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Coordinating properties of more highly preorganised ligands

De Sousa, Alvaro Silva

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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 $C_{14}H_{28}N_2O_2$ = 268.39 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.

M.w C_{15} H_{30} N_2 O_2 = 270.41 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 N_4

The macrocycle 12 ane N_4 (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 $CaCL_2$ 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 C_{14} H_{30} N_4 O = 270.42 g mol^{-1}

Mass collected = 3.0 g

Yield = 83 %

ANALYSIS	EXPECTED	OBSERVED
% C	62.18	62.59
% H	11.18	11.91
% N	20.72	19.94

CU(II)(2-HYDROXYCYCLOHEXYL)-12-ANE N_4 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.

$C_{14}H_{36}N_4O_9Mw\ Cl_2Cu$ = 532.86 g mol^{-1}

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_2 O_{10} Cl_2 Ni = 568.08 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	4.87

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.

Mw $C_{16}H_{33}N_3O_{10}Cl_2Cu$ = 561.90 g mol^{-1}

Mass collected = 0.73 g

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.

Mw C_{15} H_{30} N_2 O_{10} Cl_2 Cu = 532.86 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:

i) *Complex formation* (association) $M + L \rightarrow ML$

ii) *Breakdown of Complex* (dissociation) $ML \rightarrow M + L$

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 Φ34 pH meter equipped with a Beckman Refillable Combination electrode (Model no. 39536 (saturated KCL) or Model no. 39539 (4M KCL saturated with AgCl)).

Titrations 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 HNO_3 in 0.05M $NaNO_3$ (5ml) and 0.10M $NaNO_3$ (15ml) was titrated with 0.05M NaOH in 0.05M $NaNO_3$, to determine the standard electrode potential and the electrode calibration slope that has a value approximating the Nernstian slope (2.3026×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) :

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

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 $2.3 < pH < 3$ and $10.8 < pH < 11.8$, where $pH = -\log[H^+]$. 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±0.1 °C in aqueous solution at ionic strength, I = 0.1M. 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 Phthalate (0.01M). The acid solutions were standardised against the already standardised base solution while ligand solutions were standardised from their pKa determination titrations.

METHOD OF DETERMINING THE STABILITY CONSTANTS

$$L^{+(n-1)}H_{(n-1)} + H^+ \rightleftharpoons H_nL^n \quad pK_n$$

The protonation constants of the ligands were calculated by titrating a solution of the ligand (5×10^{-3} M, 10 ml) in 0.1M $NaNO_3$ (10 ml) 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 (5×10^{-3} 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 were 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±0.001cm) 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 $NaClO_4$ 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 nms^{-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 a accurate data set. Crystal quality was verified by, the oscillation, zero and first layer Weisenberg photographs taken using Cu-K_α radiation and a Huber Weisenberg 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-Kα 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).

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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).**

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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-THEEN

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	-319	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	-375
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	6	8	0	75	62	11	1	1	54	-55	4	3	1	207	-168
14	0	0	248	-261	6	4	0	154	160	7	8	0	54	-59	12	1	1	128	-135	5	3	1	95	94
1	1	0	1591	-1669	7	4	0	349	331	8	8	0	79	-70	13	1	1	76	-62	6	3	1	238	243
2	1	0	1239	1267	8	4	0	228	-219	1	9	0	84	87	14	1	1	199	-203	7	3	1	704	680
3	1	0	652	-657	9	4	0	66	69	2	9	0	193	-194	15	1	1	121	112	8	3	1	95	108
4	1	0	37	31	10	4	0	39	-52	3	9	0	78	-84	-14	2	1	77	76	9	3	1	189	180
5	1	0	384	370	11	4	0	302	-295	5	9	0	95	-96	-13	2	1	153	152	10	3	1	73	76
6	1	0	413	-388	14	4	0	65	64	6	9	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	3	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	508	-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	282	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	146	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	569	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	321	-343	12	2	1	184	178	12	4	1	89	86
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	169	-13	5	2	126	-136
2	5	1	109	117	10	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	-9	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
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7	2	14	211	209	2	6	14	141	-141	7	2	15	51	52	-10	0	16	81	75	-4	4	16	72	71
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10	2	14	98	94	6	6	14	127	119	-9	3	15	187	184	-6	0	16	163	153	0	4	16	44	-27
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-4	4	14	213	211
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-1	4	14	323	318
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3	4	14	122	-136
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6	4	14	63	63
7	4	14	181	174
8	4	14	52	-46
9	4	14	105	98
-7	5	14	84	83
-6	5	14	172	173
-5	5	14	122	-131
-4	5	14	118	127
-3	5	14	226	-220
-2	5	14	174	-177
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6	1	17	147	-140
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-7	2	17	124	-127
-6	2	17	230	228
-5	2	17	38	29
-3	2	17	114	118
-2	2	17	135	-146
-1	2	17	57	57
0	2	17	228	-232
1	2	17	170	-183
2	2	17	42	23
4	2	17	55	43
5	2	17	78	72
6	2	17	77	-70
-8	3	17	50	57
-7	3	17	70	-84
-5	3	17	236	-234
-3	3	17	117	124
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1	3	17	105	100
3	3	17	114	-109
7	3	17	149	129
-6	4	17	117	116
-4	4	17	76	75
5	0	15	201	193
7	0	15	42	33
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-3	1	15	52	42
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3	1	15	139	-132
6	1	15	174	-176
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10	1	15	75	77
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-9	2	15	89	-90
-8	2	15	92	-82
-7	2	15	128	-134
-6	2	15	146	140
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-2	4	17	168	-179
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3	5	17	81	-76
-2	6	17	72	-76
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-2	0	18	108	-99
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2	0	18	162	170
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-7	1	18	201	-195
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-4	4	15	96	84
-3	4	15	62	-62
-2	4	15	218	-215
-1	4	15	150	153
0	4	15	163	-155
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7	5	15	100	102
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-6	2	18	69	84
-5	2	18	133	-125
-4	2	18	108	-104
-3	2	18	93	99
-2	2	18	64	-67
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0	2	18	74	68
1	2	18	65	62
2	2	18	87	79
3	2	18	119	-108
6	2	18	55	-71
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-4	3	18	79	76
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0	3	18	143	-150
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4	3	18	152	139
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-5	4	18	65	-59
-1	4	18	204	199
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3	4	18	140	-136
-3	5	18	51	-42
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8	1	16	114	-109
-9	2	16	112	105
-8	2	16	181	185
-7	2	16	175	-170
-6	2	16	101	105
-5	2	16	225	-222
-4	2	16	92	-91
-3	2	16	86	-110
-2	2	16	79	-82
-1	2	16	172	183
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3	2	16	208	-221
4	2	16	102	-86
6	2	16	103	-95
7	2	16	127	122
8	2	16	42	-31
-7	3	16	40	-44
-6	3	16	332	336
-4	3	16	112	128
-2	3	16	96	-100
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-7	0	19	189	-178
-3	0	19	142	145
1	0	19	129	-124
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-4	2	19	73	79
-3	2	19	128	133
-2	2	19	48	-48
0	2	19	113	-116
2	2	19	66	70
3	2	19	38	-33
4	2	19	91	86
5	2	19	94	92
-5	3	19	163	-179
3	5	16	35	-43
4	5	16	103	95
5	5	16	90	-86
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1	0	17	127	-127
3	0	17	159	-165
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7	0	17	98	100
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-5	1	17	99	-89
-4	1	17	205	-212
-2	1	17	167	-164
-1	1	17	156	165
0	1	17	150	158
2	1	17	127	120
-4	3	19	48	-53
-1	3	19	135	162
2	3	19	68	63
3	3	19	108	-107
-3	4	19	72	-63
-2	4	19	81	-84
0	4	19	92	-92
1	4	19	47	54
-4	0	20	73	-79
-2	0	20	208	-203
0	0	20	89	101
2	0	20	66	52
-5	1	20	70	63
-3	1	20	165	161
-2	1	20	90	-88
-1	1	20	74	81
1	1	20	93	-100
-4	2	20	113	-108
-2	2	20	91	-93
-1	2	20	175	180
1	2	20	92	82
2	2	20	79	80
-2	3	20	113	-112
-1	3	20	63	-54
0	3	20	174	-169

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	18	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	344	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	240	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	92	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	404	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	4-15	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	8	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	183	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	284	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	1	7-15	477	474	9						
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1	3-22	310	333	12	6	6-20	42	91	42	0	6-18	41	95	40	3	3-16	408	409	8	5	7-15	269	249	12						
3	3-22	266	269	14	1	1-19	432	436	8	2	6-18	348	360	11	5	3-16	269	279	10	7	7-15	374	365	10						
5	3-22	128	142	29	3	1-19	249	255	12	4	6-18	372	393	11	7	3-16	362	373	9	9	7-15	289	291	13						
7	3-22	211	210	17	5	1-19	288	281	10	6	6-18	165	139	21	9	3-16	547	548	8	11	7-15	279	235	14						
9	3-22	337	344	12	7	1-19	439	457	8	8	6-18	93	70	47	11	3-16	595	587	8	0	8-15	42	40	41						
11	3-22	333	331	13	9	1-19	517	539	9	10	6-18	88	94	61	13	3-16	298	287	11	2	8-15	82	93	82						
0	4-22	42	46	41	11	1-19	189	200	17	1	7-18	151	180	26	15	3-16	169	152	20	4	8-15	41	70	41						
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5	1	-2	1254	1266	6	4	2	-1	1363	1345	6	8	2	0	496	525	6	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	3	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	528	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	708	7
12	2	-2	401	389	7	13	3	-1	102	110	26	17	3	0	340	337	11	3	5	1	615	607	6	9	5	2	715	740	8
14	2	-2	462	442	8	15	3	-1	277	301	11	0	4	0	1601	1604	8	5	5	1	338	385	6	11	5	2	422	422	8
16	2	-2	250	253	12	17	3	-1	234	224	14	2	4	0	350	365	5	7	5	1	356	363	7	13	5	2	176	167	17
18	2	-2	176	181	20	0	4	-1	1891	1834	7	4	4	0	529	522	5	9	5	1	33	70	33	15	5	2	303	270	12
1	3	-2	589	612	5	2	4	-1	1798	1810	7	6	4	0	163	154	10	11	5	1	35	49	35	0	6	2	437	444	7
3	3	-2	658	661	6	4	4	-1	528	452	-6	8	4	0	201	218	10	13	5	1	177	180	17	2	6	2	538	557	7
5	3	-2	1038	1047	8	6	4	-1	141	146	11	10	4	0	239	238	9	15	5	1	40	42	39	4	6	2	469	475	7
7	3	-2	890	873	7	8	4	-1	736	752	7	12	4	0	266	272	10	17	5	1	43	123	42	6	6	2	164	178	14
9	3	-2	431	430	6	10	4	-1	781	788	8	14	4	0	67	49	66	0	6	1	275	279	8	8	6	2	374	380	8
11	3	-2	629	616	7	12	4	-1	709	710	8	16	4	0	197	205	17	2	6	1	378	386	7	10	6	2	451	435	8
13	3	-2	749	738	7	14	4	-1	551	560	8	18	4	0	42	45	42	4	6	1	585	576	7	12	6	2	119	127	27
15	3	-2	417	422	9	16	4	-1	379	368	10	1	5	0	578	572	6	6	6	1	461	432	7	14	6	2	83	86	64
17	3	-2	318	318	12	18	4	-1	330	323	13	3	5	0	713	719	7	8	6	1	646	637	7	1	7	2	270	273	9
19	3	-2	241	228	16	1	5	-1	124	124	13	5	5	0	503	499	6	10	6	1	783	783	8	3	7	2	189	194	13
0	4	-2	88	89	14	3	5	-1	238	287	-9	7	5	0	413	414	7	12	6	1	317	300	10	5	7	2	253	240	10
2	4	-2	606	594	6	5	5	-1	336	331	7	9	5	0	693	692	7	14	6	1	155	149	22	7	7	2	466	479	8
4	4	-2	293	289	6	7	5	-1	287	276	8	11	5	0	468	476	8	1	7	1	434	439	8	9	7	2	378	380	9
6	4	-2	402	391	6	9	5	-1	32	45	32	13	5	0	350	361	10	3	7	1	564	569	7	11	7	2	103	126	36
8	4	-2	127	136	15	11	5	-1	152	174	17	15	5	0	453	458	10	5	7	1	618	638	7	13	7	2	137	108	27
10	4	-2	270	250	8	13	5	-1	372	352	9	17	5	0	211	213	18	7	7	1	618	619	8	0	8	2	592	606	6
12	4	-2	317	305	8	15	5	-1	90	90	46	0	6	0	463	466	6	9	7	1	619	615	8	2	8	2	528	529	8
14	4	-2	36	33	36	17	5	-1	119	32	33	2	6	0	363	351	7	11	7	1	287	263	11	4	8	2	337	324	10
16	4	-2	161	164	20	0	6	-1	253	262	8	4	6	0	288	283	8	13	7	1	196	148	17	6	8	2	312	307	10
18	4	-2	42	31	42	2	6	-1	631	623	7	6	6	0	192	209	12	0	8	1	138	153	21	8	8	2	441	457	10
1	5	-2	850	835	7	4	6	-1	987	977	8	8	6	0	261	285	10	2	8	1	36	67	36	10	8	2	451	457	10
3	5	-2	1696	1718	9	6	6	-1	477	447	7	10	6	0	490	511	8	4	8	1	205	197	14	12	8	2	322	317	13
5	5	-2	897	910	7	8	6	-1	271	275	10	12	6	0	314	306	10	6	8	1	93	90	37	1	9	2	81	71	59
7	5	-2	171	146	11	10	6	-1	499	512	8	14	6	0	40	26	40	8	8	1	258	253	13	3	9	2	132	139	26
9	5	-2	184	180	12	12	6	-1	324	322	10	16	6	0	103	113	43	10	8	1	107	146	38	5	9	2	128	159	28
11	5	-2	506	498	7	14	6	-1	367	373	11	1	7	0	364	355	8	12	8	1	131	93	29	7	9	2	153	172	23
13	5	-2	376	388	10	16	6	-1	296	305	14	3	7	0	275	271	9	1	9	1	430	434	9	9	9	2	119	110	35
15	5	-2	414	413	10	1	7	-1	414	421	7	5	7	0	35	101	34	3	9	1	421	398	9	0	10	2	325	328	12

Table 2. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fo	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	251	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	98	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	290	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	9	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	61	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	28	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	36	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	16	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	81	120	61	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	157	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	9	13	7	4	216	233	17	4	0	6	2052	2044	7	6	2	7	665	644	7	13	3	8	280	282	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
7	7	3	580	581	8	2	8	4	413	427	9	8	0	6	165	164	10	10	2	7	205	210	11	0	4	8	444	460	6
9	7	3	357	363	10	4	8	4	196	191	15	10	0	6	674	651	7	12	2	7	191	210	14	2	4	8	627	634	6
11	7	3	235	252	15	6	8	4	302	307	11	12	0	6	953	944	9	14	2	7	121	177	16	4	4	8	217	199	9
13	7	3	219	232	17	8	8	4	436	443	9	14	0	6	358	346	9	16	2	7	336	339	12	6	4	8	76	62	33
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2	8	3	329	344	10	1	9	4	39	62	39	18	0	6	321	330	13	3	3	7	1107	1082	8	10	4	8	313	295	10
4	8	3	58	79	58	3	9	4	40	68	40	1	1	6	1816	1831	6	5	3	7	431	421	6	12	4	8	163	171	19
6	8	3	424	432	9	5	9	4	63	65	62	3	1	6	372	380	5	7	3	7	399	395	7	14	4	8	164	181	22
8	8	3	39	97	39	7	9	4	101	21	42	5	1	6	362	364	6	9	3	7	261	278	10	1	5	8	1116	1123	9
10	8	3	212	210	17	9	9	4	43	79	42	7	1	6	765	758	6	11	3	7	35	38	35	3	5	8	376	409	7
12	8	3	42	78	42	0	10	4	394	410	11	9	1	6	238	235	9	13	3	7	355	348	10	5	5	8	116	97	21
1	9	3	425	424	9	2	10	4	253	265	16	11	1	6	153	124	14	15	3	7	358	387	11	7	5	8	772	753	7
3	9	3	340	306	10	4	10	4	327	326	12	13	1	6	36	24	35	0	4	7	777	779	7	9	5	8	650	634	8
5	9	3	270	273	13	1	1	5	1379	1382	6	15	1	6	262	258	12	2	4	7	1049	1071	8	11	5	8	241	266	13
7	9	3	367	363	11	3	1	5	1109	1075	7	17	1	6	210	211	17	4	4	7	1053	995	8	13	5	8	288	280	12
9	9	3	283	252	13	5	1	5	688	670	6	0	2	6	1564	1570	7	6	4	7	494	488	7	0	6	8	292	300	9
0	10	3	171	179	22	7	1	5	911	922	7	2	2	6	1114	1150	7	8	4	7	546	581	7	2	6	8	442	445	8
2	10	3	304	287	14	9	1	5	615	594	6	4	2	6	615	628	6	10	4	7	737	749	8	4	6	8	434	447	8
4	10	3	141	152	29	11	1	5	326	336	8	6	2	6	412	422	6	12	4	7	514	514	8	6	6	8	315	320	10
0	0	4	808	807	5	13	1	5	430	443	8	8	2	6	361	376	7	14	4	7	348	330	10	8	6	8	245	241	12
2	0	4	2016	2158	5	15	1	5	427	439	9	10	2	6	334	320	8	16	4	7	243	253	16	10	6	8	199	167	16
4	0	4	2304	2362	6	17	1	5	280	299	14	12	2	6	369	355	8	1	5	7	280	290	8	12	6	8	124	154	32
6	0	4	1734	1738	7	0	2	5	97	78	11	14	2	6	411	404	9	3	5	7	107	97	19	1	7	8	371	373	9
8	0	4	666	637	6	2	2	5	1076	1081	7	16	2	6	323	335	11	5	5	7	196	198	11	3	7	8	237	236	12
10	0	4	427	438	6	4	2	5	1318	1262	8	1	3	6	537	624	-5	7	5	7	222	238	12	5	7	8	106	132	30
12	0	4	869	882	8	6	2	5	967	964	7	3	3	6	608	599	6	9	5	7	103	139	30	7	7	8	253	239	13
14	0	4	872	910	9	8	2	5	119	135	15	5	3	6	900	871	7	11	5	7	117	120	27	9	7	8	214	209	16
16	0	4	367	384	10	10	2	5	99	78	23	7	3	6	904	924	8	13	5	7	40	69	39	11	7	8	42	117	42
18	0	4	188	167	19	12	2	5	302	304	9	9	3	6	530	535	7	15	5	7	109	48	39	0	8	8	413	413	9
1	1	4	52	67	19	14	2	5	286	301	11	11	3	6	365	352	8	0	6	7	727	753	7	2	8	8	635	627	8
3	1	4	386	347	4	16	2	5	222	226	15	13	3	6	389	374	9	2	6	7	875	883	8	4	8	8	425	430	10
5	1	4	1014	1024	7	18	2	5	270	281	15	15	3	6	265	275	13	4	6	7	361	371	8	6	8	8	331	314	11

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	775	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	3	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	308	295	13	1	9	11	159	146	23	12	4	13	290	290	14	5	3	15	101	90	30
11	1	9	828	798	8	0	4	10	277	278	8	3	9	11	294	290	14	1	5	13	501	526	8	7	3	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	3	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	51	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	359	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	13	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	13	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	13	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	98	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	249	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	394	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	8	2	11	76	57	42	4	6	12	260	250	11	13	3	14	353	349	12	7	3	16	297	296	11
0	8	9	38	60	38	10	2	11	442	432	8	6	6	12	255	234	12	0	4	14	108	79	23	9	3	16	487	509	10
2	8	9	40	121	40	12	2	11	360	349	10	8	6	12	96	45	42	2	4	14	163	145	16	11	3	16	403	385	11
4	8	9	107	116	34	14	2	11	200	186	17	10	6	12	133	140	29	4	4	14	36	26	35	0	4	16	387	392	9
6	8	9	103	6	40	1	3	11	676	649	7	1	7	12	184	211	17	6	4	14	37	39	37	2	4	16	126	104	23
8	8	9	42	27	41	3	3	11	339	336	7	3	7	12	408	414	10	8	4	14	39	28	38	4	4	16	252	253	12
1	9	9	312	330	12	5	3	11	68	77	43	5	7	12	269	284	14	10	4	14	59	55	58	6	4	16	146	148	22
3	9	9	222	231	17	7	3	11	373	332	8	7	7	12	112	3	35	12	4	14	43	35	42	8	4	16	40	41	40
5	9	9	238	206	16	9	3	11	287	302	10	9	7	12	177	116	21	1	5	14	623	646	8	10	4	16	42	63	42
0	0	10	1015	1022	7	11	3	11	141	138	22	0	8	12	166	193	21	3	5	14	313	311	10	1	5	16	517	522	8
2	0	10	299	268	6	13	3	11	245	251	15	2	8	12	215	221	16	5	5	14	342	353	10	3	5	16	383	390	10
4	0	10	739	774	7	15	3	11	152	150	27	4	8	12	351	363	12	7	5	14	365	373	10	5	5	16	214	211	15
6	0	10	1496	1474	10	0	4	11	467	478	7	6	8	12	532	521	10	9	5	14	316	332	12	7	5	16	239	251	15
8	0	10	937	887	8	2	4	11	282	299	8	1	9	12	128	150	32	11	5	14	327	299	12	9	5	16	308	315	14
10	0	10	744	746	9	4	4	11	573	591	7	1	1	13	1253	1288	10	0	6	14	229	236	13	0	6	16	204	223	15
12	0	10	518	497	8	6	4	11	865	891	9	3	1	13	638	628	7	2	6	14	416	425	9	2	6	16	121	100	29
14	0	10	232	253	15	8	4	11	790	758	8	5	1	13	502	509	7	4	6	14	295	302	12	4	6	16	119	120	32
16	0	10	417	418	11	10	4	11	275	271	12	7	1	13	411	410	8	6	6	14	179	149	19	6	6	16	314	316	12
1	1	10	592	595	6	12	4	11	274	262	12	9	1	13	245	239	12	8	6	14	70	139	69	1	7	16	157	154	24
3	1	10	660	650	6	14	4	11	366	367	12	11	1	13	315	315	11	1	7	14	351	347	11	3	7	16	42	29	42
5	1	10	342	339	7	1	5	11	284	306	9	13	1	13	309	315	13	3	7	14	252	266	14	5	7	16	129	135	33
7	1	10	185	199	12	3	5	11	746	701	7	0	2	13	285	304	8	5	7	14	110	113	37	0	8	16	347	360	13
9	1	10	277	280	9	5	5	11	142	138	19	2	2	13	803	784	7	7	7	14	43	46	42	1	1	17	465	465	8
11	1	10	625	633	8	7	5	11	213	220	14	4	2	13	796	792	7	0	8	14	201	216	19	3	1	17	656	666	7
13	1	10	156	147	20	9	5	11	200	191	16	6	2	13	166	165	15	2	8	14	310	317	13	5	1	17	319	302	10
15	1	10	114	113	34	11	5	11	83	111	62	8	2	13	194	193	14	4	8	14	396	415	12	7	1	17	367	359	10
0	2	10	88	90	18	13	5	11	186	195	21	10	2	13	157	165	19	1	1	15	290	304	9	9	1	17	438	444	10
2	2	10	939	882	8	0	6	11	216	229	12	12	2	13	348	335	11	3	1	15	500	507	7	11	1	17	238	223	16
4	2	10	898	891	8	2	6	11	641	629	8	14	2	13	233	230	17	5	1	15	626	622	7	0	2	17	152	177	17
6	2	10	292	292	8	4	6	11	534	533	8	1	3	13	509	503	7	7	1	15	462	449	8	2	2	17	76	101	52
8	2	10	415	431	7	6	6	11	453	458	9	3	3	13	388	403	8	9	1	15	472	469	9	4	2	17	150	140	19
10	2	10	277	286	10	8	6	11	170	194	20	5	3	13	182	182	14	11	1	15	418	414	10	6	2	17	360	358	9
12	2	10	243	238	13	10	6	11	246	244	15	7	3	13	183	187	15	13	1	15	188	210	21	8	2	17	488	498	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
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	3	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	420	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	108	36	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	379	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	439	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	3	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	477	10						

Structure Factors Table [Fo**2, Fc**2 and sigma(Fo**2)] (*=unobserved reflns.) for C(14) H(20) N(2) O(10) Cl(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)	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	-66.08	51.26
8	0	0	120.89	113.81	34.24	0	8	0	627.08	509.73	33.96	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	-47.63	43.53
2	1	0	78.73	132.08	15.26	2	8	0	1018.05	1005.66	35.99	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	38.30	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	30.40	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	331.94	370.33	27.43	1	17	0	431.07	1191.87	93.06*
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	54.40	3	17	0	69.75	49.50	56.91
2	2	0	2041.67	1962.33	70.13	4	9	0	201.04	178.32	27.58	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	19.83	4	18	0	59.18	86.26	31.86
1	3	0	2197.71	2052.18	67.95	3	10	0	41.34	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	23.72	-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	155.28	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	33.37
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	1768.21	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	45.65	58.45	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	2.69	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	0.22	23.46	49.63
7	5	0	0.67	-74.11	54.72	3	13	0	85.31	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	6.84	-21.78	49.24	-3	0	1	973.07	2124.03	79.18
1	6	0	8.96	25.49	14.26	5	13	0	58.41	66.20	30.02	-1	0	1	489.34	8052.84	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	25.41	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	[illegible]	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	[illegible]	282.07	35.90
7	6	0	0.56	29.16	52.85	4	14	0	357.70	381.32	33.90	-7	1	1	[illegible]	8.92	52.53
1	7	0	102.02	112.08	16.02	5	14	0	0.02	8.14	51.38	-6	1	1	288.81	218.51	30.51
2	7	0	6343.19	7090.04	225.03	6	14	0	26.03	51.05	56.25	-5	1	1	20.33	17.67	49.29
3	7	0	627.29	587.44	43.71	1	15	0	49.09	445.20	41.11*	-4	1	1	21.43	34.82	19.63
4	7	0	7.60	-33.72	41.40	2	15	0	141.28	320.71	31.36*	-3	1	1	185.17	289.36	17.78

Structure Factors Table (continued) (*=unobserved reflns.) for C(14) H(28) N(2) O(10) Cl(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)	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	8	1	363.11	626.68	80.86*
-1	1	1	4331.27	4588.34	142.30	6	4	1	77.15	88.37	29.35	-1	8	1	17.80	-38.13	27.42
0	1	1	314.24	137.38	11.05	7	4	1	64.14	-30.65	58.08	0	8	1	558.23	523.44	52.51
1	1	1	13642.73	14760.18	148.42	-8	5	1	19.20	19.04	59.56	1	8	1	401.11	394.47	33.18
2	1	1	4024.01	4233.57	137.70	-7	5	1	1.05	-37.12	52.99	2	8	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	8	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	8	1	6.20	28.97	43.59
5	1	1	181.55	823.72	28.89	-4	5	1	208.23	211.57	23.85	5	8	1	5.20	-53.24	50.02
6	1	1	826.58	837.57	67.15	-3	5	1	1275.57	1319.94	58.43	6	8	1	63.84	63.39	31.94
7	1	1	1.90	-40.73	56.09	-2	5	1	175.70	160.30	17.27	7	8	1	0.80	-24.28	55.92
-8	2	1	231.88	191.56	36.32	-1	5	1	1311.00	1244.26	49.93	-7	9	1	55.39	23.46	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	33.91
-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	511.34	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	62.04	-4.92	37.44
-3	2	1	835.15	850.52	44.87	4	5	1	499.68	430.81	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	992.06	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	-160.48	60.66	2	9	1	1726.80	1833.21	75.09
2	2	1	551.52	542.03	35.13	-7	6	1	59.41	41.07	51.80	3	9	1	1268.09	1198.62	65.78
3	2	1	296.17	300.19	25.36	-6	6	1	351.61	295.16	32.87	4	9	1	30.42	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	216.07	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	40.80	-3	6	1	784.29	871.69	48.56	7	9	1	125.55	153.26	38.46
7	2	1	1.21	-104.83	56.77	-2	6	1	1099.08	1121.26	50.35	-7	10	1	0.10	22.58	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	32.37
-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	22.61
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	55.77
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	87.28	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	535.29	45.80	-2	11	1	125.01	141.58	22.10
-4	4	1	99.33	121.36	21.92	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	294.84	31.60	0	11	1	2999.33	2649.03	119.07
-2	4	1	2194.47	2117.65	76.80	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	53.18	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	74.61	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

Structure Factors Table (continued) (*=unobserved reflns.) for C(14) H(28) N(2) O(10) Cl(2) Page 5

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	70.67	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	971.20	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	46.72	141.06	32.35
-2	12	1	160.07	118.44	23.54	2	16	1	0.78	-13.34	46.70	-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	98.54	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	-44.58	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	41.15	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	-139.71	158.51	-8	0	2	10.04	-46.07	55.60
-8	13	1	25.93	-28.96	50.77	1	17	1	5.55	-241.58	59.16*	-6	0	2	63.43	29.11	33.91
-4	13	1	496.42	523.77	42.86	2	17	1	1.52	31.02	27.68	-4	0	2	28.31	72.36	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	361.69
-2	13	1	446.06	403.86	35.01	4	17	1	3.41	28.32	30.43	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	36.43	83.82	33.25	4	0	2	1275.66	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	33.77
4	13	1	493.45	488.48	43.11	-1	18	1	82.99	75.92	29.05	-6	1	2	13.49	0.00	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	716.15	54.80
6	13	1	69.85	91.35	33.46	1	18	1	376.23	96.22	35.29*	-4	1	2	339.40	328.07	29.05
-6	14	1	2.40	18.61	55.54	2	18	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	-6.80	50.73	4	18	1	21.59	28.61	53.04	-1	1	2	1123.28	1296.81	49.99
-3	14	1	131.82	174.8	28.48	5	18	1	6.74	50.61	57.18	0	1	2	3695.48	3826.39	87.03
-2	14	1	6.88	13.[illegible]	43.35	-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	27.09
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	38.96	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	53.38
6	14	1	0.60	29.90	33.44	3	19	1	71.24	63.02	30.78	-7	2	2	603.66	602.82	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	-69.95	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	25.45	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	35.46
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	39.98	31.62	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	58.67	59.74	28.26	1	6	2	18.31	17.70	25.19	-2	10	2	32.20	31.77	20.29
-5	3	2	109.42	143.38	26.18	2	6	2	31.03	10.41	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	2348.14	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	365.61	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	118.67	181.90	32.25	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	10	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	39.34	28.28	58.59
3	3	2	15.80	-25.34	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	-6	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	0.02	-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	64.43	-1	7	2	370.43	348.57	32.48	-2	11	2	92.57	118.91	21.94
-7	4	2	225.81	212.72	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	42.47	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	2096.96	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	-2	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	427.38	429.46	32.45	5	8	2	358.34	312.76	33.82	4	12	2	604.89	598.71	59.13
-3	5	2	448.22	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	204.65	190.61	31.56	-7	13	2	30.82	45.56	59.64
0	5	2	1521.82	1487.83	52.39	-5	9	2	1208.78	1416.79	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	20.14	-1	9	2	1258.60	1184.14	55.69	-2	13	2	44.11	27.04	24.47
5	5	2	13.96	15.08	48.30	0	9	2	127.52	69.53	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	85.04
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	921.37	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	40.33	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	30.97
-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	-47.31	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	45.29	29.78
-1	6	2	317.75	272.61	22.90	-4	10	2	64.50	91.62	26.16	-4	14	2	116.45	72.59	29.17
0	6	2	45.57	5.19	10.92	-3	10	2	142.78	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	26.27	-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	46.68	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	10.25	27.97
-6	15	2	5.12	-0.30	34.76	-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	1999.93	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	123.69	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	0.69	-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	59.46	-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	12.47	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	649.80	693.37	28.29
-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	210.84	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	-29.99	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	103.08	105.30	27.04
-3	17	2	0.44	32.22	29.57	-5	0	3	421.35	489.09	36.85	-4	4	3	265.49	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	1397.99	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	23.30
3	17	2	17.65	5.71	52.14	-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
-6	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	388.03	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	258.93	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	638.19	652.28	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	23.97	-2	5	3	521.46	451.73	37.87
-5	19	2	1.49	23.03	32.28	4	1	3	1100.19	1038.85	68.19	-1	5	3	130.01	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	42.35	14.01
-3	19	2	73.18	37.15	54.97	6	1	3	332.91	301.93	35.38	1	5	3	347.53	293.65	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	29.91	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	2.9[illegible]	-11.27	53.96
6	5	3	133.74	30.00	58.49	4	9	3	36.33	-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	85.59	47.37	29.25	-1	14	3	338.89	325.10	30.86
-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	34.47	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	58.82
4	6	3	41.40	-8.59	49.96	3	10	3	8.58	15.16	32.18	-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	1795.63	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	31.03	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	148.13	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	160.98	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	11	3	4.22	45.08	20.14	-5	16	3	11.58	23.87	54.14
2	7	3	52.62	88.77	20.83	1	11	3	459.26	453.59	33.51	-4	16	3	83.38	97.33	30.27
3	7	3	349.02	392.31	25.87	2	11	3	11.52	41.26	42.84	-3	16	3	4.59	3.27	48.55
4	7	3	489.84	436.18	40.35	3	11	3	35.32	16.77	47.75	-2	16	3	139.41	171.54	30.15
5	7	3	0.16	28.81	35.04	4	11	3	7.34	40.14	28.88	-1	16	3	67.55	41.67	50.56
6	7	3	121.94	56.11	58.92	5	11	3	64.34	82.03	31.40	0	16	3	547.63	638.12	118.38
-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	146.52	30.24	3	16	3	0.17	-38.45	59.19
-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	32.43
-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	105.56	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	244.76	29.57	1	17	3	42.29	29.37	46.95
4	8	3	89.87	121.51	28.58	4	12	3	95.93	13.80	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	1.02	55.53
-7	9	3	34.65	50.14	56.55	-5	13	3	28.34	-63.09	52.71	-5	18	3	2.49	-13.87	56.53
-6	9	3	118.59	72.64	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	0.86	27.39	27.23	-3	18	3	38.61	9.22	53.55
-4	9	3	0.57	-10.66	45.24	-2	13	3	143.64	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	3.11	-5.54	49.25

Structure Factors Table (continued) (*=unobserved refins.) for C(14) H(28) N(2) O(10) Cl(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)	h	k	l	F^2 cal	F^2 obs	sig(F^2)
2	18	3	60.11	30.25	55.31	-3	2	4	658.88	581.24	49.07	-6	6	4	0.89	36.91	28.59
3	18	3	17.38	-13.13	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	312.90	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	3.64	18.16	35.24	-2	6	4	652.37	712.39	50.74
-1	19	3	74.21	75.25	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	96.85	29.20	1	6	4	650.14	579.91	46.30
2	19	3	169.88	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	418.63	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	322.89	26.34
-2	21	3	13.18	34.11	53.56	0	3	4	246.98	246.73	15.71	-1	7	4	357.58	414.58	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	58.17	15.16
0	21	3	5.10	-37.70	48.78	2	3	4	1246.54	1428.67	67.55	1	7	4	142.99	187.87	23.12
1	21	3	14.99	-0.56	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	384.64	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	80.50	30.06
-1	22	3	0.07	-21.35	52.15	6	3	4	2.08	35.03	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	672.77	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	60.94
-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	1 [illegible]	997.27	58.68	-2	8	4	1.20	22.49	40.98
0	0	4	657.81	609.31	31.30	-2	4	4	5 [illegible]	663.15	46.64	-1	8	4	240.12	271.53	25.66
2	0	4	970.77	1022.02	58.16	-1	4	4	888.91	896.62	50.43	0	8	4	71.43	-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	13.05	36.09
6	0	4	30.81	23.27	24.03	1	4	4	1057.33	1077.20	56.87	2	8	4	129.29	111.58	24.41
-8	1	4	13.93	62.98	30.95	2	4	4	8.89	25.82	37.72	3	8	4	2.46	-27.82	44.45
-7	1	4	696.59	733.36	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	335.14	357.67	32.25
-1	1	4	280.36	271.75	25.64	-6	5	4	156.55	115.54	30.92	-3	9	4	549.33	510.39	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	83.75	-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	28.19	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	44.91
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	39.13	55.80	2	5	4	122.84	141.23	22.86	5	9	4	34.72	-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	58.97	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	28.81
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	683.58	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	12.55	33.89	43.97	-5	16	4	35.16	18.29	58.52	1	1	5	6.08	-42.96	45.96
-3	11	4	343.22	328.42	31.07	-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	134.06	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	215.35	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	2.97	-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	1163.29	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	87.25
-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	188.36	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	-37.46	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	-3	18	4	4.29	19.48	52.64	-6	3	5	2.14	75.44	28.39
3	12	4	84.93	27.29	50.51	-2	18	4	226.33	200.56	32.65	-5	3	5	80.79	113.51	28.62
4	12	4	260.31	275.76	33.43	-1	18	4	116.90	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	82.02	84.64	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	-54.79	53.46	-1	3	5	574.09	560.57	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	53.64	-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	84.64	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	269.43	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	-6	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

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	24.76	-3	14	5	82.51	134.63	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	85.48	42.55	31.07	-1	9	5	196.74	103.18	28.49	-1	14	5	283.77	301.87	32.39
-5	5	5	0.05	23.13	34.79	0	9	5	148.77	138.22	19.19	0	14	5	8.88	-62.99	38.20
-4	5	5	46.23	8.16	33.90	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	31.59	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	987.38	72.08	-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	48.88	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	1285.65	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	1027.80	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	116.86	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	535.56	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	24.88	23.55	47.58	1	17	5	120.36	93.91	30.62
-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	-5	12	5	132.88	151.50	32.40	-3	18	5	50.34	-29.68	61.08
-1	7	5	36.41	53.40	26.62	-4	12	5	37.30	69.80	28.95	-2	18	5	155.63	322.70	36.39
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	4.89	-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	254.17	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	38.65	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	192.58	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	3	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
-7	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
-5	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	-39.00	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	33.12
0	2	6	77.27	76.30	25.10	-5	7	6	69.91	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	344.25	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	84.90	99.62	33.46
4	2	6	44.19	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	-14.89	58.67
-1	3	6	8.18	27.01	47.84	-4	8	6	2.69	12.61	53.42	-4	14	6	45.30	65.73	33.08
0	3	6	1591.82	1784.38	62.62	-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	12.9	55.89	2	8	6	0.19	-20.58	46.69	2	14	6	0.74	49.49	53.14
-6	4	6	35.4	0.	53.19	3	8	6	5.96	-65.02	47.43	-4	15	6	12.30	-4.83	56.12
-5	4	6	46	[illegible]	29.14	-6	9	6	106.44	90.37	34.01	-3	15	6	336.00	375.80	37.46
-4	4	6	121	7.44	39.10	-5	9	6	0.48	-117.01	55.86	-2	15	6	6.37	-43.13	57.87
-3	4	6	34.3	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	39.68	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	1.28	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	318.87	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	149.80	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	32.42	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	51.24
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	-8.91	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	39.02	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	48.90	-5	8	7	33.83	39.30	39.80	-4	2	8	89.32	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	33.87	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	0.02	-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	46.25	79.69	32.27	-5	10	7	7.72	-82.29	60.75	-2	4	8	24.09	-47.01	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	22.98	-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	32.61	-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	35.71	-2	11	7	52.47	52.91	54.32	1	5	8	17.88	-77.22	59.17
3	4	7	1.24	-144.00	60.73	-1	11	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	35.12	-2	12	7	268.12	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	86.45	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	67.00	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	37.18	37.54	59.59	0	7	8	157.85	182.88	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	59.38
-2	6	7	89.09	-3.90	55.69	-3	14	7	66.73	43.50	57.80	0	8	8	33.20	-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
-4	7	7	63.70	133.86	33.28	0	0	8	28.08	11.09	39.82	-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	91.41	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	12	7	-3	1	1	17	-1	-1	7	1	41	38	-3	1	2	41	41	-4	10	2	15	-19
8	0	0	67	66	-1	1	1	70	74	3	7	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	12
3	1	0	16	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
0	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	8	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	-1	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	18
-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	12	-1	7	6	12	10	-7	9	8	15	15
1	13	3	24	-28	-3	9	4	24	-30	-3	7	5	39	32	1	7	6	20	24	-6	10	8	14	12
0	14	3	20	-23	1	9	4	22	20	-1	7	5	15	18	-8	8	6	38	-39	-2	10	8	13	-6
2	14	3	14	-12	3	9	4	28	-26	5	7	5	21	14	0	8	6	23	-29	-8	14	8	14	5
-7	15	3	15	14	5	9	4	29	-29	-8	8	5	55	-56	-7	9	6	14	-11	-7	15	8	16	-6
1	15	3	21	18	2	10	4	12	18	-6	8	5	20	-25	-2	10	6	13	-9	-9	1	9	18	17
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5	1	4	13	5																				

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
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-6	8	3	62	-63	0	14	3	48	47	-11	3	4	38	-40	1	7	4	44	-46	-4	14	4	26	28							
-4	8	3	128	-119	2	14	3	35	35	-9	3	4	27	28	3	7	4	64	64	-2	14	4	40	-39							
-2	8	3	105	-95	4	14	3	46	45	-7	3	4	28	-29	5	7	4	27	34	0	14	4	75	-78							
2	8	3	143	-139	6	14	3	22	22	-5	3	4	85	-86	7	7	4	39	-35	2	14	4	28	-30							
4	8	3	53	-51	-7	15	3	31	-30	-3	3	4	29	-30	9	7	4	35	-35	4	14	4	17	-18							
-11	9	3	17	-18	-5	15	3	12	12	-1	3	4	61	57	-10	8	4	37	-38	-3	15	4	18	-16							
-9	9	3	8	-7	-1	15	3	23	22	1	3	4	49	46	-8	8	4	33	-35	-1	15	4	65	-63							
-7	9	3	55	-57	1	15	3	18	-17	3	3	4	52	-54	-6	8	4	21	14	1	15	4	63	-62							
-5	9	3	53	-55	3	15	3	31	-33	5	3	4	40	-40	-4	8	4	50	44	3	15	4	31	-33							
-3	9	3	10	-14	-6	16	3	39	-39	9	3	4	10	5	-2	8	4	50	45	-4	16	4	23	-23							
-1	9	3	48	40	-2	16	3	15	14	-12	4	4	43	-42	0	8	4	65	59	-2	16	4	13	-15							
1	9	3	71	-65	2	16	3	59	-58	-10	4	4	11	-14	2	8	4	24	22	0	16	4	32	-32							
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-2	10	3	10	11	-8	0	4	40	43	2	4	4	42	-44	-7	9	4	32	30	1	1	5	137	-131							
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5	1	5	9	-8	-3	7	5	66	63	-2	14	5	14	-13	3	5	6	33	35	1	1	7	38	36							
7	1	5	33	-38	-1	7	5	76	74	-3	15	5	17	14	5	5	6	34	42	3	1	7	33	27							
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-2	2	5	13	17	-8	8	5	8	-13	2	0	6	15	-6	6	6	6	21	-21	2	2	7	65	66							
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2	2	5	92	-89	-4	8	5	85	82	6	0	6	41	-43	-5	7	6	21	-25	-7	3	7	39	42							
4	2	5	19	16	-2	8	5	67	64	-11	1	6	32	-31	-3	7	6	13	-16	-5	3	7	24	21							
6	2	5	30	-36	0	8	5	21	-22	-9	1	6	45	-45	-1	7	6	31	27	-3	3	7	17	14							
8	2	5	45	-48	2	8	5	30	32	-7	1	6	19	-20	1	7	6	62	59	-1	3	7	13	18							
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-9	3	5	55	-56	6	8	5	22	21	-3	1	6	42	-42	5	7	6	34	-34	3	3	7	22	24							
-7	3	5	72	-71	-9	9	5	19	23	-1	1	6	27	-25	-8	8	6	16	19	5	3	7	12	-8							
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1	3	5	75	-72	-1	9	5	25	-22	-10	2	6	19	-19	0	8	6	28	-28	-2	4	7	41	39							
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0	4	5	30	28	4	10	5	27	26	-11	3	6	33	33	1	9	6	18	-19	3	5	7	16	-16							
4	4	5	47	-48	6	10	5	20	22	-7	3	6	34	-33	-8	10	6	45	-45	-8	6	7	11	-10							
6	4	5	11	14	-7	11	5	23	-25	-5	3	6	49	52	-6	10	6	51	-53	-6	6	7	35	-37							
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3	5	5	31	-31	5	11	5	26	-29	-10	4	6	47	49	-7	11	6	43	-43	-5	7	7	22	-20							
5	5	5	27	-25	-6	12	5	41	-44	-4	4	6	55	54	-5	11	6	15	-18	-3	7	7	36	-34							
7	5	5	25	26	4	12	5	40	-37	-2	4	6	60	57	-3	11	6	14	13	-1	7	7	45	-42							
-8	6	5	56	56	-2	12	5	38	-37	0	4	6	9	-6	-1	11	6	24	-22	1	7	7	37	-37							
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-4	6	5	40	40	4	12	5	58	-58	4	4	6	52	58	3	11	6	27	-27	-4	8	7	34	-33							
0	6	5	46	49	-7	13	5	29	-29	6	4	6	51	54	2	12	6	25	-25	-2	8	7	50	-48							
2	6	5	8	3	-5	13	5	38	-37	-11	5	6	30	27	-5	13	6	10	-4	0	8	7	23	-23							
4	6	5	38	-36	-3	13	5	46	-48	-9	5	6	37	37	-1	13	6	12	15	-3	9	7	42	-39							
6	6	5	24	26	1	13	5	9	7	-7	5	6	23	25	-7	1	7	39	41	-1	9	7	34	-36							
8	6	5	41	41	3	13	5	34	-35	-5	5	6	13	12	-5	1	7	40	42	1	9	7	55	52							
-7	7	5	16	12	-6	14	5	13	-10	-3	5	6	46	46	-3	1	7	16	-13	-6	10	7	13	16							
-2	10	7	30	-29	0	0	8	16	20	-6	2	8	19	19	-1	3	8	22	-23	-7	5	8	22	-22							
0	10	7	21	18	-7	1	8	17	17	-4	2	8	10	-7	-6	4	8	13	10	-3	5	8	31	-31							
-8	0	8	27	24	-3	1	8	23	22	0	2	8	10	-5	-4	4	8	17	-19	-1	5	8	18	-21							
-4	0	8	17	19	-1	1	8	22	23	-7	3	8	13	15	-2	4	8	33	-33	-6	6	8	24	-24							
-2	0	8	53	51	-8	2	8	14	15	-3	3	8	16	-15	0	4	8	12	-11	-5	7	8	11	-8							

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	8	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	39	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	590	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	1225	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	296	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	190	16	19	4	1	0	24	1	10	9	1	0	17	1	9	3	2	1161	1194	27
0	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
2	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
4	2	0	0	74	1	8	1	1	538	526	20	22	4	1	82	0	82	0	10	1	0	15	1	12	3	2	102	72	101
6	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
8	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
10	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
12	2	0	103	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	115
14	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
16	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
18	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
20	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
22	2	0	134	35	99	17	1	1	533	506	24	8	5	1	0	109	1	7	0	2	852	825	19	21	3	2	191	181	53
24	2	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
2	3	0	191	206	19	19	1	1	177	130	48	10	5	1	455	435	23	9	0	2	453	480	23	23	3	2	0	34	1
4	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
6	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	-1
8	3	0	1067	1115	26	22	1	1	0	74	1	13	5	1	0	30	1	12	0	2	349	430	18	1	4	2	265	336	18
10	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
12	3	0	459	496	24	24	1	1	148	110	148	15	5	1	303	272	29	14	0	2	122	60	122	3	4	2	736	693	23
14	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
16	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
18	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	66	6	66
20	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
22	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
24	3	0	45	218	36	4	2	1	1040	1036	21	21	5	1	0	133	1	20	0	2	0	101	1	9	4	2	168	16	34
0	4	0	1	1122	23	5	2	1	0	57	1	22	5	1	252	203	45	21	0	2	513	516	24	10	4	2	799	702	27
2	4	0	1093	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
4	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
6	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
8	4	0	195	183	35	9	2	1	0	28	1	3	6	1	293	342	24	25	0	2	171	151	171	14	4	2	290	249	31
10	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
12	4	0	447	411	21	11	2	1	1223	1186	28	5	6	1	557	521	24	2	1	2	761	785	15	16	4	2	293	285	32
14	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
16	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
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22	4	0	51	109	50	16	2	1	210	208	37	10	6	1	334	321	26	7	1	2	1029	1024	21	21	4	2	43	162	42
2	5	0	367	513	18	17	2	1	273	260	31	11	6	1	0	108	1	8	1	2	812	931	21	22	4	2	0	37	1
4	5	0	15	59	14	18	2	1	115	229	114	13	6	1	0	189	1	9	1	2	794	754	22	23	4	2	0	161	1
6	5	0	0	66	1	19	2	1	0	20	1	14	6	1	139	90	72	10	1	2	0	87	1	1	5	2	369	395	19
8	5	0	471	470	21	20	2	1	108	120	108	15	6	1	104	159	104	11	1	2	830	759	24	2	5	2	484	600	20
10	5	0	34	64	34	21	2	1	138	188	138	16	6	1	0	138	1	12	1	2	270	296	22	3	5	2	0	3	1
12	5	0	22	26	21	22	2	1	134	66	134	17	6	1	0	14	1	13	1	2	432	441	18	4	5	2	30	45	30
14	5	0	97	119	66	23	2	1	139	193	139	18	6	1	172	95	62	14	1	2	0	123	1	5	5	2	192	99	32
16	5	0	0	88	1	24	2	1	115	85	115	19	6	1	70	94	69	15	1	2	341	319	23	6	5	2	325	308	21
18	5	0	208	198	45	25	2	1	112	85	111	20	6	1	159	22	159	16	1	2	124	33	123	7	5	2	356	305	22
20	5	0	100	52	100	1	3	1	0	67	1	1	7	1	177	159	49	17	1	2	257	236	31	8	5	2	137	95	136
22	5	0	0	48	1	2	3	1	256	267	16	2	7	1	0	96	1	18	1	2	0	98	1	9	5	2	0	93	1
0	6	0	336	296	21	3	3	1	818	805	21	3	7	1	112	116	112	19	1	2	171	63	44	10	5	2	235	232	34
2	6	0	410	441	20	4	3	1	778	824	22	4	7	1	341	313	26	20	1	2	130	51	130	11	5	2	0	15	1
4	6	0	395	446	20	5	3	1	165	176	29	5	7	1	101	146	101	21	1	2	0	47	1	12	5	2	0	103	1
6	6	0	583	582	22	6	3	1	974	888	23	6	7	1	311	314	28	22	1	2	96	94	96	13	5	2	328	303	28
8	6	0	326	327	26	7	3	1	434	549	20	7	7	1	0	128	1	23	1	2	0	65	1	14	5	2	92	133	91
10	6	0	225	229	38	8	3	1	648	684	25	8	7	1	109	48	109	24	1	2	114	13	113	15	5	2	261	204	34
14	6	0	224	189	44	9	3	1	0	17	1	9	7	1	166	178	165	25	1	2	183	100	65	16	5	2	133	108	133
16	6	0	0	54	1	10	3	1	678	657	26	10	7	1	0	19	1	0	2	2	4830	4787	76	17	5	2	176	130	60
18	6	0	82	124	82	11	3	1	102	15	81	11	7	1	205	174	44	1	2	2	797	746	17	18	5	2	129	16	128
20	6	0	126	150	126	12	3	1	219	224	30	12	7	1	292	240	32	2	2	2	976	1045	19	19	5	2	0	33	1
2	7	0	772	697	32	13	3	1	339	274	23	13	7	1	0	17	1	3	2	2	1102	1112	21	20	5	2	0	83	1
4	7	0	718	754	29	14	3	1	576	469	28	14	7	1	144	209	144	4	2	2	705	825	18	21	5	2	0	36	1
6	7	0	313	353	28	15	3	1	0	139	1	15	7	1	113	19	112	5	2	2	1069	1133	21	22	5	2	143	43	143
8	7	0	209	155	43	16	3	1	135	124	155	16	7	1	174	152	173	6	2	2	791	639	20	0	6	2	197	207	34
10	7	0	0	35	1	17	3	1	457	393	24	17	7	1	132	9	132	7	2	2	449	398	22	1	6	2	104	52	104
12	7	0	382	344	26	18	3	1	224	224	38	18	7	1	102	37	101	8	2	2	86	73	86	2	6	2	284	257	24

14	7	0	0	273	1	19	3	1	88	183	87	0	8	1	150	95	66	9	2	2	447	396	18	3	6	2	284	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	330	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	179	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	49
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	809	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	18	7	3	176	16	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	575	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	34
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	3	284	272	24	1	9	3	0	40	1	24	2	4	0	25	1	1	7	4	52	41	52
0	10	2	158	66	157	10	4	3	175	225	42	2	9	3	197	241	63	25	2	4	205	39	56	2	7	4	0	166	1
1	10	2	166	30	166	11	4	3	522	462	21	3	9	3	219	145	49	1	3	4	1062	1030	22	3	7	4	270	230	33
2	10	2	0	86	1	13	4	3	514	522	26	4	9	3	246	239	40	2	3	4	1224	1225	24	4	7	4	728	801	33
3	10	2	259	187	47	14	4	3	144	50	59	5	9	3	151	11	150	3	3	4	319	285	15	5	7	4	113	30	112
4	10	2	0	3	1	15	4	3	126	198	126	6	9	3	174	151	53	4	3	4	1102	1085	23	6	7	4	763	754	31
1	1	3	1824	1845	29	16	4	3	0	109	1	7	9	3	67	47	67	5	3	4	86	23	86	7	7	4	0	57	1
2	1	3	550	553	13	17	4	3	0	108	1	8	9	3	132	72	132	6	3	4	1093	1195	24	8	7	4	140	84	139
3	1	3	1117	1000	20	18	4	3	147	66	82	9	9	3	0	50	1	7	3	4	0	40	1	9	7	4	144	249	144
4	1	3	2195	1994	35	19	4	3	131	108	131	10	9	3	0	66	1	8	3	4	448	365	19	10	7	4	318	275	34
5	1	3	354	340	14	20	4	3	0	138	1	11	9	3	117	13	116	9	3	4	146	54	35	11	7	4	0	34	1
6	1	3	1096	1063	21	21	4	3	0	114	1	0	10	3	155	47	93	10	3	4	339	335	19	12	7	4	236	226	31
7	1	3	0	53	1	22	4	3	0	10	1	1	10	3	0	119	1	11	3	4	339	333	19	13	7	4	148	132	33
8	1	3	152	155	27	23	4	3	38	95	38	2	10	3	154	51	154	12	3	4	654	631	27	14	7	4	282	345	33
9	1	3	1429	1380	27	1	5	3	719	704	24	3	10	3	169	86	168	13	3	4	0	60	1	15	7	4	109	24	109
10	1	3	0	18	1	2	5	3	473	426	21	0	0	4	1942	2104	30	14	3	4	926	858	29	16	7	4	277	259	39
11	1	3	837	774	24	3	5	3	559	566	26	1	0	4	50	63	50	15	3	4	143	211	142	17	7	4	169	51	168
12	1	3	193	181	27	4	5	3	314	360	21	2	0	4	2599	2598	40	16	3	4	584	548	24	18	7	4	160	17	160
13	1	3	348	344	20	5	5	3	439	428	22	3	0	4	1218	1083	21	17	3	4	205	29	33	0	8	4	253	240	35
14	1	3	330	345	21	6	5	3	339	369	22	4	0	4	1028	1040	19	18	3	4	162	128	59	1	8	4	0	31	1
15	1	3	0	11	1	7	5	3	919	945	28	5	0	4	32,8	3068	50	19	3	4	96	61	95	2	8	4	20	61	20
16	1	3	84	192	83	8	5	3	489	436	22	6	0	4	262	229	14	20	3	4	0	88	1	3	8	4	154	196	84
17	1	3	240	236	31	9	5	3	776	758	30	7	0	4	230	255	16	21	3	4	38	14	37	4	8	4	0	88	1
18	1	3	0	91	1	10	5	3	124	44	123	8	0	4	2198	2095	36	22	3	4	185	223	185	5	8	4	121	62	104
19	1	3	135	147	135	11	5	3	42	524	-14	9	0	4	308	335	15	23	3	4	79	32	79	6	8	4	85	76	84
20	1	3	328	320	28	12	5	3	0	30	1	10	0	4	1404	1311	27	24	3	4	178	167	178	7	8	4	99	112	99
21	1	3	264	186	29	13	5	3	184	45	43	11	0	4	415	355	20	0	4	4	1235	1188	25	8	8	4	0	67	1
22	1	3	290	289	34	14	5	3	0	154	1	12	0	4	358	438	18	1	4	4	579	678	22	9	8	4	132	54	69
23	1	3	151	114	150	15	5	3	531	417	25	13	0	4	285	270	21	2	4	4	1523	1472	29	10	8	4	0	15	1
24	1	3	145	173	123	16	5	3	151	68	150	14	0	4	242	220	27	3	4	4	254	233	22	11	8	4	0	108	1
25	1	3	0	48	1	17	5	3	469	499	27	15	0	4	734	755	27	4	4	4	628	641	24	12	8	4	64	56	64
1	2	3	2721	2664	42	18	5	3	115	38	114	16	0	4	258	214	27	5	4	4	113	124	113	13	8	4	196	146	51

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	0	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	145	22	2	6	108	2	107	19	6	6	0	85	1
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8	4	7	108	24	108	5	9	7	154	115	154	10	3	8	75	98	75	0	8	8	116	10	115	19	3	9	117	136	116
9	4	7	511	486	22	6	9	7	291	204	33	11	3	8	267	211	24	1	8	8	118	105	118	20	3	9	105	61	104
10	4	7	363	361	22	7	9	7	141	150	140	12	3	8	781	731	28	2	8	8	150	26	69	21	3	9	0	32	1
13	4	7	230	219	34	8	9	7	0	18	1	13	3	8	242	239	30	3	8	8	0	177	1	22	3	9	107	34	107
14	4	7	402	379	22	9	9	7	285	215	41	14	3	8	690	669	31	4	8	8	73	53	72	23	3	9	0	83	1
15	4	7	332	301	26	10	9	7	158	8	72	15	3	8	0	8	1	5	8	8	0	74	1	0	4	9	328	340	18
16	4	7	145	104	65	0	0	8	1870	1832	31	16	3	8	354	343	24	6	8	8	136	44	136	1	4	9	272	316	21
17	4	7	78	125	77	1	0	8	1540	1541	26	17	3	8	258	224	30	7	8	8	136	128	108	2	4	9	0	194	1
18	4	7	103	34	102	2	0	8	978	1033	20	18	3	8	0	5	1	8	8	8	0	89	1	3	4	9	394	383	18
19	4	7	102	38	101	3	0	8	461	548	18	19	3	8	121	95	120	9	8	8	100	32	160	4	4	9	112	17	111
20	4	7	220	110	44	4	0	8	197	205	19	20	3	8	141	117	140	10	8	8	75	42	74	5	4	9	0	82	1
21	4	7	0	12	1	5	0	8	1094	1160	22	21	3	8	0	42	1	11	8	8	0	84	1	6	4	9	271	265	24
22	4	7	0	115	1	6	0	8	0	78	1	22	3	8	227	232	52	12	8	8	174	75	173	7	4	9	0	130	1
23	4	7	146	43	145	7	0	8	0	23	1	23	3	8	158	41	157	13	8	8	0	35	1	8	4	9	273	210	26
1	5	7	337	293	19	8	0	8	423	456	18	0	4	8	1478	1403	29	14	8	8	0	62	1	9	4	9	225	161	31
2	5	7	293	250	22	9	0	8	461	594	24	1	4	8	338	355	18	1	9	8	169	5	168	10	4	9	137	105	59
3	5	7	343	336	19	10	0	8	1339	1317	28	2	4	8	1319	1315	27	2	9	8	51	43	50	13	4	9	445	430	21
4	5	7	334	361	20	11	0	8	319	313	20	3	4	8	822	808	24	3	9	8	0	1	1	14	4	9	137	133	136
5	5	7	0	7	1	12	0	8	578	467	26	4	4	8	540	514	19	4	9	8	0	94	1	15	4	9	130	155	86
6	5	7	333	333	22	13	0	8	101	61	100	5	4	8	721	726	25	5	9	8	0	16	1	16	4	9	147	68	71
7	5	7	309	313	25	14	0	8	148	105	148	6	4	8	675	732	28	6	9	8	171	143	170	17	4	9	0	67	1
8	5	7	0	29	1	15	0	8	339	339	21	7	4	8	217	210	28	7	9	8	0	56	1	18	4	9	176	231	175
9	5	7	187	240	36	16	0	8	0	128	1	8	4	8	1244	1211	28	8	9	8	0	40	1	19	4	9	139	67	139
10	5	7	71	116	70	17	0	8	302	272	27	9	4	8	137	141	136	9	9	8	0	51	1	20	4	9	0	86	1
12	5	7	21	74	21	18	0	8	0	65	1	10	4	8	682	729	31	1	1	9	1404	1453	25	21	4	9	141	20	111
13	5	7	238	182	36	19	0	8	538	538	28	11	4	8	769	800	31	2	1	9	398	449	15	22	4	9	110	161	110
14	5	7	0	74	1	20	0	8	571	576	28	14	4	8	300	284	27	3	1	9	402	378	20	1	5	9	621	571	26
15	5	7	111	97	111	21	0	8	120	183	119	15	4	8	260	314	33	4	1	9	1282	1297	25	2	5	9	221	243	27
16	5	7	206	252	51	22	0	8	192	172	53	16	4	8	590	512	26	5	1	9	761	750	21	3	5	9	330	332	22
17	5	7	185	195	56	23	0	8	144	71	144	17	4	8	0	22	1	6	1	9	721	733	22	4	5	9	419	374	18
18	5	7	0	12	1	24	0	8	73	21	73	18	4	8	480	505	26	7	1	9	0	53	1	5	5	9	327	332	23
19	5	7	293	264	36	25	0	8	179	13	68	19	4	8	0	59	1	8	1	9	348	310	17	6	5	9	462	469	20
20	5	7	125	137	124	1	1	8	427	424	19	20	4	8	245	140	38	9	1	9	278	270	22	7	5	9	571	546	30
21	5	7	180	149	179	2	1	8	88	110	44	21	4	8	143	173	142	10	1	9	334	372	20	8	5	9	476	453	21
0	6	7	0	50	1	3	1	8	541	529	19	22	4	8	181	56	62	11	1	9	258	283	23	9	5	9	514	566	26
1	6	7	0	48	1	4	1	8	562	530	19	1	5	8	0	87	1	12	1	9	636	630	25	10	5	9	108	107	107
2	6	7	121	154	120	5	1	8	116	76	56	2	5	8	313	324	21	13	1	9	0	168	1	11	5	9	34	314	-15
3	6	7	513	547	23	6	1	8	870	931	22	3	5	8	584	563	27	14	1	9	907	904	28	13	5	9	0	3	1
4	6	7	295	277	24	7	1	8	0	58	1	4	5	8	275	302	25	15	1	9	66	169	66	14	5	9	115	179	115
5	6	7	593	630	24	8	1	8	304	309	18	5	5	8	126	84	58	16	1	9	254	264	33	15	5	9	116	229	115
6	6	7	206	203	39	9	1	8	192	209	29	6	5	8	105	1	104	17	1	9	81	87	80	16	5	9	274	255	34
7	6	7	377	352	24	10	1	8	372	331	18	7	5	8	482	397	22	18	1	9	115	47	115	17	5	9	282	338	39
8	6	7	362	392	25	11	1	8	264	248	20	8	5	8	139	119	138	19	1	9	0	12	1	18	5	9	212	151	50
9	6	7	66	10	65	12	1	8	694	673	25	9	5	8	94	10	94	20	1	9	230	214	39	19	5	9	258	199	40
10	6	7	220	295	41	13	1	8	269	264	25	10	5	8	326	322	25	21	1	9	0	114	1	20	5	9	0	55	1

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
21	5	9	114	54	114	6	1	10	476	452	25	4	5	10	250	179	23	18	1	11	114	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	175	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	108	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	16	6	11	91	22	91
16	6	9	178	251	177	21	1	10	0	74	1	0	6	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	2	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	33	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	37	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	343	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	89	25	89	3	3	10	560	588	23	11	7	10	107	107	107	18	3	11	237	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	1	1	9	11	0	120	1
11	8	9	56	49	56	5	3	10	0	33	1	13	7	10	97	84	97	20	3	11	250	193	38	2	9	11	97	42	96
12	8	9	0	38	1	6	3	10	230	237	27	14	7	10	113	68	112	21	3	11	0	44	1	3	9	11	165	20	165
13	8	9	161	47	161	7	3	10	703	742	28	15	7	10	146	84	112	22	3	11	0	76	1	4	9	11	0	68	1
14	8	9	56	18	55	8	3	10	161	146	40	16	7	10	0	21	1	0	4	11	0	41	1	5	9	11	113	66	112
1	9	9	0	7	1	9	3	10	804	881	28	0	8	10	0	168	1	1	4	11	0	67	1	6	9	11	144	4	144
2	9	9	169	259	168	10	3	10	0	116	1	1	8	10	161	37	50	2	4	11	0	43	1	7	9	11	152	143	151
3	9	9	164	91	164	12	3	10	39	216	-13	2	8	10	81	74	80	3	4	11	461	481	19	0	0	12	2684	2722	43
4	9	9	246	264	47	13	3	10	89	188	88	3	8	10	0	90	1	4	4	11	0	105	1	1	0	12	257	253	17
5	9	9	0	67	1	14	3	10	134	180	74	4	8	10	0	4	1	5	4	11	1007	1034	27	2	0	12	2145	2117	36
6	9	9	0	176	1	15	3	10	352	366	25	5	8	10	47	214	46	6	4	11	421	426	19	3	0	12	552	532	21
7	9	9	0	8	1	16	3	10	83	103	82	6	8	10	107	2	107	7	4	11	486	443	21	4	0	12	362	371	18
8	9	9	0	54	1	17	3	10	163	148	51	7	8	10	122	68	121	8	4	11	333	326	23	5	0	12	1063	1078	24
9	9	9	175	23	175	18	3	10	130	69	130	8	8	10	0	5	1	9	4	11	0	12	1	6	0	12	349	362	18
0	0	10	1337	1316	24	19	3	10	178	183	51	9	8	10	153	28	68	10	4	11	236	304	33	7	0	12	0	167	1
1	0	10	142	115	23	20	3	10	94	74	93	10	8	10	165	90	165	13	4	11	89	182	89	8	0	12	681	647	25
2	0	10	279	298	15	21	3	10	0	199	1	11	8	10	0	60	1	14	4	11	0	139	1	9	0	12	263	287	25
3	0	10	1495	1524	27	22	3	10	91	86	90	12	8	10	58	36	58	15	4	11	0	110	1	10	0	12	1640	1605	33
4	0	10	0	22	1	23	3	10	176	71	175	13	8	10	0	100	1	16	4	11	143	177	142	11	0	12	224	172	33
5	0	10	1164	1070	24	0	4	10	978	983	25	1	9	10	159	127	159	17	4	11	146	204	146	12	0	12	950	986	28
6	0	10	370	391	16	1	4	10	131	181	131	2	9	10	0	34	1	18	4	11	0	55	1	13	0	12	88	50	88
7	0	10	316	351	16	2	4	10	583	535	24	3	9	10	129	91	128	19	4	11	0	17	1	14	0	12	932	939	29
8	0	10	602	639	23	3	4	10	494	471	26	4	9	10	0	4	1	20	4	11	164	81	164	15	0	12	317	329	26
9	0	10	675	695	24	4	4	10	349	342	20	5	9	10	89	14	88	21	4	11	0	41	1	16	0	12	765	741	32
10	0	10	396	350	17	5	4	10	372	405	20	6	9	10	146	17	146	1	5	11	663	723	28	17	0	12	135	100	73
11	0	10	516	563	20	6	4	10	832	747	27	7	9	10	125	84	123	2	5	11	589	584	28	18	0	12	436	393	23
12	0	10	357	409	19	7	4	10	304	283	23	8	9	10	32	59	31	3	5	11	233	245	29	19	0	12	0	37	1
13	0	10	1058	1029	29	8	4	10	814	871	28	1	1	11	905	892	21	4	5	11	636	636	28	20	0	12	349	418	33
14	0	10	85	138	86	9	4	10	143	3	50	2	1	11	320	255	15	5	5	11	273	263	27	21	0	12	109	60	109
15	0	10	428	452	21	10	4	10	684	698	31	3	1	11	936	906	22	6	5	11	495	535	25	22	0	12	0	7	1
16	0	10	354	338	25	11	4	10	0	378	-1	4	1	11	354	331	15	7	5	11	386	453	24	23	0	12	162	9	162
17	0	10	207	201	39	13	4	10	167	117	48	5	1	11	863	787	23	8	5	11	143	154	61	1	1	12	1015	1016	22
18	0	10	339	316	26	14	4	10	301	235	28	6	1	11	173	74	26	9	5	11	628	712	31	2	1	12	330	284	15
19	0	10	220	141	39	15	4	10	57	32	156	7	1	11	564	522	25	10	5	11	329	337	25	3	1	12	0	93	1
20	0	10	0	244	1	16	4	10	225	252	38	8	1	11	218	248	27	13	5	11	181	14	42	4	1	12	908	948	23
21	0	10	448	456	27	17	4	10	0	46	1	9	1	11	672	666	26	14	5	11	84	95	83	5	1	12	249	214	20
22	0	10	160	122	159	18	4	10	38	240	38	10	1	11	264	248	24	15	5	11	199	124	47	6	1	12	908	876	24
23	0	10	280	302	40	19	4	10	177	112	54	11	1	11	799	804	27	16	5	11	78	22	78	7	1	12	107	80	107
24	0	10	181	132	180	20	4	10	124	62	123	12	1	11	162	182	49	17	5	11	271	275	38	8	1	12	211	239	29
1	1	10	499	469	20	21	4	10	0	145	1	13	1	11	563	574	23	18	5	11	0	49	1	9	1	12	95	111	94
2	1	10	139	119	27	22	4	10	66	27	65	14	1	11	88	151	87	19	5	11	228	274	55	10	1	12	0	162	1
3	1	10	1026	1076	22	1	5	10	140	29	47	15	1	11	167	143	47	20	5	11	204	185	64	11	1	12	124	137	65
4	1	10	243	263	20	2	5	10	132	3	132	16	1	11	0	21	1	0	6	11	187	146	40	13	1	12	214	224	33
5	1	10	615	645	23	3	5	10	325	267	21	17	1	11	272	251	29	1	6	11	183	93	39	14	1	12	312	283	26

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	60	1	10	2	13	691	716	27	2	7	13	257	251	32	17	2	14	50	22	49
17	1	12	50	26	49	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	96	0	6	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	1	6	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	2	6	12	0	116	1	18	2	13	296	255	30	9	7	13	173	150	56	2	3	14	337	355	19
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	31	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	130	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	266	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
23	2	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	199	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	1273	27	7	4	14	109	23	109
3	3	12	574	554	25	12	7	12	244	191	38	2	4	13	123	26	122	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	28	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	141	77	8	4	13	354	357	23	10	0	14	424	415	19	15	4	14	147	146	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	159	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	53	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	12	208	112	49	4	5	13	1003	971	28	4	1	14	599	549	26	12	5	14	139	48	63
4	4	12	0	62	1	1	1	13	829	812	23	5	5	13	0	28	1	5	1	14	188	179	29	13	5	14	149	47	148
5	4	12	330	300	22	2	1	13	1009	1027	23	6	5	13	858	842	25	6	1	14	294	259	21	14	5	14	0	41	1
6	4	12	0	73	1	3	1	13	0	46	1	7	5	13	160	197	54	7	1	14	0	144	1	15	5	14	92	24	91
7	4	12	314	302	22	4	1	13	805	749	23	8	5	13	0	171	1	8	1	14	349	352	20	16	5	14	161	57	160
8	4	12	171	163	42	5	1	13	320	312	19	9	5	13	252	227	32	9	1	14	352	423	20	17	5	14	165	51	164
9	4	12	164	143	44	6	1	13	89	110	88	10	5	13	246	297	36	10	1	14	29	63	29	18	5	14	0	45	1
10	4	12	281	235	28	7	1	13	0	32	1	12	5	13	318	347	29	12	1	14	567	563	23	19	5	14	0	13	1
11	4	12	0	249	-1	8	1	13	75	21	74	13	5	13	109	59	109	13	1	14	158	88	48	0	6	14	123	108	123
12	4	12	0	97	1	9	1	13	119	195	70	14	5	13	395	409	26	14	1	14	39	27	39	1	6	14	147	23	48
13	4	12	360	324	21	10	1	13	0	88	1	15	5	13	226	221	43	15	1	14	147	74	146	2	6	14	99	69	98
14	4	12	156	5	56	11	1	13	312	278	23	16	5	13	196	243	56	16	1	14	59	121	59	3	6	14	161	55	45
15	4	12	237	207	34	12	1	13	0	251	-1	17	5	13	130	135	130	17	1	14	0	159	1	4	6	14	86	87	86
16	4	12	138	30	137	13	1	13	0	162	1	18	5	13	0	13	1	18	1	14	0	6	1	5	6	14	171	168	48
17	4	12	0	61	1	14	1	13	402	449	22	19	5	13	153	151	152	19	1	14	36	124	35	6	6	14	281	257	31
18	4	12	167	106	59	15	1	13	58	122	58	0	6	13	254	219	27	20	1	14	0	20	1	7	6	14	229	176	34
19	4	12	23	44	23	16	1	13	159	93	159	1	6	13	36	101	35	21	1	14	83	72	83	8	6	14	76	60	75
20	4	12	154	178	97	17	1	13	44	39	44	2	6	13	237	258	33	22	1	14	0	100	1	9	6	14	126	54	78
21	4	12	81	55	80	18	1	13	0	142	1	3	6	13	0	29	1	0	2	14	591	565	23	10	6	14	59	113	58
1	5	12	154	181	48	19	1	13	178	14	44	4	6	13	89	26	88	1	2	14	571	533	24	11	6	14	123	23	123
2	5	12	189	115	34	20	1	13	0	56	1	5	6	13	165	178	51	2	2	14	539	530	25	12	6	14	0	44	1
3	5	12	81	63	81	21	1	13	154	81	154	6	6	13	132	70	131	3	2	14	716	751	24	13	6	14	42	28	42
4	5	12	62	125	62	22	1	13	0	79	1	7	6	13	176	97	44	4	2	14	171	167	35	14	6	14	0	16	1
5	5	12	0	42	1	23	1	13	77	19	77	8	6	13	25	114	25	5	2	14	308	295	19	15	6	14	94	102	93
6	5	12	138	3	138	0	2	13	930	965	25	9	6	13	0	83	1	6	2	14	56	89	55	16	6	14	0	49	1
7	5	12	169	154	51	1	2	13	85	194	84	10	6	13	0	67	1	7	2	14	489	453	21	17	6	14	0	176	1
8	5	12	291	206	27	2	2	13	756	765	23	11	6	13	85	52	84	8	2	14	63	140	62	1	7	14	133	218	133
9	5	12	0	81	1	3	2	13	494	505	26	12	6	13	0	23	1	9	2	14	0	81	1	2	7	14	101	142	100
10	5	12	80	92	80	4	2	13	296	277	20	13	6	13	139	12	138	10	2	14	438	448	20	3	7	14	45	161	44
11	5	12	25	22	-24	5	2	13	72	69	72	14	6	13	126	50	125	12	2	14	317	333	25	4	7	14	235	216	32
12	5	12	25	111	-25	6	2	13	670	659	25	15	6	13	0	44	1	13	2	14	496	466	23	5	7	14	139	95	139
13	5	12	142	19	141	7	2	13	89	23	39	16	6	13	91	119	91	14	2	14	272	235	27	6	7	14	234	159	37
14	5	12	97	77	97	8	2	13	515	563	21	17	6	13	0	15	1	15	2	14	113	95	112	7	7	14	171	253	64

Table 7. Observed and calculated structure factors for 1

h	k	l	10Fo	10Fc	10s
8	7	14	0	96	1
9	7	14	245	208	36
10	7	14	95	11	94
11	7	14	76	130	76
12	7	14	195	8	45
13	7	14	0	14	1
14	7	14	0	102	1
0	8	14	277	269	35
1	8	14	79	66	78
2	8	14	133	69	80
3	8	14	150	130	149
4	8	14	157	54	157
5	8	14	122	119	121
6	8	14	95	175	94
7	8	14	118	20	117
8	8	14	227	203	44
9	8	14	0	46	1
10	8	14	113	173	112
1	9	14	0	128	1
1	1	15	826	837	23
2	1	15	292	294	20
3	1	15	182	167	28
4	1	15	0	32	1
5	1	15	181	156	30
6	1	15	441	446	18
7	1	15	0	56	1
8	1	15	173	187	40
9	1	15	464	476	23
10	1	15	243	216	29
11	1	15	32	838	-14
12	1	15	321	369	27
13	1	15	143	137	143
14	1	15	142	24	62
15	1	15	0	53	1
16	1	15	102	135	101
17	1	15	0	73	1
18	1	15	152	129	152
19	1	15	222	243	43
20	1	15	0	148	1
21	1	15	232	226	45
22	1	15	0	129	1
0	2	15	611	603	25
1	2	15	0	99	1
2	2	15	395	367	21
3	2	15	664	749	25
4	2	15	223	234	31
5	2	15	1347	1279	29
6	2	15	117	61	117
7	2	15	392	416	21
8	2	15	0	17	1
9	2	15	243	218	27
10	2	15	120	93	119
12	2	15	209	252	38
13	2	15	404	378	23
14	2	15	138	169	138
15	2	15	406	394	25
16	2	15	150	92	150
17	2	15	101	21	101
18	2	15	185	196	51
19	2	15	233	228	40
20	2	15	163	14	163
21	2	15	243	256	46
1	3	15	844	788	25
2	3	15	312	298	22
3	3	15	179	138	31
4	3	15	58	116	58
5	3	15	0	71	1
6	3	15	293	306	26
7	3	15	324	356	26
8	3	15	197	232	38
9	3	15	708	670	39
10	3	15	0	14	1
12	3	15	0	76	1
13	3	15	0	44	1
14	3	15	0	42	1
15	3	15	0	79	1
16	3	15	34	1	33
17	3	15	117	118	116
18	3	15	53	12	52
19	3	15	118	150	118
20	3	15	109	1	109
21	3	15	0	43	1
0	4	15	0	172	1
1	4	15	477	424	21
2	4	15	137	85	137
3	4	15	688	624	28
4	4	15	131	156	67
5	4	15	383	413	21
6	4	15	209	135	35
7	4	15	297	262	26
8	4	15	116	128	116
9	4	15	205	180	38
10	4	15	0	28	1
11	4	15	0	336	-1
12	4	15	132	173	80
13	4	15	341	300	23
14	4	15	126	76	125
15	4	15	105	88	104
16	4	15	40	18	40
17	4	15	152	50	59
18	4	15	24	59	24
19	4	15	149	46	148
20	4	15	0	57	1
1	5	15	633	669	31
2	5	15	232	159	28
3	5	15	495	459	24
4	5	15	0	39	1
5	5	15	152	161	56
6	5	15	0	105	1
7	5	15	749	720	31
8	5	15	0	140	1
9	5	15	539	583	28
10	5	15	0	185	1
11	5	15	196	265	-48
12	5	15	126	116	126
13	5	15	67	93	67
14	5	15	46	109	46
15	5	15	0	161	1
16	5	15	43	11	42
17	5	15	322	342	38
18	5	15	0	6	1
0	6	15	163	72	42
1	6	15	99	76	98
2	6	15	115	20	93
3	6	15	165	191	164
4	6	15	96	205	95
5	6	15	129	147	129
6	6	15	162	127	51
7	6	15	233	202	33
8	6	15	51	123	50
9	6	15	144	52	143
10	6	15	147	21	60
11	6	15	61	45	60
12	6	15	0	28	1
13	6	15	0	74	1
14	6	15	206	43	39
15	6	15	0	99	1
16	6	15	123	4	123
1	7	15	166	166	56
2	7	15	120	110	119
3	7	15	0	154	1
4	7	15	128	146	128
5	7	15	101	14	101
6	7	15	57	4	57
7	7	15	153	121	67
8	7	15	0	25	1
9	7	15	186	121	51
10	7	15	80	57	80
11	7	15	70	69	69
12	7	15	0	9	1
13	7	15	140	58	140
0	8	15	0	55	1
1	8	15	152	118	151
2	8	15	0	44	1
3	8	15	192	157	52
4	8	15	0	109	1
5	8	15	167	86	55
6	8	15	0	94	1
7	8	15	216	170	50
8	8	15	174	118	62
9	8	15	62	105	61
0	0	16	525	536	24
1	0	16	589	552	22
2	0	16	560	635	24
3	0	16	1142	1141	27
4	0	16	351	329	18
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14	3	18	216	241	44	0	2	19	355	345	39	8	7	19	112	21	112	1	5	20	27	39	26	3	4	21	0	78	1
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16	3	18	0	94	1	2	2	19	0	71	1	0	0	20	629	668	27	3	5	20	213	155	35	5	4	21	192	201	48
17	3	18	0	148	1	3	2	19	559	582	23	1	0	20	436	452	23	4	5	20	0	51	1	6	4	21	81	53	80
18	3	18	0	52	1	4	2	19	272	240	27	2	0	20	0	130	1	5	5	20	124	34	123	7	4	21	0	13	1
19	3	18	0	163	1	5	2	19	344	36	23	3	0	20	159	129	38	6	5	20	0	59	1	8	4	21	79	123	79
0	4	18	289	289	27	6	2	19	0	54	1	4	0	20	116	12	116	7	5	20	0	186	1	9	4	21	0	28	1
1	4	18	0	54	1	7	2	19	550	518	24	5	0	20	119	138	75	8	5	20	0	52	1	10	4	21	0	73	1
2	4	18	48	24	48	8	2	19	99	115	99	6	0	20	265	280	29	9	5	20	163	36	48	11	4	21	0	47	1
3	4	18	493	462	23	9	2	19	163	113	53	7	0	20	166	11	49	10	5	20	121	52	120	12	4	21	135	104	135
4	4	18	152	213	152	10	2	19	0	46	1	8	0	20	52	110	52	11	5	20	64	69	63	13	4	21	128	77	128
5	4	18	687	681	31	12	2	19	120	44	120	9	0	20	292	235	28	12	5	20	0	45	1	14	4	21	70	127	69
6	4	18	129	36	128	13	2	19	324	288	28	11	0	20	25	180	-24	13	5	20	0	50	1	15	4	21	0	33	1
7	4	18	257	293	32	14	2	19	135	130	73	12	0	20	240	263	38	14	5	20	0	25	1	1	5	21	144	42	144
8	4	18	0	158	1	15	2	19	158	144	158	13	0	20	154	34	154	0	6	20	209	269	41	2	5	21	104	123	103
9	4	18	26	108	28	16	2	19	0	6	1	14	0	20	0	17	1	1	6	20	157	24	156	3	5	21	0	43	1
10	4	18	120	216	120	17	2	19	145	113	144	15	0	20	0	37	1	2	6	20	215	239	43	4	5	21	147	182	70
11	4	18	209	237	41	18	2	19	0	22	1	16	0	20	191	110	49	3	6	20	179	167	54	5	5	21	120	144	119
12	4	18	0	36	1	19	2	19	64	120	64	17	0	20	85	158	84	4	6	20	0	78	1	6	5	21	141	194	82
13	4	18	365	340	26	1	3	19	124	49	124	18	0	20	121	96	120	5	6	20	314	331	34	7	5	21	99	127	98
14	4	18	0	66	1	2	3	19	0	156	1	19	0	20	208	139	50	6	6	20	113	193	113	8	5	21	0	63	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	1	5	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	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	3	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	240	31	10	0	24	520	544	25	14	1	25	126	98	126	6	3	26	148	187	137
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	1	27	0	27	1
2	2	22	248	260	31	5	2	23	394	336	25	15	1	24	0	27	1	6	3	25	0	88	1	4	1	27	0	40	1
3	2	22	244	226	32	6	2	23	133	55	133	0	2	24	225	255	37	7	3	25	116	98	116	5	1	27	119	8	119
4	2	22	94	10	94	7	2	23	302	321	31	1	2	24	0	82	1	8	3	25	0	60	1	6	1	27	198	10	42
5	2	22	61	124	61	8	2	23	0	27	1	2	2	24	199	224	46	9	3	25	160	38	160	7	1	27	142	47	142
6	2	22	250	224	33	9	2	23	166	53	50	3	2	24	0	75	1	10	3	25	145	118	72	8	1	27	81	62	81
7	2	22	83	140	82	10	2	23	118	76	117	4	2	24	53	38	52	11	3	25	0	49	1	9	1	27	100	167	99
8	2	22	238	169	31	11	2	23	239	236	38	5	2	24	0	61	1	12	3	25	200	160	50	10	1	27	169	117	64
9	2	22	67	26	66	12	2	23	128	36	127	6	2	24	244	249	38	0	4	25	185	210	51	11	1	27	160	136	73
10	2	22	67	110	66	13	2	23	224	281	47	7	2	24	142	9	141	1	4	25	0	16	1	0	2	27	0	55	1
11	2	22	0	12	1	14	2	23	143	101	143	8	2	24	0	252	1	2	4	25	171	107	171	1	2	27	0	73	1
12	2	22	116	48	116	15	2	23	159	170	159	9	2	24	0	37	1	3	4	25	0	101	1	2	2	27	0	85	1
13	2	22	173	82	50	16	2	23	0	54	1	10	2	24	0	153	1	4	4	25	149	39	148	3	2	27	315	276	28
14	2	22	0	122	1	1	3	23	0	75	1	11	2	24	0	7	1	5	4	25	30	175	29	4	2	27	0	62	1
15	2	22	0	62	1	2	3	23	100	83	99	12	2	24	0	37	1	6	4	25	0	16	1	5	2	27	331	335	32
16	2	22	183	179	60	3	3	23	137	114	136	13	2	24	0	4	1	7	4	25	0	14	1	6	2	27	0	67	1
17	2	22	154	33	154	4	3	23	134	153	134	14	2	24	85	91	85	8	4	25	168	121	58	7	2	27	168	163	168
1	3	22	263	209	27	5	3	23	105	63	105	15	2	24	0	31	1	9	4	25	0	50	1	8	2	27	243	125	36
2	3	22	379	323	23	6	3	23	113	94	113	1	3	24	279	239	30	10	4	25	109	178	109	9	2	27	132	47	132
3	3	22	123	48	122	7	3	23	212	247	43	2	3	24	139	207	138	1	5	25	98	67	98	10	2	27	0	66	1
4	3	22	317	309	26	8	3	23	0	113	1	3	3	24	0	195	1	2	5	25	0	132	1	1	3	27	185	203	56
5	3	22	0	104	1	9	3	23	195	179	47	4	3	24	219	247	44	3	5	25	152	36	151	2	3	27	121	61	121
6	3	22	198	186	40	10	3	23	0	75	1	5	3	24	131	2	130	4	5	25	287	314	39	3	3	27	0	15	1
7	3	22	129	64	74	11	3	23	0	20	1	6	3	24	257	252	36	5	5	25	174	4	173	4	3	27	158	151	158
8	3	22	0	96	1	12	3	23	0	25	1	7	3	24	214	220	45	6	5	25	322	265	34	5	3	27	116	28	115
9	3	22	203	212	45	13	3	23	135	14	135	8	3	24	117	59	117	7	5	25	57	25	57	6	3	27	134	103	101
10	3	22	69	151	69	14	3	23	46	22	45	9	3	24	0	209	1	0	0	26	335	369	27	7	3	27	0	112	1
11	3	22	143	126	67	15	3	23	0	30	1	10	3	24	35	114	35	1	0	26	155	168	55	8	3	27	0	9	1
12	3	22	0	72	1	0	4	23	0	93	1	11	3	24	166	70	56	2	0	26	335	358	27	0	4	27	125	19	125
13	3	22	139	2	139	1	4	23	125	58	79	12	3	24	116	186	115	3	0	26	323	333	28	1	4	27	0	135	1
14	3	22	0	103	1	2	4	23	125	16	72	13	3	24	45	31	44	4	0	26	190	119	42	2	4	27	120	46	119
15	3	22	0	102	1	3	4	23	189	134	45	0	4	24	103	88	103	5	0	26	264	315	37	3	4	27	263	212	39
16	3	22	99	123	99	4	4	23	150	45	150	1	4	24	34	46	34	6	0	26	309	313	34	4	4	27	93	11	93

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
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	89	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						

Structure Factors Table [Fo**2, Fc**2 and sigma(Fo**2)] (*=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)
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	47.43
3	0	0	2508.51	2302.14	65.16	-1	3	0	60130.54	60500.76	2009.27	-5	6	0	123.27	152.33	39.06
4	0	0	14.11	-33.25	50.09	0	3	0	767.26	665.91	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	481.71	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	3829.73	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	752.26	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	35.29	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	28.85	-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	539.58	564.91	61.17	8	6	0	0.66	-142.48	89.59
-3	1	0	2012.82	1888.19	80.76	-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	1504.96	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	101.61	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	4330.74	4221.50	148.24	0	7	0	3520.20	3610.32	151.01
8	1	0	518.99	515.10	52.95	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	0.11	-124.76	101.96	6	4	0	9.93	-119.15	65.48	4	7	0	5085.39	5187.56	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	56.67
-7	2	0	883.19	951.15	91.84	8	4	0	215.32	133.28	52.19	6	7	0	3141.98	3220.02	158.81
-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	66.56
-2	2	0	5047.83	5503.30	132.28	-7	5	0	2485.99	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	6238.15	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	92.52	2	8	0	2250.01	2219.61	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	2265.81	2151.29	113.30
10	2	0	12.94	-50.54	109.01	5	5	0	300.82	256.83	34.16	5	8	0	4459.78	4430.77	188.89
-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	63.95	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	30.69	-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

Structure Factors Table (continued) (*=unobserved reflns.) for C(14) H(30) Cl(2) Cu(1) N(4) O(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)	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	1	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	1	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	1	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	1	93.86	103.56	60.50
-2	9	0	4008.67	4288.74	180.61	5	12	0	22.12	-21.89	48.40	-2	-17	1	253.64	274.31	65.8*
-1	9	0	640.30	608.47	49.32	6	12	0	53.44	117.05	51.51	-1	-17	1	0.07	63.44	109.20
0	9	0	1715.82	1836.82	106.20	7	12	0	69.74	110.48	54.69	0	-17	1	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	1	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	1	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	1	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	1	83.90	54.42	107.73
5	9	0	356.41	285.21	44.95	-2	13	0	867.00	1085.24	106.65	-1	-16	1	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	1	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	1	223.10	103.81	113.08
8	9	0	273.57	418.62	58.36	1	13	0	96.02	38.43	84.00	2	-16	1	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	1	42.09	-12.40	114.56
-7	10	0	20.30	13.77	94.32	3	13	0	26.19	70.11	76.54	-5	-15	1	260.04	267.89	63.31
-6	10	0	89.96	-32.02	96.56	4	13	0	429.75	318.46	55.41	-4	-15	1	45.70	48.79	5* 85
-5	10	0	143.79	172.08	48.88	5	13	0	18.08	63.55	89.16	-3	-15	1	161.80	257.20	57.21
-4	10	0	123.01	143.95	44.97	6	13	0	134.95	147.50	57.08	-2	-15	1	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	1	33.43	-5.15	97.53
-2	10	0	186.28	209.15	39.31	-5	14	0	68.21	48.11	78.68	0	-15	1	88.21	107.32	57.82
-1	10	0	1747.49	1167.77	90.09	-4	14	0	240.12	215.12	62.69	1	-15	1	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	1	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	1	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	1	235.02	198.00	64.82
3	10	0	1.64	8.[illegible]	35.73	0	14	0	40.62	101.95	51.78	-6	-14	1	1.03	83.49	99.03
4	10	0	135.54	115.19	41.32	1	14	0	635.70	642.55	64.64	-5	-14	1	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	1	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	1	569.38	439.18	59.16
7	10	0	809.29	868.27	79.14	4	14	0	844.84	785.12	80.76	-2	-14	1	19.58	-64.80	92.48
8	10	0	8.82	-171.42	112.73	5	14	0	188.90	195.81	58.04	-1	-14	1	183.39	147.34	52.20
-7	11	0	406.30	483.37	66.83	6	14	0	188.83	201.70	63.84	0	-14	1	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	1	123.22	34.63	66.01
-5	11	0	1062.54	984.18	65.54	-3	15	0	15.16	-1.97	103.97	2	-14	1	337.62	327.77	56.66
-4	11	0	105.94	122.17	47.12	-2	15	0	163.92	18.21	107.32	3	-14	1	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	1	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	1	0.28	29.85	106.86
-1	11	0	1533.02	1636.30	112.0[illegible]	1	15	0	92.85	64.50	93.60	-7	-13	1	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	1	20.36	-74.87	94.53
1	11	0	5.23	25.68	44.50	3	15	0	146.23	146.21	56.73	-5	-13	1	324.56	352.02	55.00
2	11	0	[illegible]51	81.91	40.76	4	15	0	1.66	-80.02	95.03	-4	-13	1	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	1	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	1	218.00	208.49	50.05
5	11	0	660.24	765.57	70.50	-3	16	0	218.34	83.28	112.24	-1	-13	1	1201.97	1352.39	115.12
6	11	0	839.47	827.85	65.03	-2	16	0	234.95	243.58	63.48	0	-13	1	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	1	1.70	-115.96	84.72
8	11	0	32.97	70.23	103.84	0	16	0	21.19	39.49	102.70	2	-13	1	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	1	18.05	-48.55	90.66
-5	12	0	3.58	-86.74	96.12	2	16	0	2.26	9.63	97.98	4	-13	1	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	1	29.43	103.74	54.25
-3	12	0	1336.51	1511.4[illegible]	118.68	4	16	0	29.80	-32.20	110.82	-7	-12	1	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	1	204.41	227.34	56.15
-1	12	0	2175.38	2368.99	136.22	-1	17	0	87.06	63.93	110.33	-5	-12	1	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	1	13[illegible]3.94	1203.72	115.00

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)
-3	-12	1	264.43	172.41	46.57	4	-9	1	1761.48	2123.69	129.72	5	-6	1	2732.01	2910.10	141.16
-2	-12	1	721.05	667.57	67.24	5	-9	1	502.95	534.10	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	[illegible].35	89.90
0	-12	1	264.98	57.76	89.80	7	-9	1	154.64	178.08	59.72	8	-6	1	14.37	-36.10	96.50
1	-12	1	418.62	566.76	94.20	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	-5	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	-5	1	67.38	-22.59	101.39	-8	-5	1	3.10	11.50	69.12
4	-12	1	1331.08	1328.07	119.18	-7	-5	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	-5	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	-5	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	-5	1	382.22	394.93	40.00	-4	-5	1	104.17	111.86	28.12
-7	-11	1	8.71	25.80	94.59	-3	-5	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	-5	1	2546.06	2824.66	125.19	-2	-5	1	2719.81	2828.46	111.34
-5	-11	1	23.88	-23.41	80.59	-1	-5	1	3967.01	6442.87	231.31	-1	-5	1	1493.14	1539.23	71.03
-4	-11	1	63.88	103.30	43.56	0	-5	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	-5	1	3556.84	3273.80	138.76	1	-5	1	2911.96	3216.97	120.80
-2	-11	1	452.43	533.90	51.05	2	-5	1	1.35	46.49	48.68	2	-5	1	12124.10	13179.23	421.65
-1	-11	1	933.74	950.33	89.57	3	-5	1	187.03	39.01	3[illegible].50	3	-5	1	352.31	274.35	28.88
0	-11	1	1795.29	1789.07	126.28	4	-5	1	239.09	213.89	79.43	4	-5	1	1816.12	1943.46	98.54
1	-11	1	24.99	-9.86	63.56	5	-5	1	79.88	70.14	70.72	5	-5	1	144.66	157.03	34.47
2	-11	1	607.50	515.70	48.72	6	-5	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	-5	1	279.56	172.88	54.79	7	-5	1	150.00	191.44	47.71
4	-11	1	40.94	52.56	46.98	8	-5	1	40.39	-75.64	107.95	8	-5	1	76.53	29.03	52.94
5	-11	1	1089.29	861.58	86.41	-9	-4	1	2.41	38.90	104.11	9	-5	1	32.71	-21.54	104.56
6	-11	1	92.16	169.41	56.72	-8	-4	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	-4	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	-4	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	-4	1	541.01	615.62	53.75	-6	-4	1	55.77	94.39	37.09
-6	-10	1	83.58	90.32	48.38	-4	-4	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	-4	1	8697.59	8890.00	304.48	-4	-4	1	441.92	449.03	39.95
-4	-10	1	935.69	1020.43	92.69	-2	-4	1	144.26	222.25	29.35	-3	-4	1	3655.40	3673.62	137.08
-3	-10	1	320.77	312.45	42.57	-1	-4	1	12752.85	12910.80	419.52	-2	-4	1	4208.95	4569.44	189.76
-2	-10	1	8278.45	8422.80	315.42	0	-4	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	-4	1	2613.49	2836.89	121.56	0	-4	1	371.95	268.20	26.75
0	-10	1	1397.14	1357.74	101.40	2	-4	1	3452.73	3690.13	146.65	1	-4	1	35.34	78.24	17.44
1	-10	1	691.26	689.62	80.92	3	-4	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	-4	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	-4	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	-4	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	-4	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	-4	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	-3	1	125.72	89.95	61.98	8	-4	1	581.72	680.62	61.34
-9	-9	1	65.28	107.50	111.80	-8	-3	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	-3	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	-3	1	1294.91	1444.91	108.19	-8	-3	1	622.36	560.58	58.91
-6	-9	1	459.05	441.91	51.25	-5	-3	1	1418.59	1350.18	93.11	-7	-3	1	154.61	58.48	78.53
-5	-9	1	4802.96	4507.10	200.95	-4	-3	1	610.30	599.85	46.91	-6	-3	1	4153.40	3901.04	170.19
-4	-9	1	308.57	409.20	44.22	-3	-3	1	26.44	0.66	31.25	-5	-3	1	1194.52	1143.38	80.20
-3	-9	1	6538.12	6453.61	240.49	-2	-3	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	-3	1	276.81	151.90	24.05	-3	-3	1	165.44	167.66	20.68
-1	-9	1	558.32	575.23	40.47	0	-3	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	-3	1	3461.67	3483.21	133.29	-1	-3	1	131.30	126.49	15.19
1	-9	1	774.41	841.19	72.14	2	-3	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	-3	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	-3	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	2406.45	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	2875.38	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	10374.48	11049.27	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	691.32	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	44.18	35.59	108.81
-1	-2	1	21595.04	22882.35	697.56	-4	1	1	300.59	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	62.00	1	1	1	21907.11	22432.27	701.52	-4	4	1	12.48	27.93	48.57
5	-2	1	2147.33	2232.08	108.95	2	1	1	2635.10	2877.75	100.64	-3	4	1	282.90	510.00	49.61
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	64.28	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	47.83	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	52.91	9	1	1	186.08	181.36	55.57	4	4	1	2651.13	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	70.62*	-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	421.71
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	38.97	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	134.74	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	885.15	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	580.13	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	28.14	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	75.90
-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	52.26	6	12	1	32.04	-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	328.66	29.93	1	9	1	8.46	36.97	50.77	8	12	1	178.60	55.15	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	104.51
1	6	1	71.93	89.56	21.53	3	9	1	527.60	512.46	49.07	-4	13	1	316.33	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	0.56	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	55.24
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	233.29	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	98.49	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	274.73	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	126.40	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	140.32
-5	7	1	185.38	163.55	42.83	-2	10	1	55.80	127.94	37.79	-5	14	1	5.96	-46.09	105.39
-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	100.51
-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	811.78	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	309.87	212.42	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	50.09	4	14	1	20.20	-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	95.28
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	62.56	-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	22.71	53.47	63.00	-2	11	1	2281.43	2232.56	133.49	0	15	1	32.51	-61.59	99.95
-6	8	1	35.90	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	24.12	96.82
-3	8	1	5617.62	5334.85	206.90	2	11	1	514.31	533.29	47.63	4	15	1	61.08	174.72	55.42
-2	8	1	376.06	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	-23.00	108.08
1	8	1	83.54	38.84	49.23	6	11	1	376.91	343.73	57.22	-1	16	1	98.35	34.06	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	68.38
3	8	1	1701.62	1619.94	93.43	8	11	1	363.91	345.22	65.31	1	16	1	323.91	345.95	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	-3.30	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	15.75	-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	-12	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	186.65	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	309.74	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	88.85	96.54	33.63
-2	-16	2	4.52	73.67	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	235.34
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	43.78
1	-16	2	279.37	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
-3	-15	2	6.36	20.24	107.27	-2	-11	2	1665.55	1823.24	123.49	3	-8	2	180.15	170.32	36.25
-4	-15	2	174.67	187.38	58.01	-1	-11	2	185.67	165.73	42.51	4	-8	2	1603.76	1551.36	107.91
-3	-15	2	28.96	49.43	55.30	0	-11	2	3986.28	4290.63	295.04	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	106.66
-1	-15	2	235.77	335.89	58.28	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	16.29	103.92
2	-15	2	42.45	-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	54.50	-6	-10	2	615.88	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	2.40	-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	27.21
1	-14	2	422.71	460.10	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	2626.98	2930.45	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	606.69	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	76.14	83.17
-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	49.67	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	114.17	46.71	-4	-9	2	1003.35	892.12	87.69	-3	-6	2	87.42	94.08	27.73
2	-13	2	395.93	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	330.27	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	4791.41	4663.13	191.05	1	-6	2	4338.07	5005.64	179.05
-7	-12	2	7.64	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	38.71	94.60	2	-9	2	993.26	833.44	75.33	3	-6	2	4907.46	5546.41	203.86
-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	466.07	48 29	47.35	5	-6	2	213.29	175.68	40.95
-3	-12	2	651.54	661.95	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	332.59	47.97	6	-9	2	62.53	91.30	91.59	7	-6	2	16.56	8.61	86.72
-1	-12	2	1335.95	1297.30	110.85	7	-9	2	139.98	274.71	57.57	8	-6	2	105.47	131.76	55.55
0	-12	2	39.39	-70.18	94.73	8	-9	2	197.00	212.26	60.84	9	-6	2	37.59	37.51	105.20

Structure Factors Table (continued) (*=unobserved reflns.) for C(14) N(10) Cl(2) Cu(1) F(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	488.93	546.61	3..53
-8	-5	2	283.19	163.06	52.87	9	-3	2	9.02	-262.12	108.91	6	0	2	51.34	64.60	22.62
-7	-5	2	374.07	443.60	52.56	-9	-2	2	63.16	132.28	56.85	7	0	2	1.28	42.56	103.30
-6	-5	2	1530.09	1416.78	108.39	-8	-2	2	3.08	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	178.75	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	-9	1	2	44.64	-25.71	100.86
-2	-5	2	103.58	109.10	22.29	-4	-2	2	2638.65	2239.34	101.27	-8	1	2	94.12	84.22	52.58
-1	-5	2	1182.45	1076.63	59.95	-3	-2	2	50.82	98.14	26.29	-7	1	2	145.69	127.33	45.30
0	-5	2	6639.92	6662.61	226.91	-2	-2	2	6357.08	6318.75	208.37	-6	1	2	34.77	44.58	59.69
1	-5	2	203.66	168.72	22.25	-1	-2	2	1298.98	1300.02	54.68	-5	1	2	93.11	91.70	30.74
2	-5	2	2596.41	2106.42	92.02	0	-2	2	3675.75	4651.65	153.15	-4	1	2	6915.96	7381.63	254.03
3	-5	2	384.60	256.82	27.59	1	-2	2	28089.76	29715.52	903.88	-3	1	2	10180.83	10163.97	329.68
4	-5	2	969.51	1119.59	76.57	2	-2	2	323.33	262.95	22.52	-2	1	2	1236.52	1210.69	47.34
5	-5	2	2642.97	2441.52	124.20	3	-2	2	5.63	-5.20	32.72	-1	1	2	14909.94	15757.43	484.41
6	-5	2	252.62	271.00	43.98	4	-2	2	482.98	450.58	36.32	0	1	2	7522.61	7093.27	222.23
7	-5	2	952.55	907.09	74.40	5	-2	2	2316.49	2354.15	114.84	1	1	2	1121.82	1148.34	45.50
8	-5	2	94.92	81.61	95.21	6	-2	2	1105.13	1056.12	86.27	2	1	2	1187.30	1141.33	51.50
9	-5	2	226.97	239.10	62.07	7	-2	2	1292.62	1462.54	107.58	3	1	2	2727.55	2664.17	102.70
-9	-4	2	681.17	632.39	66.99	8	-2	2	939.40	965.00	80.26	4	1	2	1386.37	1163.80	66.63
-8	-4	2	47.21	-53.10	86.21	9	-2	2	184.00	143.20	57.52	5	1	2	3397.52	3152.92	135.70
-7	-4	2	1839.76	1922.48	130.07	-9	-1	2	322.87	302.58	62.06	6	1	2	1662.22	1595.83	99.61
-6	-4	2	1254.48	1157.26	91.95	-8	-1	2	1345.57	1472.05	125.88	7	1	2	1696.37	1574.19	109.96
-5	-4	2	84.95	-6.04	55.51	-7	-1	2	0.19	60.91	41.49	8	1	2	180.46	194.81	46.48
-4	-4	2	724.08	597.74	61.61	-6	-1	2	1261.81	1298.40	96.18	9	1	2	333.71	336.44	58.50
-3	-4	2	165.58	236.96	24.59	-5	-1	2	746.90	818.73	46.93	10	1	2	150.19	150.93	61.89
-2	-4	2	4299.14	4577.09	161.44	-4	-1	2	485.93	535.43	53.00	-9	2	2	122.44	59.27	105.78
-1	-4	2	62.70	79.80	16.93	-3	-1	2	1383.09	1144.80	62.32	-8	2	2	971.58	894.90	80.17
0	-4	2	22954.95	26268.94	809.48	-2	-1	2	179.14	138.83	16.98	-7	2	2	736.69	717.17	65.50
1	-4	2	13556.89	14221.10	446.22	-1	-1	2	22050.20	24402.95	743.45	-6	2	2	1.03	-65.61	64.68
2	-4	2	494.89	447.95	42.00	0	-1	2	2003.44	2347.01	80.79	-5	2	2	15.39	59.76	29.22
3	-4	2	8018.53	8118.90	272.97	1	-1	2	14312.21	15309.85	469.22	-4	2	2	328.96	278.65	29.88
4	-4	2	6942.44	6661.44	236.22	2	-1	2	20.41	50.14	13.79	-3	2	2	4083.51	4128.45	150.54
5	-4	2	19.81	45.51	52.75	3	-1	2	2945.44	2705.01	104.60	-2	2	2	136.91	104.33	18.21
6	-4	2	2905.31	2842.72	142.78	4	-1	2	2226.01	2577.88	108.80	-1	2	2	3865.59	4722.09	156.03
7	-4	2	54.16	81.98	43.60	5	-1	2	10876.10	9819.53	333.02	0	2	2	17593.56	15981.52	491.89
8	-4	2	168.96	128.42	54.63	6	-1	2	25.62	78.27	33.09	1	2	2	10779.00	12496.34	385.95
9	-4	2	188.06	187.39	57.70	7	-1	2	2533.93	2824.41	143.69	2	2	2	1039.41	1103.58	51.37
-9	-3	2	3.50	-26.98	99.19	8	-1	2	65.06	109.60	47.32	3	2	2	3957.79	3314.46	122.27
-8	-3	2	16.92	-31.28	85.93	9	-1	2	22.07	50.16	65.23	4	2	2	4151.07	4068.26	161.61
-7	-3	2	0.24	15.15	79.21	10	-1	2	349.75	356.76	64.61	5	2	2	530.32	474.14	43.34
-6	-3	2	1498.55	1411.68	99.45	-9	0	2	171.81	233.24	41.85	6	2	2	4220.53	3827.46	164.68
-5	-3	2	3.52	-7.78	49.38	-8	0	2	0.30	-27.08	79.84	7	2	2	6.13	-56.18	70.98
-4	-3	2	133.65	90.45	25.27	-7	0	2	1625.81	1677.04	83.73	8	2	2	208.86	211.70	48.73
-3	-3	2	2167.26	1879.05	85.81	-6	0	2	143.11	138.10	25.26	9	2	2	30.69	9.39	53.06
-2	-3	2	154.69	118.78	18.99	-5	0	2	1392.78	1335.42	59.74	10	2	2	49.68	73.02	59.80
-1	-3	2	3954.16	3540.57	123.56	-4	0	2	782.54	629.81	41.25	-9	3	2	79.40	-26.69	106.78
0	-3	2	15139.01	13455.12	420.76	-3	0	2	2.23	-1.54	19.31	-8	3	2	380.79	272.10	57.42
1	-3	2	2245.41	1884.30	74.89	-2	0	2	17354.32	18007.81	393.86	-7	3	2	106.26	151.20	45.02
2	-3	2	942.32	1063.23	55.33	-1	0	2	5535.70	5565.04	128.15	-6	3	2	990.26	1163.32	94.27
3	-3	2	3712.80	4036.73	148.69	0	0	2	25326.56	26803.02	590.67	-5	3	2	1034.22	1005.40	80.76
4	-3	2	837.34	762.32	62.68	1	0	2	112.88	41.60	6.29	-4	3	2	225.10	184.46	28.84
5	-3	2	48.49	45.53	30.26	2	0	2	12417.18	12365.35	272.44	-3	3	2	9301.80	9339.87	308.04
6	-3	2	299.59	345.33	41.60	3	0	2	19.18	11.56	21.36	-2	3	2	7778.83	8261.26	269.94
7	-3	2	34.35	8.81	68.38	4	0	2	472.81	546.35	45.24	-1	3	2	8540.93	9131.53	290.76

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	1700.23	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	134.25	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	1324.66	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	55.34	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	22.60	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	3977.22	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	251.39	49.01	6	7	2	1858.44	2109.00	125.63	-6	11	2	40.91	66.50	91.88
9	4	2	295.93	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	-83.45	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	78.18	1	11	2	493.87	587.25	57.76
-4	5	2	46.52	77.81	29.34	-4	8	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	8	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	8	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	8	2	58.55	103.78	28.00	5	11	2	65.18	-1.48	85.05
0	5	2	3342.50	2791.69	110.95	0	8	2	68.72	6.60	47.81	6	11	2	271.65	278.48	51.66
1	5	2	3193.70	2877.64	109.66	1	8	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	8	2	3212.94	3240.94	135.31	8	11	2	0.27	-133.01	103.63
3	5	2	1150.98	1025.20	62.41	3	8	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	8	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	8	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	8	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	8	2	184.80	209.12	47.31	-2	12	2	15.58	38.97	74.19
8	5	2	1.74	16.21	78.97	8	8	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	8	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	466.04	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	58.32

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)
6	12	2	0.17	-182.56	93.69	-4	-16	3	126.33	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	36.08	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	98.33	22.01	74.54	-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	3814.82	3869.93	187.50
3	13	2	183.30	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	101.37
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	109.82	192.56	55.26	-6	-14	3	120.27	232.40	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	0.66	-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	655.61	59.25
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	105.67	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	884.54	806.40	73.34	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	681.18	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	100.89
0	15	2	88.46	151.22	54.89	-3	-13	3	80.96	22.94	88.28	-7	-9	3	133.60	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	450.84	60.80	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	220.39	314.27	51.41	-2	-9	3	447.55	513.26	42.42
6	15	2	37.65	180.03	59.88	3	-13	3	3.70	-44.50	86.49	-1	-9	3	939.18	904.09	78.47
-2	16	2	0.31	-172.34	100.50	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	-33.05	94.93	-5	-12	3	52.88	-36.17	91.81	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	110.86	-1	-12	3	29.57	-40.23	74.68	8	-9	3	377.69	431.42	71.10
0	17	2	21.53	91.23	114.11	0	-12	3	84.08	75.49	46.32	-8	-8	3	304.95	281.80	63.29
1	17	2	207.08	229.84	62.79	1	-12	3	162.19	112.94	45.67	-7	-8	3	323.73	405.55	55.70
2	17	2	53.64	56.76	110.02	2	-12	3	13.77	-52.82	74.54	-6	-8	3	2111.25	1966.80	134.86
3	17	2	293.36	242.93	52.91	3	-12	3	21.80	68.48	60.03	-5	-8	3	421.34	440.87	47.56
-2	-17	3	27.25	125.46	84.00	4	-12	3	12.19	17.25	81.81	-4	-8	3	66.17	35.78	64.58
-1	-17	3	87.77	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	44.68	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	20.11	-1	-2	3	367.15	818.88	44.37
2	-8	3	4426.72	4727.47	185.81	2	-5	3	1900.10	2075.22	93.82	0	-2	3	1665.99	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	4617.98	4989.59	169.82
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	-2	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	-2	3	13.29	-23.18	91.88
-6	-7	3	211.41	182.99	47.71	-7	-4	3	352.89	294.02	50.39	-9	-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	-8	-1	3	642.41	583.50	58.95
-4	-7	3	937.86	824.94	77.96	-5	-4	3	48.38	10.66	60.69	-7	-1	3	156.07	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	6562.78	235.45	-3	-4	3	847.34	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	3937.62	144.79
1	-7	3	4979.51	4587.85	174.85	0	-4	3	6138.41	6113.00	207.37	-2	-1	3	5950.39	6103.15	203.39
2	-7	3	1773.49	1995.41	100.16	1	-4	3	47.36	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	20874.64	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	135.53	96.42	28.53	2	-1	3	6391.60	7153.06	231.47
6	-7	3	137.24	96.14	46.58	5	-4	3	3.20	23.96	51.34	3	-1	3	3651.81	3833.60	138.55
7	-7	3	8.00	-40.98	84.34	6	-4	3	253.47	266.46	41.19	4	-1	3	5.06	51.38	81.87
8	-7	3	1739.29	1987.25	142.72	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	27.80	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	23.56	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	495.42	58.38
-4	-6	3	3171.11	3163.15	139.32	-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	1548.30	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	1610.86	1524.72	84.80	-7	0	3	1144.55	1277.73	75.46
-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	1249.81	1371.77	75.95	-1	-3	3	5684.29	5593.56	187.65	-4	0	3	1393.01	1562.34	58.61
2	-6	3	4.67	-62.18	43.66	0	-3	3	6222.32	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	18014.17	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	63.77
5	-6	3	134.24	-18.78	68.34	3	-3	3	235.08	185.64	24.62	0	0	3	2001.56	7560.50	567.27*
6	-6	3	157.01	140.44	42.30	4	-3	3	1481.80	1509.82	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	1260.40	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	88.41	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	326.14	351.46	55.58	8	0	3	611.82	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	566.15	45.51
-4	-5	3	509.64	562.78	46.25	-6	-2	3	3546.01	3805.94	171.01	10	0	3	6.00	6.28	61.76
-3	-5	3	197.56	132.58	25.71	-5	-2	3	25.52	37.33	56.75	-8	1	3	92.63	34.16	101.45
-2	-5	3	572.20	520.09	51.63	-4	-2	3	29.81	-57.24	45.56	-8	1	3	608.86	597.36	89.78

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	39.17
-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	240.64	-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	383.76	465.33	48.29	-7	7	3	0.1[illegible]	70.45	89.84
0	1	3	13424.77	14329.25	433.89	-5	4	3	316.18	322.79	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	-29.38	71.14
2	1	3	22676.71	23484.72	710.05	-3	4	3	28.52	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	783.56	56.06	-3	7	3	434.98	389.68	38.39
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	1961.52	97.41	0	4	3	1680.42	1617.78	74.31	-1	7	3	4915.87	4694.40	176.45
6	1	3	302.19	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	504.58	474.00	45.58	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	155.32
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	46.91	106.97	5	4	3	1190.26	1209.81	80.58	4	7	3	1203.65	1231.80	82.80
-9	2	3	3.70	-27.00	100.60	6	4	3	66.56	90.01	56.01	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	209.24	41.96
-7	2	3	31.37	-96.95	85.64	8	4	3	268.29	301.57	51.8[illegible]	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	9.5[illegible]	-23.01	84.16	-7	8	3	2.80	-101.78	98.42
-2	2	3	1233.05	1271.35	62.74	-6	5	3	168.26	186.54	43.90	-6	8	3	35.72	60.03	47.53
-1	2	3	26984.09	28552.22	872.24	-5	5	3	415.14	463.94	43.71	-5	8	3	1491.45	1639.35	115.23
0	2	3	35.74	-2.77	24.49	-4	5	3	95.47	28.62	59.13	-4	8	3	810.69	843.51	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	146.75	-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	103.17	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	73.42
-9	3	3	148.54	72.96	109.50	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	79.24	8	5	3	15.34	-92.83	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	16.85	-4.98	55.53	-8	6	3	182.91	18.81	100.57	-6	9	3	584.72	560.82	60.58
-4	3	3	1298.46	1116.34	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	181.15	-6	6	3	401.94	357.84	51.50	-4	9	3	373.65	380.41	46.97
-2	3	3	2510.74	2927.04	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	167.72	-4	6	3	217.01	226.50	34.27	-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	1685.55	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	63.22	31.40
4	3	3	487.45	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	1172.92	94.60
6	3	3	61.34	87.38	33.49	3	6	3	3768.57	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	87.14	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	14.53	25.69	102.27
8	9	3	31.05	-95.53	98.94	1	13	3	150.50	25.57	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	-40.96	114.97
-7	10	3	172.77	225.14	62.91	3	13	3	19.28	71.08	76.79	-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	54.7	-5	-14	4	478.62	490.91	68.48
-5	10	3	25.43	-1.36	87.07	5	13	3	180.35	108.22	54.59	-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	2629.18	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	216.72	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	421.35	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	681.40	54.80	1	14	3	100.35	-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	56.36
5	10	3	80.41	93.10	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	59.39	-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	394.36	56.53
-3	11	3	208.10	226.20	46.78	0	15	3	2.32	-87.76	94.34	2	-13	4	110.60	68.51	87.95
-2	11	3	425.31	493.53	50.61	1	15	3	1.61	.51	51.31	3	-13	4	677.90	615.07	63.00
-1	11	3	1437.00	1430.45	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	109.33	38.93	6	15	3	323.29	372.89	56.66	-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	28.43	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	68.13	-2	-12	4	55.30	118.40	49.93
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	1202.61	110.75
-4	12	3	149.57	105.70	53.65	5	16	3	93.72	128.50	62.05	3	-12	4	510.00	364.41	54.83
-3	12	3	29.30	2.94	79.04	0	17	3	116.13	23.25	124.27	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	82.49	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	1361.53	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	212.07	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	43.64	150.07	41.44
-5	13	3	2.52	-67.90	98.30	-3	-15	4	3.38	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	139.15	-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	[illegible]	-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	33.25
-6	-10	4	11.96	-173.00	[illegible]	-2	-7	4	1687.02	1820.17	99.37	-3	-4	4	232.26	175.73	27.75
-5	-10	4	392.12	374.58	[illegible]	-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	78.36	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	471.45	35.00
-2	-10	4	398.06	403.51	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	32.94	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	72.50	161.63	59.60	7	-4	4	22.[illegible]	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	241.18	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	408.26	374.02	31.45
-1	-9	4	85.26	55.97	56.77	1	-6	4	5479.51	5041.93	185.43	-1	-3	4	23.88	25.19	30.86
0	-9	4	2820.24	2[illegible]9.83	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	51.36	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	67.99	-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	83.78	-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	2409.05	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	1295.05	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	1000.32	93.33	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	46.15	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	619.26	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	129.90	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	56.35	22.59	-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	884.83	608.49	62.88
-1	-1	4	2078.68	1908.14	77.22	-6	2	4	1064.88	1281.35	92.67	10	4	4	5.51	86.30	104.55
0	-1	4	9382.40	-10855.10	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	119.94	-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	57.40	-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	59.79	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	8360.54	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	167.15	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	5068.14	4467.61	180.91
-6	0	4	12.05	15.24	45.32	9	2	4	47.41	-18.91	99.49	6	5	4	346.81	315.78	40.35
-5	0	4	328.43	369.75	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	57.00	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	4762.36	117.37	-5	3	4	1286.45	1380.76	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	19.92	-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	211.62	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	188.35
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	88.88
7	0	4	30.80	51.63	31.20	2	3	4	1829.48	1676.32	72.39	0	6	4	1293.06	1151.80	71.[illegible]
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.[illegible]
9	0	4	944.54	837.95	54.29	4	3	4	976.99	952.46	64.37	2	6	4	5626.19	5640.47	199.87
10	0	4	0.20	-92.24	77.00	5	3	4	6333.22	6126.36	224.56	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	98.96	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	339.42	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	253.70	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	48.06
-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	85.86
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	339.76	-2	4	4	1336.54	1445.45	75.13	-3	7	4	3827.02	3995.94	167.69
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	3092.06	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	77.31	4	14	4	88.21	-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	603.26	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	116.90
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	1111.13	1118.69	86.53	-4	11	4	220.65	80.03	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	99.27	1	11	4	1278.59	1216.10	98.56	4	15	4	240.34	238.75	59.03
-3	8	4	2129.40	2061.53	117.36	2	11	4	1024.59	1161.65	93.07	5	15	4	8.12	52.14	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	491.41	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	0.58	-40.94	98.73
1	8	4	4656.39	4806.48	182.71	6	11	4	29.63	-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	43.54	-70.11	103.54
4	8	4	361.10	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	41.22	-59.56	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	324.79	65.60
-7	9	4	30.38	66.05	100.96	0	12	4	673.78	605.12	53.97	3	17	4	93.99	129.57	64.70
-6	9	4	0.[illegible]	-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	5.8[illegible]	10.87	79.91	2	12	4	24.48	11.25	68.80	-2	-16	5	77.61	-100.80	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	39.59	65.43	5	12	4	30.26	35.50	60.12	1	-16	5	42.23	-60.94	118.33
-1	9	4	1618.64	1490.64	90.97	6	12	4	254.76	289.69	55.18	2	-16	5	120.61	127.86	69.79
0	9	4	3763.97	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	35.89	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	97.98	-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	45.66	8.27	62.13
5	9	4	36.75	-50.51	66.09	-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	25.39	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	35.91	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	-44.53	100.43
-6	10	4	8.34	76.58	86.85	4	13	4	173.40	139.51	51.21	-2	-14	5	283.12	428.69	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	70.63	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	10	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	4.46	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	325.72	224.37	54.62	-4	-13	5	246.48	220.25	55.88
4	10	4	545.22	523.19	47.23	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	587.83	553.87	59.75	-5	-9	5	345.68	452.07	48.77	-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	58.05	1	-6	5	2804.72	2973.35	127.34
1	-13	5	928.40	1082.85	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	1324.42	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	5508.60	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	258.81	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	58.06	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	-8	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	309.[illegible]	57.08	-2	-8	5	581.03	560.87	51.60	0	-5	5	2190.42	2860.01	120.91
6	-12	5	84.77	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	39.36	-60.24	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	[illegible]	39.27	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	46.28	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	107.38	42.10	-8	-7	5	28.19	54.85	100.89	-8	-4	5	470.48	533.76	81.88
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	71.85
-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	2030.31	1680.60	98.15	0	-4	5	1246.54	1554.18	76.92
-4	-10	5	6.07	[illegible].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	35.74	36.05	2	-4	5	47.50	14.41	38.08
-2	-10	5	9.60	-28.13	67.50	3	-7	5	1325.52	1279.75	87.82	3	-4	5	41.87	70.15	24.81
-1	-10	5	703.91	547.72	51.27	[illegible]	-7	5	47.95	119.31	37.00	4	-4	5	3.98	21.88	50.99
0	-10	5	203.49	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	66.45	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	1703.54	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	108.16	-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	1782.26	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	63.42	-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	629.06	-1166.58	124.63*	-4	3	5	518.57	654.15	67.95
4	-3	5	284.96	361.57	32.60	1	0	5	300.18	339.33	20.83	-3	3	5	4614.23	5353.58	197.59
5	-3	5	451.75	373.40	35.49	2	0	5	9670.67	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	403.63	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	489.81	46.61
8	-3	5	387.23	326.77	54.38	5	0	5	2300.98	2283.62	101.60	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	84.05	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	-69.23	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	2377.58	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	53.18	-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	-34.24	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	983.13	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	86.35
-7	-1	5	208.69	221.18	83.90	8	1	5	487.64	444.79	54.03	5	4	5	92.92	94.25	32.52
-6	-1	5	63.27	20.98	74.47	9	1	5	196.58	368.14	56.98	6	4	5	480.04	464.68	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	10389.97	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	215.95	-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	450.80	-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	28.45	-1	5	5	379.62	281.29	26.80
7	-1	5	17.63	-38.03	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	2306.08	102.97
-9	0	5	93.93	212.41	71.11	6	2	5	1439.63	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	187.37	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	83.89	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	380.24	406.35	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	74.17	9	8	5	281.42	422.06	60.34	1	12	5	50.89	-50.13	72.58
9	5	5	67.26	37.75	95.13	-7	9	5	4.57	-92.99	101.24	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	89.55	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	94.47	131.87	61.84
-3	6	5	1738.16	1848.36	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	56.39
1	6	5	702.31	605.05	52.56	4	9	5	176.61	155.87	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	81.00
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	94.06	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	186.89	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	59.51
9	6	5	158.36	62.49	101.51	-4	10	5	410.89	496.81	52.82	7	13	5	58.14	125.20	60.29
-8	7	5	346.57	337.40	67.87	-3	10	5	309.45	396.58	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	80.30
-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	24.30	17.76	87.95
-1	7	5	76.33	113.50	30.37	4	10	5	825.18	823.42	65.85	3	14	5	12.05	84.04	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	880.72	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	73.53	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	522.92	54.63	1	11	5	49.46	42.33	46.96	5	15	5	225.08	230.94	63.12
-4	8	5	1366.08	1232.63	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	3872.69	164.70	4	11	5	568.48	612.87	52.13	-1	16	5	41.12	81.78	56.18
-1	8	5	8191.19	7970.97	427.55	5	11	5	141.86	150.23	48.53	0	16	5	229.77	349.39	61.43
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	53.15	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
-1	-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	105.31	4	-11	6	20.29	65.99	89.50	-5	-7	6	250.42	235.67	47.34
-4	-15	6	132.91	225.43	66.70	5	-11	6	11.17	35.23	91.00	-4	-7	6	1656.63	1815.04	113.81
-3	-15	6	11.48	-114.60	109.30	6	-11	6	17.36	-7.00	103.17	-3	-7	6	93.79	137.91	34.76
-2	-15	6	121.90	233.05	56.49	-7	-10	6	340.42	22.37	118.69	-2	-7	6	394.96	500.22	49.17
-1	-15	6	168.22	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	537.72	50.79
1	-15	6	43.71	67.81	101.86	-4	-10	6	64.34	-115.57	86.62	1	-7	6	3055.03	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	306.58	36.75
3	-15	6	31.70	146.08	60.80	-2	-10	6	0.27	-15.87	72.02	3	-7	6	3557.53	3547.68	154.90
-6	-14	6	305.29	286.65	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	376.51	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	462.14	50.86	8	-7	6	16.91	92.73	55.99
0	-14	6	32.76	-10.72	89.03	4	-10	6	0.94	-176.47	80.58	-8	-6	6	11.14	93.90	100.64
1	-14	6	0.14	-136.51	99.61	5	-10	6	591.74	610.92	60.37	-7	-6	6	89.72	41.37	87.38
2	-14	6	0.01	-99.77	100.91	6	-10	6	95.40	-15.20	98.71	-6	-6	6	12.18	35.42	44.13
3	-14	6	18.86	-41.24	95.96	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	536.79	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	86.69
-4	-13	6	458.33	591.78	64.76	-5	-9	6	51.89	43.96	57.19	-1	-6	6	1554.96	1554.94	93.91
-3	-13	6	241.74	235.77	57.68	-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	-6	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	23.17	-99.28	90.74	-1	-9	6	468.63	498.77	51.29	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	68.27	62.54	35.65
2	-13	6	415.30	392.16	58.57	1	-9	6	339.85	384.61	43.39	5	-6	6	333.79	316.40	42.77
3	-13	6	311.75	310.82	59.31	2	-9	6	2092.39	1842.35	113.56	6	-6	6	205.72	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	9	-6	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	128.07	61.18	-7	-5	6	72.75	46.39	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	143.06	-5	-5	6	1789.08	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	128.38
0	-12	6	176.59	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	450.07	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	86.53	-3	-8	6	1323.92	1510.55	107.07	0	-5	6	736.58	979.75	66.84
4	-12	6	136.74	18.24	99.11	-2	-8	6	25.54	-36.76	60.76	1	-5	6	3203.27	3321.68	136.15
5	-12	6	110.89	187.95	55.55	-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	32.73	69.74
-5	-11	6	100.73	59.29	96.45	3	-8	6	167.17	217.73	41.51	6	-5	6	949.52	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	758.44	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	75.30	6	-8	6	18.48	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	229.20	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	45.31	-8	-7	6	35.18	84.99	103.99	-6	-4	6	664.99	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	2553.34	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	2	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	2627.87	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	1132..64	368.17	0	2	6	7509.42	6637.10	225.69
6	-4	6	1448.32	1872.22	117.07	4	-1	6	350.53	375.46	32.75	1	2	6	1083.27	992.84	56.02
7	-4	6	343.53	328.64	51.21	5	-1	6	1645.86	1396.14	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	86.66	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	56.86	66.02	6	2	6	78.70	98.43	35.46
-7	-3	6	39.37	8.79	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	270.14	33.67	-7	0	6	203.38	239.38	36.06	10	2	6	1.18	-270.59	109.61
-3	-3	6	118.19	126.02	29.65	-6	0	6	107.77	106.62	29.37	-8	3	6	16.34	-24.82	96.83
-2	-3	6	2379.26	2280.81	104.98	-5	0	6	5.59	-14.70	35.05	-7	3	6	19.30	-24.63	82.21
-1	-3	6	3035.23	2469.88	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	1830.92	61.45	-3	3	6	482.65	403.88	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	96.24	-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	368.38	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	61.48	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	82.64	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	8423.42	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	2445.28	2153.92	98.64	-5	1	6	2142.28	2129.08	117.28	-7	4	6	128.19	25.00	89.96
-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	143.45	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	665.65	66.05	-3	11	6	261.66	266.06	48.27
8	4	6	0.18	-132.11	84.19	8	7	6	1417.27	1576.98	133.82	-2	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	103.92	-6	8	6	952.99	1051.58	90.33	1	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	2	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	14.23	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	36.61	-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	2846.78	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	-68.00	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	207.10	4	8	6	85.10	34.65	57.29	-3	12	6	399.54	460.68	56.58
3	5	6	14307.09	14501.41	470.49	5	8	6	224.44	186.65	41.02	-2	12	6	289.05	307.63	58.80
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	107.26
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	101.07
6	5	6	529.07	602.71	55.82	8	8	6	12.87	46.09	86.44	1	12	6	1867.95	1826.97	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	78.52
8	5	6	237.64	362.92	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	64.3[illegible]	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	66.65
-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	100.01	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	2584.42	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	425.32	49.04	3	13	6	5.13	-73.60	82.61
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	1491.10	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	34.78	-56.70	105.58
9	6	6	226.32	222.08	59.84	-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	61.57	0	14	6	72.34	-57.81	96.12
-5	7	6	2309.38	2225.68	136.43	0	10	6	79.00	67.05	13.61	1	14	6	258.41	294.52	55.97
-4	7	6	195.68	214.21	42.09	1	10	6	308.01	212.21	48.19	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	1537.43	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	-103.98	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	187.60	87.82	-3	-11	7	153.36	186.85	48.37	7	-8	7	2.27	-45.80	95.95
5	15	6	273.65	308.22	67.40	-2	-11	7	136.24	203.25	49.13	8	-8	7	8.69	79.73	101.44
6	15	6	158.31	18.09	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	46.68	-13.62	112.98	1	-11	7	211.68	167.08	49.18	-6	-7	7	308.33	388.60	54.41
1	16	6	79.56	-129.48	108.17	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	60.62	69.56	43.64	-4	-7	7	996.05	956.17	70.44
3	16	6	26.61	24.97	60.42	4	-11	7	1034.52	1192.33	114.99	-3	-7	7	2095.96	2200.31	124.17
4	16	6	54.32	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	62.31	-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	423.51	368.94	37.95
0	-16	7	141.95	207.28	67.43	-6	-10	7	0.19	-12.22	98.68	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	192.02	81.56	107.62	-3	-10	7	6.59	39.22	78.94	4	-7	7	1289.28	1402.30	101.29
0	-15	7	27.38	45.77	57.23	-2	-10	7	1231.48	1364.81	112.47	5	-7	7	74.26	-19.83	77.52
1	-15	7	3.0.	-5.79	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	102.14	111.15	2	-10	7	177.29	227.04	46.79	-8	-6	7	176.83	33.75	63.93
-3	-14	7	97.34	-33.61	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	237.42	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	59.37	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	-33.48	115.25	-4	-9	7	464.27	437.58	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	1147.74	99.46	4	-6	7	482.38	696.45	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	162.49	-108.78	105.65
3	-13	7	4.15	-54.49	98.12	4	-9	7	762.75	853.98	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	243.55
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	183.55	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)
9	-5	7	119.87	135.76	63.00	-8	-1	7	50.95	57.94	96.23	9	1	7	308.20	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	2[illegible].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	321.00	280.84	55.09
-5	-4	7	900.63	1260.56	98.13	-4	-1	7	3581.61	3951.65	166.55	-6	2	7	203.48	8.54	82.06
-4	-4	7	0.06	-27.21	60.33	-3	-1	7	155.36	209.54	31.82	-5	2	7	3202.30	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	1144.78	1144.95	89.38
-2	-4	7	6443.53	6401.13	232.42	-1	-1	7	6238.29	6769.67	235.12	-3	2	7	6047.72	6078.22	224.72
-1	-4	7	1823.94	1941.15	97.54	0	-1	7	2.47	-1469.24	150.72*	-2	2	7	2052.20	2161.95	102.87
0	-4	7	7259.71	7760.04	269.04	1	-1	7	3271.90	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	334.19	464.78	46.76	0	2	7	1839.54	2167.98	97.88
2	-4	7	831.03	980.82	67.46	3	-1	7	171.68	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	44.76	81.76	28.48	2	2	7	1057.69	1040.93	61.98
4	-4	7	111.82	46.89	53.13	5	-1	7	0.08	-54.66	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	231.07	43.02	7	-1	7	26.09	29.17	42.23	5	2	7	76.43	114.21	31.78
7	-4	7	34.34	-48.53	78.78	8	-1	7	42.83	38.93	82.31	6	2	7	23.87	-55.58	61.49
8	-4	7	134.31	72.14	93.75	9	-1	7	150.21	16.12	99.49	7	2	7	449.86	428.00	48.38
9	-4	7	14.82	71.51	59.42	10	-1	7	6.86	72.67	111.62	8	2	7	326.56	300.69	53.19
-8	-3	7	44.89	-122.59	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	151.79	237.25	37.48	10	2	7	436.40	395.10	67.39
-6	-3	7	5.07	18.83	77.39	-6	0	7	706.82	737.65	49.05	-8	3	7	15.72	-6.20	99.43
-5	-3	7	1783.24	1621.51	114.73	-5	0	7	1263.62	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	397.16	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	668.32	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	87.00	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	658.01	38.01	1	3	7	331.07	395.04	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	2382.61	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	44.22	4	3	7	473.68	386.92	33.20
7	-3	7	3.72	-85.06	79.21	7	0	7	2864.90	2843.89	106.65	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	56.22	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	8	3	7	1338.57	1542.00	121.06
-7	-2	7	256.63	293.90	71.32	-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	40.31	-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	30.01	-5	4	7	291.39	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	2490.01	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	490.15	2	1	7	5607.82	5193.65	183.16	0	4	7	6617.52	7334.60	285.37
4	-2	7	17.16	16.49	38.11	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	1569.87	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	2581.49	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	183.04	55.88	8	1	7	203.20	297.74	51.48	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	7.82	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	79.37	58.59	1	11	7	167.09	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	99.03	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	9.62	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	80.55
-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	2952.50	2583.02	132.37	8	11	7	313.94	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	7.81	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	475.55	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	86.85
2	5	7	214.22	196.03	26.90	5	8	7	89.31	72.79	39.56	0	12	7	116.11	165.42	49.32
3	5	7	564.19	539.96	44.33	6	8	7	1.41	-32.27	74.39	1	12	7	221.89	190.47	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	45.52
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	712.66	727.81	61.99
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	58.08	7	12	7	327.09	406.00	64.07
10	5	7	65.04	30.68	110.73	-3	9	7	345.39	396.24	47.51	8	12	7	47.20	-99.64	111.56
-7	6	7	12.84	13.03	93.49	-2	9	7	1181.28	1325.22	105.24	-4	13	7	5.26	-83.02	101.27
-6	6	7	470.57	523.04	56.29	-1	9	7	384.07	417.70	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	2017.65	126.07	1	9	7	367.37	423.75	42.17	-1	13	7	205.99	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	22.55	4	13	7	56.14	19.66	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	1431.26	87.41	8	9	7	735.47	760.48	69.15	6	13	7	6.59	8.00	100.98
4	6	7	2683.97	2416.06	113.32	9	9	7	58.00	-68.40	101.74	7	13	7	9.06	-31.31	109.66
5	6	7	155.64	154.91	35.96	-6	10	7	92.32	-65.15	108.54	-3	14	7	15.78	31.14	104.10
6	6	7	3.90	-16.07	71.30	-5	10	7	321.41	228.65	59.19	-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	56.89	-3	10	7	317.39	276.41	51.24	0	14	7	5.35	67.45	55.46
9	6	7	146.92	69.66	105.38	-2	10	7	448.20	350.19	51.65	1	14	7	1016.11	971.96	98.19
-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	123.88	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	144.59	102.52	40.85	6	14	7	60.70	131.01	87.64
-2	7	7	700.71	566.10	53.00	4	10	7	517.23	430.65	47.75	-2	15	7	263.75	284.19	64.49
-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	103.36
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	79.19	-1	11	7	199.75	165.05	47.06	0	16	7	7.03	93.03	106.23

Structure Factors Table (continued) (*=unobserved reflns.) for C(14) H(30) Cl(2) Cu(1) N(8) 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)
1	16	7	636.72	593.39	69.29	-6	-10	8	32.06	-90.35	100.40	3	-7	8	0.24	-43.57	50.58
2	16	7	368.00	288.58	63.93	-5	-10	8	495.33	606.55	61.60	4	-7	8	2320.75	2210.47	127.17
3	16	7	84.55	89.65	105.73	-4	-10	8	63.21	139.80	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	-15	8	1.91	-249.72	115.97	-2	-10	8	172.61	264.29	49.14	7	-7	8	211.33	239.50	55.52
-2	-15	8	23.44	62.47	108.56	-1	-10	8	109.24	-19.90	79.55	8	-7	8	6.65	36.12	101.35
-1	-15	8	57.93	-158.84	108.88	0	-10	8	260.33	187.54	51.41	-8	-6	8	24.85	78.53	105.32
0	-15	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	-15	8	27.41	79.94	113.29	2	-10	8	1.83	56.23	82.24	-6	-6	8	7.76	-30.46	91.70
2	-15	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	52.59	-3	-6	8	169.32	173.18	40.50
-2	-14	8	426.30	505.78	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	5.13	-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	452.38	51.13	4	-6	8	0.27	-34.11	67.16
-5	-13	8	212.20	70.58	83.22	-2	-9	8	314.83	276.13	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	34.75	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	56.29	100.72	2	-9	8	2446.77	2329.80	136.56	-8	-5	8	54.41	-71.26	105.03
0	-13	8	95.97	-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	-26.62	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	-141.00	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	-2	-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	393.88	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	41.01	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	91.72	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	181.71	58.23	-6	-4	8	187.57	234.15	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	68.38	-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	491.39	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	131.80	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	3.04	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	767.38	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	328.42	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	8	425.71	559.67	50.74	7	-1	8	1162.98	1127.17	102.63	6	2	8	164.62	177.73	40.35
7	-4	8	714.19	1040.34	107.14	8	-1	8	528.39	529.73	58.69	7	2	8	1753.52	1698.54	117.07
8	-4	8	150.33	85.50	97.47	9	-1	8	80.66	71.33	102.92	8	2	8	31.78	-28.47	89.49
9	-4	8	18.94	-31.58	108.70	-8	0	8	173.90	112.98	42.71	9	2	8	197.31	226.51	56.01
-8	-3	8	321.34	225.40	64.45	-7	0	8	314.90	340.94	39.28	10	2	8	18.78	111.26	58.74
-7	-3	8	90.73	37.83	97.82	-6	0	8	19.12	87.98	39.39	-8	3	8	34.27	-115.05	107.02
-6	-3	8	92.12	109.85	47.25	-5	0	8	137.99	201.15	50.38	-7	3	8	148.49	170.41	52.82
-5	-3	8	0.95	-7.00	75.92	-4	0	8	78.03	98.88	24.63	-6	3	8	1.22	32.42	74.27
-4	-3	8	1152.06	984.74	93.84	-3	0	8	1454.91	1655.25	68.97	-5	3	8	142.90	119.83	42.24
-3	-3	8	2653.25	2442.57	124.23	-2	0	8	5147.54	4731.27	128.81	-4	3	8	807.41	904.53	84.94
-2	-3	8	2315.34	2538.06	123.03	-1	0	8	2290.64	2344.18	83.86	-3	3	8	27.62	6.12	55.58
-1	-3	8	9843.07	8083.79	306.86	0	0	8	10546.02	9271.96	285.73	-2	3	8	3339.80	3352.49	146.92
0	-3	8	1164.54	1114.51	76.01	1	0	8	36.98	117.65	17.25	-1	3	8	6594.74	6259.64	227.27
1	-3	8	9091.70	7909.96	274.28	2	0	8	4670.41	4583.41	120.01	0	3	8	1737.50	1925.26	95.29
2	-3	8	660.06	517.89	43.62	3	0	8	247.71	323.08	22.66	1	3	8	11552.33	11171.78	367.70
3	-3	8	115.31	21.17	51.79	4	0	8	168.32	117.11	20.34	2	3	8	1813.07	1954.35	93.04
4	-3	8	24.67	86.06	30.91	5	0	8	79.83	19.46	42.20	3	3	8	381.28	351.76	32.15
5	-3	8	539.36	488.92	44.72	6	0	8	2234.72	2040.71	104.45	4	3	8	704.30	611.84	46.99
6	-3	8	308.57	450.34	48.03	7	0	8	267.45	286.92	33.82	5	3	8	1671.26	1757.00	104.04
7	-3	8	43.30	114.03	45.51	8	0	8	195.23	1.70	65.21	6	3	8	466.67	501.31	48.01
8	-3	8	20.06	-103.28	85.27	9	0	8	54.36	69.42	56.58	7	3	8	183.54	144.39	44.53
9	-3	8	112.65	112.84	58.49	10	0	8	403.61	474.25	49.30	8	3	8	11.92	-17.51	82.54
-8	-2	8	98.44	273.48	98.85	-8	1	8	20.76	-29.44	108.91	9	3	8	331.20	349.23	60.45
-7	-3	8	1.05	-43.38	91.93	-7	1	8	49.43	70.01	50.31	10	3	8	0.10	-26.01	114.76
-6	-2	8	137.88	189.23	48.56	-6	1	8	305.40	227.61	47.36	-8	4	8	40.14	-83.58	105.43
-5	-2	8	362.30	425.67	46.62	-5	1	8	496.71	552.67	50.81	-7	4	8	2.96	-47.31	94.16
-4	-2	8	1209.37	1143.61	90.08	-4	1	8	311.39	253.00	38.38	-6	4	8	145.00	-40.75	87.23
-3	-2	8	1674.61	1656.59	101.24	-3	1	8	1814.16	1672.35	94.46	-5	4	8	184.09	121.23	46.44
-2	-2	8	6294.50	6370.66	231.87	-2	1	8	2921.34	2635.86	121.92	-4	4	8	2.39	46.58	67.64
-1	-2	8	191.67	192.60	30.61	-1	1	8	625.96	561.20	57.98	-3	4	8	844.69	798.05	57.26
0	-2	8	2436.82	-6194.21	219.43*	0	1	8	9821.76	10032.21	338.69	-2	4	8	883.24	677.26	70.44
1	-2	8	67.34	67.84	25.56	1	1	8	201.93	173.04	26.36	-1	4	8	5290.54	5002.07	193.87
2	-2	8	46.44	29.20	43.90	2	1	8	282.73	225.37	28.18	0	4	8	58.58	2.15	35.07
3	-2	8	229.35	375.70	36.26	3	1	8	766.34	673.45	59.62	1	4	8	446.70	456.70	39.73
4	-2	8	70.74	23.14	50.91	4	1	8	2078.24	2091.08	105.70	2	4	8	66.75	31.55	44.90
5	-2	8	156.34	128.64	34.64	5	1	8	31.69	64.88	31.80	3	4	8	0.70	-66.53	47.09
6	-2	8	1249.26	1523.38	104.54	6	1	8	2789.23	2821.94	140.78	4	4	8	1076.97	1174.60	77.82
7	-2	8	791.41	799.26	70.78	7	1	8	720.63	763.49	68.12	5	4	8	622.64	580.56	53.98
8	-2	8	467.68	428.29	60.38	8	1	8	408.11	435.26	53.99	6	4	8	32.51	-13.11	66.65
9	-2	8	403.61	280.30	62.17	9	1	8	366.54	426.78	61.32	7	4	8	420.49	486.55	49.99
-8	-1	8	44.23	16.34	103.21	10	1	8	0.47	-87.68	102.89	8	4	8	337.10	404.69	54.04
-7	-1	8	156.16	143.93	53.80	-8	2	8	88.52	77.54	109.69	9	4	8	36.44	40.44	67.72
-6	-1	8	843.91	725.89	72.23	-7	2	8	10.35	55.86	44.78	10	4	8	53.18	156.40	61.17
-5	-1	8	3.82	56.23	68.71	-6	2	8	390.94	394.52	51.27	-7	5	8	205.58	112.64	59.34
-4	-1	8	747.67	687.67	56.53	-5	2	8	318.93	416.28	47.20	-6	5	8	99.72	44.51	87.03
-3	-1	8	128.16	55.57	59.69	-4	2	8	419.96	341.67	39.82	-5	5	8	49.06	-147.51	81.72
-2	-1	8	446.12	657.72	64.28	-3	2	8	2212.73	2102.95	113.09	-4	5	8	575.25	555.70	51.25
-1	-1	8	3830.09	4412.35	171.38	-2	2	8	3357.59	3553.34	149.46	-3	5	8	99.01	148.36	35.82
0	-1	8	2333.91	1925.87	107.28	-1	2	8	284.87	319.87	31.76	-2	5	8	1412.25	1348.15	87.93
1	-1	8	104.86	136.60	25.11	0	2	8	1147.93	1111.65	84.93	-1	5	8	122.97	146.17	32.26
2	-1	8	2214.67	2701.08	115.36	1	2	8	125.90	111.91	26.40	0	5	8	463.61	448.15	45.55
3	-1	8	397.82	359.08	35.77	2	2	8	1186.24	1204.11	69.96	1	5	8	676.95	825.26	65.22
4	-1	8	1405.05	1390.88	86.69	3	2	8	452.10	474.33	39.96	2	5	8	6.26	-98.87	49.22
5	-1	8	227.71	282.56	34.33	4	2	8	983.96	1073.95	76.26	3	5	8	5126.58	4821.03	184.33
6	-1	8	3049.26	3201.35	152.88	5	2	8	1881.92	1713.88	103.45	4	5	8	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	41.87	-6	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	35.22	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	997.86	888.17	72.62	-3	13	8	75.83	64.20	98.17
9	5	8	183.11	153.47	58.90	-2	9	8	1529.51	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	87.64	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	3484.02	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	53.80	4	13	8	106.04	87.38	95.05
-1	6	8	4017.92	3761.83	162.74	5	9	8	67.10	14.01	[illegible]	5	13	8	149.38	181.82	55.62
0	6	8	5640.98	5780.46	219.52	6	9	8	122.13	65.76	[illegible]	6	13	8	129.18	249.17	58.36
1	6	8	8.12	35.60	82.91	7	9	8	3.79	-100.27	98.38	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	55.29
5	6	8	83.19	105.84	37.55	-5	10	8	24.[illegible]	4.35	92.95	0	14	8	184.12	242.99	59.22
6	6	8	1431.42	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	56.20
9	6	8	1.88	-81.26	98.66	-1	10	8	883.08	1190.38	108.10	4	14	8	780.59	872.49	71.55
-7	7	8	75.93	133.58	57.36	0	10	8	50.80	42.59	77.57	5	14	8	497.37	647.05	66.08
-6	7	8	11.49	3.97	95.41	1	10	8	470.40	470.27	47.81	6	14	8	344.50	333.83	67.54
-5	7	8	215.98	185.29	53.13	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	121.48	72.30	81.13	1	15	8	24.01	-53.76	104.53
-1	7	8	2806.11	2558.13	129.81	6	10	8	435.82	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	366.58	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	15	8	4.50	37.54	109.34
8	7	8	121.60	-59.33	95.97	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	61.62	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	-[illegible]9.01	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.[illegible]	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	298.94	350.38	61.65
7	8	8	223.72	20[illegible].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	145.79	152.07	60.98	-7	-8	9	13.14	90.34	110.70	-1	-5	9	331.49	341.38	38.68
4	-13	9	2.66	135.04	57.57	-6	-8	9	205.43	215.60	60.88	0	-5	9	2905.00	2906.71	125.39
-5	-12	9	53.55	3.36	110.31	-5	-8	9	37.28	-20.33	91.48	1	-5	9	1051.27	1232.18	81.40
-4	-12	9	740.95	687.24	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	-87.94	96.03	-3	-8	9	166.47	175.47	46.30	3	-5	9	573.07	769.42	74.58
-2	-12	9	98.66	76.19	88.19	-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	6232.62	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	-103.98	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	509.96	65.55	4	-8	9	139.11	137.99	44.51	-8	-4	9	9.47	-14.33	101.00
5	-12	9	46.52	42.31	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	109.76	7	-8	9	131.95	131.39	58.57	-5	-4	9	50.59	36.04	43.87
-4	-11	9	10.33	-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	109.69	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	29.19	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	262.54	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	41.89	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	774.17	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	434.89	600.73	60.70
-6	-10	9	26.95	-57.31	107.37	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	429.31	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	2883.92	144.28
3	-10	9	397.97	384.00	51.83	-4	-6	9	1430.79	1920.41	124.97	-2	-3	9	220.30	130.96	35.91
4	-10	9	375.33	391.25	56.58	-3	-6	9	342.58	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	2375.58	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	1607.83	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	60.40	-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	-136.38	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	3327.84	-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	250.63	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	-97.38	58.70	5	1	9	3402.39	3242.42	149.84	8	4	9	34.14	-1.37	88.00
5	-2	9	104.91	138.50	36.61	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	8.06	-49.98	99.56
7	-2	9	100.01	71.98	47.66	8	1	9	1.27	10.24	83.57	-8	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	2	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	2	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	152.98	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	271.37	348.85	35.37	3	5	9	36.80	-17.39	54.20
-1	-1	9	5001.21	4680.52	183.60	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	379.56	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	54.77
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	-163.68	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	235.57	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	28.26	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	39.21	40.33	-1	3	9	59.09	119.40	32.11	3	6	9	1403.65	1287.68	88.56
-2	0	9	35.17	10.14	36.89	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	3014.92	2794.37	141.74
0	0	9	301.47	-3434.31	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	106.00	4	3	9	3345.48	3346.93	144.33	8	6	9	205.00	204.51	53.13
3	0	9	3484.87	3038.51	93.71	5	3	9	360.37	401.78	39.06	9	6	9	1.51	-74.63	102.04
4	0	9	991.13	943.55	53.02	6	3	9	2331.48	2186.88	130.20	-6	7	9	196.90	52.61	104.58
5	0	9	446.54	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	134.54	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	123.64	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	281.60	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	35.97	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	3528.71	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	66.72
-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	3669.06	3473.57	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	574.1*	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	-6	12	9	39.60	46.76	72.17	3	-13	10	534.98	387.18	65.20
-1	8	9	1902.47	1749.89	120.56	-5	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	13.29	35.93	36.34	-1	12	9	6.64	33.52	89.65	-4	-12	10	204.86	147.90	65.18
2	8	9	310.06	311.65	80.65	0	12	9	1.60	23.95	85.60	-3	-12	10	186.16	204.34	61.83
3	8	9	286.99	350.25	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	661.60	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	-11.01	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	38.58	100.27
-5	9	9	207.03	85.28	59.35	-2	13	9	21.60	39.79	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	96.18	-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	79.07	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	75.55	4	-11	10	56.55	-126.59	100.84
5	9	9	521.13	647.88	64.21	-2	14	9	274.43	292.10	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	165.25	220.96	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	102.00	-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	53.96	-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	263.93	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	477.35	63.81	-4	-9	10	3.86	41.15	65.35
-5	11	9	0.55	-27.48	108.78	3	16	9	4.71	78.34	107.46	-3	-9	10	476.44	484.12	55.30
-4	11	9	158.76	106.49	58.64	-2	-14	10	80.18	138.83	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	119.31	1	-14	10	161.67	160.79	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	-48.45	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	-8.48	54.27	0	-5	10	598.70	428.90	46.95	5	-2	10	1728.14	1821.75	110.24
7	-9	10	27.20	-34.89	110.23	1	-5	10	92.73	181.52	37.60	6	-2	10	322.21	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	96.93	9	-2	10	95.34	142.29	59.62
-3	-8	10	119.52	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	843.27	72.51	6	-5	10	1345.93	1783.35	124.44	-6	-1	10	172.97	212.90	53.16
-1	-8	10	2246.90	2417.31	143.03	7	-5	10	373.72	483.68	58.70	-5	-1	10	344.06	460.27	50.25
0	-8	10	823.42	836.93	73.37	8	-5	10	60.75	-50.40	98.48	-4	-1	10	104.91	102.34	42.78
1	-8	10	2165.28	2206.46	136.68	-7	-4	10	440.68	516.46	66.57	-3	-1	10	447.82	564.62	58.46
2	-8	10	558.81	556.24	53.41	-6	-4	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	48.96	-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	-1	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	230.81	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	292.42	306.86	56.67	2	-4	10	344.78	241.67	36.48	6	-1	10	64.05	-67.57	77.85
-4	-7	10	358.34	548.28	54.63	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	1603.97	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	1175.23	1211.48	109.98	-7	0	10	65.09	38.69	55.68
0	-7	10	199.76	220.81	43.12	7	-4	10	6.63	-23.76	82.40	-6	0	10	7.72	-35.35	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	2277.04	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	52.00	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	212.09	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	1632.23	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	65.81	2	0	10	718.51	677.61	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	91.92
-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	402.47	54.86	2	-3	10	198.48	171.32	32.90	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	-6	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	-5	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	-4	1	10	648.50	673.49	61.33
4	-6	10	465.31	502.91	47.00	-7	-2	10	4.32	60.93	98.19	-3	1	10	3031.36	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	101.73	-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	287.91	-6295.48	206.77*	4	1	10	1020.13	764.45	78.81
-4	-5	10	118.18	129.62	45.16	1	-2	10	2980.39	3031.81	136.26	5	1	10	954.79	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	127.32	275.64	36.58	7	1	10	2223.40	2240.98	139.47
-1	-5	10	1515.65	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	188.62	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
-5	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	5	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	5	10	2140.13	2193.30	112.20	9	8	10	49.06	56.79	105.71
-1	2	10	345.[illegible]	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	6.18	-21.41	126.06*	4	5	10	2919.15	3139.87	143.96	-4	9	10	108.68	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	45.73	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	1487.83	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	48.88
5	2	10	188.13	196.76	38.[illegible]	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	70.83
7	2	10	4.73	57.33	44.78	-5	6	10	17.62	-38.52	91.37	3	9	10	388.55	486.03	48.46
8	2	10	10.91	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	23.96	13.81	102.16	-2	6	10	940.07	848.55	64.57	6	9	10	172.62	-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	3.94	-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	80.15
0	3	10	138.97	158.25	34.33	5	6	10	2850.64	3001.18	156.07	-1	10	10	198.89	243.62	50.47
1	3	10	337.16	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	77.04
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	69.03
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	203.29	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	54.42	-3	7	10	1783.02	1943.89	126.13	7	10	10	252.37	305.42	59.42
9	3	10	345.27	321.29	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	12.09	-1.51	65.47	-3	11	10	138.88	97.05	53.84
-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	2724.24	2686.56	144.60	3	7	10	16.11	6.02	57.48	0	11	10	434.87	450.09	57.43
-2	4	10	5529.95	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	78.29	7	7	10	305.77	288.79	51.90	4	11	10	749.02	753.63	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	53.22	2	8	10	519.82	569.48	57.35	2	12	10	740.30	789.84	73.85

Structure Factors Table (continued) [*=unobserved refins.] 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	89.01	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	8.07	-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	60.83	-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	4.02	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	45.85	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	243.89	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	77.09
-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	98.84	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	328.27	64.92	-1	-9	11	2.51	36.21	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	178.75	54.65	-4	-5	11	55.05	-87.00	82.08
0	15	10	13.60	94.36	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	232.49	329.29	62.77	3	-5	11	642.52	798.70	63.55
0	-14	11	85.78	-7.19	116.34	7	-9	11	84.16	76.95	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	1014.53	104.99	-7	-4	11	3.70	-47.54	105.27
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	80.93	-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	89.91	93.87	-1	-4	11	955.37	803.49	82.17
-1	-12	11	26.68	106.72	54.84	6	-8	11	27.79	-127.23	88.67	0	-4	11	335.18	376.18	48.71
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	-113.55	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	47.86	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	56.37
-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	1650.35	1608.26	117.97	8	-4	11	8.80	73.17	98.44
-2	-11	11	128.93	23.94	98.81	1	-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	799.62	808.28	53.39

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	2031.16	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	38.43	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	58.98	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	206.33	67.43
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	630.76	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	68.57	-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	49.09
0	-2	11	1093.21	984.89	102.15	4	1	11	125.72	94.69	34.27	8	4	11	28.66	-93.99	97.38
1	-2	11	1286.75	980.15	82.45	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	76.32	-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	5	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	137.76	6	5	11	1.09	-27.49	79.56
-2	-1	11	786.71	827.82	84.77	2	2	11	1278.93	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	1604.89	1495.74	97.87	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	88.99	90.01	95.76
2	-1	11	1448.81	1246.46	88.06	6	2	11	831.42	565.35	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	206.69	343.07	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	64.35	-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	50.39	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	311.91	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	47.08	100.84	7	10	11	74.86	56.34	71.76	1	-12	12	64.10	89.62	101.08
-5	7	11	6.94	54.[illegible]	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	214.73	55.70	-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	500.14	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	-133.44	95.48
2	7	11	1456.45	1539.14	108.80	2	11	11	50.27	62.95	81.23	0	-11	12	106.76	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	42.37	40.83	100.53
4	7	11	1336.50	1230.38	103.22	4	11	11	2.68	-14.76	88.70	2	-11	12	255.95	102.64	106.56
5	7	11	2426.36	2495.06	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	179.48	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	462.06	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	2.68	54.03	0	12	11	509.71	422.56	62.74	-2	-10	12	12.86	41.13	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	66.05
3	8	11	613.02	544.39	61.95	7	12	11	97.27	156.82	62.13	5	-10	12	310.33	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	150.08	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	101.56
7	8	11	215.48	240.83	58.65	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	35.01	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	67.89
-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	346.80	296.91	44.65	2	14	11	86.85	144.91	59.27	6	-9	12	90.33	39.75	106.45
3	9	11	49.10	91.55	42.19	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	-2	-13	12	12.20	23.31	104.86	1	-8	12	36.67	-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	905.01	914.49	76.84	2	-13	12	14.16	-127.25	113.39	5	-8	12	4.50	28.80	86.65
2	10	11	6.86	-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	61.10	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	108.23	-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	63.40	104.87
6	10	11	192.43	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	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	-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	261.38	206.04	48.10	-6	-3	12	34.08	-101.42	97.79	-1	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	133.86	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	229.85	43.23
-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	368.09	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	182.71	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	80.94	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	12.06	23.88	59.93
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	107.12	-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	824.96	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	-54.56	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	65.69	80.67
2	-5	12	1047.07	1267.75	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	27.08
6	-5	12	288.15	236.40	55.33	-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	100.86	-2	-1	12	669.23	624.89	58.52	3	2	12	1888.79	2060.91	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	1560.54	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	48.03	69.08
-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	-42.65	86.22
1	-4	12	6.76	-62.09	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	60.35	-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	-6	7	12	87.58	-37.52	102.61	-2	11	12	126.58	12.91	105.84
4	3	12	1805.93	1822.29	113.67	-4	7	12	45.33	-33.63	88.65	-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	55.93
6	3	12	369.77	330.42	49.89	-2	7	12	12.09	-67.41	81.05	1	11	12	1091.07	1015.20	86.96
7	3	12	169.01	132.57	53.57	-1	7	12	8.08	19.71	50.97	2	11	12	95.29	41.99	60.44
8	3	12	38.66	81.46	95.85	0	7	12	2.18	14.86	66.19	3	11	12	191.96	185.46	58.92
9	3	12	167.45	71.08	63.96	1	7	12	367.42	449.23	67.79	4	11	12	291.34	341.18	57.26
-6	4	12	99.35	78.91	98.26	2	7	12	173.79	195.19	42.51	5	11	12	348.95	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	96.97
-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.[illegible]	74.00	5	7	12	160.48	167.71	47.67	-3	12	12	15.56	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	493.55	68.37
-1	4	12	1604.53	1386.29	103.39	7	7	12	426.33	373.74	60.91	-1	12	12	49.08	-30.29	107.20
0	4	12	985.76	1023.37	71.[illegible]	8	7	12	154.26	228.91	60.88	0	12	12	290.67	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	32.89	57.73	35.40	-4	8	12	497.68	518.62	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	274.26	50.97	3	12	12	63.56	59.93	66.27
4	4	12	510.74	582.61	57.14	-2	8	12	37.77	29.23	84.53	4	12	12	4.67	35.71	89.97
5	4	12	622.72	630.77	62.16	-1	8	12	132.02	-3.64	92.94	5	12	12	3.27	-14.93	98.20
6	4	12	79.08	111.86	45.81	0	8	12	327.04	389.21	51.83	6	12	12	22.00	16.13	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	102.21
8	4	12	230.28	234.80	59.99	2	8	12	2.21	-24.14	76.44	-1	13	12	483.76	601.78	70.91
9	4	12	176.54	243.91	63.50	3	8	12	332.76	341.26	46.90	0	13	12	46.25	113.65	61.80
-6	5	12	234.06	163.09	64.61	4	8	12	739.39	785.64	72.59	1	13	12	53.81	-38.73	102.21
-5	5	12	443.70	399.30	59.52	5	8	12	452.14	433.44	56.62	2	13	12	0.07	-34.22	99.02
-4	5	12	70.46	55.46	80.05	6	8	12	1846.34	1718.59	138.97	3	13	12	0.01	24.75	64.49
-3	5	12	380.67	452.71	54.89	7	8	12	5.32	-41.26	98.74	4	13	12	16.35	75.82	98.17
-2	5	12	256.74	180.93	47.65	8	8	12	225.08	173.99	64.11	5	13	12	10.13	-221.38	110.92
-1	5	12	301.64	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	0.69	14.20	97.51	0	14	12	236.17	298.71	65.24
1	5	12	642.87	605.87	36.93	-3	9	12	375.58	366.29	62.19	1	14	12	25.00	-217.84	115.09
2	5	12	336.48	347.94	42.26	-2	9	12	0.11	-80.93	91.17	2	14	12	414.38	421.41	66.54
3	5	12	189.41	249.94	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	676.43	62.85	0	9	12	32.14	61.49	87.33	4	14	12	2.80	-178.64	108.29
5	5	12	2224.81	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	1289.38	1292.72	110.80	1	-13	13	352.18	417.97	69.41
7	5	12	1289.94	1144.65	90.50	3	9	12	368.88	487.06	53.78	-2	-12	13	76.75	37.93	107.79
8	5	12	131.81	195.12	57.22	4	9	12	317.48	295.48	53.48	-1	-12	13	9.87	-79.45	104.53
9	5	12	10.29	-219.21	118.29	5	9	12	95.16	-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	58.26	2	-12	13	13.51	-124.99	109.57
-4	6	12	210.45	164.03	53.35	8	9	12	34.58	156.26	59.16	3	-12	13	141.77	107.06	65.17
-3	6	12	35.86	-71.21	81.93	-4	10	12	45.30	35.38	103.23	-3	-11	13	5.39	56.81	60.08
-2	6	12	673.80	825.19	71.29	-3	10	12	1.48	-97.91	104.09	-2	-11	13	72.29	86.98	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	105.17
0	6	12	3.68	-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	64.96
2	6	12	718.42	927.63	89.61	1	10	12	122.27	14.80	65.63	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	87.32	4	-11	13	155.67	84.29	113.31
5	6	12	284.67	338.24	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	143.33	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	34.36	101.89	-1	-10	13	1030.73	1120.42	93.95
9	6	12	80.49	36.27	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	55.00	6	-2	13	613.85	612.40	61.69
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	48.40	-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	180.54	171.08	54.01	1	-1	13	744.38	956.95	87.16
4	-9	13	997.76	976.80	92.02	7	-5	13	14.56	83.13	98.17	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	55.57	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	645.68	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	230.11	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	2218.69	147.61	-5	-3	13	258.79	58	58.00	5	0	13	861.23	838.96	50.11
-1	-7	13	592.03	751.21	61.19	-4	-3	13	537.15	650.60	61.56	6	0	13	757.02	850.98	52.12
0	-7	13	2173.22	2297.86	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	40.90	9	0	13	3.92	-3.37	75.12
3	-7	13	57.07	[illegible]	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	53.41	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	79.68
7	-7	13	28.61	72.13	104.05	4	-3	13	962.72	1036.70	99.50	-2	1	13	41.23	86.83	44.83
-6	-6	13	152.94	283.23	62.76	5	-3	13	1447.32	1677.08	124.95	-1	1	13	523.05	555.98	49.31
-5	-6	13	276.79	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	903.88	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	81.15	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	52.73	-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	55.09
-2	2	13	1944.23	1675.63	120.74	5	5	13	102.11	51.21	45.51	5	9	13	501.78	476.52	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	63.58
2	2	13	197.10	218.31	42.96	9	5	13	12.98	-172.22	102.11	-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	-2	10	13	4.13	4.39	92.23
6	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
-6	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
-5	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
-4	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
-3	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
-2	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
-1	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
0	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
1	3	13	32.09	26.10	65.14	-5	7	13	18.18	-48.55	100.42	1	11	13	2.96	-74.19	92.05
2	3	13	412.06	408.97	47.99	-4	7	13	4.72	34.10	97.91	2	11	13	8.23	57.10	51.21
3	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
4	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
5	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
6	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
7	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
8	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
9	3	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
-6	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
-5	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
-4	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
-3	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
-2	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
-1	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
0	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
1	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
2	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
3	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
4	4	13	1021.41	1369.25	101.84	1	8	13	2310.42	2712.02	155.7	2	13	13	481.64	531.48	67.28
5	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
6	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
7	4	13	87.50	78.85	51.48	4	8	13	98.84	189.24	49.70	5	13	13	78.93	68.96	107.46
8	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
9	4	13	2.84	44.14	102.30	6	8	13	1.14	128.91	51.07	2	14	13	40.30	-31.82	66.17
-6	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
-5	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
-4	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
-3	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
-2	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
-1	5	13	70.00	62.67	74.49	-1	9	13	510.24	437.21	61.42	-2	-11	14	31.83	-143.04	112.62
0	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
1	5	13	15.37	-37.41	72.55	1	9	13	40.79	21.26	91.32	0	-11	14	23.63	-8.97	76.68
2	5	13	4.77	22.60	67.62	2	9	13	667.11	847.60	76.11	1	-11	14	149.39	77.66	...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	361.56	50.28
4	-11	14	1.22	-99.51	121.15	7	-6	14	31.44	72.16	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	53.35	-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	-87.16	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	120.67	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	9.66	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	489.73	63.08	2	-1	14	1017.34	1209.09	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	223.35	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	54.72	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	52.52
-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	66.32	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	165.32	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	296.19	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	1218.08	1401.28	115.52	-3	1	14	242.60	154.32	51.92
2	-7	14	59.48	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	37.58	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	0.13	-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	116.87
-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	190.58	51.49	1	-2	14	31.56	28.30	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	62.47
-1	2	14	652.70	377.32	63.22	-2	6	14	78.56	59.74	84.92	4	10	14	373.10	288.58	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	58.89	2	6	14	79.08	37.[illegible]	84.69	-2	11	14	0.06	-179.26	107.66
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	58.06
5	2	14	509.05	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	11	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	11	14	15.32	-73.37	96.12
8	2	14	88.39	80.01	59.01	7	6	14	29.19	80.12	97.86	3	11	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	11	14	1.80	86.44	96.29
-4	3	14	80.15	-176.78	99.48	-4	7	14	7.21	-42.89	94.91	5	11	14	471.92	534.29	67.19
-3	3	14	102.91	51.40	61.95	-3	7	14	226.88	282.08	56.88	6	11	14	0.30	-22.47	103.77
-2	3	14	523.42	517.67	57.40	-2	7	14	40[illegible].33	449.00	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	21.47	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.[illegible]	-26.99	103.77	8	7	14	384.25	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	281.36	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	131.68	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	282.12	63.69
1	4	14	27.68	26.81	50.17	2	8	14	221.90	362.35	52.33	-1	-10	15	4.45	-6.27	100.98
2	4	14	2.65	-44.66	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	69.01	8	8	14	4.41	-15.19	112.56	-4	-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	95.36	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	[illegible]	[illegible]	150.61	68.61	107.43
1	5	14	96.14	164.60	45.62	4	9	14	22.48	46.11	63.35	5	[illegible]	[illegible]	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	[illegible]	[illegible]	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	[illegible]	[illegible]	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	[illegible]	[illegible]	0.36	56.09	97.61
5	5	14	18.75	44.65	78.03	-3	10	14	31.12	38.84	106.31	-1	-8	[illegible]	229.04	-37.36	103.71
6	5	14	493.53	522.09	59.17	-2	10	14	411.75	294.11	68.85	0	-8	[illegible]	[illegible]	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	29.8[illegible]	-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	[illegible].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	[illegible].78	868.10	84.69
-4	6	14	[illegible].07	14.66	100.01	2	10	14	578.54	560.82	64.67	4	-8	15	[illegible].55	[illegible].41	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
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4	8	-7	89	88	[illegible]	[illegible]	[illegible]	[illegible]	163	164	6	9	6	-5	71	79	7	10	5	-4	125	120	5	9	4	-3	88	64	4
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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
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-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	58.80	4	-3	15	392.89	307.77	54.03	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
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1	-7	15	1.81	-185.43	96.84	7	-3	15	47.13	44.50	99.89	7	1	15	3.03	-197.39	99.35
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6	-7	15	98.20	93.68	63.56	-1	-2	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	711.30	60.05	2	2	15	276.19	269.81	55.88
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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
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-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	56.11
-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*
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2	-5	15	2.04	49.51	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	110.43	50.02	5	-1	15	106.48	16.98	90.72	4	3	15	52.28	-46.71	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	101.41
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
-6	-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	13.89	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	-16.38	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	36.18	40.73	2	4	15	2080.37	2432.99	144.17
3	-4	15	89.08	137.22	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	3.33	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	229.25	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	38.96	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	-12.51	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	212.69	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	222.30	58.00
5	5	15	67.11	26.04	52.01	2	10	15	429.82	324.93	66.64	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	333.96	394.26	56.14	2	11	15	18.34	29.62	98.97	0	-5	16	350.39	300.37	60.20
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	-12[illegible]	96.22
4	6	15	41.64	45.39	82.22	0	12	15	0.50	-136.09	121.08	4	-5	16	820.18	760.34	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	2[illegible]5.10	221.16	63.68
7	6	15	470.16	451.47	66.05	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	98.36
-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	58.96	97.40	-1	-10	16	0.93	23.26	61.36	-1	-4	16	83.22	-36.85	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	111.91	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	48.14
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	133.59	64.11	4	-4	16	96.35	-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	368.06	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	373.34	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	70.29	-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	333.12	59.95	-3	-8	16	0.44	27.65	103.36	-1	-3	16	509.20	445.33	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	818.56	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	42.76	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	7.79	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	30.72	5	-8	16	205.69	146.40	67.02	7	-3	16	9[illegible].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	302.54	469.23	56.64
0	9	15	0.23	-28.19	101.99	1	-7	16	56.11	87.38	54.24	-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	-1556.99	151.72*
2	9	15	180.65	132.24	57.77	3	-7	16	7.26	86.41	95.82	1	-2	16	36.50	139.14	47.88
3	9	15	93.15	-29.96	93.96	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	264.79	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	218.86	24.84	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	38.46	-0.95	83.87	0	3	16	288.60	453.50	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	-91.31	88.12	-2	8	16	19.64	43.24	108.34
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	120.99	56.89
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	-22.89	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	24.83	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	77.87	3.88	96.26	6	8	16	52.00	2.92	76.65
-3	0	16	390.68	352.58	62.73	-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	376.21	402.61	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	1124.23	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	38.03	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	124.96	8	4	16	71.36	13.93	110.22	6	9	16	6.10	70.94	99.60
7	0	16	47.80	-10.65	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	365.82	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	225.98	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	58.89	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	1049.25	93.34	3	11	16	976.84	951.42	95.80
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	389.75	470.60	63.81	-3	6	16	323.61	297.89	65.50	2	12	16	181.22	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	-97.01	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	632.93	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	92.48	1	-9	17	217.06	183.87	67.83
-2	2	16	67.37	125.61	52.60	2	6	16	530.19	746.29	73.41	2	-9	17	29.49	-45.00	80.19
-1	2	16	385.65	389.40	58.82	3	6	16	96.48	68.43	95.73	3	-9	17	0.82	107.67	115.76
0	2	16	31.49	-993.47	434.08*	4	6	16	1.28	-126.48	91.50	-2	-8	17	2.41	0.69	108.51
1	2	16	7.82	-89.53	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	55.77	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	1.80	-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	452.48	63.23	3	-8	17	587.26	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	37.55	75.33	79.92
7	2	16	840.32	985.85	88.62	0	7	16	273.97	328.08	57.39	-2	-7	17	9.92	109.56	60.73
8	2	16	73.01	-94.16	115.89	1	7	16	267.92	238.78	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	3.54	-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	25.26	86.89
4	-7	17	21.59	-112.03	114.61	-4	-1	17	120.29	162.54	61.58	3	3	17	109.07	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	327.35	314.06	58.13
-3	-6	17	48.76	-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	730.99	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	533.09	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	353.24	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	108.67
1	-5	17	2.34	-24.51	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	32.42	-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	646.80	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	-195.01	118.21	4	0	17	61.60	110.02	76.89	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	93.46	84.43	109.78	6	0	17	463.49	486.41	48.54	3	5	17	46.38	-25.97	87.43
-2	-4	17	298.89	271.99	62.66	7	0	17	63.44	20.31	62.56	4	5	17	34.72	-22.07	94.97
-1	-4	17	32.97	-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	-160.19	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	53.02	-2	6	17	39.92	64.00	76.78
4	-4	17	123.51	114.55	60.70	1	1	17	111.52	51.88	70.11	-1	6	17	25.79	84.87	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	54.16	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	-124.23	93.00	-2	2	17	334.78	390.57	63.26	-2	7	17	80.01	77.29	108.78
3	-3	17	41.26	40.09	94.14	-1	2	17	6.55	-85.08	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	707.20	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	511.94	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	84.73	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	112.65	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	99.98	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	80.49	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	332.01	65.97	-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	837.61	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	534.28	653.82	72.18	0	-3	18	417.12	435.32	63.59	4	2	18	20.17	-133.75	103.69
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	70.91
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	84.71	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	100.90
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.[illegible]	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	63.91
4	9	17	387.23	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	91.19	89.64	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	228.79	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	68.41	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	52.54	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	-136.67	103.43	4	4	18	230.01	275.62	57.62
-1	-7	18	0.98	80.73	118.98	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	379.68	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	205.58	64.47	4	0	18	34.13	-12.64	79.29	-1	6	18	6.88	-6.58	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	58.86	5	6	18	321.91	269.21	68.53
4	-5	18	48.02	-29.86	114.82	1	1	18	103.40	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	148.61	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	103.91
-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	-15.07	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	185.70*	6	1	18	27.69	121.96	61.04	3	7	18	251.79	246.19	62.92
1	-4	18	486.18	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	29.00	49.84	110.48	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	101.84	-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	105.64	2	2	18	18.48	-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	329.01	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	312.05	67.58	4	7	19	211.71	270.60	66.44
1	9	18	355.92	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	108.98	3	8	19	10.40	-52.58	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	238.02	58.49	2	-4	20	30.62	-11.55	64.31
1	-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	64.53	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	131.56	-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	23.02	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	450.70	68.41	4	2	19	17.79	15.62	105.22	2	-2	20	10.93	-8.94	75.22
0	-4	19	1.55	-55.87	113.20	5	2	19	6.43	-33.55	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	110.49	-2	3	19	65.02	-65.71	119.41	-1	-1	20	11.36	88.77	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	111.21
-2	-3	19	98.91	112.00	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	328.19	-18.06	140.67	3	3	19	0.16	-19.34	108.50	4	-1	20	25.44	126.71	73.26
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	47.19	84.74	100.67	6	3	19	336.74	392.16	71.90	1	0	20	588.86	662.97	51.28
4	-3	19	66.63	106.36	65.70	-2	4	19	24.86	-96.89	113.70	2	0	20	142.25	42.62	76.84
5	-3	19	286.83	317.15	67.90	-1	4	19	12.99	-41.96	112.43	3	0	20	225.13	141.21	179.99
-2	-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	81.28
0	-2	19	209.04	-156.73	122.10	2	4	19	5.81	4.13	72.87	-1	1	20	5.57	-13.70	118.61
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	2.87	41.31	76.41
3	-2	19	85.28	143.23	62.24	5	4	19	29.05	-54.86	111.95	2	1	20	42.96	-60.54	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	224.91	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	12.57	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	243.46	66.98
4	-1	19	3.42	30.87	73.02	-1	6	19	94.16	156.62	66.61	4	2	20	134.37	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	28.30	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	156.78	381.41	70.74
1	0	19	35.21	-138.85	73.62	5	6	19	273.35	325.63	69.92	3	3	20	217.29	221.01	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	39.48	113.96
3	0	19	0.80	41.86	70.90	1	7	19	108.83	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	[illegible]	30	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	90	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
6	2	-14	136	135	6	1	0	-11	230	240	5	0	3	-10	240	242	5	7	4	-9	125	107	6	5	5	-8	207	219	5
0	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	191	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	208	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	183	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	60	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	339	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	0	7	-10	81	85	7	2	1	-8	277	289	5	8	1	-7	160	145	5
2	4	-13	140	127	5	1	4	-11	66	73	7	1	7	-10	179	162	7	3	1	-8	162	173	4	9	1	-7	246	241	5
3	4	-13	119	121	6	2	4	-11	178	184	6	2	7	-10	140	127	6	4	1	-8	304	285	5	10	1	-7	179	170	5
4	4	-13	99	77	6	3	4	-11	145	148	7	1	0	-9	474	471	7	5	1	-8	96	93	4	11	1	-7	220	226	6
5	4	-13	16	6	15	4	4	-11	163	153	6	3	0	-9	422	455	7	6	1	-8	92	120	4	12	1	-7	66	84	8
0	0	-12	301	293	6	5	4	-11	116	125	5	5	0	-9	255	280	5	7	1	-8	127	140	5	0	2	-7	257	258	4
2	0	-12	51	55	8	6	4	-11	206	210	6	7	0	-9	242	237	5	8	1	-8	406	406	7	1	2	-7	335	321	5
4	0	-12	181	171	5	7	4	-11	0	20	1	9	0	-9	365	348	6	9	1	-8	62	83	6	2	2	-7	290	296	5
6	0	-12	244	250	6	8	4	-11	166	173	7	11	0	-9	282	293	6	10	1	-8	254	267	6	3	2	-7	659	625	10
8	0	-12	291	273	6	0	5	-11	229	234	6	0	1	-9	248	237	5	11	1	-8	35	23	17	4	2	-7	389	381	6
0	1	-12	238	244	5	1	5	-11	44	29	12	1	1	-9	310	337	5	12	1	-8	110	110	5	5	2	-7	203	219	4
1	1	-12	135	119	6	2	5	-11	152	154	7	2	1	-9	0	16	1	0	2	-8	65	59	4	6	2	-7	215	213	5
2	1	-12	239	233	5	3	5	-11	89	86	6	3	1	-9	179	203	4	1	2	-8	141	140	4	7	2	-7	73	59	5
3	1	-12	177	184	6	4	5	-11	48	44	11	4	1	-9	161	190	5	2	2	-8	230	227	4	8	2	-7	232	227	5
4	1	-12	160	131	6	5	5	-11	72	88	8	5	1	-9	131	110	5	3	2	-8	404	407	6	9	2	-7	190	190	5
5	1	-12	128	143	5	6	5	-11	161	140	7	6	1	-9	301	311	5	4	2	-8	503	497	8	10	2	-7	102	103	4
6	1	-12	104	110	5	7	5	-11	55	65	35	7	1	-9	347	353	6	5	2	-8	375	370	6	11	2	-7	152	172	6
7	1	-12	32	38	31	0	6	-11	173	170	6	8	1	-9	210	204	5	6	2	-8	184	177	5	12	2	-7	148	149	5
8	1	-12	175	181	6	1	6	-11	69	78	8	9	1	-9	277	258	5	7	2	-8	99	97	4	0	3	-7	129	151	4
9	1	-12	70	68	7	2	6	-11	155	156	7	10	1	-9	82	87	6	8	2	-8	169	179	5	1	3	-7	253	218	5
0	2	-12	172	169	5	3	6	-11	90	86	6	11	1	-9	92	106	5	9	2	-8	66	51	6	2	3	-7	367	399	6
1	2	-12	109	92	5	4	6	-11	114	117	5	12	1	-9	43	29	14	10	2	-8	135	146	5	3	3	-7	318	326	5
2	2	-12	155	160	6	5	6	-11	0	17	1	0	2	-9	121	124	5	11	2	-8	178	182	6	4	3	-7	326	321	5
3	2	-12	139	144	6	0	0	-10	346	342	6	1	2	-9	55	87	5	12	2	-8	129	129	6	5	3	-7	80	94	4
4	2	-12	108	116	5	2	0	-10	353	356	6	2	2	-9	212	189	4	0	3	-8	194	176	4	6	3	-7	58	61	5
5	2	-12	156	152	6	4	0	-10	280	320	5	3	2	-9	295	323	5	1	3	-8	448	434	7	7	3	-7	163	159	5
6	2	-12	164	173	6	6	0	-10	0	64	-1	4	2	-9	247	259	5	2	3	-8	344	323	6	8	3	-7	159	152	5
7	2	-12	151	140	7	8	0	-10	194	200	5	5	2	-9	260	260	5	3	3	-8	159	156	5	9	3	-7	140	142	4
8	2	-12	137	139	5	10	0	-10	195	196	6	6	2	-9	58	48	6	4	3	-8	395	361	6	10	3	-7	237	228	5
9	2	-12	70	49	7	0	1	-10	202	197	5	7	2	-9	188	169	5	5	3	-8	82	68	4	11	3	-7	172	159	6

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

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	128	5	2	7	-2	158	153	5	8	5	-1	173	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	291	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	316	5
6	0	-2	484	435	7	8	7	-2	65	50	8	2	6	-1	355	370	6	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
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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
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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
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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
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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	185	210	4	8	7	-1	201	216	6	2	6	0	156	147	5	11	4	1	92	85	5
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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	6	6	6	0	82	91	5	2	5	1	262	262	5
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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
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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	4	8	0	136	131	5	7	6	1	92	99	5
7	3	-2	444	467	7	4	2	-1	191	196	3	1	1	0	332	317	5	5	8	0	91	93	5	8	6	1	141	144	6
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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	6	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
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8	4	-2	104	124	4	5	3	-1	389	379	6	2	2	0	206	198	3	13	0	1	116	106	5	3	8	1	104	104	5
9	4	-2	79	66	5	6	3	-1	180	211	4	3	2	0	47	54	3	0	1	1	290	312	4	4	8	1	91	88	5
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4	5	-2	186	175	4	0	4	-1	537	514	8	11	2	0	113	104	5	8	1	1	59	53	5	0	0	2	681	686	10
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6	6	-2	120	121	4	1	5	-1	153	139	4	11	3	0	164	151	6	8	2	1	429	436	7	7	1	2	214	195	4
7	6	-2	263	285	6	2	5	-1	269	277	5	12	3	0	87	86	6	9	2	1	254	252	5	8	1	2	361	368	6
8	6	-2	0	16	1	3	5	-1	231	228	4	13	3	0	93	93	6	10	2	1	166	160	5	9	1	2	282	303	5
9	6	-2	200	212	6	4	5	-1	278	309	5	0	4	0	146	113	4	11	2	1	121	122	5	10	1	2	170	158	5
10	6	-2	0	9	1	5	5	-1	107	93	4	1	4	0	629	689	9	12	2	1	95	101	5	11	1	2	88	97	5
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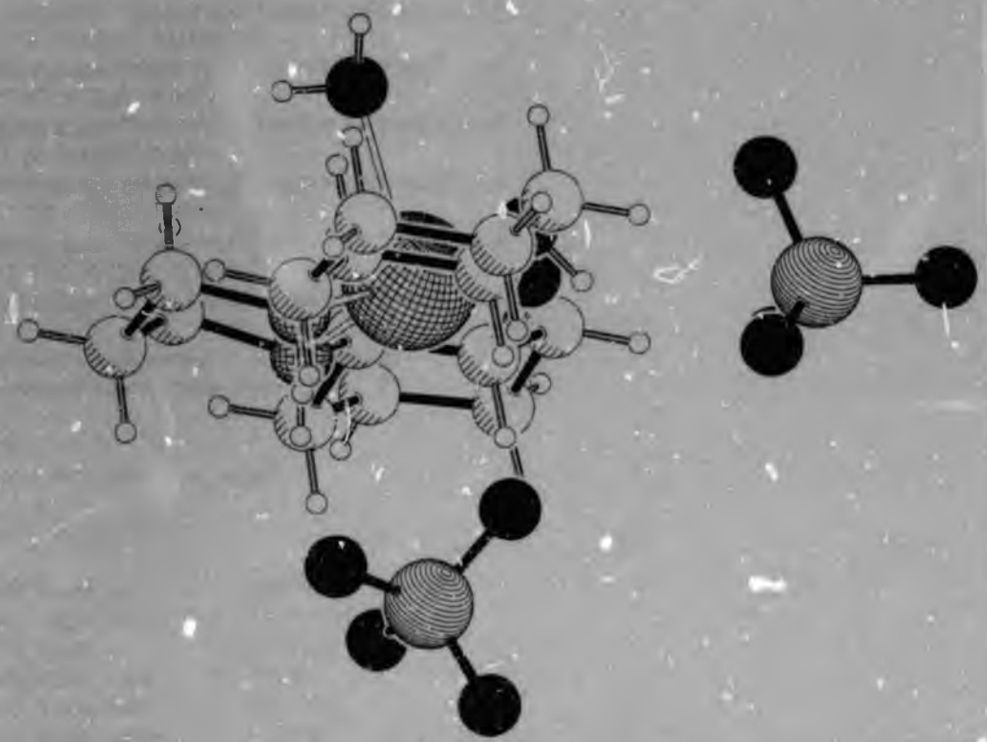
Table 1. Observed and calculated structure factors for 1

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
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	4[illegible]	7	0	1	3	677	649	10	2	9	3	111	110	5	3	8	4	178	172	6	3	8	5	115	108	5
1	2	2	732	733	[illegible]	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	2	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	449	7	4	0	4	278	297	4	0	9	4	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	1	9	4	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	1	0	5	177	177	3	6	0	6	329	326	5
6	2	2	209	190	4	6	1	3	0	14	1	10	0	4	271	275	5	3	0	5	188	172	4	8	0	6	175	160	5
7	2	2	145	137	4	7	1	3	292	331	5	12	0	4	107	106	5	5	0	5	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	7	0	5	404	366	6	0	1	6	24	9	8
9	2	2	304	318	5	9	1	3	390	386	6	1	1	4	174	163	3	9	0	5	293	282	5	1	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	5	95	101	5	2	1	6	262	242	4
11	2	2	203	224	6	11	1	3	116	116	5	3	1	4	181	192	3	0	1	5	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	5	232	270	4	4	1	6	577	543	9
13	2	2	82	72	6	0	2	3	285	235	-4	5	1	4	113	118	4	2	1	5	264	297	4	5	1	6	111	113	5
0	3	2	401	425	6	1	2	3	828	779	13	6	1	4	91	92	4	3	1	5	449	464	7	6	1	6	322	300	5
1	3	2	440	443	7	2	2	3	319	322	5	7	1	4	88	78	4	4	1	5	604	627	9	7	1	6	89	87	4
2	3	2	854	870	13	3	2	3	649	573	10	8	1	4	337	326	6	5	1	5	436	445	7	8	1	6	59	67	6
3	3	2	401	412	6	4	2	3	473	444	7	9	1	4	196	203	5	6	1	5	175	156	4	9	1	6	110	101	5
4	3	2	150	191	-4	5	2	3	236	224	4	10	1	4	279	286	6	7	1	5	149	143	5	10	1	6	152	146	6
5	3	2	301	353	5	6	2	3	277	254	5	11	1	4	0	26	1	8	1	5	118	101	6	11	1	6	61	61	8
6	3	2	83	85	3	7	2	3	106	116	4	12	1	4	40	61	40	9	1	5	196	205	5	0	2	6	324	333	5
7	3	2	236	258	5	8	2	3	136	127	5	0	2	4	393	385	6	10	1	5	69	77	6	1	2	6	454	466	7
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2	4	2	44	57	5	3	3	3	403	389	6	8	2	4	149	155	5	5	2	5	73	68	4	9	2	6	180	171	5
3	4	2	497	514	7	4	3	3	161	214	-4	9	2	4	34	37	14	6	2	5	131	148	5	10	2	6	211	201	6
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10	4	2	75	66	6	11	3	3	78	79	6	3	3	4	566	534	8	1	3	5	263	285	4	5	3	6	249	275	5
11	4	2	146	134	7	12	3	3	178	176	7	4	3	4	249	256	4	2	3	5	428	412	7	6	3	6	167	171	5
12	4	2	62	44	9	0	4	3	138	167	4	5	3	4	80	82	3	3	3	5	379	394	6	7	3	6	171	174	5
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6	1	7	77	56	4
7	1	7	116	122	4
8	1	7	100	05	4
9	1	7	100	98	4
10	1	7	89	89	5
11	1	7	104	112	5
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2	2	7	132	148	4
3	2	7	113	88	5
4	2	7	81	70	4
5	2	7	178	174	5
6	2	7	36	13	11
7	2	7	225	218	5
8	2	7	139	134	6
9	2	7	170	163	6
10	2	7	90	85	6
0	3	7	146	163	4
1	3	7	290	298	5
2	3	7	75	55	4
3	3	7	93	81	4
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6	3	7	150	175	5
7	3	7	163	165	5
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5	5	7	182	170	6
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5	7	7	132	122	5
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RH18



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_symmetry_space_group_name_H-M    'P n'

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

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_cell_angle_gamma                 90.00
_cell_volume                      1157.4(8)
_cell_formula_units_Z             2
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_diffrn_measurement_method       theta-2theta
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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^ > 2sigma(F^2^) is used only for calculating _R_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.
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_atom_sites_solution_hydrogens   geom
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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 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 . .
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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 0.3899(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 . .
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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) 0.3441(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 . .
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Cl2 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) 0.08[illegible](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) 0.050(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)
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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)
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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)
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C14 0.029(5) 0.051(6) 0.040(5) -0.006(5) 0.017(4) -0.008(5)
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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.
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Cu1 O2 1.992(9) . ?
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Cu1 N2 1.998(7) . ?
Cu1 O3 2.263(9) . ?

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Cl1 O7 1.395(10) . ?
Cl1 O6 1.406(9) . ?
Cl1 O5 1.449(9) . ?
Cl2 O8 1.390(5) . ?
Cl2 O10' 1.395(5) . ?
Cl2 O11 1.400(5) . ?
Cl2 O9 1.404(4) . ?
Cl2 O8' 1.405(5) . ?
Cl2 O11' 1.444(5) . ?
Cl2 O10 1.460(5) . ?
O1 C1 1.460(11) . ?
O2 C15 1.474(12) . ?
O8 O8' 0.67(2) . ?
O11 O11' 0.95(2) . ?
O11 O10' 1.62(2) . ?
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N1 C7 1.492(12) . ?
N1 C6 1.501(12) . ?
N2 C9 1.459(12) . ?
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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) . ?
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N1 Cu1 O3 97.2(4) . . ?
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N2 Cu1 O3 97.3(3) . . ?
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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) . . ?
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O10' Cl2 O8' 111.6(5) . . ?
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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) . . ?
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O9 Cl2 O10 105.5(4) . . ?
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C1 O1 Cu1 109.9(5) . . ?
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O11' O11 Cl2 72.9(6) . . ?
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O10' O10 Cl2 67.6(6) . . ?
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Cl2 O10' O11 54.8(5) . . ?
C7 N1 C6 114.0(8) . . ?
C7 N1 Cu1 113.0(6) . . ?
C6 N1 Cu1 108.6(6) . . ?
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C9 N2 Cu1 114.8(6) . . ?
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C6 C5 C4 109.5(8) . . ?
C1 C6 N1 107.7(7) . . ?
C1 C6 C5 110.0(7) . . ?

N1 C6 C5 114.9(7) . . ?
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