1	76	-78	11	7	1	12	11	6	12	1	19	21
5	5	0	93	-82	6	14	0	15	15	9	3	1	42	-45	-8	8	1	75	75	8	12	1	75	-76
7	5	0	93	-91	8	14	0	19	-21	11	3	1	56	-56	-6	8	1	123	116	-9	13	1	33	-34
9	5	0	65	-67	1	15	0	63	-62	-10	4	1	30	-30	-4	8	1	143	140	-7	13	1	62	-64
11	5	0	37	-36	3	15	0	79	-81	-8	4	1	41	-41	-2	8	1	75	69	-5	13	1	10	-9
0	6	0	49	54	5	15	0	23	-22	-6	4	1	44	-37	0	8	1	10	12	-3	13	1	23	-24
2	6	0	134	-125	0	16	0	27	-30	-4	4	1	16	-13	2	8	1	50	54	-1	13	1	79	-82
4	6	0	79	-82	2	16	0	20	-21	-2	4	1	17	-9	4	8	1	9	7	-1	13	1	107	-106
6	6	0	99	-95	4	16	0	17	-18	0	4	1	176	-165	6	8	1	66	61	3	13	1	54	-56
8	6	0	8	-11	6	16	0	26	-28	2	4	1	95	-88	8	8	1	65	64	7	13	1	26	-27
10	6	0	13	-15	1	17	0	31	-31	4	4	1	28	23	10	8	1	59	60	-6	14	1	21	-18
12	6	0	34	-33	5	17	0	10	10	6	4	1	49	-44	-11	9	1	10	-8	-2	14	1	55	-58
1	7	0	10	-7	0	18	0	57	-64	8	4	1	35	-34	-9	9	1	40	45	0	14	1	80	-79
3	7	0	144	-142	2	18	0	9	7	10	4	1	51	-50	-7	9	1	88	89	2	14	1	52	-53
5	7	0	28	-29	-11	1	1	92	-93	-13	5	1	12	15	-5	9	1	70	70	4	14	1	15	-15
7	7	0	30	32	-9	1	1	31	26	-11	5	1	46	45	-3	9	1	11	-5	6	14	1	20	-21
9	7	0	41	41	-7	1	1	55	45	-9	5	1	24	-28	-1	9	1	18	-7	-7	15	1	19	17
11	7	0	14	-12	-5	1	1	66	-71	-7	5	1	74	-74	-1	9	1	82	79	-5	15	1	49	-51
-3	15	1	18	-18	-8	2	2	42	-40	-6	6	2	67	68	4	10	2	124	-125	3	17	2	20	21
-1	15	1	26	26	-6	2	2	53	-48	-4	6	2	121	118	6	10	2	88	-93	-13	1	3	13	-13
1	15	1	71	73	-4	2	2	60	-58	-2	6	2	157	149	8	10	2	47	-50	-11	1	3	74	74
3	15	1	29	30	-0	2	2	41	-49	0	6	2	13	-10	-9	11	2	39	-38	-9	1	3	30	35
5	15	1	17	-18	2	2	2	12	-14	2	6	2	19	-18	-7	11	2	8	-7	-7	1	3	45	-39
7	15	1	17	-19	2	2	2	84	84	4	6	2	79	75	-5	11	2	31	-32	-3	1	3	57	56
-4	16	1	18	-19	4	2	2	10	7	6	6	2	90	82	-3	11	2	93	-88	-1	1	3	101	105
-2	16	1	22	25	6	2	2	6	-8	8	6	2	49	49	-1	11	2	23	-26	1	1	3	188	192
0	16	1	86	87	8	2	2	44	-46	10	6	2	10	8	3	11	2	45	-47	3	1	3	41	35
2	16	1	99	104	10	2	2	29	-27	-11	7	2	34	33	5	11	2	94	-95	5	1	3	46	42
4	16	1	32	34	12	2	2	20	-17	-9	7	2	14	13	7	11	2	50	-49	11	1	3	27	-26
6	16	1	32	-34	-13	3	2	24	25	-7	7	2	36	-36	-10	12	2	9	-6	-12	2	3	14	12
-5	17	1	17	17	-7	3	2	60	64	-5	7	2	14	12	-4	12	2	35	-39	-10	2	3	115	119
-3	17	1	14	13	-5	3	2	46	49	-3	7	2	76	68	-2	12	2	22	-26	-8	2	3	49	50
-1	17	1	42	43	-3	3	2	37	-36	-1	7	2	18	13	0	12	2	29	28	-4	2	3	46	46
1	17	1	37	38	-1	3	2	111	-105	1	7	2	30	-28	6	12	2	42	-43	-2	2	3	103	104
3	17	1	39	40	1	3	2	139	133	3	7	2	34	31	8	12	2	7	9	0	2	3	207	199
-2	18	1	41	43	3	3	2	36	35	5	7	2	68	65	-9	13	2	22	22	2	2	3	15	16
0	18	1	28	30	5	3	2	53	45	7	7	2	59	56	-7	13	2	39	43	4	2	3	32	35
2	18	1	14	13	7	3	2	9	-6	11	7	2	37	-38	-5	13	2	47	-48	6	2	3	58	58
-12	0	2	39	-37	9	3	2	26	25	-12	8	2	10	11	-3	13	2	40	45	8	2	3	34	30
-10	0	2	35	-38	11	3	2	24	24	-10	8	2	44	47	-1	13	2	62	64	-13	3	3	14	13
-8	0	2	122	-128	-12	4	2	21	23	-6	8	2	90	-85	1	13	2	11	-8	-11	3	3	76	74
-6	0	2	19	-29	-8	4	2	84	85	-4	8	2	60	-51	3	13	2	16	-16	-9	3	3	74	73
-4	0	2	117	111	-6	4	2	147																

1	3	5	3	68	66	4	10	3	21	-23	-2	0	4	78	82	8	4	4	11	13	-1	9	4	89	86	
3	5	5	3	52	53	8	10	3	26	27	0	0	4	5	-5	-11	5	4	27	-24	5	9	4	36	37	
5	5	5	3	67	-67	-9	11	3	16	18	2	0	4	88	80	-9	5	4	34	-36	7	9	4	26	26	
7	5	5	3	27	-28	-7	11	3	72	74	4	0	4	103	96	-7	5	4	22	-24	-10	10	4	51	51	
-12	6	6	3	34	-34	-3	11	3	55	55	6	0	4	29	24	-5	5	4	101	-100	-8	10	4	71	73	
-10	6	6	3	55	-53	-1	11	3	30	26	-13	1	4	16	13	-3	5	4	79	-80	-6	10	4	42	44	
-8	6	6	3	43	-43	1	11	3	32	29	-11	1	4	59	58	-1	5	4	94	-88	-4	10	4	34	35	
-6	6	6	3	42	-41	3	11	3	44	44	-9	1	4	21	21	1	5	4	35	-36	-2	10	4	57	57	
-4	6	6	3	31	-32	-10	12	3	11	7	-7	1	4	75	72	3	5	4	39	-41	0	10	4	29	28	
-2	6	6	3	12	-13	-8	12	3	36	37	-5	1	4	56	55	7	5	4	22	-25	6	10	4	48	53	
0	6	6	3	19	14	-6	12	3	68	71	-3	1	4	64	64	7	5	4	37	-38	-9	11	4	39	38	
2	6	6	3	26	24	-6	12	3	55	58	-1	1	4	9	9	-10	9	5	4	15	-16	-7	11	4	35	36
4	6	6	3	31	-32	-2	12	3	31	31	1	1	4	71	64	-10	6	4	21	-19	-5	11	4	14	11	
6	6	6	3	99	-103	0	12	3	23	25	3	1	4	43	48	-8	6	4	28	-26	-3	11	4	42	39	
8	6	6	3	43	-44	2	12	3	95	93	5	1	4	12	14	-6	6	4	22	21	-1	11	4	69	68	
-9	7	7	3	17	-14	4	12	3	57	60	9	1	4	16	17	-4	6	4	103	-103	1	11	4	33	35	
-7	7	7	3	11	-13	6	12	3	19	-21	-10	2	4	29	28	-2	6	4	123	-116	3	11	4	14	-1	
-5	7	7	3	116	-108	-9	13	3	23	23	-8	2	4	27	24	0	6	4	106	-104	7	11	4	39	33	
-3	7	7	3	119	-110	-7	13	3	57	57	-6	2	4	30	-31	2	6	4	11	-13	-4	12	4	21	22	
-1	7	7	3	105	-99	-5	13	3	34	32	-4	2	4	30	31	4	6	4	19	23	-2	12	4	35	36	
1	7	7	3	33	-34	-3	13	3	13	17	-2	2	4	37	40	6	6	4	9	-3	0	12	4	10	10	
3	7	7	3	76	-74	-1	13	3	15	17	0	2	4	77	75	8	6	4	42	-43	2	12	4	18	18	
5	7	7	3	34	-31	-1	13	3	63	62	2	2	4	7	9	-11	7	4	11	16	-7	13	4	41	-44	
7	7	7	3	54	-52	3	13	3	78	79	4	2	4	21	-3	-9	7	4								

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	0	0	2499	2459	39	0	8	0	295	234	31	22	3	1	263	178	36	3	8	1	207	163	41	12	2	2	105	109	75
6	0	0	200	142	17	2	8	0	431	383	25	23	3	1	0	4	1	4	8	1	102	37	101	13	2	2	296	347	22
8	0	0	2235	2077	37	4	8	0	0	122	1	24	3	1	0	43	1	5	8	1	445	418	23	14	2	2	470	446	24
10	0	0	2842	2972	46	6	8	0	279	232	30	0	4	1	428	409	17	6	8	1	0	161	1	15	2	2	322	290	25
12	0	0	140	181	41	8	8	0	509	474	22	1	4	1	99	128	98	7	8	1	203	87	39	16	2	2	344	361	25
14	0	0	927	911	27	10	8	0	127	106	89	2	4	1	882	912	22	8	8	1	0	72	1	17	2	2	212	303	45
16	0	0	910	854	28	12	8	0	69	21	68	3	4	1	300	314	17	9	8	1	0	144	1	18	2	2	192	151	43
18	0	0	597	604	26	14	8	0	264	182	37	4	4	1	211	203	27	10	8	1	132	142	131	19	2	2	119	118	118
20	0	0	312	336	31	16	8	0	145	230	145	5	4	1	919	981	25	11	8	1	0	66	1	20	2	2	141	59	140
22	0	0	121	17	120	2	9	0	161	13	161	6	4	1	451	384	21	12	8	1	204	173	43	21	2	2	239	202	39
24	0	0	341	322	34	4	9	0	0	114	1	7	4	1	573	595	28	13	8	1	0	145	1	22	2	2	168	137	71
2	1	0	185	177	11	6	9	0	80	76	80	8	4	1	127	1108	28	14	8	1	0	33	1	23	2	2	80	125	80
4	1	0	1958	1767	31	8	9	0	0	55	1	9	4	1	211	193	31	15	8	1	195	221	62	24	2	2	0	129	1
6	1	0	747	874	18	10	9	0	169	95	53	10	4	1	472	463	22	1	9	1	139	145	138	25	2	2	33	41	32
8	1	0	533	570	21	12	9	0	85	37	84	11	4	1	139	86	139	2	9	1	0	31	1	1	3	2	1325	1284	24
10	1	0	1227	1050	26	0	10	0	229	232	54	12	4	1	0	78	1	3	9	1	0	13	1	2	3	2	204	227	18
12	1	0	238	173	25	2	10	0	281	256	54	13	4	1	176	103	44	4	9	1	159	18	159	3	3	2	695	595	20
14	1	0	549	551	26	4	10	0	0	149	1	14	4	1	205	235	39	5	9	1	0	12	1	4	3	2	720	633	20
16	1	0	593	525	31	1	1	1	1381	1455	22	15	4	1	480	412	21	6	9	1	54	45	53	5	3	2	869	810	21
18	1	0	179	141	46	2	1	1	75	125	25	16	4	1	133	15	133	7	9	1	46	10	45	6	3	2	0	152	1
20	1	0	318	304	29	3	1	1	295	80	11	17	4	1	0	126	1	8	9	1	0	53	1	7	3	2	621	620	23
22	1	0	128	177	127	4	1	1	1461	1486	24	18	4	1	226	131	36	9	9	1	101	117	100	8	3	2	313	259	19
24	1	0	250	197	42	5	1	1	174	196	16	19	4	1	0	24	1	10	9	1	0	17	1	9	3	2	1161	1194	27
2	2	0	2533	2578	39	6	1	1	71	60	71	20	4	1	0	103	1	11	9	1	197	67	43	10	3	2	272	274	24
4	2	0	238	172	15	7	1	1	569	501	19	21	4	1	112	65	111	12	9	1	161	10	160	11	3	2	589	575	28
6	2	0	0	74	1	8	1	1	538	526	20	22	4	1	82	82	82	0	10	1	0	15	1	12	3	2	102	72	101
8	2	0	1474	1545	27	9	1	1	863	810	22	23	4	1	175	107	65	1	10	1	0	10	1	13	3	2	123	23	63
10	2	0	1011	1049	24	10	1	1	551	521	23	1	5	1	896	800	26	2	10	1	0	11	1	14	3	2	124	133	124
12	2	0	1302	1150	27	11	1	1	646	632	23	2	5	1	354	368	18	3	10	1	97	11	96	15	3	2	247	231	32
14	2	0	193	210	28	12	1	1	667	593	24	3	5	1	657	686	24	4	10	1	122	2	121	16	3	2	146	102	39
16	2	0	395	413	21	13	1	1	45	101	44	4	5	1	762	759	24	3	0	2	2626	2740	43	17	3	2	238	264	39
18	2	0	880	913	30	14	1	1	497	458	22	5	5	1	216	161	31	4	0	2	1985	2112	31	18	3	2	0	64	1
20	2	0	521	504	25	15	1	1	263	281	29	6	5	1	1007	1006	28	5	0	2	1594	1602	26	19	3	2	476	465	24
22	2	0	0	119	1	16	1	1	232	247	32	7	5	1	449	459	18	6	0	2	2691	2499	42	20	3	2	147	140	147
24	2	0	134	35	99	17	1	1	533	506	24	8	5	1	0	109	1	7	0	2	832	825	19	21	3	2	191	181	53
2	3	0	160	185	159	18	1	1	113	65	113	9	5	1	738	680	31	8	0	2	645	676	19	22	3	2	0	36	1
4	3	0	191	206	19	19	1	1	177	132	48	10	5	1	455	455	23	9	0	2	453	480	23	23	3	2	0	34	1
6	3	0	844	900	23	20	1	1	0	22	1	11	5	1	0	428	-1	10	0	2	338	281	18	24	3	2	109	27	108
8	3	0	1471	1343	29	21	1	1	141	143	80	12	5	1	0	571	-1	11	0	2	1100	1184	25	0	4	2	337	559	-15
10	3	0	1067	1115	26	22	1	1	0	74	1	13	5	1	0	39	-1	12	0	2	349	430	18	1	4	2	265	336	18
12	3	0	335	307	20	23	1	1	117	113	117	14	5	1	495	428	23	13	0	2	1107	1189	26	2	4	2	0	97	1
14	3	0	459	496	24	24	1	1	148	110	148	15	5	1	338	272	29	14	0	2	122	60	122	3	4	2	736	693	23
16	3	0	1108	1057	30	25	1	1	66	92	65	16	5	1	162	245	162	15	0	2	673	661	27	4	4	2	516	540	25
18	3	0	854	758	32	0	2	1	895	843	17	17	5	1	351	297	29	16	0	2	593	610	28	5	4	2	692	600	27
20	3	0	103	76	103	1	2	1	2191	2154	34	18	5	1	0	74	1	17	0	2	167	39	42	6	4	2	64	6	66
22	3	0	275	280	38	2	2	1	1529	1397	26	19	5	1	263	253	40	18	0	2	418	412	21	7	4	2	463	502	20
24	3	0	49	284	44	3	2	1	1537	1457	26	20	5	1	305	254	36	19	0	2	608	587	31	8	4	2	169	225	38
2	4	0	218	36	1	4	2	1	1040	1036	21	21	5	1	0	133	1	20	0	2	0	101	1	9	4	2	168	16	34
4	4	0	1122	23	1	5	2	1	0	57	1	22	5	1	252	203	45	21	0	2	513	516	24	10	4	2	799	702	27
6	4	0	1073	902	24	6	2	1	735	762	20	0	6	1	243	276	27	22	0	2	150	190	88	11	4	2	138	94	137
8	4	0	929	790	24	7	2	1	1596	1572	29	1	6	1	123	110	123	23	0	2	369	410	32	12	4	2	56	26	56
10	4	0	353	429	20	8	2	1	2015	2002	34	2	6	1	60	20	59	24	0	2	146	88	146	13	4	2	124	50	123
12	4	0	195	183	35	9	2	1	0	58	1	3	6	1	293	342	24	25	0	2	171	151	171	14	4	2	290	249	31
14	4	0	226	162	33	10	2	1	1731	1651	32	4	6	1	93	44	92	1	1	2	1330	1372	21	15	4	2	201	210	40
16	4	0	447	411	21	11	2	1	1223	1186	28	5	6	1	537	521	24	2	1	2	761	785	15	16	4	2	293	285	32
18	4	0	0	65	1	12	2	1	210	236	31	6	6	1	300	265	26	3	1	2	1499	1466	24	17	4	2	151	192	76
20	4	0	0	92	1	13	2	1	781	768	26	7	6	1	141	146	140	4	1	2	627	468	15	18	4	2	161	189	160
22	4	0	241	224	37	14	2	1	236	224	28	8	6	1	146	76	1												

14	7	0	0	273	1	19	3	1	88	183	37	0	8	1	150	95	66	9	2	2	447	396	18	3	6	2	264	306	26
16	7	0	176	158	66	20	3	1	265	284	38	1	8	1	0	53	1	10	2	2	776	897	24	4	6	2	211	160	31
18	7	0	108	39	107	21	3	1	0	22	1	2	8	1	17	116	17	11	2	2	269	244	22	5	6	2	826	780	29

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
6	6	2	345	530	25	1	2	3	482	445	18	19	5	3	266	268	40	17	0	4	156	190	47	6	4	4	606	606	24
7	6	2	353	368	25	2	2	3	608	568	16	20	5	3	0	98	1	18	0	4	556	596	25	7	4	4	0	190	1
8	6	2	623	537	31	3	2	3	903	900	19	21	5	3	164	128	163	19	0	4	517	501	27	8	4	4	935	952	25
9	6	2	62	48	62	4	2	3	969	913	20	22	5	3	43	59	43	20	0	4	139	237	88	9	4	4	211	227	30
10	6	2	0	99	1	5	2	3	2108	2157	34	0	6	3	297	319	23	21	0	4	27	177	27	10	4	4	908	947	28
11	6	2	25	48	25	6	2	3	78	118	78	1	6	3	0	58	1	22	0	4	311	339	31	11	4	4	560	513	23
13	6	2	0	38	1	7	2	3	1500	1529	27	2	6	3	304	266	25	23	0	4	216	103	40	13	4	4	339	268	23
14	6	2	128	41	99	8	2	3	385	387	18	3	6	3	259	199	26	24	0	4	155	64	154	14	4	4	0	128	1
15	6	2	274	201	36	9	2	3	420	428	18	4	6	3	138	96	137	25	0	4	0	55	1	15	4	4	0	99	1
16	6	2	0	155	1	10	2	3	1093	1135	25	5	6	3	571	553	21	1	1	4	189	210	11	16	4	4	671	648	35
17	6	2	143	170	142	11	2	3	646	638	26	6	6	3	192	173	41	2	1	4	2585	2600	40	17	4	4	114	6	114
18	6	2	140	124	139	12	2	3	579	556	26	7	6	3	109	64	108	3	1	4	1444	1425	24	18	4	4	573	557	28
19	6	2	141	12	140	13	2	3	835	823	26	8	6	3	627	648	24	4	1	4	0	94	1	19	4	4	0	188	1
20	6	2	82	30	82	14	2	3	46	176	46	9	6	3	0	26	1	5	1	4	100	185	99	20	4	4	244	253	42
1	7	2	280	287	29	15	2	3	792	753	29	10	6	3	157	121	57	6	1	4	70	142	70	21	4	4	48	119	48
2	7	2	209	160	39	16	2	3	289	228	27	12	6	3	52	27	15	7	1	4	321	312	16	22	4	4	0	13	1
3	7	2	190	51	39	17	2	3	225	230	33	13	6	3	254	289	37	8	1	4	432	371	22	23	4	4	0	30	1
4	7	2	107	49	107	18	2	3	0	130	1	14	6	3	97	65	97	9	1	4	173	208	26	1	5	4	145	141	38
5	7	2	0	189	1	19	2	3	186	124	49	15	6	3	273	247	37	10	1	4	1184	1180	25	2	5	4	166	140	33
6	7	2	0	61	1	20	2	3	246	199	35	16	6	3	54	18	54	11	1	4	217	186	24	3	5	4	95	63	94
7	7	2	429	478	22	21	2	3	204	268	52	17	6	3	0	52	1	12	1	4	972	968	25	4	5	4	0	52	1
8	7	2	0	44	1	22	2	3	81	13	80	18	6	3	176	156	69	13	1	4	215	153	24	5	5	4	212	126	28
9	7	2	350	381	30	23	2	3	174	154	173	19	6	3	178	56	178	14	1	4	568	536	29	6	5	4	122	52	121
10	7	2	176	206	53	24	2	3	0	51	1	20	6	3	47	5	46	15	1	4	134	76	134	7	5	4	91	9	90
11	7	2	267	258	35	25	2	3	210	141	59	1	7	3	236	259	35	16	1	4	306	347	26	8	5	4	0	47	1
12	7	2	57	88	56	1	3	3	970	965	21	2	7	3	190	123	39	17	1	4	0	55	1	9	5	4	106	131	106
13	7	2	182	39	55	2	3	3	0	136	1	3	7	3	284	226	30	18	1	4	247	216	30	10	5	4	337	280	25
14	7	2	0	80	1	3	3	3	721	628	19	4	7	3	0	147	1	19	1	4	0	220	1	12	5	4	0	291	-1
15	7	2	0	173	1	4	3	3	109	170	37	5	7	3	0	9	1	20	1	4	93	139	92	13	5	4	190	165	-9
16	7	2	0	40	1	5	3	3	119	57	34	6	7	3	0	127	1	21	1	4	209	163	43	14	5	4	90	45	89
17	7	2	251	271	47	6	3	3	314	217	17	7	7	3	328	313	26	22	1	4	243	258	41	15	5	4	199	130	49
18	7	2	0	63	1	7	3	3	329	288	17	8	7	3	0	32	1	23	1	4	0	20	1	16	5	4	0	75	1
0	8	2	277	239	37	8	3	3	128	40	40	9	7	3	171	207	55	24	1	4	149	133	149	17	5	4	99	56	98
1	8	2	113	108	112	9	3	3	759	837	24	10	7	3	217	109	39	25	1	4	0	27	1	18	5	4	44	98	43
2	8	2	268	163	31	10	3	3	96	101	96	11	7	3	0	150	1	0	2	4	594	627	17	19	5	4	168	44	61
3	8	2	326	362	32	11	3	3	339	329	21	12	7	3	141	58	140	1	2	4	2126	2109	34	20	5	4	175	137	67
4	8	2	49	33	49	12	3	3	334	329	24	13	7	3	0	10	1	2	2	4	367	314	19	21	5	4	155	14	155
5	8	2	398	367	24	13	3	3	296	250	26	14	7	3	163	36	152	3	2	4	1701	1675	29	22	5	4	103	14	102
6	8	2	113	70	112	14	3	3	57	54	56	15	7	3	67	14	66	4	2	4	262	350	14	0	6	4	849	909	27
7	8	2	301	265	28	15	3	3	280	271	30	16	7	3	88	87	88	5	2	4	809	744	20	1	6	4	94	117	94
8	8	2	161	158	53	16	3	3	204	150	40	17	7	3	143	63	142	6	2	4	685	689	20	2	6	4	558	549	20
9	8	2	0	73	1	17	3	3	0	127	1	8	7	3	176	6	176	7	2	4	426	529	21	3	6	4	150	170	150
10	8	2	0	177	1	18	3	3	142	227	141	0	8	3	0	23	1	8	2	4	161	203	24	4	6	4	148	168	50
11	8	2	0	192	1	19	3	3	245	234	38	1	8	3	0	115	1	9	2	4	164	61	27	5	6	4	375	540	30
12	8	2	131	107	130	20	3	3	0	58	1	2	8	3	152	168	152	10	2	4	290	327	20	6	6	4	271	255	28
13	8	2	204	118	44	21	3	3	0	76	1	3	8	3	230	247	42	11	2	4	832	833	25	7	6	4	252	227	30
14	8	2	95	100	94	22	3	3	59	78	59	4	8	3	129	215	129	12	2	4	469	444	21	8	6	4	508	551	26
15	8	2	189	35	51	23	3	3	0	151	1	5	8	3	283	279	29	13	2	4	514	457	20	9	6	4	390	339	24
1	9	2	70	142	69	24	3	3	139	56	138	6	8	3	112	136	111	14	2	4	182	165	37	10	6	4	683	660	35
2	9	2	96	70	96	0	4	3	682	657	-21	7	8	3	122	149	122	15	2	4	168	242	44	12	6	4	27	296	-27
3	9	2	173	210	172	1	4	3	0	173	1	8	8	3	255	285	33	16	2	4	0	13	1	13	6	4	160	97	61
4	9	2	0	25	1	2	4	3	386	392	17	9	8	3	216	90	35	17	2	4	196	174	42	14	6	4	108	168	107
5	9	2	0	52	1	3	4	3	715	681	24	10	8	3	0	51	1	18	2	4	96	20	95	15	6	4	196	78	51
6	9	2	0	47	1	4	4	3	389	385	19	11	8	3	111	37	110	19	2	4	440	463	24	16	6	4	172	219	172
7	9	2	0	21	1	5	4	3	542	491	25	12	8	3	144	71	143	20	2	4	134	64	134	17	6	4	106	62	105
8	9	2	99	3	99	6	4	3	283	267	21	13	8	3	36	176	36	21	2	4	147	143	81	18	6	4	280	273	42
9	9	2	0	26	1	7	4	3	896	947	26	14	8	3	118	49	118	22	2	4	0	211	1	19	6	4	78	162	78
10	9	2	0	17	1	8	4	3	99	170	99	15	8	3	193	136	55	23	2	4	0	59	1	20	6	4	0	219	1
11	9	2	193	82	46	9	4																						

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
14	8	4	0	57	1	23	3	5	0	56	1	5	8	5	184	271	53	15	2	6	364	411	23	12	6	6	0	238	-1
15	8	4	182	59	64	24	3	5	84	37	84	6	8	5	101	33	101	16	2	6	116	145	115	13	6	6	516	556	27
1	9	4	0	6	1	24	4	5	873	898	23	7	8	5	231	227	34	17	2	6	157	169	58	14	6	6	0	103	1
2	9	4	160	20	159	1	4	5	120	142	43	8	8	5	59	164	59	18	2	6	203	203	45	15	6	6	162	310	161
3	9	4	0	16	1	2	4	5	286	318	19	9	8	5	0	40	1	19	2	6	516	531	26	16	6	6	26	12	26
4	9	4	0	145	1	3	4	5	143	99	38	10	8	5	180	185	65	20	2	6	137	69	136	17	6	6	122	139	122
5	9	4	0	86	1	4	4	5	549	520	26	11	8	5	0	221	1	21	2	6	65	131	65	18	6	6	0	62	1
6	9	4	131	170	131	5	4	5	294	251	21	12	8	5	146	127	143	22	2	6	108	2	107	19	6	6	0	85	1
7	9	4	95	83	94	6	4	5	508	515	25	13	8	5	0	127	1	23	2	6	0	53	1	20	6	6	0	3	1
7	9	4	89	7	88	7	4	5	0	18	1	14	8	5	112	31	112	24	2	6	157	8	77	1	7	6	122	135	121
9	9	4	133	4	133	8	4	5	113	41	112	15	8	5	22	100	21	1	3	6	1238	1196	24	2	7	6	42	71	41
10	9	4	133	59	132	9	4	5	334	359	20	1	9	5	355	354	31	2	3	6	984	1040	22	3	7	6	325	310	26
11	9	4	166	2	58	10	4	5	877	901	29	2	9	5	82	104	81	3	3	6	0	40	1	4	7	6	142	18	141
0	10	4	0	169	1	11	4	5	84	180	84	3	9	5	224	165	49	4	3	6	1177	1133	25	5	7	6	143	94	39
1	10	4	0	17	1	13	4	5	105	158	105	4	9	5	75	291	75	5	3	6	792	823	22	6	7	6	193	51	41
2	10	4	108	106	108	14	4	5	222	203	37	5	9	5	112	43	111	6	3	6	352	382	16	7	7	6	516	486	24
3	10	4	29	121	28	20	4	5	294	276	31	6	9	5	195	196	54	7	3	6	669	707	23	8	7	6	0	5	1
1	1	5	3676	3674	59	16	4	5	207	213	44	7	9	5	267	200	32	8	3	6	587	502	24	9	7	6	439	456	27
2	1	5	1085	1016	20	17	4	5	158	145	57	8	9	5	0	47	1	9	3	6	967	998	26	10	7	6	123	67	122
3	1	5	197	194	15	18	4	5	0	78	1	9	9	5	122	108	122	10	3	6	334	334	21	11	7	6	0	162	1
4	1	5	913	1050	19	19	4	5	0	55	1	10	9	5	0	29	1	11	3	6	872	833	26	12	7	6	0	99	1
5	1	5	305	320	16	20	4	5	264	57	40	11	9	5	0	89	1	12	3	6	192	163	34	13	7	6	0	67	1
6	1	5	1009	979	21	21	4	5	105	14	104	0	10	5	71	143	70	13	3	6	113	14	112	14	7	6	0	97	1
7	1	5	311	313	14	22	4	5	0	50	1	1	10	5	116	4	116	14	3	6	64	13	63	15	7	6	65	108	64
8	1	5	241	201	20	23	4	5	176	142	74	0	0	6	1744	1790	28	15	3	6	124	105	124	16	7	6	0	55	1
9	1	5	1205	1203	25	1	5	5	742	698	26	1	0	6	2829	2753	44	16	3	6	110	134	110	17	7	6	165	280	164
10	1	5	766	710	23	2	5	5	337	357	20	2	0	6	280	254	11	17	3	6	268	236	32	18	7	6	87	10	86
11	1	5	449	409	19	3	5	5	372	384	18	3	0	6	2278	2368	36	18	3	6	60	64	59	0	8	6	153	16	55
12	1	5	733	734	23	4	5	5	955	854	25	4	0	6	225	257	13	19	3	6	162	216	64	1	8	6	35	163	35
13	1	5	116	155	68	5	5	5	311	281	20	5	0	6	452	443	18	20	3	6	169	82	169	2	9	6	114	50	113
14	1	5	51	84	50	6	5	5	593	554	28	6	0	6	93	9	42	21	3	6	233	167	40	3	8	6	80	27	79
15	1	5	688	670	29	7	5	5	140	30	46	7	0	6	425	461	21	22	3	6	0	33	1	4	8	6	0	40	1
16	1	5	0	137	1	8	5	5	115	72	115	8	0	6	235	202	18	23	3	6	0	5	1	5	8	6	145	109	67
17	1	5	236	259	35	9	5	5	98	35	97	9	0	6	425	503	17	24	3	6	121	7	131	6	8	6	108	48	107
18	1	5	0	57	1	10	5	5	83	129	82	10	0	6	820	774	22	0	4	6	411	411	19	7	8	6	140	35	140
19	1	5	341	295	25	11	5	5	34	44	15	11	0	6	127	165	45	1	4	6	504	418	18	8	8	6	60	42	59
20	1	5	0	142	1	12	5	5	0	215	-1	12	0	6	996	888	26	2	4	6	273	289	20	9	8	6	64	138	63
21	1	5	255	258	37	13	5	5	267	270	32	13	0	6	545	603	28	3	4	6	1023	1146	24	10	8	6	168	95	63
22	1	5	244	242	40	14	5	5	308	300	28	14	0	6	63	155	62	4	4	6	323	338	20	11	8	6	0	66	1
23	1	5	0	102	1	15	5	5	94	20	93	15	0	6	577	546	21	5	4	6	1744	1792	33	12	8	6	96	53	95
24	1	5	214	174	55	16	5	5	10	204	9	16	0	6	104	104	104	6	4	6	547	513	24	13	8	6	82	25	82
25	1	5	247	232	50	17	5	5	187	173	54	17	0	6	324	300	26	7	4	6	789	754	24	14	8	6	53	47	53
0	2	5	912	825	20	18	5	5	0	3	1	18	0	6	450	490	22	8	4	6	250	201	25	15	8	6	0	21	1
1	2	5	402	433	19	19	5	5	142	176	141	19	0	6	97	237	96	9	4	6	719	652	27	1	9	6	211	86	47
2	2	5	1367	1410	24	20	5	5	0	82	1	20	0	6	0	166	1	10	4	6	231	260	32	2	9	6	131	21	130
3	2	5	522	535	17	21	5	5	141	99	140	21	0	6	136	156	86	11	4	6	609	689	30	3	9	6	137	97	157
4	2	5	1666	1681	29	22	5	5	103	83	163	22	0	6	0	40	1	13	4	6	603	623	23	4	9	6	0	130	1
5	2	5	775	795	20	0	6	5	102	184	101	23	0	6	238	229	42	14	4	6	122	41	122	5	9	6	94	37	93
6	2	5	178	167	21	1	6	5	0	26	1	24	0	6	96	84	95	15	4	6	577	561	25	6	9	6	83	76	83
7	2	5	96	141	96	2	6	5	267	282	24	25	0	6	177	192	81	16	4	6	0	10	1	7	9	6	118	105	116
8	2	5	818	862	22	3	6	5	424	397	21	1	1	6	609	585	16	17	4	6	167	49	-7	8	9	6	0	53	1
9	2	5	91	21	90	4	6	5	151	99	40	2	1	6	558	484	16	18	4	6	0	28	1	9	9	6	145	118	145
10	2	5	805	821	25	5	6	5	386	396	23	3	1	6	335	320	14	19	4	6	436	452	29	10	9	6	136	23	135
11	2	5	184	228	31	6	6	5	277	374	33	4	1	6	404	313	20	20	4	6	0	85	1	1	1	7	2439	2522	36
12	2	5	801	760	26	7	6	5	243	286	33	5	1	6	675	745	18	21	4	6	399	384	30	2	1	7	521	507	16
13	2	5	140	205	140	8	6	5	478	444	25	6	1	6	138	208	29	22	4	6	0	42	1	3	1	7	1058	1064	21
14	2	5	197	194	36	9	6	5	229	225	38	7	1	6	406	360	16	23	4	6	129	143	129	4	1	7	987	990	21
15	2	5	702	649	30	10	6	5	144	152	75	8	1	6	197	88	22	1	5	6	313	319	21	5	1	7	75	71	75
16	2	5	428	406																									

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
12	2	7	242	258	28	12	6	7	26	29	26	14	1	8	474	510	23	12	5	8	25	37	24	22	1	9	204	281	62
13	2	7	608	559	29	13	6	7	196	282	58	15	1	8	144	122	143	13	5	8	75	182	75	23	1	9	20	80	25
14	2	7	121	105	121	14	6	7	104	77	103	16	1	8	365	374	22	14	5	8	142	32	142	24	1	9	0	154	1
15	2	7	503	502	23	15	6	7	0	161	1	17	1	8	283	295	32	15	5	8	89	230	89	0	9	2138	2122	35	
16	2	7	193	140	37	16	6	7	172	144	172	18	1	8	52	78	52	16	5	8	151	145	70	1	9	91	49	90	
17	2	7	160	247	160	17	6	7	0	12	1	19	1	8	125	114	97	17	5	8	160	101	68	2	9	1269	1209	24	
18	2	7	317	255	27	18	6	7	102	107	101	20	1	8	140	137	79	18	5	8	0	172	1	3	9	92	151	91	
19	2	7	0	145	1	19	6	7	0	105	1	21	1	8	0	43	1	19	5	8	178	10	57	4	9	322	362	16	
20	2	7	191	35	43	20	6	7	0	27	1	22	1	8	161	235	74	20	5	8	95	98	95	5	9	525	548	23	
21	2	7	348	312	29	21	6	7	163	114	51	23	1	8	119	76	118	21	5	8	65	7	34	6	9	675	602	23	
22	2	7	0	36	1	22	6	7	249	225	35	24	1	8	141	136	110	0	6	8	740	720	30	7	9	292	251	19	
23	2	7	227	226	50	23	6	7	115	35	114	0	2	8	317	335	16	1	6	8	95	91	95	8	9	352	354	17	
24	2	7	0	102	1	24	6	7	0	7	1	1	2	8	353	378	16	2	6	8	492	497	22	9	9	737	694	24	
1	3	7	764	703	21	1	6	7	141	193	141	2	2	8	199	60	-19	3	6	8	234	256	32	10	9	702	710	25	
2	3	7	372	431	17	2	6	7	171	100	53	3	2	8	1034	939	22	4	6	8	0	72	1	11	9	368	380	19	
3	3	7	539	445	20	3	6	7	248	225	39	4	2	8	297	230	15	5	6	8	681	597	1	12	9	520	515	22	
4	3	7	99	192	64	4	6	7	58	94	57	5	2	8	501	446	21	6	6	8	254	268	33	13	9	443	430	23	
5	3	7	228	272	27	5	6	7	102	95	101	6	2	8	0	16	1	7	6	8	132	145	172	14	9	262	250	29	
6	3	7	399	378	18	6	6	7	119	92	118	7	2	8	0	41	1	8	6	8	516	519	26	15	9	403	382	22	
7	3	7	148	160	37	7	6	7	0	56	1	8	2	8	385	321	20	9	6	8	323	316	30	16	9	165	170	50	
8	3	7	206	270	30	8	6	7	270	133	36	9	2	8	307	375	20	10	6	8	583	525	27	17	9	298	294	30	
9	3	7	177	110	33	9	6	7	0	85	1	10	2	8	274	199	21	13	6	8	71	175	70	18	9	120	203	120	
10	3	7	225	220	26	10	6	7	164	54	167	11	2	8	0	91	1	14	6	8	123	99	123	19	9	134	31	134	
11	3	7	0	11	1	11	6	7	274	198	33	12	2	8	90	99	89	15	6	8	139	255	139	20	9	31	288	31	
12	3	7	43	54	42	12	6	7	146	121	145	13	2	8	307	376	26	16	6	8	277	260	40	21	9	93	159	93	
13	3	7	303	295	23	13	6	7	72	99	72	14	2	8	126	133	125	17	6	8	0	82	1	22	9	53	155	53	
14	3	7	248	257	32	14	6	7	348	327	28	15	2	8	130	44	130	18	6	8	274	251	40	23	9	0	124	1	
15	3	7	168	144	44	15	6	7	195	84	42	16	2	8	0	47	1	19	6	8	222	65	49	24	9	228	136	45	
16	3	7	0	29	1	16	6	7	136	97	135	17	2	8	185	132	42	1	7	8	247	215	34	1	9	907	968	23	
17	3	7	50	13	50	17	6	7	297	318	33	18	2	8	308	332	29	2	7	8	260	273	33	2	9	496	518	23	
18	3	7	100	52	100	18	6	7	88	63	88	19	2	8	109	135	108	3	7	8	121	36	121	3	9	441	349	18	
19	3	7	0	9	1	19	6	7	447	415	25	20	2	8	186	159	53	4	7	8	459	485	22	4	9	181	221	27	
20	3	7	0	81	1	20	6	7	0	32	1	21	2	8	172	246	171	5	7	8	0	50	1	5	9	0	146	1	
21	3	7	163	49	162	21	6	7	293	282	36	22	2	8	174	164	65	6	7	8	505	447	23	6	9	45	18	45	
22	3	7	0	41	1	22	6	7	0	103	1	23	2	8	0	36	1	7	7	8	0	30	1	7	9	84	17	84	
23	3	7	0	42	1	23	6	7	0	23	1	24	2	8	173	54	74	8	7	8	0	236	1	8	9	659	687	26	
24	3	7	89	27	89	24	6	7	245	191	44	25	2	8	233	220	19	9	7	8	81	147	81	9	9	416	480	21	
0	4	7	838	901	24	0	6	7	171	156	72	26	2	8	353	394	16	10	7	8	150	120	69	10	9	127	67	53	
1	4	7	417	398	20	1	6	7	0	23	1	27	2	8	0	41	1	11	7	8	170	137	65	11	9	173	118	38	
2	4	7	194	148	28	2	6	7	208	160	60	28	2	8	1487	1477	29	12	7	8	268	177	35	12	9	268	290	28	
3	4	7	692	619	23	3	6	7	157	127	157	29	2	8	89	153	88	13	7	8	0	120	1	14	9	219	155	32	
4	4	7	769	738	25	4	6	7	336	375	30	30	2	8	1447	1433	29	14	7	8	316	285	35	15	9	0	65	1	
5	4	7	488	528	21	5	6	7	139	74	99	31	2	8	48	58	47	15	7	8	108	3	107	16	9	290	247	28	
6	4	7	343	282	22	6	6	7	192	124	53	32	2	8	475	508	19	16	7	8	229	230	51	17	9	143	140	1-2	
7	4	7	255	272	24	7	6	7	216	206	51	33	2	8	80	159	80	17	7	8	0	56	1	18	9	127	79	97	
8	4	7	108	24	108	8	6	7	154	115	154	34	2	8	75	98	75	18	6	8	116	10	115	19	9	117	136	116	
9	4	7	511	486	22	9	6	7	291	204	33	35	2	8	267	211	24	1	8	8	113	105	118	20	9	105	61	104	
10	4	7	363	361	22	10	6	7	141	250	140	36	2	8	781	731	28	2	8	8	150	26	69	21	9	0	32	1	
13	4	7	230	219	34	13	6	7	0	18	1	37	2	8	242	239	30	3	8	8	0	177	1	22	9	107	34	107	
14	4	7	402	379	22	14	6	7	285	215	41	38	2	8	690	669	31	4	8	8	73	53	72	23	9	0	83	1	
15	4	7	332	301	26	15	6	7	158	8	72	39	2	8	0	3	1	5	8	8	0	74	1	0	4	9	328	340	18
16	4	7	145	104	65	16	6	7	1870	1832	31	40	2	8	354	343	24	6	8	8	136	44	136	1	4	9	272	316	21
17	4	7	78	125	77	17	6	7	1540	1541	26	41	2	8	250	224	30	7	8	8	136	128	108	2	4	9	0	194	1
18	4	7	103	34	102	18	6	7	978	1033	20	42	2	8	0	5	1	8	8	8	89	1	1	3	4	9	394	383	18
19	4	7	102	38	101	19	6	7	461	548	18	43	2	8	121	95	120	9	8	8	160	32	160	4	4	9	112	17	111
20	4	7	220	110	44	20	6	7	197	205	19	44	2	8	141	117	140	10	8	8	75	42	74	5	4	9	0	82	1
21	4	7	0	12	1	21	6	7	1094	1160	22	45	2	8	0	42	1	11	8	8	0	84	1	6	4	9	271	265	24
22	4	7	0	115	1	22	6	7	0	78	1	46	2	8	227	232	52	12	8	8	174	75	173	7	4	9	0	130	1
23	4	7	146	43	145	23	6	7	0	23	1	47	2	8	158	41	157	13	8	8	0	35	1	8	4	9	275	210	26
1	5	7	337	293	19	1	6	7	429	456	18																		

Table 7. Observed and calculated structure factors for 1

h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10c						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s					
21	5	9	114	54	114	6	1	10	476	452	25	4	5	10	250	179	23	18	1	11	14	3	113	2	6	11	141	127	61
0	6	9	365	357	23	7	1	10	685	775	23	5	5	10	229	178	27	19	1	11	325	358	31	3	6	11	314	308	25
1	6	9	63	58	63	8	1	10	415	460	19	6	5	10	0	155	1	20	1	11	133	51	132	4	6	11	201	189	35
2	6	9	338	338	22	9	1	10	498	454	26	7	5	10	418	387	22	21	1	11	174	152	57	5	6	11	366	433	25
3	6	9	0	64	1	10	1	10	496	466	21	8	5	10	164	71	45	22	1	11	173	15	108	6	6	11	133	86	65
4	6	9	0	49	1	11	1	10	560	531	27	9	5	10	64	29	63	23	1	11	114	7	114	7	6	11	233	251	40
5	6	9	125	29	124	12	1	10	34	65	33	10	5	10	154	102	52	24	1	11	128	41	128	8	6	11	201	16	36
6	6	9	290	324	29	13	1	10	414	421	20	13	5	10	241	265	37	0	2	11	114	164	113	9	6	11	74	72	73
7	6	9	77	103	76	14	1	10	137	145	137	14	5	10	0	5	1	1	2	11	663	774	22	10	6	11	0	34	1
8	6	9	410	415	24	15	1	10	0	185	1	15	5	10	0	10	1	2	2	11	96	21	95	11	6	11	103	95	103
9	6	9	189	180	47	16	1	10	145	59	55	16	5	10	78	21	77	3	2	11	1340	1310	26	12	6	11	112	94	111
10	6	9	273	295	36	17	1	10	203	245	44	17	5	10	0	108	1	4	2	11	101	239	101	13	6	11	0	106	1
13	6	9	92	127	92	18	1	10	78	101	77	18	5	10	0	6	1	5	2	11	758	669	23	14	6	11	0	100	1
14	6	9	92	121	92	19	1	10	0	66	1	19	5	10	0	15	1	6	2	11	268	289	23	15	6	11	235	202	41
15	6	9	248	211	39	20	1	10	159	126	158	20	5	10	0	34	1	7	2	11	0	101	1	15	6	11	91	22	91
16	6	9	178	251	177	21	1	10	0	74	1	21	1	10	247	269	30	8	2	11	302	302	22	17	6	11	0	22	1
17	6	9	125	17	125	22	1	10	0	19	1	1	6	10	181	136	37	9	2	11	51	75	51	18	6	11	0	63	1
18	6	9	186	167	70	23	1	10	0	27	1	2	6	10	435	374	20	10	2	11	802	764	27	1	7	11	62	163	62
19	6	9	159	63	158	24	1	10	150	13	149	3	6	10	55	35	54	11	2	11	587	605	30	2	7	11	68	211	68
1	7	9	251	284	33	0	2	10	1001	1022	22	4	6	10	234	209	33	13	2	11	1134	1096	30	3	7	11	0	74	1
2	7	9	122	64	122	1	2	10	0	12	1	5	6	10	471	419	24	14	2	11	237	215	34	4	7	11	278	261	30
3	7	9	0	80	1	2	2	10	630	593	21	6	6	10	349	335	26	15	2	11	218	270	39	5	7	11	0	43	1
4	7	9	251	206	33	3	2	10	732	742	22	7	6	10	345	310	26	16	2	11	108	51	107	6	7	11	235	174	36
5	7	9	208	110	35	4	2	10	173	114	27	8	6	10	422	494	27	17	1	11	94	169	94	7	7	11	102	28	101
6	7	9	127	78	127	5	2	10	1024	1005	24	9	6	10	74	26	74	18	2	11	125	29	124	8	7	11	0	26	1
7	7	9	0	203	1	6	2	10	128	121	127	10	6	10	206	244	43	19	2	11	114	8	113	9	7	11	151	134	66
8	7	9	87	126	86	7	2	10	312	259	13	11	6	10	26	21	25	20	2	11	166	81	166	10	7	11	132	146	122
9	7	9	190	211	47	8	2	10	388	419	7	12	6	10	0	41	1	21	2	11	337	282	30	11	7	11	0	85	1
10	7	9	0	46	1	9	2	10	255	278	25	13	6	10	96	21	96	22	2	11	198	72	51	12	7	11	163	162	71
11	7	9	0	51	1	10	2	10	325	328	20	14	6	10	0	19	1	23	2	11	184	265	183	13	7	11	86	58	86
12	7	9	0	88	1	11	2	10	278	275	25	15	6	10	84	250	83	1	3	11	460	443	24	14	7	11	173	121	172
13	7	9	0	7	1	12	2	10	63	146	63	16	6	10	158	139	84	2	3	11	0	10	1	15	7	11	0	25	1
14	7	9	0	24	1	13	2	10	305	315	25	17	6	10	99	165	99	3	3	11	447	467	19	16	7	11	0	80	1
15	7	9	0	23	1	14	2	10	475	462	23	18	6	10	0	159	1	4	3	11	634	596	24	0	8	11	0	109	1
16	7	9	187	76	186	15	2	10	345	300	23	19	6	10	0	3	1	5	3	11	105	85	105	1	8	11	178	55	44
17	7	9	27	11	26	16	2	10	514	485	24	1	7	10	387	397	25	6	3	11	604	623	25	2	8	11	159	9	55
0	8	9	108	253	107	17	2	10	0	114	1	2	7	10	60	39	60	7	3	11	704	646	26	3	8	11	216	204	40
1	8	9	0	113	1	18	2	10	133	189	92	3	7	10	117	90	108	8	3	11	351	291	22	4	8	11	87	32	86
2	8	9	135	269	135	19	2	10	124	74	123	4	7	10	55	39	55	9	3	11	534	516	21	5	8	11	321	310	31
3	8	9	106	176	106	20	2	10	0	169	1	5	7	10	130	31	130	10	3	11	447	442	23	6	8	11	87	33	87
4	8	9	141	118	141	21	2	10	105	114	105	6	7	10	116	130	116	13	3	11	0	77	1	7	8	11	206	165	45
5	8	9	0	102	1	22	2	10	0	84	1	7	7	10	143	105	142	14	3	11	304	291	27	8	8	11	0	19	1
6	8	9	237	226	42	23	2	10	138	33	138	8	7	10	156	139	156	15	3	11	154	89	133	9	8	11	0	98	1
7	8	9	157	67	70	1	3	10	1500	1460	28	9	7	10	0	301	1	16	3	11	0	87	1	10	8	11	120	27	120
8	8	9	33	336	31	2	3	10	0	41	1	10	7	10	0	60	1	17	3	11	329	280	25	11	8	11	170	85	170
9	8	9	69	25	89	3	3	10	560	588	23	11	7	10	107	167	107	18	3	11	737	226	40	12	8	11	0	65	1
10	8	9	120	159	119	4	3	10	148	132	36	12	7	10	142	106	141	19	3	11	0	75</							

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	1	12	105	49	105	15	5	12	144	117	143	9	2	13	215	198	30	1	7	13	142	144	141	16	2	14	144	212	143
16	1	12	264	290	34	16	5	12	0	40	1	10	2	13	691	716	27	2	7	13	257	251	32	17	2	14	50	22	49
17	1	12	50	26	45	17	5	12	0	35	1	11	2	13	0	421	-1	3	7	13	154	39	59	18	2	14	114	145	114
18	1	12	0	75	1	18	5	12	0	158	1	13	2	13	387	344	22	4	7	13	235	275	38	19	2	14	56	118	56
19	1	12	143	161	142	19	5	12	0	71	1	14	2	13	119	60	119	5	7	13	89	76	89	20	2	14	113	156	112
20	1	12	68	212	67	20	5	12	0	98	1	15	2	13	125	90	124	6	7	13	0	138	1	21	2	14	138	115	138
21	1	12	97	99	56	21	5	12	267	236	28	16	2	13	341	327	27	7	7	13	130	101	130	22	2	14	0	62	1
22	1	12	186	140	49	22	5	12	241	225	32	17	2	13	60	12	60	8	7	13	35	7	34	1	3	14	624	645	24
23	1	12	71	12	70	23	5	12	0	116	1	18	2	13	296	255	30	9	7	13	173	150	56	2	3	14	337	355	16
0	2	12	909	925	22	3	6	12	303	293	26	19	2	13	0	31	1	10	7	13	119	174	119	3	3	14	333	312	19
1	2	12	0	52	1	4	6	12	326	328	26	20	2	13	240	181	39	11	7	13	117	81	116	4	3	14	637	657	27
2	2	12	913	971	23	5	6	12	0	93	1	21	2	13	0	135	1	12	7	13	0	111	1	5	3	14	232	249	27
3	2	12	127	172	127	6	6	12	0	77	1	22	2	13	35	100	34	13	7	13	0	54	1	6	3	14	660	580	25
4	2	12	0	101	1	7	6	12	234	137	32	1	3	13	208	205	23	14	7	13	170	124	69	7	3	14	474	475	22
5	2	12	0	10	1	8	6	12	0	93	1	2	3	13	244	249	24	15	7	13	113	2	113	8	3	14	234	189	29
6	2	12	657	712	26	9	6	12	0	21	1	3	3	13	715	758	25	0	8	13	215	212	43	9	3	14	717	708	30
7	2	12	141	170	45	10	6	12	153	23	60	4	3	13	417	425	21	1	8	13	0	61	1	10	3	14	0	21	1
8	2	12	995	953	27	11	6	12	240	197	39	5	3	13	80	115	79	2	8	13	0	103	1	12	3	14	292	251	27
9	2	12	162	108	40	12	6	12	0	100	1	6	3	13	442	460	22	3	8	13	0	30	1	13	3	14	25	35	25
10	2	12	596	588	30	13	6	12	125	76	124	7	3	13	472	443	22	4	8	13	92	55	92	14	3	14	118	59	117
11	2	12	93	41	93	14	6	12	247	190	38	8	3	13	0	8	1	5	8	13	0	152	1	15	3	14	0	214	1
12	2	12	0	272	-1	15	6	12	0	38	1	9	3	13	93	45	92	6	8	13	153	59	60	16	3	14	131	35	131
13	2	12	0	41	1	16	6	12	111	17	110	10	3	13	508	477	23	7	8	13	0	11	1	17	3	14	143	235	142
14	2	12	482	444	25	17	6	12	130	46	130	13	3	13	274	239	30	8	8	13	0	149	1	18	3	14	0	7	1
15	2	12	124	138	92	18	6	12	0	155	1	14	3	13	205	224	39	9	8	13	0	85	1	19	3	14	0	202	1
16	2	12	542	542	25	1	7	12	290	257	26	15	3	13	129	31	129	10	8	13	0	139	160	20	3	14	154	31	154
17	2	12	105	44	104	2	7	12	303	265	27	16	3	13	119	123	119	11	8	13	0	37	1	21	3	14	94	120	93
18	2	12	273	288	34	3	7	12	195	228	47	17	3	13	96	168	96	1	9	13	0	49	1	0	4	14	232	249	26
19	2	12	0	25	1	5	7	12	154	9	153	18	3	13	134	9	134	2	9	13	0	13	101	1	4	14	0	86	1
20	2	12	69	89	68	6	7	12	297	283	30	19	3	13	0	68	1	3	9	13	0	32	1	2	4	14	262	268	23
21	2	12	0	12	1	7	7	12	0	156	1	20	3	13	235	235	44	4	9	13	168	51	167	3	4	14	0	35	1
22	2	12	66	20	66	8	7	12	260	217	35	21	3	13	0	112	1	0	0	14	296	304	16	4	4	14	137	177	137
2	3	12	0	47	1	9	7	12	0	73	1	22	3	13	0	145	1	1	0	14	510	472	24	5	4	14	309	274	22
1	3	12	159	193	26	10	7	12	140	30	139	0	4	13	372	315	18	2	0	14	756	788	21	6	4	14	112	136	111
2	3	12	596	637	24	11	7	12	0	45	1	1	4	13	254	263	24	3	0	14	1287	1275	27	7	4	14	109	23	109
3	3	12	574	554	25	12	7	12	244	191	38	2	4	13	123	26	12	4	0	14	494	470	24	8	4	14	0	144	1
4	3	12	1484	1495	30	13	7	12	107	59	106	3	4	13	112	65	112	5	0	14	994	1058	23	9	4	14	0	134	1
5	3	12	717	699	26	14	7	12	172	213	171	4	4	13	63	179	63	6	0	14	662	642	26	10	4	14	0	36	1
6	3	12	1019	1084	26	15	7	12	163	32	163	5	4	13	741	686	27	7	0	14	407	352	19	12	4	14	129	34	129
7	3	12	0	93	1	0	8	12	221	121	37	6	4	13	0	44	1	8	0	14	1213	1229	28	13	4	14	197	150	39
8	3	12	152	204	47	1	8	12	153	30	153	7	4	13	270	276	27	9	0	14	220	223	29	14	4	14	318	287	26
9	3	12	92	167	92	2	8	12	143	41	77	8	4	13	354	357	23	10	0	14	424	415	19	15	4	14	147	166	67
10	3	12	336	360	23	3	8	12	0	59	1	9	4	13	147	74	146	12	0	14	516	508	25	16	4	14	0	110	1
11	3	12	23	349	-22	4	8	12	213	102	35	10	4	13	499	451	20	13	0	14	1075	1057	30	17	4	14	117	68	117
13	3	12	112	79	111	5	8	12	170	22	50	12	4	13	0	34	1	14	0	14	193	154	42	18	4	14	100	82	99
14	3	12	396	381	25	6	8	12	160	199	59	13	4	13	135	85	73	15	0	14	316	331	27	19	4	14	0	34	1
15	3	12	0	88	1	7	8	12	112	21	111	14	4	13	0	57	1	16	0	14	660	636	33	20	4	14	97	58	96
16	3	12	152	169	151	8	8	12	279	215	34	15	4	13	227	206	37	17	0	14	0	132	1	1	5	14	0	44	1
17	3	12	36	154	36	9	8	12	112	35	112	16	4	13	0	101	1	18	0	14	380	368	26	2	5	14	271	196	28
18	3	12	0	29	1	10	8	12	0	109	1	17	4	13	0	8	1	19	0	14	211	174	40	3	5	14	0	46	1
19	3	12	122	125	122	11	8	12	0	60	1	18	4	13	155	186	72	20	0	14	197	99	43	4	5	14	230	222	33
20	3	12	61	134	60	12	8	12	0	24	1	19	4	13	0	84	1	21	0	14	160	228	160	5	5	14	111	85	110
21	3	12	0	138	1	1	9	12	0	7	1	20	4	13	217	187	50	22	0	14	0	117	1	6	5	14	204	215	39
22	3	12	252	224	44	2	9	12	0	146	1	21	4	13	0	81	1	23	0	14	179	303	179	7	5	14	0	144	1
0	4	12	328	321	19	3	9	12	0	25	1	1	5	13	359	345	21	1	1	14	670	668	23	8	5	14	348	323	27
1	4	12	0	31	1	4	9	12	159	134	159	2	5	13	591	625	31	2	1	14	451	472	19	9	5	14	0	55	1
2	4	12	205	173	26	5	9	12	51	27	54	3	5	13	255	285	30	3	1	14	109	136	108	10	5	14	115	132	114
3	4	12	202	174	27	6	9																						

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
8	7	14	0	96	1	8	4	15	116	124	116	20	0	16	0	165	1	9	5	16	0	49	1	4	3	17	205	211	35
9	7	14	245	208	36	9	4	15	205	180	38	21	0	16	245	185	39	10	5	16	57	86	57	5	3	17	79	43	79
10	7	14	95	11	94	10	4	15	0	28	1	22	0	16	91	129	90	11	5	16	0	56	1	6	3	17	0	90	1
11	7	14	76	130	76	11	4	15	0	33	-1	1	1	16	524	530	25	12	5	16	108	98	107	7	3	17	440	384	22
12	7	14	195	8	45	12	4	15	132	173	80	2	1	16	651	642	24	13	5	16	0	32	1	8	3	17	111	117	110
13	7	14	0	14	1	13	4	15	341	300	23	3	1	16	319	329	20	14	5	16	158	96	157	9	3	17	77	115	77
14	7	14	0	102	1	14	4	15	126	76	125	4	1	16	311	246	19	15	5	16	0	55	1	10	3	17	32	35	32
0	8	14	277	269	35	15	4	15	105	88	104	5	1	16	83	88	82	16	5	16	126	39	125	12	3	17	189	174	42
1	8	14	79	66	78	16	4	15	40	18	40	6	1	16	70	103	69	17	5	16	150	29	150	13	3	17	146	19	60
2	8	14	133	69	80	17	4	15	152	50	59	7	1	16	301	286	23	0	6	16	511	482	25	14	3	17	0	100	1
3	8	14	150	130	149	18	4	15	24	59	24	8	1	16	337	297	20	1	6	16	0	62	1	3	17	0	98	1	
4	8	14	157	54	157	19	4	15	149	46	148	9	1	16	400	310	21	2	6	16	217	184	40	16	3	17	82	20	81
5	8	14	122	119	121	20	4	15	0	57	1	10	1	16	216	162	33	3	6	16	0	64	1	17	3	17	107	197	43
6	8	14	95	175	94	1	5	15	633	669	31	12	1	16	482	357	21	4	6	16	119	107	119	18	3	17	0	7	1
7	8	14	118	20	117	2	5	15	232	159	28	13	1	16	175	108	43	5	6	16	0	88	1	19	3	17	0	30	1
8	8	14	227	203	44	3	5	15	495	459	24	14	1	16	281	256	29	6	6	16	155	175	65	20	3	17	0	61	1
9	8	14	0	46	1	4	5	15	0	39	1	15	1	16	118	72	118	7	6	16	0	7	1	0	4	17	564	563	29
10	8	14	113	173	112	5	5	15	152	161	56	16	1	16	94	59	94	8	6	16	87	232	86	1	4	17	0	69	1
1	9	14	0	128	1	6	5	15	0	105	1	17	1	16	65	71	64	9	6	16	129	74	129	2	4	17	202	148	33
1	1	15	826	837	23	7	5	15	749	720	31	18	1	16	139	127	82	10	6	16	308	338	31	3	4	17	174	90	40
2	1	15	292	294	20	8	5	15	0	140	1	19	1	16	101	105	101	11	6	16	35	62	35	4	4	17	291	294	27
3	1	15	182	167	28	9	5	15	539	583	28	20	1	16	0	145	1	12	6	16	105	73	105	5	4	17	150	156	59
4	1	15	0	32	1	10	5	15	0	185	1	21	0	16	168	99	62	13	6	16	27	12	26	6	4	17	0	68	1
5	1	15	181	156	30	11	5	15	196	265	-48	1	2	16	384	365	20	14	6	16	68	99	67	7	4	17	264	292	32
6	1	15	441	446	18	12	5	15	126	116	126	1	2	16	179	194	32	15	6	16	169	24	168	8	4	17	0	24	1
7	1	15	0	56	1	13	5	15	67	93	67	2	2	16	184	187	31	1	7	16	293	312	31	9	4	17	333	281	25
8	1	15	173	187	40	14	5	15	46	109	46	3	2	16	639	661	28	2	7	16	0	16	1	10	4	17	193	211	44
9	1	15	464	476	23	15	5	15	0	161	1	4	2	16	174	158	37	3	7	16	0	52	1	11	4	17	0	43	1
10	1	15	243	216	29	16	5	15	43	11	42	5	2	16	473	470	23	4	7	16	354	352	27	12	4	17	159	184	60
11	1	15	32	838	-14	17	5	15	322	342	38	6	2	16	0	90	1	5	7	16	134	63	133	13	4	17	118	22	117
12	1	15	321	369	27	18	5	15	0	6	1	7	2	16	347	326	21	6	7	16	373	385	28	14	4	17	170	81	50
13	1	15	143	137	143	0	6	15	163	72	42	8	2	16	132	37	131	7	7	16	118	86	117	15	4	17	102	58	101
14	1	15	142	24	62	1	6	15	99	76	98	9	2	16	71	82	71	8	7	16	0	50	1	16	4	17	226	140	37
15	1	15	0	53	1	2	6	15	115	20	93	10	2	16	319	301	26	9	7	16	146	156	81	17	4	17	0	72	1
16	1	15	102	135	101	3	6	15	165	191	164	12	2	16	28	23	27	10	7	16	78	110	77	18	4	17	0	77	1
17	1	15	0	73	1	4	6	15	96	205	95	13	2	16	532	529	25	11	7	16	162	57	162	1	5	17	278	279	28
18	1	15	152	129	152	5	6	15	129	147	129	14	2	16	36	9	36	12	7	16	143	95	143	2	5	17	236	206	31
19	1	15	222	243	43	6	6	15	162	127	51	15	2	16	0	115	1	0	8	16	117	37	117	3	5	17	135	88	66
20	1	15	0	1-8	1	7	6	15	233	202	33	16	2	16	136	144	135	1	0	16	159	113	65	4	5	17	434	413	22
21	1	15	232	226	45	8	6	15	51	123	50	17	2	16	257	148	32	2	8	16	137	42	137	5	5	17	0	16	1
22	1	15	0	129	1	9	6	15	144	52	143	18	2	16	0	3	1	3	8	16	239	169	39	6	5	17	380	359	26
0	2	15	611	603	25	10	6	15	147	21	60	19	2	16	96	1-1	96	4	8	16	131	76	130	7	5	17	0	22	1
1	2	15	0	99	1	11	6	15	61	45	60	20	2	16	142	152	142	5	8	16	0	161	1	8	5	17	181	191	47
2	2	15	395	367	21	12	6	15	0	28	1	21	2	16	82	116	82	6	8	16	84	26	83	9	5	17	70	150	70
3	2	15	664	749	25	13	6	15	0	74	1	1	3	16	301	338	22	7	8	16	0	47	1	10	5	17	119	43	118
4	2	15	223	234	31	14	6	15	206	43	39	2	3	16	410	430	19	8	8	16	0	25	1	11	5	17	0	19	1
5	2	15	1347	1279	29	15	6	15	0	99	1	3	3	16	418	430	20	1	1	17	595	579	25	12	5	17	251	233	36
6	2	15	117	61	117	16	6	15	123	4	123	4	3	16	598	638	29	2	1	17	520	63	19	13	5	17	0	9	1
7	2	15	592	416	21	1	7	15	166	166	56	5	3	16	276	282	25	3	1	17	0	64	1	14	5	17	297	281	33
8	2	15	0	17	1	2	7	15	120	110	119	6	3	16	463	433	22	4	1	17	610	584	26	15	5	17	36	44	35
9	2	15	243	218	27	3	7	15	0	154	1	7	3	16	0	119	1	5	1	17	0	18	1	16	5	17	214	238	49
10	2	15	120	93	119	4	7	15	128	146	128	8	3	16	265	249	28	6	1	17	589	644	21	17	5	17	0	34	1
12	2	15	209	252	38	5	7	15	101	14	101	9	3	16	219	244	37	7	1	17	104	136	104	0	6	17	157	198	156
13	2	15	404	378	23	6	7	15	57	4	57	10	3	16	0	49	1	8	1	17	312	323	24	1	6	17	101	46	100
14	2	15	138	169	138	7	7	15	153	121	67	12	3	16	268	300	30	9	1	17	535	471	24	2	6	17	214	75	37
15	2	15	406	394	25	8	7	15	0	25	1	13	3	16	174	152	43	10	1	17	203	255	41	3	6	17	109	49	109
16	2	15	150	92	150	9	7	15	186	121	51	14	3	16	477	475	23	11	1	17	0	285	-1	4	6	17	0	156	1
17	2	15	101	21	101	10	7	15	80																				

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	0	18	117	24	116	15	4	18	268	257	33	3	3	19	196	122	33	1	1	20	261	298	27	7	6	20	0	107	1
5	0	18	345	345	22	16	4	18	0	9	1	4	3	19	0	165	1	2	1	20	161	145	43	8	6	20	177	249	62
6	0	18	308	358	25	17	4	18	0	5	1	5	3	19	29	50	29	3	1	20	299	328	26	9	6	20	0	39	1
7	0	18	0	75	1	18	4	18	113	89	112	6	3	19	133	149	132	4	1	20	457	467	24	10	6	20	221	187	38
8	0	18	625	677	23	1	5	18	0	26	1	7	3	19	248	153	28	5	1	20	0	12	1	11	6	20	0	83	1
9	0	18	293	273	26	2	5	18	45	63	45	8	3	19	146	127	146	6	1	20	167	192	51	12	6	20	81	115	80
10	0	18	626	612	24	3	5	18	199	186	38	9	3	19	152	24	151	7	1	20	279	258	29	1	7	20	0	163	1
11	0	18	36	54	35	4	5	18	97	25	96	11	3	19	117	38	117	8	1	20	0	59	1	2	7	20	121	163	120
12	0	18	0	24	1	5	5	18	78	53	77	12	3	19	0	66	1	9	1	20	0	152	1	3	7	20	0	100	1
13	0	18	64	207	63	6	5	18	0	116	1	13	3	19	154	180	59	10	1	20	0	241	-1	4	7	20	288	221	36
14	0	18	55	65	54	7	5	18	0	75	1	14	3	19	0	55	1	12	1	20	260	268	35	5	7	20	97	3	96
15	0	18	263	223	36	8	5	18	111	106	110	15	3	19	0	6	1	13	1	20	158	180	158	6	7	20	151	156	151
16	0	18	0	74	1	9	5	18	0	6	1	16	3	19	0	112	1	14	1	20	185	156	51	7	7	20	194	111	54
17	0	18	195	183	49	10	5	18	98	45	98	17	3	19	107	58	107	15	1	20	0	41	1	1	1	21	82	32	82
18	0	18	277	245	48	11	5	18	0	69	1	18	3	19	0	45	1	16	1	20	24	71	24	2	1	21	537	588	24
19	0	18	0	50	1	12	5	18	132	59	131	0	4	19	143	87	143	17	1	20	125	156	124	3	1	21	144	121	143
20	0	18	213	128	45	13	5	18	136	83	77	1	4	19	138	72	138	18	1	20	98	50	98	4	1	21	528	492	26
1	1	18	515	547	20	14	5	18	0	1	1	2	4	19	263	228	29	19	1	20	0	95	1	5	1	21	180	139	40
2	1	18	114	29	62	15	5	18	180	66	51	3	4	19	310	356	30	0	2	20	129	70	128	6	1	21	504	480	22
3	1	18	54	26	53	16	5	18	114	88	113	4	4	19	231	223	36	1	2	20	117	162	85	7	1	21	273	237	28
4	1	18	337	341	21	0	6	18	138	18	137	5	4	19	248	165	29	2	2	20	113	195	113	8	1	21	96	53	95
5	1	18	218	210	29	1	6	18	266	279	33	6	4	19	57	201	56	3	2	20	315	318	24	9	1	21	146	108	145
6	1	18	432	384	20	2	6	18	0	59	1	7	4	19	0	135	1	4	2	20	131	143	130	11	1	21	0	158	1
7	1	18	123	92	74	3	6	18	422	441	24	8	4	19	0	71	1	5	2	20	0	30	1	12	1	21	442	415	24
8	1	18	98	52	97	4	6	18	157	41	157	9	4	19	158	40	157	6	2	20	282	287	30	13	1	21	0	26	1
9	1	18	227	262	40	5	6	18	288	343	35	10	4	19	132	154	132	7	2	20	0	52	1	14	1	21	299	277	30
10	1	18	161	71	46	6	6	18	202	127	42	11	4	19	77	19	77	8	2	20	310	366	29	15	1	21	0	15	1
12	1	18	0	136	1	7	6	18	204	151	43	12	4	19	0	44	1	9	2	20	0	17	1	16	1	21	152	129	151
13	1	18	165	75	165	8	6	18	110	108	109	13	4	19	150	198	71	12	2	20	147	185	147	17	1	21	83	85	83
14	1	18	298	327	30	9	6	18	0	13	1	14	4	19	0	80	1	13	2	20	60	172	59	18	1	21	0	46	1
15	1	18	0	104	1	10	6	18	0	47	1	15	4	19	0	140	1	14	2	20	0	72	1	0	2	21	604	577	31
16	1	18	0	78	1	11	6	18	263	228	34	16	4	19	125	16	124	15	2	20	0	7	1	1	2	21	0	5	1
17	1	18	134	19	79	12	6	18	0	63	1	17	4	19	187	62	52	16	2	20	0	95	1	2	2	21	305	305	26
18	1	18	0	55	1	13	6	18	137	234	136	1	5	19	290	260	29	17	2	20	135	90	134	3	2	21	44	15	44
19	1	18	0	81	1	14	6	18	108	36	107	2	5	19	86	115	86	18	2	20	124	16	123	4	2	21	112	9	112
20	1	18	132	52	131	1	7	18	254	166	32	3	5	19	0	25	1	1	3	20	306	274	23	5	2	21	69	189	69
0	2	18	0	59	1	2	7	18	0	163	1	4	5	19	0	4	1	2	3	20	411	404	20	6	2	21	113	141	113
1	2	18	115	133	114	3	7	18	234	185	38	5	5	19	0	31	1	3	3	20	130	137	130	7	2	21	105	62	104
2	2	18	135	155	134	4	7	18	0	119	1	6	5	19	0	57	1	4	3	20	577	527	23	8	2	21	200	245	49
3	2	18	387	358	20	5	7	18	134	98	98	7	5	19	139	160	67	5	3	20	0	40	1	9	2	21	121	134	101
4	2	18	148	195	147	6	7	18	138	203	138	8	5	19	0	149	1	6	3	20	301	312	30	10	2	21	498	494	22
5	2	18	417	387	20	7	7	18	264	294	40	9	5	19	202	279	44	7	3	20	133	101	132	11	2	21	111	159	110
6	2	18	291	269	22	8	7	18	174	129	60	10	5	19	137	60	63	8	3	20	176	151	45	12	2	21	102	135	101
7	2	18	76	76	76	9	7	18	77	116	76	11	5	19	0	200	1	9	3	20	226	215	36	13	2	21	0	6	1
8	2	18	169	137	45	10	7	18	102	48	102	12	5	19	0	94	1	10	3	20	94	102	94	14	2	21	0	6	1
9	2	18	327	360	25	0	8	18	0	72	1	13	5	19	155	78	66	11	3	20	157	183	55	15	2	21	0	8	1
10	2	18	0	14	1	1	8	18	0	24	1	14	5	19	135	26	134	12	3	20	144	144	66	16	2	21	0	112	1
11	2	18	48	186	-14	2	8	18	72	73	71	15	5	19	151	13	151	13	3	20	152	151	152	17	2	21	0	26	1
12	2	18	102	42	101	3	8	18	118	60	117	0	6	19	0	18	1	14	3	20	127	107	126	18	2	21	170	187	64
13	2	18	261	224	32	4	8	18	0	27	1	1	6	19	0	77	1	15	3	20	158	13	157	1	3	21	133	138	132
14	2	18	0	70	1	1	1	19	610	627	28	2	5	19	76	13	75	16	3	20	129	126	129	2	3	21	314	313	27
15	2	18	0	45	1	2	1	19	324	378	20	3	6	19	74	159	73	17	3	20	161	131	65	3	3	21	272	232	27
16	2	18	0	38	1	3	1	19	517	434	25	4	6	19	0	120	1	0	4	20	517	545	26	4	3	21	0	90	1
17	2	18	78	79	78	4	1	19	0	67	1	5	6	19	298	335	34	1	4	20	256	277	30	5	3	21	0	9	1
18	2	18	146	88	146	5	1	19	0	8	1	6	6	19	99	142	99	2	4	20	432	416	24	6	3	21	0	127	1
19	2	18	160	103	69	6	1	19	116	129	116	7	6	19	103	115	102	3	4	20	426	451	22	7	3	21	36	164	36
20	2	18	121	86	121	7	1	19	658	605	32	8	6	19	120	3	120	4	4	20	99	175	98	8	3	21	249	208	32
1	3	18	505	472	22	8	1	19	0	43	1	9	6	19	0	71	1	5	4										

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	
9	5	21	134	112	133	0	4	22	528	507	24	5	4	23	276	282	35	2	4	24	138	29	137	7	0	26	0	87	1	
10	5	21	0	46	1	1	4	22	112	22	111	6	4	23	92	108	91	3	4	24	284	270	33	8	0	26	450	444	27	
11	5	21	0	24	1	2	4	22	360	334	24	7	4	23	0	205	1	4	4	24	138	88	138	9	0	26	225	172	38	
12	5	21	157	152	157	3	4	22	157	40	55	8	4	23	0	50	1	5	4	24	355	339	28	10	0	26	146	169	145	
13	5	21	81	82	81	4	4	22	103	45	103	9	4	23	20	53	20	6	4	24	0	13	1	11	0	26	314	272	29	
0	6	21	311	274	28	5	4	22	78	104	78	10	4	23	156	13	155	7	4	24	103	119	103	12	0	26	99	87	98	
1	6	21	15	0	15	6	4	22	228	284	43	11	4	23	162	154	162	8	4	24	0	51	1	13	0	26	306	290	37	
2	6	21	238	219	38	7	4	22	0	101	1	12	4	23	87	20	86	9	4	24	0	28	1	1	1	26	225	214	35	
3	6	21	69	32	69	8	4	22	439	383	24	13	4	23	0	35	1	10	4	24	91	63	91	2	1	26	88	142	87	
4	6	21	0	27	1	9	4	22	0	56	1	14	4	23	225	266	44	11	4	24	178	119	54	3	1	26	0	43	1	
5	6	21	127	37	127	10	4	22	266	250	35	2	5	23	207	146	43	12	4	24	0	7	1	4	1	26	128	58	127	
6	6	21	72	162	71	11	4	22	0	85	1	3	5	23	235	166	37	1	5	24	0	110	1	5	1	26	127	17	126	
7	6	21	0	17	1	12	4	22	0	120	1	4	5	23	130	64	130	2	5	24	145	61	70	6	1	26	131	69	83	
8	6	21	202	175	51	13	4	22	0	77	1	5	5	23	0	74	1	3	5	24	117	73	116	7	1	26	0	36	1	
9	6	21	0	2	1	14	4	22	0	75	1	6	5	23	0	21	1	4	5	24	135	69	134	8	1	26	181	109	50	
10	6	21	221	144	42	1	5	22	0	53	1	7	5	23	259	265	39	5	5	24	107	50	106	9	1	26	153	96	153	
1	7	21	0	113	1	2	5	22	0	33	1	8	5	23	223	47	39	6	5	24	132	58	131	10	1	26	141	3	140	
2	7	21	43	28	42	3	5	22	102	94	101	9	5	23	330	271	29	7	5	24	0	21	1	11	1	26	93	91	92	
3	7	21	0	40	1	4	5	22	60	40	60	10	5	23	0	84	1	8	5	24	138	83	138	12	1	26	209	117	45	
4	7	21	0	9	1	5	5	22	0	20	1	11	5	23	138	141	137	9	5	24	0	21	1	13	1	26	141	9	140	
5	7	21	68	23	68	6	5	22	0	32	1	0	6	23	146	86	146	0	6	24	0	49	1	0	2	26	317	344	29	
0	0	22	101	160	101	7	5	22	0	46	1	1	6	23	0	86	1	1	6	24	170	56	55	1	1	2	26	36	103	35
1	0	22	471	486	23	8	5	22	123	25	123	2	6	23	118	50	118	2	6	24	60	20	60	2	2	26	235	182	33	
2	0	22	173	101	37	9	5	22	53	96	52	3	6	23	0	173	1	3	6	24	100	127	100	3	2	26	210	229	43	
3	0	22	699	663	29	10	5	22	0	50	1	4	6	23	0	23	1	4	6	24	134	52	134	4	2	26	104	28	104	
4	0	22	0	79	1	11	5	22	52	40	51	5	6	23	0	160	1	1	1	25	0	56	1	5	2	26	269	231	33	
5	0	22	0	103	1	12	5	22	0	73	1	6	6	23	0	11	1	2	1	25	199	179	37	6	2	26	0	112	1	
6	0	22	314	291	26	0	6	22	117	145	116	7	6	23	138	100	137	3	1	25	204	5	33	7	2	26	247	148	33	
7	0	22	203	188	41	1	6	22	44	18	44	0	0	24	795	849	30	4	1	25	0	104	1	8	2	26	112	177	111	
8	0	22	0	106	1	2	6	22	171	162	66	1	0	24	120	68	119	5	1	25	116	10	115	9	2	26	96	19	96	
9	0	22	63	93	63	3	6	22	134	137	133	2	0	24	542	530	24	6	1	25	131	73	131	10	2	26	91	100	90	
10	0	22	0	143	1	4	6	22	166	134	61	3	0	24	262	255	32	7	1	25	65	81	65	11	2	26	266	183	37	
11	0	22	454	453	24	5	6	22	266	250	37	4	0	24	0	83	1	8	1	25	132	124	132	12	2	26	0	6	1	
12	0	22	328	297	30	6	6	22	0	113	1	5	0	24	200	182	44	9	1	25	123	82	122	1	3	26	161	81	57	
13	0	22	321	299	30	7	6	22	86	90	85	6	0	24	273	223	32	10	1	25	0	37	1	2	3	26	151	170	151	
14	0	22	160	199	159	8	6	22	255	214	39	7	0	24	209	107	37	11	1	25	98	4	98	3	3	26	0	22	1	
15	0	22	0	72	1	9	6	22	127	60	126	8	0	24	440	416	24	12	1	25	0	96	1	4	4	26	217	171	42	
16	0	22	50	73	50	1	1	23	287	297	27	9	0	24	185	117	45	13	1	25	0	22	1	5	3	26	0	29	1	
17	0	22	89	9	88	2	1	23	273	246	31	10	0	24	520	544	25	14	1	25	126	98	126	6	3	26	148	187	117	
1	1	22	227	254	30	3	1	23	64	55	63	11	0	24	23	33	23	0	2	25	364	411	24	7	3	26	145	68	144	
2	1	22	200	188	36	4	1	23	116	110	116	12	0	24	266	220	33	1	2	25	0	80	1	8	3	26	140	110	140	
3	1	22	260	283	32	5	1	23	0	54	1	13	0	24	0	79	1	2	2	25	325	312	26	9	3	26	126	112	125	
4	1	22	203	212	39	6	1	23	0	135	1	14	0	24	58	134	57	3	2	25	86	111	85	10	3	26	0	84	1	
5	1	22	128	4	67	7	1	23	209	177	40	15	0	24	149	125	89	4	2	25	110	99	110	0	4	26	133	43	133	
6	1	22	143	161	62	8	1	23	142	123	64	1	1	24	258	262	29	5	2	25	0	80	1	1	4	26	173	24	50	
7	1	22	254	257	33	9	1	23	410	361	25	2	1	24	112	52	93	6	2	25	209	197	44	2	4	26	0	102	1	
8	1	22	210	123	37	10	1	23	141	16	140	3	1	24	97	13	96	7	2	25	0	71	1	3	4	26	82	74	81	
9	1	22	74	78	73	11	1	23	260	294	36	4	1	24	185	138	42	8	2	25	166	267	166	4	4	26	144	76	79	
10	1	22	0	46	1	12	1	23	246	202	37	5	1	24	0	56	1	9	2	25	102	25	102	5	4	26	109	28	108	
11	1	22	0	19	1	13	1	23	113	123	113	6	1	24	218	182	39	10	2	25	250	215	35	6	4	26	122	67	121	
12	1	22	0	36	1	14	1	23	0	36	1	7	1	24	0	16	1	11	2	25	0	65	1	7	4	26	0	10	1	
13	1	22	15	49	14	15	1	23	24	17	24	8	1	24	91	9	91	12	2	25	133	117	132	8	4	26	54	103	53	
14	1	22	98	110	97	16	1	23	0	31	1	9	1	24	162	195	162	13	2	25	130	34	130	1	5	26	119	23	118	
15	1	22	32	40	31	0	2	23	320	340	25	10	1	24	109	138	108	1	3	25	0	56	1	2	5	26	0	39	1	
16	1	22	0	90	1	1	2	23	266	303	32	11	1	24	180	133	51	2	3	25	183	206	50	3	5	26	116	10	116	
17	1	22	0	75	1	2	2	23	0	24	1	12	1	24	154	169	154	3	3	25	16	29	16	1	1	27	239	198	32	
0	2	22	247	229	28	3	2	23	420	410	24	13	1	24	95	26	95	4	3	25	0	128	1	2	1	27	124	71	123	
1	2	22	148	109	51	4	2	23	78	123	78	14	1	24	100	125	100	5	3	25	134	40	134	3						

Table 7. Observed and calculated structure factors for 1

Page 10

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	4	27	114	122	114	1	1	28	61	69	61	2	2	28	121	17	121	5	3	28	90	63	90	2	2	29	139	169	138
0	0	28	0	19	1	2	1	28	60	114	60	3	2	28	267	229	36	6	3	28	155	126	155	3	2	29	57	72	57
1	0	28	192	142	40	3	1	28	80	89	80	4	2	28	57	39	56	1	1	29	0	35	1	4	2	29	97	81	97
2	0	28	0	109	1	4	1	28	90	13	89	5	2	28	241	196	42	2	1	29	0	123	1	5	2	29	0	22	1
3	0	28	334	302	27	5	1	28	198	43	42	6	2	28	36	11	35	3	1	29	88	31	87	0	0	30	160	194	159
4	0	28	131	134	131	6	1	28	123	14	122	7	2	28	141	79	141	4	1	29	174	201	174	1	0	30	82	88	82
5	0	28	308	344	36	7	1	28	0	122	1	8	2	28	69	4	89	5	1	29	0	23	1	2	0	30	130	179	129
6	0	28	0	25	1	8	1	28	0	48	1	1	3	28	193	197	53	6	1	29	182	95	52	3	0	30	0	87	1
7	0	28	204	232	54	9	1	28	0	116	1	2	3	28	185	164	55	7	1	29	0	29	1	1	1	30	41	66	40
8	0	28	166	113	70	0	2	28	103	14	102	3	3	28	95	142	95	0	2	29	216	195	43	2	1	30	0	32	1
9	0	28	102	7	102	1	2	28	87	95	86	4	3	28	201	186	53	1	2	29	0	28	1						

h	k	l	F^2 cal	F^2 obs	$\text{sig}(F^2)$	h	k	l	F^2 cal	F^2 obs	$\text{sig}(F^2)$	h	k	l	F^2 cal	F^2 obs	$\text{sig}(F^2)$
1	0	0	3065.55	3219.65	73.27	-3	3	0	226.86	313.26	29.58	-7	5	0	18.48	-57.31	81.86
2	0	0	42984.16	45874.39	1009.34	-2	3	0	829.66	711.90	45.49	-6	6	0	290.27	267.88	47.41
3	0	0	2502.51	2302.14	65.16	-1	3	0	60130.54	67500.76	2009.27	-5	6	0	123.27	153.33	39.06
4	0	0	14.11	-13.23	50.09	0	3	0	767.26	565.91	39.52	-4	6	0	1029.12	924.63	76.58
5	0	0	113.44	176.86	41.73	1	3	0	43962.80	50080.73	1515.47	-3	6	0	2894.38	3387.40	137.97
6	0	0	132.64	161.81	25.52	2	3	0	13012.43	12097.78	380.35	-2	6	0	494.30	48.71	49.91
7	0	0	1470.80	1498.33	78.15	3	3	0	3109.66	2681.61	105.77	-1	6	0	3868.15	3827.73	143.62
8	0	0	234.18	183.85	34.86	4	3	0	77.81	70.96	23.82	0	6	0	7563.06	7450.56	253.86
9	0	0	4.19	24.49	56.12	5	3	0	749.81	656.69	65.70	1	6	0	1387.83	1336.06	70.22
10	0	0	205.19	206.47	68.55	6	3	0	1287.53	1178.83	90.97	2	6	0	9454.20	9603.91	315.74
-9	1	0	321.70	276.22	62.59	7	3	0	131.05	95.74	42.34	3	6	0	1068.32	1143.06	72.59
-8	1	0	50.18	-12.57	80.77	8	3	0	8.46	-37.44	81.03	4	6	0	61.72	72.55	28.51
-7	1	0	752.24	710.44	64.32	9	3	0	2.61	-74.97	94.28	5	6	0	165.70	245.30	34.90
-6	1	0	154.37	189.53	35.39	10	3	0	3.47	9.31	102.28	6	6	0	1906.79	1934.64	116.34
-5	1	0	155.86	132.29	28.51	-9	4	0	0.02	-13.89	101.17	7	6	0	58.35	-89.31	81.50
-4	1	0	4824.13	4890.70	177.37	-8	4	0	539.59	564.91	61.17	8	6	0	0.66	-142.48	89.59
-3	1	0	2012.82	1888.19	83.76	-7	4	0	115.31	197.29	45.03	9	6	0	197.01	147.91	57.75
-2	1	0	2339.59	2613.74	94.56	-6	4	0	306.15	290.67	43.27	-8	7	0	0.17	22.10	92.75
-1	1	0	12568.67	13092.74	401.02	-5	4	0	296.27	288.47	35.74	-7	7	0	201.05	227.25	52.72
1	1	0	232.57	343.71	20.16	-4	4	0	36.18	15.77	47.64	-6	7	0	505.13	327.35	52.69
2	1	0	2189.72	2719.40	96.81	-3	4	0	2998.31	3208.80	125.70	-5	7	0	278.67	327.98	44.38
3	1	0	7.45	-20.17	30.21	-2	4	0	519.81	1192.29	62.33	-4	7	0	1504.76	1479.82	94.60
4	1	0	4005.30	4177.31	155.53	-1	4	0	482.54	404.72	27.66	-3	7	0	101.63	89.39	31.03
5	1	0	3286.10	3166.22	135.32	0	4	0	11598.98	12361.28	390.50	-2	7	0	815.50	862.32	68.00
6	1	0	3886.24	3870.86	163.89	1	4	0	9919.94	10503.88	332.18	-1	7	0	1540.86	1755.52	87.76
7	1	0	855.71	675.72	66.89	2	4	0	4336.74	4221.50	148.24	0	7	0	3520.20	3610.32	151.01
8	1	0	518.99	515.17	52.85	3	4	0	3478.28	3749.96	139.02	1	7	0	1131.76	1127.80	69.22
9	1	0	97.25	104.71	55.36	4	4	0	45.04	81.29	25.36	2	7	0	9989.35	10272.97	340.80
10	1	0	0.62	-124.57	109.16	5	4	0	4525.50	4396.91	174.94	3	7	0	101.39	93.27	29.62
-9	2	0	0.14	-127.76	101.96	6	4	0	9.93	-119.15	65.48	4	7	0	5085.39	5187.36	197.54
-8	2	0	1330.58	1456.54	122.35	7	4	0	2440.48	2532.27	143.43	5	7	0	0.74	21.45	56.87
-7	2	0	883.19	951.15	91.84	8	4	0	215.32	133.28	52.13	6	7	0	3141.98	3220.02	188.81
-6	2	0	2890.17	2715.97	135.34	9	4	0	264.12	254.74	57.84	7	7	0	243.12	288.67	48.10
-5	2	0	2056.84	1741.87	96.35	10	4	0	46.83	158.06	62.63	8	7	0	652.36	704.95	65.19
-4	2	0	1759.35	1718.55	86.68	-9	5	0	271.22	305.42	62.99	9	7	0	36.24	-37.55	100.61
-3	2	0	342.36	434.29	39.70	-8	5	0	1.32	-40.73	93.07	-8	8	0	376.02	349.79	65.56
-2	2	0	5047.83	5503.30	132.28	-7	5	0	1885.99	2702.67	154.89	-7	8	0	14.00	82.11	49.48
-1	2	0	1394.44	1168.04	48.00	-6	5	0	660.55	738.21	63.18	-6	8	0	1586.01	1519.47	125.10
0	2	0	6474.72	5238.15	167.09	-5	5	0	3269.67	3052.46	143.11	-5	8	0	165.59	148.17	43.57
1	2	0	6796.72	7033.38	221.16	-4	5	0	715.92	926.08	71.37	-4	8	0	1362.41	1357.93	95.64
2	2	0	7197.65	6952.99	224.21	-3	5	0	1184.42	1185.03	72.69	-3	8	0	16.61	38.43	31.07
3	2	0	9.43	13.90	30.74	-2	5	0	3148.00	3131.85	122.84	-2	8	0	100.86	122.30	30.62
4	2	0	1717.97	1578.03	80.77	-1	5	0	4395.47	4105.31	146.47	-1	8	0	1683.54	1411.87	83.64
5	2	0	512.52	461.91	43.01	0	5	0	513.18	490.77	45.85	0	8	0	592.26	418.28	41.50
6	2	0	17.52	43.51	58.12	1	5	0	167.03	117.41	18.75	1	8	0	182.08	230.51	30.00
7	2	0	732.17	666.60	62.07	2	5	0	2080.84	2175.95	92.32	2	8	0	2250.01	2219.62	109.66
8	2	0	550.57	528.46	57.07	3	5	0	1902.22	1579.24	79.62	3	8	0	1705.58	1652.57	98.48
9	2	0	41.41	30.79	93.32	4	5	0	2201.43	1891.51	95.80	4	8	0	2265.82	2151.29	113.30
10	2	0	12.94	-50.54	109.01	5	5	0	700.82	255.82	34.16	5	8	0	4459.78	4430.77	188.80
-9	3	0	608.19	604.86	64.88	6	5	0	2622.89	2500.38	131.08	6	8	0	103.99	41.72	79.66
-8	3	0	113.20	136.25	50.86	7	5	0	63.94	58.13	43.48	7	8	0	1053.88	923.05	80.08
-7	3	0	18.46	-16.14	41.87	8	5	0	312.99	299.53	53.04	8	8	0	10.69	-10.33	92.75
-6	3	0	211.11	275.14	40.56	9	5	0	110.03	140.90	58.37	9	8	0	2.79	-48.29	105.40
-5	3	0	67.09	35.10	53.68	-9	6	0	14.99	-56.08	108.47	-8	9	0	37.97	133.73	61.08
-4	3	0	988.68	1201.04	72.52	-8	6	0	263.05	339.63	56.11	-7	9	0	128.81	-4.53	72.19

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-6	9	0	244.92	265.19	55.58	1	12	0	245.94	309.60	44.60	1	17	0	0.56	45.52	105.61
-5	9	0	89.56	51.46	78.18	2	12	0	1318.11	1443.57	113.37	2	17	0	88.31	86.40	60.93
-4	9	0	289.75	351.45	48.04	3	12	0	151.46	115.00	48.01	3	17	0	204.50	78.77	112.50
-3	9	0	213.69	222.86	37.34	4	12	0	46.07	26.39	76.98	-3	-17	0	93.86	103.56	60.58
-2	9	0	4008.67	4288.74	180.61	5	12	0	22.12	-21.89	48.40	-2	-17	0	253.64	274.31	65.87
-1	9	0	640.30	608.47	49.32	6	12	0	53.44	117.05	51.51	-1	-17	0	9.07	63.44	109.20
0	9	0	1715.82	1836.82	106.20	7	12	0	69.74	110.48	54.69	0	-17	0	297.08	340.62	69.24
1	9	0	3068.12	3031.80	136.66	8	12	0	3.10	-51.12	109.01	1	-17	0	91.03	61.97	117.07
2	9	0	837.94	872.77	75.60	-5	13	0	88.90	-5.61	101.45	-4	-16	0	167.66	343.76	59.93
3	9	0	785.05	731.16	55.33	-4	13	0	687.11	641.92	67.39	-3	-16	0	161.64	196.53	63.16
4	9	0	59.70	-52.27	69.36	-3	13	0	25.66	-167.37	89.71	-2	-16	0	83.90	54.42	107.73
5	9	0	156.41	285.21	44.95	-2	13	0	867.00	1085.24	106.65	-1	-16	0	341.56	403.49	61.75
6	9	0	48.24	69.27	77.78	-1	13	0	7.32	40.69	58.82	0	-16	0	1.06	-146.77	107.30
7	9	0	16.08	7.35	83.08	0	13	0	21.10	18.71	63.42	1	-16	0	223.10	103.81	113.08
8	9	0	273.57	418.62	58.36	1	13	0	96.02	38.43	86.00	2	-16	0	17.73	23.81	106.38
9	9	0	92.58	168.56	64.96	2	13	0	3.02	-43.01	76.10	3	-16	0	42.09	-12.40	114.56
-7	10	0	20.30	13.77	94.32	3	13	0	28.19	70.11	76.54	-5	-15	0	260.04	247.89	63.31
-6	10	0	89.96	-32.02	96.56	4	13	0	429.75	318.46	55.41	-4	-15	0	45.70	48.79	58.85
-5	10	0	143.79	172.08	48.88	5	13	0	18.08	63.55	89.16	-3	-15	0	161.80	257.20	57.24
-4	10	0	123.01	143.95	44.97	6	13	0	134.95	147.50	57.08	-2	-15	0	235.91	281.01	56.54
-3	10	0	2580.41	2723.89	140.38	7	13	0	26.97	-73.60	103.21	-1	-15	0	33.43	-5.15	97.53
-2	10	0	186.28	209.15	33.31	-5	14	0	68.21	48.11	78.68	0	-15	0	88.21	107.32	57.82
-1	10	0	1247.49	1167.77	90.09	-4	14	0	240.12	215.12	62.69	1	-15	0	78.69	13.32	94.48
0	10	0	41.12	28.13	66.23	-3	14	0	5.81	-9.70	98.36	2	-15	0	209.86	199.54	58.87
1	10	0	136.39	42.43	64.94	-2	14	0	5.22	-108.05	91.93	3	-15	0	287.75	238.76	61.32
2	10	0	411.32	386.05	41.27	-1	14	0	279.37	285.22	53.57	4	-15	0	235.02	198.00	64.82
3	10	0	1.64	8.55	35.73	0	14	0	40.62	101.95	51.78	-6	-14	0	1.03	83.49	99.03
4	10	0	135.54	115.19	41.32	1	14	0	835.70	642.55	64.64	-5	-14	0	23.28	-91.42	102.22
5	10	0	483.79	465.17	51.74	2	14	0	188.70	151.79	51.88	-4	-14	0	78.72	40.84	63.62
6	10	0	198.40	230.20	50.73	3	14	0	51.89	7.22	62.85	-3	-14	0	569.38	439.88	59.16
7	10	0	809.29	868.27	79.14	4	14	0	844.84	785.12	80.76	-2	-14	0	19.58	-64.80	92.48
8	10	0	0.82	-171.42	112.73	5	14	0	188.90	195.81	58.04	-1	-14	0	183.39	157.14	52.20
-7	11	0	406.30	483.37	66.83	6	14	0	188.83	201.70	63.84	0	-14	0	0.02	14.84	64.20
-6	11	0	86.41	63.62	96.64	-4	15	0	106.65	124.06	65.49	1	-14	0	123.22	34.63	66.01
-5	11	0	1062.54	984.18	15.54	-3	15	0	15.16	11.97	103.97	2	-14	0	337.62	327.77	56.66
-4	11	0	105.94	122.17	47.12	-2	15	0	163.92	18.71	107.32	3	-14	0	11.82	-53.13	90.83
-3	11	0	186.61	188.99	46.12	-1	15	0	2.44	-115.60	106.45	4	-14	0	532.10	590.06	65.92
-2	11	0	69.83	19.97	66.83	0	15	0	739.39	710.94	70.00	5	-14	0	0.28	29.85	106.86
-1	11	0	1533.02	1636.30	112.09	1	15	0	92.85	64.50	93.60	-7	-13	0	0.39	70.12	76.08
0	11	0	2189.02	1979.03	128.36	2	15	0	281.62	168.36	58.14	-6	-13	0	20.26	-74.87	94.53
1	11	0	5.23	25.68	44.50	3	15	0	146.23	144.21	56.73	-5	-13	0	324.56	352.02	55.00
2	11	0	51	81.91	40.76	4	15	0	1.66	-80.02	95.03	-4	-13	0	16.10	124.60	49.42
3	11	0	4017.77	3946.19	178.94	5	15	0	0.70	56.50	95.17	-3	-13	0	2357.82	2433.67	148.75
4	11	0	1043.51	1070.33	99.43	6	15	0	0.14	-105.32	119.78	-2	-13	0	218.00	208.49	50.05
5	11	0	660.24	765.57	70.50	-3	16	0	218.34	83.28	114.24	-1	-13	0	1201.97	1352.39	115.12
6	11	0	839.47	827.85	65.03	-2	16	0	234.95	243.58	63.45	0	-13	0	419.41	377.95	57.44
7	11	0	9.08	52.13	64.05	-1	16	0	556.75	478.55	70.33	1	-13	0	1.70	-115.96	84.72
8	11	0	32.97	70.23	103.84	0	16	0	21.19	39.49	104.70	2	-13	0	16.74	28.82	83.65
-6	12	0	1.08	26.92	72.94	1	16	0	11.20	-17.32	103.45	3	-13	0	18.05	-48.35	90.66
-5	12	0	3.58	-86.74	96.12	2	16	0	2.26	9.63	97.98	4	-13	0	1.35	-25.80	95.55
-4	12	0	418.80	338.82	55.30	3	16	0	0.06	37.58	103.27	5	-13	0	29.43	103.74	54.25
-3	12	0	1336.51	1511.4	118.68	4	16	0	29.80	-32.20	110.82	-7	-12	0	165.21	71.06	109.32
-2	12	0	56.39	-25.61	75.48	5	16	0	0.85	-67.90	110.08	-6	-12	0	204.41	227.34	56.15
-1	12	0	2175.18	2368.99	136.22	-1	17	0	87.06	63.93	110.33	-5	-12	0	16.26	-39.40	84.81
0	12	0	952.57	1107.12	86.03	0	17	0	291.73	294.82	73.29	-4	-12	0	123.94	1203.72	115.80

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-3	-12	1	264.43	172.41	44.57	4	-9	1	1761.48	2123.69	125.72	5	-6	1	2732.01	2910.10	141.16
-2	-12	1	721.05	667.57	67.24	5	-9	1	502.95	534.14	53.12	6	-6	1	19.06	-94.93	74.05
-1	-12	1	1019.06	929.95	93.85	6	-9	1	33.60	45.78	86.35	7	-6	1	60.29	5.35	87.90
0	-12	1	264.98	87.76	89.80	7	-9	1	154.64	178.00	59.72	8	-6	1	14.37	-36.10	96.50
1	-12	1	418.62	566.76	54.20	8	-9	1	274.25	206.77	66.90	9	-6	1	169.93	65.88	112.73
2	-12	1	555.34	511.10	52.69	-9	-3	1	312.51	266.20	66.14	-9	-5	1	286.94	283.44	63.47
3	-12	1	1880.92	2029.98	141.36	-8	-8	1	67.51	-22.59	101.39	-8	-5	1	3.10	11.50	19.12
4	-12	1	1331.08	1328.07	119.18	-7	-8	1	185.17	90.95	91.87	-7	-5	1	15.16	-19.35	81.62
5	-12	1	33.38	137.74	52.63	-6	-8	1	129.81	121.23	46.26	-6	-5	1	256.00	258.08	40.73
6	-12	1	450.44	387.89	66.40	-5	-8	1	391.75	313.06	44.10	-5	-5	1	1458.25	1715.20	101.61
-8	-11	1	69.32	152.93	58.04	-4	-8	1	382.21	394.93	40.00	-4	-5	1	104.17	111.86	28.12
-7	-11	1	8.71	25.80	94.59	-3	-8	1	35.22	16.53	56.56	-3	-5	1	47.02	63.14	22.96
-6	-11	1	0.92	9.84	84.97	-2	-8	1	2546.06	2824.66	125.19	-2	-5	1	2719.81	2828.46	111.34
-5	-11	1	23.88	-13.41	80.59	-1	-8	1	3967.01	6442.87	231.21	-1	-5	1	1493.14	1539.23	71.03
-4	-11	1	63.88	103.30	43.56	0	-8	1	2.77	37.25	46.32	0	-5	1	9061.67	9484.70	310.61
-3	-11	1	3.45	-20.03	67.90	1	-8	1	3556.84	3273.86	138.76	1	-5	1	2911.96	3216.97	120.80
-2	-11	1	452.43	533.90	51.05	2	-8	1	1.35	46.49	48.68	2	-5	1	12124.10	13179.23	421.45
-1	-11	1	933.74	950.33	89.57	3	-8	1	187.03	39.01	3.50	3	-5	1	352.31	274.35	28.88
0	-11	1	1791.29	789.07	126.28	4	-8	1	239.09	213.89	78.43	4	-5	1	1816.12	1940.46	98.54
1	-11	1	24.99	-9.86	63.56	5	-8	1	79.88	70.14	70.71	5	-5	1	144.66	157.03	34.47
2	-11	1	607.50	515.70	48.72	6	-8	1	238.49	199.84	48.88	6	-5	1	1475.03	1401.35	108.13
3	-11	1	1267.61	1235.42	103.94	7	-8	1	278.56	172.88	54.79	7	-5	1	150.00	191.44	47.71
4	-11	1	40.94	52.56	46.98	8	-8	1	40.39	-75.64	107.95	8	-5	1	76.53	29.03	52.94
5	-11	1	1389.29	861.58	86.41	-9	-7	1	2.41	38.90	104.11	-9	-5	1	32.71	-24.54	104.56
6	-11	1	92.16	169.41	56.72	-8	-7	1	132.83	85.24	90.03	-9	-4	1	26.59	-24.78	96.15
7	-11	1	51.12	22.94	107.78	-7	-7	1	3.31	-161.10	86.06	-8	-4	1	107.20	80.15	85.47
-8	-10	1	0.19	0.36	96.37	-6	-7	1	314.22	268.08	43.81	-7	-4	1	60.13	70.48	42.06
7	-10	1	328.11	392.62	57.44	-5	-7	1	541.01	615.62	53.75	-6	-4	1	55.77	94.39	37.09
-6	-10	1	83.58	90.34	48.38	-4	-7	1	2128.79	2290.25	115.12	-5	-4	1	2803.92	2401.83	120.16
-5	-10	1	13.10	56.33	43.02	-3	-7	1	8697.59	8890.00	304.48	-4	-4	1	441.92	449.03	39.96
-4	-10	1	935.69	1020.43	92.69	-2	-7	1	144.26	221.25	29.35	-3	-4	1	3655.40	3673.62	137.08
-3	-10	1	320.77	312.45	42.57	-1	-7	1	12752.85	12970.80	419.52	-2	-4	1	4208.95	4569.44	189.76
-2	-10	1	8278.45	8422.80	315.42	0	-7	1	19.14	-73.14	49.70	-1	-4	1	4029.74	4272.10	147.20
-1	-10	1	444.28	516.08	48.89	1	-7	1	2613.49	2836.89	121.56	0	-4	1	371.95	268.20	26.75
0	-10	1	1397.14	1157.74	101.40	2	-7	1	3452.73	3690.13	146.65	1	-4	1	35.34	78.24	17.44
1	-10	1	691.26	509.62	80.92	3	-7	1	1214.82	1145.47	78.93	2	-4	1	1046.10	1074.59	59.67
2	-10	1	103.59	60.83	69.09	4	-7	1	10.60	-24.01	54.05	3	-4	1	2332.63	2576.48	107.24
3	-10	1	177.47	188.92	44.66	5	-7	1	338.07	423.99	45.28	4	-4	1	14.97	-3.44	45.08
4	-10	1	12.90	0.39	76.97	6	-7	1	53.49	1.22	55.81	5	-4	1	6.24	-8.64	54.53
5	-10	1	111.21	106.23	48.05	7	-7	1	238.08	279.29	53.33	6	-4	1	3.23	34.02	62.66
6	-10	1	112.94	62.74	80.59	8	-7	1	102.62	205.69	57.69	7	-4	1	663.05	630.88	65.67
7	-10	1	32.75	90.14	100.53	-9	-6	1	125.72	89.95	61.98	8	-4	1	581.72	680.62	61.24
-9	-9	1	65.28	107.50	111.80	-8	-6	1	0.37	59.05	87.12	-9	-4	1	273.77	185.28	63.95
-8	-9	1	58.38	33.52	93.71	-7	-6	1	639.36	531.71	53.63	-9	-3	1	134.47	-43.92	105.70
-7	-9	1	43.40	25.37	91.05	-6	-6	1	1294.91	1444.91	108.19	-8	-3	1	622.36	560.58	58.91
-6	-9	1	459.05	441.91	81.25	-5	-6	1	1418.59	1340.18	93.11	-7	-3	1	154.61	58.48	78.53
-5	-9	1	4802.96	4507.10	200.95	-4	-6	1	610.30	599.85	46.91	-6	-3	1	4153.40	3901.04	170.14
-4	-9	1	308.57	409.20	44.22	-3	-6	1	26.44	0.66	31.25	-6	-3	1	1144.52	1143.38	80.20
-3	-9	1	6538.12	6453.61	240.49	-2	-6	1	6615.10	6397.53	221.60	-4	-3	1	19.34	-8.31	41.76
-2	-9	1	3326.93	3591.84	153.10	-1	-6	1	276.81	151.90	24.05	-3	-3	1	165.44	167.66	20.68
-1	-9	1	558.32	475.23	40.47	0	-6	1	382.45	327.49	29.53	-2	-3	1	1785.71	1557.71	67.66
0	-9	1	0.06	22.59	55.20	1	-6	1	3461.67	3483.21	133.29	-1	-3	1	131.20	126.49	15.19
1	-9	1	774.41	841.19	72.14	2	-6	1	270.95	313.65	29.70	0	-3	1	1869.52	1697.21	68.74
2	-9	1	4580.50	5183.88	202.79	3	-6	1	6915.72	6850.25	242.37	1	-3	1	1.40	36.59	13.92
3	-9	1	1730.41	1846.98	111.93	4	-6	1	20.80	46.27	53.11	2	-3	1	4535.40	4327.74	150.54

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
3	-3	1	166.93	172.82	22.26	1	0	1	10489.68	11118.66	240.14	-4	3	1	9174.38	8686.74	295.45
4	-3	1	5440.34	5874.96	210.88	2	0	1	3406.45	9026.53	201.27	-3	3	1	30.60	26.06	26.22
5	-3	1	890.31	966.85	72.93	3	0	1	12652.42	12681.06	283.62	-2	3	1	2855.12	2875.28	108.51
6	-3	1	709.53	739.37	61.33	4	0	1	369.95	462.37	28.58	-1	3	1	4422.52	5327.46	175.79
7	-3	1	183.27	177.34	43.68	5	0	1	4551.85	4432.07	121.55	0	3	1	2719.57	1428.47	58.07*
8	-3	1	495.08	503.64	57.82	6	0	1	1259.33	1364.05	66.75	1	3	1	11359.43	11563.56	360.06
9	-3	1	9.97	62.62	69.86	7	0	1	65.00	46.89	48.72	2	3	1	3618.85	3619.89	126.60
-9	-2	1	86.17	180.91	54.26	8	0	1	77.04	86.34	10.64	3	3	1	137.38	144.09	19.30
-8	-2	1	287.04	439.42	54.29	9	0	1	106.38	137.38	38.85	4	3	1	14374.46	11029.27	363.23
-7	-2	1	30.85	47.94	68.09	10	0	1	9.72	-8.14	79.44	5	3	1	663.91	632.06	63.55
-6	-2	1	44.24	0.00	60.95	-9	1	1	527.10	442.94	64.22	6	3	1	994.75	822.80	76.05
-5	-2	1	1733.65	1785.46	92.92	-8	1	1	184.68	184.86	51.98	7	3	1	555.39	631.41	61.06
-4	-2	1	1498.24	1596.98	80.46	-7	1	1	348.35	417.66	47.34	8	3	1	13.90	7.28	79.04
-3	-2	1	789.70	917.96	54.91	-6	1	1	644.89	631.32	68.29	9	3	1	84.44	33.86	104.31
-2	-2	1	13079.73	13400.00	418.60	-5	1	1	36.40	39.48	28.68	10	3	1	44.15	35.59	108.81
-1	-2	1	21595.04	22882.35	697.56	-4	1	1	200.59	420.42	36.33	-9	4	1	0.52	-80.43	102.84
0	-2	1	3818.78	4453.01	144.77	-3	1	1	1.71	-9.32	32.52	-8	4	1	426.27	413.77	60.59
1	-2	1	20818.80	21586.49	658.77	-2	1	1	1635.52	1589.73	66.69	-7	4	1	253.70	206.52	47.48
2	-2	1	2912.34	2925.38	105.61	-1	1	1	11191.35	10597.07	327.33	-6	4	1	22.86	59.50	63.72
3	-2	1	9170.58	9080.66	296.00	0	1	1	7939.37	4107.67	129.39*	-5	4	1	9.71	-119.53	58.78
4	-2	1	732.70	864.98	63.00	1	1	1	21907.11	22432.27	701.52	-4	4	1	12.48	27.93	48.57
5	-2	1	2187.33	2232.08	108.95	2	1	1	2635.10	2877.75	100.64	-3	4	1	282.90	510.06	48.61
6	-2	1	100.87	140.52	35.03	3	1	1	111.52	82.06	18.04	-2	4	1	27.56	68.78	14.43
7	-2	1	49.56	64.18	41.81	4	1	1	3590.65	3824.02	143.70	-1	4	1	2051.28	2158.23	86.20
8	-2	1	132.78	152.22	50.66	5	1	1	18.98	-52.37	48.00	0	4	1	2362.98	2259.45	86.12
9	-2	1	85.15	32.67	103.69	6	1	1	772.50	675.90	54.61	1	4	1	981.57	1219.49	55.77
-9	-1	1	179.60	239.35	59.66	7	1	1	139.68	220.30	40.90	2	4	1	9369.55	8997.90	289.89
-8	-1	1	1.11	8.83	47.21	8	1	1	0.62	21.79	57.44	3	4	1	1375.09	1218.39	65.35
-7	-1	1	45.62	24.93	53.91	9	1	1	386.08	181.36	65.57	4	4	1	2681.13	2515.95	109.90
-6	-1	1	23.11	28.16	58.22	10	1	1	0.21	-127.42	109.00	5	4	1	2298.72	2210.18	108.21
-5	-1	1	22.15	87.76	27.87	-9	2	1	0.15	31.35	92.54	6	4	1	187.18	209.88	37.74
-4	-1	1	3682.00	3589.87	139.12	-8	2	1	212.37	203.82	55.26	7	4	1	260.80	317.70	45.28
-3	-1	1	4664.67	4482.77	157.37	-7	2	1	172.85	159.98	46.34	8	4	1	32.87	-6.22	59.79
-2	-1	1	7793.56	8594.85	273.14	-6	2	1	565.86	538.97	54.65	9	4	1	1.72	-80.20	98.77
-1	-1	1	12239.59	11908.33	366.29	-5	2	1	2610.18	2610.36	121.25	10	4	1	168.61	127.37	66.23
0	-1	1	5904.27	5049.77	157.91	-4	2	1	415.44	417.29	37.18	-9	5	1	39.66	148.47	59.23
1	-1	1	2946.78	2973.76	98.26	-3	2	1	6168.47	5862.95	201.14	-8	5	1	80.52	-5.15	99.34
2	-1	1	74831.59	82000.44	2514.46	-2	2	1	3249.48	3372.92	119.62	-7	5	1	162.79	150.89	47.71
3	-1	1	1118.76	1071.18	57.05	-1	2	1	953.29	1913.54	70.42*	-6	5	1	927.22	874.45	68.82
4	-1	1	433.85	563.78	50.23	0	2	1	12540.18	9368.35	291.24	-5	5	1	855.53	821.54	80.10
5	-1	1	0.71	64.87	27.74	1	2	1	21416.12	22689.64	717.61	-4	5	1	4885.31	4393.33	174.06
6	-1	1	744.52	625.53	55.00	2	2	1	3439.86	4133.72	139.78	-3	5	1	727.14	763.43	61.35
7	-1	1	2350.23	2357.90	135.71	3	2	1	2499.62	2343.99	93.94	-2	5	1	14035.31	13168.18	422.71
8	-1	1	73.94	74.96	81.88	4	2	1	221.83	181.89	24.29	-1	5	1	3243.20	3437.34	126.81
9	-1	1	752.72	662.74	68.31	5	2	1	35.93	57.39	27.18	0	5	1	3.86	-10.13	29.27
10	-1	1	235.28	271.71	66.28	6	2	1	2822.41	2639.44	127.45	1	5	1	6.84	-18.47	30.41
-9	0	1	219.61	359.76	42.32	7	2	1	813.80	758.15	64.08	2	5	1	3148.76	2935.01	114.08
-8	0	1	1.57	-42.88	59.05	8	2	1	1708.37	1909.78	128.79	3	5	1	306.46	393.76	34.21
-7	0	1	3471.28	3341.78	115.48	9	2	1	29.18	174.74	55.46	4	5	1	4781.90	4849.03	180.96
-6	0	1	364.58	266.88	38.78	10	2	1	345.33	303.21	68.70	5	5	1	43.64	55.05	56.15
-5	0	1	5348.94	4667.28	127.30	-9	3	1	25.89	-57.05	104.32	6	5	1	668.99	692.06	57.90
-4	0	1	641.60	589.52	36.92	-8	3	1	770.32	841.83	80.78	7	5	1	900.57	485.15	69.86
-3	0	1	46.93	24.90	18.65	-7	3	1	4.59	69.24	41.00	8	5	1	389.03	364.26	52.91
-2	0	1	993.95	858.14	31.24	-6	3	1	6173.26	5846.22	232.24	9	5	1	488.54	530.13	64.97
-1	0	1	27.44	38.72	5.90	-5	3	1	55.83	24.00	38.14	10	5	1	0.32	66.58	98.28

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-8	6	1	9.52	20.14	98.89	-6	9	1	1226.79	1246.09	118.59	1	12	1	85.66	40.62	53.45
-7	6	1	1368.35	1422.84	121.38	-5	9	1	287.22	330.89	48.87	2	12	1	1007.01	1027.76	71.90
-6	6	1	35.05	38.79	48.62	-4	9	1	2595.92	2489.70	136.16	3	12	1	185.50	234.78	47.19
-5	6	1	4753.53	4617.56	195.93	-3	9	1	617.01	589.31	57.66	4	12	1	98.41	139.67	46.56
-4	6	1	14.27	-55.48	58.69	-2	9	1	553.67	511.91	51.30	5	12	1	4.45	-30.49	82.25
-3	6	1	1532.44	1525.03	85.83	-1	9	1	34.65	2.34	52.24	6	12	1	32.64	-31.15	80.15
-2	6	1	2.36	-8.36	43.24	0	9	1	0.13	-194.92	59.72*	7	12	1	89.10	92.28	57.75
-1	6	1	278.96	328.64	29.93	1	9	1	8.46	36.97	50.77	8	12	1	178.60	55.55	122.52
0	6	1	5.47	-30.96	37.41	2	9	1	117.44	105.71	32.35	-5	13	1	46.00	-17.04	104.52
1	6	1	71.93	89.56	21.53	3	9	1	527.60	512.46	49.07	-4	13	1	216.33	318.73	59.60
2	6	1	450.35	431.42	35.23	4	9	1	746.23	876.60	85.02	-3	13	1	1.00	47.61	83.58
3	6	1	2874.01	3281.54	131.03	5	9	1	0.86	24.74	69.41	-2	13	1	25.03	22.29	80.21
4	6	1	1874.25	1919.47	97.44	6	9	1	223.50	293.37	46.82	-1	13	1	607.87	514.76	55.14
5	6	1	2123.35	2140.26	114.86	7	9	1	301.37	254.41	50.57	0	13	1	72.88	79.27	86.54
6	6	1	1056.05	1082.84	90.97	8	9	1	50.12	-60.18	97.85	1	13	1	2491.91	2404.59	142.19
7	6	1	60.89	95.30	41.94	9	9	1	164.82	161.41	63.83	2	13	1	186.96	270.98	50.20
8	6	1	263.17	333.29	51.80	-7	10	1	0.30	-6.37	98.43	3	13	1	2819.13	2650.51	152.94
9	6	1	78.57	28.49	98.23	-6	10	1	91.18	3.36	64.95	4	13	1	77.97	-19.19	88.61
-8	7	1	3.64	21.08	98.84	-5	10	1	299.81	443.48	53.22	5	13	1	214.56	174.73	53.38
-7	7	1	427.28	345.59	55.62	-4	10	1	0.69	73.55	74.14	6	13	1	56.50	128.40	54.85
-6	7	1	267.84	309.87	48.07	-3	10	1	1030.53	1181.85	98.10	7	13	1	57.91	-12.88	110.32
-5	7	1	185.38	163.55	42.83	-2	10	1	55.80	127.94	37.79	-8	14	1	5.96	-45.09	105.19
-4	7	1	1970.33	2077.82	112.57	-1	10	1	228.67	151.86	37.12	-4	14	1	0.77	-121.58	100.52
-3	7	1	297.18	321.29	34.79	0	10	1	2912.74	2953.22	140.44	-3	14	1	600.76	680.59	65.82
-2	7	1	81.99	82.82	26.28	1	10	1	1456.36	1668.78	101.66	-2	14	1	525.61	663.12	62.88
-1	7	1	827.42	828.68	60.76	2	10	1	7537.98	7782.08	281.24	-1	14	1	275.71	339.47	53.94
0	7	1	48.88	64.44	26.10	3	10	1	45.17	31.93	44.32	0	14	1	663.41	81.78	78.73
1	7	1	12300.72	12503.54	404.67	4	10	1	448.51	562.43	56.76	1	14	1	56.16	73.96	88.52
2	7	1	8.61	3.06	40.47	5	10	1	309.67	212.44	46.74	2	14	1	164.70	165.53	53.92
3	7	1	3877.88	3686.44	147.08	6	10	1	26.52	-70.20	87.32	3	14	1	0.63	-21.03	90.97
4	7	1	1804.91	1690.24	96.58	7	10	1	13.33	41.05	50.29	4	14	1	20.10	-64.23	94.01
5	7	1	22.99	-20.92	62.09	8	10	1	19.02	39.38	94.59	5	14	1	93.38	143.30	55.70
6	7	1	1444.74	1242.88	105.65	-7	11	1	56.81	211.50	61.79	6	14	1	5.20	-44.77	95.38
7	7	1	192.98	171.94	46.92	-6	11	1	102.38	79.65	56.98	-4	15	1	176.94	166.96	66.35
8	7	1	19.35	45.85	52.56	-5	11	1	120.14	41.76	88.53	-3	15	1	65.95	63.80	101.65
9	7	1	14.96	68.15	106.78	-4	11	1	316.77	374.38	52.25	-2	15	1	1.16	-101.79	98.44
-8	8	1	2.26	-160.92	107.26	-3	11	1	179.08	219.49	47.24	-1	15	1	162.69	231.00	54.35
-7	8	1	22.72	53.47	63.00	-2	11	1	2281.41	2232.56	133.49	0	15	1	32.51	-61.59	99.95
-6	8	1	35.93	69.48	83.11	-1	11	1	1745.11	2139.58	122.87	1	15	1	5.73	60.70	88.18
-5	8	1	294.62	314.38	46.83	0	11	1	186.01	11.70	82.05	2	15	1	28.29	-40.37	95.03
-4	8	1	374.01	433.30	44.22	1	11	1	1155.59	1032.52	95.00	3	15	1	133.47	24.17	96.82
-3	8	1	5617.62	5334.85	206.90	2	11	1	514.31	533.29	47.63	4	15	1	61.02	174.72	55.42
-2	8	1	176.06	398.12	37.12	3	11	1	25.45	39.69	40.34	5	15	1	84.14	64.23	70.72
-1	8	1	1672.39	1572.33	87.59	4	11	1	5.04	39.73	71.33	6	15	1	198.35	295.42	63.79
0	8	1	1478.29	1568.76	91.71	5	11	1	103.60	129.94	46.85	-2	16	1	36.62	-23.08	108.08
1	8	1	83.54	8.84	49.23	6	11	1	376.91	343.73	57.22	-1	16	1	98.35	34.04	104.20
2	8	1	823.63	878.06	69.53	7	11	1	183.07	228.40	54.96	0	16	1	279.98	207.11	68.35
3	8	1	1701.62	1619.94	93.43	8	11	1	163.91	345.22	65.31	1	16	1	123.91	245.95	64.00
4	8	1	41.26	95.05	32.97	-6	12	1	319.07	315.20	65.21	2	16	1	699.11	744.25	68.60
5	8	1	1.09	-1.30	61.88	-5	12	1	670.94	625.15	66.51	3	16	1	85.65	186.69	51.66
6	8	1	211.44	199.88	44.90	-4	12	1	384.19	372.63	57.70	4	16	1	308.82	329.91	64.00
7	8	1	404.87	364.51	52.96	-3	12	1	604.08	549.60	58.73	5	16	1	15.79	-100.20	136.91
8	8	1	709.39	836.55	81.28	-2	12	1	201.78	229.97	46.76	-1	17	1	42.79	105.94	107.59
9	8	1	179.29	131.35	61.47	-1	12	1	222.67	185.58	46.71	0	17	1	147.17	-91.94	125.66
-7	9	1	34.14	85.27	90.11	0	12	1	128.21	108.95	44.68	1	17	1	173.75	-93.46	118.16

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
2	17	1	3.17	24.86	103.27	1	-18	2	1412.04	1398.97	112.59	-9	-8	2	0.10	1.70	108.62
3	17	1	27.12	-53.41	110.90	2	-12	2	777.74	924.83	96.16	-8	-8	2	0.03	43.19	95.84
-2	-17	2	106.65	149.26	65.23	3	-12	2	475.62	408.93	55.00	-7	-8	2	80.66	64.69	50.31
-1	-17	2	1.31	-72.84	115.10	4	-12	2	55.69	83.14	90.08	-6	-8	2	390.74	309.00	49.25
0	-17	2	260.29	221.85	72.85	5	-12	2	30.96	69.66	94.58	-5	-8	2	217.60	266.37	42.28
-4	-16	2	80.09	123.32	64.15	6	-12	2	168.77	209.57	59.84	-4	-8	2	359.99	377.80	40.22
-3	-16	2	30.08	86.63	100.45	-8	-11	2	3.61	57.22	106.50	-3	-8	2	84.85	96.54	33.63
-2	-16	2	4.52	73.87	73.91	-7	-11	2	4.79	-146.02	100.51	-2	-8	2	460.10	450.08	44.15
-1	-16	2	156.45	194.54	58.45	-6	-11	2	33.28	66.37	50.83	-1	-8	2	3324.81	3146.19	735.34
0	-16	2	0.61	-7.19	103.07	-5	-11	2	27.76	-94.10	85.32	0	-8	2	473.19	424.77	43.79
1	-16	2	279.57	294.23	67.50	-4	-11	2	21.08	-168.62	81.43	1	-8	2	8619.98	8552.22	295.94
2	-16	2	203.62	164.40	64.46	-3	-11	2	182.51	159.11	42.63	2	-8	2	1343.02	1065.89	81.08
-5	-15	2	6.36	20.24	107.27	-2	-11	2	1665.55	1823.24	1.349	3	-8	2	180.15	170.32	36.25
-4	-15	2	174.67	187.38	58.01	-1	-11	2	185.67	165.13	42.51	4	-8	2	1603.76	1551.36	107.91
-3	-15	2	28.96	49.43	55.30	0	-11	2	1986.28	4290.63	195.04	5	-8	2	404.52	398.65	46.48
-2	-15	2	1101.72	1092.47	94.50	1	-11	2	255.71	371.35	44.98	6	-8	2	1089.14	1111.71	106.86
-1	-15	2	235.77	335.89	59.28	2	-11	2	382.42	397.00	48.43	7	-8	2	224.16	187.10	57.85
0	-15	2	647.16	735.08	69.89	3	-11	2	621.14	642.46	65.50	8	-8	2	211.38	224.83	62.94
1	-15	2	338.60	344.27	62.85	4	-11	2	0.42	9.08	82.40	-9	-7	2	24.34	14.29	103.92
2	-15	2	12.47	-113.37	102.44	5	-11	2	385.08	389.86	57.52	-8	-7	2	1491.49	1541.85	135.24
3	-15	2	2.89	63.47	97.04	6	-11	2	21.89	-14.12	98.88	-7	-7	2	251.63	235.78	49.95
4	-15	2	63.70	57.61	110.17	7	-11	2	155.69	157.56	64.26	-6	-7	2	653.55	687.51	66.16
-6	-14	2	80.03	94.29	109.01	-8	-10	2	37.80	58.31	59.37	-5	-7	2	1476.56	1322.83	96.16
-5	-14	2	0.31	59.66	94.40	-7	-10	2	885.29	746.22	68.78	-4	-7	2	11.54	40.46	32.46
-4	-14	2	181.19	213.15	54.30	-6	-10	2	618.88	641.03	60.29	-3	-7	2	199.23	207.15	31.03
-3	-14	2	396.64	445.71	58.09	-5	-10	2	110.08	60.89	78.88	-2	-7	2	903.26	884.59	68.76
-2	-14	2	2.43	-75.01	89.92	-4	-10	2	239.71	242.61	42.19	-1	-7	2	526.30	460.98	39.94
-1	-14	2	1228.13	1384.25	123.24	-3	-10	2	1330.91	1323.58	100.32	0	-7	2	1571.84	1757.35	93.43
0	-14	2	15.49	79.83	87.13	-2	-10	2	1378.27	1429.29	98.32	1	-7	2	61.00	121.42	27.31
1	-14	2	422.71	460.17	62.09	-1	-10	2	422.79	600.95	52.19	2	-7	2	5048.32	5068.83	189.78
2	-14	2	204.15	209.52	54.10	0	-10	2	93.30	-67.01	78.74	3	-7	2	2026.98	2220.45	130.47
3	-14	2	72.62	-22.43	98.00	1	-10	2	2211.96	2375.96	124.54	4	-7	2	33.68	-53.00	59.91
4	-14	2	46.43	13.88	73.61	2	-10	2	1153.55	1308.81	96.76	5	-7	2	2818.18	3248.83	155.41
5	-14	2	6.33	-99.29	109.10	3	-10	2	10.15	107.55	39.25	6	-7	2	1.05	-7.26	74.41
-7	-13	2	160.38	156.29	65.36	4	-10	2	2566.38	2957.39	157.06	7	-7	2	1318.77	1414.07	122.77
-6	-13	2	101.54	156.50	59.92	5	-10	2	835.32	754.03	73.73	8	-7	2	13.02	87.00	89.56
-5	-13	2	264.89	269.54	58.93	6	-10	2	606.65	743.21	77.50	-9	-6	2	403.38	419.19	64.15
-4	-13	2	19.58	-4.59	89.65	7	-10	2	339.16	304.38	63.12	-8	-6	2	242.91	249.26	54.55
-3	-13	2	197.90	211.19	52.22	-8	-9	2	346.87	414.04	63.71	-7	-6	2	87.19	76.74	81.17
-2	-13	2	0.81	40.54	46.49	-7	-9	2	311.71	256.67	56.58	-6	-6	2	79.51	90.20	41.32
-1	-13	2	49.47	10.99	85.77	-6	-9	2	52.59	103.36	48.32	-5	-6	2	0.15	12.72	60.88
0	-13	2	40.05	182.41	45.86	-5	-9	2	250.46	314.92	45.81	-4	-6	2	3625.91	3371.99	143.82
1	-13	2	61.30	124.17	46.72	-4	-9	2	1003.35	892.12	87.69	-3	-6	2	87.42	94.08	27.73
2	-13	2	395.91	562.86	57.09	-3	-9	2	706.64	811.13	75.39	-2	-6	2	14589.82	15758.59	502.98
3	-13	2	345.31	370.17	56.90	-2	-9	2	1574.24	1615.06	95.18	-1	-6	2	10458.30	11007.51	358.95
4	-13	2	11.98	-68.87	98.13	-1	-9	2	217.76	249.55	35.14	0	-6	2	119.30	113.12	25.09
5	-13	2	491.99	503.24	66.86	0	-9	2	4781.41	4663.13	191.05	1	-6	2	4338.07	5005.64	179.05
-7	-12	2	7.54	76.28	105.11	1	-9	2	1204.93	1230.86	84.92	2	-6	2	724.45	644.86	56.46
-6	-12	2	0.24	78.71	94.60	2	-9	2	993.16	833.44	75.33	3	-6	2	4907.46	5546.41	303.86
-5	-12	2	70.69	103.33	50.72	3	-9	2	263.41	244.11	39.43	4	-6	2	784.75	745.19	70.78
-4	-12	2	365.34	443.51	52.09	4	-9	2	465.07	48.29	47.35	5	-6	2	213.29	175.68	40.95
-3	-12	2	651.54	661.25	57.52	5	-9	2	670.95	625.70	56.39	6	-6	2	925.84	922.25	95.18
-2	-12	2	283.22	322.59	47.47	6	-9	2	62.53	91.30	91.59	7	-6	2	16.56	8.61	86.72
-1	-12	2	1375.97	1297.30	110.85	7	-9	2	139.98	274.71	57.57	8	-6	2	104.47	131.76	55.55
0	-12	2	39.39	-70.18	94.73	8	-9	2	197.80	212.26	68.84	9	-6	2	37.59	37.51	106.20

Structure Factors Table (continued) (*unobserved reflns.) for C(14) N(10) Cl(2) Cu(1) N(4) O(9)

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-9	-5	2	27.24	50.08	100.73	8	-3	2	12.53	2.95	88.55	5	0	2	486.93	546.61	31.53
-8	-5	2	283.19	163.04	52.87	9	-3	2	9.02	-262.12	108.91	4	0	2	51.34	64.60	22.62
-7	-5	2	374.07	443.60	52.56	-9	-2	2	63.86	132.28	56.85	7	0	2	1.28	42.56	103.30
-6	-5	2	1510.09	1416.78	108.99	-8	-2	2	3.80	44.08	49.14	8	0	2	39.37	58.72	73.06
-5	-5	2	897.42	817.02	80.20	-7	-2	2	38.35	-155.49	79.80	9	0	2	165.08	229.15	40.49
-4	-5	2	1581.42	1570.34	88.27	-6	-2	2	185.33	118.75	40.26	10	0	2	82.54	91.57	52.19
-3	-5	2	3926.75	3680.17	143.44	-5	-2	2	1472.06	1411.86	87.87	-3	1	2	94.12	84.22	52.55
-2	-5	2	103.55	109.10	22.29	-4	-2	2	2638.65	2239.34	101.27	-8	1	2	145.69	127.33	45.30
-1	-5	2	1182.45	1076.63	59.95	-3	-2	2	50.82	98.14	208.17	-8	1	2	34.77	44.58	59.69
0	-5	2	6639.92	6662.61	226.91	-2	-2	2	6357.08	6313.75	54.68	-5	1	2	35.11	91.70	30.74
1	-5	2	203.66	168.72	22.25	-1	-2	2	1298.98	1300.02	152.15	-4	1	2	6915.96	7381.63	254.03
2	-5	2	2596.41	2106.42	92.03	0	-2	3	3675.75	4651.65	903.88	-3	1	2	10180.83	10163.97	329.68
3	-5	2	384.60	256.82	27.99	1	-2	2	28089.76	29715.52	22.52	-2	1	2	1236.52	1210.69	27.34
4	-5	2	969.51	1119.59	76.57	2	-2	2	323.33	262.95	22.72	-1	1	2	14909.94	15757.43	484.41
5	-5	2	2642.97	2441.52	124.20	3	-2	2	5.63	-5.20	36.32	0	1	2	7522.61	7093.27	222.33
6	-5	2	252.62	271.70	43.98	4	-2	2	482.98	450.50	114.84	1	1	2	1121.82	1148.24	45.50
7	-5	2	952.55	907.09	74.40	5	-2	2	2316.49	2354.15	86.27	2	1	2	187.30	1143.33	51.50
8	-5	2	94.92	81.61	95.21	6	-2	2	1105.13	1056.12	107.58	3	1	2	2727.55	2664.17	102.70
9	-5	2	226.97	239.10	62.07	7	-2	2	1292.32	1461.54	80.26	4	1	2	1386.37	1163.80	68.63
-9	-4	2	681.17	632.39	66.99	8	-2	2	939.40	965.00	57.52	5	1	2	3397.53	3152.90	135.70
-8	-4	2	47.21	-53.10	86.21	9	-2	2	184.00	143.20	62.06	6	1	2	1662.22	1595.83	99.61
-7	-4	2	1839.76	1922.48	130.07	-9	-1	2	372.87	302.58	125.88	7	1	2	1696.37	1874.19	109.90
-6	-4	2	1254.48	1157.26	91.95	-8	-1	2	1345.57	1472.08	41.49	8	1	2	180.46	194.81	46.48
-5	-4	2	84.95	-6.04	55.51	-7	-1	2	0.19	60.91	96.18	9	1	2	333.71	336.44	58.50
-4	-4	2	724.08	597.74	61.61	-6	-1	2	1261.81	1298.40	46.93	10	1	2	180.19	150.93	61.89
-3	-4	2	165.58	236.96	24.59	-5	-1	2	746.90	518.73	53.00	-9	2	2	122.44	59.27	105.78
-2	-4	2	4299.14	4577.09	161.44	-4	-1	2	485.93	535.43	62.34	-8	2	2	971.58	894.90	80.17
-1	-4	2	62.70	79.80	16.93	-3	-1	2	1383.09	1144.80	16.98	-7	2	2	736.69	717.17	65.50
0	-4	2	22954.95	26268.94	809.48	-2	-1	2	179.14	138.93	743.45	-6	2	2	1.03	-65.61	64.68
1	-4	2	13556.89	14221.10	446.22	-1	-1	2	22050.20	24402.95	80.79	-5	2	2	15.39	59.74	29.22
2	-4	2	494.89	447.95	42.00	0	-1	2	2003.44	2347.01	469.22	-4	2	2	328.96	278.65	29.88
3	-4	2	8018.53	8112.90	272.97	1	-1	2	14312.21	15309.85	13.79	-3	2	2	4083.51	4128.45	150.54
4	-4	2	6942.44	6661.44	236.22	2	-1	2	20.41	50.14	104.60	-2	2	2	136.91	104.33	18.21
5	-4	2	19.81	45.51	52.75	3	-1	2	2945.44	2705.01	108.80	-1	2	2	3855.59	4722.09	156.03
6	-4	2	2905.31	2842.72	142.78	4	-1	2	2226.01	2577.88	333.02	0	2	2	17593.56	15981.57	491.89
7	-4	2	54.16	81.98	43.60	5	-1	2	10876.10	9819.53	33.09	1	2	2	10779.00	12496.34	385.95
8	-4	2	168.96	328.42	54.63	6	-1	2	25.62	78.27	143.69	2	2	2	1039.41	1103.58	51.37
9	-4	2	188.06	187.39	57.70	7	-1	2	2533.93	2824.41	47.32	3	2	2	3957.79	3314.46	122.27
-9	-3	2	3.50	-26.98	99.19	8	-1	2	65.06	109.60	65.23	4	2	2	4151.07	4068.26	161.68
-8	-3	2	16.97	-31.28	85.93	9	-1	2	22.07	50.16	64.61	5	2	2	530.32	474.14	43.34
-7	-3	2	0.24	15.15	79.21	10	-1	2	349.75	356.76	41.85	6	2	2	4220.53	3827.46	164.68
-6	-3	2	1498.55	1411.68	99.45	-9	0	2	171.81	233.24	79.84	7	2	2	5.13	-56.18	70.88
-5	-3	2	3.52	-7.78	49.38	-8	0	2	0.30	-27.02	83.73	8	2	2	108.86	211.70	48.73
-4	-3	2	133.65	90.45	25.27	-7	0	2	1625.81	1677.04	25.26	9	2	2	30.69	9.39	53.06
-3	-3	2	2167.26	1879.05	85.81	-6	0	2	143.11	138.10	59.74	10	2	2	49.68	73.02	59.80
-2	-3	2	154.61	118.78	18.99	-5	0	2	1392.78	1335.42	41.25	-9	3	2	79.40	-26.69	106.75
-1	-3	2	3954.16	3540.57	123.56	-4	0	2	782.54	629.81	19.31	-8	3	2	380.79	272.10	57.42
0	-3	2	15139.01	13455.12	420.76	-3	0	2	2.23	-1.54	393.86	-7	3	2	106.26	151.20	45.02
1	-3	2	2245.41	1884.30	74.89	-2	0	2	17354.32	18007.81	128.15	-6	3	2	980.26	1163.23	94.27
2	-3	2	942.32	1063.23	55.33	-1	0	2	5535.70	5565.04	590.67	-5	3	2	1034.22	1005.49	80.76
3	-3	2	3712.80	4036.73	148.69	0	0	2	25326.56	26803.02	6.29	-4	3	2	225.10	184.46	28.84
4	-3	2	897.34	762.32	62.68	1	0	2	112.88	41.60	272.44	-3	3	2	9301.80	9339.87	308.04
5	-3	2	48.49	45.53	30.26	2	0	2	12417.18	12365.35	21.36	-2	3	2	7778.83	8261.26	269.94
6	-3	2	299.59	345.37	41.60	3	0	2	19.18	11.56	45.24	-1	3	2	8540.93	9131.53	250.76
7	-3	2	34.35	8.81	68.38	4	0	2	472.81	566.35							

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
0	3	2	32023.83	20973.48	645.43*	-4	6	2	1321.61	1195.16	86.85	-2	9	2	1658.43	1780.23	102.24
1	3	2	170.54	104.06	14.46	-3	6	2	5.72	33.61	46.99	-1	9	2	11.03	30.09	29.26
2	3	2	19530.81	20950.10	645.96	-2	6	2	641.07	667.91	57.75	0	9	2	22.32	41.69	48.75
3	3	2	340.88	511.83	40.76	-1	6	2	11.74	38.37	21.53	1	9	2	2241.75	2041.42	108.11
4	3	2	161.12	173.31	24.57	0	6	2	2251.84	2164.99	96.64	2	9	2	731.03	803.46	70.34
5	3	2	85.05	134.95	29.40	1	6	2	302.28	490.83	46.85	3	9	2	170.66	128.24	84.42
6	3	2	136.21	57.90	35.48	2	6	2	11.47	-67.45	39.54	4	9	2	2458.80	2436.91	128.44
7	3	2	1.54	108.70	38.47	3	6	2	1291.58	1284.40	73.85	5	9	2	165.76	161.24	42.10
8	3	2	11.24	72.78	46.80	4	6	2	609.51	622.60	58.97	6	9	2	546.30	476.43	51.57
9	3	2	75.70	31.57	100.86	5	6	2	1305.14	1224.66	87.20	7	9	2	0.88	148.03	85.71
10	3	2	139.11	244.90	63.67	6	6	2	1277.55	1066.93	94.04	8	9	2	19.74	-14.05	92.42
-9	4	2	137.46	178.51	62.14	7	6	2	0.53	-106.81	72.02	9	9	2	77.33	82.08	104.86
-8	4	2	253.02	227.96	55.55	8	6	2	46.49	-18.78	90.09	-7	10	2	33.72	-144.09	106.01
-7	4	2	6.78	68.93	44.24	9	6	2	29.74	112.45	56.60	-6	10	2	103.25	100.69	53.97
-6	4	2	61.68	32.39	46.21	-8	7	2	21.96	52.28	104.21	-5	10	2	1488.10	1549.70	125.20
-5	4	2	3054.62	2822.06	135.07	-7	7	2	35.34	70.68	81.69	-4	10	2	23.67	-106.52	79.83
-4	4	2	1672.01	1775.68	96.58	-6	7	2	1566.42	1361.42	116.25	-3	10	2	3255.46	3166.21	158.26
-3	4	2	6.91	22.50	37.28	-5	7	2	1247.03	1319.25	102.04	-2	10	2	1683.74	1677.72	107.91
-2	4	2	10589.34	10146.46	329.25	-4	7	2	1237.35	1204.15	94.72	-1	10	2	37.41	-32.26	62.93
-1	4	2	1977.22	4330.71	150.95	-3	7	2	2135.12	2106.01	108.23	0	10	2	2177.43	2197.19	119.32
0	4	2	29335.38	31829.45	975.06	-2	7	2	110.10	32.62	45.88	1	10	2	12.87	57.54	32.82
1	4	2	26.85	18.95	27.66	-1	7	2	9531.63	8810.10	296.57	2	10	2	26.58	30.74	59.30
2	4	2	210.17	174.43	19.95	0	7	2	142.45	189.01	25.19	3	10	2	293.41	255.39	38.83
3	4	2	3.36	13.04	34.15	1	7	2	149.50	168.36	24.90	4	10	2	2333.84	2303.76	129.79
4	4	2	170.09	144.44	26.63	2	7	2	338.74	357.08	35.63	5	10	2	2444.04	2388.15	135.98
5	4	2	1657.62	1735.41	91.85	3	7	2	407.06	408.30	39.44	6	10	2	100.86	36.11	87.39
6	4	2	44.16	-28.85	58.86	4	7	2	3044.85	2943.37	129.97	7	10	2	195.52	297.85	53.40
7	4	2	70.38	159.98	41.14	5	7	2	550.34	571.19	49.95	8	10	2	339.18	272.04	62.41
8	4	2	154.49	281.39	49.01	6	7	2	1858.44	2109.00	125.63	-6	11	2	40.31	65.50	91.88
9	4	2	292.93	314.61	58.59	7	7	2	20.17	9.27	72.26	-5	11	2	71.59	-77.98	91.22
10	4	2	208.70	233.08	64.89	8	7	2	46.34	29.24	91.42	-4	11	2	19.99	22.53	46.61
-9	5	2	501.92	538.98	70.00	9	7	2	111.58	29.91	104.85	-3	11	2	843.76	752.78	66.16
-8	5	2	145.97	227.86	53.68	-8	8	2	315.64	346.58	65.05	-2	11	2	35.23	-33.45	74.55
-7	5	2	200.37	253.31	51.34	-7	8	2	6.26	62.45	91.29	-1	11	2	1107.16	1181.66	91.39
-6	5	2	114.67	97.24	42.68	-6	8	2	7.79	-159.71	90.81	0	11	2	404.11	563.10	57.07
-5	5	2	1239.13	1146.40	92.20	-5	8	2	80.98	4.40	75.12	1	11	2	493.87	587.25	57.76
-4	5	2	46.52	77.81	29.34	-4	9	2	1064.53	891.68	89.52	2	11	2	1659.72	1749.07	108.68
-3	5	2	5098.39	4852.12	181.27	-3	9	2	489.05	558.04	49.68	3	11	2	975.21	976.18	89.37
-2	5	2	5967.86	6628.99	227.68	-2	9	2	3225.89	3385.01	142.77	4	11	2	3775.75	3311.87	167.52
-1	5	2	1364.16	1728.92	77.89	-1	9	2	58.55	103.78	28.00	5	11	2	65.18	-1.48	85.05
0	5	2	3342.50	2791.49	110.95	0	9	2	68.72	6.60	47.81	6	11	2	271.65	278.41	51.66
1	5	2	3193.70	2877.64	109.66	1	9	2	4932.00	4509.17	171.58	7	11	2	2.10	41.85	94.42
2	5	2	5994.60	6215.10	210.84	2	9	2	7212.94	7240.94	135.31	8	11	2	0.27	-133.01	103.63
3	5	2	1150.98	1025.20	62.41	3	9	2	3001.46	2835.03	128.22	-6	12	2	6.94	-24.32	104.20
4	5	2	2834.62	3048.03	127.18	4	9	2	10.18	32.23	49.94	-5	12	2	42.57	-31.40	91.99
5	5	2	3855.95	3709.74	154.49	5	9	2	2194.30	2185.75	124.03	-4	12	2	0.10	-48.28	89.61
6	5	2	324.24	324.31	38.55	6	9	2	133.68	154.30	42.07	-3	12	2	184.18	211.59	47.61
7	5	2	307.02	182.50	45.15	7	9	2	184.80	205.12	47.31	-2	12	2	15.58	38.97	74.19
8	5	2	1.74	16.21	78.97	8	9	2	19.08	-13.76	89.98	-1	12	2	269.99	313.26	46.41
9	5	2	46.60	39.40	68.27	9	9	2	0.36	-38.21	100.72	0	12	2	617.96	645.62	62.29
10	5	2	0.23	84.90	99.70	-7	9	2	28.61	-103.71	99.17	1	12	2	610.65	578.53	49.51
-8	6	2	62.14	75.58	90.35	-6	9	2	6.09	10.51	46.96	2	12	2	456.04	459.43	48.42
-7	6	2	30.40	-13.03	85.17	-5	9	2	19.15	52.16	44.89	3	12	2	1311.94	1397.30	110.16
-6	6	2	8.32	44.55	42.39	-4	9	2	2.52	80.77	38.44	4	12	2	0.49	-25.06	79.18
-5	6	2	1.55	-19.37	63.08	-3	9	2	50.55	-4.70	60.77	5	12	2	499.52	560.02	58.22

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
6	12	2	0.17	-182.56	93.69	-4	-16	3	126.32	229.81	64.34	-7	-11	3	193.41	294.10	60.10
7	12	2	4.34	-54.24	97.53	-3	-16	3	329.10	328.99	66.07	-6	-11	3	36.05	20.12	97.66
8	12	2	37.89	134.37	62.57	-2	-16	3	73.43	100.02	102.57	-5	-11	3	225.86	222.36	53.36
-5	13	2	98.35	22.01	71.54	-1	-16	3	185.91	267.28	62.83	-4	-11	3	412.41	405.90	50.52
-4	13	2	1455.48	1411.65	130.02	0	-16	3	358.38	317.84	68.84	-3	-11	3	487.41	487.14	49.82
-3	13	2	101.38	89.10	89.89	1	-16	3	10.77	64.46	111.01	-2	-11	3	11.40	-98.39	70.96
-2	13	2	394.73	360.31	51.54	2	-16	3	84.24	149.40	63.47	-1	-11	3	588.38	598.44	51.17
-1	13	2	640.29	608.35	56.68	-5	-15	3	120.78	89.27	62.68	0	-11	3	968.25	1151.67	107.35
0	13	2	467.89	684.61	69.12	-4	-15	3	214.27	189.21	62.33	1	-11	3	2347.77	2542.10	139.90
1	13	2	356.92	445.93	51.10	-3	-15	3	143.97	57.95	107.21	2	-11	3	688.15	828.60	69.21
2	13	2	3.95	-83.88	83.24	-2	-15	3	115.77	130.58	56.52	3	-11	3	1814.82	1863.93	187.50
3	13	2	182.30	211.37	50.32	-1	-15	3	46.30	75.60	102.53	4	-11	3	19.36	3.01	80.47
4	13	2	758.43	808.62	73.82	0	-15	3	5.21	108.59	51.83	5	-11	3	270.62	379.85	56.06
5	13	2	50.92	-28.62	92.13	1	-15	3	61.95	4.58	97.91	6	-11	3	76.75	-16.66	101.17
6	13	2	122.57	78.60	99.31	2	-15	3	8.20	-137.92	105.15	7	-11	3	27.99	62.16	75.02
7	13	2	141.67	19.82	101.92	3	-15	3	193.88	231.37	59.33	-8	-10	3	8.48	-25.10	59.19
-4	14	2	3.94	60.72	98.48	4	-15	3	14.11	-158.16	121.79	-7	-10	3	20.86	-23.77	99.88
-3	14	2	109.02	192.56	55.26	-6	-14	3	120.27	222.40	63.02	-6	-10	3	346.94	283.00	54.57
-2	14	2	0.02	-126.02	88.90	-5	-14	3	61.30	146.40	58.15	-5	-10	3	5.37	-38.30	78.50
-1	14	2	402.33	336.81	55.97	-4	-14	3	0.09	49.07	54.00	-4	-10	3	515.26	523.00	51.44
0	14	2	6.12	-86.50	97.13	-3	-14	3	0.64	-39.85	92.39	-3	-10	3	34.82	-8.02	72.74
1	14	2	867.81	1087.31	109.13	-2	-14	3	2.19	33.95	62.69	-2	-10	3	248.01	393.07	42.10
2	14	2	151.90	219.59	52.19	-1	-14	3	33.56	36.18	94.64	-1	-10	3	662.44	656.61	95.25
3	14	2	421.63	517.00	58.38	0	-14	3	119.27	197.70	53.94	0	-10	3	1178.96	1040.92	96.25
4	14	2	109.14	214.85	54.32	1	-14	3	130.36	199.62	56.44	1	-10	3	152.40	147.99	37.07
5	14	2	130.02	114.59	56.23	2	-14	3	1553.13	1522.73	135.67	2	-10	3	1466.26	1216.57	98.15
6	14	2	48.06	10.16	163.67	3	-14	3	45.48	-17.13	96.08	3	-10	3	1.00	-91.69	71.29
7	14	2	77.05	137.68	61.82	4	-14	3	854.54	806.40	73.14	4	-10	3	21.60	55.50	74.61
-4	15	2	10.96	-143.28	113.04	5	-14	3	0.58	50.44	107.66	5	-10	3	12.91	-105.76	89.49
-3	15	2	8.03	-16.75	103.70	-6	-13	3	1.13	6.41	101.16	6	-10	3	13.06	-1.28	91.38
-2	15	2	275.49	295.71	60.84	-5	-13	3	737.96	702.59	68.23	7	-10	3	633.98	481.18	70.36
-1	15	2	21.24	71.61	54.21	-4	-13	3	214.43	240.07	55.95	-8	-9	3	1.30	-122.20	103.89
0	15	2	88.46	151.22	54.89	-3	-13	3	80.96	22.94	88.28	-7	-9	3	153.60	218.66	54.81
1	15	2	362.50	300.00	58.37	-2	-13	3	729.11	671.00	60.01	-6	-9	3	1.95	64.09	46.69
2	15	2	72.27	8.96	98.32	-1	-13	3	409.92	432.90	56.72	-5	-9	3	1052.90	991.83	100.22
3	15	2	538.48	540.27	64.70	0	-13	3	276.62	183.85	51.16	-4	-9	3	785.30	911.18	87.83
4	15	2	425.62	480.84	60.89	1	-13	3	736.74	820.29	76.50	-3	-9	3	1367.06	1493.95	100.32
5	15	2	123.27	69.83	103.85	2	-13	3	240.39	314.27	51.41	-2	-9	3	447.55	513.16	42.42
6	15	2	37.65	186.02	59.88	3	-13	3	3.70	-46.50	86.49	-1	-9	3	939.18	904.09	78.47
-2	16	2	0.31	-172.34	101.50	4	-13	3	0.00	18.12	87.41	0	-9	3	591.37	608.90	53.14
-1	16	2	124.28	92.21	59.13	5	-13	3	18.49	112.15	57.51	1	-9	3	281.30	266.25	37.68
0	16	2	170.30	84.98	105.50	-7	-12	3	3.44	9.18	99.51	2	-9	3	5.67	37.79	32.96
1	16	2	59.04	78.85	57.09	-6	-12	3	367.16	454.83	61.65	3	-9	3	50.64	131.03	37.77
2	16	2	0.49	-13.05	94.97	-5	-12	3	52.88	-36.17	91.01	4	-9	3	115.70	138.38	40.36
3	16	2	14.59	68.53	100.27	-4	-12	3	554.59	730.93	71.30	5	-9	3	104.84	22.49	44.16
4	16	2	86.35	63.61	75.05	-3	-12	3	115.07	175.85	47.79	6	-9	3	404.59	507.11	50.32
5	16	2	163.76	211.66	64.42	-2	-12	3	290.76	246.97	49.35	7	-9	3	294.16	329.47	57.70
-1	17	2	30.17	5.93	116.86	-1	-12	3	29.57	-40.23	74.68	8	-9	3	377.69	431.42	71.10
0	17	2	21.53	9.23	114.11	0	-12	3	84.08	75.49	46.12	-8	-8	3	304.95	281.80	63.29
1	17	2	207.08	221.84	62.79	1	-12	3	162.19	112.94	45.67	-7	-8	3	323.73	405.55	55.70
2	17	2	52.64	56.71	110.02	2	-12	3	13.77	-52.82	74.54	-6	-8	3	2111.25	1966.80	123.86
3	17	2	293.36	242.93	52.91	3	-12	3	21.88	88.48	60.03	-5	-8	3	421.34	520.87	47.56
-2	-17	3	27.25	125.46	54.00	4	-12	3	12.19	17.25	81.81	-4	-8	3	68.17	35.78	64.58
-1	-17	3	37.77	33.60	109.62	5	-12	3	91.48	76.06	104.97	-3	-8	3	155.47	136.14	33.42
0	-17	3	44.63	15.99	116.01	6	-12	3	47.32	-8.98	105.48	-2	-8	3	1261.20	1493.70	88.85

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-1	-8	3	1347.57	1329.00	86.66	-1	-5	3	31.31	69.09	20.76	-3	-2	3	395.31	519.98	47.51
0	-8	3	299.46	367.91	35.56	0	-5	3	6127.55	6425.54	221.73	-2	-2	3	213.19	214.32	20.81
1	-8	3	356.15	397.49	37.30	1	-5	3	51.86	56.70	20.16	-1	-2	3	367.15	818.88	44.37
2	-8	3	4426.72	4727.47	185.81	2	-5	3	1900.10	2079.22	93.82	0	-2	3	1565.99	1308.71	58.10
3	-8	3	199.42	219.40	35.40	3	-5	3	7515.01	7473.84	258.54	1	-2	3	24269.13	25327.79	774.52
4	-8	3	2088.79	2415.81	130.99	4	-5	3	18.53	21.77	34.68	2	-2	3	4617.94	4989.59	168.82
5	-8	3	16.13	-45.94	71.33	5	-5	3	222.53	262.20	35.42	3	-2	3	5560.91	5708.65	196.34
6	-8	3	30.23	-24.29	79.98	6	-5	3	205.95	288.47	42.55	4	-2	3	4669.86	4915.43	180.79
7	-8	3	8.10	66.73	81.19	7	-5	3	346.54	274.47	50.83	5	-2	3	229.41	200.78	30.96
8	-8	3	47.58	74.21	62.17	8	-5	3	69.38	72.19	89.33	6	-2	3	250.75	271.47	36.90
9	-7	3	13.35	-177.84	111.59	9	-5	3	61.96	54.36	60.23	7	-2	3	1122.12	1136.02	99.96
-8	-7	3	16.58	26.60	98.50	-9	-4	3	8.26	156.23	57.84	8	-1	3	313.20	262.11	53.22
-7	-7	3	89.51	162.27	48.91	-8	-4	3	0.27	-11.47	86.59	9	-1	3	13.19	-23.18	81.88
-6	-7	3	211.41	182.99	47.71	-7	-4	3	252.89	294.02	50.39	-8	-1	3	1.37	71.29	97.43
-5	-7	3	2237.91	2193.61	119.94	-6	-4	3	1141.91	1065.98	95.55	-6	-1	3	642.41	513.50	58.95
-4	-7	3	937.86	824.94	77.96	-5	-4	3	48.13	10.66	60.69	-7	-1	3	56.07	130.72	46.89
-3	-7	3	707.00	630.41	48.89	-4	-4	3	100.92	101.93	29.03	-6	-1	3	186.89	-7.06	69.09
-2	-7	3	6698.32	6567.78	235.45	-3	-4	3	847.14	686.58	57.61	-5	-1	3	326.20	278.30	34.10
-1	-7	3	568.66	469.67	42.93	-2	-4	3	1312.09	1452.92	71.93	-4	-1	3	212.50	240.87	27.27
0	-7	3	3228.25	3494.29	145.03	-1	-4	3	4519.12	4174.86	149.34	-3	-1	3	3742.27	2937.62	144.79
1	-7	3	4979.51	4587.85	174.85	0	-4	3	6138.41	6113.00	207.37	-2	-1	3	5950.79	6103.15	203.39
2	-7	3	1773.49	1995.41	100.16	1	-4	3	47.16	23.70	30.38	-1	-1	3	3463.23	4133.82	139.84
3	-7	3	184.26	156.64	32.56	2	-4	3	360.27	394.77	32.49	0	-1	3	19369.10	20974.64	639.48
4	-7	3	144.40	209.26	34.40	3	-4	3	1722.28	2103.70	95.53	1	-1	3	2976.36	3367.77	114.80
5	-7	3	214.43	358.32	42.66	4	-4	3	131.53	96.42	28.53	2	-1	3	6391.60	7151.06	221.47
6	-7	3	137.24	96.14	46.58	5	-4	3	3.20	23.94	51.34	3	-1	3	3651.81	3833.60	138.55
7	-7	3	8.00	-40.98	85.34	6	-4	3	253.47	266.46	41.19	4	-1	3	5.06	51.38	71.87
8	-7	3	1739.29	1987.25	142.73	7	-4	3	163.78	127.71	45.51	5	-1	3	1035.97	891.45	72.94
9	-6	3	66.02	137.13	60.28	8	-4	3	41.88	-50.83	88.74	6	-1	3	70.05	6.53	60.95
-8	-6	3	162.24	27.86	105.69	9	-4	3	468.87	472.63	65.62	7	-1	3	39.20	-5.49	69.75
-7	-6	3	9.24	-16.91	77.59	-9	-3	3	82.24	23.55	100.74	8	-1	3	174.95	228.50	48.43
-6	-6	3	1665.90	1813.67	116.75	-8	-3	3	321.64	416.21	55.41	9	-1	3	1.71	8.69	87.80
-5	-6	3	64.14	54.73	36.59	-7	-3	3	142.83	133.45	44.50	10	-1	3	438.62	494.42	68.28
-4	-6	3	3171.11	3163.15	139.12	-6	-3	3	734.62	654.78	60.71	-9	0	3	236.18	269.70	68.64
-3	-6	3	42.99	34.84	44.11	-5	-3	3	1548.10	1356.67	51.81	-8	0	3	31.58	126.16	47.56
-2	-6	3	8543.24	9058.11	305.07	-4	-3	3	1618.86	1524.72	84.80	-7	0	3	1144.55	1277.73	75.16
-1	-6	3	126.10	133.73	25.28	-3	-3	3	2904.57	2395.35	103.21	-6	0	3	18.49	44.96	36.29
0	-6	3	1966.44	2022.34	86.48	-2	-3	3	905.11	801.59	51.56	-5	0	3	587.55	412.84	84.06
1	-6	3	1449.81	1371.77	75.95	-1	-3	3	5684.29	5593.56	187.65	-4	0	3	1393.01	1562.34	58.65
2	-6	3	4.67	-61.18	43.66	0	-3	3	6122.12	5022.21	170.76	-3	0	3	2648.82	2786.58	102.88
3	-6	3	513.24	563.25	47.61	1	-3	3	511.32	426.35	37.51	-2	0	3	18009.23	18074.17	395.71
4	-6	3	986.75	864.56	73.47	2	-3	3	3127.26	2926.25	110.98	-1	0	3	1742.87	1540.76	43.77
5	-6	3	134.24	-18.78	68.34	3	-3	3	235.08	185.64	24.62	0	0	3	2001.96	7560.50	567.27
6	-6	3	157.01	140.44	42.30	4	-3	3	1481.80	1809.82	85.52	1	0	3	714.32	773.51	26.68
7	-6	3	1305.97	1324.76	118.87	5	-3	3	1054.17	1038.12	75.30	2	0	3	794.84	1013.24	63.89
8	-6	3	256.88	212.98	57.44	6	-3	3	744.76	721.99	58.95	3	0	3	1868.97	1712.71	53.19
9	-6	3	262.09	153.12	65.44	7	-3	3	493.28	471.68	49.97	4	0	3	1153.09	1260.46	50.25
-9	-5	3	5.93	147.54	56.61	8	-3	3	1578.88	1494.74	134.42	5	0	3	555.73	517.26	50.63
-8	-5	3	47.80	-12.57	88.38	9	-3	3	140.88	156.14	57.49	6	0	3	1866.78	1838.40	74.57
-7	-5	3	696.75	774.97	72.44	-9	-2	3	88.44	56.75	101.73	7	0	3	448.95	623.97	41.35
-6	-5	3	3.60	113.01	40.29	-8	-2	3	226.14	351.45	55.58	8	0	3	613.82	625.47	43.48
-5	-5	3	1715.12	1833.83	108.95	-7	-2	3	106.04	36.38	54.30	9	0	3	551.83	546.15	45.51
-4	-5	3	509.64	562.78	46.25	-6	-2	3	1546.01	1805.44	171.01	10	0	3	6.70	6.29	61.76
-3	-5	3	197.56	132.58	25.71	-5	-2	3	25.52	37.33	56.75	-5	1	3	92.63	34.16	101.45
-2	-5	3	572.20	510.09	51.63	-4	-2	3	29.81	-57.24	45.56	-8	1	3	608.86	597.16	59.78

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-7	1	3	730.25	673.82	69.60	8	3	3	251.25	214.44	46.72	5	6	3	414.14	454.00	59.17
-6	1	3	811.50	747.64	61.29	9	3	3	26.47	20.38	80.17	6	6	3	4646.22	4387.94	189.53
-5	1	3	556.08	478.77	47.40	10	3	3	118.46	94.25	108.64	7	6	3	2.20	42.89	38.66
-4	1	3	84.31	56.71	26.86	-9	4	3	335.32	423.95	67.57	8	6	3	161.32	58.65	54.65
-3	1	3	95.11	44.57	22.10	-8	4	3	0.59	12.99	92.30	9	6	3	27.36	63.94	55.16
-2	1	3	7628.00	7346.55	140.64	-7	4	3	1136.28	1232.11	111.62	-8	7	3	175.45	194.21	63.59
-1	1	3	4152.75	4759.40	158.14	-6	4	3	103.76	465.33	48.29	-7	7	3	0.14	70.45	89.84
0	1	3	17424.77	14329.25	433.89	-5	4	3	316.18	322.19	37.99	-6	7	3	730.33	978.26	99.81
1	1	3	445.56	418.36	28.27	-4	4	3	381.46	478.90	42.71	-5	7	3	4.64	-29.34	71.14
2	1	3	22876.71	23484.72	10.05	-3	4	3	28.54	27.10	42.69	-4	7	3	672.24	751.53	78.44
3	1	3	6747.79	6657.67	222.07	-2	4	3	755.73	753.56	56.06	-3	7	3	424.98	389.68	38.59
4	1	3	4414.36	3769.89	143.62	-1	4	3	378.19	364.09	27.83	-2	7	3	408.18	410.16	41.97
5	1	3	1801.73	1941.52	97.41	0	4	3	1680.42	1617.78	74.31	-1	7	3	4915.87	4694.40	176.45
6	1	3	301.19	345.47	39.25	1	4	3	2875.78	2543.15	97.55	0	7	3	1189.77	1246.05	72.22
7	1	3	504.18	474.00	45.68	2	4	3	1175.29	1220.42	61.44	1	7	3	376.79	250.23	28.09
8	1	3	410.78	467.02	51.89	3	4	3	14024.16	14263.94	453.86	2	7	3	4516.01	4431.01	145.32
9	1	3	55.16	77.09	88.59	4	4	3	1869.00	1627.19	85.37	3	7	3	1522.54	1328.42	78.36
10	1	3	32.96	46.01	106.97	5	4	3	1190.26	1209.81	80.58	4	7	3	1293.65	1231.80	82.80
-9	2	3	3.70	-247.00	100.60	6	4	3	66.56	90.01	46.01	5	7	3	639.95	681.41	54.66
-8	2	3	12.99	29.66	89.17	7	4	3	598.88	578.48	59.61	6	7	3	231.15	269.24	41.96
-7	2	3	31.37	-96.95	85.64	8	4	3	268.29	301.57	51.87	7	7	3	13.73	59.90	42.40
-6	2	3	1.34	-25.13	65.80	9	4	3	42.30	-14.64	98.50	8	7	3	1.61	-51.77	89.75
-5	2	3	382.58	391.91	37.17	10	4	3	21.19	72.91	94.41	9	7	3	89.60	27.13	102.12
-4	2	3	1455.45	1356.38	81.00	-8	5	3	0.52	72.43	91.19	-8	8	3	67.22	12.91	108.69
-3	2	3	5.61	-23.91	40.03	-7	5	3	9.56	-23.01	84.16	-7	8	3	2.80	-101.78	98.42
-2	2	3	1233.05	1271.35	61.74	-6	5	3	168.26	186.54	43.90	-6	8	3	25.72	60.03	47.53
-1	2	3	26984.09	28552.12	872.14	-5	5	3	415.14	463.94	43.71	-5	8	3	1491.45	1639.38	115.23
0	2	3	35.74	-2.77	24.49	-4	5	3	95.47	28.62	59.13	-4	8	3	810.59	743.51	94.22
1	2	3	29674.56	31703.83	964.08	3	5	3	31.20	28.41	26.57	-3	8	3	937.37	926.74	79.93
2	2	3	4078.82	4307.96	148.75	-2	5	3	2131.25	2090.49	95.70	-2	8	3	1121.71	1306.55	97.93
3	2	3	592.36	423.95	43.27	-1	5	3	569.71	782.93	52.13	-1	8	3	22.51	45.08	29.00
4	2	3	1560.61	1356.33	74.41	0	5	3	1826.90	1724.35	82.00	0	8	3	2500.61	2697.67	123.69
5	2	3	1216.37	1424.91	83.02	1	5	3	2318.42	2232.78	91.35	1	8	3	237.89	196.88	30.24
6	2	3	1604.27	1623.49	102.17	2	5	3	3800.98	3879.78	143.06	2	8	3	1250.97	1230.88	80.60
7	2	3	17.39	113.77	38.09	3	5	3	1010.15	791.62	57.73	3	8	3	626.97	604.42	48.26
8	2	3	25.35	-34.22	77.84	4	5	3	1018.10	1199.52	72.08	4	8	3	1562.10	1537.65	95.13
9	2	3	125.56	144.56	53.34	5	5	3	2225.84	2108.95	108.19	5	8	3	39.52	126.51	34.23
10	2	3	30.72	10.65	107.34	6	5	3	57.75	50.46	59.93	6	8	3	89.53	60.78	73.41
-9	3	3	148.54	72.94	108.50	7	5	3	720.80	739.87	65.98	7	8	3	92.60	87.96	46.29
-8	3	3	692.68	827.94	78.24	8	5	3	15.34	-82.83	82.23	8	8	3	297.02	301.79	56.47
-7	3	3	1183.75	1185.36	109.34	9	5	3	117.27	90.91	56.99	9	8	3	0.34	-104.06	104.42
-6	3	3	2029.44	2041.09	123.07	10	5	3	55.39	54.59	112.75	-7	9	3	291.85	324.27	59.06
-5	3	3	16.86	-4.98	68.53	-8	6	3	182.91	18.81	100.57	-6	9	3	584.72	560.82	60.58
-4	3	3	1298.46	1114.34	74.24	-7	6	3	773.98	742.39	74.82	-5	9	3	36.29	56.93	46.49
-3	3	3	5195.29	5005.70	161.15	-6	6	3	401.94	357.84	51.50	-4	9	3	373.65	380.41	46.97
-2	3	3	2510.74	2921.04	112.95	-5	6	3	1728.60	1785.89	110.56	-3	9	3	935.72	976.04	85.70
-1	3	3	4708.13	4919.61	167.70	6	6	3	217.01	226.50	34.17	-2	9	3	48.27	34.09	60.38
0	3	3	7969.52	6837.67	224.62	-3	6	3	4.74	34.90	48.43	-1	9	3	1586.32	1686.55	97.90
1	3	3	3946.27	3200.16	112.79	-2	6	3	2051.72	1997.37	99.01	0	9	3	94.83	-87.23	58.21
2	3	3	6055.89	6259.17	207.17	-1	6	3	2020.95	1926.00	90.28	1	9	3	0.45	12.88	49.23
3	3	3	1529.72	1475.57	72.00	0	6	3	377.88	292.69	26.87	2	9	3	86.41	63.12	31.40
4	3	3	457.45	516.46	49.01	1	6	3	389.50	498.37	47.01	3	9	3	0.31	34.10	51.16
5	3	3	138.03	163.28	29.36	2	6	3	140.47	162.50	24.81	4	9	3	1192.69	1172.82	94.60
6	3	3	61.34	87.38	33.49	3	6	3	3768.97	3556.43	141.13	5	9	3	1918.37	1755.23	113.91
7	3	3	1778.58	1796.40	116.14	4	6	3	77.14	29.16	34.35	6	9	3	1126.97	1165.86	108.42

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
7	9	3	1913.96	2149.62	134.11	0	13	3	7.73	40.33	78.21	2	-15	4	14.55	25.69	102.27
8	9	3	31.05	-95.53	98.94	1	13	3	150.50	25.17	79.17	3	-15	4	4.27	-83.05	105.79
9	9	3	262.56	273.01	63.52	2	13	3	7.15	-203.78	83.31	4	-15	4	84.71	-40.36	114.97
-7	10	3	172.77	225.14	62.91	3	13	3	19.28	71.08	76.77	-6	-14	4	39.23	104.09	61.15
-6	10	3	27.04	78.29	52.28	4	13	3	356.95	438.87	54.71	-5	-14	4	478.62	490.91	68.48
-5	10	3	35.43	-1.36	87.07	5	13	3	180.35	108.22	54.89	-4	-14	4	19.87	30.09	99.64
-4	10	3	646.81	707.97	67.11	6	13	3	42.11	-87.13	97.53	-3	-14	4	1313.33	1640.88	131.67
-3	10	3	167.24	119.47	43.02	7	13	3	42.91	68.11	98.76	-2	-14	4	135.14	192.63	53.85
-2	10	3	2429.18	3009.49	144.89	-4	14	3	75.58	-43.55	101.06	-1	-14	4	23.41	-2.42	90.68
-1	10	3	216.74	230.43	39.14	-3	14	3	312.09	369.34	60.01	0	-14	4	1.84	67.98	85.11
0	10	3	2503.17	2523.36	127.99	-2	14	3	461.24	431.35	58.58	1	-14	4	19.47	29.20	92.13
1	10	3	87.22	69.45	33.36	-1	14	3	41.40	65.48	90.17	2	-14	4	258.38	257.86	58.98
2	10	3	57.28	49.87	32.68	0	14	3	1503.75	1608.56	125.25	3	-14	4	2.36	53.30	66.91
3	10	3	634.92	671.40	54.80	1	14	3	103.35	-63.57	90.83	4	-14	4	40.16	-6.83	105.14
4	10	3	1046.30	1165.63	98.24	2	14	3	453.54	410.76	54.86	5	-14	4	233.78	239.55	66.36
5	10	3	80.41	33.10	42.25	3	14	3	10.58	1.92	84.90	-6	-13	4	33.58	-74.33	103.99
6	10	3	438.16	380.15	53.21	4	14	3	4.69	28.89	89.15	-5	-13	4	27.01	-112.65	94.80
7	10	3	12.40	39.80	52.70	5	14	3	24.99	37.29	96.13	-4	-13	4	65.71	83.16	52.63
8	10	3	9.06	-13.49	101.40	6	14	3	3.39	-29.25	97.03	-3	-13	4	59.19	-32.23	89.35
9	10	3	1.78	-63.77	106.63	7	14	3	67.86	144.49	63.53	-2	-13	4	0.78	-178.44	84.27
-6	11	3	0.63	-80.85	95.15	-3	15	3	195.04	60.28	105.47	-1	-13	4	159.81	138.61	52.28
-5	11	3	123.53	329.51	53.73	-2	15	3	13.01	-228.92	104.40	0	-13	4	201.92	226.48	53.75
-4	11	3	369.13	356.80	53.22	-1	15	3	108.98	92.99	54.54	1	-13	4	399.33	394.16	56.52
-3	11	3	208.10	226.20	46.78	0	15	3	2.32	-87.76	94.34	2	-13	4	116.60	68.51	87.95
-2	11	3	425.31	493.53	50.61	1	15	3	1.61	7.51	51.31	3	-13	4	677.90	615.87	63.00
-1	11	3	1437.00	1410.45	102.88	2	15	3	3.14	46.48	89.81	4	-13	4	21.20	57.53	94.06
0	11	3	521.20	450.71	54.31	3	15	3	284.36	323.17	56.82	5	-13	4	211.69	231.35	61.76
1	11	3	818.51	798.29	63.74	4	15	3	475.53	470.33	64.54	-7	-12	4	3.29	32.14	99.66
2	11	3	251.32	261.60	39.65	5	15	3	64.54	115.25	57.70	-6	-12	4	5.81	-45.86	99.54
3	11	3	89.20	103.33	38.93	6	15	3	323.29	372.89	66.66	-5	-12	4	0.51	22.70	91.19
4	11	3	1.03	-41.31	78.00	-2	16	3	400.68	406.05	67.91	-4	-12	4	234.73	255.04	51.12
5	11	3	1.83	-38.61	80.32	-1	16	3	23.43	6.13	100.07	-3	-12	4	96.08	67.61	47.45
6	11	3	35.52	-25.28	90.73	0	16	3	447.69	449.12	65.13	-2	-12	4	55.30	118.40	47.93
7	11	3	103.74	25.58	96.64	1	16	3	6.59	79.91	90.12	-1	-12	4	1410.11	1614.56	121.24
8	11	3	83.84	-39.72	107.09	2	16	3	282.69	239.23	61.71	0	-12	4	89.72	172.10	46.00
-6	12	3	79.19	123.58	60.26	3	16	3	187.95	32.85	105.85	1	-12	4	682.28	784.17	72.11
-5	12	3	275.15	133.94	60.01	4	16	3	0.66	-192.42	106.15	2	-12	4	1087.68	1202.81	110.75
-4	12	3	149.57	105.70	53.61	5	16	3	93.72	128.50	62.05	3	-12	4	510.00	364.41	51.83
-3	12	3	29.30	2.94	79.04	0	17	3	116.13	23.25	114.27	4	-12	4	55.70	-12.26	92.14
-2	12	3	1064.56	1281.00	103.62	1	17	3	366.89	99.66	122.97	5	-12	4	805.43	716.20	71.82
-1	12	3	764.38	792.89	68.13	2	17	3	13.50	-4.29	109.28	6	-12	4	33.57	177.51	59.24
0	12	3	92.49	74.94	40.32	3	17	3	50.61	-210.04	117.25	-7	-11	4	127.89	183.18	57.86
1	12	3	152.45	113.70	43.53	-3	-16	4	0.46	-67.11	76.08	-6	-11	4	125.70	159.37	54.03
2	12	3	376.41	454.70	48.93	-2	-16	4	0.08	-87.98	107.61	-5	-11	4	226.09	206.00	52.31
3	12	3	77.23	15.70	75.46	-1	-16	4	9.72	55.96	59.87	-4	-11	4	2146.72	2274.00	140.78
4	12	3	18.55	41.02	77.91	0	-16	4	50.86	40.44	108.04	-3	-11	4	24.22	4.00	76.33
5	12	3	910.29	998.51	80.08	1	-16	4	53.13	8.57	113.50	-2	-11	4	1761.53	1650.27	116.04
6	12	3	828.78	836.00	79.43	2	-16	4	193.66	169.55	67.40	-1	-11	4	191.90	231.33	44.76
7	12	3	116.60	211.07	55.53	-5	-15	4	3.06	-71.55	108.98	0	-11	4	242.96	185.21	46.26
8	12	3	708.76	735.46	77.11	-4	-15	4	45.13	-107.69	101.40	1	-11	4	49.64	150.07	41.44
-5	13	3	2.52	-67.80	98.30	-3	-13	4	3.15	59.89	71.24	2	-11	4	693.67	633.19	65.16
-4	13	3	124.99	128.86	57.60	-2	-15	4	416.22	425.03	64.34	3	-11	4	702.48	930.99	75.09
-3	13	3	473.76	551.93	59.34	-1	-15	4	423.66	442.30	62.51	4	-11	4	19.31	-15.26	84.27
-2	13	3	68.39	93.73	47.05	0	-15	4	142.14	37.24	104.21	5	-11	4	75.74	86.10	52.92
-1	13	3	1181.97	1248.02	109.96	1	-15	4	261.58	273.74	62.85	6	-11	4	309.32	329.87	58.00

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
7	-11	4	11.95	146.13	119.15	-5	-7	4	27.06	93.18	68.83	-6	-4	4	342.69	399.73	45.16
-8	-10	4	94.39	151.35	88.81	-4	-7	4	486.63	600.59	55.23	-5	-4	4	315.37	234.94	38.78
-7	-10	4	0.80	-107.06	98.90	-3	-7	4	67.17	63.25	32.40	-4	-4	4	409.45	320.71	31.25
-6	-10	4	11.96	-173.00	119.15	-2	-7	4	1687.02	1820.17	99.37	-3	-4	4	232.26	175.73	27.75
-5	-10	4	192.12	174.58	192.12	-1	-7	4	12.50	36.44	28.65	-2	-4	4	568.78	700.55	54.41
-4	-10	4	6.73	-50.27	72.46	0	-7	4	430.79	375.35	35.44	-1	-4	4	7.57	-45.08	35.37
-3	-10	4	218.35	238.21	42.22	1	-7	4	36.82	33.01	35.15	0	-4	4	403.55	171.45	35.00
-2	-10	4	198.06	403.61	44.32	2	-7	4	41.82	145.01	30.81	1	-4	4	958.11	999.51	59.02
-1	-10	4	166.78	146.71	38.82	3	-7	4	3656.71	3911.46	162.59	2	-4	4	7297.14	8427.85	279.24
0	-10	4	620.59	601.65	59.75	4	-7	4	19.77	46.64	55.84	3	-4	4	34.07	47.05	23.66
1	-10	4	467.23	488.10	46.82	5	-7	4	699.09	765.80	63.18	4	-4	4	9661.00	10464.43	351.33
2	-10	4	2131.62	2054.46	119.44	6	-7	4	19.32	-92.32	79.41	5	-4	4	0.68	12.94	53.88
3	-10	4	171.95	233.23	42.71	7	-7	4	30.94	-130.72	90.58	6	-4	4	10.36	51.91	64.16
4	-10	4	264.84	256.74	46.64	8	-7	4	72.53	161.63	59.00	7	-4	4	22.57	45.49	70.98
5	-10	4	216.49	278.31	50.79	-9	-6	4	268.52	211.71	64.29	8	-4	4	67.76	66.12	49.92
6	-10	4	4.56	-41.44	87.38	-8	-6	4	159.39	165.98	56.59	9	-4	4	1.74	87.64	55.08
7	-10	4	58.07	63.80	105.47	-7	-6	4	383.48	398.00	53.37	-9	-3	4	1.33	0.92	96.44
-8	-9	4	147.42	83.45	105.67	-6	-6	4	68.00	-53.56	77.24	-8	-3	4	595.98	668.53	62.79
-7	-9	4	103.82	186.63	52.06	-5	-6	4	296.94	307.85	41.09	-7	-3	4	36.48	-44.30	83.60
-6	-9	4	29.48	31.86	58.37	-4	-6	4	969.73	973.26	81.02	-6	-3	4	3.85	40.43	37.82
-5	-9	4	227.93	220.89	48.11	-3	-6	4	637.17	666.39	62.03	-5	-3	4	241.19	173.84	35.78
-4	-9	4	204.43	221.56	41.15	-2	-6	4	2572.24	2894.83	123.25	-4	-3	4	657.32	612.11	62.58
-3	-9	4	401.77	399.74	41.60	-1	-6	4	10708.62	10982.63	364.04	-3	-3	4	1281.00	1217.23	71.77
-2	-9	4	334.24	364.10	41.16	0	-6	4	2013.80	2147.66	103.76	-2	-3	4	108.26	374.02	31.45
-1	-9	4	85.26	55.97	56.77	1	-6	4	5479.51	5042.93	185.43	-1	-3	4	13.88	25.19	30.86
0	-9	4	2820.24	2899.83	137.42	2	-6	4	5277.44	6151.72	218.99	0	-3	4	2183.64	1930.23	82.96
1	-9	4	2768.74	2979.12	143.53	3	-6	4	2077.99	2223.06	108.39	1	-3	4	9344.15	7391.65	243.02
2	-9	4	591.58	462.19	41.92	4	-6	4	212.34	252.09	36.49	2	-3	4	53.18	23.94	31.66
3	-9	4	549.69	832.49	82.10	5	-6	4	1303.11	1327.56	97.21	3	-3	4	3249.50	2989.69	119.75
4	-9	4	574.37	637.13	31.36	6	-6	4	84.35	90.30	42.21	4	-3	4	0.34	-29.40	45.16
5	-9	4	80.99	72.29	77.23	7	-6	4	10.45	69.50	79.66	5	-3	4	59.27	35.59	29.35
6	-9	4	526.06	608.26	58.50	8	-6	4	22.46	83.06	99.57	6	-3	4	261.32	341.31	38.44
7	-9	4	18.13	-36.50	102.37	9	-6	4	292.40	314.74	64.60	7	-3	4	105.57	46.42	75.96
8	-9	4	107.94	103.57	108.44	-9	-5	4	34.77	40.29	76.60	8	-3	4	25.04	44.76	85.94
-8	-8	4	1.29	-45.18	97.67	-8	-5	4	136.80	147.84	55.00	9	-3	4	5.13	-60.08	96.86
-7	-8	4	4.56	-20.16	88.52	-7	-5	4	184.87	275.57	87.99	-9	-2	4	14.08	-96.46	104.71
-6	-8	4	177.47	197.26	49.17	-6	-5	4	30.95	36.88	74.90	-8	-2	4	30.76	-69.34	91.19
-5	-8	4	1796.04	1501.99	112.47	-5	-5	4	1060.81	1115.36	81.78	-7	-2	4	275.04	266.26	50.05
-4	-8	4	85.70	76.36	37.73	-4	-5	4	2082.03	1923.19	105.52	-6	-2	4	1431.52	1337.51	102.62
-3	-8	4	4604.06	4835.05	194.31	-3	-5	4	6.68	0.26	43.30	-5	-2	4	27.19	48.25	55.50
-2	-8	4	163.78	222.37	33.08	-2	-5	4	7948.46	8221.44	278.47	-4	-2	4	651.66	642.71	58.46
-1	-8	4	7247.61	8415.01	298.30	-1	-5	4	1282.98	1496.85	77.09	-3	-2	4	4871.59	4823.49	175.34
0	-8	4	260.84	286.21	37.10	0	-5	4	908.12	875.18	61.21	-2	-2	4	1398.26	1636.40	75.46
1	-8	4	111.86	56.55	29.42	1	-5	4	31.69	31.37	38.47	-1	-2	4	47.17	23.41	28.29
2	-8	4	1.17	-22.96	55.19	2	-5	4	2659.63	2471.54	106.99	0	-2	4	1056.89	1071.81	54.72
3	-8	4	119.31	51.24	36.10	3	-5	4	2409.65	1966.29	97.60	1	-2	4	9939.07	10486.28	332.53
4	-8	4	391.67	542.52	47.40	4	-5	4	121.83	107.25	30.94	2	-2	4	1479.31	1565.93	69.06
5	-8	4	36.62	57.58	73.70	5	-5	4	1369.39	1795.05	91.37	3	-2	4	1131.01	1296.09	67.98
6	-8	4	280.55	359.64	50.58	6	-5	4	715.62	1300.32	93.13	4	-2	4	993.58	825.45	61.50
7	-8	4	850.12	1063.63	86.57	7	-5	4	102.84	66.28	82.43	5	-2	4	32.98	26.69	47.23
8	-8	4	104.06	46.57	104.51	8	-5	4	444.42	469.79	60.70	6	-2	4	77.08	-100.86	62.07
-9	-7	4	19.85	105.09	108.46	9	-5	4	20.64	-50.15	107.14	7	-2	4	104.76	106.25	40.98
-8	-7	4	162.10	89.36	99.65	9	-4	4	82.12	-207.43	109.22	8	-2	4	8.26	-134.46	80.65
-7	-7	4	14.80	10.95	84.83	-8	-4	4	22.30	70.48	51.43	9	-2	4	111.28	60.78	69.36
-6	-7	4	9.28	-97.68	81.53	-7	-4	4	137.37	135.51	45.15	10	-2	4	84.61	-4.38	114.56

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-9	-1	4	52.68	-99.07	102.33	6	1	4	258.10	212.32	37.45	2	4	4	4154.70	4429.37	156.79
-8	-1	4	270.27	202.13	56.56	7	1	4	9.18	-102.17	68.65	3	4	4	1827.06	1622.37	80.08
-7	-1	4	685.63	419.26	58.55	8	1	4	664.64	711.09	59.74	4	4	4	491.01	403.84	38.83
-6	-1	4	557.77	577.81	58.39	9	1	4	13.81	40.60	89.47	5	4	4	441.21	440.89	36.58
-5	-1	4	1798.03	1990.81	103.79	10	1	4	86.81	129.30	59.48	6	4	4	402.28	486.23	41.70
-4	-1	4	131.14	120.21	27.03	-9	2	4	1.57	-2.29	101.56	7	4	4	1172.77	1156.26	101.17
-3	-1	4	88.34	56.13	22.19	-8	2	4	5.95	1.98	91.63	8	4	4	98.94	282.29	45.01
-2	-1	4	2512.34	2215.67	92.04	-7	2	4	217.77	208.22	49.11	9	4	4	884.27	608.49	62.88
-1	-1	4	2078.68	1508.14	77.22	-6	2	4	1064.88	1281.35	92.67	10	4	4	5.53	84.30	104.55
0	-1	4	9382.40	-18855.10	275.50*	-5	2	4	342.17	377.73	39.29	-8	5	4	25.81	64.71	92.51
1	-1	4	3666.43	3447.68	119.84	-4	2	4	1503.09	1351.60	84.81	-7	5	4	210.97	239.79	52.67
2	-1	4	1165.51	1207.57	57.42	-3	2	4	129.08	135.72	24.85	-6	5	4	546.55	514.60	50.47
3	-1	4	7627.72	7522.16	249.87	-2	2	4	237.87	211.91	22.82	-5	5	4	3761.78	3705.94	169.54
4	-1	4	67.22	59.75	23.80	-1	2	4	2084.86	2055.13	84.88	-4	5	4	697.29	716.10	71.49
5	-1	4	6497.18	6167.35	224.27	0	2	4	656.38	589.58	41.16	-3	5	4	4511.83	4382.86	171.25
6	-1	4	34.47	16.26	58.90	1	2	4	7861.15	8260.54	267.25	-2	5	4	96.52	136.30	25.68
7	-1	4	314.55	247.43	42.76	2	2	4	1658.01	1537.39	67.07	-1	5	4	5.61	39.93	20.68
8	-1	4	372.52	376.64	51.89	3	2	4	27.73	50.81	18.91	0	5	4	119.39	167.13	23.57
9	-1	4	217.72	61.38	103.62	4	2	4	11787.95	11742.63	382.41	1	5	4	3390.17	3099.64	120.24
10	-1	4	24.87	51.43	104.24	5	2	4	1706.76	1794.35	95.89	2	5	4	10920.74	11897.47	383.09
-9	0	4	319.90	369.67	45.44	6	2	4	2446.39	2179.24	117.70	3	5	4	2145.25	2060.15	94.97
-8	0	4	210.39	252.10	38.81	7	2	4	7.44	-40.20	69.38	4	5	4	2502.21	2687.03	119.42
-7	0	4	72.89	103.22	66.80	8	2	4	10.19	-8.89	55.82	5	5	4	3008.14	4467.61	180.91
-6	0	4	12.05	15.24	44.32	9	2	4	47.41	-18.91	99.49	6	5	4	346.81	315.78	40.35
-5	0	4	328.43	367.75	51.30	10	2	4	132.90	203.22	60.26	7	5	4	454.38	476.83	48.95
-4	0	4	4037.39	3714.13	105.63	-9	3	4	17.85	32.51	105.33	8	5	4	563.22	620.29	57.35
-3	0	4	1649.02	1786.75	60.12	-8	3	4	154.07	197.14	54.63	9	5	4	90.14	57.06	93.01
-2	0	4	2645.03	2917.36	78.70	-7	3	4	141.82	228.33	45.57	10	5	4	5.69	5.27	105.91
-1	0	4	999.16	906.20	34.67	-6	3	4	97.64	86.15	41.27	-8	6	4	18.56	-126.86	102.32
0	0	4	5782.52	4762.16	117.37	-5	3	4	1286.45	1380.16	93.46	-7	6	4	63.44	64.78	88.35
1	0	4	4227.27	4320.20	102.43	-4	3	4	1437.97	1293.40	81.54	-6	6	4	4.47	-85.16	78.09
2	0	4	18601.33	20237.89	441.58	-3	3	4	9424.27	9714.09	323.60	-5	6	4	145.00	166.92	40.06
3	0	4	111.72	95.66	13.92	-2	3	4	84.13	57.53	20.09	-4	6	4	1409.85	1233.69	93.81
4	0	4	14507.73	14979.57	338.81	-1	3	4	2109.82	2146.70	88.34	-3	6	4	21.42	177.59	32.27
5	0	4	657.06	677.96	46.13	0	3	4	1348.58	1095.90	57.48	-2	6	4	5391.44	5008.79	188.38
6	0	4	12.85	-48.66	39.78	1	3	4	448.24	513.95	38.28	-1	6	4	2049.37	2101.06	98.88
7	0	4	30.80	51.63	31.20	2	3	4	1829.48	1676.32	72.39	0	6	4	1293.06	1157.80	71.11
8	0	4	36.54	86.89	40.08	3	3	4	10935.26	11248.88	362.60	1	6	4	9572.25	8981.13	297.11
9	0	4	944.54	817.95	54.29	4	3	4	976.99	952.46	64.37	2	6	4	5626.49	5640.47	199.87
10	0	4	0.20	-92.24	77.09	5	3	4	6333.22	6126.36	324.56	3	6	4	4032.71	3873.40	151.16
-9	1	4	0.39	-32.17	104.95	6	3	4	0.14	52.63	55.81	4	6	4	5480.89	5744.17	211.40
-8	1	4	172.39	84.98	54.42	7	3	4	42.89	-12.73	72.42	5	6	4	204.39	223.05	34.89
-7	1	4	811.65	822.06	70.51	8	3	4	610.98	710.94	70.62	6	6	4	58.96	99.02	39.72
-6	1	4	30.20	7.78	68.13	9	3	4	86.83	199.82	53.06	7	6	4	348.35	329.42	47.81
-5	1	4	1677.48	1627.36	99.14	10	3	4	635.19	731.01	72.93	8	6	4	129.88	201.31	50.95
-4	1	4	313.20	257.70	29.47	-8	4	4	36.55	-112.39	99.90	9	6	4	533.01	480.91	66.01
-3	1	4	9639.76	8863.52	295.70	-7	4	4	44.48	-63.10	93.26	-8	7	4	39.52	79.04	61.75
-2	1	4	15262.70	16004.44	502.75	-6	4	4	598.52	662.99	63.67	-7	7	4	3.56	13.11	88.06
-1	1	4	1062.73	1306.38	60.56	-5	4	4	38.91	-5.75	59.33	-6	7	4	64.28	-127.36	35.86
0	1	4	16398.64	16782.42	521.58	-4	4	4	4120.56	4169.90	168.33	-5	7	4	1275.85	1259.89	104.41
1	1	4	389.69	454.75	33.21	-3	4	4	2108.61	2191.46	104.31	-4	7	4	223.03	194.21	39.56
2	1	4	11398.11	12742.45	399.76	-2	4	4	1336.54	1445.45	75.13	-3	7	4	3827.02	3995.94	167.61
3	1	4	573.77	817.81	52.15	-1	4	4	70.52	108.51	21.03	-2	7	4	1056.94	1128.04	84.31
4	1	4	475.03	683.51	54.51	0	4	4	2895.95	3092.05	118.66	-1	7	4	3101.71	3070.31	131.61
5	1	4	1629.32	1723.71	93.84	1	4	4	234.26	273.91	25.13	0	7	4	9.95	77.33	27.33

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
1	7	4	2.35	11.33	23.22	5	10	4	32.31	24.81	76.21	3	14	4	737.74	773.54	75.73
2	7	4	922.13	814.55	62.00	6	10	4	26.88	0.92	77.11	4	14	4	88.1	-16.80	69.48
3	7	4	1016.96	957.36	70.18	7	10	4	23.66	-18.97	94.25	5	14	4	567.50	803.26	65.17
4	7	4	15.25	18.54	53.28	8	10	4	470.47	448.58	63.61	6	14	4	98.94	185.60	60.85
5	7	4	20.02	40.90	41.49	9	10	4	170.72	274.45	66.85	7	14	4	7.64	-102.23	115.90
6	7	4	1492.29	1329.21	105.33	-6	11	4	124.76	70.00	98.69	-3	15	4	114.56	54.91	104.94
7	7	4	560.67	541.89	51.99	-5	11	4	550.43	586.81	62.01	-2	15	4	0.94	35.28	93.25
8	7	4	1117.13	1118.69	86.53	-4	11	4	220.65	80.0	87.78	-1	15	4	352.33	352.28	61.53
9	7	4	71.72	141.75	56.20	-3	11	4	185.48	195.17	47.01	0	15	4	608.12	624.59	63.59
-7	8	4	141.94	201.87	53.36	-2	11	4	209.20	200.58	44.85	1	15	4	421.37	498.13	59.41
-6	8	4	530.17	590.40	57.19	-1	11	4	74.06	153.41	39.68	2	15	4	681.69	616.06	67.95
-5	8	4	1450.19	1298.92	115.94	0	11	4	412.08	362.81	45.42	3	15	4	108.87	98.31	98.78
-4	8	4	1158.47	1184.73	99.17	1	11	4	1278.59	1216.10	98.56	4	15	4	247.34	238.75	59.03
-3	8	4	2129.40	2061.13	117.35	2	11	4	1024.59	1161.65	93.07	5	15	4	8.12	51.14	57.25
-2	8	4	1975.55	1862.31	106.04	3	11	4	358.54	437.79	45.23	6	15	4	10.87	60.16	106.95
-1	8	4	492.41	505.17	47.68	4	11	4	2850.23	2814.33	153.15	-2	16	4	141.28	173.58	61.32
0	8	4	37.00	75.06	30.47	5	11	4	594.37	664.94	67.53	-1	16	4	0.88	-40.94	98.73
1	8	4	4656.38	4806.48	182.71	6	11	4	19.63	-22.41	87.74	0	16	4	388.55	303.77	63.91
2	8	4	13.99	23.48	33.36	7	11	4	285.62	268.27	57.05	1	16	4	8.36	-72.65	101.30
3	8	4	1437.04	1407.15	88.98	8	11	4	139.88	162.67	62.85	2	16	4	48.54	-70.11	103.54
4	8	4	161.10	425.60	36.89	-6	12	4	0.79	-120.51	109.38	3	16	4	3.75	6.03	58.95
5	8	4	1230.29	1243.86	94.94	-5	12	4	41.12	-59.55	97.89	4	16	4	0.10	41.28	58.50
6	8	4	771.15	865.22	69.50	-4	12	4	54.53	-40.94	91.47	5	16	4	80.57	-4.34	113.56
7	8	4	25.06	74.14	79.00	-3	12	4	101.90	144.25	46.82	0	17	4	8.45	-297.74	118.81
8	8	4	5.47	-102.16	89.41	-2	12	4	212.67	12.71	82.40	1	17	4	404.59	346.48	70.54
9	8	4	71.17	38.25	104.64	-1	12	4	700.22	700.50	68.60	2	17	4	279.90	314.79	65.60
-7	9	4	30.38	66.05	100.96	0	12	4	673.78	505.12	53.97	3	17	4	93.99	129.57	64.70
-6	9	4	0.78	-27.25	90.70	1	12	4	2775.05	3118.00	155.42	-3	16	5	219.23	167.68	66.34
-5	9	4	5.81	10.87	79.91	2	12	4	24.48	11.25	68.80	-2	16	5	77.61	-100.86	114.68
-4	9	4	360.71	275.41	45.94	3	12	4	120.97	123.97	42.95	-1	16	5	26.83	44.59	73.37
-3	9	4	967.70	925.50	86.70	4	12	4	11.93	20.12	78.06	0	16	5	302.03	310.82	68.46
-2	9	4	80.82	89.59	65.43	5	12	4	30.26	35.50	60.12	1	16	5	42.23	-60.94	118.37
-1	9	4	1618.64	1490.64	90.97	6	12	4	254.78	289.69	55.18	2	16	5	120.61	127.86	69.79
0	9	4	1763.97	3623.84	158.04	7	12	4	0.78	88.49	55.33	-4	15	5	434.35	490.28	71.88
1	9	4	408.47	360.24	35.09	8	12	4	261.08	382.50	67.52	-3	15	5	104.63	54.28	110.51
2	9	4	3226.60	3141.18	139.23	-5	13	4	7.80	2.70	101.80	-2	15	5	56.52	84.46	101.84
3	9	4	99.25	7.91	41.21	-4	13	4	72.19	12.56	97.92	-1	15	5	123.18	62.16	61.62
4	9	4	23.09	65.09	34.35	-3	13	4	146.82	125.25	52.53	0	15	5	48.66	8.27	62.13
5	9	4	36.75	-50.51	66.08	-2	13	4	6.89	1.83	85.88	1	15	5	16.46	-183.43	103.48
6	9	4	320.20	330.09	46.45	-1	13	4	717.79	771.61	73.60	2	15	5	57.20	115.41	58.13
7	9	4	173.66	83.07	90.24	0	13	4	91.50	25.19	58.54	3	15	5	72.74	46.85	63.87
8	9	4	145.17	51.42	104.68	1	13	4	66.20	60.89	46.27	-5	14	5	89.36	63.69	107.73
9	9	4	212.80	287.06	63.87	2	13	4	38.72	-67.24	79.18	-4	14	5	38.91	23.00	101.98
-7	10	4	75.13	31.54	105.39	3	13	4	38.44	5.92	82.20	-3	14	5	7.21	-44.43	100.43
-6	10	4	8.34	76.58	86.95	4	13	4	173.40	139.51	51.21	-2	14	5	283.12	428.89	59.38
-5	10	4	171.91	50.51	91.61	5	13	4	93.92	120.33	51.78	-1	14	5	10.65	-64.59	98.34
-4	10	4	245.72	327.29	50.97	6	13	4	64.25	70.67	98.81	0	14	5	857.11	654.71	69.51
-3	10	4	186.26	215.83	45.14	7	13	4	341.25	363.41	64.03	1	14	5	1.18	-17.52	94.60
-2	10	4	1659.19	1611.47	110.10	-4	14	4	79.49	-6.54	105.52	2	14	5	283.71	24.22	108.20
-1	0	4	223.41	139.94	39.22	-3	14	4	285.66	205.80	59.63	3	14	5	85.00	7.52	104.06
0	10	4	660.20	698.00	55.70	-2	14	4	16.70	63.70	50.16	4	14	5	5.59	96.27	103.18
1	10	4	191.63	226.02	35.86	-1	14	4	63.70	119.81	50.92	-6	13	5	4.48	46.97	102.13
2	10	4	0.11	22.92	57.41	0	14	4	128.92	220.69	50.10	-5	13	5	42.40	147.44	56.28
3	10	4	130.06	35.61	66.15	1	14	4	323.72	224.37	54.62	-4	13	5	246.48	220.25	55.88
4	10	4	545.22	523.19	47.27	2	14	4	60.74	-72.94	91.99	-3	13	5	41.29	15.41	90.29

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-2	-13	5	507.03	553.97	59.75	-5	-9	5	345.68	452.07	40.77	-1	-6	5	147.67	159.69	20.29
-1	-13	5	840.17	928.13	83.36	-4	-9	5	342.54	317.52	45.95	0	-6	5	5822.30	5555.24	205.26
0	-13	5	25.45	-75.80	92.86	-3	-9	5	594.06	536.04	55.05	1	-6	5	2804.72	2973.35	127.34
1	-13	5	928.40	1092.05	86.97	-2	-9	5	100.09	124.13	36.86	2	-6	5	372.13	374.31	33.23
2	-13	5	49.79	60.72	83.78	-1	-9	5	1224.42	1454.48	98.64	3	-6	5	1596.06	1827.76	97.97
3	-13	5	200.12	164.74	54.71	0	-9	5	384.78	339.39	42.11	4	-6	5	2989.25	2943.86	137.97
4	-13	5	0.78	-65.43	88.89	1	-9	5	170.40	112.79	37.20	5	-6	5	4848.26	5508.50	221.35
5	-13	5	161.39	156.39	62.35	2	-9	5	16.37	-22.41	62.42	6	-6	5	19.25	-74.85	75.94
-7	-12	5	49.35	130.94	63.03	3	-9	5	830.80	670.27	63.61	7	-6	5	1928.02	1870.16	139.09
-6	-12	5	177.05	358.81	68.28	4	-9	5	1014.59	1257.73	107.54	8	-6	5	280.66	275.58	58.93
-5	-12	5	609.71	672.97	64.68	5	-9	5	1.71	-20.61	79.93	9	-6	5	1.63	0.94	107.94
-4	-12	5	14.29	-14.71	89.76	6	-9	5	1083.90	1154.93	87.89	-9	-5	5	277.97	280.94	67.08
-3	-12	5	72.18	20.47	59.39	7	-9	5	91.73	51.31	98.22	-8	-5	5	42.05	84.09	53.80
-2	-12	5	462.04	506.16	54.06	8	-9	5	137.62	151.20	64.55	-7	-5	5	244.57	261.86	50.28
-1	-12	5	763.30	716.35	70.35	-8	-9	5	478.75	538.28	68.06	-6	-5	5	748.16	800.60	70.32
0	-12	5	41.48	49.02	57.41	-7	-8	5	5.34	-129.38	97.19	-5	-5	5	245.75	198.75	41.67
1	-12	5	22.67	81.38	45.97	-6	-8	5	176.53	205.06	49.73	-4	-5	5	75.90	85.86	32.22
2	-12	5	355.47	384.85	53.26	-5	-8	5	11.06	28.32	75.17	-3	-5	5	69.27	84.90	27.95
3	-12	5	92.27	46.91	82.47	-4	-8	5	2.01	3.30	67.14	-2	-5	5	1077.18	1096.00	73.04
4	-12	5	10.77	72.84	89.20	-3	-8	5	381.92	328.88	42.01	-1	-5	5	3.56	17.16	41.92
5	-12	5	201.73	209.85	57.08	-2	-8	5	581.53	560.87	51.60	0	-5	5	2190.42	2860.01	120.91
6	-12	5	34.77	212.52	57.88	-1	-8	5	822.50	917.22	84.51	1	-5	5	3241.17	3281.37	120.80
-7	-11	5	39.38	-50.24	118.71	0	-8	5	4334.99	4069.70	171.53	2	-5	5	695.58	708.15	60.91
-6	-11	5	22.59	-157.66	98.58	1	-8	5	24.57	-28.27	28.27	3	-5	5	4680.98	4749.34	179.35
-5	-11	5	24.64	-35.62	86.41	2	-8	5	1884.76	1847.98	106.46	4	-5	5	1080.74	1190.37	80.82
-4	-11	5	34.10	21.03	88.14	3	-8	5	31.81	28.29	42.24	5	-5	5	34.04	-52.63	64.77
-3	-11	5	103.48	8.64	76.86	4	-8	5	46.38	77.14	38.40	6	-5	5	1846.35	1949.44	120.24
-2	-11	5	37.68	-2.00	71.00	5	-8	5	1257.32	1058.71	100.14	7	-5	5	7.99	55.88	83.86
-1	-11	5	1560.80	1530.38	119.74	6	-8	5	5.11	-4.18	78.15	8	-5	5	27.89	31.85	62.62
0	-11	5	30.91	87.71	41.96	7	-8	5	135.57	174.78	56.04	9	-5	5	55.61	127.51	59.11
1	-11	5	2354.46	2127.45	132.09	8	-8	5	10.74	34.98	61.90	-9	-4	5	1.06	-108.32	106.52
2	-11	5	56.72	107.48	42.10	-8	-7	5	28.19	54.85	100.89	-8	-4	5	470.48	533.76	61.88
3	-11	5	206.75	200.45	46.94	-7	-7	5	47.63	82.36	50.01	-7	-4	5	148.55	237.98	48.14
4	-11	5	32.13	66.84	74.35	-6	-7	5	194.21	122.43	48.62	-6	-4	5	19.79	-3.51	42.03
5	-11	5	0.03	10.30	88.88	-5	-7	5	268.88	325.74	43.58	-5	-4	5	184.53	206.56	38.63
6	-11	5	44.41	49.10	93.57	-4	-7	5	1095.65	1085.51	91.61	-4	-4	5	406.11	332.52	35.78
7	-11	5	71.35	11.82	103.63	-3	-7	5	0.36	-62.71	55.27	-3	-4	5	4050.16	3766.92	151.12
-7	-10	5	9.55	-259.94	109.34	-2	-7	5	1683.62	1537.92	94.55	-2	-4	5	1080.58	1196.88	71.83
-6	-10	5	1.84	51.05	87.94	-1	-7	5	1041.76	1175.71	79.99	-1	-4	5	11423.51	12102.07	392.28
-5	-10	5	36.87	-11.97	82.68	0	-7	5	2020.31	1680.60	98.15	0	-4	5	1246.54	1554.18	76.92
-4	-10	5	6.07	8.43	73.99	1	-7	5	4110.61	3946.13	161.93	1	-4	5	218.06	226.29	23.90
-3	-10	5	268.41	228.25	44.83	2	-7	5	25.29	33.74	35.05	2	-4	5	47.50	14.41	38.08
-2	-10	5	9.60	-28.12	67.50	3	-7	5	1325.52	1279.75	87.82	3	-4	5	41.87	70.15	24.81
-1	-10	5	703.41	547.72	51.27	4	-7	5	47.95	119.31	37.00	4	-4	5	3.98	21.88	50.99
0	-10	5	303.49	360.08	44.68	5	-7	5	33.73	32.09	71.17	5	-4	5	191.42	163.90	24.53
1	-10	5	185.62	165.94	40.61	6	-7	5	755.76	694.02	58.51	6	-4	5	26.76	66.25	37.03
2	-10	5	2845.04	2908.73	151.42	7	-7	5	126.69	109.95	51.94	7	-4	5	1306.74	1407.00	106.24
3	-10	5	584.35	630.17	63.31	8	-7	5	1306.98	1185.06	93.96	8	-4	5	156.16	235.47	51.22
4	-10	5	373.15	423.46	50.59	-8	-6	5	430.03	405.07	63.18	9	-4	5	298.98	103.44	104.08
5	-10	5	33.47	37.80	87.91	-7	-6	5	3.97	18.02	81.54	-9	-3	5	8.14	92.85	60.96
6	-10	5	9.12	43.74	52.87	-6	-6	5	1701.54	1743.53	120.09	-8	-3	5	221.55	341.47	55.37
7	-10	5	431.01	378.77	64.65	-5	-6	5	898.18	1041.46	91.86	-7	-3	5	1372.63	1524.71	115.17
-8	-9	5	1.87	-143.84	108.76	-4	-6	5	134.88	159.84	36.92	-6	-3	5	0.27	16.60	71.50
-7	-9	5	453.07	465.10	63.36	-3	-6	5	165.90	134.89	31.84	-5	-3	5	4347.30	4400.53	184.02
-6	-9	5	18.97	34.48	87.75	-2	-6	5	1.44	0.64	50.05	-4	-3	5	1783.26	1693.16	94.60

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-3	-3	5	1.08	-25.55	43.42	-6	0	5	1517.88	1426.25	74.86	9	2	5	1008.45	987.68	83.16
-2	-3	5	1351.39	1489.04	74.75	-5	0	5	1373.55	1273.34	65.63	10	2	5	88.66	-0.88	106.03
-1	-3	5	6626.72	6741.50	229.22	-4	0	5	1436.50	1362.17	68.14	-8	3	5	256.98	135.25	59.67
0	-3	5	1699.98	1447.97	74.54	-3	0	5	1417.22	1136.68	50.39	-7	3	5	33.92	-46.52	83.56
1	-3	5	79.94	59.50	18.39	-2	0	5	351.60	358.08	32.50	-6	3	5	10.35	-14.85	70.99
2	-3	5	1531.44	1620.66	76.86	-1	0	5	195.38	190.69	14.46	-5	3	5	764.91	765.86	60.51
3	-3	5	1359.86	1169.27	68.45	0	0	5	625.06	-1166.58	124.63*	-4	3	5	518.57	654.18	67.95
4	-3	5	284.96	361.57	32.60	1	0	5	300.18	339.33	20.83	-3	3	5	4614.22	5353.58	197.59
5	-3	5	451.75	373.40	35.49	2	0	5	9670.07	9616.00	218.33	-2	3	5	2816.27	2707.18	113.50
6	-3	5	3862.39	4175.30	178.91	3	0	5	1949.51	2459.11	70.91	-1	3	5	403.62	382.23	31.78
7	-3	5	99.27	89.09	41.89	4	0	5	6942.98	7228.05	175.96	0	3	5	468.67	509.81	46.61
8	-3	5	387.23	326.77	54.38	5	0	5	2300.98	2283.62	201.60	1	3	5	877.41	1012.18	53.93
9	-3	5	13.26	-3.77	103.59	6	0	5	640.75	631.01	91.05	2	3	5	793.03	960.70	54.92
-9	-2	5	42.68	50.34	105.44	7	0	5	1005.18	1067.49	83.74	3	3	5	6260.95	6138.12	211.22
-8	-2	5	725.69	636.22	67.12	8	0	5	181.36	195.70	34.09	4	3	5	325.50	308.69	29.67
-7	-2	5	5.90	-18.52	94.05	9	0	5	289.00	5.67	71.51	5	3	5	5498.96	5129.45	194.83
-6	-2	5	521.78	558.57	48.62	10	0	5	21.34	-19.18	74.16	6	3	5	157.97	205.30	36.98
-5	-2	5	15.71	50.16	61.59	-9	1	5	18.81	11.71	98.90	7	3	5	51.29	24.71	68.63
-4	-2	5	1.72	8.30	51.86	-8	1	5	191.68	319.35	55.67	8	3	5	613.24	544.22	54.57
-3	-2	5	209.12	201.64	27.51	-7	1	5	157.22	137.47	48.18	9	3	5	70.04	7.23	91.91
-2	-2	5	1268.66	1354.95	71.51	-6	1	5	1162.21	972.30	96.06	10	3	5	25.97	16.48	108.52
-1	-2	5	2339.90	2577.72	102.55	-5	1	5	2.32	-69.27	61.27	-8	4	5	10.94	7.48	66.03
0	-2	5	1355.52	1447.86	69.32	-4	1	5	532.04	539.92	45.76	-7	4	5	403.78	461.08	56.76
1	-2	5	2377.56	2366.38	99.63	-3	1	5	115.71	144.11	26.92	-6	4	5	26.10	34.43	72.07
2	-2	5	3795.20	4010.25	144.39	-2	1	5	775.63	695.69	53.10	-5	4	5	22.09	-28.15	61.82
3	-2	5	0.06	11.21	27.27	-1	1	5	39.58	207.02	21.05*	-4	4	5	38.08	37.76	32.25
4	-2	5	4463.41	4957.52	184.72	0	1	5	864.94	-3476.12	113.74*	-3	4	5	9.85	-14.24	49.32
5	-2	5	1815.02	1727.23	95.50	1	1	5	7487.87	7053.72	230.28	-2	4	5	2910.16	3330.33	133.27
6	-2	5	152.20	165.13	37.03	2	1	5	6236.92	6457.83	214.34	-1	4	5	2480.47	2779.70	113.71
7	-2	5	1603.96	1507.08	112.70	3	1	5	1794.46	2082.88	89.58	0	4	5	1424.70	1353.47	72.89
8	-2	5	579.94	550.02	58.46	4	1	5	596.34	599.59	58.55	1	4	5	4437.36	4412.72	156.28
9	-2	5	2.25	-29.62	98.55	5	1	5	741.36	792.64	72.56	2	4	5	1094.65	933.13	59.96
-9	-1	5	195.69	174.27	62.38	6	1	5	1725.58	1590.06	100.54	3	4	5	1328.52	1126.16	66.83
-8	-1	5	61.88	1.84	88.64	7	1	5	958.87	1050.86	98.49	4	4	5	1706.51	1526.74	84.35
-7	-1	5	208.69	221.18	52.90	8	1	5	487.64	444.79	54.03	5	4	5	92.92	94.25	32.52
-6	-1	5	61.27	20.58	74.47	9	1	5	196.58	368.14	56.98	6	4	5	480.04	464.88	43.76
-5	-1	5	33.19	74.72	33.44	10	1	5	139.22	113.66	60.88	7	4	5	1041.02	938.30	96.26
-4	-1	5	1116.55	1012.83	75.96	-9	2	5	5.01	19.47	106.11	8	4	5	19.07	14.99	84.22
-3	-1	5	2204.06	2185.24	98.38	-8	2	5	347.94	250.40	58.98	9	4	5	1.19	14.60	95.70
-2	-1	5	10989.97	10308.78	335.31	-7	2	5	114.76	139.26	49.11	10	4	5	13.51	-79.32	118.46
-1	-1	5	4639.54	5383.91	184.36	-6	2	5	12.06	55.62	73.14	-8	5	5	11.49	-53.15	100.73
0	-1	5	3100.17	-17523.42	253.19*	-5	2	5	13.51	-15.25	58.89	-7	5	5	186.94	79.67	95.50
1	-1	5	1057.75	1099.77	55.64	-4	2	5	848.65	877.87	71.87	-6	5	5	50.90	134.48	42.07
2	-1	5	540.09	620.89	42.72	-3	2	5	1421.82	1327.51	77.18	-5	5	5	97.59	-15.80	67.16
3	-1	5	428.64	454.28	43.59	-2	2	5	7523.88	7534.16	11.95	-4	5	5	272.03	184.64	36.34
4	-1	5	30.03	-74.70	44.99	-1	2	5	14669.92	14226.64	430.80	-3	5	5	186.41	156.46	29.83
5	-1	5	907.15	1008.40	74.70	0	2	5	5477.54	5450.76	186.34	-2	5	5	11995.23	11826.67	390.23
6	-1	5	12.19	38.85	55.29	1	2	5	16.42	-17.71	28.48	-1	5	5	379.62	281.29	26.80
7	-1	5	17.63	58.03	39.96	2	2	5	934.90	887.96	51.63	0	5	5	9515.17	9030.34	302.75
8	-1	5	584.41	796.49	73.78	3	2	5	241.11	154.09	21.31	1	5	5	224.29	277.04	28.01
9	-1	5	17.05	-101.86	96.09	4	2	5	0.05	-2.24	43.26	2	5	5	16.93	13.74	37.61
10	-1	5	161.04	239.44	64.34	5	2	5	710.90	700.68	65.07	3	5	5	2363.10	2306.05	102.97
-9	0	5	93.93	212.41	71.11	6	2	5	1429.63	1367.80	96.55	4	5	5	1241.74	1146.30	74.49
-8	0	5	66.00	48.97	63.98	7	2	5	154.27	187.39	39.82	5	5	5	759.04	732.62	69.91
-7	0	5	0.69	-111.51	61.46	8	2	5	8.20	67.53	46.33	6	5	5	83.88	155.53	37.88

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
7	5	5	390.24	406.25	48.04	8	8	5	132.93	159.70	54.13	0	13	5	304.46	274.20	49.68
8	5	5	739.67	736.18	74.87	9	8	5	281.42	422.06	60.34	1	12	5	50.89	-50.13	72.58
9	5	5	67.26	27.75	95.13	-7	9	5	4.57	-92.99	131.24	2	12	5	537.49	421.24	61.41
10	5	5	299.96	284.54	67.61	-6	9	5	178.42	147.00	55.59	3	12	5	41.68	63.62	43.80
-8	6	5	1.70	45.27	101.63	-5	9	5	718.72	815.45	71.26	4	12	5	700.99	538.94	56.55
-7	6	5	1.84	13.14	91.84	-4	9	5	1.34	-20.94	70.00	5	12	5	879.67	751.56	74.25
-6	6	5	313.66	293.89	49.65	-3	9	5	54.78	5.51	69.55	6	12	5	937.34	800.88	83.19
-5	6	5	8.83	31.42	66.05	-2	9	5	57.30	44.40	67.43	7	12	5	34.98	-11.71	97.61
-4	6	5	735.09	890.30	76.82	-1	9	5	585.19	678.72	58.25	8	12	5	91.47	131.87	61.82
-3	6	5	1738.16	1848.35	102.14	0	9	5	147.64	101.27	37.24	-5	13	5	16.06	53.71	100.98
-2	6	5	692.57	610.09	62.95	1	9	5	889.25	827.99	77.07	-4	13	5	1.36	112.95	54.96
-1	6	5	1536.25	1691.55	90.56	2	9	5	255.93	185.72	33.72	-3	13	5	0.54	-43.25	95.29
0	6	5	345.80	477.90	39.12	3	9	5	1292.57	1226.40	90.31	-2	13	5	381.29	292.01	56.19
1	6	5	702.31	605.05	52.56	4	9	5	176.61	171.87	38.50	-1	13	5	1.36	-41.06	58.60
2	6	5	12.36	6.84	29.52	5	9	5	1945.47	1816.76	118.39	0	13	5	2.63	35.04	84.30
3	6	5	759.61	748.40	65.55	6	9	5	1248.27	1184.84	109.31	1	13	5	0.46	-22.60	61.00
4	6	5	4818.30	4426.06	173.35	7	9	5	607.99	656.39	68.07	2	13	5	110.01	153.76	46.52
5	6	5	48.81	61.22	31.12	8	9	5	6.24	-64.09	94.66	3	13	5	10.11	-20.61	82.13
6	6	5	1802.01	1803.99	109.39	9	9	5	20.40	90.00	106.03	4	13	5	556.61	526.26	59.95
7	6	5	170.72	185.89	46.57	-6	10	5	23.67	91.83	52.01	5	13	5	855.34	786.91	67.91
8	6	5	280.71	279.73	52.95	-5	10	5	16.05	-39.26	91.16	6	13	5	29.53	21.87	69.51
9	6	5	158.35	62.49	101.51	-4	10	5	410.89	496.81	52.82	7	13	5	58.12	125.27	60.29
-8	7	5	345.57	337.40	67.87	-3	10	5	309.45	396.88	48.31	-4	14	5	386.89	400.00	66.32
-7	7	5	1.95	16.39	91.17	-2	10	5	184.48	22.31	68.65	-3	14	5	7.52	-156.70	103.18
-6	7	5	240.73	192.37	53.64	-1	10	5	3.61	-209.89	70.24	-2	14	5	802.62	775.71	80.70
-5	7	5	125.75	33.35	77.66	0	10	5	4.92	-115.87	67.48	-1	14	5	224.98	73.01	94.87
-4	7	5	153.18	8.25	70.86	1	10	5	2275.85	2124.25	110.48	0	14	5	533.69	438.01	56.84
-3	7	5	81.55	38.65	58.85	2	10	5	121.22	21.84	44.31	1	14	5	548.73	430.69	57.22
-2	7	5	228.22	158.83	34.31	3	10	5	1675.08	1597.21	106.18	2	14	5	74.30	17.76	87.95
-1	7	5	76.33	113.50	30.37	4	10	5	625.18	823.42	65.85	3	14	5	12.05	54.04	87.10
0	7	5	1849.29	2268.13	109.28	5	10	5	551.76	474.26	53.50	4	14	5	40.38	91.63	92.09
1	7	5	789.99	980.72	63.47	6	10	5	1024.64	948.95	76.47	5	14	5	68.30	-22.78	96.91
2	7	5	8067.07	8198.11	281.70	7	10	5	0.17	-21.84	88.56	6	14	5	223.19	215.58	60.94
3	7	5	2264.15	2320.81	110.00	8	10	5	92.58	49.64	97.84	7	14	5	6.66	-46.73	109.83
4	7	5	750.60	676.78	51.68	9	10	5	0.41	-73.12	110.62	-3	15	5	216.68	183.42	63.24
5	7	5	322.23	257.65	38.76	-6	11	5	108.78	41.69	109.53	-2	15	5	22.12	-21.96	98.81
6	7	5	342.85	298.69	45.32	-5	11	5	104.13	79.53	100.48	-1	15	5	88.47	-104.62	106.20
7	7	5	302.59	347.89	48.40	-4	11	5	77.93	131.73	48.92	0	15	5	7.91	67.82	94.38
8	7	5	1.13	1.63	90.72	-3	11	5	852.17	710.53	71.93	1	15	5	35.26	119.33	54.29
9	7	5	10.27	113.46	56.81	-2	11	5	88.65	138.45	41.16	2	15	5	6.54	0.74	88.46
-7	8	5	5.29	70.10	95.32	-1	11	5	1442.17	1555.10	108.31	3	15	5	49.61	79.67	97.87
-6	8	5	21.89	-82.40	95.24	0	11	5	1015.52	918.92	70.62	4	15	5	253.94	265.26	60.16
-5	8	5	542.77	523.92	54.63	1	11	5	49.46	42.33	46.96	5	15	5	215.08	230.94	63.12
-4	8	5	1366.08	1332.63	103.41	2	11	5	189.78	195.22	39.58	6	15	5	11.30	171.05	59.93
-3	8	5	1033.81	1083.15	87.42	3	11	5	74.33	28.59	74.45	-2	16	5	54.78	109.51	59.99
-2	8	5	3572.40	3872.09	164.70	4	11	5	568.48	612.87	52.13	-1	16	5	41.12	81.78	56.15
-1	8	5	8191.19	7970.97	425.55	5	11	5	141.86	150.23	48.53	0	16	5	229.77	349.39	61.41
0	8	5	41.74	35.03	36.78	6	11	5	0.03	27.56	86.04	1	16	5	321.06	256.73	62.47
1	8	5	904.15	694.99	61.93	7	11	5	485.30	529.92	64.96	2	16	5	20.57	63.49	103.07
2	8	5	280.18	278.49	32.15	8	11	5	90.15	7.78	109.34	3	16	5	900.39	855.10	76.15
3	8	5	38.16	61.09	30.69	-5	12	5	82.01	-104.24	104.64	4	16	5	179.99	161.13	61.98
4	8	5	21.20	43.87	32.25	-4	12	5	229.56	307.95	56.62	5	16	5	85.54	128.12	66.04
5	8	5	126.40	124.81	40.14	-3	12	5	87.81	26.47	88.44	1	17	5	44.39	-18.76	104.28
6	8	5	951.58	958.74	99.04	-2	12	5	328.39	415.23	52.15	2	17	5	0.72	-57.94	111.35
7	8	5	18.90	-77.69	82.56	-1	12	5	2.00	66.58	71.36	-2	16	6	100.90	-115.21	121.48

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
1	-16	6	0.57	-65.22	116.33	2	-11	6	381.84	424.62	52.66	-7	-7	6	937.55	194.16	58.90
-16	6		23.79	-21.46	113.11	3	-11	6	126.10	159.93	47.88	-6	-7	6	475.96	605.84	56.47
1	-16	6	66.58	80.09	105.71	4	-11	6	20.29	65.99	89.50	-5	-7	6	250.42	235.67	47.34
-4	-15	6	122.91	225.43	62.70	5	-11	6	11.17	35.23	91.00	-4	-7	6	1656.63	1815.04	113.81
-3	-15	6	13.48	-114.60	109.30	6	-11	6	17.36	-7.00	103.77	-3	-7	6	91.79	137.91	24.76
-2	-15	6	121.90	233.05	56.49	-7	-10	6	140.42	22.33	118.69	-2	-7	6	394.96	500.22	48.17
-1	-15	6	169.22	234.04	62.41	-6	-10	6	3.37	-102.48	101.43	-1	-7	6	2.63	-114.32	52.91
0	-15	6	281.72	174.87	62.13	-5	-10	6	978.70	925.03	83.11	0	-7	6	527.68	527.72	50.79
1	-15	6	43.71	67.81	101.86	-4	-10	6	64.34	-115.57	86.62	1	-7	6	1055.03	3671.40	155.25
2	-15	6	622.04	513.98	72.05	-3	-10	6	488.09	528.04	51.47	2	-7	6	287.17	206.58	36.75
3	-15	6	31.70	146.08	60.80	-2	-10	6	0.27	-15.77	72.02	3	-7	6	1657.51	3517.68	154.90
-5	-14	6	305.26	286.45	66.57	-1	-10	6	230.33	247.38	42.55	4	-7	6	2397.67	2448.09	131.65
-4	-14	6	11.51	17.23	101.22	0	-10	6	3401.53	3428.38	167.16	5	-7	6	309.91	378.51	48.47
-3	-14	6	514.35	442.79	67.89	1	-10	6	6.33	108.13	37.78	6	-7	6	1940.64	2025.83	132.41
-2	-14	6	206.23	204.62	59.54	2	-10	6	3765.75	4059.57	187.50	7	-7	6	627.27	787.50	78.92
-1	-14	6	51.50	150.57	54.62	3	-10	6	407.49	452.14	50.86	8	-7	6	16.91	92.73	55.89
0	-14	6	32.76	-10.72	89.03	4	-10	6	0.94	-176.47	80.58	-6	-6	6	11.14	93.90	100.64
1	-14	6	0.14	-136.51	98.61	5	-10	6	591.74	610.92	60.37	-7	-6	6	82.72	11.37	87.38
2	-14	6	0.01	-99.77	100.91	6	-10	6	95.40	-15.20	98.71	-8	-6	6	12.18	35.42	44.13
3	-14	6	18.86	-41.24	95.98	7	-10	6	56.80	-18.47	110.49	-5	-6	6	104.54	11.51	72.47
4	-14	6	5.32	-110.54	109.89	-8	-9	6	4.24	-77.75	104.32	-4	-6	6	627.81	526.79	59.25
-6	-13	6	464.62	396.16	72.40	-7	-9	6	41.93	28.10	58.40	-3	-6	6	510.72	417.89	39.67
-5	-13	6	156.31	143.19	60.27	-6	-9	6	45.96	7.04	93.16	-2	-6	6	1349.50	1379.03	86.64
4	-13	6	458.33	591.78	64.76	-5	-9	6	51.89	43.96	57.19	-1	-6	6	1554.96	1554.84	93.91
-3	-13	6	241.74	235.77	67.68	-4	-9	6	58.66	-47.30	75.89	0	-6	6	6110.27	7316.31	258.98
-2	-13	6	0.00	-74.00	94.09	-3	-9	6	632.83	847.58	86.82	1	-3	6	125.27	122.52	28.27
-1	-13	6	265.62	261.15	55.34	-2	-9	6	64.01	111.28	38.71	2	-6	6	272.42	523.76	64.34
0	-13	6	13.17	-99.28	20.74	-1	-9	6	468.63	498.77	51.23	3	-6	6	57.60	-71.45	56.03
1	-13	6	755.51	713.63	65.08	0	-9	6	845.38	841.58	65.02	4	-6	6	68.17	62.54	35.65
2	-13	6	425.30	392.16	58.57	1	-9	6	339.85	384.61	43.39	5	-6	6	313.79	316.40	42.77
3	-13	6	311.75	310.82	59.31	2	-9	6	1092.39	1842.35	113.56	6	-6	6	204.72	264.46	49.07
4	-13	6	649.87	564.93	63.01	3	-9	6	307.96	326.39	44.15	7	-6	6	438.81	376.75	56.69
5	-13	6	1.24	28.64	102.31	4	-9	6	414.38	331.76	48.96	8	-6	6	60.16	98.63	54.11
-6	-12	6	113.01	147.57	62.26	5	-9	6	511.55	514.56	55.02	-7	-5	6	191.10	123.42	64.48
-5	-12	6	87.75	37.88	100.77	6	-9	6	6.66	24.74	62.35	-8	-5	6	5.41	-10.92	99.22
-4	-12	6	4.99	-158.26	95.83	7	-9	6	217.85	123.07	61.18	-7	-5	6	72.75	46.19	51.71
-3	-12	6	73.39	211.21	50.74	8	-9	6	56.34	-7.04	106.82	-6	-5	6	1.92	13.15	78.59
-2	-12	6	213.35	258.00	50.61	-8	-8	6	2.65	45.83	123.06	-5	-5	6	1789.09	1621.69	109.58
-1	-12	6	7.86	47.99	82.13	-7	-8	6	129.98	-67.02	97.93	-4	-5	6	2477.94	2540.02	128.18
0	-12	6	126.59	190.72	47.11	-6	-8	6	37.46	19.41	47.18	-3	-5	6	966.09	1045.40	79.09
1	-12	6	456.07	454.21	58.53	-5	-8	6	188.84	202.18	48.11	-2	-5	6	935.61	1123.03	73.32
2	-12	6	358.47	324.92	53.64	-4	-8	6	558.07	421.65	48.16	-1	-5	6	775.29	843.20	66.23
3	-12	6	1306.37	1183.56	66.53	-3	-8	6	1323.92	1518.55	107.07	0	-5	6	726.58	979.75	66.84
4	-12	6	136.74	18.24	99.11	-2	-8	6	25.54	-38.76	60.76	1	-5	6	1203.27	1321.88	126.15
5	-12	6	110.89	187.95	55.35	-1	-8	6	634.40	532.32	44.76	2	-5	6	8.31	-71.96	47.29
6	-12	6	109.17	149.93	62.03	0	-8	6	218.46	84.03	36.18	3	-5	6	1349.93	1700.08	92.80
-7	-11	6	42.05	95.16	103.83	1	-8	6	338.23	372.91	40.25	4	-5	6	2168.32	2257.58	117.24
-6	-11	6	538.03	371.33	67.03	2	-8	6	745.87	634.81	51.74	5	-5	6	58.55	32.72	69.74
-5	-11	6	100.73	59.29	96.45	3	-8	6	167.17	217.73	41.51	6	-5	6	949.62	893.52	66.97
-4	-11	6	573.23	689.54	60.87	4	-8	6	56.37	31.63	41.04	7	-5	6	313.07	759.44	71.67
-3	-11	6	84.76	56.78	47.38	5	-8	6	7.29	14.36	74.28	8	-5	6	523.15	532.59	61.76
-2	-11	6	67.54	46.90	75.10	6	-8	6	18.45	57.75	81.37	9	-5	6	609.21	646.10	69.13
-1	-11	6	7.96	-26.93	78.20	7	-8	6	147.16	91.04	54.13	-8	-4	6	202.09	223.20	58.66
0	-11	6	8.43	-62.23	79.00	8	-8	6	509.18	317.26	66.53	-7	-4	6	5.40	63.94	84.64
1	-11	6	180.56	154.57	45.11	-8	-7	6	35.18	84.99	133.99	-6	-4	6	684.99	720.59	67.74

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-5	-4	6	2031.46	2132.69	124.94	-7	-1	6	2473.63	2853.34	154.87	9	1	6	518.27	613.81	62.67
-4	-4	6	14.26	14.95	58.01	-6	-1	6	874.24	882.96	91.23	10	1	6	60.91	88.04	108.78
-3	-4	6	2079.15	2310.89	113.73	-5	-1	6	12.83	19.42	59.46	-8	2	6	427.98	344.72	62.83
-2	-4	6	168.14	232.10	28.65	-4	-1	6	2070.33	1900.36	105.90	-7	2	6	42.59	75.61	84.55
-1	-4	6	1015.35	1216.96	73.78	-3	-1	6	2281.84	2375.42	109.27	-6	3	6	905.11	1003.71	96.96
0	-4	6	1110.70	1099.16	67.03	-2	-1	6	284.28	232.99	26.37	-5	2	6	3.52	3.60	37.47
1	-4	6	2526.72	2827.87	117.54	-1	-1	6	1117.75	1061.42	63.49	-4	2	6	1.22	10.53	29.78
2	-4	6	4897.28	5038.39	182.97	0	-1	6	3787.93	-1672.62	160.31*	-3	2	6	1437.68	1266.20	78.61
3	-4	6	1364.39	1459.25	81.73	1	-1	6	10387.87	10834.59	348.27	-2	2	6	413.83	439.52	37.64
4	-4	6	361.06	209.67	32.49	2	-1	6	78.74	56.08	19.97	-1	2	6	167.85	177.82	23.98
5	-4	6	1649.10	1507.29	99.28	3	-1	6	10648.39	11321.64	368.17	0	2	6	7509.42	6637.10	225.69
6	-4	6	1448.32	1872.22	117.07	4	-1	6	359.53	378.46	32.75	1	2	6	1083.27	992.84	56.02
7	-4	6	343.53	328.84	51.21	5	-1	6	1645.86	2396.14	93.96	2	2	6	4334.92	4329.25	154.84
8	-4	6	387.69	399.01	58.34	6	-1	6	983.68	886.52	86.61	3	2	6	103.22	113.04	22.81
9	-4	6	0.20	-29.30	100.44	7	-1	6	608.55	638.23	62.59	4	2	6	15611.38	15714.54	504.67
-9	-3	6	49.31	3.33	103.85	8	-1	6	454.40	316.63	55.22	5	2	6	8.50	-59.23	53.18
-8	-3	6	4.35	89.85	50.80	9	-1	6	54.05	56.56	66.02	6	2	6	78.70	98.43	35.46
-7	-3	6	39.37	74.79	85.22	10	-1	6	11.99	-84.19	109.66	7	2	6	188.41	195.89	43.85
-6	-3	6	228.99	161.83	45.77	-9	0	6	25.56	66.24	75.47	8	2	6	93.37	225.89	45.85
-5	-3	6	18.73	15.46	63.74	-8	0	6	1.03	-6.68	63.55	9	2	6	21.00	35.22	90.96
-4	-3	6	190.99	170.14	33.67	-7	0	6	203.38	239.38	36.06	10	2	6	1.18	-270.59	109.61
-3	-3	6	118.16	126.02	29.65	-6	0	6	107.77	106.43	29.37	-8	3	6	16.34	-21.82	96.83
-2	-3	6	2379.26	2280.81	104.98	-5	0	6	5.59	-14.54	35.05	-7	3	6	19.30	-24.63	82.21
-1	-3	6	3025.23	2469.84	107.83	-4	0	6	35.26	4.23	37.99	-6	3	6	82.11	38.32	43.80
0	-3	6	2279.33	2105.84	95.88	-3	0	6	1946.82	2067.33	79.31	-5	3	6	46.89	28.92	68.43
1	-3	6	3029.76	2572.59	107.69	-2	0	6	4321.17	4164.89	110.77	-4	3	6	67.23	60.57	61.17
2	-3	6	520.34	525.37	50.01	-1	0	6	1899.64	1930.92	61.45	-3	3	6	482.65	403.85	35.50
3	-3	6	158.13	149.47	35.31	0	0	6	867.37	172.27	70.04*	-2	3	6	742.86	801.08	63.33
4	-3	6	244.43	165.08	30.74	1	0	6	3979.51	3752.05	98.24	-1	3	6	5487.57	5405.86	193.24
5	-3	6	16.91	67.27	32.91	2	0	6	12536.13	11872.15	768.38	0	3	6	4807.60	5164.92	184.02
6	-3	6	460.56	446.59	43.65	3	0	6	2846.98	3057.21	86.00	1	3	6	2281.06	2341.08	96.50
7	-3	6	185.83	263.71	47.15	4	0	6	9619.14	9192.90	218.91	2	3	6	182.48	236.38	23.67
8	-3	6	75.80	54.83	49.26	5	0	6	9.60	-8.91	34.82	3	3	6	8251.86	8006.05	269.57
9	-3	6	1.42	-48.93	96.20	6	0	6	29.16	23.66	61.45	4	3	6	963.75	1044.13	70.64
-9	-2	6	0.56	-135.62	108.37	7	0	6	179.11	159.87	30.23	5	3	6	385.55	308.94	35.91
-8	-2	6	18.13	-133.28	97.90	8	0	6	16.32	100.74	47.41	6	3	6	340.88	292.23	39.11
-7	-2	6	209.29	76.62	32.64	9	0	6	163.12	121.89	40.50	7	3	6	172.78	234.12	42.13
-6	-2	6	1944.63	2013.98	127.65	10	0	6	98.85	171.05	43.23	8	3	6	196.14	250.64	49.51
-5	-2	6	337.06	62.94	40.49	-8	1	6	1.30	-107.46	94.54	9	3	6	19.49	-19.64	93.54
-4	-2	6	297.13	289.42	35.34	-7	1	6	1510.67	1386.21	122.10	10	3	6	124.73	58.43	112.76
-3	-2	6	8423.44	7763.39	270.28	-6	1	6	79.83	93.50	42.75	-8	4	6	0.16	12.85	53.91
-2	-2	6	2445.25	2153.92	38.64	-5	1	6	2142.28	2129.08	117.28	-7	4	6	128.19	25.00	89.46
-1	-2	6	4514.05	4263.04	157.23	-4	1	6	1519.73	1479.23	88.91	-6	4	6	1410.94	1524.26	114.93
0	-2	6	10035.23	9926.50	324.81	-3	1	6	2802.82	2693.58	119.42	-5	4	6	143.43	131.52	40.27
1	-2	6	1842.76	2128.40	89.76	-2	1	6	5805.39	5647.85	201.07	-4	4	6	4841.21	4939.78	197.18
2	-2	6	633.62	520.80	48.56	-1	1	6	1816.05	1508.49	73.81	-3	4	6	275.32	298.11	32.16
3	-2	6	6046.92	6645.05	230.65	0	1	6	4853.09	4395.63	161.00	-2	4	6	3485.95	3597.84	145.97
4	-2	6	3.31	-3.77	43.74	1	1	6	8132.36	7579.48	250.41	-1	4	6	500.45	575.30	53.10
5	-2	6	105.52	177.93	31.96	2	1	6	389.12	288.36	28.84	0	4	6	744.91	678.77	56.47
6	-2	6	27.73	81.50	34.66	3	1	6	2604.38	2363.34	100.26	1	4	6	659.93	731.18	54.23
7	-2	6	1310.64	1441.75	108.50	4	1	6	1.93	-18.06	46.42	2	4	6	4847.28	4398.12	159.19
8	-2	6	99.54	94.07	50.14	5	1	6	4585.92	4262.46	169.55	3	4	6	1897.57	1906.36	90.40
9	-2	6	494.38	557.42	61.64	6	1	6	679.93	569.17	53.19	4	4	6	1554.05	1596.91	87.60
-9	-1	6	190.13	65.37	113.90	7	1	6	292.66	268.72	44.15	5	4	6	4.24	39.12	31.14
-8	-1	6	2.44	-64.87	92.39	8	1	6	1026.46	1063.95	108.70	6	4	6	5452.43	4965.68	201.32

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
7	4	6	1759.43	1634.44	113.23	7	7	6	617.28	645.65	66.05	-3	11	6	261.66	266.06	48.27
8	4	6	0.18	-122.11	84.19	8	7	6	1417.27	1576.98	133.89	-3	11	6	475.45	462.24	49.05
9	4	6	474.65	462.92	62.38	9	7	6	5.67	80.95	105.18	-1	11	6	18.40	-32.64	74.08
10	4	6	100.55	84.01	118.13	-7	8	6	137.27	67.16	107.07	0	11	6	1011.63	775.47	70.80
-8	5	6	63.97	52.85	193.92	-6	8	6	952.99	1051.58	90.33	2	11	6	8.56	27.97	69.58
-7	5	6	706.51	828.87	77.47	-5	8	6	268.91	248.09	51.56	3	11	6	697.74	636.90	60.34
-6	5	6	56.30	56.67	44.43	-4	8	6	277.87	292.14	47.50	3	11	6	79.08	134.77	41.45
-5	5	6	210.51	160.75	43.59	-3	8	6	669.91	632.92	60.15	4	11	6	5.73	-19.35	73.85
-4	5	6	5.08	14.49	60.16	-2	8	6	0.05	-90.16	60.45	5	11	6	237.46	277.01	49.37
-3	5	6	0.21	-1.65	36.41	-1	8	6	1722.69	1733.42	104.22	6	11	6	99.47	12.67	64.38
-2	5	6	97.53	109.36	27.00	0	8	6	371.93	347.73	38.82	7	11	6	150.10	155.48	57.62
-1	5	6	200.44	199.23	27.85	1	8	6	2946.78	2444.03	118.98	8	11	6	221.44	111.41	114.46
0	5	6	3061.44	2822.03	122.03	2	8	6	1195.26	1064.85	78.54	-5	12	6	37.38	-64.00	97.16
1	5	6	325.83	245.57	26.10	3	8	6	26.07	11.29	54.27	-4	12	6	12.85	-13.40	97.64
2	5	6	5156.42	5871.29	207.18	4	8	6	85.10	34.65	57.29	-3	12	6	399.54	460.88	56.58
3	5	6	14307.09	14581.41	470.49	5	8	6	224.44	186.65	41.02	-2	12	6	289.05	307.62	52.80
4	5	6	8.32	-32.34	51.62	6	8	6	24.96	30.54	75.02	-1	12	6	836.35	1112.77	27.26
5	5	6	1157.49	1181.63	85.06	7	8	6	16.63	20.47	81.70	0	12	6	937.69	1004.09	181.07
6	5	6	529.07	602.71	53.82	8	8	6	12.87	46.09	86.44	1	12	6	1867.95	1826.77	121.47
7	5	6	21.55	26.16	75.20	9	8	6	4.55	21.07	105.59	2	12	6	71.20	53.03	74.52
8	5	6	137.64	162.92	52.91	-7	9	6	41.66	84.68	99.44	3	12	6	42.25	117.07	43.12
9	5	6	117.11	160.76	54.41	-6	9	6	4.78	64.37	85.09	4	12	6	15.75	6.15	80.24
10	5	6	23.77	20.31	64.34	-5	9	6	83.87	69.15	50.47	5	12	6	1.14	55.38	92.43
-8	6	6	16.47	21.21	74.06	-4	9	6	22.81	-10.24	86.83	6	12	6	1.38	56.53	51.86
-7	6	6	79.97	44.88	93.15	-3	9	6	351.41	438.76	45.36	7	12	6	15.29	9.43	101.04
-6	6	6	205.58	206.37	47.84	-2	9	6	2055.72	2208.29	128.68	8	12	6	223.55	234.87	166.65
-5	6	6	0.24	78.80	40.67	-1	9	6	144.58	116.41	37.33	-4	13	6	2.54	-58.59	106.52
-4	6	6	9.64	-155.09	68.52	0	9	6	4346.61	4519.52	191.39	-3	13	6	686.22	701.67	66.58
-3	6	6	6.53	14.81	58.52	1	9	6	206.74	122.05	36.64	-2	13	6	203.87	238.07	52.22
-2	6	6	200.01	57.65	29.83	2	9	6	1936.24	1925.10	105.71	-1	13	6	69.66	-141.93	86.96
-1	6	6	2398.90	2884.42	119.74	3	9	6	688.44	713.52	56.05	0	13	6	513.10	410.79	55.18
0	6	6	643.17	615.57	45.60	4	9	6	331.65	362.46	40.76	1	13	6	232.21	7.59	88.27
1	6	6	1953.04	1977.95	95.48	5	9	6	60.18	20.01	66.96	2	13	6	2.61	-7.29	78.61
2	6	6	4332.75	4852.20	180.23	6	9	6	382.67	425.31	49.04	3	13	6	5.13	-73.60	92.61
3	6	6	80.54	127.33	29.13	7	9	6	51.87	33.08	49.57	4	13	6	194.98	251.96	53.30
4	6	6	1566.27	1431.10	92.74	8	9	6	71.07	57.72	70.59	5	13	6	670.54	779.50	66.25
5	6	6	1691.53	1781.45	107.24	9	9	6	96.08	15.70	109.25	6	13	6	136.11	172.93	58.10
6	6	6	230.85	200.34	42.84	-6	10	6	327.71	380.94	60.27	7	13	6	477.26	441.09	69.23
7	6	6	719.03	738.91	71.26	-5	10	6	54.30	-161.08	98.91	-4	14	6	16.63	-1.54	113.49
8	6	6	75.07	169.94	48.20	-4	10	6	2113.58	2219.47	139.67	-3	14	6	14.78	-56.70	105.58
9	6	6	226.32	222.08	59.54	-3	10	6	41.39	-6.18	70.76	-2	14	6	53.94	61.72	93.72
-7	7	6	94.80	47.85	69.88	-2	10	6	991.34	813.82	69.42	-1	14	6	0.81	0.99	92.68
-6	7	6	83.89	101.68	53.04	-1	10	6	748.25	601.21	61.97	0	14	6	72.34	-57.81	96.13
-5	7	6	2309.38	2225.68	136.43	0	10	6	79.00	67.05	3.61	1	14	6	228.41	294.52	55.97
-4	7	6	195.68	214.21	42.09	1	10	6	308.01	212.21	33.19	2	14	6	3.41	41.25	91.17
-3	7	6	2554.69	2569.74	131.97	2	10	6	403.89	425.44	42.41	3	14	6	34.43	59.10	92.64
-2	7	6	2537.43	1497.07	92.60	3	10	6	304.84	190.84	42.32	4	14	6	2.83	-205.42	95.90
-1	7	6	700.44	689.04	71.67	4	10	6	55.83	-97.39	75.11	5	14	6	5.18	40.69	68.82
0	7	6	762.89	874.48	72.49	5	10	6	146.61	226.17	44.13	6	14	6	252.48	229.18	65.14
1	7	6	454.22	402.89	34.20	6	10	6	1752.08	2084.34	131.47	-3	15	6	74.66	-115.25	110.36
2	7	6	309.14	392.38	39.11	7	10	6	182.52	229.89	54.98	-2	15	6	144.76	104.63	108.69
3	7	6	50.36	59.32	29.44	8	10	6	573.65	551.81	67.70	-1	15	6	702.11	690.39	70.39
4	7	6	2019.77	2082.09	110.37	-6	11	6	60.49	28.00	107.39	0	15	6	648.57	628.50	69.66
5	7	6	3904.00	3518.57	158.57	-5	11	6	233.85	361.53	61.44	1	15	6	730.19	707.07	67.21
6	7	6	2599.62	2517.28	138.77	-4	11	6	2.32	-103.95	90.57	2	15	6	560.62	623.39	62.97

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
3	15	6	11.43	-189.24	103.79	-4	-11	7	31.12	54.05	50.31	6	-8	7	125.36	89.19	52.93
4	15	6	88.53	167.60	57.82	-3	-11	7	152.36	185.85	48.37	7	-8	7	2.17	-45.80	95.9F
5	15	6	273.65	308.22	67.40	-2	-11	7	136.24	203.25	49.13	8	-8	7	0.69	79.73	101.44
6	15	6	158.31	19.09	113.21	-1	-11	7	383.57	394.16	51.56	-8	-7	7	4.34	-19.89	107.37
-1	16	6	145.34	81.51	107.94	0	-11	7	7.07	9.60	79.01	-7	-7	7	11.39	23.29	66.65
0	16	6	46.58	-13.62	112.98	1	-11	7	211.68	167.08	49.18	-6	-7	7	308.33	388.60	94.41
1	16	6	79.56	-129.48	102.17	2	-11	7	1290.15	1568.68	124.87	-5	-7	7	37.04	62.58	72.97
2	16	6	10.70	-17.49	111.08	3	-11	7	60.65	69.56	49.64	-4	-7	7	996.05	956.17	70.44
3	16	6	26.51	24.97	60.43	4	-11	7	1034.52	1192.33	114.99	-3	-7	7	2095.96	2200.31	124.17
4	16	6	84.32	72.35	61.37	5	-11	7	67.22	71.97	55.04	-2	-7	7	415.35	307.55	41.41
2	17	6	419.87	316.78	69.01	6	-11	7	83.27	56.87	62.33	-1	-7	7	2716.14	3188.81	146.50
-1	-16	7	165.70	304.41	66.92	-7	-10	7	47.56	-33.98	100.49	0	-7	7	422.51	368.94	37.95
0	-16	7	141.95	207.28	67.43	-6	-10	7	0.19	-12.22	98.62	1	-7	7	1911.63	1812.54	107.92
-3	-15	7	267.85	255.35	66.67	-5	-10	7	298.19	12.01	107.47	2	-7	7	101.18	114.29	34.04
-2	-15	7	0.20	-16.55	102.42	-4	-10	7	470.49	502.49	58.36	3	-7	7	413.50	520.58	53.67
-1	-15	7	152.03	81.56	107.62	-3	-10	7	6.59	39.22	78.94	4	-7	7	1289.28	1402.90	101.29
0	-15	7	37.38	45.77	87.23	-2	-10	7	1231.48	1364.81	112.47	5	-7	7	74.26	-19.83	77.52
1	-15	7	3.01	-6.79	134.35	-1	-10	7	185.49	189.01	41.96	6	-7	7	235.00	232.56	52.32
2	-15	7	140.89	-176.04	122.05	0	-10	7	435.72	532.74	54.30	7	-7	7	19.93	24.16	96.95
3	-15	7	99.64	-278.58	122.57	1	-10	7	48.22	74.72	43.04	8	-7	7	19.48	-32.72	100.84
-4	-14	7	41.35	102.18	111.15	2	-10	7	177.29	227.04	46.79	-8	-6	7	176.83	33.75	61.93
-3	-14	7	97.34	-133.61	106.56	3	-10	7	123.84	197.44	44.92	-7	-6	7	17.27	206.96	51.19
-2	-14	7	128.52	146.61	58.90	4	-10	7	45.81	41.65	80.92	-6	-6	7	64.69	0.45	85.13
-1	-14	7	24.28	91.14	91.95	5	-10	7	384.42	413.39	57.84	-5	-6	7	138.19	64.24	79.46
0	-14	7	337.42	185.12	51.94	6	-10	7	1.85	-13.19	94.19	-4	-6	7	296.44	347.18	44.36
1	-14	7	191.27	247.32	39.37	7	-10	7	3.03	-62.29	102.03	-3	-6	7	1037.17	1008.23	87.15
2	-14	7	2.86	-63.71	99.89	-7	-9	7	32.97	5.57	103.94	-2	-6	7	1291.61	1355.87	89.96
3	-14	7	601.22	476.55	64.99	-6	-9	7	63.79	121.24	55.11	-1	-6	7	998.06	1117.69	82.20
4	-14	7	158.18	102.55	106.58	-5	-9	7	0.33	-21.62	88.88	0	-6	7	376.32	314.27	37.77
-5	-13	7	155.00	-33.43	115.25	-4	-9	7	464.27	437.50	51.85	1	-6	7	40.25	36.62	50.92
-4	-13	7	219.26	42.99	114.24	-3	-9	7	408.03	519.11	49.02	2	-6	7	1512.72	1850.66	100.96
-3	-13	7	760.74	904.99	86.12	-2	-9	7	1047.70	1154.34	92.41	3	-6	7	780.67	956.90	78.23
-2	-13	7	69.66	-158.08	102.12	-1	-9	7	1222.32	1117.74	99.46	4	-6	7	482.38	698.45	56.28
-1	-13	7	708.43	770.70	68.42	0	-9	7	515.21	372.77	44.85	5	-6	7	4235.82	4771.75	201.80
0	-13	7	319.15	318.31	59.48	1	-9	7	192.19	205.05	42.37	6	-6	7	128.72	27.03	82.58
1	-13	7	164.87	186.60	56.06	2	-9	7	2.06	-19.35	64.39	7	-6	7	616.95	678.60	62.47
2	-13	7	11.88	57.46	61.43	3	-9	7	331.09	384.82	46.26	8	-6	7	162.43	-108.78	105.65
3	-13	7	4.15	-58.49	98.12	4	-9	7	762.75	852.98	70.21	9	-6	7	1.94	64.28	109.81
4	-13	7	185.02	-113.56	108.06	5	-9	7	179.45	52.46	84.18	-8	-5	7	0.65	71.61	96.30
5	-13	7	22.72	-43.23	109.27	6	-9	7	674.37	754.50	78.07	-7	-5	7	398.12	426.84	55.06
6	-12	7	35.30	64.73	104.77	7	-9	7	93.52	28.85	105.03	-6	-5	7	2.23	99.57	44.28
-5	-12	7	116.70	72.49	59.86	-8	-8	7	161.76	151.58	66.61	-5	-5	7	176.47	226.65	43.08
-4	-12	7	424.39	356.81	61.09	-7	-8	7	232.60	165.29	63.02	-4	-5	7	46.27	30.38	48.51
-3	-12	7	118.87	-33.81	92.83	-6	-8	7	7.83	-17.85	91.78	-3	-5	7	47.98	32.41	34.01
-2	-12	7	281.04	365.20	58.26	-5	-8	7	493.06	431.62	54.20	-2	-5	7	381.14	371.20	36.69
-1	-12	7	35.19	14.63	89.78	-4	-8	7	159.60	186.36	47.09	-1	-5	7	28.90	91.39	25.98
0	-12	7	115.44	52.13	49.96	-3	-8	7	0.78	-6.84	70.97	0	-5	7	4919.02	5505.27	206.27
1	-12	7	815.15	868.04	80.55	-2	-8	7	159.41	143.59	39.32	1	-5	7	5135.85	5208.91	195.60
2	-12	7	11.90	-165.31	91.17	-1	-8	7	1229.28	1263.14	92.81	2	-5	7	519.95	500.75	42.68
3	-12	7	368.96	387.61	57.99	0	-8	7	1162.69	989.14	84.12	3	-5	7	808.84	581.45	48.06
4	-12	7	40.17	-147.38	96.41	1	-8	7	68.43	55.48	67.04	4	-5	7	2901.58	3168.17	243.35
5	-12	7	317.91	199.11	62.50	2	-8	7	2310.74	2106.70	117.54	5	-5	7	18.02	14.64	64.78
6	-12	7	313.73	184.21	66.82	3	-8	7	2675.69	2953.15	144.94	6	-5	7	153.60	10.12	72.01
-6	-11	7	197.32	-172.78	120.87	4	-8	7	48.60	42.82	40.75	7	-5	7	7.46	-139.67	83.89
-5	-11	7	153.85	263.41	58.48	5	-8	7	971.60	1073.00	108.48	8	-5	7	222.26	188.55	58.20

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
8	-5	7	119.87	135.76	63.00	-8	-1	7	50.95	57.94	96.23	9	1	7	100.20	280.43	59.11
-8	-4	7	109.80	17.03	109.93	-7	-1	7	0.06	78.55	86.53	10	1	7	21.23	78.09	118.61
-7	-4	7	99.82	151.99	52.18	-6	-1	7	1737.17	1683.47	122.73	-8	2	7	19.64	74.51	95.63
-6	-4	7	66.88	21.96	93.93	-5	-1	7	187.92	174.56	40.77	-7	2	7	121.00	250.84	55.09
-5	-4	7	900.63	1260.56	98.13	-4	-1	7	3581.61	3951.65	166.55	-1	2	7	203.48	8.54	82.06
-4	-4	7	0.06	-27.21	60.33	-3	-1	7	155.16	209.54	31.82	-5	2	7	1207.30	3110.02	153.33
-3	-4	7	839.99	867.91	76.90	-2	-1	7	1722.39	2225.64	103.59	-4	2	7	114.78	1144.95	89.38
-2	-4	7	6443.53	6401.13	232.42	-1	-1	7	6218.29	6769.67	235.12	-3	2	7	4047.72	6078.21	224.72
-1	-4	7	1823.94	1941.15	97.54	0	-1	7	2.47	-4469.24	150.72*	2	2	7	2052.20	2161.95	102.87
0	-4	7	7259.71	7760.04	269.04	1	-1	7	1271.90	3197.59	135.47	-1	2	7	2670.05	3017.82	124.59
1	-4	7	1698.24	1738.30	89.20	2	-1	7	124.19	464.78	46.76	0	2	7	1839.54	2167.93	97.88
2	-4	7	831.03	980.82	67.46	3	-1	7	171.63	147.74	26.95	1	2	7	1181.66	1340.75	70.29
3	-4	7	875.90	906.08	66.92	4	-1	7	84.76	81.76	28.48	2	2	7	1057.69	1040.90	61.98
4	-4	7	111.82	46.89	53.13	5	-1	7	0.08	-54.60	54.27	3	2	7	65.99	24.71	30.61
5	-4	7	1800.58	1772.29	110.36	6	-1	7	268.64	316.42	39.23	4	2	7	890.73	1076.36	74.34
6	-4	7	147.89	331.07	43.02	7	-1	7	26.09	29.17	42.23	5	2	7	76.43	114.71	31.78
7	-4	7	34.34	-48.53	78.78	8	-1	7	42.83	78.93	82.31	6	2	7	23.87	-55.58	61.49
8	-4	7	134.31	72.14	93.75	9	-1	7	150.41	16.12	99.49	7	2	7	449.86	428.00	42.38
9	-4	7	14.82	71.51	59.42	10	-1	7	6.86	72.67	111.62	8	2	7	326.50	300.69	53.19
-8	-3	7	44.89	-121.59	103.01	-8	0	7	44.02	-102.84	146.77	9	2	7	237.39	199.82	57.14
-7	-3	7	347.06	237.32	53.91	-7	0	7	141.79	237.25	37.48	10	2	7	436.40	395.10	67.39
-6	-3	7	5.07	18.87	77.39	-6	0	7	706.82	737.65	49.05	-8	3	7	15.72	-6.10	99.43
-5	-3	7	1783.24	1621.51	114.73	-5	0	7	1262.62	1331.47	70.77	-7	3	7	284.08	367.25	53.44
-4	-3	7	2095.03	2063.87	110.82	-4	0	7	74.29	84.03	25.50	-6	3	7	311.01	279.27	52.03
-3	-3	7	2177.64	1841.10	102.86	-3	0	7	775.75	712.62	47.36	-5	3	7	1598.37	1723.03	118.02
-2	-3	7	297.16	501.00	43.56	-2	0	7	994.43	770.64	72.39	-4	3	7	2088.54	2095.41	115.67
-1	-3	7	2052.13	1798.80	92.87	-1	0	7	4919.23	4851.33	125.38	-3	3	7	2566.48	2600.73	122.89
0	-3	7	868.32	923.65	65.64	0	0	7	1452.45	-292.92	157.83*	-2	3	7	7154.08	7538.27	264.39
1	-3	7	29.44	18.68	24.05	1	0	7	962.33	766.29	37.93	-1	3	7	248.76	220.78	28.70
2	-3	7	124.78	87.60	25.09	2	0	7	4402.02	4732.42	120.11	0	3	7	1641.95	1830.19	91.09
3	-3	7	1093.72	1199.68	75.04	3	0	7	511.16	653.01	38.01	1	3	7	331.07	345.04	34.85
4	-3	7	2097.35	2011.66	103.04	4	0	7	1208.88	1297.29	103.22	2	3	7	3597.47	3599.66	137.56
5	-3	7	406.51	175.03	41.42	5	0	7	2618.78	2382.81	83.52	3	3	7	4792.33	4504.38	167.80
6	-3	7	1888.71	1871.09	118.27	6	0	7	294.40	349.08	44.24	4	3	7	473.68	386.92	33.20
7	-3	7	1.72	-85.06	79.21	7	0	7	2864.90	2843.89	106.85	5	3	7	5659.53	5881.51	221.03
8	-3	7	419.02	497.48	58.58	8	0	7	3.72	-20.92	56.23	6	3	7	1849.80	1960.94	115.64
9	-3	7	24.21	91.66	56.46	9	0	7	299.69	368.22	41.43	7	3	7	143.03	121.27	42.39
-8	-2	7	629.80	461.17	65.57	10	0	7	77.75	42.91	54.25	4	3	7	1338.57	1542.00	121.06
-7	-2	7	256.63	293.90	74.32	-8	1	7	4.89	-68.72	103.04	9	3	7	113.04	76.18	96.07
-6	-2	7	11.06	-68.76	75.54	-7	1	7	360.68	325.36	58.14	10	3	7	5.46	-51.91	100.46
-5	-2	7	515.08	518.54	48.13	-6	1	7	378.49	405.45	50.72	-8	4	7	55.19	-50.20	104.76
-4	-2	7	326.67	412.03	40.11	-5	1	7	41.44	104.26	37.99	-7	4	7	97.80	63.67	90.67
-3	-2	7	626.15	679.75	63.64	-4	1	7	2.87	-30.55	54.32	-6	4	7	4.11	-84.21	80.44
-2	-2	7	154.33	193.54	28.76	-3	1	7	73.54	71.29	30.02	-5	4	7	281.39	381.75	44.85
-1	-2	7	718.99	724.55	59.31	-2	1	7	10.13	-22.81	43.74	-4	4	7	83.98	-106.21	72.72
0	-2	7	6048.82	5131.60	210.95	-1	1	7	2275.13	2420.01	104.61	-3	4	7	308.64	335.80	34.19
1	-2	7	1574.54	1403.54	74.07	0	1	7	347.95	3264.24	125.74*	-2	4	7	420.29	430.79	42.30
2	-2	7	1774.84	1978.53	90.66	1	1	7	4156.87	4360.73	158.23	-1	4	7	9463.62	8506.97	293.71
3	-2	7	6346.18	5193.19	190.15	2	1	7	5607.82	5193.65	183.16	0	4	7	6617.52	7334.60	285.37
4	-2	7	17.16	16.79	18.11	3	1	7	1741.53	1652.98	84.43	1	4	7	5.62	26.66	40.05
5	-2	7	3147.75	3005.12	139.02	4	1	7	1568.87	1293.89	76.83	2	4	7	1211.19	1346.07	74.26
6	-2	7	17.90	-12.53	60.47	5	1	7	621.75	918.90	46.86	3	4	7	2463.28	2588.49	114.33
7	-2	7	29.56	-34.68	70.68	6	1	7	1226.06	1208.90	91.10	4	4	7	530.62	651.70	60.04
8	-2	7	96.99	77.47	80.83	7	1	7	309.09	326.23	46.59	5	4	7	3808.65	3741.48	158.40
9	-2	7	75.43	183.64	55.88	8	1	7	203.20	297.74	61.48	6	4	7	1.14	48.84	66.01

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
7	4	7	3.14	52.98	41.28	8	7	7	7.22	59.71	92.13	0	11	7	608.35	615.31	55.32
8	4	7	62.31	103.80	45.29	9	7	7	38.00	79.27	58.59	1	11	7	167.03	174.20	43.71
9	4	7	235.16	287.35	59.87	-7	8	7	14.40	1.60	99.04	2	11	7	838.17	818.15	65.64
10	4	7	93.03	197.82	62.36	-6	8	7	0.51	8.24	93.13	3	11	7	347.95	323.55	48.09
-8	5	7	37.77	26.47	110.15	-5	8	7	0.36	-86.89	89.44	4	11	7	28.88	9.64	78.54
-7	5	7	14.46	-50.43	91.86	-4	8	7	640.27	673.68	66.04	5	11	7	49.37	72.57	20.55
-6	5	7	229.80	249.27	50.98	-3	8	7	987.52	891.33	69.25	6	11	7	19.39	79.72	89.49
-5	5	7	761.42	696.24	64.65	-2	8	7	524.45	577.54	56.68	7	11	7	31.23	-44.00	99.54
-4	5	7	1648.90	1675.87	112.30	-1	8	7	2552.50	2583.02	132.37	8	11	7	113.94	161.36	60.33
-3	5	7	1768.88	1604.53	102.47	0	8	7	885.86	875.70	83.18	-5	12	7	5.41	5.29	102.09
-2	5	7	2388.02	2261.70	112.19	1	8	7	258.55	217.48	35.44	-4	12	7	264.97	334.78	58.27
-1	5	7	29.68	31.83	47.81	2	8	7	1234.74	1458.73	69.56	-3	12	7	252.43	241.12	55.38
0	5	7	857.33	1024.42	72.32	3	8	7	241.20	196.56	34.72	-2	12	7	355.12	479.55	53.78
1	5	7	1969.00	2104.92	99.34	4	8	7	294.62	237.73	40.11	-1	12	7	155.24	48.81	86.95
2	5	7	214.22	196.03	26.90	5	3	7	89.31	72.79	39.56	0	12	7	116.11	165.47	48.32
3	5	7	564.19	539.96	44.33	6	8	7	1.41	-32.27	74.39	1	12	7	221.89	150.47	49.59
4	5	7	13.74	-111.86	53.66	7	8	7	103.28	26.34	59.34	2	12	7	114.17	147.89	45.89
5	5	7	120.14	110.05	33.84	8	8	7	26.40	34.60	95.62	3	12	7	591.58	607.41	57.17
6	5	7	46.02	74.03	39.04	9	8	7	357.90	74.90	115.46	4	12	7	712.06	727.81	61.98
7	5	7	178.98	204.70	46.71	-6	9	7	8.13	-17.14	99.91	5	12	7	37.72	17.79	85.29
8	5	7	484.33	427.81	55.90	-5	9	7	982.77	837.36	84.57	6	12	7	426.56	497.44	62.32
9	5	7	349.17	284.81	60.53	-4	9	7	705.19	636.55	58.88	7	12	7	322.09	405.00	64.07
10	5	7	65.04	30.68	110.73	-3	9	7	345.39	396.24	47.51	8	12	7	27.20	-99.64	121.56
-7	6	7	12.84	13.03	93.49	-2	9	7	1181.28	1325.22	105.24	-4	13	7	5.26	-53.02	101.27
-6	6	7	470.57	523.04	56.29	-1	9	7	384.07	417.78	46.02	-3	13	7	42.11	-36.47	99.58
-5	6	7	739.56	826.65	70.05	0	9	7	11.34	-51.91	70.93	-2	13	7	104.76	16.73	90.59
-4	6	7	1900.86	2017.55	126.07	1	9	7	367.37	423.75	42.17	-1	13	7	205.98	38.77	101.16
-3	6	7	2580.79	3112.80	145.99	2	9	7	500.49	494.54	42.18	0	13	7	815.53	617.97	66.60
-2	6	7	1253.01	1256.13	86.67	3	9	7	298.80	228.23	41.32	1	13	7	187.36	44.33	90.13
-1	6	7	1167.13	1072.37	79.39	4	9	7	219.17	217.57	42.33	2	13	7	656.85	679.88	69.56
0	6	7	60.59	2.94	51.73	5	9	7	170.70	214.08	42.84	3	13	7	499.41	444.32	58.35
1	6	7	1450.75	1374.56	83.05	6	9	7	19.50	45.53	32.55	4	13	7	56.14	59.66	51.07
2	6	7	662.29	705.31	63.14	7	9	7	0.89	-53.69	86.69	5	13	7	344.52	267.29	58.64
3	6	7	1327.25	1431.28	87.41	8	9	7	735.47	760.48	69.15	6	13	7	6.52	8.60	100.98
4	6	7	2683.97	2416.06	113.32	9	9	7	58.00	-68.40	10.74	7	13	7	9.06	-31.31	109.66
5	6	7	158.64	154.91	35.96	-6	10	7	92.32	-65.15	108.54	-3	14	7	15.78	31.14	104.20
6	6	7	3.90	-16.07	71.30	-5	10	7	321.41	228.65	53.17	-2	14	7	164.75	83.42	105.19
7	6	7	2077.70	2014.49	135.40	-4	10	7	17.25	-107.52	86.92	-1	14	7	211.21	250.09	57.23
8	6	7	510.81	392.76	58.89	-3	10	7	317.39	276.41	51.24	0	14	7	5.35	67.45	85.46
9	6	7	146.92	69.66	105.38	-2	10	7	448.20	356.11	51.65	1	14	7	1016.11	971.96	88.10
-7	7	7	101.89	143.10	56.20	-1	10	7	2695.18	2696.09	143.19	2	14	7	183.50	110.49	55.23
-6	7	7	145.37	180.13	53.78	0	10	7	2691.48	2515.99	141.17	3	14	7	188.34	213.68	55.99
-5	7	7	396.88	363.10	53.04	1	10	7	2247.07	2296.12	123.86	4	14	7	131.34	30.30	95.73
-4	7	7	246.48	314.58	45.06	2	10	7	1831.33	1718.18	108.95	5	14	7	19.90	11.19	100.90
-3	7	7	433.05	474.06	43.71	3	10	7	144.89	102.52	40.85	6	14	7	60.70	131.01	87.64
-2	7	7	706.71	566.10	53.00	4	10	7	517.23	430.65	47.75	-2	15	7	263.75	284.19	64.45
-1	7	7	1322.63	1298.09	88.08	5	10	7	104.07	79.79	46.53	-1	15	7	0.41	-149.77	103.34
0	7	7	1401.93	1150.34	84.83	6	10	7	1.50	38.43	77.80	0	15	7	9.87	-42.19	102.56
1	7	7	3037.00	2912.51	130.84	7	10	7	27.15	39.91	90.41	1	15	7	4.70	58.13	93.42
2	7	7	933.21	799.59	70.95	8	10	7	91.42	109.66	59.17	2	15	7	360.79	394.07	62.54
3	7	7	4768.20	4646.15	183.27	-5	11	7	96.55	204.85	58.10	3	15	7	421.85	343.81	63.46
4	7	7	1351.19	1400.91	95.67	-4	11	7	6.51	19.30	90.03	4	15	7	71.37	12.43	108.06
5	7	7	13.58	-90.16	68.25	-3	11	7	175.06	230.77	51.74	5	15	7	387.30	428.19	69.22
6	7	7	26.60	-15.60	69.93	-2	11	7	14.67	13.52	77.62	-1	16	7	144.57	41.97	117.50
7	7	7	3.66	6.54	79.79	-1	11	7	198.75	165.05	47.06	0	16	7	7.03	93.03	106.23

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
1	16	7	626.72	593.39	69.29	-6	-10	8	32.04	-80.35	100.40	3	-7	8	0.24	-43.57	52.58
2	16	7	348.00	288.59	63.93	-5	-10	8	495.33	606.85	61.60	4	-7	8	2320.75	2210.47	127.17
3	16	7	84.55	49.05	105.73	-4	-10	8	63.21	139.20	49.72	5	-7	8	537.19	562.81	51.54
4	16	7	397.73	357.93	70.52	-3	-10	8	871.68	827.21	74.01	6	-7	8	565.29	749.79	74.19
-3	-16	8	1.94	-249.72	115.97	-2	-10	8	172.61	264.29	49.14	7	-7	8	211.33	239.50	55.52
-2	-16	8	23.44	52.47	106.56	-1	-10	8	109.24	-19.90	79.55	8	-7	8	6.65	36.12	101.35
-1	-16	8	57.93	-138.84	108.88	0	-10	8	260.33	187.54	51.41	-8	-6	8	24.85	78.53	105.32
0	-16	8	614.08	709.00	70.13	1	-10	8	203.32	195.86	47.55	-7	-6	8	389.16	435.37	62.27
1	-16	8	17.41	78.94	113.29	2	-10	8	1.83	56.23	82.24	-6	-6	8	7.76	-30.46	91.70
2	-16	8	359.66	309.39	68.62	3	-10	8	540.49	545.39	52.64	-5	-6	8	64.03	174.50	43.86
-4	-14	8	365.90	312.42	71.25	4	-10	8	22.20	-72.50	81.07	-4	-6	8	24.64	76.82	41.67
-3	-14	8	2.61	75.40	60.68	5	-10	8	84.67	120.94	52.55	-3	-6	8	159.32	173.18	40.50
-2	-14	8	426.30	305.78	65.33	6	-10	8	69.85	1.48	104.62	-2	-6	8	3512.55	3654.94	161.35
-1	-14	8	507.44	467.18	67.74	7	-10	8	0.00	30.12	107.66	-1	-6	8	126.45	127.78	34.24
0	-14	8	0.56	108.31	55.85	-7	-9	8	11.06	-145.09	112.63	0	-6	8	9078.92	9496.05	332.95
1	-14	8	86.32	-40.89	105.70	-6	-9	8	174.94	219.15	60.88	1	-6	8	2764.89	2389.31	123.06
2	-14	8	5.23	-21.23	110.21	-5	-9	8	96.09	23.79	89.52	2	-6	8	5733.92	5509.29	211.75
3	-14	8	64.37	-112.58	110.81	-4	-9	8	13.21	61.21	81.26	3	-6	8	911.36	819.97	81.08
4	-14	8	177.20	73.49	77.64	-3	-9	8	512.35	482.33	51.13	4	-6	8	0.27	-34.11	67.16
-5	-13	8	212.28	70.58	83.22	-2	-9	8	314.83	276.11	47.39	5	-6	8	3.26	60.72	70.04
-4	-13	8	87.23	-21.46	108.98	-1	-9	8	1559.39	1587.84	115.44	6	-6	8	133.81	232.65	48.02
-3	-13	8	18.11	-26.68	91.62	0	-9	8	3150.98	3160.66	160.20	7	-6	8	36.68	21.24	87.85
-2	-13	8	0.05	34.35	67.06	1	-9	8	1488.10	1380.64	111.24	8	-6	8	87.59	93.89	96.00
-1	-13	8	74.24	36.29	100.72	2	-9	8	2446.77	2329.80	136.56	-8	-5	8	54.41	-71.26	105.03
0	-13	8	35.97	-13.81	89.85	3	-9	8	210.52	139.18	45.74	-7	-5	8	316.91	82.05	109.64
1	-13	8	6.97	-26.63	94.05	4	-9	8	165.31	160.22	47.68	-6	-5	8	617.17	703.31	60.13
2	-13	8	357.05	323.09	62.52	5	-9	8	3.53	-141.09	91.55	-5	-5	8	1.89	40.53	53.58
3	-13	8	177.83	141.00	59.89	6	-9	8	18.44	-17.52	66.38	-4	-5	8	2489.19	2662.89	144.10
4	-13	8	108.13	-3.72	104.89	7	-9	8	1.92	65.34	100.24	-3	-5	8	3566.64	3775.83	166.88
5	-13	8	84.90	92.21	106.40	-7	-8	8	313.99	379.03	63.50	8	-5	8	21.37	33.40	58.25
-5	-12	8	3.49	-114.88	108.96	-6	-8	8	124.31	58.48	100.29	-1	-5	8	709.42	642.33	47.66
-4	-12	8	0.16	-247.99	101.34	-5	-8	8	390.88	385.22	55.10	0	-5	8	1174.64	1217.67	86.77
-3	-12	8	0.08	12.96	66.68	-4	-8	8	239.58	208.64	51.04	1	-5	8	198.79	225.63	33.61
-2	-12	8	227.94	186.75	53.98	-3	-8	8	32.16	24.83	68.04	2	-5	8	124.26	134.52	31.07
-1	-12	8	954.50	1034.54	88.11	-2	-8	8	1304.36	1208.87	102.30	3	-5	8	179.76	120.64	31.67
0	-12	8	920.96	843.93	79.74	-1	-8	8	1003.48	899.23	69.33	4	-5	8	1269.55	1084.18	92.37
1	-12	8	902.43	859.65	82.43	0	-8	8	260.85	310.52	41.82	5	-5	8	1350.97	1644.16	108.75
2	-12	8	665.30	596.53	61.28	1	-8	8	98.54	107.69	40.83	6	-5	8	1326.02	1241.77	105.56
3	-12	8	637.64	640.00	64.31	2	-8	8	0.28	-56.40	62.50	7	-5	8	2502.50	2643.18	157.82
4	-12	8	0.41	-86.06	96.51	3	-8	8	9.47	17.19	66.49	8	-5	8	93.82	128.59	54.66
5	-12	8	0.06	-4.71	103.78	4	-8	8	648.85	750.97	70.68	9	-5	8	130.31	81.29	111.71
-6	-11	8	418.57	377.69	69.98	5	-8	8	73.08	111.96	48.62	-8	-4	8	192.09	208.84	64.58
-5	-11	8	210.79	256.48	59.37	6	-8	8	1437.41	1418.94	132.90	-7	-4	8	294.72	282.84	57.81
-4	-11	8	18.77	44.57	52.76	7	-8	8	152.72	111.71	58.23	-6	-4	8	187.57	234.16	47.71
-3	-11	8	399.00	571.52	55.61	8	-8	8	541.41	493.67	68.39	-5	-4	8	1200.24	1180.49	104.33
-2	-11	8	671.58	809.73	75.74	-7	-7	8	15.53	19.81	68.35	-4	-4	8	38.78	17.48	49.59
1	-11	8	31.24	36.81	84.12	-6	-7	8	939.73	960.69	84.71	-3	-4	8	491.59	466.67	42.69
0	-11	8	891.98	977.16	79.46	-5	-7	8	252.02	255.88	50.49	-2	-4	8	391.73	460.07	38.28
1	-11	8	108.22	131.83	50.15	-4	-7	8	1919.71	2037.74	130.98	-1	-4	8	337.76	270.39	33.29
2	-11	8	3.66	3.64	79.38	-3	-7	8	390.11	429.43	46.45	0	-4	8	248.74	201.26	32.72
3	-11	8	40.72	163.42	47.88	-2	-7	8	72.23	24.52	63.80	1	-4	8	1093.48	1154.73	79.88
4	-11	8	71.05	71.42	50.96	-1	-7	8	959.31	974.06	88.81	2	-4	8	4.23	30.06	45.70
5	-11	8	1074.22	915.38	91.91	0	-7	8	6.34	-148.12	63.71	3	-4	8	658.40	767.35	68.58
6	-11	8	2.87	43.66	99.51	1	-7	8	11.52	7.53	60.16	4	-4	8	509.51	632.27	52.66
-7	-10	8	228.42	418.02	68.74	2	-7	8	10.03	-15.25	61.57	5	-4	8	1846.88	2109.41	119.96

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
6	-4	0	425.71	559.67	50.74	7	-1	0	1162.98	1127.17	102.63	6	2	0	164.62	177.73	40.35
7	-4	0	714.19	1040.34	107.14	8	-1	0	520.39	529.73	50.69	7	2	0	1753.52	1698.54	117.07
8	-4	0	150.33	85.50	97.47	9	-1	0	80.64	71.33	102.92	8	2	0	31.78	-28.47	89.49
9	-4	1	18.94	-31.58	108.70	-8	0	0	173.90	112.95	42.71	9	2	0	197.31	226.51	56.01
-8	-3	0	321.34	225.40	64.45	-7	0	0	314.90	340.94	39.28	10	2	0	12.70	111.26	58.74
-7	-3	0	90.73	37.83	97.82	-6	0	0	19.12	87.98	39.39	-8	3	0	34.27	-115.05	109.02
-6	-3	0	93.12	109.85	47.25	-5	0	0	137.99	201.15	50.38	-7	3	0	148.49	170.41	52.82
-5	-3	0	0.95	-7.00	75.92	-4	0	0	78.03	98.88	24.63	-6	3	0	1.22	32.42	74.27
-4	-3	0	1152.06	984.74	93.84	-3	0	0	1454.91	1655.25	68.97	-5	3	0	142.90	119.83	42.24
-3	-3	0	2653.25	2442.57	124.23	-2	0	0	5147.54	4731.17	128.81	-4	3	0	807.41	904.53	84.94
-2	-3	0	2315.34	2538.06	123.03	-1	0	0	2290.64	2344.18	82.86	-3	3	0	27.62	6.12	55.58
-1	-3	0	9843.07	8083.79	306.86	0	0	0	10546.02	9271.96	185.73	-2	3	0	3333.80	3352.49	146.92
0	-3	0	1164.54	1114.51	76.01	1	0	0	38.95	117.65	17.25	-1	3	0	6594.74	6259.64	227.27
1	-3	0	9091.70	7909.96	274.28	2	0	0	4670.41	4583.41	120.01	0	3	0	1737.50	1925.26	95.29
2	-3	0	660.06	517.89	43.62	3	0	0	242.57	323.08	22.66	1	3	0	11552.33	11171.78	367.70
3	-3	0	115.31	21.17	51.79	4	0	0	168.82	117.11	20.34	2	3	0	1813.07	1954.35	93.04
4	-3	0	24.67	86.06	30.91	5	0	0	79.83	19.46	42.20	3	3	0	381.28	351.76	32.15
5	-3	0	539.36	488.92	44.72	6	0	0	2234.72	2040.71	104.45	4	3	0	704.30	611.84	46.99
6	-3	0	308.57	430.34	48.03	7	0	0	267.45	286.92	33.82	5	3	0	1671.26	1757.00	104.04
7	-3	0	43.30	114.03	45.51	8	0	0	195.23	1.70	65.21	6	3	0	466.67	501.31	48.01
8	-3	0	20.06	-103.28	85.27	9	0	0	54.36	69.42	56.50	7	3	0	183.54	144.39	44.53
9	-3	0	112.65	112.84	58.49	10	0	0	403.61	474.25	49.30	8	3	0	11.92	-17.51	82.54
-8	-2	0	98.44	273.40	78.85	-8	1	0	20.76	-29.44	108.91	9	3	0	331.20	349.23	60.45
-7	-2	0	1.05	-43.38	91.93	-7	1	0	49.43	70.01	50.31	10	3	0	0.10	-26.01	114.76
-6	-2	0	137.88	189.23	48.56	-6	1	0	305.40	227.61	47.36	-8	4	0	40.14	-83.58	105.43
-5	-2	0	362.30	425.67	46.62	-5	1	0	456.71	552.67	50.81	-7	4	0	2.96	-47.31	94.16
-4	-2	0	1209.37	1143.61	90.08	-4	1	0	311.39	253.00	38.38	-6	4	0	145.00	-40.75	87.23
-3	-2	0	1674.61	1656.59	101.24	-3	1	0	1814.16	1672.35	94.46	-5	4	0	184.09	121.23	48.44
-2	-2	0	6294.50	6370.66	231.87	-2	1	0	2921.34	2635.86	121.92	-4	4	0	2.39	46.58	67.64
-1	-2	0	191.67	192.60	30.61	-1	1	0	625.96	561.20	57.98	-3	4	0	844.69	798.05	57.26
0	-2	0	2436.82	-6194.21	219.43	0	1	0	9821.76	10032.21	338.69	-2	4	0	883.24	677.26	70.44
1	-2	0	67.34	67.84	25.56	1	1	0	201.93	173.04	26.36	-1	4	0	5290.54	5002.07	192.87
2	-2	0	46.44	29.20	43.90	2	1	0	282.73	225.37	28.18	0	4	0	58.58	2.15	35.07
3	-2	0	229.35	375.70	36.26	3	1	0	766.34	673.45	59.62	1	4	0	446.70	456.70	39.73
4	-2	0	70.74	23.14	50.91	4	1	0	2078.24	2091.08	105.70	2	4	0	66.75	31.55	44.90
5	-2	0	156.34	128.64	34.64	5	1	0	31.69	64.88	31.80	3	4	0	0.70	-66.53	47.09
6	-2	0	1249.26	1523.38	104.54	6	1	0	789.23	2821.94	140.78	4	4	0	1076.97	1174.60	77.82
7	-2	0	791.41	799.26	70.78	7	1	0	720.63	763.49	68.12	5	4	0	622.64	580.56	53.98
8	-2	0	467.68	428.29	60.38	8	1	0	408.11	435.26	53.99	6	4	0	32.51	-13.11	66.65
9	-2	0	403.61	280.30	62.17	9	1	0	366.54	426.78	61.32	7	4	0	420.49	486.55	49.99
-8	-1	0	44.23	16.34	103.21	10	1	0	0.47	-87.68	102.89	8	4	0	337.10	404.69	54.04
-7	-1	0	156.16	143.93	53.80	-8	2	0	88.52	77.54	109.69	9	4	0	36.44	40.44	67.72
-6	-1	0	843.91	725.89	72.23	-7	2	0	10.35	55.84	44.78	10	4	0	53.18	356.40	61.17
-5	-1	0	3.82	56.23	68.71	-6	2	0	390.94	394.52	51.27	-7	5	0	205.58	112.64	59.34
-4	-1	0	747.67	687.67	56.53	-5	2	0	318.93	416.28	47.20	-6	5	0	99.72	44.51	87.03
-3	-1	0	128.16	55.57	59.69	-4	2	0	419.96	341.67	39.82	-5	5	0	49.06	-147.51	81.72
-2	-1	0	446.12	657.72	64.28	-3	2	0	2212.73	2101.95	113.09	-4	5	0	575.25	555.70	51.25
-1	-1	0	3830.09	4412.15	171.38	-2	2	0	3357.59	3553.34	149.46	-3	5	0	99.01	148.36	35.82
0	-1	0	2333.91	1925.87	107.28	-1	2	0	284.87	319.87	31.76	-2	5	0	1412.25	1348.15	87.93
1	-1	0	104.86	136.60	25.11	0	2	0	1147.93	1111.65	84.93	-1	5	0	122.97	146.17	32.26
2	-1	0	2214.67	2701.08	115.36	1	2	0	125.90	111.91	26.40	0	5	0	483.61	448.15	45.55
3	-1	0	397.82	359.08	35.77	2	2	0	1186.24	1204.11	69.96	1	5	0	676.95	825.26	65.22
4	-1	0	1405.05	1390.88	86.69	3	2	0	452.10	474.33	39.96	2	5	0	4.26	-98.87	49.22
5	-1	0	227.71	282.56	34.33	4	2	0	983.96	1073.95	76.26	3	5	0	5126.58	4821.03	184.33
6	-1	0	3049.26	3201.35	152.88	5	2	0	1881.92	1713.88	103.45	4	5	0	3176.14	3367.54	146.50

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
5	5	8	415.71	428.87	41.27	-5	9	8	0.52	63.94	56.73	6	12	8	1.44	56.02	67.66
6	5	8	2331.50	2100.80	128.19	-5	9	8	67.77	-69.60	98.30	7	12	8	15.22	64.33	98.70
7	5	8	108.01	36.41	82.86	-4	9	8	54.85	22.65	58.62	-4	13	8	49.86	-168.11	112.30
8	5	8	63.14	56.06	86.01	-3	9	8	297.86	888.17	72.62	-3	13	8	75.83	64.20	98.17
9	5	8	183.11	183.47	58.90	-2	9	8	18.9.51	1436.70	111.44	-2	13	8	346.47	296.16	61.59
-7	6	8	4.60	-17.93	69.93	-1	9	8	637.40	588.18	61.38	-1	13	8	1.71	43.95	84.36
-6	6	8	3.20	-103.00	85.64	0	9	8	527.70	426.68	46.94	0	13	8	435.84	516.47	62.63
-5	6	8	13.86	-75.40	81.04	1	9	8	3691.60	3360.14	176.26	1	13	8	16.81	31.67	89.53
-4	6	8	659.89	712.28	65.85	2	9	8	20.78	-7.57	58.90	2	13	8	239.68	282.37	52.88
-3	6	8	542.82	457.71	45.82	3	9	8	3448.54	3482.02	159.52	3	13	8	4.88	78.63	87.03
-2	6	8	6.98	22.80	41.67	4	9	8	1.23	-4.26	57.88	4	13	8	106.04	87.38	95.05
-1	6	8	4017.92	3761.83	162.74	5	9	8	67.10	14.81	57.88	5	13	8	149.38	181.82	95.62
0	6	8	5640.98	5780.46	219.52	6	9	8	122.13	65.76	57.88	6	13	8	129.18	249.17	58.36
1	6	8	8.12	35.60	42.91	7	9	8	3.79	-100.27	108.38	7	13	8	21.69	-147.23	113.58
2	6	8	3086.18	3010.39	130.31	8	9	8	23.73	-90.97	101.68	-3	14	8	129.07	26.45	109.34
3	6	8	41.38	-14.73	52.36	9	9	8	4.94	12.15	108.51	-2	14	8	2.35	51.80	96.62
4	6	8	58.01	6.16	56.76	-6	10	8	186.21	169.15	63.65	-1	14	8	30.72	62.23	95.29
5	6	8	83.19	185.24	37.55	-5	10	8	24.15	4.35	92.95	0	14	8	184.12	242.99	59.22
6	6	8	1431.82	1632.37	112.98	-4	10	8	39.43	55.26	57.96	1	14	8	129.22	67.34	57.43
7	6	8	162.74	9.95	88.47	-3	10	8	274.12	243.27	51.00	2	14	8	126.74	157.35	53.41
8	6	8	26.06	49.55	63.52	-2	10	8	57.12	31.88	79.14	3	14	8	185.70	234.19	56.23
9	6	8	1.88	-81.26	98.66	-1	10	8	833.08	1180.38	108.10	4	14	8	780.59	872.49	71.55
-7	7	8	75.93	133.58	57.36	0	10	8	56.80	42.59	77.57	5	14	8	497.37	64.05	66.08
-6	7	8	11.49	3.97	95.41	1	10	8	400.40	470.27	47.81	6	14	8	344.50	333.83	67.54
-5	7	8	215.98	185.29	53.12	2	10	8	87.66	113.38	41.76	-2	15	8	200.31	159.95	62.29
-4	7	8	62.50	37.04	71.94	3	10	8	346.10	352.91	44.98	-1	15	8	41.05	157.87	60.87
-3	7	8	202.50	246.51	41.90	4	10	8	1.25	-37.62	69.27	0	15	8	124.11	262.94	61.78
-2	7	8	646.37	774.87	58.89	5	10	8	131.48	72.30	81.13	1	15	8	24.01	-53.76	104.53
-1	7	8	2806.11	2558.71	129.81	6	10	8	439.25	386.39	54.73	2	15	8	55.46	131.82	58.11
0	7	8	49.89	51.83	57.69	7	10	8	200.66	331.96	55.00	3	15	8	231.70	-125.80	120.52
1	7	8	45.60	114.57	30.02	8	10	8	110.08	194.34	60.23	4	15	8	24.22	-57.91	105.28
2	7	8	0.45	-17.95	52.36	-5	11	8	255.19	266.58	58.48	5	15	8	166.69	-32.90	117.45
3	7	8	20.99	46.13	32.14	-4	11	8	71.56	123.47	51.52	0	16	8	32.35	-204.47	123.87
4	7	8	1931.04	2086.85	113.47	-3	11	8	53.38	-135.20	96.29	1	16	8	150.93	166.00	62.10
5	7	8	1.96	23.00	47.18	-2	11	8	69.37	179.00	45.26	2	16	8	16.54	3.01	77.54
6	7	8	260.12	290.73	46.00	-1	11	8	46.26	-9.71	83.10	3	16	8	6.61	78.38	104.65
7	7	8	8.74	54.62	82.80	0	11	8	76.68	121.30	46.62	4	16	8	4.50	37.54	109.34
8	7	8	121.60	-59.33	95.77	1	11	8	101.76	18.81	72.80	-2	-15	9	147.51	204.03	65.20
9	7	8	67.83	-6.33	102.16	2	11	8	12.49	69.72	72.81	-1	-15	9	83.46	33.38	110.47
-6	8	8	399.65	435.99	63.56	3	11	8	543.89	613.13	53.91	0	-15	9	81.16	133.99	62.10
-5	8	8	348.59	272.87	53.78	4	11	8	830.21	1127.48	100.27	1	-15	9	9.54	-158.24	117.56
-4	8	8	129.89	69.09	81.72	5	11	8	1530.33	1530.29	126.90	-3	-14	9	25.23	39.21	104.03
-3	8	8	158.24	-37.11	78.97	6	11	8	885.55	839.40	81.91	-2	-14	9	0.82	39.64	103.96
-2	8	8	335.19	335.75	44.86	7	11	8	44.91	95.98	96.99	-1	-14	9	161.48	136.27	61.99
-1	8	8	30.44	-9.04	71.20	8	11	8	272.94	210.02	64.02	0	-14	9	26.20	10.66	103.26
0	8	8	189.54	227.54	38.52	-4	12	8	77.82	145.52	55.27	1	-14	9	339.51	392.63	62.34
1	8	8	203.82	241.17	36.24	-3	12	8	512.47	547.35	61.63	2	-14	9	200.14	40.40	106.51
2	8	8	1146.87	1037.31	87.46	-2	12	8	12.78	45.40	86.16	3	-14	9	103.23	130.81	62.97
3	8	8	383.15	402.01	40.80	-1	12	8	36.12	-14.01	83.31	-4	-13	9	27.10	15.53	108.92
4	8	8	1170.55	1047.13	95.16	0	12	8	263.56	139.88	53.30	-3	-13	9	535.70	453.49	68.07
5	8	8	1481.38	1338.64	102.84	1	12	8	89.50	62.20	86.72	-2	-13	9	49.68	-55.38	96.55
6	8	8	235.07	260.92	45.82	2	12	8	1117.62	994.59	78.30	-1	-13	9	298.04	350.38	61.65
7	8	8	223.72	203.60	52.59	3	12	8	101.04	66.63	85.89	0	-13	9	194.12	196.79	58.08
8	8	8	8.86	5.06	96.80	4	12	8	129.55	40.40	86.78	-1	-13	9	5.55	17.23	89.55
9	8	8	74.22	-12.55	114.78	5	12	8	6.31	35.56	83.49	2	-13	9	79.02	-94.24	98.99

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
3	-13	9	145.75	152.07	60.98	-7	-8	9	13.14	30.34	110.70	-1	-5	9	331.49	341.38	38.68
4	-13	9	2.66	135.04	57.57	-8	-8	9	205.43	215.60	60.88	0	-5	9	2905.00	2906.71	125.39
-5	-12	9	53.55	3.36	118.31	-5	-8	9	37.28	-20.33	91.48	1	-5	9	1051.27	1232.78	81.40
-4	-12	9	740.95	687.54	75.57	-4	-8	9	36.73	14.08	57.44	2	-5	9	3897.37	3881.32	164.15
-3	-12	9	3.31	89.94	96.03	-3	-8	9	166.47	175.47	46.30	3	-5	9	573.07	769.42	74.58
-2	-12	9	78.66	76.19	88.15	-2	-8	9	3.73	38.38	71.53	4	-5	9	489.98	602.18	55.21
-1	-12	9	134.42	191.53	53.91	-1	-8	9	773.06	843.67	67.81	5	-5	9	69.18	50.74	70.95
0	-12	9	92.09	-146.78	98.76	0	-8	9	8.42	-86.00	69.39	6	-5	9	43.74	-255.31	85.60
1	-12	9	422.45	315.84	61.04	1	-8	9	6234.62	6573.88	259.50	7	-5	9	23.21	31.13	84.30
2	-12	9	181.38	216.18	53.80	2	-8	9	0.07	0.70	67.82	8	-5	9	49.73	-193.98	100.73
3	-12	9	664.28	619.73	65.50	3	-8	9	1270.13	1371.99	106.30	9	-5	9	0.54	-19.06	102.86
4	-12	9	611.58	509.98	65.55	4	-8	9	139.11	137.99	46.51	-8	-4	9	9.47	-14.33	101.00
5	-12	9	46.52	42.32	104.76	5	-8	9	11.17	57.85	58.18	-7	-4	9	14.19	-15.89	101.97
-6	-11	9	2.55	77.87	112.06	6	-8	9	166.37	183.26	53.45	-6	-4	9	337.12	313.10	57.37
-5	-11	9	32.37	-234.06	109.74	7	-8	9	131.95	131.39	58.57	-5	-4	9	50.59	36.04	43.87
-4	-11	9	10.13	-1.84	101.71	8	-8	9	4.29	-90.71	111.28	-4	-4	9	21.33	28.60	71.79
-3	-11	9	2.22	-101.99	92.54	-7	-7	9	18.12	169.69	58.58	-3	-4	9	1060.65	1049.61	96.82
-2	-11	9	128.82	120.32	52.77	-6	-7	9	71.41	147.64	55.19	-2	-4	9	3565.34	4138.59	176.57
-1	-11	9	95.17	143.15	48.64	-5	-7	9	19.19	74.44	79.62	-1	-4	9	78.40	32.53	53.30
0	-11	9	434.91	436.95	61.25	-4	-7	9	385.93	326.05	50.67	0	-4	9	2766.91	3146.13	140.33
1	-11	9	10.78	-113.39	85.78	-3	-7	9	2144.91	2399.58	138.29	1	-4	9	4737.26	4771.65	187.35
2	-11	9	362.54	301.09	56.09	-2	-7	9	158.28	83.26	41.43	2	-4	9	33.43	73.20	28.58
3	-11	9	77.40	12.01	64.24	-1	-7	9	2038.91	2254.43	124.84	3	-4	9	11.89	46.38	52.69
4	-11	9	136.13	89.45	93.45	0	-7	9	1011.75	1066.22	95.27	4	-4	9	74.17	858.32	81.05
5	-11	9	229.74	164.18	61.64	1	-7	9	67.10	24.26	55.50	5	-4	9	97.76	43.99	74.43
6	-11	9	17.16	35.98	113.39	2	-7	9	1657.49	1607.24	107.98	6	-4	9	434.99	600.73	60.70
-6	-10	9	26.95	-57.31	107.17	3	-7	9	1348.68	1416.34	102.83	7	-4	9	40.76	50.40	85.32
-5	-10	9	96.54	52.72	75.36	4	-7	9	196.05	190.67	44.11	8	-4	9	1047.46	1058.66	92.43
-4	-10	9	189.50	205.59	53.95	5	-7	9	107.31	166.37	46.91	9	-4	9	14.70	41.75	103.24
-3	-10	9	63.82	2.37	48.78	6	-7	9	111.33	42.49	91.82	-8	-3	9	48.31	-13.24	111.55
-2	-10	9	771.95	808.74	75.26	7	-7	9	317.00	276.13	59.08	-7	-3	9	3.33	-52.15	102.58
-1	-10	9	141.34	152.55	45.92	8	-7	9	42.13	65.95	60.83	-6	-3	9	660.57	721.05	72.65
0	-10	9	197.38	16.25	84.07	-7	-6	9	435.34	419.31	66.87	-5	-3	9	180.66	288.98	48.22
1	-10	9	99.35	199.09	44.36	-6	-6	9	526.82	581.03	61.83	-4	-3	9	1928.68	1972.56	122.46
2	-10	9	156.02	278.92	47.62	-5	-6	9	492.16	444.79	56.50	-3	-3	9	2796.53	2800.92	114.28
3	-10	9	397.97	384.00	51.83	-4	-6	9	1430.79	1928.41	124.97	-2	-3	9	220.30	130.96	35.91
4	-10	9	375.33	391.25	56.59	-3	-6	9	142.58	290.76	44.04	-1	-3	9	338.46	327.85	38.26
5	-10	9	11.45	35.24	65.23	-2	-6	9	358.11	301.57	44.85	0	-3	9	1379.05	1687.92	96.35
6	-10	9	51.84	91.90	97.31	-1	-6	9	44.06	23.13	34.56	1	-3	9	280.62	274.28	35.11
7	-10	9	52.81	-24.57	104.26	0	-6	9	519.99	515.23	47.32	2	-3	9	431.67	335.36	34.01
-7	-9	9	58.69	93.07	112.48	1	-6	9	1275.61	1308.89	96.74	3	-3	9	646.11	550.18	46.86
-6	-9	9	322.20	263.27	64.56	2	-6	9	5.19	12.77	62.66	4	-3	9	2375.54	2076.15	111.27
-5	-9	9	1179.56	1231.39	93.01	3	-6	9	2145.80	2134.91	120.79	5	-3	9	130.00	130.61	38.17
-4	-9	9	559.60	464.87	58.54	4	-6	9	595.92	599.98	50.43	6	-3	9	66.00	80.91	40.76
-3	-9	9	534.50	551.24	55.58	5	-6	9	1661.97	1607.81	117.11	7	-3	9	501.09	394.19	52.68
-2	-9	9	22.77	14.70	78.75	6	-6	9	839.73	1090.83	106.81	8	-3	9	119.10	215.05	55.24
-1	-9	9	165.57	168.74	45.28	7	-6	9	78.99	-60.45	100.63	9	-3	9	46.75	-129.95	108.47
0	-9	9	242.16	286.56	44.99	8	-6	9	104.73	43.14	102.56	8	-2	9	114.04	36.06	118.46
1	-9	9	186.60	144.45	45.94	-8	-5	9	47.02	10.89	116.12	-7	-2	9	63.40	-13.55	95.23
2	-9	9	383.57	546.33	52.32	-7	-5	9	8.66	34.24	98.38	-6	-2	9	45.31	-34.54	85.34
3	-9	9	16.13	-119.31	79.53	-6	-5	9	1.16	-126.38	93.77	-5	-2	9	82.06	-111.18	78.05
4	-9	9	837.89	807.43	75.47	-5	-5	9	1.10	-179.73	84.93	-4	-2	9	1183.97	1318.61	97.53
5	-9	9	641.89	624.52	62.29	-4	-5	9	437.21	493.84	50.30	-3	-2	9	437.10	502.11	51.75
6	-9	9	0.61	34.62	52.09	-3	-5	9	26.26	32.74	71.63	-2	-2	9	1739.48	1839.55	105.61
7	-9	9	90.74	-63.43	106.18	-2	-5	9	338.80	349.21	39.35	-1	-2	9	1097.29	1008.68	77.77

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
0	-2	9	3227.84	-319.78	183.34*	1	1	9	6572.01	6659.08	236.60	4	4	9	3230.03	3183.56	141.43
1	-2	9	3238.13	2798.44	124.86	2	1	9	7146.72	7136.70	250.62	5	4	9	1321.28	1388.94	97.62
2	-2	9	3216.96	3016.77	131.73	3	1	9	3729.22	3255.88	137.56	6	4	9	19.30	-68.41	70.15
3	-2	9	4249.74	4331.31	170.92	4	1	9	2286.02	2373.63	116.58	7	4	9	13.33	81.65	78.30
4	-2	9	52.03	-97.22	58.70	5	1	9	1402.39	1245.42	149.88	8	4	9	34.14	-1.37	88.00
5	-2	9	104.91	138.50	35.61	6	1	9	308.82	330.48	44.88	9	4	9	11.60	5.91	101.21
6	-2	9	66.34	-72.36	73.88	7	1	9	236.03	334.60	49.43	-9	5	9	2.06	-49.98	99.56
7	-2	9	100.01	71.98	47.66	8	1	9	1.27	10.24	83.57	-6	5	9	41.77	-87.07	89.44
8	-2	9	156.60	31.35	100.81	9	1	9	24.53	-40.06	96.89	-5	5	9	516.78	541.07	55.32
9	-2	9	14.16	16.96	103.25	-8	1	9	43.78	36.55	108.22	-4	5	9	1116.46	1322.03	101.63
-8	-1	9	3.16	-93.90	113.22	-7	1	9	1.57	-21.66	98.45	-3	5	9	48.80	30.58	45.81
-7	-1	9	97.94	43.56	98.46	-6	2	9	468.98	390.91	56.85	-2	5	9	33.33	-49.11	61.36
-6	-1	9	93.37	57.31	59.08	-5	2	9	450.24	398.61	50.43	-1	5	9	2817.42	2707.23	131.03
-5	-1	9	341.76	417.10	49.66	-4	2	9	336.93	341.65	40.93	0	5	9	263.73	328.20	36.03
-4	-1	9	264.95	258.46	41.58	-3	2	9	139.53	37.76	63.82	1	5	9	278.73	159.98	32.36
-3	-1	9	2330.28	2243.79	121.12	-2	2	9	2050.50	1980.02	108.64	2	5	9	1153.33	1243.97	83.01
-2	-1	9	91.28	142.04	33.13	-1	2	9	272.37	348.85	35.37	3	5	9	36.88	-17.39	54.20
-1	-1	9	5001.21	4680.52	181.60	0	2	9	6783.78	6395.52	235.19	4	5	9	216.48	199.90	38.26
0	-1	9	2366.39	-534.29	131.40*	1	2	9	4061.77	3294.05	136.82	5	5	9	132.50	180.41	38.57
1	-1	9	2735.99	2886.42	124.95	2	2	9	349.56	499.32	38.91	6	5	9	920.62	867.12	88.99
2	-1	9	5974.91	5635.32	207.61	3	2	9	4653.46	4564.62	175.08	7	5	9	412.78	567.40	54.72
3	-1	9	34.78	-45.44	53.93	4	2	9	0.18	-5.55	50.40	8	5	9	466.23	462.52	57.76
4	-1	9	353.64	379.56	36.00	5	2	9	114.16	34.54	42.68	9	5	9	575.42	637.12	66.22
5	-1	9	171.31	132.14	36.54	6	2	9	319.71	365.46	43.65	-7	6	9	247.33	256.58	62.19
6	-1	9	210.58	228.94	43.91	7	2	9	1164.56	1114.60	104.83	-6	6	9	65.23	-163.88	97.41
7	-1	9	1193.33	1327.48	113.53	8	2	9	1574.01	1422.53	128.30	-5	6	9	1252.86	1179.20	84.65
8	-1	9	226.46	233.57	54.11	9	2	9	4.99	-48.35	100.64	-4	6	9	190.24	225.38	46.48
9	-1	9	872.76	857.96	74.02	-7	3	9	37.74	-13.35	90.38	-3	6	9	249.86	218.63	43.57
-8	0	9	24.37	42.00	73.27	-6	3	9	822.17	729.55	65.12	-2	6	9	371.98	364.79	40.54
-7	0	9	550.84	490.63	44.97	-5	3	9	50.86	-62.61	77.73	-1	6	9	1.33	68.25	33.65
-6	0	9	9.49	28.76	55.73	-4	3	9	1156.94	1037.21	95.59	0	6	9	331.15	363.07	40.44
-5	0	9	423.03	425.97	34.45	-3	3	9	56.46	-10.12	61.43	1	6	9	25.98	9.39	51.58
-4	0	9	1017.40	1158.03	64.83	-2	3	9	768.75	875.90	79.20	2	6	9	101.56	136.52	31.32
-3	0	9	25.20	19.21	40.37	-1	3	9	59.09	119.40	32.11	3	6	9	1403.65	1287.88	88.56
-2	0	9	35.17	10.14	36.39	0	3	9	42.44	30.06	45.81	4	6	9	278.31	300.80	39.81
-1	0	9	4.70	-10.87	33.60	1	3	9	1312.77	1281.64	82.65	5	6	9	1014.92	2794.37	141.74
0	0	9	301.47	-3454.31	105.41*	2	3	9	70.29	-9.63	46.88	6	6	9	1021.18	1119.56	99.96
1	0	9	45.37	44.60	23.25	3	3	9	42.68	26.16	28.62	7	6	9	440.33	417.40	55.21
2	0	9	4122.11	3859.03	106.06	4	3	9	3345.48	3346.93	144.33	8	6	9	205.00	204.51	53.13
3	0	9	3184.87	3038.51	93.71	5	3	9	160.37	31.78	39.06	9	6	9	1.51	-74.63	102.04
4	0	9	991.33	943.65	53.02	6	3	9	2331.48	2186.88	130.20	-6	7	9	196.90	52.61	104.58
5	0	9	445.54	437.27	29.27	7	3	9	315.08	348.83	49.82	-5	7	9	153.15	106.90	53.84
6	0	9	1512.16	1581.35	76.15	8	3	9	41.37	-77.03	87.51	-4	7	9	61.70	107.91	45.27
7	0	9	52.42	-39.14	56.81	9	3	9	54.98	24.16	102.58	-3	7	9	104.11	-1.37	78.85
8	0	9	446.79	397.18	39.24	-7	4	9	218.92	38.96	109.33	-2	7	9	20.34	8.63	58.40
9	0	9	61.04	-32.59	93.13	-6	4	9	147.73	96.14	99.10	-1	7	9	114.54	23.58	64.67
-8	1	9	79.40	22.20	74.25	-5	4	9	19.74	41.83	73.96	0	7	9	259.80	295.28	43.71
-7	1	9	142.47	123.44	56.49	-4	4	9	206.58	269.37	42.59	1	7	9	1355.35	1411.13	92.55
-6	1	9	215.47	281.61	50.90	-3	4	9	19.89	-23.89	62.97	2	7	9	255.21	196.85	36.71
-5	1	9	12.32	-73.21	75.07	-2	4	9	181.87	129.82	38.97	3	7	9	4671.93	4895.61	197.22
-4	1	9	2.59	67.30	34.91	-1	4	9	228.41	149.72	34.34	4	7	9	3129.60	3525.71	160.62
-3	1	9	330.92	263.33	37.97	0	4	9	4519.50	5011.54	194.24	5	7	9	1.64	19.06	64.72
-2	1	9	811.54	787.98	74.69	1	4	9	1306.95	1137.17	77.93	6	7	9	382.33	336.74	50.33
-1	1	9	1838.56	2112.55	105.82	2	4	9	1669.06	1473.57	142.48	7	7	9	100.91	76.33	84.63
0	1	9	1631.03	-2076.81	135.30*	3	4	9	2447.28	2338.73	111.85	8	7	9	8.66	-13.97	98.84

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
9	7	9	0.24	36.99	60.78	4	11	9	34.34	35.36	65.78	-2	-13	10	29.64	48.71	106.35
-6	8	9	38.89	63.09	102.66	5	11	9	65.06	52.55	84.68	-1	-13	10	11.59	20.80	100.87
-5	8	9	91.55	59.48	93.46	6	11	9	434.51	414.44	58.01	0	-13	10	147.00	60.36	71.99
-4	8	9	20.17	-30.58	84.75	7	11	9	162.98	38.44	105.61	1	-13	10	15.12	110.07	58.30
-3	8	9	574.3	645.97	67.39	8	11	9	168.31	70.19	111.85	2	-13	10	274.64	261.40	62.91
-2	8	9	607.99	752.55	65.55	-4	12	9	39.60	45.76	72.17	3	-13	10	534.98	387.18	65.20
-1	8	9	1902.47	1749.89	120.56	-3	12	9	207.82	217.51	56.53	4	-13	10	60.81	92.33	63.02
0	8	9	4910.64	5126.33	212.69	-2	12	9	27.18	-119.14	93.30	-5	-12	10	0.35	40.09	79.92
1	8	9	13.28	35.93	36.34	-1	12	9	6.64	33.52	89.65	-4	-12	10	204.86	147.90	65.19
2	8	9	910.06	911.65	80.65	0	12	9	1.60	23.95	85.60	-3	-12	10	106.16	204.24	61.83
3	8	9	286.99	358.25	41.87	1	12	9	162.02	79.79	90.62	-2	-12	10	275.98	294.44	61.24
4	8	9	88.25	-29.86	68.49	2	12	9	0.90	10.36	82.13	-1	-12	10	747.51	661.40	68.25
5	8	9	60.77	12.02	82.36	3	12	9	18.64	68.10	86.03	0	-12	10	59.15	83.90	99.72
6	8	9	98.74	67.21	83.33	4	12	9	2.26	55.06	59.74	1	-12	10	103.16	-21.01	98.46
7	8	9	900.91	814.24	78.24	5	12	9	345.62	341.68	58.71	2	-12	10	2.61	-126.20	100.81
8	8	9	333.08	344.36	59.59	6	12	9	21.04	55.78	67.55	3	-12	10	0.67	-86.25	98.99
9	8	9	274.05	272.91	63.61	7	12	9	333.39	106.87	107.75	4	-12	10	23.32	-57.13	100.68
-6	9	9	510.36	488.17	70.63	-3	13	9	9.77	50.30	93.23	5	-12	10	17.25	38.54	108.27
-5	9	9	207.03	85.28	59.35	-2	13	9	21.60	29.79	66.85	-5	-11	10	177.80	57.28	103.01
-4	9	9	938.63	1225.75	114.41	-1	13	9	1.82	92.04	94.18	-4	-11	10	10.69	72.33	96.45
-3	9	9	31.21	-54.01	80.81	0	13	9	327.81	399.58	56.71	-3	-11	10	141.80	214.77	54.45
-2	9	9	99.72	145.57	42.87	1	13	9	333.09	373.32	57.62	-2	-11	10	383.99	337.48	57.80
-1	9	9	44.65	63.32	73.51	2	13	9	421.99	420.68	58.71	-1	-11	10	57.34	78.07	91.90
0	9	9	229.68	71.46	81.75	3	13	9	915.84	1084.69	110.89	0	-11	10	1000.13	1065.57	87.92
1	9	9	128.35	108.33	42.39	4	13	9	70.34	150.88	52.72	1	-11	10	77.04	58.46	64.88
2	9	9	6.37	25.19	66.04	5	13	9	47.12	-73.77	102.60	2	-11	10	37.04	-78.30	93.81
3	9	9	89.85	202.24	40.60	6	13	9	177.63	83.58	105.49	3	-11	10	370.27	422.21	60.03
4	9	9	902.70	974.25	95.31	7	13	9	49.92	54.21	75.95	4	-11	10	56.55	-126.59	100.84
5	9	9	521.13	647.88	64.21	-2	14	9	274.43	292.18	63.34	5	-11	10	538.62	542.13	68.17
6	9	9	788.63	803.94	75.49	-1	14	9	335.93	328.84	62.73	6	-11	10	2.78	-64.41	113.08
7	9	9	79.69	20.82	94.60	0	14	9	524.43	494.05	69.79	-6	-10	10	96.80	80.53	109.42
8	9	9	465.54	437.78	63.29	1	14	9	212.40	167.63	57.67	-5	-10	10	9.20	-43.49	98.76
-5	10	9	171.71	162.23	59.04	2	14	9	145.25	221.96	55.62	-4	-10	10	28.39	57.45	53.81
-4	10	9	59.38	90.67	51.46	3	14	9	0.03	93.74	94.10	-3	-10	10	402.73	542.85	59.42
-3	10	9	69.22	112.49	47.37	4	14	9	0.26	43.41	98.50	-2	-10	10	26.79	73.46	48.85
-2	10	9	0.78	-1.87	54.30	5	14	9	12.01	54.36	102.08	-1	-10	10	288.43	334.08	54.16
-1	10	9	831.88	676.45	70.14	6	14	9	0.17	-3.51	103.70	0	-10	10	51.96	-17.13	83.09
0	10	9	1278.54	1219.24	108.56	-1	15	9	0.20	99.06	104.65	1	-10	10	512.43	439.06	56.88
1	10	9	150.88	161.04	46.24	0	15	9	0.75	-92.92	115.03	2	-10	10	408.36	531.66	53.35
2	10	9	1886.75	1736.66	118.34	1	15	9	21.26	-222.82	108.20	3	-10	10	286.36	288.91	56.91
3	10	9	24.07	-52.42	70.12	2	15	9	2.90	45.80	58.72	4	-10	10	871.56	837.43	80.62
4	10	9	486.09	417.26	53.77	3	15	9	173.23	26.21	109.66	5	-10	10	163.93	204.41	59.14
5	10	9	284.44	214.98	52.40	4	15	9	258.85	242.77	64.61	6	-10	10	461.93	298.65	67.10
6	10	9	108.61	13.99	92.25	5	15	9	33.14	-72.14	117.66	-6	-9	10	2.46	-127.60	114.06
7	10	9	97.03	9.59	95.83	1	16	9	220.85	29.35	125.84	-5	-9	10	3.88	2.18	96.12
8	10	9	50.47	74.15	101.13	2	16	9	460.70	677.35	63.81	-4	-9	10	3.86	41.15	65.58
-5	11	9	0.55	-27.48	108.78	3	16	9	4.71	78.34	107.46	-3	-9	10	476.74	484.12	55.00
-4	11	9	158.76	106.49	58.64	-2	-14	10	80.18	158.83	63.50	-2	-9	10	760.08	805.17	74.89
-3	11	9	248.95	287.17	53.57	-1	-14	10	421.02	533.12	69.42	-1	-9	10	856.57	790.34	76.80
-2	11	9	424.52	346.07	55.42	0	-14	10	17.35	-2.63	107.87	0	-9	10	559.24	548.43	55.27
-1	11	9	1175.39	1358.50	149.31	1	-14	10	161.67	162.79	63.78	1	-9	10	132.10	148.38	47.40
0	11	9	104.70	18.84	81.47	2	-14	10	4.26	-37.18	108.86	2	-9	10	138.72	116.33	46.02
1	11	9	924.52	963.48	100.11	3	-14	10	1.26	-45.45	106.70	3	-9	10	109.13	65.26	83.81
2	11	9	52.66	23.84	56.52	-4	-13	10	74.15	9.39	113.35	4	-9	10	22.22	45.36	48.12
3	11	9	178.27	130.54	47.97	-3	-13	10	5.46	-100.52	111.61	5	-9	10	4.34	47.87	90.67

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
6	-9	10	0.00	54.48	54.27	0	-5	10	598.70	428.96	45.95	5	-2	10	1728.14	1821.75	110.24
7	-9	10	17.20	-34.89	110.23	1	-5	10	92.73	181.52	37.60	6	-2	10	122.21	378.85	46.71
-6	-8	10	16.16	34.22	98.04	2	-5	10	818.34	647.07	55.94	7	-2	10	145.97	128.13	50.83
-5	-8	10	24.67	-1.78	63.46	3	-5	10	170.06	232.62	36.46	8	-2	10	213.75	229.72	54.50
-4	-8	10	467.92	608.34	58.51	4	-5	10	1207.39	1187.26	96.91	9	-2	10	95.34	142.29	59.62
-3	-8	10	118.52	34.11	82.55	5	-5	10	699.20	832.48	68.89	-7	-1	10	0.31	-103.21	100.29
-2	-8	10	845.10	842.27	72.51	5	-5	10	1345.93	1783.35	124.44	-6	-1	10	172.97	212.90	53.16
-1	-8	10	2245.90	2417.31	143.03	7	-5	10	373.72	483.68	58.70	-5	-2	10	344.06	460.27	50.25
0	-8	10	827.42	826.93	73.37	8	-5	10	60.73	-50.40	98.48	-4	-1	10	104.91	102.34	42.78
1	-8	10	2165.28	2206.46	136.68	-7	-1	10	440.68	516.46	66.57	-3	-1	10	447.32	564.62	58.46
2	-8	10	558.81	556.24	53.41	-6	-1	10	36.57	69.01	52.71	-2	1	10	1339.06	1363.97	98.12
3	-8	10	419.62	377.57	52.13	-5	-4	10	127.52	124.83	42.96	-1	-1	10	27.60	-66.17	57.07
4	-8	10	329.28	287.92	49.87	-4	-4	10	2.85	-41.62	75.84	0	-4	10	1083.56	-871.29	125.85*
5	-8	10	468.22	553.78	57.10	-3	-4	10	686.11	813.05	66.99	1	-1	10	192.46	199.83	30.99
6	-8	10	339.94	445.06	59.07	-2	-4	10	2.25	58.61	59.96	2	-1	10	7151.82	7550.56	269.43
7	-8	10	83.25	130.82	58.28	-1	-4	10	192.90	213.85	36.00	3	-1	10	2918.35	2691.83	125.91
-7	-7	10	25.96	-87.88	113.30	0	-4	10	334.63	430.81	39.20	4	-1	10	2579.76	2670.61	130.29
-6	-7	10	68.37	136.57	55.88	1	-4	10	3284.76	3915.12	165.52	5	-1	10	2352.70	2480.79	129.97
-5	-7	10	232.42	306.86	56.67	2	-4	10	344.78	241.67	36.48	6	-1	10	64.05	-87.87	77.85
-4	-7	10	358.34	548.28	54.53	3	-4	10	5614.96	6388.99	242.29	7	-1	10	402.76	446.84	50.90
-3	-7	10	68.32	-18.34	82.35	4	-4	10	1833.97	1609.04	110.58	8	-1	10	40.68	23.11	92.76
-2	-7	10	1015.08	1313.91	102.71	5	-4	10	1436.59	1367.96	108.07	9	-1	10	29.05	-94.84	102.95
-1	-7	10	8.97	-76.33	73.81	6	-4	10	1175.11	1211.48	109.98	-7	0	10	65.09	18.69	55.68
0	-7	10	199.76	220.21	43.12	7	-4	10	6.63	-23.76	82.40	-6	0	10	7.72	-35.38	60.37
1	-7	10	574.40	557.96	49.32	8	-4	10	31.77	-6.33	95.20	-5	0	10	25.06	-23.74	55.11
2	-7	10	2177.04	2062.34	128.78	9	-4	10	2.93	75.41	106.86	-4	0	10	19.86	-28.46	84.54
3	-7	10	595.83	693.52	63.95	-7	-3	10	20.91	50.90	100.90	-3	0	10	76.34	66.85	34.81
4	-7	10	434.93	375.96	50.50	-6	-3	10	3.79	-100.96	92.42	-2	0	10	1288.64	1563.03	67.57
5	-7	10	1583.97	1620.01	128.98	-5	-3	10	199.53	329.24	48.85	-1	0	10	212.05	168.23	23.25
6	-7	10	57.07	83.25	51.81	-4	-3	10	58.91	54.85	43.80	0	0	10	22.47	-256.16	46.88*
7	-7	10	515.32	437.37	64.06	-3	-3	10	1574.22	1672.23	112.53	1	0	10	138.33	184.19	22.28
8	-7	10	44.80	62.41	73.43	-2	-3	10	54.59	-149.41	65.31	2	0	10	718.51	671.61	40.89
-7	-6	10	20.84	24.66	110.21	-1	-3	10	242.30	263.89	34.33	3	0	10	2666.33	2858.31	91.91
-6	-6	10	7.37	-25.87	101.21	0	-3	10	86.38	-83.42	62.06	4	0	10	3175.45	3033.33	98.05
-5	-6	10	3.05	46.82	59.12	1	-3	10	1.87	-62.45	54.79	5	0	10	773.56	755.44	46.58
-4	-6	10	467.04	502.47	54.86	2	-3	10	198.48	171.32	22.90	6	0	10	174.08	225.22	31.47
-3	-6	10	40.06	76.92	44.19	3	-3	10	2107.07	2200.80	115.97	7	0	10	233.65	311.38	34.74
-2	-6	10	1446.52	1165.35	100.88	4	-3	10	226.51	202.37	33.06	8	0	10	322.59	301.60	40.18
-1	-6	10	638.32	637.74	55.68	5	-3	10	993.65	1132.61	91.90	9	0	10	119.94	91.71	46.10
0	-6	10	253.73	-24.31	73.36	6	-3	10	220.06	205.69	48.63	7	1	10	15.09	43.45	93.75
1	-6	10	1264.57	1283.20	98.59	7	-3	10	135.20	81.53	86.19	-5	1	10	36.19	43.15	59.65
2	-6	10	210.31	205.94	42.22	8	-3	10	154.65	179.30	56.90	-4	1	10	522.16	638.37	58.78
3	-6	10	561.98	623.62	60.44	9	-3	10	59.57	-160.90	113.45	-3	1	10	648.50	673.49	61.33
4	-6	10	465.31	502.91	47.00	-7	-2	10	4.32	63.93	98.19	-3	1	10	3031.25	3262.91	154.46
5	-6	10	49.15	60.71	81.72	-6	-2	10	32.28	49.76	94.65	-2	1	10	1734.26	1689.14	100.45
6	-6	10	0.05	44.30	87.77	-5	-2	10	107.73	136.09	46.43	-1	1	10	947.68	818.41	79.56
7	-6	10	449.54	442.09	61.42	-4	-2	10	342.53	328.40	45.74	0	1	10	1008.69	131.01	56.83*
8	-6	10	0.52	-72.64	102.73	-3	-2	10	724.70	674.51	61.22	1	1	10	820.67	915.90	76.15
-7	-5	10	0.16	-160.73	107.25	-2	-2	10	1365.07	1275.80	94.27	2	1	10	1635.94	1666.21	92.20
-6	-5	10	7.68	-11.39	53.16	-1	-2	10	606.30	481.05	40.10	3	1	10	514.65	443.77	38.46
-5	-5	10	330.88	333.31	51.84	0	-2	10	287.01	-6295.48	206.77*	4	1	10	1020.13	764.45	78.81
-4	-5	10	118.18	179.62	45.16	1	-2	10	2980.39	3031.81	136.26	5	1	10	954.74	1008.37	85.22
-3	-5	10	2115.75	1947.24	123.29	2	-2	10	481.75	150.54	32.16	6	1	10	662.46	620.87	62.98
-2	-5	10	309.33	320.04	42.24	3	-2	10	327.32	275.64	36.58	7	1	10	2223.40	2240.98	139.47
-1	-5	10	515.65	1554.13	109.78	4	-2	10	70.93	102.33	33.42	8	1	10	65.97	-113.82	94.10

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
8	1	10	202.19	182.62	59.54	-4	5	10	2.81	72.57	75.38	3	8	10	2567.50	2503.79	136.07
-7	2	10	317.89	479.04	60.42	-3	5	10	1326.78	1239.97	103.18	4	8	10	173.38	210.45	44.98
-6	2	10	22.48	-79.66	92.27	-2	5	10	9.96	-69.60	67.79	5	8	10	439.23	440.41	48.21
-8	2	10	26.27	-6.03	77.96	-1	5	10	59.27	57.26	61.15	6	8	10	163.23	161.60	47.38
-4	2	10	692.57	696.39	64.47	0	5	10	48.59	54.50	61.89	7	8	10	2.42	-90.96	86.97
-3	2	10	175.27	230.13	39.97	1	8	10	459.48	393.82	37.77	8	8	10	77.30	121.49	56.53
-2	2	10	899.12	909.44	83.10	2	8	10	2140.13	2193.30	112.20	9	8	10	49.06	56.79	105.71
-1	2	10	345.77	335.06	38.27	3	5	10	286.11	294.60	36.06	-5	9	10	1.44	-47.16	102.48
0	2	10	6.12	-212.41	128.06*	4	5	10	2919.15	3139.87	143.96	-4	9	10	106.68	64.95	54.20
1	2	10	4344.77	3735.25	155.31	5	5	10	698.63	698.52	60.06	-3	9	10	4.43	-122.47	84.11
2	2	10	14.66	8.01	48.73	6	5	10	127.27	88.53	44.26	-2	9	10	0.89	33.78	79.39
3	2	10	2671.07	2659.11	122.50	7	5	10	477.43	507.11	54.68	-1	9	10	1289.67	1467.83	114.40
4	2	10	738.84	707.50	72.53	8	5	10	1.12	-30.58	97.33	0	9	10	255.65	197.45	48.98
5	2	10	188.13	196.76	38.77	9	5	10	0.45	17.39	104.27	1	9	10	1753.96	1820.48	123.41
6	2	10	644.81	668.30	64.86	-6	6	10	10.30	-72.48	101.16	2	9	10	191.28	69.12	70.87
7	2	10	4.73	57.33	44.78	-5	6	10	17.62	-38.52	91.37	3	9	10	388.55	485.03	48.46
8	2	10	10.51	87.32	87.53	-4	6	10	0.32	-14.71	75.54	4	9	10	1420.31	1475.69	110.47
9	2	10	76.90	87.39	97.83	-3	6	10	402.89	366.99	51.13	5	9	10	252.66	329.10	50.28
-7	3	10	22.96	13.81	102.16	-2	6	10	940.07	848.55	63.57	6	9	10	172.42	-62.04	89.84
-6	3	10	170.59	274.29	54.14	-1	6	10	88.38	56.41	38.30	7	9	10	3.10	10.94	93.20
-5	3	10	108.43	1.62	55.16	0	6	10	2337.31	2303.31	126.08	8	9	10	3.95	-118.96	97.89
-4	3	10	0.34	-211.27	78.73	1	6	10	110.77	87.82	35.11	-5	10	10	271.38	365.23	66.60
-3	3	10	541.60	386.33	45.40	2	6	10	483.63	556.57	51.68	-4	10	10	97.33	181.09	52.12
-2	3	10	127.32	169.50	37.41	3	6	10	582.61	621.11	51.51	-3	10	10	311.18	339.34	56.88
-1	3	10	2212.64	2001.38	112.58	4	6	10	36.49	108.49	36.79	-2	10	10	998.38	808.79	90.15
0	3	10	138.97	158.25	34.33	5	6	10	2850.84	3001.18	156.07	-1	10	10	198.89	243.62	50.47
1	3	10	339.16	267.55	35.43	6	6	10	876.99	930.36	74.37	0	10	10	492.59	642.22	57.38
2	3	10	2305.89	2230.38	112.90	7	6	10	177.79	60.88	64.60	1	10	10	37.11	67.61	77.84
3	3	10	679.66	728.06	64.81	8	6	10	133.95	70.13	55.01	2	10	10	2.80	-49.92	69.63
4	3	10	491.67	472.01	42.65	9	6	10	35.36	77.15	56.85	3	10	10	14.15	-40.88	78.33
5	3	10	5.43	-122.79	64.26	-6	7	10	145.68	203.19	58.94	4	10	10	294.16	388.21	53.83
6	3	10	2556.89	2359.24	134.42	-5	7	10	124.85	86.15	89.70	5	10	10	652.47	678.63	60.30
7	3	10	17.72	60.97	86.36	-4	7	10	1001.34	1452.93	114.77	6	10	10	3.98	-34.95	93.69
8	3	10	308.45	305.03	51.42	-3	7	10	1783.02	1943.89	126.13	7	10	10	252.37	305.42	59.42
9	3	10	345.27	331.29	61.63	-2	7	10	855.81	768.12	68.89	8	10	10	419.71	366.72	66.23
-7	4	10	0.88	60.73	97.28	-1	7	10	1938.60	2375.77	136.86	-4	11	10	24.35	16.73	58.58
-6	4	10	1.31	2.54	91.96	0	7	10	12.08	-1.51	65.47	-3	11	10	138.88	97.05	52.84
-5	4	10	1039.07	963.66	78.72	1	7	10	41.05	41.42	44.32	-2	11	10	11.30	-6.88	64.88
-4	4	10	1613.88	1754.55	121.85	2	7	10	42.12	-88.74	67.74	-1	11	10	0.43	9.83	86.26
-3	4	10	2734.24	2685.56	144.60	3	7	10	16.11	6.02	57.48	0	11	10	434.87	450.09	57.43
-2	4	10	5579.95	6091.63	238.15	4	7	10	216.44	20.58	74.47	1	11	10	579.23	476.96	56.64
-1	4	10	274.52	230.04	36.83	5	7	10	1.58	64.87	69.34	2	11	10	788.36	828.00	73.55
0	4	10	168.21	197.14	35.33	6	7	10	167.00	216.99	48.22	3	11	10	607.43	639.01	57.46
1	4	10	1134.28	976.25	76.29	7	7	10	305.77	288.79	81.90	4	11	10	749.02	755.63	73.17
2	4	10	44.72	46.61	52.36	8	7	10	2.96	44.24	96.76	5	11	10	134.47	171.65	54.47
3	4	10	98.44	101.21	31.48	9	7	10	546.38	564.10	69.06	6	11	10	100.74	145.83	54.89
4	4	10	71.34	106.71	33.95	-6	8	10	3.72	7.91	105.70	7	11	10	40.02	57.79	56.43
5	4	10	455.57	424.41	44.99	-5	8	10	360.08	357.89	61.00	8	11	10	0.66	-2.01	113.47
6	4	10	62.32	101.10	42.05	-4	8	10	502.55	524.91	56.67	-4	12	10	0.05	73.34	94.65
7	4	10	99.84	131.96	45.64	-3	8	10	44.87	71.63	47.15	-3	12	10	3.01	2.63	99.12
8	4	10	780.42	873.44	80.76	-2	8	10	497.55	474.00	51.16	-2	12	10	163.06	133.05	59.08
9	4	10	85.73	158.84	56.62	-1	8	10	463.61	595.23	52.03	-1	12	10	45.06	43.71	93.01
-7	5	10	0.31	-5.31	102.63	0	8	10	811.68	771.04	67.32	0	12	10	911.10	883.53	85.20
-6	5	10	312.02	293.64	60.93	1	8	10	1964.19	2156.98	128.00	1	12	10	1.64	-219.41	94.10
-5	5	10	449.24	253.11	52.22	2	8	10	519.82	569.48	57.35	2	12	10	740.30	789.84	73.85

Structure Factors Table (continued) [*-unobserved reflns.] for C(14) H(30) Cl(2) Cu(1) N(4) O(9)

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
3	12	10	176.67	140.86	52.19	1	-11	11	53.52	39.66	97.32	4	-7	11	83.59	139.90	47.21
4	12	10	105.58	80.02	98.35	2	-11	11	334.14	278.09	59.01	5	-7	11	213.62	215.50	52.10
5	12	10	208.56	154.97	55.29	3	-11	11	655.76	566.12	65.64	6	-7	11	211.11	244.15	56.68
6	12	10	0.18	51.33	95.13	4	-11	11	53.48	39.99	103.83	7	-7	11	99.67	114.96	59.28
7	12	10	0.07	-136.81	109.85	5	-11	11	156.78	108.55	111.33	-7	-6	11	107.02	111.91	112.53
-3	13	10	1.09	126.97	57.02	-5	-10	11	0.15	-40.19	113.61	-6	-6	11	237.42	322.70	60.61
-2	13	10	302.66	333.14	68.83	-4	-10	11	158.27	116.28	61.16	-5	-6	11	28.98	-113.45	95.45
-1	13	10	310.59	128.36	62.81	-3	-10	11	31.71	174.90	51.05	-4	-6	11	192.93	214.89	52.45
0	13	10	4.92	62.54	56.90	-2	-10	11	26.47	90.02	50.60	-3	-6	11	84.66	62.00	46.11
1	13	10	45.55	154.59	51.12	-1	-10	11	459.90	440.41	59.14	-2	-6	11	14.34	76.59	42.37
2	13	10	8.03	55.08	95.11	0	-10	11	862.01	1028.53	83.92	-1	-6	11	123.54	193.71	43.66
3	13	10	33.67	47.25	63.00	1	-10	11	375.45	529.18	55.55	0	-6	11	223.10	185.62	43.37
4	13	10	193.28	243.85	58.82	2	-10	11	224.45	208.43	56.35	1	-6	11	22.37	-156.29	71.61
5	13	10	24.65	51.52	100.57	3	-10	11	29.07	49.90	92.70	2	-6	11	401.34	423.22	48.53
6	13	10	191.45	74.00	112.21	4	-10	11	51.69	94.83	97.37	3	-6	11	28.83	61.13	40.68
-2	14	10	65.73	130.35	61.00	5	-10	11	94.24	34.86	59.27	4	-6	11	14.05	-77.97	77.00
-1	14	10	133.80	53.90	74.06	6	-10	11	182.47	158.92	64.99	5	-6	11	50.24	4.16	84.65
0	14	10	2.98	66.81	60.09	-6	-9	11	43.65	58.69	116.42	6	-6	11	524.97	434.72	58.82
1	14	10	153.44	70.84	108.25	-5	-9	11	143.46	105.69	107.21	7	-6	11	457.42	409.37	62.94
2	14	10	383.79	232.92	61.75	-4	-9	11	3.17	-46.68	91.82	8	-6	11	350.64	131.24	67.02
3	14	10	727.29	680.60	70.98	-3	-9	11	5.84	-1.25	87.75	-7	-5	11	464.16	447.38	70.18
4	14	10	213.54	192.80	61.93	-2	-9	11	206.67	312.80	52.85	-6	-5	11	7.92	38.44	66.47
5	14	10	281.72	128.27	64.92	-1	-9	11	2.51	18.51	55.52	-5	-5	11	627.59	687.22	64.97
-1	15	10	157.38	171.93	64.05	0	-9	11	283.06	172.75	54.65	-4	-5	11	55.05	-87.00	82.08
0	15	10	12.60	94.34	105.71	1	-9	11	116.17	231.50	48.41	-3	-5	11	30.05	-74.66	78.44
1	15	10	497.08	387.80	67.89	2	-9	11	146.89	23.97	85.48	-2	-5	11	633.94	653.87	63.63
2	15	10	0.13	11.18	103.93	3	-9	11	112.33	7.57	92.19	-1	-5	11	22.33	18.53	67.31
3	15	10	535.67	391.82	70.62	4	-9	11	9.93	51.33	81.62	0	-5	11	2600.82	2908.23	146.53
4	15	10	211.17	12.80	114.00	5	-9	11	33.61	116.42	51.95	1	-5	11	23.31	-89.98	63.33
-1	-14	11	80.64	100.09	64.51	6	-9	11	322.49	329.29	62.77	3	-5	11	642.52	798.70	63.55
0	-14	11	85.78	-7.19	115.34	7	-9	11	84.16	76.05	78.73	3	-5	11	995.91	1075.12	97.57
1	-14	11	190.84	184.78	65.49	-6	-8	11	491.18	442.67	69.94	4	-5	11	17.61	10.58	69.62
2	-14	11	240.90	98.56	70.02	-5	-8	11	68.87	184.86	55.47	5	-5	11	1791.38	1969.55	129.73
-3	-13	11	62.10	-110.05	117.44	-4	-8	11	102.38	157.25	54.16	6	-5	11	27.92	64.78	84.32
-2	-13	11	182.09	52.45	113.26	-3	-8	11	18.93	108.72	48.46	7	-5	11	44.15	-41.08	93.86
-1	-13	11	150.57	47.81	109.98	-2	-8	11	330.09	400.67	55.12	8	-5	11	2.46	-0.12	102.39
0	-13	11	341.08	413.47	63.20	-1	-8	11	931.79	1044.53	104.99	-7	-4	11	3.70	-47.54	135.27
1	-13	11	496.40	363.91	67.34	0	-8	11	119.11	95.50	46.96	-6	-4	11	1.34	-69.00	99.84
2	-13	11	43.75	-53.82	107.93	1	-8	11	2153.10	2177.62	144.05	-5	-4	11	45.58	5.34	90.52
3	-13	11	96.45	-99.16	118.34	2	-8	11	2927.60	2969.35	159.02	-4	-4	11	323.81	337.53	50.92
-4	-12	11	54.49	103.31	116.02	3	-8	11	23.85	20.25	30.93	-3	-4	11	1.00	58.14	73.31
-3	-12	11	57.64	51.26	59.61	4	-8	11	1384.46	1231.73	124.51	-2	-4	11	421.25	411.81	46.36
-2	-12	11	44.81	81.48	61.24	5	-8	11	224.16	87.91	93.87	-1	-4	11	955.37	803.49	82.17
-1	-12	11	26.58	106.72	54.84	6	-8	11	27.79	-127.23	88.67	0	-4	11	335.18	176.18	42.71
0	-12	11	6.01	-100.00	103.01	7	-8	11	1.97	31.46	75.64	1	-4	11	1064.98	1060.13	82.67
1	-12	11	92.68	96.08	58.28	-6	-7	11	20.20	-44.68	100.60	2	-4	11	63.05	-27.91	63.02
2	-12	11	36.61	-25.74	97.87	-5	-7	11	100.17	84.77	55.96	3	-4	11	821.67	741.98	63.00
3	-12	11	51.42	-111.55	108.89	-4	-7	11	17.84	9.77	86.59	4	-4	11	52.22	37.20	70.59
4	-12	11	100.99	47.56	107.79	-3	-7	11	260.41	271.57	48.25	5	-4	11	5.87	28.66	82.07
-5	-11	11	56.41	32.38	80.05	-2	-7	11	1022.68	1054.22	78.10	6	-4	11	438.55	390.96	54.27
-4	-11	11	155.38	186.93	64.48	-1	-7	11	329.29	213.92	47.30	7	-4	11	333.34	411.39	58.00
-3	-11	11	25.78	-19.85	96.44	0	-7	11	1630.35	1608.26	117.97	8	-4	11	8.80	73.17	98.44
-2	-11	11	128.93	23.94	98.81	-7	-7	11	3177.14	3124.10	164.67	-7	-3	11	1.52	10.35	102.71
-1	-11	11	75.45	65.32	99.54	2	-7	11	134.97	-12.64	82.22	-6	-3	11	164.74	-64.59	105.90
0	-11	11	582.20	585.12	64.06	3	-7	11	31.21	-72.02	78.22	-5	-3	11	399.62	308.28	53.19

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-4	-3	11	22.56	97.25	42.34	0	0	11	583.92	419.17	33.24	4	3	11	1542.29	1472.06	101.54
-3	-3	11	2031.14	2044.68	128.03	1	0	11	45.74	-37.84	79.16	5	3	11	916.76	976.39	92.58
-2	-3	11	267.50	212.21	40.46	2	0	11	0.96	-52.77	39.74	6	3	11	61.60	32.43	45.30
-1	-3	11	512.48	549.82	51.17	3	0	11	1093.96	1073.60	60.33	7	3	11	1916.87	2092.37	133.50
0	-3	11	641.27	545.27	49.13	4	0	11	3.36	-19.28	42.67	8	3	11	204.10	274.11	54.63
1	-3	11	144.36	28.35	58.88	5	0	11	1.51	-40.81	47.00	9	3	11	228.71	249.56	61.12
2	-3	11	933.51	694.86	56.22	6	0	11	1215.85	1190.32	76.10	-7	4	11	255.01	405.33	67.42
3	-3	11	16.97	38.76	35.71	7	0	11	838.14	905.13	175.13	-6	4	11	62.49	55.97	100.91
4	-3	11	797.41	805.34	63.82	8	0	11	430.76	709.10	81.52	-5	4	11	0.36	-49.67	88.90
5	-3	11	196.23	100.78	42.46	9	0	11	315.86	316.39	47.18	-4	4	11	180.80	142.87	48.61
6	-3	11	97.27	0.42	82.17	-7	1	11	48.25	-154.27	110.56	-3	4	11	103.00	194.18	44.36
7	-3	11	972.91	895.23	84.72	-6	1	11	93.50	56.84	77.91	-2	4	11	1099.82	1308.35	102.66
8	-3	11	404.41	476.73	65.57	-5	1	11	642.79	574.13	58.62	-1	4	11	552.49	556.14	46.98
9	-3	11	160.90	283.21	62.88	-4	1	11	192.53	173.70	46.05	0	4	11	2842.67	2657.50	137.82
-7	-2	11	244.46	278.96	65.27	-3	1	11	20.77	3.35	66.56	1	4	11	1760.05	1932.98	107.63
-6	-2	11	742.99	844.28	79.39	-2	1	11	344.00	806.54	62.07	2	4	11	0.37	-8.83	58.66
-5	-2	11	1.26	-92.63	88.35	-1	1	11	4197.52	4168.61	178.45	3	4	11	1213.92	1011.50	85.40
-4	-2	11	386.77	469.90	50.25	0	1	11	1453.59	512.37	62.85*	4	4	11	933.34	961.20	86.05
-3	-2	11	25.64	21.89	72.11	1	1	11	295.30	361.42	36.51	5	4	11	229.32	241.75	42.59
-2	-2	11	1446.69	1579.65	106.93	2	1	11	1722.75	1860.43	101.26	6	4	11	932.57	1090.86	99.08
-1	-2	11	1186.77	1105.38	88.33	3	1	11	2727.20	2746.70	131.94	7	4	11	127.11	52.96	43.09
0	-2	11	1093.21	984.89	102.15	4	1	11	125.72	94.69	14.27	8	4	11	28.66	-93.99	97.38
1	-2	11	1286.75	980.15	81.45	5	1	11	729.26	782.15	59.74	9	4	11	0.95	32.18	100.83
2	-2	11	245.03	240.88	37.04	6	1	11	419.95	412.02	48.67	-6	5	11	0.67	-96.65	101.72
3	-2	11	294.06	366.59	39.56	7	1	11	259.24	326.40	52.21	-5	5	11	23.03	60.72	87.00
4	-2	11	3492.62	3685.07	164.38	8	1	11	1.28	-117.37	88.97	-4	5	11	1.99	-142.70	79.86
5	-2	11	539.39	592.59	57.12	9	1	11	47.44	-14.05	105.40	-3	5	11	1173.50	1171.71	105.87
6	-2	11	949.11	959.22	76.33	-7	2	11	35.09	86.97	101.37	-2	5	11	1061.27	998.25	98.78
7	-2	11	316.24	333.40	55.40	-6	2	11	38.58	107.15	53.76	-1	5	11	320.56	306.77	43.57
8	-2	11	75.60	75.19	56.41	-5	2	11	13.70	16.76	79.43	0	5	11	654.12	668.09	53.13
9	-2	11	7.06	-30.97	108.60	-4	2	11	289.29	324.44	48.22	1	6	11	94.76	82.92	35.98
-7	-1	11	52.24	56.19	103.25	-3	2	11	163.51	57.59	74.63	2	5	11	854.56	938.48	82.44
-6	-1	11	32.75	-150.40	94.13	-2	2	11	2726.68	2860.13	141.00	3	5	11	928.31	1062.55	82.50
-5	-1	11	161.93	146.85	53.35	-1	2	11	1056.59	1038.61	92.24	4	5	11	180.54	225.78	40.41
-4	-1	11	478.86	525.67	53.54	0	2	11	1570.34	1591.38	111.81	5	5	11	743.26	741.09	64.85
-3	-1	11	1189.33	1188.90	99.93	1	2	11	2645.48	2885.90	137.78	6	5	11	1.09	-27.49	79.56
-2	-1	11	786.71	827.82	84.77	2	2	11	1278.33	1186.54	84.53	7	5	11	51.37	-33.46	81.88
-1	-1	11	265.11	191.19	33.97	3	2	11	1604.19	1495.74	97.07	8	5	11	0.20	47.50	93.49
0	-1	11	1821.10	1427.31	123.79	4	2	11	737.31	718.00	57.58	9	5	11	148.61	123.11	60.73
1	-1	11	644.12	570.48	50.01	5	2	11	24.07	-2.22	64.18	-6	6	11	28.99	90.01	95.76
2	-1	11	1448.81	1246.46	88.06	6	2	11	83.42	565.25	52.66	-5	6	11	224.67	284.04	55.27
3	-1	11	3.00	-34.51	56.73	7	2	11	0.18	72.91	44.55	-4	6	11	349.55	455.24	55.69
4	-1	11	23.28	37.75	40.81	8	2	11	70.53	90.55	93.42	-3	6	11	526.71	453.97	54.45
5	-1	11	185.92	205.74	42.72	9	2	11	138.58	119.31	59.51	-2	6	11	1680.64	2047.15	131.50
6	-1	11	21.86	0.74	71.69	-7	3	11	75.13	-95.79	109.01	-1	6	11	1229.74	1259.72	105.77
7	-1	11	404.37	463.04	54.87	-6	3	11	306.68	343.87	60.07	0	6	11	1408.85	1406.64	103.28
8	-1	11	65.23	26.76	90.38	-5	3	11	17.79	74.46	45.47	1	6	11	1.81	-12.44	63.02
9	-1	11	47.45	90.34	57.52	-4	3	11	5.31	-122.84	76.07	2	6	11	157.84	194.63	37.51
-7	0	11	230.82	249.97	43.57	-3	3	11	1637.35	1493.75	119.30	3	6	11	1326.91	1439.87	98.37
-6	0	11	5.64	-58.23	84.35	-2	3	11	1515.37	1560.26	110.46	4	6	11	190.04	170.16	40.13
-5	0	11	31.96	-20.73	108.69	-1	3	11	1774.59	1668.70	105.68	5	6	11	1591.93	1671.97	119.18
-4	0	11	327.15	318.65	54.02	0	3	11	1978.43	2277.56	123.82	6	6	11	384.34	386.52	51.44
-3	0	11	176.53	122.85	29.21	1	3	11	0.19	50.59	55.44	7	6	11	46.12	148.73	49.78
-2	0	11	436.69	300.81	29.28	2	3	11	615.72	753.44	77.02	8	6	11	315.83	311.31	59.90
-1	0	11	1388.94	1363.72	64.82	3	3	11	306.87	271.36	39.09	9	6	11	56.47	-44.67	107.92

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-6	7	11	48.92	47.01	100.84	7	10	11	74.86	58.34	71.76	1	-12	12	64.10	89.62	101.08
-5	7	11	6.94	54.92	64.41	8	10	11	2.83	-25.60	105.32	2	-12	12	329.24	337.65	64.86
-4	7	11	20.34	-2.85	86.07	-4	11	11	135.79	83.93	64.31	3	-12	12	60.55	14.13	183.34
-3	7	11	2.17	-141.23	84.38	-3	11	11	230.97	189.56	60.80	4	-12	12	212.73	224.61	63.38
-2	7	11	87.22	71.67	47.53	-2	11	11	236.47	114.73	85.70	-4	-11	12	468.07	508.76	70.91
-1	7	11	614.56	675.74	65.81	-1	11	11	337.46	320.20	60.07	-3	-11	12	1.35	26.21	101.49
0	7	11	38.18	58.66	70.12	0	11	11	7.59	-120.42	93.08	-2	-11	12	900.14	441.87	67.83
1	7	11	586.68	509.14	47.76	1	11	11	64.44	-93.01	93.15	-1	-11	12	1.27	-132.44	95.46
2	7	11	1456.45	1539.14	108.80	2	11	11	50.27	62.95	81.23	0	-11	12	166.76	27.00	104.06
3	7	11	208.72	247.98	42.62	3	11	11	98.66	82.91	86.55	1	-11	12	43.37	40.83	100.83
4	7	11	1336.50	1230.38	103.22	4	11	11	2.68	-14.76	88.70	2	-11	12	235.95	102.64	106.56
5	7	11	2426.36	1495.06	144.44	5	11	11	0.19	-115.35	93.50	3	-11	12	214.71	-88.02	104.36
6	7	11	81.09	57.35	79.74	6	11	11	198.77	175.48	59.17	4	-11	12	26.69	9.85	96.09
7	7	11	130.14	130.73	52.11	7	11	11	137.40	108.11	61.65	5	-11	12	51.94	2.69	63.79
8	7	11	2.06	32.09	68.71	-3	12	11	38.84	48.31	100.23	-5	-10	12	158.44	165.18	67.63
9	7	11	55.50	7.64	106.92	-2	12	11	496.02	402.06	61.22	-4	-10	12	0.34	47.05	61.25
-5	8	11	40.95	26.97	93.76	-1	12	11	27.87	-69.91	90.73	-3	-10	12	129.06	75.25	102.84
-4	8	11	64.65	2.48	54.03	0	12	11	509.71	422.56	62.74	-2	-10	12	12.86	42.13	91.51
-3	8	11	2.01	15.99	82.69	1	12	11	85.24	-19.09	98.13	-1	-10	12	9.40	37.41	91.99
-2	8	11	308.93	181.79	47.70	2	12	11	8.99	-45.71	94.21	0	-10	12	8.92	80.21	91.59
-1	8	11	392.56	362.02	52.57	3	12	11	436.62	290.47	56.81	1	-10	12	7.92	-8.69	66.30
0	8	11	2645.89	2570.70	147.43	4	12	11	10.72	14.87	65.38	2	-10	12	173.16	124.38	55.57
1	8	11	881.89	869.59	69.34	5	12	11	1005.53	985.70	91.17	3	-10	12	92.85	114.03	84.38
2	8	11	720.94	847.45	87.63	6	12	11	274.50	140.03	62.27	4	-10	12	439.56	392.93	86.05
3	8	11	613.02	544.39	51.95	7	12	11	97.27	156.82	62.13	5	-10	12	110.33	43.64	127.69
4	8	11	133.06	166.48	46.01	-2	13	11	20.54	106.08	57.54	6	-10	12	143.75	105.90	116.07
5	8	11	44.90	56.75	84.33	-1	13	11	250.08	21.67	104.58	-5	-9	12	41.08	-72.35	107.69
6	8	11	44.68	20.63	59.86	0	13	11	0.16	-53.06	113.50	-4	-9	12	32.85	-4.41	191.56
7	8	11	215.48	240.83	55.65	1	13	11	50.14	42.53	97.44	-3	-9	12	671.99	673.91	63.74
8	8	11	103.52	91.96	58.01	2	13	11	70.81	-45.08	98.53	-2	-9	12	135.60	133.22	52.47
-5	9	11	39.03	-153.28	110.10	3	13	11	46.89	35.07	95.38	-1	-9	12	111.28	64.33	85.24
-4	9	11	147.33	171.09	55.65	4	13	11	414.92	343.08	62.01	0	-9	12	437.32	485.73	87.89
-3	9	11	515.26	508.92	61.41	5	13	11	160.30	140.84	59.95	1	-9	12	1218.01	1273.75	127.30
-2	9	11	503.84	543.11	54.42	6	13	11	168.05	130.52	64.90	2	-9	12	34.38	150.24	50.24
-1	9	11	1003.67	1027.58	80.90	-1	14	11	112.09	141.11	61.40	3	-9	12	472.04	322.30	57.17
0	9	11	493.95	680.17	70.17	0	14	11	197.49	189.42	66.76	4	-9	12	956.80	694.34	68.77
1	9	11	57.87	-63.44	82.10	1	14	11	18.83	-61.07	107.08	5	-9	12	3.26	84.66	97.26
2	9	11	346.86	296.91	44.65	2	14	11	86.85	144.91	59.27	6	-9	12	90.33	39.75	106.46
3	9	11	49.10	91.55	44.19	3	14	11	50.82	-72.96	100.75	-6	-8	12	91.43	136.63	63.89
4	9	11	2212.39	2367.12	145.34	4	14	11	14.16	-68.75	102.07	-5	-8	12	238.60	178.59	65.00
5	9	11	358.41	337.77	53.62	5	14	11	40.64	47.56	115.67	-4	-8	12	77.16	55.79	97.78
6	9	11	1349.18	1233.59	91.35	0	15	11	14.07	38.73	68.08	-3	-8	12	1374.33	1365.99	129.05
7	9	11	614.91	541.07	66.31	1	15	11	1.24	11.68	104.75	-2	-8	12	39.40	59.01	85.34
8	9	11	23.41	-139.68	97.06	2	15	11	69.08	97.09	65.99	-1	-8	12	917.67	864.66	80.52
-4	10	11	7.18	-150.42	102.98	3	15	11	31.17	97.69	104.54	0	-8	12	2.24	-37.00	80.83
-3	10	11	25.82	0.51	92.87	-3	-13	12	12.20	23.31	104.86	1	-8	12	16.67	-11.35	84.30
-2	10	11	226.15	439.94	53.60	-1	-13	12	7.67	-18.78	117.86	2	-8	12	278.12	299.46	53.14
-1	10	11	7.26	60.71	90.77	0	-13	12	2.14	-0.82	110.09	3	-8	12	624.50	606.87	59.90
0	10	11	921.91	1012.91	83.04	1	-13	12	91.07	54.59	112.35	4	-8	12	8.76	-29.67	91.49
1	10	11	905.31	914.49	76.84	2	-13	12	14.16	-127.25	112.39	5	-8	12	4.80	58.80	86.65
2	10	11	6.85	-163.04	80.50	3	-13	12	129.47	74.40	116.75	6	-8	12	1.56	111.45	57.00
3	10	11	875.13	898.14	74.65	-3	-12	12	51.48	87.45	61.20	7	-8	12	306.04	286.48	68.17
4	10	11	601.90	639.19	59.00	-2	-12	12	92.21	37.74	108.21	-6	-7	12	104.87	152.70	62.11
5	10	11	558.74	557.12	59.33	-1	-12	12	230.46	213.55	62.83	-5	-7	12	74.93	43.40	104.87
6	10	11	192.42	294.62	55.58	0	-12	12	198.89	208.66	61.09	-4	-7	12	408.84	434.99	59.13

h	k	l	F ² cal	F ² obs	nig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-3	-7	12	0.28	-135.46	88.53	8	-4	12	7.16	77.12	99.85	-3	0	12	690.41	620.69	42.22
-2	-7	12	103.89	-15.55	86.53	-7	-3	12	56.22	76.40	109.65	-2	0	12	1181.82	1170.67	71.86
-1	-7	12	261.35	206.04	45.10	-6	-3	12	34.08	-101.42	97.79	-	0	12	907.69	634.94	42.77
0	-7	12	68.77	-84.52	84.85	-5	-3	12	7.04	-135.10	99.95	0	0	12	1004.42	739.88	44.07
1	-7	12	713.94	745.62	70.93	-4	-3	12	53.83	40.49	48.72	1	0	12	5580.59	6262.24	169.34
2	-7	12	104.03	-129.44	92.13	-3	-3	12	242.31	286.15	45.86	2	0	12	7166.67	6543.40	174.91
3	-7	12	223.68	263.68	47.94	-2	-3	12	111.82	131.86	41.32	3	0	12	3596.67	4017.17	122.63
4	-7	12	171.58	166.20	49.09	-1	-3	12	2.02	-69.48	66.52	4	0	12	3367.20	3355.84	112.29
5	-7	12	582.13	550.85	58.58	0	-3	12	799.11	431.69	70.27	5	0	12	75.87	57.27	36.94
6	-7	12	68.74	106.31	56.68	1	-3	12	3243.97	3063.92	149.84	6	0	12	224.28	238.93	33.22
7	-7	12	111.78	174.44	60.34	2	-3	12	2636.06	2809.60	146.35	7	0	12	86.98	166.10	48.29
-6	-6	12	28.70	72.44	103.00	3	-3	12	3129.67	3368.44	160.71	8	0	12	293.59	228.85	41.23
-5	-6	12	47.45	72.44	96.72	4	-3	12	123.60	114.20	44.03	9	0	12	251.29	300.67	58.94
-4	-6	12	360.09	376.98	56.05	5	-3	12	1166.63	1124.31	105.41	-7	1	12	63.63	77.47	99.60
-3	-6	12	65.62	119.11	47.12	6	-3	12	79.30	153.97	47.16	-6	1	12	175.50	146.12	58.51
-2	-6	12	351.06	392.36	53.74	7	-3	12	173.64	152.71	56.72	-5	1	12	283.87	294.13	53.19
-1	-6	12	68.40	131.39	44.65	8	-3	12	243.42	178.78	52.22	-4	1	12	5.84	12.61	77.18
0	-6	12	1020.48	1176.45	106.85	-7	-2	12	80.54	145.13	65.20	-3	1	12	510.62	548.27	52.62
1	-6	12	354.13	465.86	51.37	-6	-2	12	349.33	402.47	60.75	-2	1	12	1225.50	1253.20	105.21
2	-6	12	4993.66	5444.71	231.25	-5	-2	12	21.70	79.37	50.87	-1	1	12	11.52	-157.10	74.10
3	-6	12	3.74	53.85	74.27	-4	-2	12	228.57	233.72	50.96	0	1	12	1226.63	947.33	82.81
4	-6	12	1070.88	1158.98	103.86	-3	-2	12	56.42	40.13	74.90	1	1	12	22.06	23.88	59.92
5	-6	12	428.13	418.55	55.81	-2	-2	12	595.26	664.02	64.52	2	1	12	368.23	356.42	42.63
6	-6	12	46.85	-90.82	94.97	-1	-2	12	460.21	638.00	57.91	3	1	12	45.88	32.48	45.74
7	-6	12	10.79	7.01	90.26	0	-2	12	507.12	-1635.70	130.42*	4	1	12	8.70	-147.26	70.56
8	-6	12	3.67	-92.71	109.17	1	-2	12	15.00	42.35	62.44	5	1	12	22.30	43.90	67.50
-6	-5	12	2.53	-194.45	97.98	2	-2	12	105.90	108.08	37.82	6	1	12	1276.75	1188.90	112.30
-5	-5	12	238.10	234.72	58.19	3	-2	12	597.47	689.37	61.86	7	1	12	47.50	18.23	87.69
-4	-5	12	655.05	824.95	79.38	4	-2	12	41.06	-36.24	73.54	8	1	12	809.70	876.10	84.70
-3	-5	12	194.65	138.00	48.64	5	-2	12	55.61	68.42	72.26	9	1	12	0.16	118.22	55.77
-2	-5	12	1397.71	1382.21	119.15	6	-2	12	192.93	199.04	48.12	-6	2	12	205.42	148.34	59.36
-1	-5	12	255.00	199.49	44.45	7	-2	12	1188.43	1321.97	118.95	-5	2	12	126.68	137.60	50.01
0	-5	12	117.95	-54.36	91.79	8	-2	12	120.03	159.19	56.58	-4	2	12	882.91	1053.59	109.07
1	-5	12	127.74	82.05	40.49	9	-2	12	339.21	250.26	67.21	-3	2	12	96.83	65.63	80.67
2	-5	12	1047.07	1267.73	102.22	-7	-1	12	17.54	54.12	113.11	-2	2	12	186.02	198.31	44.79
3	-5	12	999.58	1020.02	97.17	-6	-1	12	23.27	-1.43	94.57	-1	2	12	23.94	-110.87	79.38
4	-5	12	720.02	904.55	71.06	-5	-1	12	1023.75	1039.93	84.77	0	2	12	1040.95	391.80	62.86*
5	-5	12	16.86	-26.34	82.99	-4	-1	12	76.29	74.90	80.86	1	2	12	696.23	678.31	87.08
6	-5	12	288.15	236.40	45.33	-3	-1	12	2450.26	2851.15	149.95	2	2	12	195.13	247.48	39.08
7	-5	12	49.50	-11.50	100.84	-2	-1	12	669.23	624.89	58.52	3	2	12	1888.79	3060.91	118.34
8	-5	12	795.84	689.08	76.27	-1	-1	12	156.35	146.38	39.97	4	2	12	1588.94	1860.54	107.55
-6	-4	12	242.67	34.92	115.67	0	-1	12	177.88	-1322.70	124.00*	5	2	12	212.12	101.89	43.36
-5	-4	12	97.80	187.94	51.60	1	-1	12	36.11	6.67	60.58	6	2	12	325.42	313.76	51.16
-4	-4	12	212.61	353.62	52.18	2	-1	12	887.16	947.53	80.30	7	2	12	51.39	45.03	49.08
-3	-4	12	199.11	211.68	46.77	3	-1	12	3045.23	3042.79	147.65	8	2	12	13.80	5.65	90.79
-2	-4	12	980.12	1112.74	97.12	4	-1	12	586.97	532.12	47.41	9	2	12	26.77	-127.31	105.55
-1	-4	12	208.11	223.79	44.46	5	-1	12	652.71	673.25	62.95	-6	3	12	0.28	-116.98	101.85
0	-4	12	1125.41	1142.59	98.04	6	-1	12	4.44	60.51	75.81	-5	3	12	17.33	-42.84	86.22
1	-4	12	0.76	-42.09	63.39	7	-1	12	24.35	-32.24	92.75	-4	3	12	194.91	151.75	46.78
2	-4	12	490.19	419.30	44.80	8	-1	12	53.63	65.41	55.34	-3	3	12	1580.44	1489.70	117.44
3	-4	12	292.24	282.95	43.98	9	-1	12	100.37	104.97	63.91	-2	3	12	15.52	63.04	72.91
4	-4	12	1778.07	1853.89	120.35	-7	0	12	24.20	-157.69	78.38	-1	3	12	385.82	330.01	45.81
5	-4	12	6.08	8.49	75.58	-6	0	12	38.67	57.84	70.87	0	3	12	3023.60	3004.71	158.46
6	-4	12	610.89	572.66	60.38	-5	0	12	57.57	67.06	144.63	1	3	12	1678.47	1779.83	112.26
7	-4	12	8.19	50.77	51.21	-4	0	12	296.11	287.25	35.08	2	3	12	4779.40	5079.89	204.42

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
3	3	12	3897.39	3698.34	154.58	-5	7	12	87.58	-37.52	102.61	-2	11	12	126.58	11.51	105.84
4	3	12	1805.93	1822.29	113.67	-4	7	12	45.33	-32.63	88.55	-1	11	12	44.54	-142.71	100.37
5	3	12	91.30	60.68	71.56	-3	7	12	199.79	183.93	50.02	0	11	12	1.19	-23.95	55.92
6	3	12	369.77	330.42	49.89	-2	7	12	12.09	-57.41	81.05	1	11	12	1091.07	1015.20	86.96
7	3	12	169.01	192.57	53.57	-1	7	12	8.08	19.71	70.97	2	11	12	95.29	41.99	64.44
8	3	12	39.66	81.46	95.85	0	7	12	2.18	14.86	66.19	3	11	12	191.96	185.46	58.91
9	3	12	167.45	71.08	63.96	1	7	12	167.42	449.23	47.79	4	11	12	291.34	141.14	57.36
-6	4	12	99.35	70.91	98.26	2	7	12	173.79	195.19	42.51	5	11	12	148.95	266.33	61.51
-5	4	12	201.97	239.34	55.40	3	7	12	46.02	0.33	74.23	6	11	12	66.80	62.51	56.97
-4	4	12	396.76	322.23	52.21	4	7	12	131.92	135.21	44.63	7	11	12	448.31	509.84	67.97
-3	4	12	67.58	22.5	74.00	5	7	12	160.48	167.71	47.67	-3	12	12	15.55	99.84	61.24
-2	4	12	4.14	-3.15	74.84	6	7	12	65.84	49.17	45.48	-2	12	12	466.04	492.55	68.37
-1	4	12	1604.53	1386.29	103.19	7	7	12	426.33	373.74	60.61	-1	12	12	49.08	-30.29	107.20
0	4	12	985.76	1023.37	71.11	8	7	12	154.26	218.91	60.88	0	12	12	290.97	285.13	62.34
1	4	12	30.91	33.32	36.98	-5	8	12	209.59	297.82	59.80	1	12	12	252.95	249.32	61.66
2	4	12	22.89	57.73	35.40	-4	8	12	497.68	518.63	62.82	2	12	12	3.41	-73.44	89.24
3	4	12	24.23	113.42	38.09	-3	8	12	240.86	276.25	50.97	3	12	12	63.55	59.93	66.37
4	4	12	510.74	542.81	57.14	-2	8	12	37.77	29.33	84.53	4	12	12	4.67	35.71	89.97
5	4	12	622.72	630.77	62.18	-1	8	12	132.02	-3.64	92.94	5	12	12	3.27	-14.93	98.20
6	4	12	79.08	111.66	45.81	0	8	12	327.06	389.21	51.83	6	12	12	22.06	16.11	102.91
7	4	12	100.09	79.34	51.51	1	8	12	200.58	102.97	48.13	-2	13	12	9.38	-26.35	102.24
8	4	12	239.28	234.80	59.99	2	8	12	2.21	-24.14	76.44	-1	13	12	483.76	601.78	70.21
9	4	12	176.54	243.91	63.56	3	8	12	332.76	343.26	46.96	0	13	12	46.25	113.65	61.80
-6	5	12	234.06	162.09	64.61	4	8	12	739.39	784.64	72.59	1	13	12	52.81	-38.73	102.21
-5	5	12	443.70	399.30	59.52	5	8	12	452.14	493.44	56.62	2	13	12	0.07	-34.22	99.02
-4	5	12	70.46	55.46	90.65	6	8	12	1846.34	1718.59	138.97	3	13	12	0.01	24.75	64.49
-3	5	12	380.67	652.71	54.88	7	8	12	5.32	-41.26	98.74	4	13	12	16.35	75.62	98.17
-2	5	12	256.74	160.93	47.65	8	8	12	225.08	173.99	64.11	5	13	12	10.12	-221.38	110.92
-1	5	12	302.64	277.53	45.80	-5	9	12	0.33	1.16	75.20	6	13	12	2.73	-181.06	117.32
0	5	12	39.00	67.58	69.78	-4	9	12	0.59	14.20	97.51	0	14	12	236.17	298.71	69.24
1	5	12	642.87	605.87	58.93	-3	9	12	375.58	366.29	62.19	1	14	12	25.00	-217.84	115.09
2	5	12	336.48	147.94	42.24	-2	9	12	0.11	-80.92	91.17	2	14	12	414.98	421.41	66.54
3	5	12	189.81	248.94	39.60	-1	9	12	1107.54	1270.35	120.88	3	14	12	214.69	109.51	109.56
4	5	12	646.76	676.42	62.85	0	9	12	32.14	61.49	87.32	4	14	12	2.80	-178.64	108.29
5	5	12	2221.81	2195.14	136.68	1	9	12	282.84	286.68	50.13	0	-13	13	60.85	89.18	110.09
6	5	12	17.98	11.04	84.16	2	9	12	1289.98	1292.72	110.80	1	-13	13	352.18	417.97	69.41
7	5	12	1289.94	1144.85	90.50	3	9	12	368.88	487.04	53.78	-2	-12	13	76.75	37.93	107.79
8	5	12	131.81	195.12	57.23	4	9	12	317.48	295.48	53.46	-1	-12	13	9.87	-79.45	104.53
9	5	12	10.29	-219.21	118.29	5	9	12	95.14	-161.78	92.74	0	-12	13	52.13	188.71	61.25
-6	6	12	0.22	-78.66	112.15	6	9	12	10.48	1.69	94.32	1	-12	13	51.32	63.97	106.06
-5	6	12	0.03	45.45	88.14	7	9	12	149.24	241.49	58.96	2	-12	13	13.51	-124.99	109.57
-4	6	12	210.45	164.03	53.35	8	9	12	34.68	156.25	59.16	3	-12	13	141.77	107.86	65.17
-3	6	12	35.86	-71.21	81.43	-4	10	12	45.30	35.38	103.23	-3	-11	13	5.32	56.81	60.05
-2	6	12	673.80	825.19	71.29	-3	10	12	1.48	-97.91	104.09	-2	-11	13	72.29	86.88	100.66
-1	6	12	174.05	267.26	48.28	-2	10	12	468.18	454.27	60.41	-1	-11	13	110.73	62.95	109.17
0	6	12	2.68	-43.72	71.52	-1	10	12	0.92	16.69	86.99	0	-11	13	63.32	6.61	102.22
1	6	12	1408.81	1402.61	110.56	0	10	12	748.24	679.46	63.44	1	-11	13	395.64	354.72	64.56
2	6	12	718.42	927.63	89.61	1	10	12	122.27	14.80	65.43	2	-11	13	27.71	-41.77	105.85
3	6	12	2210.22	2349.40	134.17	2	10	12	25.71	27.06	84.76	3	-11	13	64.48	68.90	105.83
4	6	12	396.89	431.55	49.10	3	10	12	64.09	47.18	87.33	4	-11	13	155.57	84.29	113.31
5	6	12	284.67	328.24	49.70	4	10	12	31.46	-5.89	83.90	-4	-10	13	3.46	2.24	101.62
6	6	12	6.83	56.56	81.05	5	10	12	116.42	149.52	54.29	-3	-10	13	154.06	163.33	61.43
7	6	12	105.38	102.24	51.02	6	10	12	502.26	529.01	63.93	-2	-10	13	79.83	170.78	57.02
8	6	12	600.42	574.33	67.33	7	10	12	13.11	34.35	101.69	-1	-10	13	1030.73	1120.42	93.95
9	6	12	80.49	26.27	80.53	-3	11	12	168.65	36.08	113.58	0	-10	13	305.93	289.01	61.72

h	k	l	F^2 cal	F^2 obs	sig(F^2)	h	k	l	F^2 cal	F^2 obs	sig(F^2)	h	k	l	F^2 cal	F^2 obs	sig(F^2)
1	-10	13	379.03	380.65	60.54	7	-6	13	378.38	344.71	67.34	3	-2	13	228.44	302.67	44.06
2	-10	13	125.23	77.30	57.41	-6	-5	13	5.21	-236.68	112.64	4	-2	13	3324.39	3572.54	170.83
3	-10	13	95.34	95.26	98.79	-5	-5	13	0.23	-128.72	98.90	5	-2	13	625.09	597.45	56.49
4	-10	13	11.14	77.21	108.65	-4	-5	13	162.74	235.77	85.00	6	-2	13	613.85	612.40	61.64
5	-10	13	12.86	91.13	108.05	-3	-5	13	150.72	192.32	48.34	7	-2	13	66.11	200.32	54.51
-5	-9	13	52.23	-23.83	116.28	-2	-5	13	290.18	255.40	49.73	8	-2	13	9.57	188.48	55.38
-4	-9	13	342.35	287.37	67.61	-1	-5	13	48.48	-130.12	70.60	-6	-1	13	33.47	83.48	57.90
-3	-9	13	183.19	61.76	72.02	0	-5	13	514.53	559.96	54.95	-5	-1	13	116.20	44.55	70.87
-2	-9	13	16.41	51.54	64.87	1	-5	13	546.11	534.23	53.82	-4	-1	13	225.02	237.94	49.89
-1	-9	13	525.75	443.07	62.47	2	-5	13	0.32	25.72	74.65	-3	-1	13	50.57	30.83	57.91
0	-9	13	1.56	-99.69	91.96	3	-5	13	272.68	266.53	49.67	-2	-1	13	764.34	857.89	67.16
1	-9	13	26.64	-95.65	99.50	4	-5	13	47.88	-9.54	83.14	-1	-1	13	9.59	15.74	64.46
2	-9	13	48.16	-13.23	91.16	5	-5	13	659.53	677.72	62.17	0	-1	13	1826.59	1824.49	128.91
3	-9	13	45.82	41.34	66.34	6	-5	13	183.54	177.08	54.01	1	-1	13	744.38	956.95	87.16
4	-9	13	397.76	976.80	92.02	7	-5	13	14.56	83.13	96.17	2	-1	13	155.89	37.56	70.10
5	-9	13	87.63	21.04	108.68	8	-5	13	36.10	77.26	109.95	3	-1	13	160.43	183.08	42.92
6	-9	13	636.08	543.06	73.15	-6	-4	13	9.01	-73.11	108.12	4	-1	13	1704.89	1932.03	117.74
-5	-8	13	7.39	-20.48	100.05	-5	-4	13	1.94	12.71	97.23	5	-1	13	31.65	121.79	43.56
-4	-8	13	38.04	-28.88	108.05	-4	-4	13	90.81	99.81	52.10	6	-1	13	151.41	130.92	49.19
-3	-8	13	53.96	33.23	95.61	-3	-4	13	520.59	575.11	58.23	7	-1	13	67.71	70.58	93.07
-2	-8	13	271.29	274.13	55.54	-2	-4	13	90.36	36.95	45.57	8	-1	13	614.10	586.61	68.35
-1	-8	13	172.21	-8.00	92.57	-1	-4	13	1147.69	1295.33	114.89	-6	0	13	325.61	238.36	46.51
0	-8	13	84.85	55.00	89.31	0	-4	13	136.92	213.68	45.89	-5	0	13	246.76	223.87	40.34
1	-8	13	1.53	56.43	58.55	1	-4	13	1536.00	1828.37	124.08	-4	0	13	608.75	648.68	42.83
2	-8	13	572.84	580.14	59.75	2	-4	13	313.95	489.56	51.72	-3	0	13	208.96	248.66	57.05
3	-8	13	482.05	377.11	58.48	3	-4	13	0.16	26.56	76.90	-2	0	13	166.31	123.35	43.86
4	-8	13	5.87	-59.95	96.54	4	-4	13	340.78	287.51	51.89	-1	0	13	11.36	-109.38	51.77
5	-8	13	181.17	730.11	57.25	5	-4	13	476.61	500.08	58.20	0	0	13	90.27	-884.26	81.28
6	-8	13	40.07	14.77	95.47	6	-4	13	0.57	4.36	89.46	1	0	13	47.03	-89.40	49.68
-5	-7	13	46.28	-128.79	110.79	7	-4	13	41.46	-9.68	89.31	2	0	13	929.05	826.30	66.15
-4	-7	13	61.43	30.86	94.33	8	-4	13	1.73	-317.31	125.59	3	0	13	150.77	226.53	32.17
-3	-7	13	0.73	136.82	49.46	-6	-3	13	20.14	29.78	103.19	4	0	13	2066.95	2317.71	108.79
-2	-7	13	2001.75	2318.69	147.61	-5	-3	13	258.79	58	58.00	5	0	13	861.23	838.96	59.11
-1	-7	13	592.03	751.21	61.19	-4	-3	13	537.15	850.60	61.56	6	0	13	757.02	850.98	52.12
0	-7	13	2173.22	1297.86	143.94	-3	-3	13	0.63	86.09	44.66	7	0	13	583.38	571.70	43.53
1	-7	13	569.46	609.24	60.53	-2	-3	13	392.91	333.04	48.58	8	0	13	4.87	-37.46	69.40
2	-7	13	7.08	-48.12	79.48	-1	-3	13	63.24	75.73	40.10	9	0	13	3.92	-3.37	75.12
3	-7	13	57.07	48.63	0	-3	13	0.15	-1498.48	133.21	-6	1	13	50.73	105.17	58.63	
4	-7	13	70.02	99.52	80.95	1	-3	13	3.67	0.71	76.14	-5	1	13	143.99	-3.95	97.44
5	-7	13	21.62	53.43	88.58	2	-3	13	151.65	149.90	43.73	-4	1	13	25.42	0.65	86.04
6	-7	13	23.43	-27.59	101.40	3	-3	13	1531.76	1782.34	120.41	-3	1	13	3.19	-68.28	79.83
7	-7	13	28.61	72.13	104.09	4	-3	13	962.72	1035.70	99.50	-2	1	13	41.23	86.83	44.83
-6	-6	13	152.94	283.23	62.78	5	-3	13	1447.32	1677.08	124.95	-1	1	13	523.05	555.98	49.31
-5	-6	13	278.79	298.41	61.89	6	-3	13	1049.64	1078.57	82.97	0	1	13	5.00	-863.62	105.47
-4	-6	13	4.26	127.20	50.92	7	-3	13	136.29	198.09	55.71	1	1	13	343.98	350.43	42.58
-3	-6	13	431.13	419.45	55.15	8	-3	13	27.34	68.49	105.32	2	1	13	674.48	596.70	59.83
-2	-6	13	911.14	903.86	83.13	-6	-2	13	164.80	96.59	64.04	3	1	13	3501.56	3575.66	168.32
-1	-6	13	12.22	6.99	74.79	-5	-2	13	58.41	-16.73	95.77	4	1	13	10.98	44.00	39.21
0	-6	13	124.45	22.72	46.39	-4	-2	13	0.47	-90.63	87.64	5	1	13	924.85	1084.25	99.92
1	-6	13	11.40	69.83	76.42	-3	-2	13	2.72	-53.70	81.75	6	1	13	23.23	5.43	82.08
2	-6	13	135.03	141.15	51.43	-2	-2	13	712.44	795.76	67.91	7	1	13	254.19	208.98	55.26
3	-6	13	1416.50	1303.29	113.73	-1	-2	13	41.68	75.66	38.52	8	1	13	2.79	14.56	99.24
4	-6	13	55.57	148.35	47.99	0	-2	13	13.05	-153.02	75.39	9	1	13	52.79	-144.52	117.06
5	-6	13	2072.66	1886.81	141.94	1	-2	13	29.09	21.63	46.83	-6	2	13	2.05	-54.65	105.08
6	-6	13	258.93	332.78	59.89	2	-2	13	2172.80	2339.03	134.84	-5	2	13	40.66	44.74	91.03

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-4	2	13	526.02	570.33	59.30	3	5	13	15.78	27.17	51.11	3	9	13	244.17	309.25	52.04
-3	2	13	285.14	236.13	49.75	4	5	13	548.50	702.26	62.17	4	9	13	450.56	422.60	39.09
-2	2	13	1944.23	1675.63	120.74	5	5	13	102.11	51.21	45.51	5	9	13	501.78	478.52	60.56
-1	2	13	4593.99	4793.11	208.67	6	5	13	1.02	58.06	83.62	6	9	13	62.46	22.92	93.32
0	2	13	9.34	452.63	95.58*	7	5	13	32.38	75.25	89.67	7	9	13	193.81	-33.04	114.09
1	2	13	867.31	817.47	66.16	8	5	13	234.06	200.66	62.78	8	9	13	187.79	192.95	62.58
2	2	13	197.10	218.31	42.96	9	5	13	12.98	-172.22	105.11	-3	10	13	71.92	-66.96	103.35
3	2	13	75.15	-12.20	71.36	-5	6	13	48.72	80.02	56.95	-3	10	13	4.13	4.39	92.23
4	2	13	20.76	-39.56	74.38	-4	6	13	347.57	397.77	59.16	-1	10	13	26.89	-163.64	100.94
5	2	13	1056.08	1187.76	98.59	-3	6	13	312.64	296.92	51.24	0	10	13	10.26	8.74	60.86
6	2	13	158.36	231.44	48.88	-2	6	13	230.88	184.14	51.36	1	10	13	505.23	430.10	59.64
7	2	13	258.80	184.69	53.98	-1	6	13	101.33	101.41	45.68	2	10	13	135.16	125.81	53.47
8	2	13	8.47	14.72	70.26	0	6	13	165.40	275.68	47.85	3	10	13	737.59	733.31	74.54
9	2	13	246.18	72.25	117.13	1	6	13	352.40	326.46	50.62	4	10	13	360.00	296.22	56.85
-5	3	13	1.10	-147.68	107.67	2	6	13	196.43	169.89	45.97	5	10	13	494.29	502.56	62.10
-4	3	13	327.42	310.34	59.15	3	6	13	6.45	-89.55	75.69	6	10	13	101.12	128.18	59.91
-3	3	13	426.19	403.16	54.64	4	6	13	548.33	572.72	53.80	7	10	13	1.01	5.88	105.10
-2	3	13	516.28	467.89	55.32	5	6	13	8.29	56.40	56.95	-3	11	13	248.01	310.48	66.32
-1	3	13	320.42	280.36	48.78	6	6	13	102.25	51.35	90.68	-2	11	13	153.32	47.38	104.86
0	3	13	2.59	52.51	41.64	7	6	13	11.57	86.15	51.12	-1	11	13	188.12	328.68	60.15
1	3	13	535.91	-570.99	126.78*	8	6	13	43.17	35.68	70.80	0	11	13	528.39	580.37	68.16
2	3	13	32.09	26.10	65.14	-5	7	13	18.18	-58.55	100.42	1	11	13	2.96	-74.19	92.05
3	3	13	411.06	408.97	47.99	-4	7	13	4.72	34.10	97.91	2	11	13	8.33	57.10	51.21
4	3	13	1629.28	1688.10	111.12	-3	7	13	11.40	10.17	84.81	3	11	13	1.49	27.63	87.17
5	3	13	52.79	112.79	39.47	-2	7	13	17.80	91.35	46.07	4	11	13	286.83	361.99	58.79
6	3	13	1371.32	1292.72	106.81	-1	7	13	12.18	35.67	80.36	5	11	13	41.53	-72.44	102.18
7	3	13	1370.41	1430.32	118.86	0	7	13	5.09	52.97	71.08	6	11	13	26.93	-224.77	113.35
8	3	13	172.43	189.57	55.25	1	7	13	73.25	128.57	45.11	7	11	13	153.43	23.35	109.66
9	3	13	161.74	156.02	58.10	2	7	13	465.01	481.02	51.42	-2	12	13	331.21	364.44	68.95
-6	4	13	0.83	1.77	103.72	3	7	13	331.54	280.65	49.33	-1	12	13	3.06	6.19	105.06
-5	4	13	96.28	-20.71	105.70	4	7	13	579.91	392.82	55.66	0	12	13	243.16	69.12	110.94
-4	4	13	14.01	15.60	54.88	5	7	13	654.40	780.14	75.39	1	12	13	8.44	91.47	100.90
-3	4	13	0.20	77.57	83.83	6	7	13	0.18	39.93	86.03	2	12	13	0.82	132.64	55.40
-2	4	13	9.23	-4.12	58.21	7	7	13	268.72	252.36	60.67	3	12	13	280.42	258.77	60.85
-1	4	13	661.73	570.86	57.33	8	7	13	99.23	190.42	59.71	4	12	13	74.50	45.99	60.19
0	4	13	11.62	-83.67	75.86	-4	8	13	28.62	-139.53	101.21	5	12	13	229.32	323.15	60.82
1	4	13	515.81	550.77	53.30	-3	8	13	68.92	69.59	93.83	6	12	13	86.30	33.22	62.93
2	4	13	456.05	446.81	46.95	-2	8	13	212.74	212.54	54.96	-1	13	13	10.50	52.65	112.18
3	4	13	265.36	301.16	40.73	-1	8	13	904.09	1175.60	118.02	0	13	13	18.81	53.62	110.87
4	4	13	1261.74	1189.61	99.91	0	8	13	748.51	736.77	72.94	1	13	13	9.55	-73.34	109.93
5	4	13	1021.41	1369.25	101.84	1	8	13	2310.42	2712.02	155.4	2	13	13	481.64	531.48	67.28
6	4	13	8.60	-10.01	75.25	2	8	13	63.96	104.79	47.02	3	13	13	27.54	-49.20	108.30
7	4	13	244.55	271.31	51.42	3	8	13	15.62	-44.17	83.23	4	13	13	582.86	667.39	71.94
8	4	13	89.50	78.85	51.48	4	8	13	98.84	189.24	49.70	5	13	13	78.93	68.96	107.46
9	4	13	6.96	60.21	96.64	5	8	13	614.91	633.12	62.10	1	14	13	380.76	404.44	71.27
-6	5	13	2.84	44.14	102.30	6	8	13	15.14	128.91	51.07	2	14	13	40.30	-31.82	66.17
-5	5	13	42.44	-60.16	110.68	7	8	13	14.01	-92.02	102.90	3	14	13	0.59	55.62	74.31
-4	5	13	64.16	-32.50	104.55	8	8	13	89.99	-35.85	115.98	-1	-12	14	4.69	-224.15	115.60
-3	5	13	56.43	93.77	49.59	-4	9	13	9.74	-51.95	104.42	0	-12	14	454.56	315.43	70.43
-2	5	13	412.10	534.75	55.90	-3	9	13	667.08	587.55	66.12	1	-12	14	109.86	-55.01	115.21
-1	5	13	2421.64	2373.87	152.36	-2	9	13	39.79	-35.28	90.40	2	-12	14	188.07	-61.05	124.63
0	5	13	70.00	62.67	74.49	-1	9	13	510.24	427.21	61.42	-2	-11	14	31.83	-143.04	112.62
1	5	13	1250.38	1541.84	113.48	0	9	13	134.27	128.61	53.89	-1	-11	14	47.64	61.93	107.59
2	5	13	15.37	-37.41	72.53	1	9	13	40.79	21.26	91.32	0	-11	14	23.63	-8.97	76.68
3	5	13	4.77	22.60	67.62	2	9	13	667.11	847.60	76.11	1	-11	14	149.39	77.66	81.90

Structure Factors Table (continued) (*unobserved reflns.) for C(14) H(30) Cl(2) Cu(1) N(4) O(9)

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
2	-11	14	93.44	10.16	115.76	5	-6	14	2.19	-40.61	94.13	3	-2	14	423.60	434.46	50.59
3	-11	14	136.87	62.41	110.27	6	-6	14	89.93	48.28	98.17	4	-2	14	253.55	361.55	50.28
4	-11	14	1.22	-99.51	121.15	7	-6	14	31.44	71.16	75.99	5	-2	14	209.69	265.03	51.65
-3	-10	14	14.32	-41.35	107.54	-5	-5	14	299.54	293.18	64.50	6	-2	14	16.56	62.47	52.27
-2	-10	14	31.17	105.13	55.70	-4	-5	14	368.05	426.91	61.74	7	-2	14	791.85	833.09	86.22
-1	-10	14	13.35	-112.70	108.90	-3	-5	14	113.35	53.54	94.09	8	-2	14	14.19	-11.93	106.31
0	-10	14	312.29	261.15	59.45	-2	-5	14	712.49	1052.21	79.17	-6	-1	14	36.02	8.53	116.37
1	-10	14	11.64	25.83	102.66	-1	-5	14	37.46	-117.86	85.94	-5	-1	14	268.50	357.15	61.68
2	-10	14	479.22	406.71	67.47	0	-5	14	180.29	206.33	49.14	-4	-1	14	434.26	388.58	58.88
3	-10	14	127.16	0.52	110.84	1	-5	14	340.11	494.25	56.20	-3	-1	14	5.61	94.35	43.93
4	-10	14	164.23	161.49	60.24	2	-5	14	443.87	434.97	56.81	-2	-1	14	76.01	-124.35	79.04
5	-10	14	307.04	24.76	20.67	3	-5	14	62.01	130.23	48.80	-1	-1	14	221.75	147.71	46.64
-4	-9	14	0.28	17.45	106.10	4	-5	14	264.65	390.06	52.48	0	-1	14	1196.85	-47.63	151.53
-3	-9	14	9.46	38.73	104.73	5	-5	14	129.34	107.40	55.16	1	-1	14	1931.78	1731.59	122.80
-2	-9	14	39.84	-27.28	109.09	6	-5	14	531.51	499.73	63.08	2	-1	14	1017.34	1209.05	102.42
-1	-9	14	465.12	517.40	64.09	7	-5	14	4.92	-72.79	106.72	3	-1	14	2974.40	2936.82	187.55
0	-9	14	116.40	197.77	54.85	-6	-4	14	228.54	229.32	70.64	4	-1	14	100.36	133.42	45.65
1	-9	14	527.56	575.78	64.61	-5	-4	14	293.75	359.84	63.67	5	-1	14	23.20	13.49	84.96
2	-9	14	239.10	268.20	58.27	-4	-4	14	9.46	-157.87	98.81	6	-1	14	512.68	539.09	60.21
3	-9	14	51.54	70.01	56.08	-3	-4	14	71.34	26.16	93.31	7	-1	14	188.99	233.35	56.72
4	-9	14	224.93	247.08	62.00	-2	-4	14	70.62	15.02	89.76	8	-1	14	106.58	68.80	106.00
5	-9	14	4.59	-29.85	112.53	-1	-4	14	191.48	203.63	49.22	-6	0	14	31.70	13.69	61.32
-4	-8	14	64.08	17.21	107.40	0	-4	14	266.03	246.77	52.50	-5	0	14	56.72	96.01	48.71
-3	-8	14	302.94	303.90	64.03	1	-4	14	449.68	526.05	54.63	-4	0	14	65.31	18.95	45.80
-2	-8	14	21.61	154.91	52.68	2	-4	14	2156.57	2214.72	142.89	-3	0	14	2.85	36.13	52.54
-1	-8	14	8.82	75.52	52.27	3	-4	14	1.13	77.18	80.52	-2	0	14	508.00	595.36	39.59
0	-8	14	95.06	81.91	53.17	4	-4	14	535.60	610.28	57.66	-1	0	14	1152.72	1201.74	74.16
1	-8	14	107.61	48.55	66.42	5	-4	14	778.04	660.91	62.90	0	0	14	1979.44	1892.77	96.90
2	-8	14	233.53	170.41	57.48	6	-4	14	129.74	191.98	55.76	1	0	14	1776.68	1868.46	88.07
3	-8	14	69.66	-5.37	98.27	7	-4	14	165.80	185.32	58.42	2	0	14	423.55	387.28	33.45
4	-8	14	23.36	-53.69	105.05	8	-4	14	304.95	213.98	70.48	3	0	14	324.26	256.19	33.64
5	-8	14	385.86	283.11	63.83	-6	-3	14	45.13	-166.14	114.32	4	0	14	3.30	-7.14	78.95
6	-8	14	23.20	-34.42	106.03	-5	-3	14	4.63	48.90	97.20	5	0	14	114.29	140.02	32.10
-5	-7	14	54.42	-25.78	114.08	-4	-3	14	11.58	13.15	35.65	6	0	14	16.04	36.94	61.26
-4	-7	14	240.06	190.36	65.34	-3	-3	14	106.98	128.74	49.58	7	0	14	25.37	-15.53	65.17
-3	-7	14	81.07	134.13	54.07	-2	-3	14	3.37	25.33	73.68	8	0	14	0.05	-92.95	73.71
-2	-7	14	21.97	75.86	95.68	-1	-3	14	563.20	758.34	70.37	-6	1	14	95.14	129.92	62.59
-1	-7	14	0.00	12.65	84.21	0	-3	14	558.68	570.10	54.74	-5	1	14	362.53	303.63	62.58
0	-7	14	30.51	75.37	87.80	1	-3	14	809.83	746.83	68.46	-4	1	14	217.30	298.47	54.67
1	-7	14	1085.03	963.75	86.52	2	-3	14	1288.08	1401.28	115.52	-3	1	14	242.60	154.32	51.92
2	-7	14	59.44	49.87	85.28	3	-3	14	61.69	-23.31	82.51	-2	1	14	863.83	911.78	75.03
3	-7	14	776.76	687.91	65.13	4	-3	14	2.41	-1.14	82.33	-1	1	14	413.21	441.90	54.24
4	-7	14	592.11	486.61	61.53	5	-3	14	358.98	312.52	53.84	0	1	14	464.87	449.21	50.64
5	-7	14	2.57	10.01	97.20	6	-3	14	17.58	44.94	93.69	1	1	14	1158.43	997.72	75.22
6	-7	14	140.09	215.51	60.01	7	-3	14	13.32	-39.14	102.46	2	1	14	2.05	59.62	69.11
-5	-6	14	18.17	-16.68	113.47	8	-3	14	101.44	61.99	63.58	3	1	14	0.33	-6.83	77.02
-4	-6	14	0.10	65.35	99.11	-6	-2	14	116.41	-18.31	122.47	4	1	14	125.39	79.21	45.32
-3	-6	14	50.07	106.55	51.53	-5	-2	14	118.35	109.57	60.18	5	1	14	122.27	84.15	84.37
-2	-6	14	399.99	501.53	58.11	-4	-2	14	266.78	263.04	56.95	6	1	14	1117.56	1151.11	146.87
-1	-6	14	23.16	54.61	89.85	-3	-2	14	415.53	301.68	55.81	7	1	14	329.51	261.84	58.33
0	-6	14	674.47	570.37	60.54	-2	-2	14	126.42	129.55	47.46	8	1	14	936.89	958.51	93.68
1	-6	14	41.26	-9.22	82.33	-1	-2	14	129.17	89.27	44.16	-6	2	14	380.90	276.59	69.50
2	-6	14	11.52	-103.82	81.12	0	-2	14	429.17	252.36	52.58	-5	2	14	64.54	18.20	101.27
3	-6	14	196.33	190.88	51.49	1	-2	14	31.56	28.20	74.08	-4	2	14	62.37	156.23	51.19
4	-6	14	34.88	19.09	89.61	2	-2	14	270.30	278.01	49.99	-3	2	14	102.12	87.80	49.11

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
-2	2	14	50.55	5.40	82.97	-3	6	14	50.80	29.17	86.95	3	10	14	25.80	50.74	42.47
-1	2	14	652.70	377.32	53.22	-2	6	14	72.56	59.74	84.92	4	10	14	373.10	298.58	59.37
0	2	14	16.91	-176.68	82.29	-1	6	14	299.10	320.98	50.87	5	10	14	7.13	-63.19	102.49
1	2	14	595.18	644.37	54.83	0	6	14	58.08	-31.79	84.81	6	10	14	814.71	842.57	87.82
2	2	14	3219.24	3359.14	165.65	1	6	14	691.65	651.51	57.03	7	10	14	186.23	191.70	67.84
3	2	14	530.33	566.22	52.89	2	6	14	79.08	37.21	84.69	-2	11	14	0.06	-179.26	107.86
4	2	14	643.71	668.52	67.84	3	6	14	1300.79	1426.33	112.03	-1	11	14	12.44	138.93	59.06
5	2	14	509.08	580.74	56.51	4	6	14	96.10	151.72	48.09	0	11	14	21.38	87.37	99.09
6	2	14	77.39	16.75	88.61	5	6	14	12.19	59.74	80.23	1	12	14	28.90	53.36	70.97
7	2	14	440.93	468.60	60.57	6	6	14	45.34	48.43	88.30	2	12	14	15.32	-73.37	96.12
8	2	14	88.39	20.01	59.01	7	6	14	29.19	80.12	97.86	3	12	14	475.49	483.84	64.89
-5	3	14	7.10	29.24	101.32	8	6	14	64.10	69.22	73.84	4	12	14	1.80	86.44	96.29
-4	3	14	80.15	-176.78	99.48	-4	7	14	7.21	-42.89	94.71	5	12	14	471.92	534.39	67.19
-3	3	14	102.91	51.40	61.95	-3	7	14	226.28	282.08	56.88	6	12	14	0.30	-22.47	103.77
-2	3	14	523.42	517.67	57.40	-2	7	14	48.33	449.03	60.55	-1	12	14	95.04	79.27	111.34
-1	3	14	694.13	827.13	72.76	-1	7	14	0.03	34.99	77.81	0	12	14	52.62	185.36	60.62
0	3	14	2094.14	1698.59	140.78	0	7	14	260.75	357.32	53.04	1	12	14	179.72	109.80	63.31
1	3	14	589.54	491.23	51.56	1	7	14	392.64	542.10	55.80	2	12	14	64.75	-48.98	107.07
2	3	14	2129.23	2249.51	130.72	2	7	14	389.23	450.55	54.01	3	12	14	7.29	-0.56	99.26
3	3	14	4.07	38.84	76.77	3	7	14	271.14	361.41	48.94	4	12	14	102.40	154.19	61.82
4	3	14	331.34	225.89	47.95	4	7	14	11.47	44.76	59.97	5	12	14	0.74	-115.96	104.61
5	3	14	382.07	302.08	51.46	5	7	14	934.70	826.42	79.39	0	13	14	51.92	92.22	63.12
6	3	14	13.14	24.42	91.31	6	7	14	64.10	30.26	101.68	1	13	14	64.88	-63.76	108.34
7	3	14	2.86	27.97	65.91	7	7	14	392.15	353.33	65.92	2	13	14	15.14	-200.92	119.92
8	3	14	4.11	-26.99	103.77	8	7	14	364.25	460.36	68.42	3	13	14	26.98	-74.99	104.81
-5	4	14	0.08	50.86	96.76	-4	8	14	10.68	138.02	104.18	4	13	14	24.34	65.94	114.90
-4	4	14	281.16	290.36	56.43	-3	8	14	10.86	-45.09	97.05	-1	-11	15	119.04	108.92	109.46
-3	4	14	314.60	407.30	55.50	-2	8	14	131.69	200.70	54.23	0	-11	15	16.74	-206.26	112.38
-2	4	14	41.34	0.64	86.98	-1	8	14	2.92	-75.89	93.22	1	-11	15	182.10	72.44	116.67
-1	4	14	811.46	859.07	77.97	0	8	14	59.96	51.37	59.39	2	-11	15	211.76	55.45	68.26
0	4	14	1015.10	1261.05	115.06	1	8	14	52.12	24.70	90.55	-2	-10	15	170.83	182.12	63.69
1	4	14	27.68	26.37	50.17	2	8	14	221.90	162.35	52.33	-1	-10	15	4.45	-6.27	190.98
2	4	14	2.65	-44.68	73.01	3	8	14	4.86	2.02	82.13	0	-10	15	69.39	40.69	62.43
3	4	14	38.29	51.52	73.14	4	8	14	842.99	870.03	79.67	1	-10	15	38.55	176.23	56.78
4	4	14	538.65	530.29	54.15	5	8	14	7.66	10.50	87.35	2	-10	15	33.72	-70.59	113.35
5	4	14	443.79	443.57	53.77	6	8	14	237.11	287.28	57.87	3	-10	15	10.93	-24.38	110.75
6	4	14	947.18	837.38	81.82	7	8	14	57.81	37.70	103.63	4	-10	15	0.27	56.26	109.84
7	4	14	663.32	734.20	62.01	8	8	14	4.41	-15.19	112.56	-1	-9	15	122.02	73.58	80.16
8	4	14	177.21	95.85	61.69	-3	9	14	42.80	52.80	57.50	-2	-9	15	16.04	-115.40	97.99
-3	5	14	140.32	33.26	76.02	-2	9	14	84.03	75.82	101.74	-1	-9	15	130.57	139.81	60.63
-4	5	14	0.45	68.33	92.18	-1	9	14	90.14	93.77	96.15	0	-9	15	36.45	-157.20	101.18
-3	5	14	149.44	133.05	51.84	0	9	14	349.16	201.81	58.35	1	-9	15	5.23	70.70	56.28
-2	5	14	135.28	24.99	89.91	1	9	14	33.50	88.78	51.46	2	-9	15	140.78	95.16	60.88
-1	5	14	513.42	449.27	54.61	2	9	14	1008.82	1032.45	84.37	3	-9	15	26.31	40.35	74.72
0	5	14	137.86	58.84	85.78	3	9	14	196.17	217.98	50.39	4	-9	15	150.61	68.61	107.43
1	5	14	96.14	164.60	45.62	4	9	14	22.48	46.11	63.15	5	-9	15	87.19	75.07	119.06
2	5	14	56.47	98.99	44.38	5	9	14	28.66	-50.11	99.81	-4	-8	15	187.22	135.39	67.09
3	5	14	353.53	473.07	48.96	6	9	14	64.40	135.57	56.63	-3	-8	15	5.12	-128.58	110.31
4	5	14	90.13	70.00	82.52	7	9	14	4.34	64.97	101.33	-2	-8	15	0.36	56.99	97.61
5	5	14	18.75	44.65	78.03	-3	10	14	31.12	38.84	106.11	-1	-8	15	229.04	-37.16	102.71
6	5	14	493.53	522.09	59.17	-2	10	14	411.75	294.11	68.85	0	-8	15	100.97	528.51	64.30
7	5	14	1.40	31.70	88.73	-1	10	14	276.62	223.21	64.24	1	-8	15	29.81	-128.27	102.78
8	5	14	208.03	220.51	65.03	0	10	14	17.89	-8.71	98.17	2	-8	15	13.89	321.30	59.06
-5	6	14	0.71	-95.97	102.36	1	10	14	130.08	172.68	56.90	3	-8	15	620.78	868.10	84.69
-4	6	14	0.07	14.66	100.01	2	10	14	578.54	560.82	64.67	4	-8	15	49.55	27.44	72.00

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	4	-7	236	233	5	9	3	-6	87	99	5	2	3	-5	173	164	4	6	2	-4	287	320	5	6	1	-3	139	146	4
1	4	-7	228	231	5	10	3	-6	116	117	5	3	3	-5	341	335	5	7	2	-4	74	64	4	7	1	-3	423	420	6
2	4	-7	167	180	5	11	3	-6	176	186	6	4	3	-5	315	322	5	8	2	-4	178	197	5	8	1	-3	254	243	5
3	4	-7	130	117	5	12	3	-6	132	127	5	5	3	-5	126	135	5	9	2	-4	248	241	5	9	1	-3	217	229	5
4	4	-7	384	369	6	0	4	-6	174	165	4	6	3	-5	233	254	4	10	2	-4	166	160	5	10	1	-3	154	173	5
5	4	-7	98	78	5	1	4	-6	291	286	5	7	3	-5	61	70	5	11	2	-4	197	188	5	11	1	-3	99	102	4
6	4	-7	328	337	6	2	4	-6	228	344	5	8	3	-5	69	68	5	12	2	-4	193	212	6	12	1	-3	71	61	6
7	4	-7	85	94	5	3	4	-6	421	379	7	9	3	-5	171	183	5	13	2	-4	74	66	7	13	1	-3	196	189	6
8	4	-7	174	185	5	4	4	-6	193	218	5	10	3	-5	153	155	6	0	3	-4	176	154	4	0	2	-3	317	250	-5
9	4	-7	184	173	6	5	4	-6	384	370	6	11	3	-5	68	75	6	1	3	-4	429	387	6	1	1	-3	412	386	6
10	4	-7	146	142	7	6	4	-6	143	140	5	12	3	-5	220	225	6	2	3	-4	223	201	4	2	2	-3	295	354	-4
11	4	-7	148	141	7	7	4	-6	160	148	5	U	4	-5	489	464	7	3	3	-4	94	112	4	3	1	-3	228	213	4
0	5	-7	127	137	6	8	4	-6	59	47	7	1	4	-5	180	181	4	4	3	-4	385	346	6	4	2	-3	370	342	6
1	5	-7	162	177	5	9	4	-6	151	133	6	2	4	-5	378	355	6	5	3	-4	297	288	5	5	1	-3	152	93	-4
2	5	-7	126	120	6	10	4	-6	153	169	7	3	4	-5	262	244	5	6	3	-4	119	114	5	6	2	-3	214	160	-4
3	5	-7	274	256	5	11	4	-6	196	208	6	4	4	-5	508	322	5	7	3	-4	384	360	6	7	1	-3	251	234	4
4	5	-7	261	236	5	0	5	-6	79	69	4	5	4	-5	276	251	5	8	3	-4	168	165	5	8	2	-3	126	130	5
5	5	-7	184	190	5	1	5	-6	242	230	5	6	4	-5	226	217	5	9	3	-4	225	240	5	9	1	-3	215	216	5
6	5	-7	333	331	6	2	5	-6	126	111	5	7	4	-5	330	336	6	10	3	-4	180	177	5	10	2	-3	142	150	6
7	5	-7	135	140	6	3	5	-6	264	240	5	8	4	-5	236	250	5	11	3	-4	128	120	5	11	1	-3	128	134	5
8	5	-7	153	168	6	4	5	-6	155	141	5	9	4	-5	30	35	29	12	3	-4	144	154	7	12	2	-3	149	151	6
9	5	-7	40	58	39	5	5	-6	285	283	5	10	4	-5	211	213	5	13	3	-4	212	204	6	13	1	-3	221	223	6
10	5	-7	134	127	5	6	5	-6	187	193	5	11	4	-5	109	98	5	0	4	-4	247	218	4	0	1	-3	555	561	8
0	6	-7	169	146	6	7	5	-6	231	233	5	12	4	-5	223	214	5	1	4	-4	517	332	5	1	2	-3	237	221	4
1	6	-7	117	132	5	8	5	-6	71	78	6	0	5	-5	237	228	5	2	4	-4	154	140	4	2	1	-3	360	377	5
2	6	-7	365	360	6	9	5	-6	154	134	6	1	5	-5	141	130	5	3	4	-4	112	158	-5	3	2	-3	109	197	-4
3	6	-7	103	91	4	10	5	-6	94	81	6	2	5	-5	343	345	6	4	4	-4	199	195	4	4	1	-3	193	168	4
4	6	-7	233	228	5	11	5	-6	169	170	7	3	5	-5	136	115	5	5	4	-4	313	295	5	5	2	-3	302	317	5
5	6	-7	52	14	8	0	6	-6	185	186	5	4	5	-5	343	345	6	6	4	-4	325	327	6	6	1	-3	430	407	7
6	6	-7	97	74	5	1	6	-6	241	226	5	5	5	-5	183	171	5	7	4	-4	389	411	6	7	2	-3	105	112	4
7	6	-7	67	49	7	2	6	-6	114	105	4	6	5	-5	261	292	5	8	4	-4	155	173	5	8	1	-3	420	413	7
8	6	-7	157	163	7	3	6	-6	302	299	6	7	5	-5	111	108	5	9	4	-4	114	137	5	9	2	-3	246	246	5
9	6	-7	44	44	13	4	6	-6	0	51	1	8	5	-5	165	156	6	10	4	-4	80	78	6	10	3	-3	189	172	5
0	7	-7	120	131	5	5	6	-6	240	222	5	9	5	-5	110	122	5	11	4	-4	191	191	6	11	2	-3	200	193	6
1	7	-7	90	90	5	6	6	-6	77	78	5	10	5	-5	173	172	6	12	4	-4	77	75	7	12	1	-3	144	128	7
2	7	-7	150	158	6	7	6	-6	78	86	6	11	5	-5	17	60	16	0	5	-4	145	148	5	13	3	-3	154	147	4
3	7	-7	90	77	5	8	6	-6	153	164	7	0	6	-5	276	167	5	1	5	-4	317	356	5	0	4	-3	150	177	4
4	7	-7	200	197	6	9	6	-6	162	163	7	1	6	-5	17	65	27	2	5	-4	31	44	11	1	3	-3	286	263	5
5	7	-7	85	90	6	0	7	-6	155	154	6	2	6	-5	182	190	5	3	5	-4	416	447	7	2	4	-3	99	144	-5
6	7	-7	96	80	6	1	7	-6	187	178	6	3	6	-5	72	73	5	4	5	-4	92	95	4	3	4	-3	364	288	-6
7	7	-7	112	114	5	2	7	-6	35	18	16	4	6	-5	354	359	6	5	5	-4	283	293	5	4	4	-3	287	264	5
0	8	-7	0	69	1	3	7	-6	87	78	5	5	6	-5	118	122	4	6	5	-4	90	65	4	5	4	-3	171	174	5
1	8	-7	75	64	1	4	7	-6	64	61	7	6	6	-5	264	284	6	7	5	-4	214	229	5	6	4	-3	487	497	8
2	8	-7	140	139	5	5	7	-6	165	172	5	7	6	-5	185	199	6	8	5	-4	123	111	4	7	4	-3	377	366	8
3	8	-7	146	131	5	6	7	-6	113	104	5	8	6	-5	93	100	5	9	5	-4	162	171	6	8	4	-3	169	170	5
4	8	-7	89	88	5	7	7	-6	163	164	6	9	6	-5	71	79	7	10	5	-4	125	120	5	9	4	-3	88	64	6
0	0	-6	232	239	5	8	7	-6	105	50	5	10	6	-5	117	111	6	11	5	-4	144	152	7	10	4	-3	137	122	6
1	0	-6	233	268	5	9	7	-6	67	74	8	0	7	-5	229	219	5	12	5	-4	162	157	5	11	4	-3	58	54	7
2	0	-6	453	479	5	0	8	-6	120	113	6	1	7	-5	80	75	5	1	6	-4	127	133	5	0	3	-3	155	160	7
3	0	-6	514	483	8	1	8	-6	234	236	6	2	7	-5	146	126	6	2	6	-4	58	46	6	1	2	-3	290	315	5
4	0	-6	283	307	5	2	8	-6	76	66	7	3	7	-5	97	93	4	3	6	-4	253	248	5	2	1	-3	303	290	5
5	0	-6	0	14	5	3	8	-6	214	225	6	4	7	-5	166	166	6	4	6	-4	169	164	5	3	2	-3	329	323	5
6	0	-6	175	194	6	4	8	-6	96	106	6	5	7	-5	54	39	9	5	6	-4	399	411	7	4	1	-3	191	182	5
7	0	-6	64	46	3	5	8	-6	235	272	4	6	7	-5	171	173	6	6	6	-4	79	89	5	5	2	-3	460	429	7
8	0	-6	270	270	4	6	7	-5	336	371	5	7	7	-5	86	72	6	7	6	-4	215	217	5	6	1	-3	157	168	5
9	0	-6	301	326	4	7	7	-5	686	584	-10	8	7	-5	100	108	6	8	6	-4	32	44	31	7	2	-3	391	405	6
0	1	-6	176	154	4	8	7	-5	361	390	6	9	8	-5	115	100	6	9	6	-4	33	42	20	8	1	-3	87	103	4
1	1	-6	695	752	10	9	8	-5	352	338	6	0	8	-5	157	163	6	0	6	-4	86	91	6	9	2	-3	68	85	5
2	1	-6	127	107	4	10	8	-5	253	274	5	1	8	-5	104	105	5	1	7	-4	217	222	5	0	3	-3	92	99	5
3	1	-6	135	147	4	11	9	-5	111	112	5	2	8	-5	217														

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
5	-8	15	614.98	576.39	70.77	1	-3	15	5.47	-62.98	84.28	1	1	15	2896.11	2931.62	159.01
-4	-7	15	367.77	403.01	68.62	2	-3	15	53.16	53.07	81.99	2	1	15	86.38	111.72	45.92
-3	-7	15	223.58	102.06	103.16	3	-3	15	1129.87	1073.89	83.55	3	1	15	1127.04	1318.22	114.27
-2	-7	15	256.64	149.58	58.84	4	-3	15	392.89	307.77	84.03	4	1	15	1148.38	1098.22	106.60
-1	-7	15	445.92	388.98	58.92	5	-3	15	415.46	423.68	58.23	5	1	15	85.76	-130.93	87.52
0	-7	15	32.13	51.26	52.56	6	-3	15	164.92	65.82	104.15	6	1	15	58.69	100.73	54.93
1	-7	15	1.81	-183.43	96.84	7	-3	15	47.13	44.50	99.89	7	1	15	3.03	-197.39	99.35
2	-7	15	106.76	173.10	51.58	-1	-2	15	120.27	109.70	63.21	8	1	15	18.06	-280.57	110.58
3	-7	15	88.95	56.06	94.92	-4	-2	15	115.98	30.73	96.97	-5	2	15	50.56	197.48	61.08
4	-7	15	177.43	177.40	58.27	-3	-2	15	77.29	134.53	48.84	-4	2	15	176.31	68.63	98.59
5	-7	15	0.81	-22.72	103.53	-2	-1	15	152.82	172.74	49.84	-3	2	15	370.80	337.91	57.02
6	-7	15	98.20	93.68	63.56	-1	-1	15	124.62	142.78	49.32	-2	2	15	258.11	211.52	50.33
-4	-6	15	17.97	31.71	73.88	0	-2	15	1397.68	1528.48	136.31	-1	2	15	245.05	-131.84	93.98
-3	-6	15	263.96	346.12	59.42	1	-2	15	446.20	452.14	54.88	0	2	15	737.11	903.11	75.88
-2	-6	15	568.38	634.47	68.53	2	-2	15	2075.03	2373.45	145.73	1	2	15	163.92	209.80	47.08
-1	-6	15	57.67	110.53	51.34	3	-2	15	718.86	711.33	60.05	2	2	15	276.19	269.81	55.88
0	-6	15	34.76	-31.96	96.51	4	-2	15	75.94	61.24	84.85	3	2	15	228.00	32.99	81.11
1	-6	15	146.42	173.21	50.47	5	-2	15	1234.42	1172.64	119.96	4	2	15	362.30	336.91	52.77
2	-6	15	93.85	11.48	63.70	6	-2	15	112.56	62.45	87.27	5	2	15	20.66	66.26	82.64
3	-6	15	244.34	208.12	55.32	7	-2	15	0.33	-4.05	99.93	6	2	15	114.20	-54.63	94.06
4	-6	15	271.84	304.20	57.94	8	-2	15	9.56	138.49	59.75	7	2	15	505.56	517.26	65.72
5	-6	15	307.56	222.98	61.96	-5	-1	15	68.96	-20.76	99.42	8	2	15	29.39	45.92	73.29
6	-6	15	1.23	-138.50	107.14	-4	-1	15	372.58	396.31	63.20	-5	3	15	554.60	634.01	72.70
-5	-5	15	55.54	128.71	61.83	-3	-1	15	0.84	-40.07	83.77	-4	3	15	227.47	186.33	60.37
-4	-5	15	3.68	-38.52	102.75	-2	-1	15	3.75	-30.15	83.25	-3	3	15	206.95	245.12	51.90
-3	-5	15	61.68	-85.09	100.95	-1	-1	15	24.19	-22.54	77.80	-2	3	15	67.88	136.71	51.81
-2	-5	15	48.41	81.83	91.89	0	-1	15	190.45	-592.55	124.41*	-1	3	15	265.81	275.68	16.11
-1	-5	15	288.93	322.10	56.38	1	-1	15	410.43	384.00	53.78	0	3	15	0.61	-1822.19	151.96*
0	-5	15	0.84	-86.88	84.60	2	-1	15	318.65	234.34	47.44	1	3	15	135.46	106.81	48.00
1	-5	15	712.44	1361.04	109.65	3	-1	15	1.85	-96.20	85.54	2	3	15	139.64	113.19	46.85
2	-5	15	2.04	49.52	89.78	4	-1	15	63.13	-12.62	83.15	3	3	15	1085.73	1185.85	109.74
3	-5	15	94.10	118.43	50.02	5	-1	15	106.48	16.98	90.72	4	3	15	52.28	-44.71	83.14
4	-5	15	531.97	659.68	63.26	6	-1	15	271.03	296.85	57.70	5	3	15	500.90	606.01	60.34
5	-5	15	6.50	10.04	94.89	7	-1	15	77.94	50.70	94.86	6	3	15	741.36	748.17	70.56
6	-5	15	416.89	282.46	63.17	8	-1	15	161.24	187.03	63.83	7	3	15	2.27	-43.76	101.42
7	-5	15	87.40	102.92	108.63	-5	0	15	223.57	188.30	45.44	8	3	15	263.53	290.91	66.35
-5	-4	15	283.70	344.17	66.73	-4	0	15	189.99	240.00	126.49	-5	4	15	70.48	8.97	105.41
-4	-4	15	16.01	-54.38	101.76	-3	0	15	450.20	476.86	82.54	-4	4	15	2.92	48.57	93.34
-3	-4	15	519.15	509.25	64.38	-2	0	15	12.89	88.15	39.63	-3	4	15	3.60	-32.46	98.18
-2	-4	15	80.99	44.56	59.75	-1	0	15	137.44	-16.34	67.36	-2	4	15	63.25	140.91	49.35
-1	-4	15	49.54	79.62	83.14	0	0	15	376.76	-917.05	111.12*	-1	4	15	670.66	679.17	62.71
0	-4	15	13.49	-341.88	104.14*	1	0	15	4.40	-5.10	73.61	0	4	15	1073.31	1006.02	85.97
1	-4	15	19.45	-4.23	80.24	2	0	15	225.28	296.74	34.71	1	4	15	81.41	-41.07	81.17
2	-4	15	17.91	21.04	58.67	3	0	15	62.50	35.18	40.73	2	4	15	2080.37	2432.99	144.17
3	-4	15	89.08	177.22	48.06	4	0	15	655.83	673.23	53.33	3	4	15	34.17	-27.03	76.92
4	-4	15	33.30	76.30	86.89	5	0	15	28.63	18.90	55.10	4	4	15	362.51	452.92	52.31
5	-4	15	25.95	3.30	88.38	6	0	15	157.32	62.25	83.30	5	4	15	409.62	449.53	55.21
6	-4	15	1.87	-41.20	93.13	7	0	15	239.25	289.25	64.24	6	4	15	6.00	-13.02	86.63
7	-4	15	82.65	69.90	102.83	8	0	15	176.16	199.22	56.27	7	4	15	0.48	96.31	57.19
-5	-3	15	103.01	104.89	109.91	-5	1	15	16.45	8.13	105.14	8	4	15	11.70	30.44	101.63
-4	-3	15	276.62	258.43	58.34	-4	1	15	192.60	250.62	59.13	-4	5	15	129.53	57.61	100.13
-3	-3	15	78.17	33.10	66.26	-3	1	15	23.20	38.95	89.26	-3	5	15	111.02	141.41	57.01
-2	-3	15	260.82	98.98	52.24	-2	1	15	54.02	92.79	49.72	-2	5	15	189.88	190.08	53.87
-1	-3	15	207.83	145.07	57.60	-1	1	15	428.83	354.08	60.64	-1	5	15	31.98	59.63	79.18
0	-3	15	158.33	-410.46	116.32*	0	1	15	42.34	-254.72	97.12	0	5	15	100.04	136.63	48.32

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
1	5	15	176.41	69.16	85.28	-2	10	15	6.33	-12.54	106.99	-1	-6	16	78.10	32.24	55.98
2	5	15	206.72	237.54	51.11	-1	10	15	357.40	208.27	69.02	0	-6	16	503.02	552.26	64.47
3	5	15	31.44	73.99	83.07	0	10	15	222.53	228.32	60.25	1	-6	16	177.42	212.49	55.77
4	5	15	5.73	72.75	46.01	1	10	15	252.61	220.09	65.10	2	-6	16	237.35	222.10	55.00
5	5	15	67.11	26.04	52.01	2	10	15	429.82	324.93	56.64	3	-6	16	480.11	492.66	63.04
6	5	15	576.25	669.14	63.04	3	10	15	17.59	72.38	98.15	4	-6	16	4.12	-48.03	98.03
7	5	15	49.01	8.86	97.70	4	10	15	192.31	48.56	111.58	5	-6	16	0.26	-19.45	72.47
8	5	15	103.11	-31.49	112.29	5	10	15	72.30	34.10	104.00	6	-6	16	6.82	-26.80	110.27
-4	6	15	404.86	441.32	68.38	6	10	15	1.25	-0.86	75.54	-4	-5	16	223.11	256.05	64.65
-3	6	15	105.11	-65.44	101.16	-1	11	15	36.63	-95.57	109.28	-3	-5	16	331.89	345.45	62.94
-2	6	15	40.68	62.64	51.47	0	11	15	137.21	20.02	117.58	-2	-5	16	19.72	31.99	92.22
-1	6	15	2.48	63.25	48.97	1	11	15	4.98	-30.23	76.58	-1	-5	16	869.07	718.77	69.27
0	6	15	333.26	394.26	56.14	2	11	15	18.34	29.62	98.97	0	-5	16	350.39	300.37	68.20
1	6	15	9.28	44.59	60.83	3	11	15	80.10	143.87	61.36	1	-5	16	102.90	81.35	94.50
2	6	15	18.55	3.54	80.46	4	11	15	27.95	-22.78	103.81	2	-5	16	6.61	-59.02	92.36
3	6	15	29.02	-17.43	81.41	5	11	15	10.77	67.37	107.32	3	-5	16	0.09	-178.13	96.12
4	6	15	41.64	45.39	82.22	0	12	15	0.50	-136.09	121.08	4	-5	16	820.18	760.14	72.61
5	6	15	34.45	78.13	82.61	1	12	15	0.37	63.55	99.90	5	-5	16	142.13	86.66	101.12
6	6	15	105.35	68.22	56.67	2	12	15	45.14	95.03	98.57	6	-5	16	235.10	221.16	63.68
7	6	15	470.16	451.47	66.35	3	12	15	111.34	-23.35	112.22	-4	-4	16	2.79	-111.85	105.61
8	6	15	0.53	21.73	107.15	4	12	15	106.60	181.06	61.92	-3	-4	16	29.08	-84.70	95.36
-4	7	15	12.28	57.26	104.59	2	13	15	298.35	369.81	71.54	-2	-4	16	16.73	-42.50	93.77
-3	7	15	7.89	55.96	97.40	-1	-10	16	0.93	23.26	61.26	-1	-4	16	83.22	-26.85	90.76
-2	7	15	110.07	167.37	54.53	0	-10	16	77.53	-62.35	116.74	0	-4	16	332.12	269.66	55.41
-1	7	15	179.71	146.09	54.24	1	-10	16	3.94	-92.50	111.21	1	-4	16	57.59	38.50	88.26
0	7	15	289.44	358.20	57.06	2	-10	16	9.73	0.78	109.29	2	-4	16	70.95	119.15	88.14
1	7	15	477.98	558.83	60.80	3	-10	16	40.99	80.96	81.59	3	-4	16	18.52	-8.66	95.73
2	7	15	49.26	-58.40	97.99	-2	-9	16	48.64	123.59	64.11	4	-4	16	96.34	-20.35	93.04
3	7	15	254.63	267.22	53.34	-1	-9	16	182.65	73.04	120.60	5	-4	16	265.06	394.45	61.75
4	7	15	1.25	-38.17	88.31	0	-9	16	13.21	44.55	103.37	6	-4	16	263.75	246.16	60.95
5	7	15	1.94	43.97	81.32	1	-9	16	173.34	412.54	64.62	7	-4	16	241.93	245.05	70.68
6	7	15	172.47	173.00	57.40	2	-9	16	552.30	394.49	70.39	-4	-3	16	198.66	235.85	66.27
7	7	15	10.18	-53.33	101.72	3	-9	16	31.12	-69.65	122.29	-3	-3	16	96.28	132.12	56.48
-3	8	15	137.77	91.51	60.20	4	-9	16	83.43	39.18	64.67	-2	-3	16	557.20	600.93	64.94
-2	8	15	241.18	233.12	59.95	-3	-8	16	0.44	27.65	103.36	-1	-3	16	509.20	445.32	62.48
-1	8	15	266.93	228.59	58.89	-2	-8	16	318.54	425.48	65.14	0	-3	16	27.18	-218.07	97.91
0	8	15	23.57	71.55	87.71	-1	-8	16	282.82	153.91	63.63	1	-3	16	818.86	825.48	78.44
1	8	15	62.21	-59.38	93.08	0	-8	16	98.32	185.98	57.03	2	-3	16	845.09	1066.72	86.74
2	8	15	762.01	734.88	65.60	1	-8	16	65.03	1.57	101.39	3	-3	16	137.68	181.41	51.87
3	8	15	17.10	42.74	86.38	2	-8	16	1.65	-102.67	109.25	4	-3	16	270.91	350.23	56.56
4	8	15	475.84	538.33	62.01	3	-8	16	116.36	-41.40	105.96	5	-3	16	7.78	0.02	98.23
5	8	15	1.02	1.30	92.17	4	-8	16	24.50	10.54	102.14	6	-3	16	5.70	106.93	53.32
6	8	15	6.93	83.22	90.72	5	-8	16	205.69	146.40	67.02	7	-3	16	8.12	8.96	111.63
7	8	15	229.41	363.25	66.10	-3	-7	16	26.84	-0.34	101.93	-5	-2	16	84.19	178.33	63.03
-3	9	15	334.81	301.06	65.91	-2	-7	16	3.68	91.45	103.01	-4	-2	16	49.06	-7.15	101.79
-2	9	15	228.21	141.33	64.37	-1	-7	16	0.24	22.50	98.08	-3	-2	16	31.12	61.88	92.82
-1	9	15	6.19	-164.58	103.10	0	-7	16	65.01	3.15	69.92	-2	-2	16	302.84	469.23	56.64
0	9	15	0.13	-28.19	101.89	1	-7	16	56.11	87.38	54.14	-1	-2	16	234.82	237.98	53.98
1	9	15	238.09	78.54	106.62	2	-7	16	1.30	-206.56	101.19	0	-2	16	6.47	-1556.93	151.72*
2	9	15	180.65	192.24	57.77	3	-7	16	7.26	86.41	95.82	1	-2	16	16.50	139.14	47.88
3	9	15	93.15	-29.96	93.36	4	-7	16	151.05	134.81	61.40	2	-2	16	0.78	-164.87	91.67
4	9	15	71.22	62.35	92.16	5	-7	16	152.12	121.16	64.75	3	-2	16	43.05	26.85	59.84
5	9	15	254.79	105.08	62.50	-4	-6	16	0.97	29.81	103.60	4	-2	16	2.16	33.75	81.19
6	9	15	332.41	295.01	65.82	-3	-6	16	158.00	139.49	62.20	5	-2	16	630.95	685.56	65.30
7	9	15	0.58	-28.41	113.99	-2	-6	16	331.60	383.55	62.34	6	-2	16	25.14	63.91	93.53

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
7	-2	16	213.93	169.70	63.68	-4	3	16	115.78	164.47	59.13	2	7	16	234.92	254.79	56.23
5	-1	16	33.61	-70.30	110.42	-3	3	16	0.60	38.32	92.20	3	7	16	30.14	67.54	88.68
-4	-1	16	18.86	14.84	107.31	-2	3	16	725.66	801.52	78.90	4	7	16	3.50	-9.08	90.03
-3	-1	16	17.24	45.33	88.11	-1	3	16	153.80	106.20	55.82	5	7	16	199.70	204.46	57.49
-2	-1	16	38.44	-0.95	83.87	0	3	16	288.60	433.50	55.20	6	7	16	56.93	-43.82	108.54
-1	-1	16	0.21	-191.16	92.57	1	3	16	883.90	837.53	78.49	7	7	16	7.52	138.45	61.95
0	-1	16	16.35	-106.37	90.16	2	3	16	144.95	112.80	50.87	-3	8	16	123.99	216.77	63.59
1	-1	16	120.63	25.89	62.17	3	3	16	8.18	-91.21	88.12	-2	8	16	19.64	43.24	105.34
2	-1	16	55.01	6.85	82.41	4	3	16	586.70	728.17	73.63	-1	8	16	102.20	83.45	103.74
3	-1	16	36.47	-69.09	85.80	5	3	16	40.57	-18.31	91.96	0	8	16	1.83	129.89	58.88
4	-1	16	623.49	654.90	60.95	6	3	16	4.46	-91.52	94.36	1	8	16	7.72	-14.24	98.47
5	-1	16	149.99	-23.89	98.60	7	3	16	17.48	87.70	99.93	2	8	16	610.94	537.82	67.09
6	-1	16	745.25	862.40	82.11	8	3	16	19.75	101.34	113.20	3	8	16	2.98	-49.16	92.86
7	-1	16	92.19	23.29	63.07	-4	4	16	0.10	20.29	99.25	4	8	16	497.28	598.07	63.67
-5	0	16	24.53	16.22	78.72	-3	4	16	232.58	282.12	58.75	5	8	16	508.14	600.27	68.17
-4	0	16	8.36	-76.00	88.37	-2	4	16	77.47	3.88	96.26	6	8	16	52.00	2.93	76.65
-3	0	16	190.68	152.58	42.73	-1	4	16	460.97	529.98	63.09	7	8	16	209.72	268.15	67.17
-2	0	16	118.24	24.78	62.89	0	4	16	587.49	436.49	65.01	-2	9	16	319.28	321.19	70.51
-1	0	16	376.22	482.61	46.84	1	4	16	212.48	258.54	54.59	-1	9	16	15.59	83.17	107.88
0	0	16	955.76	752.25	133.88	2	4	16	28.92	27.18	85.92	0	9	16	81.86	120.21	53.08
1	0	16	153.24	227.62	37.67	3	4	16	171.13	147.27	50.25	1	9	16	735.73	887.74	98.15
2	0	16	56.67	123.09	34.27	4	4	16	83.34	60.37	51.50	2	9	16	0.32	40.47	102.17
3	0	16	900.14	1124.12	79.26	5	4	16	427.06	426.57	60.20	3	9	16	395.51	452.31	62.04
4	0	16	91.81	55.10	49.46	6	4	16	0.13	44.45	96.45	4	9	16	109.82	9.72	104.09
5	0	16	133.95	157.55	28.03	7	4	16	177.13	167.91	63.87	5	9	16	1.55	-228.80	108.94
6	0	16	108.61	173.18	124.95	8	4	16	71.36	13.93	110.22	6	9	16	6.10	70.94	99.60
7	0	16	47.80	-10.85	74.49	4	5	16	128.45	50.05	106.64	-1	10	16	176.33	270.02	67.26
8	0	16	5.19	20.17	77.07	-3	5	16	26.88	106.92	54.16	0	10	16	112.31	56.15	115.31
-5	1	16	63.78	87.98	110.72	-2	5	16	189.91	414.41	56.44	1	10	16	123.58	168.83	63.74
-4	1	16	272.14	165.82	62.51	-1	5	16	56.34	-78.30	97.15	2	10	16	14.72	-180.26	107.67
-3	1	16	64.54	91.51	93.28	0	5	16	20.12	-61.27	93.76	3	10	16	104.96	95.50	62.04
-2	1	16	9.12	-104.77	90.51	1	5	16	183.33	229.76	53.97	4	10	16	165.87	205.97	62.37
-1	1	16	402.02	497.54	59.51	2	5	16	28.19	-85.22	91.82	5	10	16	13.32	48.12	72.84
0	1	16	0.51	-24.41	61.25	3	5	16	199.00	33.28	97.10	0	11	16	2.89	49.79	103.56
1	1	16	272.52	225.95	57.21	4	5	16	26.99	13.86	86.64	1	11	16	212.46	73.66	122.98
2	1	16	2.36	21.71	78.73	5	5	16	108.30	17.89	95.87	2	11	16	6.48	-106.77	115.97
3	1	16	4.92	-37.81	86.06	6	5	16	970.51	1729.25	93.34	3	11	16	976.84	951.42	95.88
4	1	16	313.97	231.62	53.71	7	5	16	19.71	-39.02	103.12	4	11	16	11.98	-7.63	106.26
5	1	16	8.60	-75.67	93.62	-4	6	16	2.33	-47.09	113.30	5	11	16	330.68	291.40	70.32
6	1	16	189.75	470.60	63.81	-3	6	16	333.61	297.89	65.50	2	12	16	181.23	443.00	72.46
7	1	16	41.78	28.67	108.54	-2	6	16	11.57	-37.27	103.72	3	12	16	40.82	-37.01	115.49
8	1	16	156.49	196.66	64.03	-1	6	16	617.78	678.78	66.64	-1	-9	17	16.77	-39.44	114.91
-4	2	16	13.13	-140.67	112.82	0	6	16	432.93	503.88	63.33	0	-9	17	7.02	28.98	101.76
-3	2	16	236.56	320.13	59.85	1	6	16	28.26	59.75	52.48	1	-9	17	217.06	183.87	57.83
-2	2	16	67.37	125.61	52.60	2	6	16	530.19	740.29	73.41	2	-9	17	29.49	-45.00	80.19
-1	2	16	185.65	389.40	58.82	3	6	16	96.48	63.43	95.73	3	-9	17	0.82	107.67	115.76
0	2	16	31.49	-993.47	134.08	4	6	16	1.28	-126.48	91.50	-2	-8	17	2.41	0.69	108.51
1	2	16	7.82	-19.53	83.96	5	6	16	204.99	228.04	57.91	-1	-8	17	55.72	83.93	99.79
2	2	16	29.90	29.87	78.11	6	6	16	35.89	137.07	55.79	0	-8	17	0.56	29.97	103.32
3	2	16	26.91	5.18	81.92	7	6	16	28.64	18.21	108.03	1	-8	17	269.83	298.84	61.49
4	2	16	4.33	-136.95	82.48	-3	7	16	1.50	-84.10	109.07	2	-8	17	4.30	-151.56	111.38
5	2	16	1328.58	1399.93	128.16	-2	7	16	311.75	432.48	63.23	3	-8	17	587.25	429.39	78.22
6	2	16	24.19	102.37	52.57	-1	7	16	226.70	267.43	58.34	4	-8	17	17.55	75.33	99.42
7	2	16	840.32	985.85	88.62	0	7	16	273.97	338.08	57.39	-2	-7	17	9.92	199.56	68.73
8	2	16	73.01	-94.16	115.89	1	7	16	267.92	248.78	60.55	-1	-7	17	170.80	261.68	61.35

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
0	-7	17	448.22	454.72	65.99	4	-2	17	9.76	-84.39	102.88	-1	3	17	37.88	40.54	95.21
1	-7	17	25.46	36.40	98.67	5	-2	17	1.97	66.46	67.99	0	3	17	42.06	-15.04	105.10
2	-7	17	447.44	455.13	68.33	6	-2	17	4.97	-44.08	105.08	1	3	17	5.54	-71.20	96.06
3	-7	17	122.57	201.89	62.48	7	-2	17	23.96	52.03	63.85	2	3	17	56.46	29.26	86.89
4	-7	17	21.59	-112.03	114.61	-4	-1	17	120.29	162.54	61.58	3	3	17	209.07	52.76	96.39
5	-7	17	20.24	73.74	80.78	-3	-1	17	33.50	-27.41	102.05	4	3	17	327.75	314.06	58.13
-3	-6	17	48.78	-2.74	112.10	-2	-1	17	3.11	73.60	50.48	5	3	17	80.19	72.14	98.03
-2	-6	17	176.11	168.33	62.79	-1	-1	17	720.99	859.42	83.34	6	3	17	465.38	376.32	66.70
-1	-6	17	15.25	30.62	99.73	0	-1	17	461.02	415.14	59.84	7	3	17	369.26	387.67	69.18
0	-6	17	133.41	12.74	108.71	1	-1	17	651.95	673.31	65.18	-3	4	17	13.48	11.30	101.28
1	-6	17	4.81	-70.97	98.30	2	-1	17	833.09	492.95	62.50	-2	4	17	31.80	-225.55	113.55
2	-6	17	168.01	223.66	60.30	3	-1	17	2.42	-55.00	93.80	-1	4	17	6.96	-75.97	104.63
3	-6	17	154.77	41.93	108.86	4	-1	17	16.80	-62.32	93.16	0	4	17	157.42	56.69	112.05
4	-6	17	77.66	55.73	107.47	5	-1	17	21.96	24.66	96.45	1	4	17	62.44	-7.82	102.15
5	-6	17	114.33	41.14	78.62	6	-1	17	88.17	-110.27	111.88	2	4	17	663.32	627.75	67.77
-3	-5	17	4.92	34.62	77.96	7	-1	17	144.72	177.76	64.00	3	4	17	253.24	402.93	56.69
-2	-5	17	41.30	95.49	58.31	4	0	17	132.83	12.08	75.97	4	4	17	289.01	317.54	55.41
-1	-5	17	33.09	-283.76	110.35	-3	0	17	55.60	43.53	69.27	5	4	17	290.51	374.62	62.00
0	-5	17	195.82	-82.61	110.68	-2	0	17	112.42	67.76	66.44	6	4	17	15.60	-128.72	106.67
1	-5	17	2.34	-24.31	99.23	-1	0	17	4.86	-51.02	56.14	7	4	17	43.41	74.12	114.12
2	-5	17	518.34	496.69	61.88	0	0	17	32.12	-755.65	93.92	-3	5	17	15.11	11.04	109.55
3	-5	17	1.86	49.52	90.24	1	0	17	45.50	32.91	65.36	-2	5	17	49.07	19.97	101.24
4	-5	17	367.76	246.54	66.07	2	0	17	80.56	31.01	45.61	-1	5	17	546.80	739.32	72.70
5	-5	17	3.36	-101.36	110.09	3	0	17	70.24	91.93	50.82	0	5	17	11.79	55.36	90.79
6	-5	17	24.15	-195.04	118.21	4	0	17	51.60	110.02	75.89	1	5	17	1316.84	1367.08	137.88
-4	-4	17	0.29	94.22	112.32	5	0	17	38.07	-14.00	69.22	2	5	17	215.32	253.87	56.52
-3	-4	17	93.45	54.43	109.78	6	0	17	463.49	486.41	48.54	3	5	17	46.38	-25.97	87.13
-2	-4	17	298.89	271.99	52.66	7	0	17	62.44	20.31	62.56	4	5	17	34.72	-27.07	94.97
-1	-4	17	12.97	-20.35	101.81	-4	1	17	40.15	-12.06	112.10	5	5	17	14.38	32.15	92.45
0	-4	17	645.00	404.78	77.30	-3	1	17	0.88	64.36	67.28	6	5	17	346.71	278.81	65.46
1	-4	17	221.52	239.27	58.01	-2	1	17	3.70	18.71	89.19	7	5	17	41.92	9.23	110.98
2	-4	17	216.71	196.16	55.82	-1	1	17	69.12	-140.19	109.35	-3	6	17	54.88	-56.95	114.57
3	-4	17	255.04	182.58	61.51	0	1	17	106.41	170.04	57.02	-2	6	17	39.92	64.03	76.78
4	-4	17	133.51	114.55	60.70	1	1	17	111.53	51.88	70.11	-1	6	17	25.79	84.57	100.29
5	-4	17	29.36	25.08	110.02	2	1	17	173.50	97.50	53.69	0	6	17	52.41	108.26	57.58
6	-4	17	45.50	96.69	104.99	3	1	17	164.08	193.12	50.78	1	6	17	45.25	51.56	71.44
-4	-3	17	122.63	44.88	105.82	4	1	17	216.59	26.19	99.32	2	6	17	96.28	-14.41	100.66
-3	-3	17	217.25	207.31	62.07	5	1	17	54.15	55.65	67.92	3	6	17	174.48	221.68	56.59
-2	-3	17	4.27	-204.25	99.55	6	1	17	96.21	165.36	59.55	4	6	17	54.22	-69.64	102.36
-1	-3	17	26.92	-43.66	98.96	7	1	17	30.37	22.37	112.12	5	6	17	363.12	248.76	64.20
0	-3	17	0.19	3.56	98.25	-4	2	17	36.24	102.68	113.24	6	6	17	76.38	33.26	107.86
1	-3	17	201.05	174.92	60.36	-3	2	17	75.46	62.50	70.99	7	6	17	228.92	175.69	67.90
2	-3	17	23.20	-124.13	93.00	-2	2	17	234.78	390.57	63.26	-2	7	17	80.01	77.29	108.78
3	-3	17	41.26	40.89	94.14	-1	2	17	6.55	-85.88	103.71	-1	7	17	3.54	-7.49	102.53
4	-3	17	312.78	324.23	61.88	0	2	17	2677.51	2976.32	180.18	0	7	17	73.77	-53.31	105.52
5	-3	17	707.30	639.66	71.68	1	2	17	336.39	94.89	97.12	1	7	17	240.41	236.01	63.21
6	-3	17	42.76	-46.56	107.06	3	2	17	811.94	434.25	60.86	2	7	17	15.40	-35.37	103.92
-4	-2	17	0.71	9.10	76.02	3	2	17	210.24	154.01	58.02	3	7	17	427.39	517.52	64.31
-3	-2	17	1.09	111.10	54.73	4	2	17	5.89	-6.40	95.86	4	7	17	128.94	149.40	58.41
-2	-2	17	9.34	-21.73	102.65	5	2	17	17.82	-204.24	98.20	5	7	17	109.29	77.71	60.95
-1	-2	17	4.18	12.30	69.98	6	2	17	1.07	-121.67	104.71	6	7	17	267.23	289.58	67.19
0	-2	17	532.79	537.71	62.39	7	2	17	121.33	80.40	106.03	-2	8	17	124.34	64.33	116.14
1	-2	17	174.85	8.66	97.53	-4	3	17	159.31	132.01	65.77	-1	8	17	80.94	-51.59	110.19
2	-2	17	199.56	181.65	54.31	-3	3	17	98.46	71.22	104.70	0	8	17	827.41	836.17	76.99
3	-2	17	569.92	607.09	61.87	-2	3	17	2.16	-163.56	101.45	1	8	17	58.77	62.88	59.61

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
2	8	17	594.28	653.82	72.18	0	-3	18	417.12	435.32	63.59	4	2	18	20.17	-133.75	103.89
3	8	17	18.27	-35.00	101.28	1	-3	18	0.27	14.08	89.99	5	2	18	726.24	612.95	70.81
4	8	17	44.65	100.89	58.63	2	-3	18	180.78	128.21	59.70	6	2	18	151.15	227.08	60.91
5	8	17	0.74	-49.10	121.17	3	-3	18	60.19	21.21	73.26	7	2	18	04.71	113.50	66.78
6	8	17	31.38	144.50	63.15	4	-3	18	3.96	19.42	104.21	-3	3	18	20.82	-238.61	116.40
-1	9	17	30.36	3.47	107.45	5	-3	18	19.30	-33.31	110.43	-2	3	18	0.13	-22.57	108.90
0	9	17	0.16	41.80	107.14	6	-3	18	8.84	51.45	71.41	-1	3	18	21.76	44.40	71.30
1	9	17	6.31	79.07	98.08	-3	-2	18	29.82	-197.59	110.11	0	3	18	5.03	24.64	106.63
2	9	17	27.49	34.87	109.42	-2	-2	18	627.85	663.22	71.79	1	3	18	169.17	179.43	57.47
3	9	17	34.99	63.67	107.43	-1	-2	18	11.27	-93.50	98.28	2	3	18	373.37	461.92	63.93
4	9	17	357.23	287.74	67.87	0	-2	18	151.92	-534.44	138.55*	3	3	18	11.42	59.67	91.70
5	9	17	2.72	91.17	59.64	1	-2	18	0.90	-6.50	100.51	4	3	18	446.95	543.87	65.34
0	10	17	79.33	225.00	65.32	2	-2	18	35.43	99.64	55.63	5	3	18	67.92	154.27	56.65
1	10	17	5.57	-107.16	111.54	3	-2	18	0.02	-16.77	98.49	6	3	18	257.34	227.77	69.75
2	10	17	225.79	245.97	68.73	4	-2	18	0.19	81.52	103.80	-3	4	18	180.19	75.67	79.32
3	10	17	80.31	95.10	109.08	5	-2	18	110.12	117.85	62.01	-2	4	18	337.03	380.25	61.38
4	10	17	106.84	44.07	65.41	6	-2	18	311.92	387.87	70.70	-1	4	18	88.25	-78.59	105.53
2	11	17	3.52	62.01	114.88	-3	-1	18	22.04	51.54	63.91	0	4	18	429.04	375.95	65.54
3	11	17	42.94	-96.11	114.73	-2	-1	18	117.04	116.08	61.41	1	4	18	59.94	-10.69	96.89
0	-8	18	7.65	95.50	105.76	-1	-1	18	0.05	-267.42	113.27	2	4	18	74.88	23.17	101.05
1	-8	18	54.00	47.39	113.42	0	-1	18	0.04	-389.40	121.60*	3	4	18	31.26	-23.03	98.67
2	-8	18	74.63	-41.67	116.49	1	-1	18	12.82	-126.67	103.43	4	4	18	237.01	275.62	57.82
-1	-7	18	0.98	80.73	112.95	2	-1	18	200.78	145.46	59.21	5	4	18	96.72	74.25	107.20
0	-7	18	0.42	40.35	105.50	3	-1	18	170.03	191.40	56.27	6	4	18	161.94	44.57	84.22
1	-7	18	0.02	-80.96	110.94	4	-1	18	527.55	659.27	67.47	-2	5	18	1.79	-147.67	117.53
2	-7	18	400.24	61.73	123.97	5	-1	18	373.58	332.30	65.65	-1	5	18	0.65	-175.31	110.94
3	-7	18	206.41	188.74	67.41	6	-1	18	35.25	-30.38	107.90	0	5	18	8.64	46.13	101.33
4	-7	18	255.33	85.56	69.74	-3	0	18	61.16	76.90	77.43	1	5	18	106.32	32.79	73.72
-2	-6	18	17.36	-40.85	114.21	-2	0	18	41.58	7.42	72.70	2	5	18	474.93	514.27	66.61
1	-6	18	231.76	226.20	64.59	-1	0	18	75.55	-92.25	98.58	3	5	18	7.77	72.34	56.38
0	-6	18	0.36	-45.00	112.54	0	0	18	110.14	70.18	57.13	4	5	18	880.01	1044.18	92.54
1	-6	18	366.42	441.45	65.03	1	0	18	193.65	210.70	41.10	5	5	18	47.44	42.24	96.00
2	-6	18	38.62	77.67	109.90	2	0	18	15.54	-18.87	63.96	6	5	18	296.86	399.25	68.48
3	-6	18	33.38	101.16	103.89	3	0	18	70.88	91.67	47.99	-2	6	18	17.98	-38.27	109.20
4	-6	18	137.96	203.58	64.47	4	0	18	34.13	-12.64	79.29	-1	6	18	6.88	-5.58	100.61
-2	-5	18	15.74	-99.14	62.87	5	0	18	67.81	-2.56	74.02	0	6	18	202.10	302.55	61.31
1	-5	18	435.44	478.39	70.16	6	0	18	1.55	-7.37	97.17	1	6	18	67.57	-18.14	105.68
0	-5	18	179.78	149.58	65.02	-3	1	18	409.14	415.64	69.16	2	6	18	88.53	74.53	109.17
1	-5	18	3.83	35.11	100.84	-2	1	18	55.68	124.23	58.48	3	6	18	576.39	619.28	70.46
2	-5	18	54.37	12.45	107.80	-1	1	18	401.09	261.09	67.20	4	6	18	27.67	66.53	73.35
3	-5	18	51.57	20.81	110.30	0	1	18	38.83	-4.23	98.86	5	6	18	321.91	269.21	58.53
4	-5	18	48.02	-29.86	114.82	1	1	18	105.40	89.72	99.61	6	6	18	55.67	99.66	108.39
5	-5	18	71.80	48.18	65.94	2	1	18	183.40	148.01	58.20	-1	7	18	258.32	267.76	67.73
-3	-4	18	47.04	-4.74	114.52	3	1	18	34.36	-11.36	101.27	0	7	18	0.12	-52.06	103.93
-2	-4	18	22.34	-131.84	110.31	4	1	18	1.02	-130.36	99.99	1	7	18	4.23	-116.15	111.15
-1	-4	18	63.97	-19.07	103.50	5	1	18	24.26	75.47	56.88	2	7	18	36.84	112.09	59.25
0	-4	18	59.69	-1060.91	155.70*	6	1	18	27.69	131.96	61.04	3	7	18	251.79	246.19	62.92
1	-4	18	486.16	350.29	66.92	7	1	18	273.53	230.26	68.62	4	7	18	23.42	64.55	100.83
2	-4	18	134.56	102.77	111.65	-3	2	18	23.00	49.54	110.42	5	7	18	1.37	-92.67	106.63
3	-4	18	714.52	530.59	72.85	-2	2	18	1.16	-41.56	103.56	6	7	18	101.99	55.23	80.18
4	-4	18	379.79	318.93	67.96	-1	2	18	0.64	-165.44	101.94	-1	8	18	0.71	-48.66	113.42
5	-4	18	215.91	107.72	117.73	0	2	18	0.35	-2311.72	193.25*	0	8	18	68.27	87.35	113.10
-3	-3	18	83.65	44.94	64.73	1	2	18	85.16	126.27	54.07	1	8	18	61.79	20.78	105.51
-2	-3	18	16.59	-65.32	105.84	2	2	18	18.28	-44.79	104.95	2	8	18	203.37	243.07	67.31
-1	-3	18	77.01	2.97	99.02	3	2	18	705.37	710.01	70.62	3	8	18	516.70	524.00	71.75

h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)	h	k	l	F ² cal	F ² obs	sig(F ²)
4	8	18	39.81	80.67	109.63	4	0	19	229.34	89.84	55.31	2	7	19	499.03	611.73	74.93
5	8	18	251.21	229.01	68.60	5	0	19	66.35	61.14	81.48	3	7	19	24.04	-28.17	108.87
0	9	18	1.59	-13.64	112.92	6	0	19	232.74	712.05	47.58	4	7	19	211.71	270.60	66.44
1	9	18	755.92	416.41	71.65	-2	1	19	10.90	-6.69	114.64	1	8	19	20.88	-3.89	115.34
2	9	18	73.23	-76.66	124.73	-1	1	19	205.93	108.12	113.58	2	8	19	29.03	191.61	63.54
3	9	18	71.29	-159.95	117.90	0	1	19	120.33	-24.51	104.98	3	8	19	10.40	-53.58	111.65
4	9	18	73.07	-52.97	119.76	1	1	19	13.83	17.48	70.21	0	-4	20	2.79	45.32	114.18
2	10	18	28.48	-82.35	117.48	2	1	19	28.78	-90.67	101.71	1	-4	20	108.50	84.25	67.46
0	-6	19	3.94	19.13	110.81	3	1	19	108.20	238.0	58.49	2	-4	20	20.62	-11.55	64.31
-6	-6	19	105.64	139.43	65.70	4	1	19	15.35	-89.49	108.43	3	-4	20	58.74	87.78	116.66
2	-6	19	5.14	65.72	112.70	5	1	19	539.95	565.77	72.38	0	-3	20	333.92	3.66	142.37
3	-6	19	21.09	8.30	64.83	6	1	19	3.88	-153.28	119.16	1	-3	20	119.99	-3.87	118.12
-1	-5	19	49.70	104.01	104.38	-2	2	19	310.13	462.24	68.02	2	-3	20	83.10	91.98	61.57
0	-5	19	199.79	-95.79	121.56	-1	2	19	61.60	63.58	74.46	3	-3	20	363.89	477.20	67.99
1	-5	19	0.08	-177.93	114.91	0	2	19	288.89	296.45	63.67	4	-3	20	8.10	47.08	103.52
2	-5	19	279.86	103.49	124.72	1	2	19	23.01	2.98	73.93	-1	-2	20	243.16	389.17	67.30
3	-5	19	302.57	205.18	70.79	2	2	19	67.49	61.38	100.22	0	-2	20	53.31	-168.77	129.09
4	-5	19	2.29	53.19	63.66	3	2	19	55.00	90.40	58.52	1	-2	20	74.46	-136.51	113.94
-1	-4	19	321.56	450.77	68.41	4	2	19	17.79	15.62	105.22	2	-2	20	10.93	-8.64	75.22
0	-4	19	1.25	-55.87	113.20	5	2	19	6.43	-33.35	115.88	3	-2	20	5.41	-148.00	112.57
1	-4	19	163.14	-16.42	127.62	6	2	19	10.49	40.46	63.53	4	-2	20	56.15	-8.65	120.24
2	-4	19	89.40	91.30	110.43	-2	3	19	65.02	-65.71	119.41	-1	-1	20	11.36	88.27	116.17
3	-4	19	57.67	46.06	63.61	-1	3	19	85.57	-56.47	108.37	0	-1	20	0.54	-302.55	128.69
4	-4	19	3.58	99.88	110.81	0	3	19	119.63	102.34	105.27	1	-1	20	2.11	-19.10	111.31
-2	-3	19	98.91	112.80	66.79	1	3	19	51.64	61.83	69.06	2	-1	20	63.24	37.38	114.00
-1	-3	19	18.31	-184.40	112.39	2	3	19	14.00	85.56	103.51	3	-1	20	11.14	-112.99	111.00
0	-3	19	338.19	-18.06	140.67	3	3	19	0.16	-19.34	108.50	4	-1	20	25.44	126.71	110.26
1	-3	19	23.10	95.64	58.10	4	3	19	263.13	288.29	66.72	-1	0	20	224.48	141.99	49.27
2	-3	19	5.02	-13.76	109.37	5	3	19	170.48	150.06	63.93	0	0	20	47.85	-15.63	108.44
3	-3	19	47.29	84.74	100.67	6	3	19	336.74	392.16	71.90	1	0	20	588.88	662.97	51.28
4	-3	19	66.63	106.36	65.70	-2	4	19	24.88	-96.89	113.70	2	0	20	142.25	42.62	76.84
5	-3	19	286.23	317.15	67.90	-1	4	19	12.44	-41.96	112.43	3	0	20	225.13	141.21	179.99
-3	-2	19	115.66	56.47	112.67	0	4	19	87.71	-78.87	119.55	4	0	20	190.51	293.47	51.89
-1	-2	19	26.59	33.08	103.40	1	4	19	204.48	150.41	64.60	5	0	20	0.36	-144.75	81.26
0	-2	19	209.04	-156.73	122.10	2	4	19	5.81	4.13	72.87	-1	1	20	5.57	-13.76	115.61
1	-2	19	568.43	548.98	69.99	3	4	19	359.93	389.74	63.06	0	1	20	229.13	133.27	71.28
2	-2	19	67.00	-63.18	111.06	4	4	19	477.44	508.68	69.36	1	1	20	1.87	41.31	78.41
3	-2	19	85.44	143.23	62.24	5	4	19	29.05	-54.86	111.95	2	1	20	42.96	-68.54	112.67
4	-2	19	452.73	464.27	71.15	6	4	19	394.30	224.95	69.43	3	1	20	22.67	-107.05	104.67
5	-2	19	52.69	53.43	63.96	-1	5	19	245.83	466.75	66.13	4	1	20	6.62	12.98	111.98
-2	-1	19	129.20	92.74	102.71	0	5	19	8.44	-89.70	105.59	5	1	20	80.01	132.37	68.15
-1	-1	19	288.91	307.03	65.26	1	5	19	180.62	90.64	112.16	-1	2	20	1.99	73.52	113.03
0	-1	19	204.36	224.51	61.80	2	5	19	28.22	48.82	104.74	0	2	20	2.06	-75.42	118.78
1	-1	19	51.50	-26.71	103.65	3	5	19	41.01	132.92	62.00	1	2	20	112.68	12.53	115.58
2	-1	19	1.21	29.94	97.27	4	5	19	1.06	17.07	108.86	2	2	20	26.52	-9.24	98.12
3	-1	19	13.85	-2.74	101.24	5	5	19	22.14	-49.31	121.16	3	2	20	165.47	243.44	66.98
4	-1	19	3.42	30.87	73.02	-1	6	19	94.16	156.62	66.61	4	2	20	134.57	71.88	81.76
5	-1	19	114.01	144.32	64.18	0	6	19	133.62	52.84	78.76	5	2	20	34.18	-0.21	113.29
6	-1	19	22.66	20.00	114.82	1	6	19	21.81	17.86	105.52	-1	3	20	83.49	-55.03	122.85
-2	0	19	75.90	131.28	55.50	2	6	19	2.14	26.30	103.06	0	3	20	193.94	188.90	68.86
-1	0	19	213.87	-13.22	82.84	3	6	19	300.53	291.37	69.06	1	3	20	4.42	-286.33	114.05
0	0	19	14.35	-86.09	77.46	4	6	19	34.19	-75.74	117.45	2	3	20	358.78	351.41	70.74
1	0	19	38.21	-138.85	73.62	5	6	19	273.35	325.63	69.92	3	3	20	217.29	221.81	66.84
2	0	19	114.74	74.76	59.01	0	7	19	43.74	-85.34	114.66	4	3	20	61.70	19.48	113.96
3	0	19	0.80	41.86	70.90	1	7	19	108.82	122.35	64.88	5	3	20	51.18	-3.02	110.59

Table 1. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	0-15	99	86	6		1	3-12	211	199	6		2	1-10	239	242	5		9	2-9	153	147	6		7	3-8	222	220	5	
3	0-15	200	191	6		2	3-12	56	61	8		3	1-10	49	41	7		10	2-9	131	136	5		8	3-8	49	27	8	
1	1-15	71	85	8		3	3-12	70	61	6		4	1-10	209	233	5		11	2-9	102	101	5		9	3-8	263	258	6	
2	1-15	37	40	19		4	3-12	161	150	6		5	1-10	201	197	5		0	3-9	269	264	5		10	3-8	194	178	6	
3	1-15	114	113	5		5	3-12	79	75	6		6	1-10	222	228	5		1	3-9	105	101	4		11	3-8	126	119	5	
0	0-14	53	38	10		6	3-12	78	78	7		7	1-10	149	131	5		2	3-9	231	203	5		0	4-8	268	255	5	
2	0-14	256	255	6		7	3-12	115	113	5		8	1-10	192	192	5		3	3-9	430	433	7		1	4-8	353	326	6	
4	0-14	206	227	6		8	3-12	123	118	6		9	1-10	57	45	9		4	3-9	221	213	5		2	4-8	294	279	5	
6	0-14	141	141	5		0	4-12	62	67	8		10	1-10	147	146	7		5	3-9	205	184	5		3	4-8	180	192	5	
0	1-14	180	164	6		1	4-12	201	177	6		11	1-10	18	57	17		6	3-9	175	173	5		4	4-8	152	175	5	
1	1-14	86	76	6		2	4-12	195	184	6		0	2-10	207	181	5		7	3-9	116	99	5		5	4-8	148	169	5	
2	1-14	151	125	7		3	4-12	75	85	7		1	2-10	299	312	5		8	3-9	215	216	5		6	4-8	144	165	6	
3	1-14	56	53	9		4	4-12	137	128	5		2	2-10	141	143	5		9	3-9	91	101	5		7	4-8	181	186	5	
4	1-14	0	48	1		5	4-12	107	116	5		3	2-10	181	169	5		10	3-9	128	137	5		8	4-8	121	116	5	
5	1-14	69	53	7		6	4-12	20	21	20		4	2-10	83	90	4		11	3-9	118	117	5		9	4-8	216	220	6	
6	1-14	142	144	5		7	4-12	138	133	7		5	2-10	17	29	16		0	4-9	280	265	5		10	4-8	95	87	5	
0	2-14	150	140	7		0	5-12	36	64	21		6	2-10	82	68	5		1	4-9	142	158	6		11	4-8	128	118	5	
1	2-14	60	49	9		1	5-12	131	124	5		7	2-10	172	176	6		2	4-9	399	373	7		0	5-8	147	157	6	
2	2-14	100	89	5		2	5-12	91	82	34		8	2-10	282	266	6		3	4-9	67	58	6		1	5-8	171	179	5	
3	2-14	118	111	6		3	5-12	10	97	5		9	2-10	182	201	6		4	4-9	334	304	6		2	5-8	74	85	5	
4	2-14	67	71	8		4	5-12	91	82	6		10	2-10	182	180	6		5	4-9	229	199	5		3	5-8	172	194	5	
5	2-14	101	105	5		5	5-12	131	139	6		11	2-10	17	65	17		6	4-9	56	58	7		4	5-8	50	50	8	
0	2-14	136	135	6		1	5-12	230	240	5		0	3-10	240	242	5		7	4-9	125	107	6		5	5-8	207	219	5	
6	3-14	42	64	41		3	0-11	202	190	5		1	3-10	160	176	5		8	4-9	202	187	6		6	5-8	0	26	1	
1	3-14	118	126	5		5	0-11	34	10	34		2	3-10	234	218	5		9	4-9	64	53	7		7	5-8	167	164	6	
2	3-14	73	71	7		7	0-11	342	357	6		3	3-10	306	289	6		10	4-9	162	177	7		8	5-8	57	45	9	
3	3-14	30	28	30		9	0-11	249	261	6		4	3-10	91	114	5		0	5-9	210	205	5		9	5-8	134	145	5	
4	3-14	73	70	7		0	1-11	90	83	4		5	3-10	286	299	6		1	5-9	229	217	5		10	5-8	61	57	9	
1	0-13	164	138	5		1	1-11	146	122	5		6	3-10	157	160	6		2	5-9	291	273	6		0	6-8	61	59	7	
3	0-13	95	109	5		2	1-11	167	164	5		7	3-10	208	223	6		3	5-9	172	156	6		1	6-8	151	203	6	
5	0-13	95	86	5		3	1-11	295	283	5		8	3-10	218	226	6		4	5-9	112	103	5		2	6-8	111	120	5	
7	0-13	188	169	6		4	1-11	156	154	5		9	3-10	86	99	6		5	5-9	146	137	6		3	6-8	213	206	5	
0	1-13	50	55	10		5	1-11	254	260	5		10	3-10	98	111	6		6	5-9	105	117	5		4	6-8	138	117	7	
1	1-13	228	222	6		6	1-11	177	181	5		0	4-10	89	82	5		7	5-9	130	145	5		5	6-8	145	151	7	
2	1-13	51	53	9		7	1-11	198	201	5		1	4-10	298	296	6		8	5-9	152	147	7		6	6-8	78	83	6	
3	1-13	151	162	6		8	1-11	67	70	7		2	4-10	195	209	5		9	5-9	115	119	5		7	6-8	165	156	6	
4	1-13	116	113	5		9	1-11	142	148	5		3	4-10	269	229	5		0	6-9	235	216	6		8	6-8	19	12	19	
5	1-13	0	18	1		10	1-11	114	112	5		4	4-10	79	105	6		1	6-9	46	46	11		0	7-8	206	198	6	
6	1-13	33	13	32		0	2-11	300	291	6		5	4-10	200	180	6		2	6-9	32	37	31		1	7-8	77	96	7	
7	1-13	168	166	7		1	2-11	250	225	5		6	4-10	58	84	8		3	6-9	0	12	1		2	7-8	96	94	5	
8	1-13	0	54	1		2	2-11	214	214	5		7	4-10	89	90	5		4	6-9	146	139	6		3	7-8	225	231	6	
0	2-13	113	122	5		3	2-11	161	142	5		8	4-10	36	21	36		5	6-9	0	55	1		4	7-8	73	66	7	
1	2-13	72	72	6		4	2-11	82	89	5		9	4-10	128	130	6		6	6-9	220	231	6		5	7-8	200	193	6	
2	2-13	139	134	6		5	2-11	56	56	8		0	5-10	115	116	4		7	6-9	0	35	1		6	7-8	90	74	6	
3	2-13	145	149	7		6	2-11	161	159	6		1	5-10	270	260	6		0	7-9	85	74	6		1	0-7	256	265	4	
4	2-13	248	238	6		7	2-11	146	143	6		2	5-10	168	163	6		1	7-9	158	143	7		3	0-7	224	233	4	
5	2-13	185	192	6		8	2-11	202	187	6		3	5-10	239	218	6		2	7-9	127	121	6		5	0-7	396	487	-6	
6	2-13	207	207	6		9	2-11	186	193	6		4	5-10	121	117	5		3	7-9	123	121	6		7	0-7	629	607	9	
7	2-13	140	136	5		10	2-11	140	124	5		5	5-10	130	107	5		4	7-9	178	172	7		9	0-7	187	187	5	
8	2-13	56	61	10		0	3-11	60	55	7		6	5-10	0	18	1		5	7-9	63	54	9		11	0-7	160	139	6	
0	3-13	222	210	6		1	3-11	281	267	5		7	5-10	98	108	5		0	0-8	512	511	8		13	0-7	218	214	6	
1	3-13	62	67	8		2	3-11	182	198	5		8	5-10	64	66	9		2	0-8	371	367	6		0	1-7	231	222	4	
2	3-13	95	84	5		3	3-11	159	135	6		0	6-10	102	94	5		4	0-8	330	283	5		1	1-7	190	178	4	
3	3-13	41	43	13		4	3-11	298	295	6		1	6-10	92	100	5		6	0-8	355	361	6		2	1-7	286	276	5	
4	3-13	98	79	5		5	3-11	83	78	5		2	6-10	65	72	8		8	0-8	212	182	5		3	1-7	320	330	5	
5	3-13	163	166	7		6	3-11	218	212	6		3	6-10	60	52	9		10	0-8	189	207	6		4	1-7	66	116	-4	
6	3-13	106	95	5		7	3-11	166	161	6		4	6-10	24	22	24		12	0-8	194	194	6		5	1-7	303	351	5	
7	3-13	127	135	6		8	3-11	101	94	5		5	6-10	153	148	7		0	1-8	359	359	6		6	1-7	228	238	4	
0	4-13	169	171	7		9	3-11	128	120	5		6	6-10	52	44	11		1	1-8	100	85	5		7	1-7	261	249	5	
1	4-13	80	83	7		0	4-11	122	122	5		7	7-10	81	85	7		2	1-8	277	289	5		8	1-7	160	145	5	
2	4-13	140	127	5		1																							

0 3-12 0 23 1 1 1-10 235 232 5 8 2 -9 27 23 27 6 3 -8 254 235 5 12 3 -7 1 2 108 5



Table 1. Observed and calculated structure factors for 1

Page 3

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	9	-3	41	82	41	1	7	-2	110	87	5	7	5	-1	76	82	5	3	4	0	344	370	5	0	3	1	304	304	5
1	9	-3	133	122	5	2	7	-2	158	153	5	8	5	-1	170	159	5	4	4	0	110	116	5	1	3	1	344	353	5
2	9	-3	72	70	8	3	7	-2	70	82	5	9	5	-1	109	90	5	5	4	0	73	74	3	2	3	1	340	311	5
3	9	-3	187	168	7	4	7	-2	283	274	6	10	5	-1	125	115	5	6	4	0	66	64	4	3	3	1	630	619	9
0	0	-2	696	688	10	5	7	-2	131	142	5	11	5	-1	22	24	21	7	4	0	379	382	6	4	3	1	293	272	5
2	0	-2	935	907	14	6	7	-2	147	133	6	0	6	-1	251	299	5	8	4	0	156	148	5	5	3	1	271	280	5
4	0	-2	1169	1146	18	7	7	-2	246	251	6	1	6	-1	110	114	4	9	4	0	264	265	5	6	3	1	341	315	5
6	0	-2	482	435	7	8	7	-2	65	50	8	2	6	-1	355	370	5	10	4	0	151	140	6	7	3	1	23	20	22
8	0	-2	135	147	4	9	7	-2	109	115	5	3	6	-1	64	54	5	11	4	0	130	134	5	8	3	1	218	225	5
10	0	-2	166	173	5	0	8	-2	72	86	6	4	6	-1	241	245	5	12	4	0	140	145	5	9	3	1	240	223	5
12	0	-2	376	386	6	1	8	-2	94	78	5	5	6	-1	191	183	5	0	5	0	375	360	6	10	3	1	86	75	5
0	1	-2	937	904	14	2	8	-2	111	106	4	6	6	-1	137	159	6	1	5	0	467	496	7	11	3	1	114	103	5
1	1	-2	1099	1069	16	3	8	-2	52	37	9	7	6	-1	67	78	6	2	5	0	370	372	6	12	3	1	151	162	7
2	1	-2	655	644	10	4	8	-2	251	241	6	8	6	-1	181	176	6	3	5	0	103	97	5	0	4	1	529	516	8
3	1	-2	880	828	13	5	8	-2	126	108	5	9	6	-1	36	43	35	4	5	0	460	448	7	1	4	1	178	182	4
4	1	-2	342	343	5	6	8	-2	33	22	33	10	6	-1	173	171	6	5	5	0	138	143	5	2	4	1	461	443	7
5	1	-2	171	173	3	7	8	-2	164	149	7	0	7	-1	252	238	5	6	5	0	260	273	5	3	4	1	166	165	4
6	1	-2	512	441	-8	0	9	-2	81	86	7	1	7	-1	127	119	6	7	5	0	283	289	5	4	4	1	193	183	4
7	1	-2	408	396	6	1	9	-2	95	83	6	2	7	-1	87	77	4	8	5	0	139	141	6	5	4	1	220	197	4
8	1	-2	242	247	5	2	9	-2	85	90	6	3	7	-1	94	82	4	9	5	0	239	244	5	6	4	1	389	403	6
9	1	-2	252	261	5	3	9	-2	54	44	10	4	7	-1	171	159	5	10	5	0	127	124	5	7	4	1	199	192	5
10	1	-2	141	129	5	1	0	-1	1123	1078	17	5	7	-1	245	242	5	11	5	0	175	165	6	8	4	1	282	279	5
11	1	-2	149	146	6	3	0	-1	405	372	6	6	7	-1	338	346	6	0	6	0	33	35	11	9	4	1	65	42	6
12	1	-2	232	239	6	5	0	-1	636	564	9	7	7	-1	136	130	7	1	6	0	249	245	5	10	4	1	159	161	6
13	1	-2	0	47	1	7	0	-1	165	210	4	8	7	-1	201	216	6	2	6	0	156	147	5	11	4	1	92	85	5
0	2	-2	504	488	7	9	0	-1	245	245	5	9	7	-1	78	77	7	3	6	0	382	384	6	12	4	1	127	112	5
1	2	-2	367	292	-5	11	0	-1	226	252	5	0	8	-1	83	90	5	4	6	0	184	172	5	0	5	1	502	487	8
2	2	-2	268	278	4	13	0	-1	213	208	6	1	8	-1	342	334	6	5	6	0	304	316	6	1	5	1	117	120	5
3	2	-2	149	141	3	0	1	-1	292	304	4	2	8	-1	103	94	4	6	6	0	82	91	5	2	5	1	262	262	5
4	2	-2	92	41	-3	1	1	-1	1034	1010	15	3	8	-1	262	254	6	7	6	0	264	252	5	3	5	1	243	233	5
5	2	-2	326	347	5	2	1	-1	460	446	7	4	8	-1	43	50	12	8	6	0	68	76	7	4	5	1	201	199	4
6	2	-2	381	328	6	3	1	-1	484	460	7	5	8	-1	138	134	5	9	6	0	93	79	5	5	5	1	31	5	31
7	2	-2	123	157	-4	4	1	-1	281	283	4	6	8	-1	185	168	6	10	6	0	75	91	7	6	5	1	190	205	5
8	2	-2	500	481	8	5	1	-1	247	213	4	7	8	-1	34	64	33	0	7	0	405	406	7	7	5	1	154	142	5
9	2	-2	128	131	5	6	1	-1	197	188	4	0	9	-1	113	119	5	1	7	0	172	183	5	8	5	1	301	307	6
10	2	-2	140	139	5	7	1	-1	269	311	-5	1	9	-1	103	109	6	2	7	0	175	168	5	9	5	1	82	76	6
11	2	-2	169	169	5	8	1	-1	46	39	6	2	9	-1	116	119	5	3	7	0	229	217	5	10	5	1	182	195	6
12	2	-2	60	66	8	9	1	-1	384	374	6	3	9	-1	84	76	7	4	7	0	129	114	6	11	5	1	141	131	5
13	2	-2	84	92	6	10	1	-1	141	125	5	4	9	-1	145	143	5	5	7	0	89	87	5	0	6	1	290	303	5
0	3	-2	422	433	6	11	1	-1	180	187	5	2	0	0	1073	1017	16	6	7	0	137	142	5	1	6	1	202	215	5
1	3	-2	425	438	6	12	1	-1	79	68	6	4	0	0	411	426	6	7	7	0	211	210	6	2	6	1	361	358	6
2	3	-2	559	424	-8	13	1	-1	180	184	6	6	0	0	341	355	5	8	7	0	136	143	5	3	6	1	135	129	5
3	3	-2	339	325	5	0	2	-1	1032	984	15	8	0	0	461	459	7	9	7	0	119	121	6	4	6	1	268	259	5
4	3	-2	285	306	5	1	2	-1	318	336	5	10	0	0	385	419	6	0	8	0	137	127	6	5	6	1	180	173	5
5	3	-2	390	382	6	2	2	-1	414	439	6	12	0	0	177	164	6	1	8	0	75	86	6	6	6	1	287	265	6
6	3	-2	340	347	5	3	2	-1	296	261	4	0	1	0	761	740	11	7	7	0	136	131	6	7	6	1	92	99	5
7	3	-2	444	467	7	4	2	-1	191	196	3	1	1	0	332	317	5	8	6	0	91	93	5	8	6	1	141	144	6
8	3	-2	483	480	8	5	2	-1	542	473	8	2	1	0	393	391	6	4	8	0	195	207	6	9	6	1	142	128	6
9	3	-2	241	239	5	6	2	-1	427	419	7	3	1	0	624	631	9	5	8	0	134	131	5	10	6	1	168	163	7
10	3	-2	126	139	4	7	2	-1	457	456	7	4	1	0	330	329	5	6	8	0	37	50	9	0	7	1	234	224	5
11	3	-2	85	87	5	8	2	-1	313	318	5	5	1	0	341	312	5	7	8	0	84	92	7	1	7	1	154	159	6
12	3	-2	78	76	6	9	2	-1	261	258	5	6	1	0	170	248	-4	0	9	0	124	112	5	2	7	1	478	469	8
13	3	-2	124	118	6	10	2	-1	216	208	5	7	1	0	189	175	4	1	9	0	113	118	5	3	7	1	110	125	5
0	4	-2	205	220	4	11	2	-1	56	59	7	8	1	0	346	334	4	2	9	0	136	119	5	4	7	1	220	207	5
1	4	-2	402	358	6	12	2	-1	144	133	6	9	1	0	127	127	5	3	9	0	73	76	8	5	7	1	59	63	7
2	4	-2	232	291	-4	13	2	-1	153	144	7	10	1	0	202	215	5	1	0	1	1138	1094	17	6	7	1	84	89	5
3	4	-2	305	292	5	0	3	-1	282	283	4	11	1	0	89	105	5	3	0	1	211	268	3	7	7	1	156	148	6
4	4	-2	274	299	5	1	3	-1	212	277	-4	12	1	0	214	224	6	5	0	1	46	63	4	8	7	1	139	143	5
5	4	-2	420	425	7	2	3	-1	475	459	7	13	1	0	122	119	5	7	0	1	490	465	7	0	8	1	78	93	6
6	4	-2	74	79	4	3	3	-1	179	144	-																		

Table 1. Observed and calculated structure factors for 1

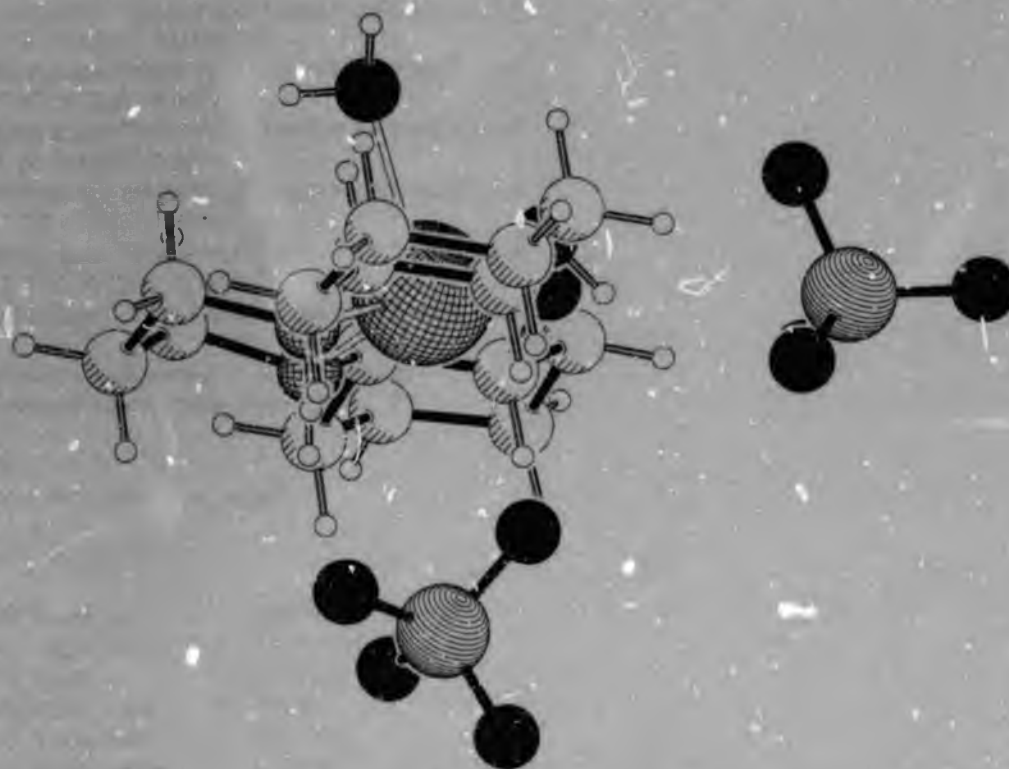
Page 4

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
13	1	2	40	18	39	13	0	3	94	99	6	1	9	3	131	133	6	2	8	4	219	213	5	2	8	5	153	143	7
0	2	2	473	471	7	0	1	3	677	649	10	2	9	3	111	110	5	3	8	5	178	172	6	3	8	5	115	108	5
1	2	2	732	733	1	1	1	3	1403	1383	22	0	0	4	635	663	9	4	8	4	77	75	7	4	8	5	126	134	6
2	2	2	839	834	13	2	1	3	164	165	3	0	0	4	441	444	6	5	8	4	104	93	5	0	0	6	189	200	3
3	2	2	629	668	9	3	1	3	471	469	7	4	0	4	278	297	4	0	0	6	197	199	6	2	0	6	652	669	10
4	2	2	573	561	8	4	1	3	190	133	-3	6	0	4	317	350	5	4	0	6	104	111	6	4	0	6	618	617	9
5	2	2	200	180	4	5	1	3	135	129	4	8	0	4	312	303	5	5	0	6	177	177	3	6	0	6	322	326	5
6	2	2	209	190	4	6	1	3	0	14	1	10	0	4	271	275	5	6	0	6	188	172	4	6	0	6	175	160	5
7	2	2	145	137	4	7	1	3	292	331	5	12	0	4	107	106	5	7	0	6	506	490	8	10	0	6	127	122	5
8	2	2	330	330	6	8	1	3	245	249	5	0	1	4	676	681	10	8	0	6	404	366	6	0	1	6	24	9	8
9	2	2	304	318	5	9	1	3	390	386	6	0	1	4	174	163	3	9	0	6	293	282	5	0	1	6	250	265	4
10	2	2	184	183	5	10	1	3	96	94	4	2	1	4	593	611	9	11	0	6	95	101	5	2	1	6	262	242	4
11	2	2	203	224	6	11	1	3	116	116	5	3	1	4	187	192	3	0	1	6	133	159	3	3	1	6	159	160	4
12	2	2	106	103	5	12	1	3	33	35	33	4	1	4	733	737	11	1	1	6	232	270	4	4	1	6	577	543	9
13	0	1	82	72	6	0	2	3	285	235	-4	5	1	4	113	118	4	2	1	6	264	297	4	5	1	6	111	113	5
0	1	1	401	425	6	1	2	3	828	775	13	6	1	4	91	92	4	3	1	6	449	464	7	6	1	6	322	300	5
1	1	1	440	443	7	2	2	3	319	322	5	7	1	4	88	78	4	4	1	6	604	627	9	7	1	6	89	87	4
2	1	1	854	870	13	3	2	3	649	573	10	8	1	4	337	326	6	5	1	6	436	445	7	8	1	6	59	67	6
3	1	1	401	412	6	4	2	3	473	444	7	9	1	4	196	203	5	6	1	6	175	156	4	9	1	6	110	101	5
4	1	1	150	191	-4	5	2	3	236	224	4	10	1	4	279	286	6	7	1	6	149	143	5	10	1	6	152	146	6
5	1	1	301	353	5	6	2	3	277	254	5	11	1	4	0	26	1	8	1	6	118	101	6	11	1	6	61	61	8
6	1	1	83	85	3	7	2	3	106	116	4	12	1	4	40	61	40	9	1	6	196	205	5	0	2	6	324	333	5
7	1	1	236	258	5	8	2	3	136	127	5	0	2	4	393	385	6	10	1	6	69	77	6	1	2	6	454	466	7
8	1	1	178	174	5	9	2	3	205	198	5	1	2	4	334	327	5	11	1	6	149	137	6	2	2	6	393	379	6
9	1	1	144	141	6	10	2	3	23	31	22	2	2	4	317	348	5	12	1	6	102	95	5	3	2	6	277	308	5
10	1	1	152	163	6	11	2	3	111	108	4	3	2	4	734	686	11	0	2	6	246	270	4	4	2	6	232	226	4
11	1	1	30	44	30	12	2	3	93	83	5	4	2	4	372	379	6	1	2	6	517	583	8	5	2	6	112	103	5
12	1	1	15	31	15	0	3	3	553	572	8	5	2	4	253	232	4	2	2	6	420	379	6	6	2	6	89	84	4
0	1	1	218	234	4	1	3	3	353	329	5	6	2	4	147	158	4	3	2	6	201	268	-4	7	2	6	163	157	5
1	1	1	225	205	5	2	3	3	504	548	7	7	2	4	216	206	5	4	2	6	199	210	4	8	2	6	204	213	5
2	1	1	44	57	5	3	3	3	403	389	6	8	2	4	149	155	5	5	2	6	73	68	4	9	2	6	180	171	5
3	1	1	497	514	7	4	3	3	161	214	-4	9	2	4	34	37	14	6	2	6	131	148	5	10	2	6	211	201	6
4	1	1	110	99	4	5	3	3	208	202	4	10	2	4	98	104	5	7	2	6	73	71	4	11	2	6	65	67	3
5	1	1	477	474	7	6	3	3	192	176	4	11	2	4	95	76	5	8	2	6	72	77	5	0	3	6	378	399	6
6	1	1	187	201	5	7	3	3	141	125	5	12	2	4	145	146	7	9	2	6	150	164	6	1	3	6	243	278	4
7	1	1	179	172	5	8	3	3	133	127	5	0	3	4	193	177	4	10	2	6	88	73	5	2	3	6	496	502	8
8	1	1	216	232	5	9	3	3	30	90	5	1	3	4	739	713	11	11	2	6	175	166	6	3	3	6	254	291	5
9	1	1	129	138	6	10	3	3	168	160	6	2	3	4	343	318	5	0	3	6	394	375	6	4	3	6	93	99	4
10	1	1	75	66	6	11	3	3	78	79	6	3	3	4	566	534	8	1	3	6	263	285	5	5	3	6	249	275	5
11	1	1	146	134	7	12	3	3	178	176	7	4	3	4	249	256	4	2	3	6	428	412	7	6	3	6	167	171	5
12	1	1	62	44	9	0	4	3	138	167	4	5	3	4	80	82	3	3	3	6	379	394	6	7	3	6	171	174	5
0	1	1	73	65	3	1	4	3	256	277	4	6	3	4	233	239	5	4	3	6	295	278	5	8	3	6	206	200	5
1	1	1	468	458	7	2	4	3	361	396	6	7	3	4	187	169	4	5	3	6	97	100	4	9	3	6	74	63	6
2	1	1	179	194	4	3	4	3	71	57	3	8	3	4	97	105	4	6	3	6	153	143	5	10	3	6	159	165	7
3	1	1	312	221	5	4	4	3	404	428	6	9	3	4	160	149	5	7	3	6	65	68	5	11	3	6	128	128	6
4	1	1	55	44	5	5	4	3	59	74	5	10	3	4	81	71	6	8	3	6	112	105	5	0	4	6	178	175	4
5	1	1	229	248	5	6	4	3	129	129	5	11	3	4	179	177	6	9	3	6	134	140	7	1	4	6	164	156	4
6	1	1	0	29	1	7	4	3	157	164	5	0	4	4	247	220	4	10	3	6	216	212	6	2	4	6	225	233	5
7	1	1	146	149	5	8	4	3	196	204	5	1	4	4	419	427	6	11	3	6	145	141	7	3	4	6	316	335	5
8	1	1	96	100	4	9	4	3	172	188	6	2	4	4	281	262	5	0	4	6	478	464	7	4	4	6	243	254	5
9	1	1	239	236	5	10	4	3	195	182	6	3	4	4	242	258	4	1	4	6	164	165	4	5	4	6	324	330	6
10	1	1	0	4	1	11	4	3	99	98	5	4	4	4	162	171	4	2	4	6	234	230	4	6	4	6	154	129	5
11	1	1	253	256	6	0	5	3	276	296	5	5	4	4	68	68	4	3	4	6	462	459	7	7	4	6	133	121	6
0	1	1	187	194	7	1	5	3	271	269	5	6	4	4	0	13	1	4	4	6	188	204	5	8	4	6	78	76	6
1	1	1	444	420	7	2	5	3	388	420	6	7	4	4	190	172	5	5	4	6	138	134	5	9	4	6	32	46	32
2	1	1	30	40	29	3	5	3	179	166	4	8	4	4	89	76	5	6	4	6	207	197	5	10	4	6	33	45	32
3	1	1	176	168	5	4	5	3	314	321	5	9	4	4	230	227	6	7	4	6	60	57	6	0	5	6	66	67	5
4	1	1	62	68	6	5	5	3	167	144	5	10	4	4	116	116	5	8	4	6	210	214	5	1	5	6	162	168	5
5	1	1	121	120	4	6	5	3	258	251	5	11	4	4	187	194	6	9	4	6	65	63	7	2	5	6	0	25	1
6	1	1	44	57	10	7	5	3	61	58	7	0	5	4</															

Table 1. Observed and calculated structure factors for 1

h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s						h k l 10Fo 10Fc 10s												
9	0	7	139	150	6	2	0	8	344	359	6	0	1	9	236	230	5	3	2	10	81	71	5	3	5	11	49	38	11	
1	0	7	185	171	6	4	0	8	472	501	7	1	1	9	213	227	4	4	2	10	160	146	6	4	5	11	141	128	5	
0	1	7	232	231	4	6	0	8	106	102	4	2	1	9	241	248	5	5	2	10	139	142	6	5	6	11	162	176	7	
1	1	7	252	242	4	8	0	8	113	106	5	3	1	9	159	159	5	6	2	10	130	124	5	6	7	11	59	56	9	
2	1	7	0	27	1	10	0	8	153	151	7	4	1	9	145	144	5	7	2	10	104	105	5	7	8	11	81	71	6	
3	1	7	249	234	4	0	1	8	354	362	4	5	1	9	203	205	5	8	2	10	88	87	6	8	9	12	287	294	5	
4	1	7	372	380	6	1	1	8	70	83	4	6	1	9	184	176	6	0	3	10	232	240	5	0	0	12	245	251	5	
5	1	7	364	373	6	2	1	8	274	274	5	7	1	9	182	185	6	1	3	10	101	118	5	1	0	12	81	92	6	
6	1	7	77	56	4	3	1	8	116	124	5	8	1	9	70	48	6	2	3	10	94	95	4	2	0	12	32	37	31	
7	1	7	116	122	4	4	1	8	112	140	4	9	1	9	126	127	5	3	3	10	83	97	5	3	0	12	232	252	5	
8	1	7	100	05	4	5	1	8	80	80	4	0	2	9	108	109	5	4	3	10	105	112	4	4	1	12	161	146	6	
9	1	7	100	98	4	6	1	8	198	194	5	1	2	9	126	133	5	5	3	10	199	200	6	5	2	12	113	127	5	
10	1	7	89	89	5	7	1	8	216	208	5	2	2	9	264	271	5	6	3	10	68	70	7	6	3	12	81	08	5	
11	1	7	104	112	5	8	1	8	131	140	5	3	2	9	266	258	5	7	3	10	74	88	7	7	4	12	112	109	5	
0	2	7	253	261	4	9	1	8	90	72	5	4	2	9	220	237	5	8	3	10	87	84	6	8	5	12	100	104	5	
1	2	7	258	231	5	10	1	8	119	115	6	5	2	9	243	250	5	9	4	10	77	74	5	9	6	12	119	115	6	
2	2	7	132	148	4	0	0	8	89	67	4	6	2	9	154	150	6	0	1	4	10	27	27	27	0	0	12	173	176	6
3	2	7	113	88	5	1	0	8	276	255	5	7	2	9	119	116	6	1	2	4	10	122	132	5	1	1	12	52	51	9
4	2	7	81	70	4	2	2	8	58	82	5	8	2	9	92	91	5	2	3	4	10	168	188	6	2	2	12	22	48	21
5	2	7	178	174	5	3	3	8	308	290	5	9	3	9	0	44	1	3	4	4	10	121	109	5	3	3	12	64	55	7
6	2	7	36	13	11	4	4	8	245	272	5	0	3	9	263	264	5	4	5	4	10	212	203	6	4	4	12	92	94	5
7	2	7	225	218	5	5	5	8	279	273	5	6	4	9	93	89	4	5	6	4	10	0	35	1	5	5	12	81	88	5
8	2	7	139	134	6	6	6	8	328	335	6	7	5	9	245	226	5	6	7	4	10	120	130	5	6	6	12	157	158	7
9	2	7	170	163	6	7	7	8	85	87	5	8	6	9	252	243	5	7	0	5	10	111	118	5	7	7	12	0	26	1
10	2	7	90	85	6	8	8	8	125	114	5	9	7	9	114	117	5	8	1	5	10	116	127	5	8	8	12	139	121	6
0	3	7	146	163	4	9	9	8	50	40	10	0	8	9	213	217	5	9	2	5	10	91	104	5	9	9	12	69	70	5
1	3	7	290	298	5	10	0	8	41	64	15	1	9	9	155	145	6	0	3	5	10	111	119	5	0	0	12	102	97	5
2	3	7	75	55	4	0	1	8	192	190	4	2	0	9	142	137	7	1	4	4	10	0	37	1	1	4	12	69	58	7
3	3	7	93	81	4	1	2	8	308	313	5	3	0	9	178	165	6	2	5	5	10	166	160	6	2	5	12	117	110	5
4	3	7	262	259	5	2	3	8	231	239	5	4	1	9	270	260	5	3	6	5	10	91	83	6	3	6	12	207	215	6
5	3	7	69	80	5	3	4	8	155	157	5	5	2	9	194	202	5	4	0	6	10	88	89	6	4	7	12	26	17	25
6	3	7	150	175	5	4	5	8	316	322	6	6	3	9	173	167	5	5	1	6	10	211	217	6	5	8	12	153	145	7
7	3	7	163	165	5	5	6	8	107	114	6	7	4	9	162	146	5	6	2	6	10	40	50	15	6	9	12	65	56	8
8	3	7	117	119	5	6	7	8	172	181	6	8	5	9	126	138	4	7	3	6	10	159	174	7	7	1	12	38	61	38
9	3	7	147	153	7	7	8	8	184	176	6	9	6	9	46	48	10	8	4	7	10	0	17	8	8	1	12	180	188	7
10	3	7	100	102	5	8	9	8	75	36	6	0	7	9	225	238	6	9	5	7	10	75	67	8	9	2	12	80	95	7
0	4	7	207	213	5	9	0	8	88	93	6	1	8	9	52	52	10	0	6	0	11	195	193	5	0	3	12	196	195	6
1	4	7	62	65	5	0	1	8	256	255	6	2	9	9	162	161	7	1	7	0	11	131	137	6	1	4	12	113	112	4
2	4	7	258	270	5	1	2	8	287	292	27	3	0	9	205	207	5	2	8	0	11	138	148	7	2	5	12	70	60	8
3	4	7	96	106	4	2	3	8	307	307	6	4	1	9	86	93	5	3	9	0	11	68	60	4	3	6	12	188	195	6
4	4	7	408	408	7	3	4	8	0	46	1	5	2	9	111	113	5	4	0	1	11	99	86	4	4	7	12	53	50	9
5	4	7	86	105	4	4	5	8	0	46	5	3	3	9	67	72	7	5	1	1	11	216	221	5	5	8	12	55	45	9
6	4	7	142	139	6	5	6	8	87	96	5	4	4	9	159	176	6	6	2	1	11	90	89	4	6	9	12	35	54	34
7	4	7	38	58	37	6	7	8	34	40	33	7	4	9	13	40	13	7	3	1	11	192	196	5	7	0	12	64	69	9
8	4	7	129	136	5	7	8	8	199	193	6	8	5	9	108	128	5	8	3	1	11	87	102	5	8	1	12	109	116	4
9	4	7	72	65	7	8	9	8	0	22	1	9	6	9	77	67	7	9	4	2	11	209	208	6	9	2	12	69	70	5
0	5	7	108	114	4	9	0	8	89	98	6	0	7	9	220	204	6	0	5	1	11	29	33	29	0	3	12	127	137	5
1	5	7	360	363	6	0	1	8	145	156	5	1	8	9	113	122	5	1	6	2	11	106	89	5	1	4	12	136	135	5
2	5	7	264	276	5	1	2	8	0	21	1	2	9	9	227	233	6	2	7	1	11	284	290	5	2	5	12	143	136	5
3	5	7	276	276	5	2	3	8	108	120	5	3	0	9	108	101	5	3	8	2	11	235	230	5	3	6	12	104	10	5
4																														

RH18



data_rh18

_audit_creation_method	SHELXL
_chemical_name_systematic	?
_chemical_name_common	?
_chemical_formula_moiety	?
_chemical_formula_structural	?
_chemical_formula_analytical	?
_chemical_formula_sum	'C15 H32 Cl2 Cu N2 O11'
_chemical_formula_weight	550.87
_chemical_melting_point	?
_chemical_compound_source	?

loop_

_atom_type_symbol	
_atom_type_description	
_atom_type_scatter_dispersion_real	

_atom_type_scatter_dispersion_imag
 _atom_type_scatter_source
 'C' 'C' 0.0033 0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H' 'H' 0.0000 0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N' 'N' 0.0061 0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O' 'O' 0.0106 0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cl' 'Cl' 0.1484 0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cu' 'Cu' 0.3201 1.2651
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting 'Monoclinic'
 _symmetry_space_group_name_H-M 'P n'

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 'x+1/2, -y, z+1/2'

_cell_length_a 11.627(2)
 _cell_length_b 7.8950(10)
 _cell_length_c 12.737(8)
 _cell_angle_alpha 90.00
 _cell_angle_beta 98.15(3)
 _cell_angle_gamma 90.00
 _cell_volume 1157.4(8)
 _cell_formula_units_Z 2
 _cell_measurement_temperature 163(2)
 _cell_measurement_reflns_used ?
 _cell_measurement_theta_min ?
 _cell_measurement_theta_max ?

_exptl_crystal_description 'plate'
 _exptl_crystal_colour 'blue'
 _exptl_crystal_size_max 0.41
 _exptl_crystal_size_mid 0.33
 _exptl_crystal_size_min 0.12
 _exptl_crystal_density_meas ?
 _exptl_crystal_density_diffn 1.581
 _exptl_crystal_density_method ?
 _exptl_crystal_F_000 574
 _exptl_absorpt_coefficient_mu 1.231
 _exptl_absorpt_correction_type Psi-scans
 _exptl_absorpt_correction_T_min 0.8513
 _exptl_absorpt_correction_T_max 0.9999

_exptl_special_details

;
 ?
 ;

```

_diffra_ambient_temperature 163(2)
_diffra_radiation_wavelength 0.71073
_diffra_radiation_source 'rotating anode'
_diffra_radiation_monochromator graphite
_diffra_measurement_device 'Rigaku AFC5'
_diffra_measurement_method theta-2theta
_diffra_standards_number 3
_diffra_standards_interval_count 150
_diffra_standards_interval_time ?
_diffra_standards_decay_% <1
_diffra_reflns_number 2161
_diffra_reflns_av_R_equivalents 0.0000
_diffra_reflns_av_sigma/netI 0.0440
_diffra_reflns_limit_h_min 0
_diffra_reflns_limit_h_max 13
_diffra_reflns_limit_k_min 0
_diffra_reflns_limit_k_max 9
_diffra_reflns_limit_l_min -15
_diffra_reflns_limit_l_max 15
_diffra_reflns_theta_min 2.22
_diffra_reflns_theta_max 25.06
_reflns_number_total 2161
_reflns_number_observed 2003
_reflns_observed_criterion >2sigma(I)

_computing_data_collection 'MSC CTR (4:1:0)'
_computing_cell_refinement 'MSC CTR (4:1:0)'
_computing_data_reduction 'MSC TEXSAN PROCESS'
_computing_structure_solution 'SHELXS-86 (Sheldrick, 1990)'
_computing_structure_refinement 'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics 'Siemens XP SHELXTL-PLUS'
_computing_publication_material 'SHELXL-93 CIFTAB'

```

refine_special_details

Refinement on F^2 for ALL reflections except for 31 with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating $R_{\text{factor_obs}}$ etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

```

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme
'calc w=1/[s^2*(Fo^2)+( 0.0888P)^2+2.5066P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment riding

```

```

_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details
'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack -0.02(3)
_refine_ls_number_reflns 2130
_refine_ls_number_parameters 308
_refine_ls_number_restraints 63
_refine_ls_R_factor_all 0.0619
_refine_ls_R_factor_obs 0.0524
_refine_ls_wR_factor_all 0.1594
_refine_ls_wR_factor_obs 0.1359
_refine_ls_goodness_of_fit_all 1.062
_refine_ls_goodness_of_fit_obs 1.053
_refine_ls_restrained_S_all 1.287
_refine_ls_restrained_S_obs 1.171
_refine_ls_shift/esd_max 0.093
_refine_ls_shift/esd_mean 0.007

```

loop_

```

_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_group
Cu1 Cu 0.25084(13) 0.04861(12) 0.35383(11) 0.0248(3) Uani 1 d . .
Cl1 Cl 0.3800(2) -0.3793(3) 0.1717(2) 0.0378(6) Uani 1 d . .
Cl2 Cl 0.3656(2) -0.1875(3) 0.5914(2) 0.0412(6) Uani 1 d . .
O1 O 0.1647(6) -0.1425(8) 0.2759(5) 0.0304(14) Uani 1 d . .
H1D H 0.1309(6) -0.1071(8) 0.2164(5) 0.080 Uiso 1 d R .
O2 O 0.3899(8) 0.0278(12) 0.2796(7) 0.046(2) Uani 1 d . .
H2C H 0.3763 0.1554 0.5077 0.080 Uiso 1 d . .
H2C H 0.4124 -0.0738 0.2941 0.050 Uiso 1 d . .
O3 O 0.1725(8) 0.2381(12) 0.2308(8) 0.053(2) Uani 1 d . .
H3C H 0.2014(8) 0.3039(12) 0.1899(8) 0.050 Uiso 1 d R .
H3D H 0.1322(8) 0.3028(12) 0.2646(8) 0.080 Uiso 1 d R .
O4 O 0.4668(10) -0.3303(14) 0.2527(10) 0.081(3) Uani 1 d . .
O5 O 0.2770(8) -0.4320(10) 0.2151(8) 0.057(2) Uani 1 d . .
O6 O 0.4194(10) -0.5099(13) 0.1107(8) 0.066(3) Uani 1 d . .
O7 O 0.3515(12) -0.2337(14) 0.1115(10) 0.088(4) Uani 1 d . .
O8 O 0.5899(15) -0.3354(10) 0.6496(7) 0.047(5) Uani 0.52(3) d PDU .
O8' O 0.4430(15) -0.3060(19) 0.6450(8) 0.059(6) Uani 0.48(3) d PDU .
O9 O 0.3513(8) -0.2144(10) 0.4814(3) 0.064(3) Uani 1 d DU .
O11 O 0.2717(11) -0.0986(23) 0.6220(9) 0.086(8) Uani 0.52(3) d PDU .
O11' O 0.2536(8) -0.2164(33) 0.6247(10) 0.108(10) Uani 0.48(3) d PDU .
O10 O 0.4672(12) -0.0778(20) 0.6142(9) 0.071(7) Uani 0.52(3) d PDU .
O10' O 0.3998(21) -0.0218(10) 0.6177(10) 0.100(9) Uani 0.48(3) d PDU .
N1 N 0.1219(8) 0.0470(9) 0.4398(7) 0.024(2) Uani 1 d . .

```

H1A H 0.1473(8) -0.0067(9) 0.5010(7) 0.080 Uiso 1 d R.
 N2 N 0.3477(7) 0.2119(10) 0.4482(6) 0.025(2) Uani 1 d..
 C1 C 0.0774(7) -0.2082(11) 0.3372(7) 0.025(2) Uani 1 d..
 H1B H 0.1167(7) -0.2764(11) 0.3936(7) 0.080 Uiso 1 d R.
 C2 C -0.0125(8) -0.3139(12) 0.2699(8) 0.031(2) Uani 1 d..
 H2A H -0.0472(8) -0.2493(12) 0.2098(8) 0.080 Uiso 1 d R.
 H2B H 0.0236(8) -0.4113(12) 0.2441(8) 0.080 Uiso 1 d R.
 C3 C -0.1056(9) -0.3724(12) 0.3362(9) 0.037(2) Uani 1 d..
 H3A H -0.1656(9) -0.4311(12) 0.2908(9) 0.080 Uiso 1 d R.
 H3B H -0.0726(9) -0.4499(12) 0.3904(9) 0.080 Uiso 1 d R.
 C4 C -0.1577(9) -0.2247(14) 0.3860(9) 0.041(2) Uani 1 d..
 H4A H -0.2005(9) -0.1562(14) 0.3317(9) 0.080 Uiso 1 d R.
 H4B H -0.2113(9) -0.2660(14) 0.4309(9) 0.080 Uiso 1 d R.
 C5 C -0.0645(8) -0.1165(13) 0.4527(8) 0.032(2) Uani 1 d..
 H5A H -0.1008(8) -0.0198(13) 0.4798(8) 0.080 Uiso 1 d R.
 H5B H -0.0268(8) -0.1806(13) 0.5117(8) 0.080 Uiso 1 d R.
 C6 C 0.0247(7) 0.0584(11) 0.3837(7) 0.024(2) Uani 1 d..
 H6A H -0.0147(7) 0.0079(11) 0.3264(7) 0.080 Uiso 1 d R.
 C7 C 0.0859(9) 0.2205(13) 0.4683(10) 0.040(2) Uani 1 d..
 H7A H 0.0619(9) 0.2841(13) 0.4047(10) 0.080 Uiso 1 d R.
 H7B H 0.0204(9) 0.2103(13) 0.5060(10) 0.080 Uiso 1 d R.
 C8 C 0.1811(9) 0.3147(14) 0.5363(9) 0.041(2) Uani 1 d..
 H8A H 0.1499(9) 0.4161(14) 0.5628(9) 0.080 Uiso 1 d R.
 H8B H 0.2098(9) 0.2452(14) 0.5962(9) 0.080 Uiso 1 d R.
 C9 C 0.2853(9) 0.3604(13) 0.4785(9) 0.034(2) Uani 1 d..
 H9A H 0.3377(9) 0.4322(13) 0.5235(9) 0.080 Uiso 1 d R.
 H9B H 0.2561(9) 0.4242(13) 0.4162(9) 0.080 Uiso 1 d R.
 C10 C 0.4504(8) 0.2575(11) 0.3948(7) 0.026(2) Uani 1 d..
 H10A H 0.4238(8) 0.3340(11) 0.3379(7) 0.080 Uiso 1 d R.
 C11 C 0.5496(9) 0.3426(15) 0.4647(9) 0.039(2) Uani 1 d..
 H11A H 0.5239(9) 0.4488(15) 0.4898(9) 0.080 Uiso 1 d R.
 H11B H 0.5757(9) 0.2725(15) 0.5250(9) 0.080 Uiso 1 d R.
 C12 C 0.6497(10) 0.3751(15) 0.4018(10) 0.046(3) Uani 1 d..
 H12A H 0.6236(10) 0.4502(15) 0.5441(10) 0.080 Uiso 1 d R.
 H12B H 0.7132(10) 0.4290(15) 0.4458(10) 0.080 Uiso 1 d R.
 C13 C 0.6895(8) 0.2104(15) 0.3553(9) 0.042(2) Uani 1 d..
 H13A H 0.7526(8) 0.2333(15) 0.3163(9) 0.080 Uiso 1 d R.
 H13B H 0.7164(8) 0.1340(15) 0.4122(9) 0.080 Uiso 1 d R.
 C14 C 0.5896(9) 0.1308(15) 0.2821(8) 0.039(2) Uani 1 d..
 H14A H 0.5637(9) 0.2069(15) 0.2248(8) 0.080 Uiso 1 d R.
 H14B H 0.6136(9) 0.0270(15) 0.2526(8) 0.080 Uiso 1 d R.
 C15 C 0.4916(8) 0.0976(13) 0.3482(8) 0.033(2) Uani 1 d..
 H15A H 0.5182(8) 0.0190(13) 0.4059(8) 0.080 Uiso 1 d R.

loop_

_atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12

Cu1 0.0219(5) 0.0222(5) 0.0317(5) -0.0059(5) 0.0086(3) -0.0046(5)
 Cl1 0.0435(13) 0.0304(12) 0.0438(13) 0.0024(10) 0.0215(11) 0.0051(11)

C12 0.061(2) 0.0312(12) 0.0289(11) 0.0009(9) -0.0018(10) 0.0153(12)
 O1 0.030(3) 0.032(3) 0.032(3) -0.008(3) 0.013(3) -0.007(3)
 O2 0.036(5) 0.055(5) 0.050(5) -0.027(4) 0.017(4) -0.025(4)
 O3 0.043(5) 0.043(5) 0.068(5) 0.020(4) -0.008(4) -0.007(4)
 O4 0.070(7) 0.069(7) 0.100(9) -0.024(6) 0.001(6) 0.001(6)
 O5 0.062(6) 0.035(4) 0.087(6) 0.004(4) 0.040(5) 0.002(4)
 O6 0.075(6) 0.054(5) 0.075(6) -0.022(5) 0.032(5) 0.007(5)
 O7 0.117(9) 0.062(6) 0.099(8) 0.048(6) 0.065(7) 0.031(6)
 O8 0.056(9) 0.039(7) 0.047(8) 0.025(6) 0.009(6) 0.004(7)
 O8' 0.056(10) 0.039(8) 0.075(10) 0.012(7) -0.020(8) -0.001(7)
 O9 0.095(7) 0.050(5) 0.044(5) -0.005(4) 0.003(5) 0.018(5)
 O11 0.103(12) 0.091(12) 0.070(10) 0.028(8) 0.035(8) 0.047(9)
 O11' 0.092(13) 0.111(14) 0.129(14) 0.039(10) 0.044(10) 0.016(10)
 O10 0.066(10) 0.030(9) 0.084(10) 0.011(7) -0.032(8) -0.006(8)
 O10' 0.125(14) 0.062(11) 0.100(12) -0.004(9) -0.030(10) 0.022(10)
 N1 0.022(4) 0.021(4) 0.031(4) -0.006(3) 0.009(3) -0.004(3)
 N2 0.027(4) 0.020(3) 0.029(4) -0.001(3) 0.002(3) -0.006(3)
 C1 0.020(4) 0.024(4) 0.032(4) 0.001(4) 0.002(3) -0.007(3)
 C2 0.027(5) 0.028(5) 0.038(5) -0.006(4) 0.003(4) -0.005(4)
 C3 0.034(5) 0.028(5) 0.050(6) -0.010(4) 0.014(4) -0.016(4)
 C4 0.035(5) 0.039(5) 0.052(6) -0.009(5) 0.019(5) -0.014(5)
 C5 0.027(5) 0.033(5) 0.038(5) -0.003(4) 0.011(4) -0.003(4)
 C6 0.019(4) 0.025(4) 0.027(4) -0.003(3) 0.004(3) -0.002(3)
 C7 0.025(5) 0.028(5) 0.072(7) -0.014(5) 0.020(5) -0.001(4)
 C8 0.038(6) 0.034(5) 0.053(6) -0.015(5) 0.017(5) -0.006(4)
 C9 0.029(5) 0.027(4) 0.047(5) -0.008(4) 0.008(4) -0.002(4)
 C10 0.023(4) 0.026(4) 0.030(4) 0.005(4) 0.004(4) -0.005(4)
 C11 0.025(5) 0.045(6) 0.049(6) -0.016(5) 0.008(4) -0.010(4)
 C12 0.037(6) 0.041(6) 0.062(7) -0.012(5) 0.012(5) -0.015(5)
 C13 0.026(5) 0.047(6) 0.055(5) -0.008(5) 0.008(5) 0.000(5)
 C14 0.029(5) 0.051(6) 0.040(5) -0.006(5) 0.017(4) -0.008(5)
 C15 0.022(4) 0.037(5) 0.043(5) -0.008(4) 0.008(4) -0.009(4)

geom_special_details

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
 Cu1 N1 1.977(9) . ?
 Cu1 O2 1.992(9) . ?
 Cu1 O1 1.996(6) . ?
 Cu1 N2 1.998(7) . ?
 Cu1 O3 2.263(9) . ?

C11 O4 1.392(11) . ?
 C11 O7 1.395(10) . ?
 C11 O6 1.406(9) . ?
 C11 O5 1.449(9) . ?
 C12 O8 1.390(5) . ?
 C12 O10' 1.395(5) . ?
 C12 O11 1.400(5) . ?
 C12 O9 1.404(4) . ?
 C12 O8' 1.405(5) . ?
 C12 O11' 1.444(5) . ?
 C12 O10 1.460(5) . ?
 O1 C1 1.460(1) . ?
 O2 C15 1.474(12) . ?
 O8 O8' 0.67(2) . ?
 O11 O11' 0.95(2) . ?
 O11 O10' 1.62(2) . ?
 O10 O10' 0.91(2) . ?
 N1 C7 1.492(12) . ?
 N1 C6 1.501(12) . ?
 N2 C9 1.459(12) . ?
 N2 C10 1.499(12) . ?
 C1 C6 1.492(13) . ?
 C1 C2 1.507(12) . ?
 C2 C3 1.535(13) . ?
 C3 C4 1.497(15) . ?
 C4 C5 1.538(14) . ?
 C5 C6 1.522(12) . ?
 C7 C8 1.502(15) . ?
 C8 C9 1.547(14) . ?
 C10 C15 1.503(14) . ?
 C10 C11 1.511(13) . ?
 C11 C12 1.53(2) . ?
 C12 C13 1.53(2) . ?
 C13 C14 1.519(14) . ?
 C14 C15 1.531(13) . ?

loop_

_geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
 N1 Cu1 O2 172.8(4) . . ?
 N1 Cu1 O1 84.5(3) . . ?
 O2 Cu1 O1 94.9(3) . . ?
 N1 Cu1 N2 94.5(3) . . ?
 O2 Cu1 N2 85.0(3) . . ?
 O1 Cu1 N2 170.9(3) . . ?
 N1 Cu1 O3 97.2(4) . . ?
 O2 Cu1 O3 90.0(4) . . ?
 O1 Cu1 O3 91.8(3) . . ?
 N2 Cu1 O3 97.3(3) . . ?

O4 Cl1 O7 105.6(8) . . ?
O4 Cl1 O6 110.8(7) . . ?
O7 Cl1 O6 111.8(7) . . ?
O4 Cl1 O5 110.4(7) . . ?
O7 Cl1 O5 107.5(6) . . ?
O6 Cl1 O5 110.6(6) . . ?
O8 Cl2 O10' 129.1(7) . . ?
O8 Cl2 O11 112.3(5) . . ?
O10' Cl2 O11 70.7(9) . . ?
O8 Cl2 O9 113.0(4) . . ?
O10' Cl2 O9 111.8(5) . . ?
O11 Cl2 O9 111.6(4) . . ?
O8 Cl2 O8' 27.7(7) . . ?
O10' Cl2 O8' 111.6(5) . . ?
O11 Cl2 O8' 132.0(7) . . ?
O9 Cl2 O8' 111.2(4) . . ?
O8 Cl2 O11' 80.5(8) . . ?
O10' Cl2 O11' 108.4(5) . . ?
O11 Cl2 O11' 39.2(9) . . ?
O9 Cl2 O11' 106.5(5) . . ?
O8' Cl2 O11' 107.1(5) . . ?
O8 Cl2 O10 107.2(4) . . ?
O10' Cl2 O10 36.9(9) . . ?
O11 Cl2 O10 106.7(4) . . ?
O9 Cl2 O10 105.5(4) . . ?
O8' Cl2 O10 81.7(7) . . ?
O11' Cl2 O10 140.6(8) . . ?
C1 O1 Cu1 109.9(5) . . ?
C15 O2 Cu1 109.0(6) . . ?
O8' O8 Cl2 77.4(7) . . ?
O8 O8' Cl2 74.9(6) . . ?
O11' O11 Cl2 72.9(6) . . ?
O11' O11 O10' 125.1(8) . . ?
Cl2 O11 O10' 54.5(5) . . ?
O11 O11' Cl2 67.9(6) . . ?
O10' O10 Cl2 67.6(6) . . ?
O10 O10' Cl2 75.5(6) . . ?
O10 O10' O11 128.8(7) . . ?
Cl2 O10' O11 54.8(5) . . ?
C7 N1 C6 114.0(8) . . ?
C7 N1 Cu1 113.0(6) . . ?
C6 N1 Cu1 108.6(6) . . ?
C9 N2 C10 112.6(7) . . ?
C9 N2 Cu1 114.8(6) . . ?
C10 N2 Cu1 107.4(5) . . ?
O1 C1 C6 106.6(7) . . ?
O1 C1 C2 111.8(7) . . ?
C6 C1 C2 111.9(7) . . ?
C1 C2 C3 109.9(8) . . ?
C4 C3 C2 111.0(8) . . ?
C3 C4 C5 111.8(8) . . ?
C6 C5 C4 109.5(8) . . ?
C1 C6 N1 107.7(7) . . ?
C1 C6 C5 110.0(7) . . ?

N1 C6 C5 114.9(7) .. ?
N1 C7 C8 112.7(9) .. ?
C7 C8 C9 113.8(9) .. ?
N2 C9 C8 113.0(8) .. ?
N2 C10 C15 107.3(7) .. ?
N2 C10 C11 115.5(8) .. ?
C15 C10 C11 110.3(8) .. ?
C10 C11 C12 110.0(8) .. ?
C11 C12 C13 110.3(9) .. ?
C14 C13 C12 110.1(9) .. ?
C13 C14 C15 107.3(8) .. ?
O2 C15 C10 105.9(8) .. ?
O2 C15 C14 109.6(8) .. ?
C10 C15 C14 112.2(8) .. ?

_refine_diff_density_max 1.616
_refine_diff_density_min -0.655
_refine_diff_density_rms 0.105



Collection Number: A2084

SUZMAN, Helen, Papers, 1944-2009

PUBLISHER:

Publisher:- Historical Papers Research Archive

Location:- Johannesburg

©2014

LEGAL NOTICES:

Copyright Notice: All materials on the Historical Papers website are protected by South African copyright law and may not be reproduced, distributed, transmitted, displayed, or otherwise published in any format, without the prior written permission of the copyright owner.

Disclaimer and Terms of Use: Provided that you maintain all copyright and other notices contained therein, you may download material (one machine readable copy and one print copy per page) for your personal and/or educational non-commercial use only.

People using these records relating to the archives of Historical Papers, The Library, University of the Witwatersrand, Johannesburg, are reminded that such records sometimes contain material which is uncorroborated, inaccurate, distorted or untrue. While these digital records are true facsimiles of paper documents and the information contained herein is obtained from sources believed to be accurate and reliable, Historical Papers, University of the Witwatersrand has not independently verified their content. Consequently, the University is not responsible for any errors or omissions and excludes any and all liability for any errors in or omissions from the information on the website or any related information on third party websites accessible from this website.

This document forms part of the Helen Suzman Papers, a private collection deposited with the Historical Papers Research Archive at The University of the Witwatersrand, Johannesburg.