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Chemical and structural studies of substituted transition metal carbonyl complexes

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2015-01-23
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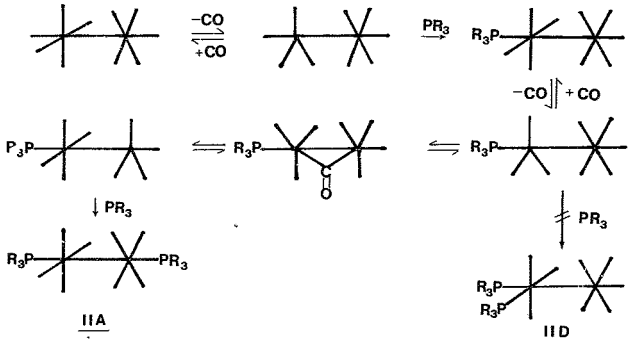


Figure 15.4: Schematic representation of the mechanism for the formation of diax-$Re_2(CO)_8(PR_3)_2$ (IIA)

105-125°]. Slow isomerization of the 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ (R = Bu^n, Ph) complexes to diax-$Re_2(CO)_8(PR_3)_2$ was observed in toluene solution at room temperature (half-life of 10 h (PPh_3) or 1-2 days (PBu^n_3)). The 1,2-eq,eq-$Re_2(CO)_8(PR_3)_2$ complexes appear to be stable towards isomerization.

(ii) The Me_3NO-assisted reaction of $Re_2(CO)_{10}$ and PMe_2Ph in MeCN (80°C) resulted in the formation of 1,2-ax,eq-$Re_2(CO)_8(PMe_2Ph)_2$ (vide supra).

(iii) The thermal reaction between $Re_2(CO)_{10}$ and PR_3 (PR_3 = PMe_2Ph[183], $PMePh_2$[184]) at elevated temperatures and for extended reaction times (eg. PMe_2Ph, 80-100°C, 60-96 h;[183] $PMePh_2$, 140°C, 15 h[184]) yielded a product identified as 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ (vide supra).

(iv) The photochemical reaction between $Re_2(CO)_{10}$ and PR_3 (PR_3 = PMe_2Ph,[183] $PMePh_2$[184]) has also been reported to yield the 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$. An analogous arsine derivative, 1,2-ax,eq-$Re_2(CO)_8(AsMe_2Ph)_2$, has also been prepared by the photochemical reaction of $Re_2(CO)_{10}$ with $AsMe_2Ph$.[183]

The first two cases can be explained in terms of replacement of equatorial ligand(s) from 1,2-eq,eq-$Re_2(CO)_8(L)_2$ ((i) (L)$_2$ = μ-olefin; (ii) L = NCMe), to give 1,2-eq,eq-$Re_2(CO)_8(PR_3)_2$, or 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$, depending on the size of the phosphine ligand.

In the third case, formation of 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ products in thermal reactions of $Re_2(CO)_{10}$ with PR_3 at elevated temperatures and extended reaction times, can be explained in terms of the initial formation of diax-$Re_2(CO)_8(PR_3)_2$ (obtained from thermal reactions under less forcing conditions (shorter reaction times)[185] and from the Pd-catalysed and Me_3NO-assisted (solvent CH_2Cl_2 or $CHCl_3$[177]) reactions of $Re_2(CO)_{10}$ with PR_3), followed by metal-metal bond cleavage, and rearrangement and recombination to give the electronically favoured 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ isomer. The formation of 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ products photochemically (case (iv)), where Re-Re bond cleavage is likely,[266a] is consistent with this proposal. Further, traces

of 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ *isomer can* be detected by IR spectroscopy in the cases of the reactions which give the diax-$Re_2(CO)_8(PR_3)_2$ *isomer* (*vide supra*), suggesting that a small amount of isomerization to the 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ *isomer occurs even under milder reaction conditions.* As described above, partial isomerization of diax-$Re_2(CO)_8(PMe_2Ph)_2$ to 1,2-ax,eq-$Re_2(CO)_8(PMe_2Ph)_2$ in toluene solution (80°C, 4 h) has also been observed (under normal laboratory light). Thus a slow thermal isomerization of diax-$Re_2(CO)_8(PR_3)_2$ to 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ can occur, provided the phosphine is not too large (*vide infra*).

Steric factors determine whether the 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ isomer is stable for a particular phosphine. Thus for PMe_2Ph and $PMePh_2$ (Tolman cone angles[83] of 122° and 136° respectively), the 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ isomers are obtained from the thermal reaction of $Re_2(CO)_{10}$ with PR_3 (case (ii)), but the thermal reaction between $Re_2(CO)_{10}$ and PPh_3 (Tolman cone angle[83]: 145°) yields only diax-$Re_2(CO)_8(PPh_3)_2$ (140°C, 16 h).[182] Further, no 1,2-ax,eq-$Re_2(CO)_8(PPh_3)_2$ (as evidenced by sidebands in the IR spectrum of the diax-$Re_2(CO)_8(PPh_3)_2$ product) is formed in the Pd0-catalysed reaction of $Re_2(CO)_{10}$ and PPh_3 (*vide supra*).

Thus it would appear that the particular synthetic method employed, and the size of the phosphine ligand used, determine whether the diax-, 1,2-eq,eq- or 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ isomer will be obtained. For a synthetic method predisposed towards the formation of equatorially substituted $Re_2(CO)_8(PR_3)_2$ isomers (cases *(i)-(iv) above*), 1,2-eq,eq-$Re_2(CO)_8(PR_3)_2$ is obtained for small phosphines (Tolman cone angle *range:* 105°-121°), *while large phosphines* (Tolman cone angle range: 122°-145°) yield 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$. *For the larger phosphine* ligands (Tolman cone angle range: 130°-145°), the 1,2-ax,eq-$Re_2(CO)_8(PR_3)_2$ isomers are *unstable, and* slowly isomerize (rate increases with the size of the PR_3 ligand) to diax-$Re_2(CO)_8(PR_3)_2$.

15D.2 Experimental

15D.2.1 Synthesis of $Re_2(CO)_{10-n}(PR_3)_n$ ($n = 1,2$) from the reaction of $Re_2(CO)_{10}$ and PR_3 in the presence of Pd-catalysts

$Re_2(CO)_{10}$ (163 mg, 0.25 mmol) and 50 mg Pd-catalyst (Pd/C (10% Pd), $Pd/CaCO_3$ (10% Pd) or PdO) were stirred in xylene (10 mℓ), to which was added PR_3 (0.75 mmol). The reaction solution was refluxed at 140°C for 1 to 9 h, depending on the phosphine used (see Table 15.5). The progress of the reaction was monitored by TLC (Silica; eluent: ethylacetate: petroleum ether (80-100°C), 1:3). The product(s) were isolated by preparative layer chromatography (Silica; eluent as for TLC), extracted with benzene, and crystallized from benzene-hexane solution, to yield colourless to yellow solids.

15D.2.2 Synthesis of $Re_2(CO)_{10-n}(PR_3)_n$ ($n = 1,2$) by the NMe_3O-assisted reaction of $Re_2(CO)_{10}$ with PR_3 and $CH_2Cℓ_2$

$Re_2(CO)_{10}$ (163 mg, 0.25 mmol) was dissolved in $CH_2Cℓ_2$ (10 mℓ), to which PR_3 (0.75 mmol) was added, followed by $NMe_3O \cdot 2H_2O$ (60 mg, 0.54 mmol) dissolved in degassed MeOH (5 mℓ). The reaction solution was heated at 40°C for 8 h. The progress of the reaction was monitored by TLC (Silica; eluent: ethylacetate: petroleum ether (80-100°C), 1:3). The products were isolated by preparative layer chromatography (Silica; eluent as for TLC), extracted with $CH_2Cℓ_2$, and recrystallized from $CH_2Cℓ_2$-pentane solution, to yield colourless to yellow solids.

15D.2.3 Preparation of an isomer of $Re_2(CO)_8(PMe_2Ph)_2$

$Re_2(CO)_{10}$ (653 mg, 1 mmol), was dissolved in acetonitrile, MeCN (10 mℓ), and the solution heated at 80°C. To this solution was added $NMe_3O \cdot 2H_2O$ (234 mg, 2.1 mmol) dissolved in degassed MeOH (10 mℓ). Reaction was instantaneous, as evidenced by the colour change of the reaction solution from colourless to pale yellow. Then PMe_2Ph (2.1 mmol) was added to the reaction solution, and the mixture heated at 80°C for 2 h. The product was isolated by column chromatography (2cm x 40cm column, silica; gradient elution with hexane-

benzene solutions, starting with hexane and ending with benzene). Recrystallization from CH_2Cl_2-pentane solution gave a cream solid.

15D.2.4 Preparation of an isomer of $Re_2(CO)_8(PMePh_2)_2$

$Re_2(CO)_{10}$ (667 mg, 1.02 mmol) and $PMePh_2$ (4.0 mmol) were refluxed in xylene (17 mℓ) at 138°C for 15 h. During this time the solution changed from colourless to an intense yellow. The xylene was removed on a rotary evaporator, and the yellow oily residue pumped under vacuum for several days to remove excess phosphine, to give a yellow solid.

15E. The Crystal and Molecular Structure of diax[$Re_2(CO)_8(PMe_2Ph)_2$]

15E.1 Introduction

Although the crystal and molecular structures of three $Mn_2(CO)_{10-n}(PR_3)_n$ ($n = 1$,[224] 2[255-6]) compounds have been determined by X-ray crystallography, no analogous dirhenium carbonyl-phosphine complexes have been studied crystallographically.

From IR spectral data (see section 15B), the geometry of the majority of $Re_2(CO)_9(PR_3)$ and $Re_2(CO)_8(PR_3)_2$ products is expected to be the same as that of the analogous $Mn_2(CO)_9(PR_3)$ and $Mn_2(CO)_8(PR_3)_2$ complexes, viz. axial and diaxial phosphine substitution respectively. An X-ray crystallographic study of the complex diax[$Re_2(CO)_8(PMe_2Ph)_2$], product of the PdO-catalysed reaction between $Re_2(CO)_{10}$ and PMe_2Ph (see section 15D), was undertaken with a view to confirming this prediction.

Further, the structural investigation of diax[$Re_2(CO)_8(PMe_2Ph)_2$] was undertaken as part of an extension of the chemical, mechanistic and structural studies of isonitrile derivatives of dirhenium decacarbonyl (see chs. XI and XIV) to other donor ligands. Specifically, the structural effect (if any) of the bulkier phosphine ligand (Tolman cone angle[81] for PMe_2Ph: 122°; values from MO calculations[254]: 139.8° (staggered), 155.6° (eclipsed)) on the $Re_2(CO)_8$ unit was of interest. For example, increased

steric bulk could affect the phenomenon of the bending in of the equatorial carbonyl ligands towards the metal-metal bond, observed in the parent carbonyl, $Re_2(CO)_{10}$,[118] and in a series of dirhenium decacarbonyl-isonitrile derivatives, $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-4) (see ch. XIV).

15E.2 Discussion of related $Mn_2(CO)_{10-n}(PR_3)_n$ (n = 1,2) Structures

As has been mentioned, no crystallographic studies of $Re_2(CO)_{10-n}(PR_3)_n$ (n = 1-4) complexes have been reported. However, X-ray crystallography has been used to determine the structures of the related manganese complexes, ax-$Mn_2(CO)_9(PMe_2Ph)$,[224] diax-$Mn_2(CO)_8(PMePh_2)_2$[255] and diax-$Mn_2(CO)_8(PEt_3)_2$.[256] Although bond length values for the manganese complexes cannot be compared to those of $[Re_2(CO)_8(PMe_2Ph)_2]$, overall molecular conformation is comparable. The salient structural features of the $Mn_2(CO)_{10-n}(PR_3)_n$ (n = 1,2) complexes will thus be discussed.

Crystal data and selected bond parameters for the $Mn_2(CO)_{10-n}(PR_3)_n$ (n = 1,2) structures are given in Table 15.8. In all three cases, the dimer adopts a staggered conformation, with C-Mn-Mn-C torsion angles close to the ideal 45°. For the mono-substituted $Mn_2(CO)_9(PMe_2Ph)$, the phosphine ligand occupies an axial position; for the bisphosphine complexes, $Mn_2(CO)_8(PR_3)_2$ (PR_3 = $PMePh_2$, PEt_3), phosphine substitution is diaxial. The observation that phosphine ligands occupy axial sites, rather than electronically favoured equatorial positions, is rationlized in terms of the steric requirements [Tolman cone angles[65]: PMe_2Ph, 122°; PEt_3, 132°; $PMePh_2$, 136°] of the bulky phosphine ligands[112] (see Section 15D; see also ch. XII for a discussion of electronic and steric factors governing ligand site preference in $M_2(CO)_{10}$ (M = Re,Mn) complexes).

Interestingly, an X-ray crystallographic structure determination of $Mn_2(CO)_8(AsMe_2Ph)_2$[255] has shown that this molecule has an eclipsed conformation, with an arsine ligand occupying an equatorial site on each Mn-atom. This crucial difference is ascribed to the longer Mn-As bond distance (av. 2.46Å, cf. av. Mn-P, 2.23Å, for diax-$Mn_2(CO)_8$-

$(PMePh_2)_2$[235]) which reduces repulsion between substituent groups and the carbonyls, hence permitting the electronically favoured equatorial substitution. Steric strain in this molecule is however reflected in the marked angular distortions (eg. Mn-Mn-As: 103°, instead of the ideal 90°) caused by close contacts between the phenyl ring and two of the equatorial carbonyls on the other Mn-atom. The unusual eclipsed conformation is probably adopted in order to minimize repulsions between the arsine substituents and the equatorial CO ligands, as repulsive interactions between the two sets of carbonyl groups is expected to be greater in the eclipsed than in the staggered conformation.[126]

Significantly, for all the three $Mn_2(CO)_{10-n}(PR_3)_n$ (n = 1,2) structures, the Mn'-Mn-COeq bond angles are less than 90°, ie. the equatorial carbonyls bend in towards the Mn-Mn bond. The significance of this will be discussed in section 15E.3.4.

In all three structures, the Mn-C-O bond angles are in the range 171 - 178°, as expected.[19]

15E.3 Discussion of the structure of diax[$Re_2(CO)_8(PPhMe_2)_2$](VII)

The molecular structre of diax[$Re_2(CO)_8(PPhMe_2)_2$](VII), and the numbering system used in the crystal structure determination, is shown in Fig. 15.5. The compound crystallizes in the monoclinic centrosymmetric space group C2/c, with Z = 4. A view of the unit cell, looking down the b-axis, is shown in Fig. 15.6. Bond lengths and bond angles are given in Tables 15.9 and 15.10 respectively. Average bond angle and bond length data is summarized in Table 15.11. The molecule adopts a staggered conformation, with diaxial phosphine substitution. The main structural features will be discussed in detail.

15E.3.1 Diaxial phosphine substitution

The two phosphine ligands occupy the axial positions, as expected from IR data (section 15D). This is in contrast to the structure of $Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ (see ch. XIV), where the two isonitrile ligands occupy electronically favoured equatorial sites. This is an example of the

TABLE 15.8: Crystal data and selected bond parameters for $Mn_2(CO)_{10-n}(PR_3)_n$ structures (n = 1,2) (Bond lengths in Å, bond angles in °)

Complex	$Mn_2(CO)_9(PMe_2Ph)$	$Mn_2(CO)_8(PMePh_2)_2$	$Mn_2(CO)_8(PEt_3)_2$
Space group, Z	C2/c,8	$P2_1/c$,4	Aba2,16
Mn-Mn	2.904	2.90	2.913(6)
Mn-P	2.239	2.23[a]	2.247(7)
Mn-CO[a]	1.76	1.75	1.81(4)
Mn'-Mn-COeq[a]	87.5	86	87.6(5)
Mn-C-O[a]	177.5	176	171(2)
Mn-P-C[a]	114(1)	[b]	116.0(6)
C-P-C[a]	104(1)	102	[b]
P-C[a]	1.84	1.83	1.85(2)
Reference	224	255	256

[a] Average value

[b] Not quoted in reference

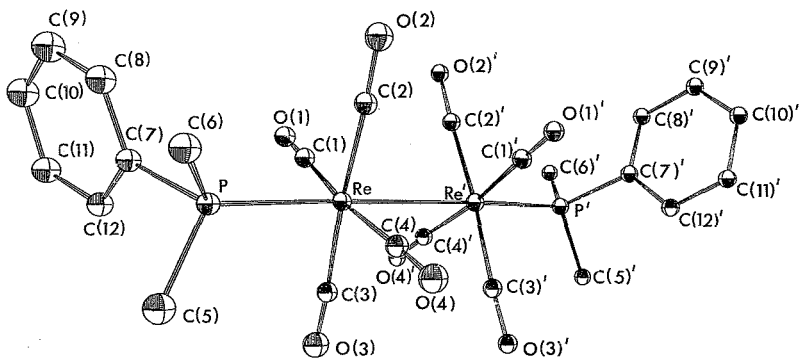


Figure 15.6: ORTEP[45] view of the diax $[Re_2(CO)_8(PMe_2Ph)_2]$ molecule (VII), showing the numbering system used. (Re related to Re' by a 2-fold axis, generating the equivalent position $(-x, y, \frac{1}{2}-z)$, and similarly for the other atoms).

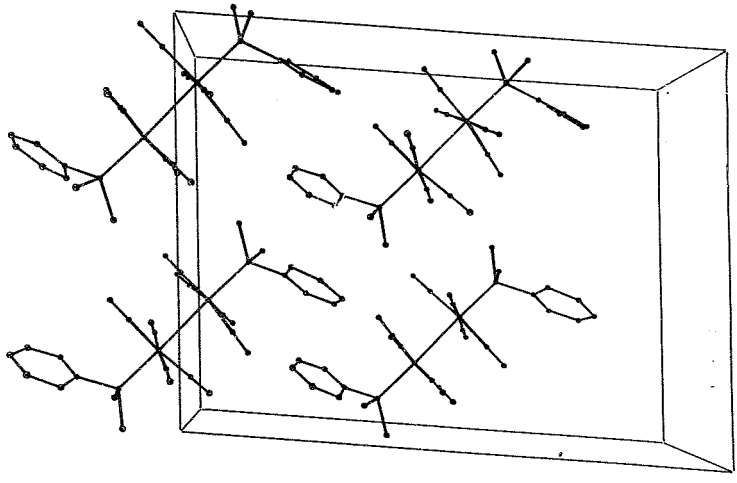


Figure 15.6: ORTEP[45] view of the unit cell of diax-$[Re_2(CO)_8(PMe_2Ph)_2]$ (..I), looking down the b-axis.

dominance of steric factors over electronic site preference in the case of the bulky phosphine ligand. (For the $Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ and $Re_2(CO)_8(PPhMe_2)_2$ structures, the bulky $C_6H_3Me_2$-2,6 groups are much further removed from the Re atom than the $PPhMe_2$ groups viz. adding the av. bond lengths for the linear Re-CN (2.05Å), C-N (1.15Å) and N-C(R) (1.43Å) bonds gives an effective av. Re...C(R) distance of 4.63Å, cf. Re-P distance of 2.35Å; the lesser steric bulk of the isonitrile ligand is also reflected in the "fan-shaped" angles[44] for $CNC_6H_3Me_2$-2,6 of 106° (wideness) and 53° (thickness)).

Axial substitution has also been observed in related $Mn_2(CO)$ (n = 1,2) structures (see section 15E.2). The di- derivative, $Mn_2(CO)_8(CNBu^t)_2$ ("fan-shaped" angles[44] for $CNBu^t$: 70° (wideness) and 68° (thickness)) is again equatorially substituted (see ch.XIV). Hence the size of the metal atom seemingly has no effect on the substitution geometry.

15E.3.2 The Re-Re, Re-P and Re-CO bond lengths

In diax$[Re_2(CO)_8(PMe_2Ph)_2]$ the Re-Re bond length is 3.044(1)Å, only fractionally longer than that of 3.041(1)Å in the parent carbonyl, $Re_2(CO)_{10}$.[158] The substitution of a carbonyl trans to the metal-metal bond by a poorer π-accepting[43a] phosphine ligand, and the consequent increase in electron density on the metal atoms, perhaps in anti-bonding orbitals,[274] might be expected to result in an increase in metal-metal bond length. Such effects have been observed for phosphine-substituted metal clusters eg. $Fe_3(CO)_{11}(PPh_3)$,[275] $Ru_3(CO)_{11}(PPh_3)$,[276] $Os_3(CO)_{11}$-$[P(OMe)_3]$,[277] $(Os_3(CO)_{17}[P(OMe)_3]_4)$,[278] and has also been ascribed to ligand packing effects, ie. congestion between phosphine and carbonyl groups causes expansion of the metal core.[279-281] Further, kinetic studies[282] have shown that the Mn-Mn bond strength in $Mn_2(CO)_8(PR_3)_2$ is less than in $Mn_2(CO)_{10}$.

The av. Re-CO bond length is 1.94(2)Å, similar to that of 1.976(6)Å for the av. Re-CO(trans to CO) bond length

TABLE 15.9 : Bond lengths (Å) for diax$[Re_2(CO)_8(PMe_2Ph)_2]$(VII)

R(x,y,z)-Re(x,y,½-z)	3.044(1)
Re-P	2.349(5)
Re-C(1)	1.954(21)
Re-C(2)	1.949(21)
Re-C(3)	1.946(20)
Re-C(4)	1.921(21)
C(1)-O(1)	1.163(24)
C(2)-O(2)	1.201(24)
C(3)-O(3)	1.178(24)
C(4)-O(4)	1.180(22)
P-C(5)	1.836(28)
P-C(6)	1.836(23)
P-C(7)	1.826(22)
C(7)-C(8)	1.387(31)
C(8)-C(9)	1.434(33)
C(9)-C(10)	1.339(34)
C(10)-C(11)	1.411(36)
C(11)-C(12)	1.419(31)
C(12)-C(7)	1.378(29)

TABLE 15.10 : Bond angles (°) for dimx$[Re_2(CO)_8(PMe_2Ph)_2]$ (VII)

Re-C(1)-O(1)	178.0(18)
Re-C(2)-O(2)	177.6(19)
Re-C(3)-O(3)	177.2(17)
Re-C(4)-O(4)	177.1(18)
P-Re-Re^{1a}	177.2(5)
P-Re-C(1)	93.7(6)
P-Re-C(2)	91.7(6)
P-Re-C(3)	92.4(6)
P-Re-C(4)	93.7(6)
C(1)-Re-Re^{1a}	85.0(5)
C(1)-Re-C(2)	90.5(8)
C(1)-Re-C(3)	90.4(8)
C(1)-Re-C(4)	172.3(8)
C(2)-Re-Re^{1a}	90.7(5)
C(2)-Re-C(3)	175.7(8)
C(2)-Re-C(4)	87.1(9)
C(3)-Re-Re^{1a}	85.2(5)
C(3)-Re-C(4)	91.5(8)
C(4)-Re-Re^{1a}	87.8(5)
Re-P-C(5)	116.0(8)
Re-P-C(6)	116.7(8)
Re-P-C(7)	113.8(6)
C(12)-C(7)-C(8)	120.7(22)
C(7)-C(8)-C(9)	119.2(23)
C(8)-C(9)-C(10)	121.9(28)
C(9)-C(10)-C(11)	117.6(27)
C(10)-C(11)-C(12)	122.3(24)
C(11)-C(12)-C(7)	117.9(22)
P-C(7)-C(8)	119.1(18)
P-C(7)-C(12)	120.2(17)
C(5)-P-C(6)	101.0(11)
C(5)-P-C(7)	102.7(11)
C(6)-P-C(7)	104.8(10)

[a] Re^1 is related to Re by a 2-fold axis, generating the equivalent position ($\bar{x}$ y, $\frac{1}{2}-z$)

TABLE 15.11 : Average bond length (Å) and bond angle (°) data for diax$[Re_2(CO)_8(PMe_2Ph)_2]$ (V.I)

Re-Re	3.044(1)
Re-P	2.349(5)
Re-C	1.94(2)
P-C	1.83(2)
Re-Re-P	177.2(5)
Re-Re-C	87.2(5)
P-Re-C	92.9(6)
C-Re-C(cis)	89.9(8)
Re-C-O	177.5(18)
Re-P-C	115.5(8)
C-P-C	102.8(11)

in $Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ (ch. XIV). The Re-P bond length is 2.349(5)Å.

15E.3.3 Molecular conformation

Although the two sets of eq-carbonyl groups are staggered with respect to each other, the C-Re-Re-C torsional angles (see Appendix C,(VII)) deviate an av. of 6.9° from the ideal 45° (see Fig. 15.7). This is probably due to the influence of crystal packing forces (see section 15E.3.6).

The conformation of the ax-(PMe_2Ph) groups with respect to the eq-CO groups is interesting in that the phenyl rings of the axial phosphine groups each eclipses a carbonyl ligand (see Fig. 15.8), with torsional angle (see Appendix C,(VII)) of 0.0 for C(1)-Re-P-C(7). This feature could be due to :-

(i) steric factors: the methyl groups are then in staggered positions with respect to the eq CO's (see Fig. 15.8(b)), with the smallest OC-Re-P-CH_3 torsional angle being 27.7°. However, in diax-$Mn_2(CO)_8(PEt_3)_2$,[236] all three ethyl groups are staggered with respect to the eq CO ligands.

(ii) electronic factors: possible interactions between the π-cloud of a phenyl ring and an eclipsed CO.

(iii) crystal packing forces (see section 15E.3.6).

The phenyl rings align parallel to the plane of the eq carbonyl groups, as necessitated by steric factors. The two phenyl rings deviate from co-planarity by 30.8° The phenyl rings are slightly puckered (see Table 15.12).

The av. Re-P-C and C-P-C bond angles of 115.5(8)° and 102.8(11)° respectively, and the av. P-C bond length of 1.83(2)Å, are similar to those for the related $Mn_2(CO)_{10-n}(PR_3)_n$ (n = 1,2) structures (see Table 15.8).

15E.3.4. P-Re-CO, OC-Re-CO and Re-Re-CO bond angles

The axP-Re-COeq bond angles are obtuse (av. 92.9(6)° the eqOC-Re-COeq bond angles close to 90° (av. 89.9(8)°, and the Re-Re-COeq bond angles acute (av. 87.2(5)°, ie. the equatorial carbonyls bend in towards the Re-Re bond. This

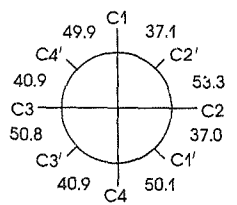


Figure 15.7: Newman projection of diax[$Re_2(CO)_8(PMe_2Ph)_2$] looking down the Re-Re' bond (phosphine groups omitted for clarity). Torsional angles (°). C-Re-Re'-C, between C-atoms adjacent in projection shown.

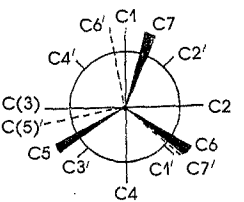
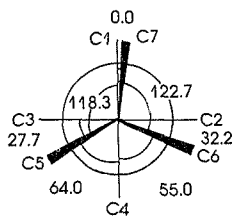


Figure 15.8: Newman projections of diax[$Re_2(CO)_8(PMe_2Ph)_2$], showing conformation of phosphine groups relative to eq carbonyl ligands[a]
(a) Newman projection of diax[$Re_2(CO)_8(PMe_2Ph)_2$], looking down the P-Re-Re'-P' axis.

Figure 15.8 (contd)



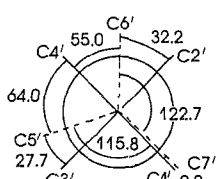


Figure 15.8: (b) *Newman projection* of ax[$Re(CO)_4P(Me_2Ph)$] fragment[a] looking down the P-Re bond.

[a] Selected OC-Re-P-C torsional angles (°) shown.

TABLE 15.12 : *Least squares planes* for phenyl rings in diax$[Re_2(CO)_8(PMe_2Ph)_2]$ (VII)

(a) Phenyl ring on P (i.e. C(7) to C(12))[a]

Atom	deviation(Å)
P	0.120
C(7)	0.022
C(8)	-0.034
C(9)	0.011
C(10)	0.[illegible]
C(11)	-0.037
C(12)	0.013

[a] Equation of plane : $(9.7474)x + (-1.9024)y + (14.1819)g = -0.5419$

(b) Phenyl ring on P' (i.e. C(7)' to C(12)')[b]

Atom	deviation(Å)
P'	-0.117
C(7)'	-0.022
C(8)'	0.034
C(9)'	-0.012
C(10)'	-0.024
C(11)'	0.037
C(12)'	-0.014

[b] Equation of plane : $(9.7334)x + (1.9013)y + (14.1888)g = 7.6319$

effect of the bending in of the equatorial CO ligands towards the metal-metal bond is observed for related $Mn_2(CO)_{10-n}(PR_3)_n$ (n = 1,2) complexes (section 15E.2), as well as for a series of $M_2(CO)_{10-n}(CNR)_n$ (M = Re, n = 1-4; M = Mn, n = 2,4) complexes (ch. XIV) and the parent carbonyls, $M_2(CO)_{10}$ (M = Re,Mn).[138] Hence this phenomenon would appear to be an electronic effect, unaffected by steric considerations. Various explanations have been proposed (see ch. XII), and Elian and Hoffmann[98] have predicted the effect on the basis of MO calculations.

15E.3.5 Re-C-O bond angles

The Re-C-O bond angles are in the range 177(2)° to 178(2)° (av. 177.5°). Slight deviations from linearity (ca. 5°) of M-C-O ligands is expected.[39]

15E.3.6 Packing

The overall conformation adopted by the molecule could be governed largely by crystal packing forces. The molecules pack in a regular fashion (Fig. 15.6). A notable feature is the way in which the phenyl rings of different molecules line up in rows down the cell.

According to Johnson's[248] model of close-packing of CO's for metal carbonyl complexes, packing forces are responsible for distortions from ideal geometry. Crystal packing forces could account for several observed distortions in the diax-$[Re_2(CO)_8(PMe_2Ph)_2]$ molecule:-

(i) An av. 6.0° deviation from ideal 45° C-Re-Re-C torsional angle.

(ii) The slight deviation of the P-Re-Re-P unit from linearity, as evidenced by the P-Re-Re bond angle of 177.2(5)°

(iii) The deviation of the phenyl rings from co-planarity. (Angle between mean planes of the two phenyl rings: 30.8°).

(iv) The deviation from parallel alignment of the phenyl rings with the planes of the C-atoms of the eq carbonyl groups. (Angles between mean planes: Ph(C(7) to C(12)) and eq C-atoms (C(1) to C((4)): 21.3°; Ph(C(7)′ to C(12))′ and eq C-atoms (C(1)′ to C(4)′: 21.3°).

Other structural features that could be largely determined by crystal packing forces are the orientation of the PMe_2Ph groups with respect to the eq CO's such that the phenyl rings eclipse an eq carbonyl, and the position of the phenyl groups relative to each other (ie. which CO ligand is eclipsed by the Ph rings). The role of crystal packing forces in determining overall molecular conformation should not be neglected.

15E.4 Experimental

15E.4.1 Data collection

The compound diex$[Re_2(CO)_8(PMe_2Ph)_2]$ was synthesized in the PdO-catalysed reaction between $Re_2(CO)_{10}$ and PMe_2Ph (section 15D). Recrystallization from diethylether-pentane solution under nitrogen at 20°C yielded fine colourless needlelike crystals.

Preliminary investigation by standard Weissenberg photography established the space group as the centred monoclinic C2/c, or the non-centrosymmetric Cc, from the absences $hk\ell$, $h + k = 2n$, $h0\ell$, $\ell = 2n$ ($h = 2n$) and $0k0$, $k = 2n$. Refined cell constants were obtained during data collection on a Philips PW1100 four-circle diffractometer, using graphite-monochromated MoKα radiation ($\lambda = 0.7107$Å) at room temperature (20°C). Lorentz and polarization corrections were applied, and the data were empirically corrected for absorption effects using the program DIFABS, written by N. Walker and D. Stuart,[117a] and adapted by G. Kruger.[117b] Crystal data and details of the structure analysis are summarized in Table 15.13.

15E.4.2 Structure solution and refinement

Structure analysis and refinement were carried out using the program SHELX82.[116a] Initial co-ordinates for the rhenium atoms were derived from a Patterson synthesis, and the positions of the other non-hydrogen atoms were found by difference Fourier syntheses. The structure was refined in the centrosymmetric space group C2/c (No. 15).* The two halves of the molecule being related by a crystallographic 2-fold axis. Positional parameters for all atoms,

and anisotropic temperature factors for the rhenium and phosphorous atoms, were refined by full-matrix least-squares analyses. In the initial stages, the phenyl rings were treated as rigid hexagons, but all restraints were removed in the later stages of refinement. Least-squares refinement was considered completed when all parameter shifts were less than 0.5σ. At this stage the R-value was 0.0602, Unit Weights were used. Scattering factors for Re(0) were taken from "International Tables for X-ray Crystallography",[46b] and anomalous dispersion corrections[46c] for rhenium were made.

Final atomic co-ordinates for all atoms, and isotropic temperature factors of the carbon and oxygen atoms are given in Table 15.14, and Table 15.15 gives the anisotropic temperature factors of the rhenium and phosphorous atoms. A listing of the Structure Factors is to be found in Appendix D.

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* The structure was also refined in the non-centrosymmetric space group, Cc (No. 9), and Hamilton's Statistical Significance Test on the Crystallographic R Factor[285] applied. At the 0.005 significance level, it was found that the hypothesis that the space group is C2/c and not Cc, could not be rejected.

TABLE 15.13: Crystal data and details of structure analysis for *diax*$[Re_2(CO)_8(PMe_2Ph)_2]$(VII)

Formula	$Re_2C_{24}H_{22}O_6P_2$
Mr	872.76
Crystal dimensions (mm)	0.19 x 0.09 x 0.09
Space group	C2/c (No. 15)
a(Å)	22.779(9)
b(Å)	7.166(3)
c(Å)	17.249(7)
β(°)	95.13(3)
U(Å^3)	2804.33
Z	4
F(000)	1639.61
Dc (gcm^{-3})	2.07
μ(cm^{-1})	84.01
λ(Å)	MoKα (0.7107)
Scan mode	ω/2θ
Range (°)	3≤θ≤23
Scan width (°)	0.90
Scan speed (°sec^{-1})	0.030
Range of hkℓ	±h, +k,+ℓ
Measured intensities	1768
Unique reflections	1473
Internal consistency R-index	0.0314
Omitted reflections	103
Cut-off criterion	F<σF
R	0.0602

Table 15.14 : Final atomic co-ordinates, and isotropic temperature factors for the C and O atoms, of diax-$[Re_2(CO)_8(PMe_2Ph)_2]$ (VII)

Atom	x/a	y/b	c/z	$U(Å^2)$
Re	-0.0480(1)	0.1879(1)	0.1827(1)	-
P	-0.1249(2)	0.1968(8)	0.0824(3)	-
O(1)	-0.1253(6)	0.0013(20)	0.3011(8)	0.060(4)
O(2)	-0.0078(7)	-0.2067(24)	0.1269(9)	0.078(5)
O(3)	0.9174(8)	0.5811(25)	0.2423(9)	0.085(5)
O(4)	0.0[illegible]2(7)	0.3659(24)	0.0789(9)	0.082(5)
C(1)	-0.0963(9)	0.0679(29)	0.2563(11)	0.051(5)
C(2)	-0.0218(9)	-0.0551(30)	0.1486(11)	0.054(5)
C(3)	-0.0685(9)	0.4325(28)	0.2215(10)	0.051(5)
C(4)	0.0085(9)	0.2956(30)	0.1194(11)	0.053(5)
C(5)	-0.1479(12)	0.4299(39)	0.0475(14)	0.082(7)
C(6)	-0.1112(10)	0.0815(34)	-0.0093(13)	0.071(6)
C(7)	-0.1937(9)	0.0952(30)	0.1093(11)	0.054(5)
C(8)	-0.2067(11)	-0.0889(35)	0.0896(13)	0.072(6)
C(9)	-0.2580(12)	-0.1741(41)	0.1166(15)	0.089(8)
C(10)	-0.2959(12)	-0.0782(41)	0.1564(15)	0.085(8)
C(11)	-0.2843(11)	0.1131(36)	0.1697(13)	0.074(7)
C(12)	-0.2320(10)	0.2001(33)	0.1490(12)	0.062(6)

Table 15.15 : Anisotropic temperature factors ($Å^2$) for the Re and P atoms of diax-$[Re_2(CO)_8(PMe_2Ph)_2]$ (VII)

Atom	U11	U22	U33	U23	U13	U12
Re	0.0412(6)	0.0422(5)	0.0419(4)	0.0019(4)	0.0043(3)	0.004(4)
P	0.048(4)	0.063(3)	0.040(3)	0.005(3)	0.001(2)	0.004(3)

Page 333 omitted in the pagination.

XVI. Conclusion

The synthetic utility of catalysts such as PdO (alone or in combination with $[(\eta^5C_5Me_5)Fe(CO)_2]_2$) to bring about the substitution of CO by RNC ligands in transition metal carbonyl complexes under mild thermal conditions has been demonstrated for a wide variety of metal carbonyl complexes, including $(Arene)Cr(CO)_3$, $(C_5H_5)Mn(CO)_3$ and $Re_2(CO)_{10}$. This catalytic synthetic route provided access to novel isonitrile-substituted derivatives of these carbonyl complexes, thus making the derivatives available for further chemical and structural studies.

X-ray crystallographic studies of representative isonitrile-substituted metal carbonyl derivatives were undertaken to establish the stereochemistry of the products. From an analysis of the bond data from these studies, together with a comparison of the structure to that of the unsubstituted parent carbonyl complex, the structural effect of ligand substitution was evaluated. Trends were rationalized in terms of electronic effects, and deviations explained by the influence of steric factors and/or crystal packing forces. Further, with the backing of the crystallographic studies, the relationship between molecular structure and IR spectral data was examined.

The crystal and molecular structures of $(\eta^5C_5H_5CO_2Me)$-$Cr(CO)_2(CNBu^t)$ and $(\eta^5C_5H_5)Mn(CO)_2(CNBu^t)$ were undertaken largely in order to establish whether the anomalous IR spectra of these complexes could be explained in terms of molecular structure. No definite conclusion could be reached in this regard, but possible explanations for the anomalous IR data were advanced. If the effect is due to the bent C-N-C bond, crystal structure determinations of similar complexes which do not show the anomalous IR spectral behaviour, eg. $Cr(CNC_6H_3Me_2\text{-}2,6)$ (attempts to solve this structure unsuccessful), $(\eta^5C_5H_5)Mn(CO)_2(CNC_6H_3Me_2\text{-}2,$ may help clarify the issue, as such complexes would thus be expected to have a linear C-N-C bond. No explanation of the anomalous IR spectra of

the $Fe(CO)_3(CNR)_2$ complexes could be found from the crystal and molecular structure of $Fe(CO)_3(CNMe)_2$. The reason for the anomalous IR data is unclear.

A systematic study (spectral, structural and mechanistic) was conducted of the $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-4) complexes. From an X-ray crystallographic study of a series of representative derivatives, viz. $Re_2(CO)_9(CNBu^t)$, $Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$, $Re_2(CO)_7(CNMe)_3$ and $Re_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$, it was shown that the increasing degree of isonitrile substitution has little structural effect on the dimer, relative to the parent carbonyl, $Re_2(CO)_{10}$. In particular, the equatorial ligands (both CO and CNR) bend in towards the rhenium-rhenium bond, as in $Re_2(CO)_{10}$, despite the increased steric bulk of the isonitrile ligands. Further, the poorer π-accepting RNC ligands do not result in an increase in the Re-Re bond length for the $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-3) complexes, although a slight lengthening is observed for $Re_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$. A shortening of the Re-CO bonds trans to an RNC is however a general trend. The structures of two manganese analogues, $Mn_2(CO)_8(CNBu^t)_2$ and $Mn_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$, were also determined crystallographically. The above features are applicable, but here a lengthening of the Mn-Mn bond relative to that in $Mn_2(CO)_{10}$ is observed.

It was found that the differences in the IR and ^1H NMR spectra of the $Re_2(CO)_8(CNR)_2$ and $Mn_2(CO)_8(CNR)_2$ derivatives could be explained in terms of differences in the substitution geometry, as demonstrated by the crystal structure determinations of 1,2-dieq-$Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ and 1,1-cis-dieq-$Mn_2(CO)_8(CNBu^t)_2$. Kinetic studies on $M_2(CO)_{10-n}(CNBu^t)_n$ (M = Mn, Re; n = 1-3) are in progress[23] and should provide information on the formation of isomers and the reaction pathways.

An X-ray crystal structure determination confirmed the diax-substitution of $Re_2(CO)_8(PMe_2Ph)_2$, obtained from the PdO-catalysed reaction of $Re_2(CO)_{10}$ and PMe_2Ph. However, an ax-eq isomer was prepared by alternate methods.

The substitution geometry of the latter isomer was established by IR spectral methods.

From a consideration of IR spectral data of $M_2(CO)_8(L)_2$ (M = Re,Mn) complexes, backed up by X-ray crystallographic structural information, it was found to be possible to establish a correlation between IR spectral data (number of ν(CO) bands, and intensity pattern) and molecular geometry. This has been done for all known isomers of $M_2(CO)_8(L)_2$, viz. 1,2-diax, 1,2-ax,eq, 1,2-eq,eq, 1,1-ax,eq and 1,1-cis-dieq. A synthetic challenge would be to tailor-make the missing isomer, 1,1-trans-dieq-$M_2(CO)_8(L)_2$, to complete the set.

This work demonstrated that the catalytic synthetic route opens up new areas of metal carbonyl-isonitrile chemistry. Extensions of this method to other complexes can be invisaged, for exa[illegible]he full potential of the reaction between $(\eta^5C_5H_5)V$[illegible]RNC in the presence of Pd-catalyst, is being further explored.[279]

The approach of investigating substitution geometry and and structural effects of increasing ligand substitution, exemplified by the $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-4) study, could be extended to other systems. Specifically, the $Re_2(CO)_{10-n}$[illegible]$_n$ system could be further investigated. With str[illegible]ural data from X-ray studies of isomers of $Re_2(CO)_7(PR_3)_3$, together with IR spectra, a correlation could be established between IR data and substitution geometry, as has been demonstrated for the $M_2(CO)_8(L')_2$ case.

In this work, monomeric and dimeric metal carbonyl complexes were studied. A logical extension would be to trimeric complexes. Trimers can be of two types, viz. triangular (closed) eg. $Os_3(CO)_{12}$[illegible] or oper, linear eg. $[Mn_3(CO)_{14}]^-$,[277] or bent eg. [illegible]$Mn(CO)_{14}]$.[281] Few systematic investigations have been reported on this latter class of compounds. Structural studies on these higher clusters along the lines of the $Re_2(CO)_{10}$/RNC structural study would be expected to provide valuable information regarding the substitution geometry, molecular conformation and structural trends.

Appendix A

The Sources of Chemicals used in this study

All materials were used as obtained from the manufacturers, without further purification

(A) General Chemicals

(a) Strem Chemicals Incorporated: $Re_2(CO)_{10}$, $[(C_5H_5)Fe(CO)_2]_2$, $(C_6H_6)Cr(CO)_3$, $(C_6H_5Me)Cr(CO)_3$, $(C_5H_5)Mn(CO)_3$, $(C_5H_5)V(CO)_4$, $Cr(CO)_6$, $Fe(CO)_5$, PMe_2Ph, $PMePh_2$, PMe_3, $P(CH_2C_6H_5)$, $AsMe_2Ph$.

(b) Fluka AG: ^tBuNC, 2,6-$Me_2C_6H_4NC$, $C_6H_{11}NC$, $NMe_3O.2H_2O$.

(c) Merck Chemicals: PPh_3, $LiAlH_4$.

(d) British Drug Houses Ltd.: $P(OMe)_3$, $CaCO_3$, $C_6H_5CO_2Me$.

(e) Aldrich Chemical Co. Ltd.: $C_6H_5CH_2NC$.

(f) Schuch: $CClCO_2Me$

(B) Catalysts Supported metals, metals and metal oxides.

(a) Strem Chemicals Incorporated: Re/C(5% Re), Pd/$BaCO_3$(5% Pd), Pd/$BaSO_4$(5% Pd), Pd/Al_2O_3(5% Pd), Pt/Al_2O_3(5%Pt).

(b) Engelhard: Pd/C(5% Pd), Pt/C(5% Pt), Rh/C(5% Rh), Ru/C(5% Ru).

(c) Merck Chemicals: Pd/$CaCO_3$(10% Pd), Pd/C(10% Pd), Pt/C(10% Pt).

(d) Johnson Matthey Chemicals Ltd.: PdO, PtO_2, Pd(metal).

(e) Analar: Zn(metal).

(f) Pierce Chemical Co. Ltd.: Pd-impregnated polymer (40 mesh).

(g) In addition, Activated Carbon, "Bergswerksverband", GmbH Type PK221, was a gift from Dr. G.J. McDougal.

(C) Other Sources

(a) The following compounds were gifts from Dr. M.O. Albers: $[(C_5Me_5)Fe(CO)_2]_2$,[21] $[(C_5H_5)Fe(CNC_6H_3Me_2\text{-}2,6)_2]_2$,[23] $(C_6H_5Cl)Cr(CO)_3$,[11a] $CoCl_2.2H_2O$,[142] MeNC,[262] and the $Fe(CO)_3(CNMe)_2$[142] used in the X-ray structure analysis.

Appendix A (contd)

(b) The *following* compounds were gifts from Dr. N.J. Coville: The samples of $Mn_2(CO)_8(CNBu^t)_2$ and $Mn_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$[220] used in the X-ray structure analyses, and the isotopically labelled $Re_2(^{13}CO)_{10}$.[221]

(c) The sample of ax-$Mn_2(CO)_9(PMe_2Ph)$ used for recording the IR spectrum (Fig. 11.2(b)) was a gift from Dr. E. Singleton.[133]

Appendix B

General Experimental Details

(a) Synthetic Methods

All reactions were routinely carried out under an inert atmosphere of argon in an appropriate round-bottomed flask. Oil baths (pre-set to the appropriate temperature) were used for the heating of the reaction solution. Generally, all solvents were deoxygenated prior to use by a rapid stream of nitrogen passed through the solvent.

Column chromatography was carried out using silica gel (Merck, "Kieselgel 60", 60-200μm). Thin layer chromatography (TLC) was carried out on silica gel (Merck, silica gel 60 F-254), and preparative layer chromatography was performed using silica gel plates (Merck, silica gel 60 F-254, 20 x 20cm, layer thickness 2 mm).

Operations such as filtration, chromatography and routine recrystallizations, were generally carried out in air, unless otherwise stated.

For the purposes of obtaining crystals suitable for X-ray analysis, slow recrystallizations were carried out either under nitrogen in a suitable solvent system at room temperature, of in a deoxygenated solution at -5°C.

(b) Solvents

The following solvents were distilled under an atmosphere of nitrogen, prior to use:

(i) benzene and tetrahydrofuran (THF), from sodium benzophenone ketyl

(ii) toluene and xylene, from sodium

(iii) hexane, heptane and dichloromethane, from calcium hydride

(iv) pentane, from sodium benzophenone ketyl, with diglyme (diethylene glycol dimethyl ether).

(c) Instrumentation

Infra red spectra were recorded using either a Pye Unicam SP300 or a Jasco IRA 1 instrument. The IR spectra of the $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-4) derivatives were recorded on a Pye Unicam SP300

Appendix B (contd)

spectrophotometer, at X5 expansion.

FTIR spectra were run on a Bruker IFS 85 FTIR spectrophotometer.

All ^{1}H NMR spectra were recorded using a Bruker WP80 FTNMR spectrometer. Spectra were run in C_6D_6, relative to TMS (tetramethylsilane).

ss spectra were all obtained using a Varian MAT CH5 spectrometer (operating at 70eV).

Melting points were determined using a Kofler micro-hotstage apparatus, and are all uncorrected.

Microanalyses were all performed by the Microanalytical Division of the National Chemical Research Laboratories, South African Council for Scientific and Industrial Research (Pretoria).

(d) X-ray data collection

Preliminary investigations were by standard Weissenberg and precession methods. For the photographic work a Seifert X-ray generator, using Ni-filtered monochromatic CuKα radiation(λ = 1.5418Å), was employed. The Space Group was determined from the systematic absences, and cell constants were measured from the photographs.

Refined cell constants were obtained during data collection on a Philips PW1100 four-circle diffractometer with MoKα (λ= 0.7107Å) or CuKα (λ= 1.5418Å) graphite-monochromated radiation, using $\omega/2\theta$ scans. The cell constants were obtained by least-squares refinement of the θ values of 25 general reflections in the measured θ range. During data collection, the intensity of certain standard reflections were checked at intervals, to ensure that crystal deterioration was not observed. The data collection was performed at the National Physical Research Laboratories, South African Council for Scientific and Industrial Research (Pretoria).

(e) Crystallographic Computing Programs

SHELX82: Program for Crystal Structure Determination, by G. Sheldrick - used for structure solution and refinement.

XANADU : Program for crystallographic calculations by P. Roberts and G. Sheldrick - used to calculate torsional angles and the best least-squares plane through atoms, with deviations of atoms from the mean plane.

Appendix B (contd)

DIFABS : Program for correcting diffractometer data for absorption effects, by N. Walker and D. Stuart,[217a] adapted by G.J. Kruger[217b] - used to correct data for absorption in the case of the Re_2 structures.

ORTEP : A Fortran Thermal-Ellipsoid Plot Program for Crystal Structure Illustrations by C.K. Johnson[45] - used to plot diagrams of the molecules and unit cells for the crystal structures.

(f) Crystallographic R-indices

(i) The internal consistency R-index: R is defined as $R = [\Sigma(N.\Sigma(w(F(mean)-F)^2))/\Sigma((N-1).\Sigma(wF^2))]^{\frac{1}{2}}$ where the inner summations are over the N equivalent reflections averaged to give F(mean), and the outer summations are over all unique reflections.

(ii) The conventional R, $R = \Sigma||Fo|-|Fc||/\Sigma|Fo|$, where Fo is the observed structure factor, and Fc the calculated structure factor.

(iii) The weighted R, Rw, $Rw = \Sigma|Fo-Fc|w^{\frac{1}{2}}/\Sigma|Fo|w^{\frac{1}{2}}$, where w is the weighted used ($w = k/(\sigma^2 F)$, k being redetermined after each structure factor calculation).

Appendix C

Torsional Angles for the $M_2(CO)_{10-n}(L)_n$ Structures (M = Re, L = RNC, n = 1-4; M = Mn, L = RNC, n= 2,4; M = Re, L = PMe_2Ph, n = 2)

The program XANADU, written by Paul Roberts and G. Sheldrick, was used to calculate torsional angles for the $M_2(CO)_{10-n}(L)_n$ structures, using the SHELX[348a] output of the final atomic co-ordinates from the crystal structure determinations to perform the calculations.

The torsional angle C(n)-Re(1)-Re(2)-C(m) is defined as the angle between the vector Re(1)-C(n) and the vector Re(2)-C(m), when viewed down Re(1)-Re(2). The sign of the torsional angle is positive if Re(1)-C(n) is to be rotated clockwise into Re(2)-C(m), and negative if anticlockwise.

In the case of the structure diax[$Re_2(CO)_8(PMe_2Ph)_2$](VII), the C(x)-Re-P-C(y) torsional angles are [illegible]ly defined.

Torsional angles (°) are listed [illegible]ructures:-

(I) $Re_2(CO)_9(CNBu^t)$

(II) $Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$

(III) $Re_2(CO)_7(CNMe)_3$

(IV) $Re_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$

(V) $Mn_2(CO)_8(CNBu^t)_2$

(VI) $MN_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$

(VII) diax[$Re_2(CO)_8(PMe_2Ph)_2$]

(I) $Re_2(CO)_8(CNBu^t)$		(II) $Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$	
C(1)-Re(1)-Re(2)-C(5)	42.8	CN(1)-Re(1)-Re(2)-CN(2)	137.6
C(1)-Re(1)-Re(2)-C(6)	-45.1	CN(1)-Re(1)-Re(2)-CO(5)	46.6
C(1)-Re(1)-Re(2)-C(7)	156.9	CN(1)-Re(1)-Re(2)-CO(6)	-134.4
C(1)-Re(1)-Re(2)-C(8)	-138.2	CN(1)-Re(1)-Re(2)-CO(7)	-44.9
C(1)-Re(1)-Re(2)-C(9)	135.8	CN(1)-Re(1)-Re(2)-CO(8)	101.2
C(2)-Re(1)-Re(2)-C(5)	-57.4	CO(1)-Re(1)-Re(1)-CN(2)	-134.2
C(2)-Re(1)-Re(2)-C(6)	-145.2	CO(1)-Re(2)-Re(2)-CO(5)	134.8
C(2)-Re(1)-Re(2)-C(8)	121.6	CO(1)-Re(2)-Re(2)-CO(6)	-46.2
C(2)-Re(1)-Re(2)-C(9)	35.6	CO(1)-Re(1)-Re(2)-CO(7)	43.4
C(3)-Re(1)-Re(2)-C(5)	132.9	CO(1)-Re(1)-Re(2)-CO(8)	-170.6
C(3)-Re(1)-Re(2)-C(6)	45.1	CO(2)-Re(1)-Re(2)-CN(2)	37.7
C(3)-Re(1)-Re(2)-C(7)	-113.0	CO(2)-Re(1)-Re(2)-CO(5)	-53.3
C(3)-Re(1)-Re(2)-C(8)	-48.1	CO(2)-Re(1)-Re(2)-CO(6)	125.7
C(3)-Re(1)-Re(2)-C(9)	-134.1	CO(2)-Re(1)-Re(2)-CO(7)	-144.8
C(4)-Re(1)-Re(2)-C(5)	-47.1	CO(3)-Re(1)-Re(2)-CN(2)	49.3
C(4)-Re(1)-Re(2)-C(6)	-134.9	CO(3)-Re(1)-Re(2)-CO(5)	-41.7
C(4)-Re(1)-Re(2)-C(7)	67.1	CO(3)-Re(1)-Re(2)-CO(6)	137.3
C(4)-Re(1)-Re(2)-C(8)	131.9	CO(3)-Re(1)-Re(2)-CO(7)	-133.2
C(4)-Re(1)-Re(2)-C(9)	45.9	CO(3)-Re(1)-Re(2)-CO(8)	12.9
C(10)-Re(1)-Re(2)-C(5)	-137.4	CO(4)-Re(1)-Re(2)-CN(2)	-43.0
C(10)-Re(1)-Re(2)-C(6)	134.8	CO(4)-Re(1)-Re(2)-CO(5)	-134.0
C(10)-Re(1)-Re(2)-C(7)	-23.2	CO(4)-Re(1)-Re(2)-CO(6)	45.0
C(10)-Re(1)-Re(2)-C(8)	41.6	CO(4)-Re(1)-Re(2)-CO(7)	134.5
C(10)-Re(1)-Re(2)-C(9)	-44.4	CO(4)-Re(1)-Re(2)-CO(8)	-79.4

(III) $Re_2(CO)_7(CNMe)_3$		(IV) $Re_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$ [a]	
C(1)-Re(1)-Re(2)-C(6)	-127.9	C(1)-Re-Re'-C(2)'	-98.0
C(1)-Re(1)-Re(2)-C(7)	-37.8	C(1)-Re-Re'-C(3)'	171.4
C(1)-Re(1)-Re(2)-C(9)	53.7	C(1)-Re-Re'-C(4)'	-8.6
C(1)-Re(1)-Re(2)-C(10)	140.6	C(1)-Re-Re'-C(5)'	84.1
C(2)-Re(1)-Re(2)-C(5)	-133.0	C(2)-Re-Re'-C(1)'	-95.9
C(2)-Re(1)-Re(2)-C(6)	-44.3	C(2)-Re-Re'-C(2)'	-48.9
C(2)-Re(1)-Re(2)-C(7)	45.9	C(2)-Re-Re'-C(3)'	-139.4
C(2)-Re(1)-Re(2)-C(9)	137.4	C(2)-Re-Re'-C(4)'	40.6
C(2)-Re(1)-Re(2)-C(10)	-135.7	C(2)-Re-Re'-C(5)'	133.2
C(3)-Re(1)-Re(2)-C(5)	45.9	C(3)-Re-Re'-C(1)'	173.6
C(3)-Re(1)-Re(2)-C(6)	134.6	C(3)-Re-Re'-C(2)'	-139.4
C(3)-Re(1)-Re(2)-C(7)	-135.3	C(3)-Re-Re'-C(3)'	130.0
C(3)-Re(1)-Re(2)-C(9)	-43.8	C(3)-Re-Re'-C(4)'	-50.0
C(3)-Re(1)-Re(2)-C(10)	43.1	C(3)-Re-Re'-C(5)'	42.6
C(4)-Re(1)-Re(2)-C(5)	136.9	C(4)-Re-Re'-C(1)'	-6.4
C(4)-Re(1)-Re(2)-C(6)	-134.4	C(4)-Re-Re'-C(2)'	40.6
C(4)-Re(1)-Re(2)-C(7)	-44.2	C(4)-Re-Re'-C(3)'	-50.0
C(4)-Re(1)-Re(2)-C(9)	47.3	C(4)-Re-Re'-C(4)'	130.0
C(4)-Re(1)-Re(2)-C(10)	134.2	C(4)-Re-Re'-C(5)'	-137.3
C(8)-Re(1)-Re(2)-C(5)	-44.4	C(5)-Re-Re'-C(1)'	86.2
C(8)-Re(1)-Re(2)-C(6)	44.3	C(5)-Re-Re'-C(2)'	133.2
C(8)-Re(1)-Re(2)-C(7)	134.5	C(5)-Re-Re'-C(3)'	42.7
C(8)-Re(1)-Re(2)-C(9)	-134.1	C(5)-Re-Re'-C(4)'	-137.4
C(8)-Re(1)-Re(2)-C(10)	-47.1	C(5)-Re-Re'-C(5)'	-44.7

[a] Atom Re' is related to atom Re by a 2-fold axis, generating the equivalent position ($\frac{1}{4}$-x, $\frac{1}{4}$-y, z), and similarly for C(n)' and C(m) atoms (n = 1-5)

(V) $Mn_2(CO)_8(CNBu^t)_2$		(VI) $Mn_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$ [a]	
C(1)-Mn(1)-Mn(2)-C(6)	46.1	C(1)-Mn-Mn'-C(1)'	45.0
C(1)-Mn(1)-Mn(2)-C(7)	-36.1	C(1)-Mn-Mn'-C(2)'	114.8
C(1)-Mn(1)-Mn(2)-C(8)	137.0	C(1)-Mn-Mn'-C(3)'	-137.0
C(1)-Mn(1)-Mn(2)-C(9)	-43.7	C(1)-Mn-Mn'-C(4)'	-134.8
C(1)-Mn(1)-Mn(2)-C(10)	-134.2	C(1)-Mn-Mn'-C(5)'	-43.7
C(2)-Mn(1)-Mn(2)-C(6)	132.1	C(2)-Mn-Mn'-C(1)'	114.1
C(2)-Mn(1)-Mn(2)-C(7)	50.0	C(2)-Mn-Mn'-C(3)'	-153.9
C(2)-Mn(1)-Mn(2)-C(8)	-137.0	C(2)-Mn-Mn'-C(4)'	-65.7
C(2)-Mn(1)-Mn(2)-C(9)	42.3	C(2)-Mn-Mn'-C(5)'	25.5
C(2)-Mn(1)-Mn(2)-C(10)	-48.1	C(3)-Mn-Mn'-C(1)'	137.0
C(3)-Mn(1)-Mn(2)-C(6)	-102.3	C(3)-Mn-Mn'-C(2)'	-153.2
C(3)-Mn(1)-Mn(2)-C(8)	-11.4	C(3)-Mn-Mn'-C(3)'	-131.0
C(3)-Mn(1)-Mn(2)-C(9)	167.9	C(3)-Mn-Mn'-C(4)'	-42.8
C(3)-Mn(1)-Mn(2)-C(10)	77.5	C(3)-Mn-Mn'-C(5)'	48.4
C(4)-Mn(1)-Mn(2)-C(6)	-44.9	C(4)-Mn-Mn'-C(1)'	-134.8
C(4)-Mn(1)-Mn(2)-C(7)	-127.1	C(4)-Mn-Mn'-C(2)'	-64.9
C(4)-Mn(1)-Mn(2)-C(8)	46.0	C(4)-Mn-Mn'-C(3)'	-42.8
C(4)-Mn(1)-Mn(2)-C(9)	-134.7	C(4)-Mn-Mn'-C(4)'	45.5
C(4)-Mn(1)-Mn(2)-C(10)	134.8	C(4)-Mn-Mn'-C(5)'	136.6
C(5)-Mn(1)-Mn(2)-C(6)	-136.4	C(5)-Mn-Mn'-C(1)'	-43.6
C(5)-Mn(1)-Mn(2)-C(7)	141.5	C(5)-Mn-Mn'-C(2)'	26.2
C(5)-Mn(1)-Mn(2)-C(8)	-45.5	C(5)-Mn-Mn'-C(3)'	48.4
C(5)-Mn(1)-Mn(2)-C(9)	133.8	C(5)-Mn-Mn'-C(4)'	136.6
C(5)-Mn(1)-Mn(2)-C(10)	43.3	C(5)-Mn-Mn'-C(5)'	-132.3

[a] Atom Mn' is related to atom Mn by a 2-fold axis, generating the equivalent position (1-x, 1-y, z), and similarly for the C(n)' and C(n) atoms (n = 1-5)

(VII) diax[$Re_2(CO)_6(PMe_2Ph)_2$]

C(n)-Re(1)-Re'-C(m)[a]		C(x)-Re-P-C(y)	
P-Re-Re'-C(1)'	-172.1	C(1)-Re-P-C(5)	118.3
P-Re-Re'-C(2)'	97.5	C(1)-Re-P-C(6)	-122.7
P-Re-Re'-C(3)'	-81.2	C(1)-Re-P-C(7)	0.0
P-Re-Re'-C(4)'	10.5	C(2)-Re-P-C(5)	-151.1
C(1)-Re-Re'-P'	-171.8	C(2)-Re-P-C(6)	-32.2
C(1)-Re-Re'-C(1)'	127.5	C(2)-Re-P-C(7)	90.1
C(1)-Re-Re'-C(2)'	37.1	C(3)-Re-P-C(5)	27.7
C(1)-Re-Re'-C(3)'	-141.6	C(3)-Re-P-C(6)	146.7
C(1)-Re-Re'-C(4)'	-49.9	C(3)-Re-P-C(7)	-91.1
C(2)-Re-Re'-P'	97.7	C(4)-Re-P-C(5)	-64.0
C(2)-Re-Re'-C(1)'	37.0	C(4)-Re-P-C(6)	55.0
C(2)-Re-Re'-C(2)'	-53.3	C(4)-Re-P-C(7)	177.2
C(2)-Re-Re'-C(3)'	128.0		
C(2)-Re-Re'-C(4)'	-40.7		
C(3)-Re-Re'-P'	-81.1		
C(3)-Re-Re'-C(1)'	-141.7		
C(3)-Re-Re'-C(2)'	127.9		
C(3)-Re-Re'-C(3)'	-50.8		
C(3)-Re-Re'-C(4)'	40.9		
C(4)-Re-Re'-P'	10.7		
C(4)-Re-Re'-C(1)'	-50.0		
C(4)-Re-Re'-C(2)'	-140.4		
C(4)-Re-Re'-C(3)'	40.9		
C(4)-Re-Re'-C(4)'	132.6		

[a] Atom Re' is related to atom Re by a 2-fold axis, generating the *equivalent position* $(x,y,\frac{1}{2}-z)$, and similarly for atoms P' and P and C(n)' and C(n) (n = 1-4).

Appendix D

Structure Factor Tables

The Structure Factor Tables from the ten crystal structure determinations are bound as a separate volume (105 pages).

List of Contents

Code name	(no of pages)	Structure
LS2H	(9)	$(\eta^6\text{-}C_6H_5CO_2Me)Cr(CO)_2(CNBu^t)$
CPMN	(4)	$(\eta^5\text{-}C_5H_5)Mn(CO)_2(CNBu^t)$
FEME	(6)	$Fe(CO)_3(CNMe)_2$
RECO	(8)	$Re_2(CO)_9(CNBu^t)$ (I)
REX2	(20)	$Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ (II)
REM3	(15)	$Re_2(CO)_7(CNMe)_3$ (III)
REX4	(13)	$Re_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$ (IV)
MNTB	(18)	$Mn_2(CO)_8(CNBu^t)_2$ (V)
MNXY	(7)	$Mn_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$ (VI)
REP2	(7)	diax$[Re_2(CO)_8(PMe_2Ph)_2]$ (VII)

Appendix E

List of Publications

The following is a list of publications that have arisen from the work carried out in this thesis.

(a) G.W. Harris, M.O. Albers, J.C.A. Boeyens and N.J. Coville, "Metal Dimers as Catalysts: 5. Catalytic Synthesis of $(\eta^6\text{-Arene})Cr(CO)_2(CNR)$ and the Crystal and Molecular Structure of $(\eta^6\text{-}C_6H_5CO_2Me)Cr(CO)_2(CNBu^t)$," Organometallics, 2 (1983) 609.

(b) G.W. Harris, J.C.A. Boeyens and N.J. Coville, "Structure of Dimethylisonitriletetracarbonyliron(0): $Fe(CO)_3(CNCH_3)_2$," Acta Cryst., C39 (1983) 1180.

(c) G.W. Harris, J.C.A. Boeyens and N.J. Coville, "Catalytic Synthesis of $(\eta^5\text{-}C_5H_5)Mn(CO)_2(CNR)$ complexes and the Crystal and Molecular Structure of $(\eta^5\text{-}C_5H_5)Mn(CO)_2(CNBu^t)$," J. Organomet. Chem., 255 (1983) 87.

(d) M.O. Albers, J.C.A. Boeyens, N.J. Coville and G.W. Harris, "Synthesis and Crystal Structure of t-butylisocyanidenona-carbonyldirhenium(0): $Re_2(CO)_9(CNBu^t)$," J. Organomet. Chem., 260 (1984) 99.

(e) D.J. Robinson, G.W. Harris, J.C.A. Boeyens and N.J. Coville, "A Structural and Kinetic Investigation of the Isomers of $M_2(CO)_8(CNBu^t)_2$ (M = Mn,Re)," J. Chem. Soc., Chem. Commun., (1984) 1307.

(f) G.W. Harris and N.J. Coville, "The PdO catalysed reaction between $[Re_2(CO)_{10}]$ and isontriles," Organometallics, 4, (1985) 908.

(g) G.W. Harris, J.C.A. Boeyens and N.J. Coville, "Synthetic substitution of $[Re_2(CO)_{10}]$. The crystal and molecular structures of a series of $[Re_2(CO)_{10-n}(CNR)_n]$ complexes (n = 1, R = ^{t}Bu; n = 2,4, R = 2,6-$Me_2C_6H_4$; n = 3, R = Me)," Organometallics, 4, (1985) 914.

Appendix E (contd)

(h) G.W. Harris, J.C.A. Boeyens and N.J. Coville, "The Pd catalysed reaction between $Re_2(CO)_{10}$ and phosphines and the crystal and molecular structure of *diax*-$Re_2(CO)_8(PMe_2Ph)_2$," J. Chem. Soc., Dalton Trans., submitted.

(i) G.W. Harris and N.J. Coville, "$Re_2(CO)_{10}$ and its derivatives," Coord. Chem. Rev., in preparation.

(j) N.J. Coville, G.W. Harris and D. Reader, "Synthesis and characterisation of a series of Vanadium isonitrile complexes," J. Organomet. Chem., 293, (1985) 365.

(k) D.J. Robinson, G.W. Harris, J.C.A. Boeyens and N.J. Coville, "A kinetic investigation of the reactions of $M_2(CO)_{10}$ (M = Mn,Re) with isonitriles, and the crystal and molecular structures of $Mn_2(CO)_8(CNBu^t)_2$ and $Mn_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$," J. Chem. Soc., Dalton Trans., in preparation.

(l) P.D. Harvey, I.S. Butler, N.J. Coville and G.W. Harris, "Application of Raman microprobe technique (MOLE) to the study of vibrational spectroscopy of rhenium carbonyl and its isonitrile derivatives," Can. J. Chem., in preparation.

Appendix F

Molecular Mechanics Calculations

In ch XIV, the results of the X-ray crystal structure determinations of a series of dirhenium carbony_-isonitrile complexes viz. $Re_2(CO)_9(CNBu^t)$ (I), $Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ (II) $Re_2(CO)_7(CNMe)_3$ (III) and $Re_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$ (IV), were presented. In order to quantify the relative importance of the various steric and electronic factors in these structures, molecular mechanics calculations were performed on the complexes (I) - (IV).

The molecular mechanics calculations were carried out using the Energy Minimization Program bMPMDS[285], written by M.I.J. Haneef, and based on the molecular mechanics program of White[286]. The force field used was based on that developed by Koolman et al[287]. (see equation I)

$$E_{total} = \sum_{bonds} K_r(r-r_{eq})^2 + \sum_{angles} K_\theta(\theta-\theta_{eq}) + \sum_{dihedrals} \frac{V_n}{2}[1 + \cos(n\phi-\gamma)]$$
$$+ \sum_{i<j} \frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^{6}} + \frac{q_i q_j}{\varepsilon R_{ij}} \qquad (I)$$

The sources of the force field parameters are discussed below.

(a) Non-bonded parameters

The non-bonded parameters were based on the Lennard-Jones potential (see equation II).

$$V(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$
$$\text{where } A = \sqrt{\varepsilon^*}\,(2r^*)^6 \qquad (II)$$
$$\text{and } B = \sqrt{\varepsilon^*}\,(2r^*)^3$$

r^* is the van der Waals minimum, and ε^* the van der Waals well depth (see Figure E.1).

Figure E.1. Plot of V(r) against r, showing r^* and ε^*.

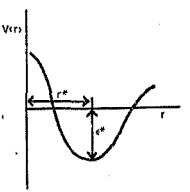

Table E.1 : Values of the force field parameters used in the calculations.

E.1.1. r^* and ε^*

Atom type	r^*(Å)	ε^*(kcal/mol)
C	1.850	0.120
C(CN)	2.025	0.120
O	1.600	0.200
N	1.750	0.160
Re	2.761	0.250

E.1.2. K_r and r_{eq}

Bond Type	Kr (kcal/mol Å^2)	req (Å)
C O	570	1.130
C Re	350	1.987
C N (double)	570	1.130
(single)	367	1.450
C C (single)	317	1.552
(aromatic)	512	1.388
Re Re	118	3.048

E.1.3. θ_r and θ_{eq}

Angle type	K_θ(kcal/mol rad^2)	θ_{eq}(°)
eqOC-Re-COeq trans	58.0	172.5
cis	58.0	89.8
axOC-Re-COeq	58.0	93.7
eqOC-Re-CN trans	58.0	174.9
cis	58.0	89.9
axOC-Re-CN	58.0	92.1
NC-Re-CN	58.0	89.3
eqCO-Re-Re	58.0	86.4
axCO-Re-Re	58.0	176.3
CN-Re-Re	58.0	87.5
Re-C-O(eq)	72.0	178.0
Re-C-O(ax)	72.0	177.5
Re-C-N	72.0	175.5
C-N-C	90.0	175.0
N-C-C(^{t}Bu)	80.0	103.7
C-C-C(^{t}Bu)	63.0	109.1
C-C-C(benzene)	85.0	120.0
N-C-C(benzene)	70.0	120.0

Table E2 : Observed and calulated Re-Re bond lengths for the $Re_2(CO)_{10-n}(CNR)_n$ (n = 0-4) structures.

Structure	Re-Re bond length (Å) Crystal Structure	Calculated
$Re_2(CO)_{10}$	3.041(1)	3.041
$Re_2(CO)_9(CNBu^t)$ (I)	3.048(1)	3.039
$Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ (II)	3.047(1)	3.048
$Re_2(CO)_7(CNMe)_3$ (III)	3.049(1)	3.048
$Re_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$ (IV)	3.081(2)	3.051

The calculated results indicate a slight increase in the Re-Re bond length down the series $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-4), but this effect is not as large as might be expected from the crystal structure data. Hence the role of non-bonded interactions, or steric effects, which might be expected to increase the Re-Re bond length, is not the dominant factor in these structures. The differences between the crystallographic Re-Re bond distance, and the calculated values, can be ascribed to electronic effects which are not adequately modelled by using the force field for the parent $Re_2(CO)_{10}$. In particular, replacing carbonyls by isonitriles, which are poorer π-acceptors[63], would be expected to cause a weakening, and hence a lengthening, of the Re-Re bond. Hence electronic i.e. bonding interactions, rather than steric effects i.e. non-bonded interactions, would appear to be the dominant factor influencing the length of the Re-Re bond in the $Re_2(CO)_{10-n}(CNR)_n$ structures.

The values of r* and ε* for the C,O and N atoms were obtained from Kollman[287]. For Re, the r* value was taken as the shortest Re-Re distance in rhenium metal[288]. The values of r* and ε* used in the calculations are given in Table E.1.1.

(b) Bond length and bond angle parameters.

The values for the equilibrium bond length r_{eq}, and bond angle θ_{eq}, were obtained from X-ray crystal structures of $Re_2(CO)_{10}$[158], and $Re_2(CO)_{10-n}(CNR)_n$ (ch XIV). For the parent compound, $Re_2(CO)_{10}$, the Re-Re equilibrium bond distance was adjusted until the observed structure of $Re_2(CO)_{10}$[158] was reproduced (K_r = 118 kcal mol $\AA^2$). This value of r_{eq} (Re-Re) (3.048$\AA$) was then used in the subsequent calculations for the $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-4) derivatives. The values of r_{eq} and θ_{eq} used in the calculations are given in Tables E.1.2 and E.1.3 respectively.

(c) Force constants.

The bond and angle force constants, K_r and K_θ, were obtained from Infrared[146b] and Raman[147b] Spectroscopic studies on $Re_2(CO)_{10}$. The value used for the force constant for the Re-Re bond was 118 kcal/mol $\AA^2$, obtained from the Raman study of $Re_2(CO)_{10}$ by Spiro et al[147b]. The values of the force constants K_r and K_θ used in the calculations are given in Tables E.1.2 and E.1.3 respectively.

The force field parameters were established by an analysis of the parent $Re_2(CO)_{10}$ structure, the X-ray crystal structure of which has been reported[158]. These force field parameters were then kept constant for the subsequent calculations on the derived $Re_2(CO)_{10-n}(CNR)_n$ (n = 1-4) structures.

Results and discussion.

An analysis of the results revealed a variation in the Re-Re bond length. The values of the bond angles and the other bond lengths did not change significantly. Table E.2 below shows the calculated Re-Re bond lengths, compared to the crystal structure values.

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CHEMICAL AND STRUCTURAL STUDIES OF SUBSTITUTED TRANSITION METAL CARBONYL COMPLEXES

APPENDIX D

STRUCTURE FACTOR TABLES

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November 1984

Appendix D

Structure Factor Tables

Code name	(no. of pages)	Structure	Pages
LS2H	(9)	$(\eta^5C_5H_5CO_2Me)Cr(CO)_2(CNBu^t)$	1-9
CPMN	(4)	$(\eta^5C_5H_5)Mn(CO)_2(CNBu^t)$	10-13
FEME	(6)	$Fe(CO)_3(CNMe)_2$	14-15
RECO	(8)	$Re_2(CO)_9(CNBu^t)$ (I)	20-27
REX2	(20)	$Re_2(CO)_8(CNC_6H_3Me_2\text{-}2,6)_2$ (II)	28-47
REM3	(15)	$Re_2(CO)_7(CNMe)_3$ (III)	48-62
REX4	(13)	$Re_2(CO)_6(CNC_6H_3Me\text{-}2,6)_4$ (IV)	63-75
MNTB	(16)	$Mn_2(CO)_8(CNBu^t)_2$ (V)	76-91
MNXY	(7)	$Mn_2(CO)_6(CNC_6H_3Me_2\text{-}2,6)_4$ (VI)	92-98
REP2	(7)	diax-$[Re_2(CO)_8(PMe_2Ph)_2]$ (VII)	99-105

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR L52H CHCOHSCUOMLICU)2T-BUTIC

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	0	0	28	-24	-3	2	0	24	31	-3	4	0	6	-4	-3	6	0	6	6	-9	9	0	14	-13
4	0	0	47	45	-2	2	0	41	-39	-4	4	0	21	-21	-3	6	0	17	17	-8	9	0	7	7
5	0	0	13	-14	-1	2	0	101	101	-5	4	0	11	9	-2	6	0	25	-23	-7	9	0	3	0
6	0	0	13	-11	0	2	0	9	-3	-6	4	0	33	32	-1	6	0	1	-1	-6	9	0	14	-13
7	0	0	3	-3	1	2	0	17	13	-1	5	0	17	-17	0	6	0	19	19	-5	9	0	13	12
8	0	0	21	-21	2	2	0	3	-2	0	5	0	20	17	1	6	0	17	-17	-4	9	0	3	-3
9	0	0	4	4	3	2	0	1	-2	1	5	0	14	14	2	6	0	13	14	-3	9	0	4	4
10	0	0	7	-7	4	2	0	54	53	2	5	0	11	-12	3	6	0	4	-4	-2	9	0	10	9
10	0	0	10	-10	5	2	0	13	13	3	5	0	27	27	4	6	0	1	-7	-1	9	0	11	-11
11	0	0	9	9	6	2	0	21	-21	4	5	0	17	-16	5	6	0	1	11	0	9	0	2	-2
12	0	0	9	-9	7	2	0	10	10	5	5	0	11	-11	6	6	0	1	10	1	9	0	4	2
13	1	0	1	1	8	2	0	16	-15	6	5	0	10	10	7	6	0	7	8	2	9	0	2	4
13	1	0	3	-3	9	2	0	13	-15	7	5	0	13	-13	8	6	0	1	1	-5	10	0	10	8
12	1	0	8	-8	10	2	0	8	9	8	5	0	9	8	-11	7	0	7	-6	-5	10	0	8	10
11	1	0	4	4	11	2	0	8	-8	9	5	0	8	8	-10	7	0	8	-8	-4	10	0	10	-8
10	1	0	15	-15	12	2	0	6	8	10	5	0	5	-4	-9	7	0	10	10	-3	10	0	3	-9
9	1	0	19	19	-13	3	0	7	-5	-13	6	0	4	5	-8	7	0	5	-5	1	-10	1	3	3
9	1	0	3	-3	-12	3	0	7	-7	-12	6	0	12	-12	-7	7	0	4	4	2	-10	1	3	3
-7	1	0	17	-17	-11	3	0	32	-31	-11	6	0	6	7	-6	7	0	2	0	3	-10	1	3	-2
-6	1	0	2	2	-10	3	0	18	19	-10	6	0	5	-5	-5	7	0	24	-24	4	-10	1	6	7
-5	1	0	47	-47	-9	3	0	5	5	-9	6	0	21	-21	-4	7	0	22	20	5	-10	1	2	-2
-4	1	0	19	19	-8	3	0	21	-21	-8	6	0	11	11	-3	7	0	19	-9	6	-10	1	5	4
-3	1	0	96	95	-7	3	0	20	21	-7	6	0	20	-23	-2	7	0	7	-7	-3	-9	1	5	-5
-2	1	0	31	-33	-6	3	0	31	-31	-6	6	0	4	-4	-1	7	0	21	19	-2	-9	1	5	5
-1	1	0	41	-42	-5	3	0	2	-2	-5	6	0	22	22	0	7	0	2	1	-1	-9	1	3	-3
0	1	0	2	2	-4	3	0	50	50	-4	6	0	11	-13	1	7	0	1	-2	0	-9	1	3	3
2	1	0	17	16	-3	3	0	12	-13	-3	6	0	46	44	2	7	0	10	10	1	-9	1	14	14
3	1	0	50	-50	-1	3	0	14	-14	-2	6	0	20	-19	3	7	0	11	-10	2	-9	1	7	-8
4	1	0	2	3	0	3	0	34	32	-1	6	0	1	-1	4	7	0	3	7	3	-9	1	1	1
5	1	0	8	-8	1	3	0	24	25	0	6	0	32	31	5	7	0	4	-3	4	-9	1	13	12
6	1	0	8	8	2	3	0	6	5	1	6	0	7	7	6	7	0	8	-8	5	-9	1	12	-12
7	1	0	17	17	3	3	0	21	19	2	6	0	8	8	7	7	0	5	6	6	-9	1	3	3
8	1	0	29	-28	4	3	0	9	10	3	6	0	10	11	-11	8	0	10	-9	7	-9	1	4	-4
9	1	0	4	4	5	3	0	38	-37	4	6	0	11	-10	-10	8	0	11	11	8	-9	1	9	-9
10	1	0	3	-3	6	3	0	4	-4	5	6	0	9	9	-9	8	0	8	-8	9	-9	1	6	6
12	1	0	5	-5	7	3	0	13	13	6	6	0	4	-4	-8	8	0	10	-9	-5	-8	1	5	6
13	1	0	6	6	9	3	0	27	-27	7	6	0	11	-11	-7	8	0	10	9	-4	-8	1	5	-5
14	1	0	3	-2	9	3	0	8	8	8	6	0	12	12	-6	8	0	15	-15	-3	-8	1	4	6
15	2	0	2	-2	10	3	0	3	3	9	6	0	3	-2	-5	8	0	10	9	-2	-8	1	6	6
12	2	0	12	12	11	3	0	3	-2	-13	6	0	8	-8	-4	8	0	5	-5	-1	-8	1	13	-13
11	2	0	19	-19	-13	4	0	7	7	-12	6	0	2	-2	-3	8	0	5	5	0	-8	1	22	23
-10	2	0	1	-1	-12	4	0	7	-7	-11	6	0	9	9	-2	8	0	8	-8	1	-8	1	12	-12
-9	2	0	9	-9	-11	4	0	9	9	-10	6	0	19	-18	-1	8	0	12	12	2	-8	1	18	18
-8	2	0	39	-39	-10	4	0	15	15	-9	6	0	1	-2	1	8	0	5	-5	4	-8	1	11	-11
-7	2	0	1	-1	-9	4	0	17	-17	-7	6	0	4	4	2	8	0	9	-8	5	-8	1	15	-16
-6	2	0	1	-1	-8	4	0	6	6	-6	6	0	2	-2	3	8	0	8	-8	6	-8	1	6	5
-5	2	0	25	-25	-7	4	0	12	11	-5	6	0	26	25	4	8	0	9	10	7	-8	1	3	-2
-4	2	0	6	7	-6	4	0	21	-21	-3	6	0	21	-20	5	8	0	7	-7	8	-8	1	6	5

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR L53B CRCOHBCDOAE(CO)2F-B.M.C

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
9	-4	1	6	6	-9	-5	1	2	-2	-7	-3	1	9	-7	-14	-1	1	1	1	12	0	1	2	2
10	-4	1	10	-10	-5	-5	1	15	-13	-6	-3	1	2	-4	-11	-1	1	4	4	13	0	1	2	3
11	-4	1	3	6	-4	-5	1	11	11	-5	-3	1	20	20	-10	-1	1	20	-21	-13	1	1	8	8
7	-5	1	4	-4	-3	-5	1	6	-7	-4	-3	1	2	-22	-9	-1	1	17	17	-12	1	1	2	0
8	-5	1	5	5	-2	-5	1	6	5	-3	-3	1	19	18	-8	-1	1	7	-11	-11	1	1	12	-12
5	-5	1	5	-4	-1	-5	1	11	12	-2	-3	1	14	14	-7	-1	1	10	-10	-10	1	1	6	6
4	-5	1	5	-6	0	-5	1	11	-12	-1	-3	1	21	-25	-6	-1	1	13	14	-9	1	1	18	-18
2	-5	1	15	16	1	-5	1	16	17	0	-3	1	4	4	-5	-1	1	14	-20	-8	1	1	4	-4
0	-5	1	9	-7	2	-5	1	13	14	1	-3	1	4	-4	-4	-1	1	3	-4	-7	1	1	11	13
-1	-5	1	3	3	3	-5	1	16	-15	2	-3	1	10	-11	-3	-1	1	14	-14	-5	1	1	17	-17
0	-6	1	25	26	4	-5	1	20	22	3	-3	1	3	3	-2	-1	1	26	-27	-3	1	1	32	32
1	-6	1	19	-19	5	-5	1	7	-7	4	-3	1	5	-5	-1	-1	1	78	79	-4	1	1	11	12
2	-6	1	1	-2	6	-5	1	19	-20	5	-3	1	1	0	0	-1	1	38	39	-3	1	1	19	-19
3	-6	1	11	11	7	-5	1	14	11	6	-3	1	22	21	1	-1	1	33	-35	-2	1	1	74	74
4	-6	1	20	-21	8	-5	1	9	-23	7	-3	1	21	-21	2	-1	1	7	3	-1	1	1	5	6
5	-6	1	20	19	9	-5	1	1	-2	8	-3	1	12	12	3	-1	1	23	-20	0	1	1	53	-51
6	-6	1	3	3	10	-5	1	16	15	9	-3	1	8	7	4	-1	1	10	-11	1	1	1	3	-3
7	-6	1	12	-11	11	-5	1	12	-12	10	-3	1	17	-17	5	-1	1	3	-1	2	1	1	59	-57
8	-6	1	11	10	12	-5	1	7	7	11	-3	1	20	20	6	-1	1	40	-41	3	1	1	2	2
9	-6	1	13	-12	13	-5	1	9	-9	12	-3	1	8	-8	7	-1	1	20	23	4	1	1	52	-51
10	-6	1	7	6	-10	-4	1	5	5	13	-3	1	6	-9	8	-1	1	12	12	5	1	1	29	-30
11	-6	1	7	6	-9	-4	1	9	-10	14	-3	1	8	7	9	-1	1	17	-18	6	1	1	1	2
12	-6	1	13	-12	-8	-4	1	7	-6	-12	-2	1	7	-6	10	-1	1	25	25	7	1	1	15	15
-3	-6	1	4	-4	-7	-4	1	7	6	-11	-2	1	7	-8	11	-1	1	2	-1	8	1	1	19	-20
-7	-6	1	5	-7	-6	-4	1	21	-21	-10	-2	1	15	-15	12	-1	1	1	-1	9	1	1	5	4
-6	-6	1	8	7	-5	-4	1	4	5	-9	-2	1	9	-9	13	-1	1	6	6	10	1	1	4	4
-5	-6	1	9	-9	-4	-4	1	12	13	-8	-2	1	15	15	-14	0	1	10	10	11	1	1	1	2
-4	-6	1	7	7	-3	-4	1	1	1	-7	-2	1	19	-20	13	0	1	13	-12	12	1	1	9	8
-3	-6	1	19	19	-2	-4	1	21	22	-6	-2	1	11	11	-10	0	1	3	3	-13	2	1	2	2
-2	-6	1	15	-15	-1	-4	1	14	15	-5	-2	1	11	-11	-9	0	1	17	19	-12	2	1	16	-16
-1	-6	1	23	24	0	-4	1	3	-3	-4	-2	1	1	-4	-8	0	1	25	-25	-11	2	1	13	13
0	-6	1	1	-2	1	-4	1	39	41	-3	-2	1	29	30	-7	0	1	2	2	-10	2	1	7	7
1	-6	1	14	-30	2	-4	1	30	-31	-2	-2	1	10	-10	-6	0	1	28	-27	-9	2	1	12	-12
2	-6	1	27	27	3	-4	1	19	19	-1	-2	1	54	-55	-5	0	1	13	-13	-8	2	1	22	22
3	-6	1	12	-13	4	-4	1	9	-7	0	-2	1	73	76	-4	0	1	6	7	-7	2	1	29	-28
4	-6	1	8	7	5	-4	1	27	-27	1	-2	1	2	-2	-3	0	1	21	20	-6	2	1	18	16
5	-6	1	5	5	6	-4	1	1	1	2	-2	1	39	41	-2	0	1	20	-20	-5	2	1	48	47
6	-6	1	21	-21	7	-4	1	6	6	3	-2	1	5	6	-1	0	1	54	-54	-4	2	1	40	-40
7	-6	1	7	7	8	-4	1	18	-19	4	-2	1	2	-3	1	0	1	23	23	-3	2	1	13	-13
8	-6	1	9	10	9	-4	1	22	22	5	-2	1	24	23	2	0	1	33	34	-2	2	1	5	5
9	-6	1	32	-31	10	-4	1	8	-9	6	-2	1	26	-25	3	0	1	82	-82	-1	2	1	71	-70
10	-6	1	10	10	11	-4	1	5	-5	7	-2	1	5	-6	4	0	1	48	48	0	2	1	19	-17
11	-6	1	7	8	12	-4	1	11	11	8	-2	1	22	22	5	0	1	6	-7	1	2	1	26	25
12	-6	1	1	3	13	-4	1	8	-9	9	-2	1	20	-19	6	0	1	1	1	2	2	1	30	-30
13	-6	1	12	11	-11	-3	1	1	0	10	-2	1	1	2	7	0	1	37	35	3	2	1	45	45
-5	-5	1	1	3	-10	-3	1	6	6	11	-2	1	9	-9	8	0	1	7	-7	4	2	1	24	-23
-4	-5	1	12	-12	-9	-3	1	20	-20	12	-2	1	10	-11	9	0	1	1	-2	5	2	1	11	-11
-3	-5	1	10	10	-8	-3	1	7	7	13	-2	1	6	7	10	0	1	4	3	6	2	1	25	24

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
7	2	1	10	-10	5	4	1	12	12	7	6	1	4	3	3-10	2	5	5	5	11	-7	2	5	-5
9	2	1	3	2	6	4	1	13	-13	8	6	1	4	-4	4-10	2	5	-4	12	-7	2	12	12
5	3	1	8	8	10	4	1	21	21	-12	7	1	10	-10	5-10	2	5	2	13	-6	2	4	4
10	3	1	4	4	9	4	1	6	6	-11	7	1	7	7	-2	-9	2	-5	3	-6	2	10	-6
11	3	1	6	4	9	4	1	7	-4	-10	7	1	8	9	-1	-9	2	3	1	-5	2	8	9
12	3	1	3	2	10	4	1	7	8	-9	7	1	2	-1	0	-9	2	5	-5	-4	2	5	-5
-11	4	1	4	-3	-11	5	1	1	0	-8	7	1	5	5	1	-9	2	5	-5	-3	2	6	-6
-12	4	1	4	-7	-12	5	1	11	10	-7	7	1	2	-2	2	-9	2	6	6	-2	2	15	15
-11	5	1	4	4	-11	5	1	12	-13	-6	7	1	6	-7	3	-9	2	1	0	-1	2	7	-7
-10	5	1	24	-25	-10	5	1	6	6	-5	7	1	12	12	4	-9	2	12	-12	1	2	17	-19
-9	5	1	9	8	-9	5	1	7	7	-4	7	1	19	-13	5	-9	2	5	5	1	2	22	23
-8	5	1	17	17	-8	5	1	2	1	-3	7	1	5	3	6	-9	2	6	-6	2	2	25	-26
-7	5	1	23	-23	-7	5	1	10	10	-2	7	1	10	11	7	-9	2	3	3	3	2	22	22
-6	5	1	19	17	-6	5	1	6	6	-1	7	1	12	-11	8	-9	2	9	9	4	2	5	6
-5	5	1	3	-2	-5	5	1	28	-27	0	7	1	4	4	9	-9	2	7	-7	5	2	15	-16
-4	5	1	56	-57	-4	5	1	40	40	1	7	1	8	-9	-5	-8	2	4	-4	6	2	5	5
-3	5	1	76	-75	-3	5	1	22	-25	2	7	1	13	-12	-4	-8	2	1	1	7	2	9	-9
-2	5	1	28	-29	-2	5	1	7	-9	3	7	1	11	11	-3	-8	2	1	1	8	2	12	-11
0	5	1	34	33	-1	5	1	8	9	4	7	1	7	-7	-2	-8	2	2	-2	9	2	23	23
1	5	1	14	-15	0	5	1	27	-27	5	7	1	2	0	-1	-8	2	13	13	10	2	1	1
2	5	1	7	7	1	5	1	11	11	6	7	1	8	8	0	-8	2	1	-2	11	2	4	-5
3	5	1	7	6	2	5	1	2	-1	-10	8	1	9	-8	1	-8	2	12	-13	12	2	8	8
4	5	1	22	22	3	5	1	21	-21	-9	8	1	2	2	2	-8	2	3	3	13	2	2	-1
5	5	1	14	-14	4	5	1	20	20	-8	8	1	12	13	3	-8	2	21	-22	2	2	7	7
6	5	1	11	-10	5	5	1	1	-3	-7	8	1	20	-20	4	-8	2	11	11	-7	2	12	-12
7	5	1	11	-10	6	5	1	1	-1	-6	8	1	10	10	5	-8	2	5	5	-6	2	6	6
8	5	1	19	19	7	5	1	1	7	-5	8	1	5	5	6	-8	2	12	-11	-5	2	18	18
9	5	1	5	5	8	5	1	1	2	-4	8	1	2	1	7	-8	2	2	2	-4	2	18	-18
10	5	1	1	0	9	5	1	1	2	-3	8	1	11	11	8	-8	2	2	2	-3	2	7	7
11	5	1	9	9	-11	6	1	1	2	-2	8	1	9	-9	9	-8	2	4	-3	-2	2	7	8
-13	4	1	13	-13	-11	6	1	10	-10	-1	8	1	2	-1	10	-8	2	8	9	-1	2	23	-24
-12	4	1	9	9	-10	6	1	4	4	0	8	1	3	-1	11	-8	2	3	-7	0	2	16	17
-11	4	1	2	-2	-9	6	1	9	9	1	8	1	11	-11	-5	-7	2	7	6	1	2	4	-4
-10	4	1	5	-5	-8	6	1	8	-9	2	8	1	4	4	-4	-7	2	7	-7	2	2	9	-10
-9	4	1	15	-15	-7	6	1	15	15	3	8	1	2	2	-3	-7	2	7	-7	3	2	2	-2
-8	4	1	19	-19	-6	6	1	12	-12	4	8	1	10	-10	-2	-7	2	5	5	4	2	31	-31
-7	4	1	12	-11	-5	6	1	21	21	-8	9	1	6	6	-1	-7	2	3	3	5	2	3	3
-6	4	1	31	28	-4	6	1	7	-9	-7	9	1	2	-1	0	-7	2	23	-24	6	2	19	19
-5	4	1	17	-18	-3	6	1	21	-22	-6	9	1	19	19	1	-7	2	9	9	7	2	14	-14
-4	4	1	17	15	-2	6	1	14	14	-5	9	1	9	-8	2	-7	2	2	1	8	2	8	9
-3	4	1	12	13	-1	6	1	5	-4	-4	9	1	2	-3	3	-7	2	15	-17	9	2	20	20
-2	4	1	31	-30	0	6	1	10	-10	-3	9	1	3	2	4	-7	2	14	14	10	2	9	-9
-1	4	1	13	13	1	6	1	11	11	-2	9	1	7	-7	5	-7	2	6	-9	11	2	17	17
0	4	1	5	-5	2	6	1	15	-15	-1	9	1	5	6	6	-7	2	17	-17	12	2	3	-3
1	4	1	26	-27	3	6	1	3	-4	0	9	1	11	-11	7	-7	2	20	-20	13	2	6	-7
2	4	1	13	14	4	6	1	7	8	1	9	1	7	7	8	-7	2	7	-7	-10	-4	2	2
3	4	1	31	-30	5	6	1	19	-16	2	9	1	12	11	9	-7	2	4	-4	-7	-4	4	5
4	4	1	7	-5	6	6	1	9	9	2-10	2	6	-5	10	-7	2	9	9	-6	-4	2	1	1

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
-7	-4	2	9	-8	-9	-2	2	1	-2	-11	0	2	9	8	11	1	2	9	9	9	3	2	5	-5
-8	-4	2	17	17	-7	-2	2	16	16	-10	0	2	5	5	12	1	2	5	5	5	3	2	4	4
-9	-4	2	14	-14	-6	-2	2	6	-6	-9	0	2	3	-4	-13	2	2	10	-9	10	3	2	2	2
-3	-4	2	27	27	-5	-2	2	4	4	-8	0	2	21	21	-12	2	2	9	8	11	3	2	8	-8
-2	-4	2	11	-11	-4	-2	2	1	1	-7	0	2	13	-13	-11	2	2	6	-6	-13	4	2		
-1	-4	2	23	-22	-3	-2	2	43	-43	-6	0	2	3	3	-10	2	2	4	-5	-12	4	2	9	-9
0	-4	2	5	5	-2	-2	2	14	14	-5	0	2	43	43	-9	2	2	28	29	-11	4	2	6	-6
1	-4	2	39	-41	-1	-2	2	2	-1	-4	0	2	23	-24	-8	2	2	5	-6	-10	4	2	5	-4
2	-4	2	31	31	0	-2	2	65	-68	-3	0	2	5	4	-7	2	2	4	5	-9	4	2	4	-4
3	-4	2	17	-17	1	-2	2	28	25	-2	0	2	11	-11	-6	2	2	35	36	-8	4	2	17	18
4	-4	2	19	-21	2	-2	2	16	15	-1	0	2	3	3	-5	2	2	31	-31	-7	4	2	8	8
5	-4	2	29	31	3	-2	2	51	-53	0	0	2	34	-33	-4	2	2	24	24	-6	4	2	29	-29
6	-4	2	6	-6	4	-2	2	15	16	1	0	2	46	-46	-3	2	2	33	-34	-5	4	2	40	40
7	-4	2	1	-1	5	-2	2	10	-16	2	0	2	24	-24	-2	2	2	6	-8	-4	4	2	3	-3
8	-4	2	3	-3	6	-2	2	14	13	3	0	2	29	27	-1	2	2	10	10	-3	4	2	29	-27
10	-4	2	2	1	8	-2	2	23	22	4	0	2	30	-30	0	2	2	33	-32	-2	4	2	33	33
11	-4	2	3	1	9	-2	2	16	-17	5	0	2	24	24	1	2	2	27	-26	-1	4	2	18	-17
12	-4	2	11	-10	9	-2	2	25	23	6	0	2	41	41	2	2	2	27	27	0	4	2	35	-33
13	-4	2	6	6	10	-2	2	2	2	7	0	2	32	-32	3	2	2	32	-32	1	4	2	19	19
-11	-3	2	3	-3	11	-2	2	5	-8	8	0	2	21	21	4	2	2	1	2	2	4	2	20	-19
-10	-3	2	7	-7	12	-2	2	10	9	9	0	2	2	-2	5	2	2	11	11	3	4	2	3	-3
-9	-3	2	9	9	13	-2	2	6	-5	10	0	2	2	-2	6	2	2	35	-36	4	4	2	17	16
-8	-3	2	4	-2	-12	-1	2	3	-3	11	0	2	9	9	7	2	2	18	13	5	4	2	14	-14
-7	-3	2	2	2	-11	-1	2	12	-14	12	0	2	3	-4	8	2	2	6	7	6	4	2	7	7
-6	-3	2	23	20	-10	-1	2	10	10	-13	1	2	2	-3	9	2	2	3	3	7	4	2	3	-3
-5	-3	2	5	-5	-7	-1	2	8	-9	-12	1	2	2	3	10	2	2	7	7	9	4	2	4	4
-4	-3	2	27	27	-6	-1	2	17	-18	-11	1	2	15	13	11	2	2	5	-4	10	4	2	7	7
-3	-3	2	17	-16	-5	-1	2	17	17	-10	1	2	14	-13	-13	3	2	2	-1	11	4	2	12	-11
-2	-3	2	14	-14	-4	-1	2	6	6	-9	1	2	6	5	-12	3	2	13	13	-12	5	2	11	-11
-1	-3	2	47	43	-3	-1	2	27	-27	-8	1	2	10	11	-11	3	2	3	-4	-11	5	2	13	14
0	-3	2	34	-34	-2	-1	2	54	57	-7	1	2	24	-23	-10	3	2	12	-12	-10	5	2	3	-3
1	-3	2	13	-13	-1	-1	2	18	-17	-6	1	2	32	32	-9	3	2	2	-2	-9	5	2	5	6
2	-3	2	1	1	0	-1	2	4	-4	-5	1	2	13	12	-8	3	2	7	-7	-8	5	2	17	17
3	-3	2	33	-36	1	-1	2	23	-23	-4	1	2	11	-11	-7	3	2	24	24	-7	5	2	10	-10
4	-3	2	12	13	2	-1	2	37	-33	-3	1	2	22	23	-6	3	2	4	-5	-6	5	2	9	9
5	-3	2	15	16	3	-1	2	10	-10	-2	1	2	36	-37	-5	3	2	14	-14	-5	5	2	22	22
6	-3	2	23	-22	4	-1	2	5	5	-1	1	2	17	-17	-4	3	2	28	29	-4	5	2	35	-35
7	-3	2	13	13	5	-1	2	23	-23	0	1	2	62	58	-3	3	2	50	-51	-3	5	2	14	14
8	-3	2	7	8	6	-1	2	31	31	1	1	2	21	19	-2	3	2	5	5	-2	5	2	16	16
9	-3	2	7	7	7	-1	2	3	-2	2	1	2	55	53	-1	3	2	17	17	-1	5	2	27	-26
10	-3	2	10	10	8	-1	2	2	2	3	1	2	17	-17	0	3	2	93	-97	0	5	2	13	13
11	-3	2	19	-10	9	-1	2	21	21	4	1	2	30	-30	1	3	2	32	32	1	5	2	5	-4
12	-3	2	7	7	10	-1	2	18	-15	5	1	2	40	36	2	3	2	4	4	2	5	2	10	-15
13	-3	2	11	11	11	-1	2	3	3	6	1	2	11	-13	3	3	2	49	-47	3	5	2	17	16
-12	-2	2	5	5	12	-1	2	13	13	7	1	2	12	-12	4	3	2	13	13	4	5	2	3	3
-11	-2	2	9	-9	13	-1	2	11	-11	8	1	2	10	11	5	3	2	1	1	5	5	2	9	9
-10	-2	2	4	4	-13	0	2	5	5	9	1	2	2	-3	6	3	2	17	17	6	5	2	5	6
-9	-2	2	13	-14	-12	0	2	10	-10	10	1	2	1	-1	7	3	2	5	5	7	5	2	5	-6

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR LS2H1 CRC6H8C1O8ME(CO)2T-BUNC

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
0	0	2	1	1	1	2	2	19	17	5	-7	3	3	-1	-7	-4	3	13	13	-3	-2	3	11	11
0	0	4	1	0	2	2	2	1	-1	7	-7	3	16	-14	-6	-4	3	6	-6	-7	-2	3	10	-10
-12	0	6	3	-3	3	2	2	5	-3	8	-7	3	15	14	-5	-4	3	9	10	-5	-2	3	2	1
-11	0	8	3	3	4	2	2	6	6	9	-7	3	2	1	-4	-4	3	1	-2	-3	-2	3	11	10
-10	0	10	10	-11	5	2	2	6	6	10	-7	3	6	-5	-3	-4	3	36	-36	-4	-2	3	31	-31
-9	0	12	15	16	6	2	2	5	-2	11	-7	3	11	10	-2	-4	3	16	15	-3	-2	3	19	20
-8	0	14	6	7	7	2	2	5	-2	-7	-6	4	4	-4	-1	-4	3	10	10	-2	-2	3	6	6
-7	0	16	21	-21	8	2	2	11	11	-6	-6	4	12	12	0	-4	3	34	-34	-1	-2	3	2	-1
-6	0	18	9	8	9	2	2	10	9	-5	-6	4	6	-6	1	-4	3	7	9	0	-2	3	10	12
-5	0	20	3	-3	10	2	2	0	0	-4	-6	4	2	-1	2	-4	3	7	-7	1	-2	3	36	-37
-4	0	22	0	-2	11	2	2	3	3	-3	-6	4	3	2	3	-4	3	15	-16	2	-2	3	15	-15
-3	0	24	19	19	-1	-1	3	2	2	-2	-6	4	7	-7	4	-4	3	34	34	3	-2	3	38	38
-2	0	26	4	-9	0	-1	3	2	-2	-1	-6	4	2	-1	5	-4	3	11	-12	4	-2	3	30	-31
-1	0	28	2	3	1	-1	3	9	-9	0	-6	4	5	-5	6	-4	3	12	11	5	-2	3	1	0
0	0	30	1	1	2	-1	3	4	-5	1	-6	4	3	-3	7	-4	3	5	5	6	-2	3	24	23
1	2	0	13	-13	3	-1	3	4	4	2	-6	4	13	14	8	-4	3	13	-13	7	-2	3	17	-18
2	2	0	14	14	4	-1	3	5	-5	3	-6	4	14	-14	9	-4	3	10	10	8	-2	3	14	14
3	2	0	11	-11	5	-1	3	7	-7	4	-5	4	10	-10	10	-4	3	3	-9	9	-2	3	8	-7
4	2	0	7	7	6	-1	3	3	3	5	-5	4	24	23	11	-4	3	3	-2	10	-2	3	3	-2
5	2	0	2	-1	7	-1	3	6	-6	6	-5	4	11	-11	12	-4	3	7	7	11	-2	3	9	-7
6	2	0	4	-5	8	-1	3	4	-4	7	-5	4	1	0	13	-4	3	4	-4	12	-2	3	7	-7
-11	0	7	3	-3	9	-1	3	4	4	8	-5	4	9	8	-10	-3	3	4	4	13	-2	3	8	-8
-10	0	9	4	-2	-3	0	3	2	-2	9	-5	4	4	-4	-9	-3	3	2	-1	-12	-1	3	2	6
-9	0	11	16	17	-2	0	3	3	-3	10	-5	4	11	10	-8	-3	3	12	11	-11	-1	3	6	8
-8	0	13	16	-17	-1	0	3	2	-2	-7	-4	5	8	-8	-7	-3	3	4	-4	-10	-1	3	2	-3
-7	0	15	1	0	0	0	3	3	3	-6	-4	5	4	5	-6	-3	3	11	-12	-9	-1	3	11	11
-6	0	17	14	15	1	0	3	7	-7	-5	-4	5	6	6	-5	-3	3	14	14	-8	-1	3	12	-12
-5	0	19	3	-2	2	0	3	4	4	-4	-4	5	2	-2	-4	-3	3	3	-5	-7	-1	3	10	-9
-4	0	21	2	1	3	0	3	5	-5	-3	-4	5	2	2	-3	-3	3	24	-23	-6	-1	3	10	12
-3	0	23	2	-2	4	0	3	5	5	-2	-4	5	18	17	-2	-3	3	42	43	-5	-1	3	2	-2
-2	0	25	7	7	5	0	3	8	-8	-1	-4	5	1	-1	-1	-3	3	42	-43	-4	-1	3	14	-14
-1	0	27	15	-15	6	0	3	4	4	-5	-3	6	14	-13	0	-3	3	17	19	-3	-1	3	28	28
0	1	1	21	-20	7	0	3	3	-3	-6	-3	6	14	15	1	-3	3	16	17	-2	-1	3	30	-30
1	2	1	9	-9	8	0	3	3	3	-7	-3	6	22	-22	2	-3	3	24	-25	-1	-1	3	21	21
2	2	1	11	11	9	0	3	3	-3	-8	-3	6	7	7	3	-3	3	13	14	0	-1	3	22	-22
3	2	1	13	-13	10	0	3	7	-7	-2	-4	7	12	13	4	-3	3	1	2	1	-1	3	22	-24
4	2	1	7	7	-10	-1	3	4	4	-3	-4	7	24	-25	5	-3	3	12	-12	2	-1	3	41	40
5	2	1	5	5	-9	-1	3	4	-4	-4	-4	7	6	7	6	-3	3	15	17	3	-1	3	3	-5
-9	0	9	2	1	-7	-1	3	7	-7	-5	-4	7	2	2	7	-3	3	14	-14	4	-1	3	11	-11
-8	0	11	11	-11	-5	-1	3	4	4	-6	-4	7	8	-8	8	-3	3	1	-1	5	-1	3	39	40
-7	0	13	11	11	-3	-1	3	3	-3	-7	-4	7	10	-10	9	-3	3	1	1	6	-1	3	5	-8
-6	0	15	2	-3	-1	-1	3	8	-8	-8	-4	7	15	15	10	-3	3	10	-11	7	-1	3	5	5
-5	0	17	5	-5	1	-1	3	5	5	-9	-4	8	2	2	11	-3	3	1	1	8	-1	3	3	3
-4	0	19	10	10	3	-1	3	9	-9	-10	-3	8	1	1	12	-3	3	7	6	9	-1	3	9	-9
-3	0	21	13	-13	5	-1	3	9	9	-11	-3	8	12	-12	13	-3	3	7	-7	10	-1	3	5	-5
-2	0	23	4	4	7	-1	3	9	-9	-12	-3	8	1	2	-11	-2	3	9	9	11	-1	3	3	-2
-1	0	25	6	-6	9	-1	3	12	-12	-9	-3	8	2	1	-10	-2	3	5	-5	12	-1	3	10	-10
0	0	3	13	-14	4	-7	3	6	7	-3	-3	3	2	1	-9	-2	3	6	6	-12	0	3	9	9

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
-11	0	3	11	-10	-12	2	3	4	-3	-7	4	3	5	-6	-1	6	3	4	3	3	-8	4	2	-2
-10	0	3	7	6	-11	2	3	2	-1	-3	4	3	15	16	0	6	3	18	-19	5	-8	4	8	9
-9	0	3	7	6	-10	2	3	4	4	-2	4	3	22	-23	1	6	3	16	17	6	-8	4	5	-8
-8	0	3	9	-9	-9	2	3	10	-10	-4	4	3	4	-3	2	6	3	6	-1	7	-8	4	9	2
-7	0	3	9	-9	-7	2	3	12	-11	-3	4	3	9	-9	3	6	3	25	-5	8	-8	4	2	-9
-6	0	3	15	16	-6	2	3	36	-32	-2	4	3	12	-13	4	6	3	3	-4	9	-8	4	8	-7
-5	0	3	24	-23	-5	2	3	20	20	-1	4	3	24	24	5	6	3	3	-4	10	-8	4	7	6
-4	0	3	15	18	-4	2	3	7	-10	0	4	3	10	10	6	6	3	12	-1	11	-8	4	3	-3
-3	0	3	14	-19	-3	2	3	7	-7	1	4	3	21	-20	7	6	3	4	-6	12	-8	4	4	-4
-2	0	3	15	19	-2	2	3	18	18	2	4	3	19	19	8	6	3	6	3	13	-8	4	1	-1
-1	0	3	13	-12	-1	2	3	8	-13	3	4	3	10	10	-9	7	3	23	-24	0	-7	4	4	-3
0	1	3	27	-28	0	2	3	47	45	4	4	3	2	-1	-8	7	3	10	10	1	-7	4	12	12
1	1	3	43	38	1	2	3	6	5	5	4	3	10	10	-7	7	3	1	-1	2	-7	4	2	-1
2	1	3	9	9	2	2	3	31	-30	6	4	3	6	-9	-6	7	3	10	-10	3	-7	4	2	-2
3	1	3	15	-15	3	2	3	5	5	7	4	3	10	-11	-5	7	3	16	16	4	-7	4	7	-7
4	1	3	17	17	4	2	3	3	-4	8	4	3	6	3	-4	7	3	4	-4	5	-7	4	6	6
5	1	3	13	13	5	2	3	17	17	9	4	3	9	-11	-3	7	3	9	-9	6	-7	4	6	-5
6	1	3	27	-27	6	2	3	21	-21	-11	5	3	7	-9	-2	7	3	6	7	7	-7	4	7	6
7	1	3	7	7	7	2	3	2	-1	-10	5	3	2	3	-1	7	3	10	-10	8	-7	4	10	-11
8	1	3	14	-15	8	2	3	13	13	-9	5	3	19	20	0	7	3	10	10	9	-7	4	6	5
9	1	3	10	-9	9	2	3	18	-17	-8	5	3	21	-22	1	7	3	11	12	10	-7	4	6	6
10	1	3	11	11	10	2	3	6	-9	-7	5	3	6	6	2	7	3	10	-10	11	-7	4	8	-8
11	1	3	4	4	11	2	3	6	5	-6	5	3	9	-9	3	7	3	7	-7	12	-7	4	8	8
12	1	3	4	4	-10	3	3	15	-15	-5	5	3	4	4	4	7	3	1	-1	13	-7	4	2	6
-12	1	3	7	-7	-9	3	3	5	-4	-4	5	3	18	19	5	7	3	5	9	14	-7	4	10	-10
-11	1	3	9	-9	-8	3	3	12	12	-3	5	3	8	-5	6	7	3	13	13	15	-7	4	3	3
-10	1	3	15	15	-7	3	3	13	-13	-2	5	3	14	-14	7	7	3	7	-5	16	-7	4	3	-3
-9	1	3	6	5	-6	3	3	8	6	-1	5	3	21	21	-6	8	3	1	-1	0	-8	4	7	7
-8	1	3	33	-33	-5	3	3	5	-5	0	5	3	7	-6	-5	8	3	2	2	1	-8	4	8	-7
-7	1	3	22	22	-4	3	3	14	13	1	5	3	2	3	-4	8	3	13	-13	2	-8	4	5	5
-6	1	3	7	-8	-3	3	3	2	-3	2	5	3	17	17	-3	8	3	3	4	3	-8	4	4	-4
-5	1	3	17	-17	-2	3	3	22	-21	3	5	3	14	-14	-2	8	3	6	3	4	-8	4	5	5
-4	1	3	19	19	-1	3	3	20	21	4	5	3	2	2	-1	8	3	10	-10	5	-8	4	15	-15
-3	1	3	40	-40	0	3	3	15	-15	5	5	3	6	1	0	8	3	13	13	6	-8	4	12	12
-2	1	3	23	23	1	3	3	2	1	6	5	3	2	-6	1	8	3	4	-4	7	-8	4	3	3
-1	1	3	13	-12	2	3	3	26	-22	7	5	3	4	4	2	8	3	5	5	8	-8	4	8	-8
0	1	3	15	-15	3	3	3	21	21	8	5	3	5	-5	3	8	3	2	-1	9	-8	4	13	13
1	1	3	42	41	4	3	3	11	-11	9	5	3	2	-1	4	8	3	10	-10	10	-8	4	17	-17
2	1	3	7	7	5	3	3	7	8	-11	6	3	8	-8	1	9	4	4	4	11	-8	4	3	-3
3	1	3	17	16	6	3	3	7	-7	-10	6	3	16	16	2	9	4	5	5	12	-8	4	7	7
4	1	3	9	8	7	3	3	10	-10	-9	6	3	15	-14	3	9	4	5	-5	13	-8	4	6	-6
5	1	3	34	-34	8	3	3	11	-12	-8	6	3	14	-14	5	9	4	7	7	0	-9	4	2	1
6	1	3	16	17	10	3	3	2	-2	-7	6	3	22	22	6	9	4	3	-3	1	-9	4	6	-6
7	1	3	4	3	-11	4	3	2	0	-6	6	3	14	-15	-2	9	4	3	-7	2	-9	4	10	9
8	1	3	10	-11	-10	4	3	4	-3	-5	6	3	4	-8	-1	9	4	3	3	3	-9	4	11	-11
9	1	3	12	-13	-9	4	3	10	-10	-4	6	3	6	-7	0	9	4	3	-3	4	-9	4	12	12
10	1	3	5	-5	-8	4	3	1	-2	-3	6	3	18	19	1	9	4	2	-1	5	-9	4	7	-7
11	1	3	12	-12	-7	4	3	1	-2	-2	6	3	19	19	2	9	4	10	10	2	-9	4	7	-7

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR L52H CRC6H5COOME(C3)2T-BUNC

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
1	-5	4	13	15	9	-3	4	6	-6	10	-1	4	2	-1	-10	2	4	9	-5	-4	4	4	4	-5
4	-5	4	1	0	10	-3	4	8	7	11	-1	4	4	-4	-9	2	4	3	3	-3	4	4	10	-10
5	-5	4	1	1	11	-3	4	3	-3	-11	0	4	7	7	-8	2	4	10	-11	-2	4	4	15	15
6	-5	4	14	14	12	-3	4	9	-9	-10	0	4	4	-4	-7	2	4	5	-5	-1	4	4	7	-7
7	-5	4	20	-20	-10	-2	4	5	5	-9	0	4	17	-17	-6	2	4	4	5	0	4	4	7	4
8	-5	4	6	6	-9	-2	4	4	-3	-8	0	4	13	13	-5	2	4	17	-17	1	4	4	19	19
9	-5	4	5	-5	-8	-2	4	17	-16	-7	0	4	3	-2	-4	2	4	9	10	2	4	4	16	-17
10	-5	4	12	6	-7	-2	4	5	9	-6	0	4	14	-14	-3	2	4	24	22	3	4	4	14	15
11	-5	4	6	6	-6	-2	4	4	-5	-5	0	4	12	13	-2	2	4	24	-23	4	4	4	3	-3
-9	-4	4	2	-1	-5	-2	4	13	-13	-4	0	4	17	-17	-1	2	4	22	23	5	4	4	11	-12
-8	-4	4	4	-4	-4	-2	4	24	24	-3	0	4	2	2	0	2	4	14	14	6	4	4	4	4
-7	-4	4	7	-6	-3	-2	4	3	-3	-2	0	4	17	17	1	2	4	13	-17	7	4	4	4	5
-6	-4	4	1	1	-2	-2	4	2	-1	-1	0	4	27	-28	2	2	4	10	15	8	4	4	10	-11
-5	-4	4	3	3	-1	-2	4	14	14	0	0	4	48	48	3	2	4	10	-10	-10	5	4	5	4
-4	-4	4	5	-6	0	-2	4	16	-15	1	0	4	25	28	4	2	4	9	8	-9	5	4	19	-19
-3	-4	4	11	11	1	-2	4	6	15	2	0	4	14	-15	5	2	4	5	5	-3	5	4	11	11
-2	-4	4	17	-17	2	-2	4	7	7	3	0	4	17	17	6	2	4	3	-3	-7	5	4	3	-3
-1	-4	4	3	3	3	-2	4	16	-16	4	0	4	13	-14	7	2	4	5	5	-6	5	4	10	-10
0	-4	4	22	22	4	-2	4	12	12	5	0	4	4	-4	8	2	4	9	9	-5	5	4	4	4
1	-4	4	10	-10	5	-2	4	2	3	6	0	4	3	3	9	2	4	13	-13	-4	5	4	3	-4
2	-4	4	2	2	6	-2	4	11	-12	7	0	4	11	-12	10	2	4	9	10	-3	5	4	20	21
3	-4	4	22	23	7	-2	4	10	12	8	0	4	7	-7	-11	3	4	8	-8	-2	5	4	4	4
4	-4	4	11	-10	8	-2	4	12	12	9	0	4	7	7	-10	3	4	4	3	1	5	4	16	-17
5	-4	4	4	4	9	-2	4	7	-7	10	0	4	10	-10	-9	3	4	5	-5	2	5	4	13	18
6	-4	4	1	-1	10	-2	4	7	4	11	0	4	6	6	-8	3	4	11	-11	3	5	4	1	0
7	-4	4	10	10	11	-2	4	4	-5	-11	1	4	5	5	-7	3	4	11	-11	4	5	4	9	-8
8	-4	4	12	-12	12	-2	4	4	5	-10	1	4	9	-9	-6	3	4	11	-12	5	5	4	12	13
9	-4	4	21	-22	-11	-1	4	5	-5	-9	1	4	3	3	-5	3	4	3	-3	6	5	4	7	-7
10	-4	4	0	9	-10	-1	4	11	12	-8	1	4	7	8	-4	3	4	10	12	7	5	4	8	-8
11	-4	4	9	-9	-9	-1	4	17	-16	-7	1	4	17	-17	-3	3	4	2	-1	8	5	4	8	8
12	-4	4	4	-4	-8	-1	4	2	1	-6	1	4	6	6	-1	3	4	15	15	-9	6	4	6	-7
-9	-3	4	3	3	-7	-1	4	12	12	-5	1	4	7	-8	0	3	4	15	-15	-8	6	4	6	6
-8	-3	4	7	-7	-6	-1	4	17	-17	-4	1	4	11	-11	1	3	4	7	6	-7	6	4	9	-9
-7	-3	4	2	-2	-5	-1	4	7	7	-3	1	4	22	22	2	3	4	3	-4	-6	6	4	12	13
-6	-3	4	15	-14	-4	-1	4	10	10	-2	1	4	7	-7	3	3	4	4	4	-5	6	4	3	3
-5	-3	4	2	-2	-3	-1	4	15	-15	-1	1	4	7	-7	4	3	4	16	17	-4	6	4	10	-10
-4	-3	4	11	11	-2	-1	4	7	3	0	1	4	55	54	5	3	4	10	-10	-3	6	4	9	9
-3	-3	4	8	-8	-1	-1	4	3	-2	1	1	4	31	-30	6	3	4	10	-10	-2	6	4	10	-11
-2	-3	4	21	21	0	-1	4	13	-12	2	1	4	7	-6	7	3	4	11	11	-1	6	4	2	-2
0	-3	4	1	0	1	-1	4	29	29	3	1	4	15	15	8	3	4	12	-12	0	6	4	16	17
1	-3	4	15	-17	2	-1	4	11	-11	4	1	4	14	-15	9	3	4	2	-1	1	6	4	14	-14
2	-3	4	23	23	3	-1	4	22	22	5	1	4	5	5	-11	4	4	4	-4	2	6	4	3	3
3	-3	4	4	3	4	-1	4	21	21	6	1	4	20	-19	-10	4	4	14	13	3	6	4	5	4
4	-3	4	7	-7	5	-1	4	25	-26	7	1	4	3	3	-9	4	4	7	-9	4	6	4	7	-7
5	-3	4	15	17	6	-1	4	6	6	8	1	4	19	19	-8	4	4	12	-12	-7	7	4	3	-3
6	-3	4	17	-17	7	-1	4	2	-3	9	1	4	10	-11	-7	4	4	6	6	-6	7	4	2	2
7	-3	4	7	6	8	-1	4	7	-7	10	1	4	3	-3	-6	4	4	3	-3	-5	7	4	5	-5
8	-3	4	5	-5	9	-1	4	2	3	-11	2	4	1	1	-5	4	4	3	8	-4	7	4	15	16

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR LS2H CRC6H5C00HE(CO)2T-BUNC

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
-3	7	4	10	10	3	-5	5	4	-5	-6	-2	5	2	-2	2	0	5	16	16	-8	3	5	12	12
-2	7	4	15	-14	4	-5	5	3	3	-5	-2	5	6	6	3	0	5	19	-19	-7	3	5	7	-7
-1	7	4	5	5	5	-5	5	3	2	-4	-2	5	9	-9	4	0	5	1	2	-6	3	5	4	4
0	7	4	7	7	6	-5	5	8	-8	-3	-2	5	15	15	5	0	5	4	-5	-5	3	5	4	5
1	7	4	2	-2	7	-5	5	13	13	-2	-2	5	3	-2	6	0	5	2	-1	-4	3	5	15	-15
2	7	4	5	5	8	-5	5	10	-10	-1	-2	5	16	-15	7	0	5	16	15	-3	3	5	12	12
0	-8	5	4	4	9	-5	5	11	-11	0	-2	5	11	11	9	0	5	8	-8	-2	3	5	6	6
1	-8	5	8	8	10	-5	5	13	12	1	-2	5	4	-4	10	0	5	3	8	-1	3	5	17	-17
2	-8	5	7	-7	-7	-4	5	3	2	2	-2	5	6	6	-10	1	5	1	1	0	3	5	9	8
3	-8	5	3	4	-6	-4	5	2	-1	3	-2	5	17	18	-9	1	5	2	1	1	3	5	4	-3
4	-8	5	3	2	-5	-4	5	7	-7	4	-2	5	20	-20	-8	1	5	9	-10	2	3	5	2	-1
5	-8	5	10	-9	-4	-4	5	7	7	5	-2	5	2	1	[illegible]	1	5	15	15	3	3	5	9	8
6	-8	5	3	2	-3	-4	5	2	-2	6	-2	5	6	3			5	13	-13	4	3	5	11	-11
-3	-7	5	4	4	-2	-4	5	10	10	7	-2	5	7	-7			5	1	1	5	3	5	2	-3
-2	-7	5	5	4	-1	-4	5	3	3	8	-2	5	5	5			5	13	12	6	3	5	5	5
-1	-7	5	9	-8	0	-4	5	7	-7	9	-2	5	4	4			5	6	-6	7	3	5	8	-7
0	-7	5	15	15	1	-4	5	13	13	10	-2	5	9	-9			5	5	4	-9	4	5	6	6
1	-7	5	4	-3	2	-4	5	5	-5	-9	-1	5	2	0			5	22	21	-8	4	5	5	4
2	-7	5	7	-5	3	-4	5	1	-1	-8	-1	5	8	8	1		5	21	-20	-7	4	5	11	-10
3	-7	5	9	9	4	-4	5	11	11	-7	-1	5	10	-9	1	1	5	7	-8	-6	4	5	10	11
4	-7	5	6	-5	5	-4	5	14	-14	-6	-1	5	17	16	2	1	5	2	-2	-5	4	5	3	2
5	-7	5	2	-3	6	-4	5	8	-7	-5	-1	5	9	-9	3	1	5	12	-12	-4	4	5	4	-4
6	-7	5	6	5	7	-4	5	10	10	-4	-1	5	2	-2	4	1	5	13	13	-3	4	5	9	9
7	-7	5	2	-2	8	-4	5	10	-10	-3	-1	5	7	7	5	1	5	6	-6	-2	4	5	14	-15
8	-7	5	6	6	9	-4	5	6	5	-2	-1	5	13	-13	6	1	5	1	-1	-1	4	5	1	1
-5	-6	5	2	-2	10	-4	5	7	9	-1	-1	5	3	3	7	1	5	8	9	0	4	5	6	6
-4	-6	5	1	-2	-8	-3	5	3	-3	0	-1	5	25	26	8	1	5	7	-7	1	4	5	18	-17
-3	-6	5	13	13	-7	-3	5	6	5	1	-1	5	17	-16	9	1	5	5	5	2	4	5	9	9
-2	-6	5	11	-11	-6	-3	5	7	-5	2	-1	5	4	-4	-10	2	5	11	10	3	4	5	5	-6
-1	-6	5	4	5	-5	-3	5	7	7	3	-1	5	2	-2	-9	2	5	7	-6	4	4	5	9	-9
0	-6	5	13	13	-4	-3	5	1	-1	4	-1	5	5	-7	-8	2	5	4	3	5	4	5	8	8
1	-6	5	13	-13	-3	-3	5	2	3	5	-1	5	13	13	-7	2	5	1	-2	5	4	5	5	-6
2	-6	5	1	0	-2	-3	5	2	2	6	-1	5	18	-18	-6	2	5	9	-9	-8	5	5	4	-4
3	-6	5	4	3	-1	-3	5	8	-9	7	-1	5	1	-2	-5	2	5	19	19	-7	5	5	3	2
4	-6	5	1	-1	0	-3	5	10	10	8	-1	5	13	13	-4	2	5	1	-1	-6	5	5	10	10
5	-6	5	6	3	1	-3	5	5	5	9	-1	5	5	-5	-3	2	5	13	-12	-5	5	5	12	-12
6	-6	5	4	-3	2	-3	5	22	-22	10	-1	5	6	6	-2	2	5	9	9	-4	5	5	5	5
7	-6	5	1	-1	3	-3	5	8	3	-9	0	5	11	10	-1	2	5	8	-7	-3	5	5	1	1
8	-6	5	4	3	4	-3	5	4	4	-8	0	5	9	-8	0	2	5	14	-15	-2	5	5	9	-9
9	-6	5	12	-11	5	-3	5	14	-14	-7	0	5	1	0	1	2	5	12	12	-1	5	5	9	10
-6	-5	5	3	2	6	-3	5	16	15	-6	0	5	4	4	2	2	5	17	-16	0	5	5	10	-11
-5	-5	5	5	-5	7	-3	5	3	-3	-5	0	5	18	-18	3	2	5	10	9	1	5	5	1	2
-4	-5	5	4	4	8	-3	5	6	-8	-4	0	5	12	12	4	2	5	4	4	2	5	5	5	6
-2	-5	5	8	-8	9	-3	5	10	10	-3	0	5	6	6	5	2	5	5	-4	3	5	5	13	-13
-1	-5	5	13	12	10	-3	5	2	-1	-2	0	5	17	-16	6	2	5	5	5	4	5	5	2	3
0	-5	5	5	-5	-9	-2	5	10	-9	-1	0	5	15	15	7	2	5	2	1	-5	6	5	3	-3
1	-5	5	5	-4	-8	-2	5	7	5	0	0	5	7	7	8	2	5	2	-3	-5	6	5	2	-2
2	-5	5	11	10	-7	-2	5	4	-3	1	0	5	14	-14	-9	3	5	11	-11	-4	6	5	11	12

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR ES2H CRC6H5C03NE(CO)2T-BUNC

H	K	L	FO	FC
-3	9	5	19	-11
-2	9	5	1	1
-1	9	5	3	2
0	9	5	7	-5
1	9	5	7	6
2	9	5	5	5
3	-7	6	7	-7
4	-7	6	3	3
-2	-6	6	7	6
-1	-6	6	1	1
0	-6	6	13	-12
1	-6	6	3	2
2	-6	6	1	-1
3	-6	6	1	-1
4	-6	6	3	3
5	-6	6	3	-3
6	-6	6	2	1
-4	-5	6	5	-4
-3	-5	6	1	0
-2	-5	6	7	6
-1	-5	6	7	-7
0	-5	6	3	-3
1	-5	6	5	5
2	-5	6	10	-10
3	-5	6	3	3
4	-5	6	1	-1
5	-5	6	7	-5
6	-5	6	1	1
7	-5	6	2	-2
-4	-4	6	1	0
-3	-4	6	3	-3
-2	-4	6	6	6
-1	-4	6	6	-6
0	-4	6	3	3
1	-4	6	5	-5
2	-4	6	1	1
3	-4	6	7	-7
4	-4	6	3	3
5	-4	6	1	-1
6	-4	6	1	0
7	-4	6	3	-3
8	-4	6	5	5
-3	-3	6	4	-4
-2	-3	6	5	5
-1	-3	6	7	-7
0	-3	6	7	5
1	-3	6	7	-8
2	-3	6	5	5
3	-3	6	3	-3
4	-3	6	1	1
5	-3	6	3	-3
6	-3	6	1	1
7	-3	6	3	-3
8	-3	6	1	0
-4	-2	6	4	-4
-3	-2	6	5	5
-2	-2	6	7	-7
-1	-2	6	7	6
0	-2	6	7	-7
1	-2	6	7	7
2	-2	6	7	-7
3	-2	6	5	5
4	-2	6	3	-3
5	-2	6	1	1
6	-2	6	3	-3
7	-2	6	1	1
8	-2	6	3	-3
9	-2	6	1	0
-4	-1	6	12	-12
-3	-1	6	5	5
-2	-1	6	9	-9
-1	-1	6	7	7
0	-1	6	9	-9
1	-1	6	11	11
2	-1	6	12	-11
3	-1	6	10	-10
4	-1	6	5	5
5	-1	6	7	-7
6	-1	6	7	8
7	-1	6	11	-11
8	-1	6	2	2
9	-1	6	3	-3
-4	0	6	7	-7
-3	0	6	2	2
-2	0	6	5	-5
-1	0	6	10	9
0	0	6	9	-9
1	0	6	12	12
2	0	6	13	-13
3	0	6	12	-11
4	0	6	2	2
5	0	6	3	-3
6	0	6	10	10
7	0	6	1	-1
8	0	6	4	3
9	0	6	2	-3
-4	1	6	13	-12
-3	1	6	1	0
-2	1	6	6	-5
-1	1	6	9	9
0	1	6	14	-13
1	1	6	7	7
2	1	6	4	-3
3	1	6	6	-5
4	1	6	2	1
5	1	6	1	1
6	1	6	3	-3
7	1	6	4	4
8	1	6	3	-3
9	1	6	4	4
-4	2	6	6	-6
-3	2	6	4	4
-2	2	6	6	-6
-1	2	6	6	6
0	2	6	6	-6
1	2	6	4	4
2	2	6	5	-5
3	2	6	1	1
4	2	6	3	-3
5	2	6	1	1
6	2	6	3	-3
7	2	6	1	0
-4	3	6	6	6
-3	3	6	3	-3
-2	3	6	5	5
-1	3	6	7	-7
0	3	6	7	7
1	3	6	7	-7
2	3	6	5	5
3	3	6	3	-3
4	3	6	1	1
5	3	6	3	-3
6	3	6	1	1
7	3	6	3	-3
8	3	6	1	0
-4	4	6	7	7
-3	4	6	5	-5
-2	4	6	3	3
-1	4	6	5	-5
0	4	6	3	3
1	4	6	5	-4
2	4	6	1	1
3	4	6	3	-3
4	4	6	1	1
5	4	6	3	-3
6	4	6	1	0
-3	5	6	4	-4
-2	5	6	5	5
-1	5	6	7	-7
0	5	6	7	7
1	5	6	7	-8
2	5	6	5	5
3	5	6	3	-3
4	5	6	1	1
5	5	6	3	-3
6	5	6	1	0
-2	6	6	3	3
-1	6	6	1	1
0	6	6	3	-3
1	6	6	1	1
2	6	6	3	-3
3	6	6	1	0
-1	7	6	3	-3
0	7	6	1	1
1	7	6	3	-3
2	7	6	1	0
0	8	6	1	0
-4	-7	7	6	5
-3	-7	7	5	-5
-2	-7	7	1	2
-1	-7	7	1	-1
0	-7	7	1	-2
1	-7	7	4	3
2	-7	7	4	-3
3	-7	7	2	2
4	-7	7	1	-1
-3	-6	7	7	6
-2	-6	7	5	-5
-1	-6	7	7	7
0	-6	7	7	-8
1	-6	7	5	5
2	-6	7	3	-3
3	-6	7	1	1
4	-6	7	3	-4
5	-6	7	1	1
-4	-5	7	5	-5
-3	-5	7	1	2
-2	-5	7	1	-1
-1	-5	7	1	-2
0	-5	7	4	3
1	-5	7	4	-3
2	-5	7	2	2
3	-5	7	1	-1
-4	-4	7	6	5
-3	-4	7	5	-5
-2	-4	7	1	2
-1	-4	7	1	-1
0	-4	7	1	-2
1	-4	7	4	3
2	-4	7	4	-3
3	-4	7	2	2
4	-4	7	1	-1
-3	-3	7	7	6
-2	-3	7	5	-5
-1	-3	7	7	7
0	-3	7	7	-7
1	-3	7	7	8
2	-3	7	5	5
3	-3	7	3	-3
4	-3	7	1	1
5	-3	7	3	-4
6	-3	7	1	1
-4	-2	7	5	-5
-3	-2	7	1	2
-2	-2	7	1	-1
-1	-2	7	1	-2
0	-2	7	4	3
1	-2	7	4	-3
2	-2	7	2	2
3	-2	7	1	-1
-4	-1	7	6	5
-3	-1	7	5	-5
-2	-1	7	1	2
-1	-1	7	1	-1
0	-1	7	1	-2
1	-1	7	4	3
2	-1	7	4	-3
3	-1	7	2	2
4	-1	7	1	-1
-3	0	7	6	5
-2	0	7	5	-5
-1	0	7	7	7
0	0	7	7	-8
1	0	7	5	5
2	0	7	3	-3
3	0	7	1	1
4	0	7	3	-4
5	0	7	1	1
-4	1	7	6	5
-3	1	7	5	-5
-2	1	7	1	2
-1	1	7	1	-1
0	1	7	1	-2
1	1	7	4	3
2	1	7	4	-3
3	1	7	2	2
4	1	7	1	-1
-3	2	7	7	6
-2	2	7	5	-5
-1	2	7	7	7
0	2	7	7	-8
1	2	7	5	5
2	2	7	3	-3
3	2	7	1	1
4	2	7	3	-4
5	2	7	1	1
-4	3	7	5	-5
-3	3	7	1	2
-2	3	7	1	-1
-1	3	7	1	-2
0	3	7	4	3
1	3	7	4	-3
2	3	7	2	2
3	3	7	1	-1
-4	4	7	6	5
-3	4	7	5	-5
-2	4	7	1	2
-1	4	7	1	-1
0	4	7	1	-2
1	4	7	4	3
2	4	7	4	-3
3	4	7	2	2
4	4	7	1	-1
-3	5	7	7	6
-2	5	7	5	-5
-1	5	7	7	7
0	5	7	7	-8
1	5	7	5	5
2	5	7	3	-3
3	5	7	1	1
4	5	7	3	-4
5	5	7	1	1
-4	6	7	5	-5
-3	6	7	1	2
-2	6	7	1	-1
-1	6	7	1	-2
0	6	7	4	3
1	6	7	4	-3
2	6	7	2	2
3	6	7	1	-1
-3	7	7	6	5
-2	7	7	5	-5
-1	7	7	1	2
0	7	7	1	-1
1	7	7	1	-2
2	7	7	4	3
3	7	7	4	-3
-2	8	7	5	-5
-1	8	7	1	2
0	8	7	1	-1
1	8	7	1	-2
2	8	7	4	3
-1	9	7	6	5
0	9	7	5	-5
1	9	7	1	2
2	9	7	1	-1
3	9	7	1	-2

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CPRN

H	K	L	FO	FC
4	0	0	116	114
6	0	0	109	104
8	0	0	39	36
10	0	0	42	42
12	0	0	6	6
14	0	0	11	10
16	0	0	33	31
20	0	0	29	28
1	1	0	70	70
2	1	0	20	23
4	1	0	75	76
5	1	0	25	25
6	1	0	77	79
7	1	0	57	59
8	1	0	72	72
9	1	0	18	18
10	1	0	51	53
11	1	0	11	9
12	1	0	39	40
13	1	0	30	31
14	1	0	7	7
15	1	0	18	19
16	1	0	7	7
17	1	0	16	16
19	1	0	7	4
0	2	0	16	17
1	2	0	56	54
2	2	0	24	24
3	2	0	18	17
4	2	0	31	33
5	2	0	60	62
6	2	0	11	10
7	2	0	61	65
8	2	0	67	70
9	2	0	7	6
10	2	0	29	29
11	2	0	9	9
12	2	0	10	11
13	2	0	7	8
14	2	0	11	12
15	2	0	8	8
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR CPMN

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
9	3	9	14	16	1	1	10	10	10	1	2	10	9	4	5	3	10	8	10	2	1	11	15	14
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4	4	9	10	7	4	1	10	14	15	3	2	10	8	5	2	0	11	8	10	1	2	11	10	10
0	0	10	43	43	5	1	10	7	7	4	2	10	7	9	4	0	11	14	10	0	0	12	13	12
2	0	10	22	23	6	1	10	12	13	7	2	10	6	10	6	0	11	12	10	2	0	12	7	9
4	0	10	15	14	7	1	10	8	8	8	2	10	6	4	8	0	11	14	11	4	0	12	12	10
6	0	10	7	7	8	1	10	9	11	9	2	10	14	15	10	0	11	11	12	6	0	12	8	10
10	0	10	5	6	10	1	10	11	9	1	3	10	7	9	12	0	11	16	13	8	0	12	12	8
12	0	10	5	4	11	1	10	8	3	3	3	10	8	9	0	1	11	11	9					



OBSERVED AND CALCULATED STRUCTURE FACTORS FOR FEME

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	125	-120	11	3	0	7	-8	3	1	1	54	-55	-1	3	1	29	-29	2	5	1	31	-31
3	0	0	30	28	12	3	0	6	-6	4	1	1	59	61	0	3	1	63	-62	3	5	1	13	13
4	0	0	18	16	1	4	0	5	6	5	1	1	28	26	1	3	1	19	19	4	5	1	22	22
5	0	0	10	-10	2	4	0	4	-2	6	1	1	24	-25	2	3	1	20	20	5	5	1	8	-7
6	0	0	64	-63	3	4	0	3	-4	7	1	1	2	3	3	3	1	18	-18	6	5	1	20	-19
7	0	0	3	3	4	4	0	6	-1	8	1	1	15	16	4	3	1	22	-24	7	5	1	3	2
8	0	0	42	40	5	4	0	4	-3	9	1	1	4	-7	5	3	1	7	6	8	5	1	23	23
9	0	0	4	2	6	4	0	12	13	10	1	1	16	-15	6	3	1	49	49	9	5	1	4	-4
10	0	0	39	-38	7	4	0	2	-1	11	1	1	4	3	7	3	1	19	-20	-7	6	1	8	-9
11	0	0	11	-9	8	4	0	9	-7	12	1	1	10	9	8	3	1	37	-37	-6	6	1	4	4
12	0	0	20	19	9	4	0	2	4	13	1	1	6	-3	9	3	1	10	8	-5	6	1	14	11
1	1	0	109	-109	10	4	0	2	0	-13	2	1	3	4	10	3	1	25	24	-4	6	1	15	-15
2	1	0	13	-13	11	4	0	5	1	-12	2	1	11	-8	11	3	1	4	2	-3	6	1	12	-10
3	1	0	101	100	1	5	0	21	21	-11	2	1	17	-17	12	3	1	10	-12	-2	6	1	17	17
4	1	0	28	-26	2	5	0	2	3	-10	2	1	9	11	-11	4	1	5	7	-1	6	1	18	18
5	1	0	66	-65	3	5	0	20	-21	-9	2	1	19	18	-10	4	1	16	-14	0	6	1	10	-8
6	1	0	11	-11	4	5	0	5	6	-8	2	1	18	-16	-9	4	1	19	-19	1	6	1	16	-16
7	1	0	29	28	5	5	0	16	14	-7	2	1	12	-13	-8	4	1	19	20	2	6	1	7	7
8	1	0	7	6	6	5	0	9	-12	-6	2	1	3	3	-7	4	1	36	36	3	6	1	10	10
9	1	0	40	-39	7	5	0	6	-8	-5	2	1	40	41	-6	4	1	18	-17	4	6	1	5	-6
10	1	0	7	-9	9	5	0	12	10	-4	2	1	29	-28	-5	4	1	34	-32	5	6	1	17	-16
11	1	0	23	22	0	6	0	31	29	-3	2	1	42	-43	-4	4	1	15	13	6	6	1	7	6
12	1	0	9	7	1	6	0	3	-1	-2	2	1	95	94	-3	4	1	22	23	7	6	1	11	11
13	1	0	19	-13	2	6	0	22	-21	-1	2	1	43	41	-2	4	1	35	-36	-9	7	1	6	4
0	2	0	17	-17	3	6	0	5	4	0	2	1	16	17	-1	4	1	49	-50	-8	7	1	4	4
1	2	0	46	-45	4	6	0	16	15	1	2	1	16	-17	0	4	1	16	15	-7	7	1	7	-9
2	2	0	13	13	5	6	0	1	-3	2	2	1	32	-30	1	4	1	44	43	0	7	1	5	-3
3	2	0	4	3	6	6	0	12	-12	3	2	1	36	36	2	4	1	7	7	1	7	1	1	2
4	2	0	45	-45	7	6	0	4	-2	4	2	1	18	-18	3	4	1	34	-34	2	7	1	5	5
5	2	0	2	1	1	7	0	14	-14	5	2	1	63	-63	4	4	1	21	22	-13	0	2	23	22
6	2	0	50	50	2	7	0	5	-4	6	2	1	4	5	5	4	1	30	31	-12	0	2	8	8
7	2	0	17	18	3	7	0	15	14	7	2	1	37	36	6	4	1	4	-5	-11	0	2	35	-34
8	2	0	29	-29	-13	1	1	5	3	8	2	1	5	-6	7	4	1	24	-22	-10	0	2	16	-16
9	2	0	7	-6	-12	1	1	9	9	9	2	1	25	-25	8	4	1	4	6	-9	0	2	40	40
10	2	0	14	14	-11	1	1	15	-14	11	2	1	16	15	9	4	1	33	33	-8	0	2	29	29
11	2	0	12	13	-10	1	1	7	-6	12	2	1	3	-3	10	4	1	6	-7	-7	0	2	72	-72
12	2	0	10	-10	-9	1	1	10	10	13	2	1	9	11	11	4	1	20	-19	-6	0	2	29	-27
13	2	0	5	-5	-8	1	1	8	6	-12	3	1	4	-3	-7	5	1	4	7	-5	0	2	61	60
1	3	0	21	20	-7	1	1	5	-7	-11	3	1	9	10	-8	5	1	14	14	-4	0	2	15	-14
2	3	0	15	15	-6	1	1	4	5	-10	3	1	19	19	-7	5	1	14	-14	-3	0	2	86	-86
3	3	0	9	-1	-5	1	1	11	-10	-9	3	1	7	-6	-6	5	1	16	-15	-2	0	2	38	-32
4	3	0	9	-8	-4	1	1	28	-28	-8	3	1	30	-30	-5	5	1	15	16	-1	0	2	53	53
5	3	0	20	21	-3	1	1	34	34	-7	3	1	25	25	-4	5	1	16	14	0	0	2	61	59
6	3	0	7	-6	-2	1	1	16	-16	-6	3	1	50	51	-3	5	1	11	-12	1	0	2	99	-98
7	3	0	11	-9	-1	1	1	59	59	-5	3	1	41	-41	-2	5	1	25	-25	2	0	2	20	-20
8	3	0	4	2	0	1	1	37	37	-4	3	1	48	-49	-1	5	1	17	17	3	0	2	173	172
9	3	0	7	9	1	1	1	18	-18	-3	3	1	41	41	0	5	1	39	39	4	0	2	41	41
10	3	0	14	15	2	1	1	44	-43	-2	3	1	37	38	1	5	1	10	-10	5	0	2	21	-21



OBSERVED AND CALCULATED STRUCTURE FACTORS FOR FEME

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
6	0	2	24	-23	1	2	2	0	8	3	4	2	5	-5	-11	1	3	7	-8	-12	3	3	5	4
7	0	2	11	11	3	2	2	13	13	4	4	2	3	-3	-10	1	3	4	-7	-11	3	3	8	12
8	0	2	26	24	4	2	2	18	-18	5	4	2	12	11	-9	1	3	13	14	-10	3	3	6	-6
9	0	2	13	-14	6	2	2	45	-46	6	4	2	5	-3	-7	1	3	11	-14	-9	3	3	14	-14
10	0	2	22	-21	9	2	2	39	34	7	4	2	12	-11	-6	1	3	17	-17	-8	3	3	11	-10
11	0	2	5	5	0	2	2	22	22	8	4	2	10	7	-5	1	3	15	15	-7	3	3	38	39
12	0	2	12	12	7	2	2	45	-46	9	4	2	5	0	-4	1	3	27	28	-6	3	3	14	-10
13	0	2	12	-14	8	2	2	16	-17	10	4	2	6	-2	-3	1	3	25	-25	-5	3	3	40	-41
-13	1	2	4	4	9	2	2	20	21	11	4	2	5	-1	-2	1	3	44	-44	-4	3	3	25	24
-12	1	2	24	-25	10	2	2	16	16	-9	5	2	3	-1	-1	1	3	49	49	-3	3	3	50	58
-11	1	2	15	-14	11	2	2	3	-3	-8	5	2	17	18	0	1	3	50	51	-2	3	3	7	4
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-7	1	2	19	-20	-9	3	2	3	4	-4	5	2	6	7	4	1	3	14	-14	2	3	3	10	12
-6	1	2	42	43	-8	3	2	17	17	-3	5	2	26	19	5	1	3	24	-23	3	3	3	26	-28
-5	1	2	34	35	-7	3	2	7	-5	-2	5	2	16	-16	6	1	3	32	-32	4	3	3	23	-24
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7	1	2	18	17	6	3	2	5	-3	-6	6	2	4	-1	-8	2	3	29	-30	-7	4	3	3	-3
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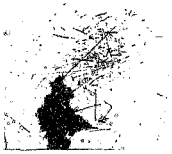
-2	2	2	73	73	0	4	2	15	-14	2	7	2	'	7	9	2	3	20	-21	10	4	3	10	-11
-1	2	2	37	-37	1	4	2	10	9	-13	1	;	.	6	10	2	3	19	19	-9	5	3	18	18
0	2	2	93	-90	2	4	2	5	4	-12	1	;	.	2	12	2	3	10	-11	-7	5	3	17	-18



OBSERVED AND CALCULATED STRUCTURE FACTORS FOR FEME

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
-6	5	3	3	-5	5	0	4	75	-75	2	2	4	10	-12	8	4	4	11	7	3	1	5	4	3
-5	5	3	18	15	6	0	4	74	24	3	2	4	43	-44	9	4	4	5	-3	4	1	5	34	-34
-4	5	3	4	-2	7	0	4	72	72	4	2	4	3	2	10	4	4	8	-2	5	1	5	17	17
-3	5	3	35	-34	8	0	4	12	13	5	2	4	12	12	-9	5	4	9	2	6	1	5	19	18
-2	5	3	3	9	9	0	4	18	-20	6	2	4	2	-1	-8	5	4	10	8	7	1	5	10	11
-1	5	3	38	36	10	0	4	8	-6	7	2	4	28	-29	-7	5	4	6	-7	8	1	5	4	2
0	5	3	8	8	11	0	4	13	12	8	2	4	3	2	-6	5	4	4	-2	9	1	5	19	-19
1	5	3	29	-28	12	0	4	2	-1	9	2	4	13	13	-5	5	4	16	15	11	1	5	8	10
2	5	3	28	29	-13	1	4	3	-8	10	2	4	9	-9	-4	5	4	9	6	12	1	5	6	-1
3	5	3	3	-2	-12	1	4	14	-15	11	2	4	9	-11	-3	5	4	5	-7	-11	2	5	9	-7
4	5	3	19	-21	-11	1	4	10	11	-12	3	4	4	-2	-2	5	4	16	-16	-10	2	5	8	9
5	5	3	3	-3	-10	1	4	28	28	-10	3	4	6	-1	-1	5	4	4	-3	-10	2	5	8	7
7	5	3	13	14	-9	1	4	24	-24	-9	3	4	5	-4	0	5	4	11	11	-9	2	5	17	-18
8	5	3	9	-9	-8	1	4	39	-39	-8	3	4	7	5	1	5	4	4	3	-8	2	5	13	-13
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-6	6	3	12	12	-5	1	4	24	-25	-5	3	4	27	26	4	5	4	12	11	-5	2	5	25	-24
-5	6	3	5	-3	-4	1	4	62	-63	-4	3	4	9	9	5	5	4	3	-4	-4	2	5	49	-49
-4	6	3	9	-9	-3	1	4	45	49	-3	3	4	8	-7	6	5	4	6	-6	-3	2	5	26	28
-3	6	3	3	5	-2	1	4	81	81	-2	3	4	32	-31	7	5	4	3	1	-2	2	5	37	38
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2	6	3	12	10	3	1	4	8	9	3	3	4	10	10	-2	6	4	4	-3	3	2	5	34	-41
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-12	0	4	12	-13	11	1	4	7	-2	11	3	4	3	4	6	6	4	5	0	11	2	5	12	-10
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-9	0	4	25	25	-11	2	4	6	6	-7	4	4	5	4	-10	1	5	13	13	-9	3	5	12	-11
-8	0	4	22	-24	-10	2	4	3	2	-6	4	4	8	-9	-9	1	5	13	13	-8	3	5	5	4
-7	0	4	32	-33	-9	2	4	18	-19	-5	4	4	8	-10	-8	1	5	5	-7	-7	3	5	12	11
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-5	0	4	34	35	-7	2	4	39	40	-3	4	4	0	1	-6	1	5	29	29	-5	3	5	27	-30
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-3	0	4	34	-34	-5	2	4	34	-35	0	4	4	7	8	-4	1	5	21	-22	-3	3	5	47	47
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-1	0	4	57	56	-3	2	4	47	48	3	4	4	5	6	-2	1	5	4	7	-1	3	5	38	-39
0	0	4	12	12	-2	2	4	34	-32	4	4	4	0	-2	-1	1	5	20	20	0	3	5	36	37
1	0	4	29	-28	-1	2	4	38	-39	5	4	4	3	-2	0	1	5	21	-19	1	3	5	50	50
2	0	4	12	13	0	2	4	17	17	6	4	4	3	2	1	1	5	25	-26	2	3	5	46	-47
3	0	4	40	38	1	2	4	58	57	7	4	4	1	0	2	1	5	25	26	3	3	5	38	-38



OBSERVED AND CALCULATED STRUCTURE FACTORS FOR FEME

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
4	2	5	16	17	-1	6	5	5	3	6	1	6	35	36	9	3	6	2	-3	-6	1	7	16	16
5	2	5	20	22	0	6	5	6	-4	7	1	6	20	-21	10	3	6	3	-2	-5	1	7	3	3
6	2	5	19	-19	1	6	5	6	4	8	1	6	19	-19	-8	4	6	5	-4	-4	1	7	16	-16
7	2	5	25	-26	2	6	5	4	4	9	1	6	17	17	-7	4	6	4	6	-3	1	7	5	3
8	2	5	10	10	3	6	5	3	-5	10	1	6	9	7	-6	4	6	1	-2	-2	1	7	4	-1
9	2	5	7	8	4	6	5	9	-9	11	1	6	17	-17	-5	4	6	1	2	-1	1	7	8	8
10	3	5	6	-9	5	6	5	5	4	-11	2	6	4	1	-4	4	6	3	1	0	1	7	25	-25
11	3	5	11	-10	-12	0	6	9	-8	-10	2	6	14	-13	-3	4	6	18	-13	1	1	7	8	-9
-10	4	5	12	-11	-11	0	6	1	2	-9	2	6	5	-5	-2	4	6	4	5	2	1	7	22	22
-9	4	5	18	18	-10	0	6	24	24	-8	2	6	7	7	-1	4	6	4	3	3	1	7	1	1
-8	4	5	11	12	-9	0	6	3	11	-7	2	6	9	9	0	4	6	4	-4	4	1	7	18	-17
-7	4	5	12	-14	-8	0	6	36	-37	-6	2	6	29	-32	1	4	6	1	-2	5	1	7	2	-4
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-5	4	5	19	18	-6	0	6	36	38	-4	2	6	53	53	3	4	6	3	-6	7	1	7	10	-10
-4	4	5	19	20	-5	0	6	8	7	-3	2	6	3	0	4	4	6	5	-7	8	1	7	4	-2
-3	4	5	26	-29	-4	0	6	53	-52	-2	2	6	18	-17	5	4	6	11	12	9	1	7	5	6
-2	4	5	45	-44	-3	0	6	39	-39	-1	2	6	8	6	6	4	6	1	1	10	1	7	11	8
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0	4	5	29	29	-1	0	6	37	37	1	2	6	4	-2	8	4	6	4	2	-11	2	7	16	17
1	4	5	25	-24	0	0	6	42	-41	2	2	6	16	-15	9	4	6	3	2	-10	2	7	3	-2
2	4	5	24	-24	1	0	6	38	-37	3	2	6	23	-23	-7	5	6	6	-6	-9	2	7	19	19
3	4	5	16	16	2	0	6	66	65	4	2	6	29	28	-6	5	6	3	-4	-8	2	7	10	11
4	4	5	18	19	4	0	6	24	-25	5	2	6	31	29	-5	5	6	4	4	-7	2	7	14	15
5	4	5	19	-21	5	0	6	19	-19	6	2	6	21	-21	-4	5	6	6	-6	-6	2	7	18	-20
6	4	5	20	-20	6	0	6	23	25	7	2	6	18	-19	-3	5	6	9	-9	-5	2	7	25	-27
7	4	5	8	7	7	0	6	32	32	8	2	6	2	3	-2	5	6	4	6	-4	2	7	5	-5
8	4	5	16	15	8	0	6	32	-31	9	2	6	8	5	-1	5	6	10	11	-3	2	7	47	47
9	4	5	5	-4	9	0	6	10	-9	10	2	6	10	-12	0	5	6	4	-2	-2	2	7	7	-4
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-7	5	5	3	-5	11	0	6	14	16	-11	3	6	3	-8	2	5	6	15	-14	0	2	7	10	7
-6	5	5	22	20	-12	1	6	5	-2	-10	3	6	3	0	3	5	6	9	-9	1	2	7	19	
-5	5	5	7	8	-11	1	6	13	13	-9	3	6	13	11	4	5	6	10	9	2	2	7	2	
-4	5	5	15	-15	-10	1	6	7	7	-8	3	6	4	3	5	5	6	7	-7	3	2	7	20	-20
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0	5	5	17	-17	-6	1	6	4	5	-4	3	6	5	4	-3	6	6	4	4	7	2	7	15	-14
1	5	5	11	-8	-5	1	6	51	-52	-3	3	6	20	-20	-2	6	6	11	12	8	2	7	5	3
2	5	5	17	17	-4	1	6	29	-29	-2	3	6	11	11	-1	6	6	10	6	9	2	7	8	9
3	5	5	13	12	-3	1	6	36	37	-1	3	6	15	15	0	6	6	9	9	10	2	7	2	1
4	5	5	11	-10	-2	1	6	20	21	0	3	6	5	6	1	6	6	5	-4	-10	3	7	14	-15
5	5	5	5	-4	-1	1	6	43	-45	1	3	6	23	-22	2	6	6	13	13	-9	3	7	5	2
6	5	5	4	5	0	1	6	4	2	2	3	6	22	-21	4	6	6	12	-14	-8	3	7	22	22
7	5	5	15	14	1	1	6	35	36	3	3	6	17	18	-11	1	7	4	2	-7	3	7	4	-4
-5	6	5	10	-12	2	1	6	21	21	4	3	6	7	4	-10	1	7	12	11	-6	3	7	35	-35
-4	6	5	8	-7	3	1	6	18	-18	5	3	6	12	-12	-9	1	7	20	-19	-5	3	7	8	8
-3	6	5	9	8	4	1	6	19	-18	7	3	6	5	5	-8	1	7	3	-6	-4	3	7	31	30
-2	6	5	6	5	5	1	6	48	42	8	3	6	4	-1	-7	1	7	14	14	-3	3	7	10	-10



OBSERVED AND CALCULATED STRUCTURE FACTORS FOR *FEME*

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	3	7	32	-32	-11	0	8	10	7	-6	2	8	1.	-18	-3	5	8	12	-12	5	3	9	25	25
-1	3	7	12	11	-10	0	8	4	9	-4	2	8	26	25	-2	5	8	2	2	-4	3	9	6	6
0	3	7	39	40	-9	0	8	6	-7	-3	2	8	9	-10	-1	5	8	12	10	-3	3	9	18	-17
1	3	7	3	-4	-8	0	8	9	-10	-2	2	8	15	-16	0	5	8	11	-11	-1	3	9	9	9
2	3	7	34	-34	-7	0	8	23	24	-1	2	8	23	24	1	5	8	4	-4	0	3	9	5	6
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-2	5	7	11	9	2	1	8	17	-17	-5	4	8	8	-8	-1	2	9	10	-10	-6	0	10	4	4
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3	5	7	18	-18	7	1	8	13	-14	0	4	8	4	3	4	2	9	2	5	-1	0	10	31	-31
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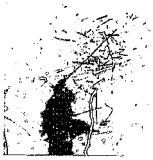
1



OBSERVED AND CALCULATED STRUCTURE FACTORS FOR FEHE

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
7	0	10	17	-17	0	2	10	5	-4	0	4	10	5	-2	4	2	11	14	12	-5	1	12	10	12
8	0	10	5	-2	1	2	10	19	-19	1	4	10	3	-3	5	2	11	4	-2	-4	1	12	5	7
-9	1	10	5	5	2	2	10	8	6	2	4	10	5	4	6	2	11	11	-10	-3	1	12	14	-13
-8	1	10	16	18	3	2	10	16	17	3	4	10	5	2	-5	3	11	16	15	-2	1	12	13	-12
-7	1	10	2	-1	4	2	10	4	4	4	4	10	3	-4	-4	3	11	6	-5	-1	1	12	10	12
-6	1	10	22	-22	5	2	10	9	-7	-7	1	11	10	8	-3	3	11	17	-18	0	1	12	12	13
-5	1	10	8	-9	6	2	10	7	1	-6	1	11	6	1	-2	3	11	9	8	1	1	12	15	-15
-4	1	10	19	18	7	2	10	8	8	-5	1	11	6	-6	-1	3	11	17	14	2	1	12	12	-13
-3	1	10	7	7	-7	3	10	2	4	-4	1	11	13	14	0	3	11	2	-4	3	1	12	10	10
-2	1	10	31	-32	-6	3	10	7	6	-3	1	11	6	-4	1	3	11	11	-12	4	1	12	8	8
-1	1	10	4	1	-5	3	10	3	-3	-2	1	11	10	-8	2	3	11	3	-2	5	1	12	12	-10
0	1	10	34	35	-4	3	10	6	-4	-1	1	11	5	-5	3	3	11	13	13	-5	2	12	8	8
1	1	10	4	-2	-3	3	10	4	3	0	1	11	4	0	-1	4	11	6	-7	-4	2	12	14	-13
2	1	10	29	-31	-2	3	10	4	3	1	1	11	14	13	0	4	11	15	-16	-3	2	12	7	-7
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6	1	10	15	-13	2	3	10	9	6	-7	2	11	7	-5	-3	0	12	9	7	1	2	12	12	-11
7	1	10	4	2	3	3	10	3	-4	-6	2	11	11	-11	-2	0	12	12	-11	2	2	12	4	3
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-3	2	10	15	-14	-3	4	10	8	-7	0	2	11	8	7	4	0	12	13	12	-1	1	13	4	2
-2	2	10	5	-5	-2	4	10	6	-3	1	2	11	4	-4	5	0	12	5	6	0	1	13	5	3
-1	2	10	20	20	-1	4	10	9	5	2	2	11	17	-16	-6	1	12	4	-4	1	1	13	6	3

6

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 0KEO

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
4	A	0	90	-43	18	K	0	64	46	10	11	0	238	236	6	1	1	69	65	3	4	1	32	-28
K	0	C	245	-284	C	K	0	K4	-48	12	11	0	130	-122	6	1	1	493	485	4	4	1	273	-287
0	0	C	429	422	2	K	0	620	660	14	11	0	30	-35	7	1	1	115	-112	5	4	1	77	-71
10	0	C	101	-97	4	K	0	644	-658	0	12	0	70	125	8	1	1	542	-540	6	4	1	186	183
12	0	C	363	-361	6	K	0	178	184	2	12	0	108	-115	9	1	1	141	140	7	4	1	92	-83
14	0	C	247	254	8	K	0	214	207	4	12	0	69	82	10	1	1	117	119	8	4	1	155	158
16	0	C	60	37	10	K	0	126	-124	6	12	C	42	-38	11	1	1	139	-141	9	4	1	90	90
4	1	C	87	-90	12	K	0	87	-83	8	12	0	26	26	12	1	1	139	-129	10	4	1	110	-112
6	1	C	488	511	14	K	C	62	-38	12	12	C	48	-72	13	1	1	57	55	12	4	1	64	-58
8	1	C	294	-279	16	K	0	204	209	14	12	0	27	40	14	1	1	231	238	13	4	1	73	-76
12	1	C	72	-72	18	K	0	147	-146	0	13	0	224	226	16	1	1	117	-118	14	4	1	53	-54
14	1	C	264	264	2	K	0	215	-214	4	13	C	151	-147	18	1	1	38	-40	15	4	1	34	20
16	1	C	157	-155	4	K	0	200	191	6	13	0	78	80	1	2	1	153	153	16	4	1	155	152
18	1	C	52	-48	6	K	0	218	-224	8	13	C	175	-183	2	2	1	475	487	18	4	1	105	-105
2	2	C	172	-171	8	K	0	275	268	10	13	0	263	261	3	2	1	297	-288	1	5	1	66	-47
4	2	C	299	310	10	K	0	297	-302	12	13	0	182	-177	4	2	1	242	229	2	5	1	317	-319
6	2	C	176	-177	12	K	0	219	218	14	13	0	24	17	5	2	1	244	247	3	5	1	220	226
8	2	C	49	-42	14	K	0	101	-104	0	14	0	61	47	6	2	1	80	71	4	5	1	154	164
10	2	C	28	-17	16	K	0	70	44	2	14	0	124	123	7	2	1	36	-38	5	5	1	317	-316
12	2	C	67	67	0	L	0	167	171	4	14	0	342	-345	8	2	1	427	-431	6	5	1	303	-303
14	2	C	21	27	2	L	0	145	-148	6	14	C	128	130	9	2	1	87	-81	7	5	1	177	179
16	2	C	40	-29	4	L	0	132	-137	8	14	0	167	162	10	2	1	40	40	8	5	1	296	300
18	2	C	48	42	6	L	0	127	132	10	14	C	76	68	11	2	1	84	81	9	5	1	135	-139
2	3	C	30	27	10	K	0	89	-94	12	14	C	105	-101	12	2	1	106	108	10	5	1	187	186
4	3	C	138	-120	12	K	0	46	-48	0	15	0	191	-187	13	2	1	21	13	11	5	1	120	114
6	3	C	427	447	14	K	0	67	48	8	15	0	232	232	14	2	1	230	-224	12	5	1	197	195
8	3	C	472	-473	16	K	0	43	46	8	15	0	70	-63	15	2	1	58	58	13	5	1	77	-79
10	3	C	171	167	2	L	0	362	-375	10	15	0	142	-142	17	2	1	90	-96	14	5	1	133	-133
12	3	C	169	-167	4	L	0	212	209	12	15	0	41	47	19	2	1	96	-96	15	5	1	66	65
14	3	C	284	284	6	L	0	174	170	0	16	0	282	-272	1	3	1	979	984	17	5	1	72	-72
16	3	C	107	-112	8	L	0	45	49	2	16	0	152	149	2	3	1	373	392	0	6	1	423	458
0	4	C	384	-377	10	L	0	375	-378	4	16	0	45	45	3	3	1	127	128	1	6	1	154	153
2	4	C	292	305	12	L	0	177	175	6	16	0	124	-127	4	3	1	77	71	2	6	1	338	-337
4	4	C	108	102	14	L	0	84	84	4	17	0	77	72	5	3	1	114	-110	3	6	1	174	172
6	4	C	14	24	0	K	0	41	-31	6	17	0	42	-47	6	3	1	476	-467	4	6	1	79	-76
8	4	C	351	-351	2	K	0	211	-214	8	17	0	48	44	7	3	1	108	-94	5	6	1	120	-115
10	4	C	81	82	2	L	0	240	-244	10	17	0	46	-40	8	3	1	174	163	6	6	1	30	-37
12	4	C	308	318	4	L	0	634	647	0	18	0	106	-98	9	3	1	83	-78	8	6	1	261	272
14	4	C	172	-167	6	L	0	236	-238	4	18	0	107	102	10	3	1	182	181	9	6	1	32	36
16	4	C	44	-38	8	L	0	204	-221	6	18	0	78	-71	11	3	1	124	118	10	6	1	78	-84
2	5	C	407	421	10	L	0	107	110	8	18	0	84	-71	12	3	1	34	-38	12	6	1	179	-186
4	5	C	19	19	12	L	0	79	82	2	19	0	123	128	14	3	1	196	-197	14	6	1	118	114
6	5	C	368	-374	14	L	0	27	29	4	19	0	204	-202	15	3	1	26	-27	17	6	1	59	61
8	5	C	72	69	16	L	0	211	-212	0	20	0	260	269	16	3	1	49	47	1	7	1	52	57
10	5	C	118	117	2	L	0	260	267	2	20	C	119	-118	18	3	1	81	82	2	7	1	452	-458
12	5	C	158	-151	4	L	0	71	-72	2	1	1	248	-240	0	4	1	192	190	3	7	1	60	-59
14	5	C	170	-174	6	L	0	58	-57	3	1	1	157	-147	1	4	1	211	215	4	7	1	130	129
16	5	C	70	69	8	L	0	60	-59	4	1	1	317	-325	2	4	1	335	334	5	7	1	129	-133

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
6	7	1	211	209	2	11	1	65	-35	10	14	1	41	10	4	0	2	491	-496	2	3	2	26	-31
7	7	1	119	108	3	11	1	314	302	12	14	1	88	81	6	0	2	117	104	3	3	2	212	212
8	7	1	62	30	4	11	1	107	-200	2	15	1	102	-98	8	0	2	535	521	4	3	2	300	310
9	7	1	93	-76	5	11	1	184	186	3	15	1	38	38	10	0	2	177	188	5	3	2	52	-58
10	7	1	256	-348	6	11	1	74	-30	5	15	1	58	58	12	0	2	357	-383	6	3	2	425	-434
11	7	1	168	168	7	11	1	134	-137	6	15	1	77	-73	0	0	2	192	-196	7	3	2	149	161
12	7	1	48	-51	8	11	1	174	-181	8	15	1	67	-66	10	0	2	131	136	8	3	2	232	223
14	7	1	114	114	9	11	1	60	61	9	15	1	104	-97	12	0	2	92	0	9	3	2	352	-368
15	7	1	61	66	10	11	1	288	288	8	15	1	113	121	12	0	2	244	248	10	3	2	126	-124
16	7	1	79	-88	11	11	1	48	-39	8	15	1	54	-46	13	0	2	92	16	11	3	2	251	247
0	8	1	60	-65	12	11	1	189	-189	10	15	1	141	-150	14	0	2	152	-162	12	3	2	98	106
1	8	1	196	-198	13	11	1	56	46	11	15	1	28	32	15	0	2	174	187	13	3	2	133	133
2	8	1	322	-306	14	11	1	98	-13	12	15	1	108	107	17	0	2	145	-140	14	3	2	136	-135
3	8	1	58	49	15	11	1	84	-69	0	16	1	72	-74	19	0	2	71	-11	15	3	2	49	41
4	8	1	566	607	0	12	1	86	79	1	16	1	59	-64	1	1	2	272	-265	16	3	2	74	78
5	8	1	220	-221	1	12	1	154	163	2	16	1	41	-36	2	1	2	263	267	17	3	2	30	-37
7	8	1	115	108	2	12	1	108	141	4	16	1	147	150	3	1	2	206	224	18	3	2	37	29
8	8	1	136	-105	3	12	1	22	-22	5	16	1	70	-70	4	1	2	64	94	0	4	2	558	575
9	8	1	102	-101	4	12	1	458	-455	7	16	1	43	47	5	1	2	207	-205	1	4	2	42	-78
10	8	1	109	94	5	12	1	178	172	8	16	1	127	-131	6	1	2	398	-388	2	4	2	188	-173
11	8	1	77	-70	7	12	1	80	-86	9	16	1	29	-37	7	1	2	36	32	3	4	2	418	414
12	8	1	110	108	8	12	1	150	148	10	16	1	63	60	8	1	2	194	175	4	4	2	181	-187
13	8	1	102	101	9	12	1	60	66	11	16	1	24	-12	9	1	2	258	-247	6	4	2	368	-359
14	8	1	40	20	10	12	1	96	-91	12	16	1	58	58	10	1	2	104	100	8	4	2	31	-9
15	8	1	36	-42	11	12	1	61	31	0	17	1	155	156	11	1	2	268	270	9	4	2	309	297
16	8	1	182	184	12	12	1	105	-100	3	17	1	55	55	13	1	2	40	-48	0	4	2	135	134
17	8	1	0	14	13	12	1	77	-69	4	17	1	40	0	14	1	2	164	-166	10	4	2	72	-67
0	9	1		98	15	12	1	41	24	5	17	1	227	-230	15	1	2	25	-20	12	4	2	211	213
3	9	1			1	13	1	28	40	7	17	1	30	-17	16	1	2	89	61	14	4	2	142	139
4	9	1			2	13	1	244	-232	8	17	1	88	86	17	1	2	41	-35	15	4	2	105	-104
5	9	1			3	13	1	61	-71	9	17	1	84	84	18	1	2	60	62	17	4	2	150	146
6	9	1			4	13	1	71	50	10	17	1	77	79	0	2	2	42	-40	1	M	2	96	98
7	9	1			5	13	1	52	-44	0	18	1	246	246	1	2	2	227	216	2	M	2	316	-334
8	9	1	194		6	13	1	150	153	1	18	1	52	-26	2	2	2	34	32	3	M	2	138	-132
9	9	1	80	61	7	13	1	54	64	2	18	1	110	-102	4	2	2	408	-408	4	M	2	94	86
10	9	1	273	272	8	13	1	23	-20	3	18	1	40	26	6	2	2	95	-91	5	M	2	114	-104
11	9	1	157	-153	9	13	1	143	-134	4	18	1	52	-52	8	2	2	189	188	6	M	2	258	303
12	9	1	38	38	11	13	1	50	-25	5	18	1	67	-73	9	2	2	31	-29	7	M	2	238	230
14	9	1	28	22	12	13	1	70	75	8	18	1	114	115	8	2	2	46	37	9	M	2	116	-108
15	9	1	44	-44	14	13	1	52	54	9	18	1	22	14	9	2	2	58	17	9	M	2	56	57
16	9	1	42	-7	0	14	1	226	-216	10	18	1	52	-16	11	2	2	83	57	10	M	2	255	-251
1	10	1	28	-23	1	14	1	28	10	3	19	1	28	-24	12	2	2	47	-44	11	M	2	170	-132
4	10	1	80	78	2	14	1	180	178	4	19	1	48	-34	13	2	2	92	-92	12	M	2	100	98
5	10	1	28	20	3	14	1	77	-70	5	19	1	102	96	14	2	2	29	23	13	M	2	67	-54
8	10	1	54	-50	4	14	1	22	-21	0	20	1	54	78	15	2	2	66	60	14	M	2	114	114
9	10	1	37	-47	5	14	1	54	53	0	0	2	422	-428	17	2	2	40	-15	15	M	2	103	99
15	10	1	24	-2	8	14	1	52	39	1	0	2	214	194	18	2	2	60	-40	16	M	2	79	-64
16	10	1	31	-28	9	14	1	109	-106	3	0	2	242	270	1	3	2	178	-175	18	M	2	79	-71

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 0F00

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
0	6	2	142	-140	2	9	2	300	321	2	12	2	26	39	2	15	2	94	-91	6	2	3	95	*
1	6	2	469	-479	3	9	2	41	75	3	12	2	131	-128	3	15	2	144	140	8	2	3	225	217
2	6	2	104	-104	4	9	2	328	-321	4	12	2	25	-12	4	15	2	24	-24	9	2	3	231	233
3	6	2	131	115	5	9	2	224	244	5	12	2	74	76	5	15	2	132	-135	10	2	3	50	-52
4	6	2	394	416	6	9	2	101	-103	6	12	2	78	-70	6	15	2	24	-23	11	2	3	20	14
5	6	2	31	-25	7	9	2	234	-248	7	12	2	20	-19	7	15	2	24	-7	12	2	3	130	-133
6	6	2	116	-115	8	9	2	49	-74	8	12	2	27	-19	8	15	2	93	96	13	2	3	44	-44
7	6	2	174	160	9	9	2	71	73	10	12	2	31	7	9	15	2	49	44	14	2	3	101	95
8	6	2	151	-151	10	9	2	260	286	12	12	2	28	30	1	17	2	24	17	15	2	3	169	-171
9	6	2	184	-187	11	9	2	24	-21	14	12	2	41	-25	2	17	2	44	-44	17	2	3	223	223
10	6	2	53	72	12	9	2	119	-122	1	13	2	24	20	4	17	2	60	-66	1	3	3	260	230
11	6	2	104	-106	13	9	2	99	102	2	13	2	168	-177	5	17	2	56	47	2	3	3	197	185
12	6	2	66	76	14	9	2	56	-63	3	13	2	28	26	6	17	2	52	61	3	3	3	221	-221
13	6	2	184	185	15	9	2	118	-124	4	13	2	32	29	7	17	2	80	-77	4	3	3	139	134
15	6	2	67	68	16	9	2	46	29	6	13	2	140	-142	8	17	2	67	-64	6	3	3	93	-97
16	6	2	161	-164	0	10	2	43	43	7	13	2	210	208	9	17	2	71	69	8	3	3	216	242
17	6	2	69	78	1	10	2	384	387	8	13	2	83	80	0	18	2	74	70	9	3	3	329	327
1	7	2	21	36	2	10	2	157	165	9	13	2	69	-91	1	18	2	54	49	8	3	3	89	-97
2	7	2	157	154	3	10	2	46	-59	10	13	2	176	-175	3	18	2	26	30	9	3	3	195	194
3	7	2	150	-163	4	10	2	415	-437	11	13	2	54	63	4	18	2	101	-94	10	3	3	207	-200
4	7	2	154	-157	5	10	2	42	18	12	13	2	114	111	5	18	2	49	-54	12	3	3	264	-263
5	7	2	184	206	6	10	2	148	159	13	13	2	47	-45	6	18	2	24	36	13	3	3	22	34
6	7	2	114	124	7	10	2	167	-172	0	14	2	110	-119	7	18	2	28	-31	14	3	3	102	98
7	7	2	249	-253	8	10	2	158	166	1	14	2	227	-221	1	19	2	75	73	15	3	3	91	92
8	7	2	101	-118	9	10	2	146	161	2	14	2	81	-80	2	19	2	137	-130	16	3	3	41	-50
9	7	2	178	179	10	10	2	80	*	3	14	2	38	33	3	19	2	97	-94	17	3	3	29	37
10	7	2	146	144	11	10	2	87	91	4	14	2	267	247	1	1	3	233	-247	18	3	3	69	-56
11	7	2	174	-177	12	10	2	71	77	5	14	2	61	-54	2	1	3	211	211	0	4	3	54	-51
12	7	2	111	-108	13	10	2	124	-147	7	14	2	114	116	3	1	3	341	353	3	4	3	427	-433
13	7	2	112	122	14	10	2	41	24	8	14	2	116	-117	4	1	3	148	152	2	4	3	33	20
14	7	2	50	51	15	10	2	152	147	9	14	2	42	-45	5	1	3	123	-127	3	4	3	182	185
15	7	2	74	-81	1	11	2	62	67	10	14	2	66	58	6	1	3	246	-253	4	4	3	218	215
17	7	2	28	34	2	11	2	220	-242	11	14	2	32	-40	7	1	3	84	80	5	4	3	22	-34
0	8	2	260	-272	3	11	2	28	-47	12	14	2	74	79	8	1	3	85	79	6	4	3	77	-69
1	8	2	58	-44	4	11	2	76	79	13	14	2	101	103	9	1	3	193	-204	7	4	3	168	163
2	8	2	32	45	5	11	2	126	-161	1	15	2	42	-48	10	1	3	43	39	8	4	3	71	-77
3	8	2	154	-160	6	11	2	47	42	2	15	2	162	161	11	1	3	133	143	9	4	3	176	-172
4	8	2	114	109	7	11	2	174	174	3	15	2	101	108	12	1	3	114	-118	10	4	3	64	66
5	8	2	142	138	8	11	2	28	28	4	15	2	24	-31	14	1	3	92	-91	11	4	3	89	-90
8	8	2	98	-104	9	11	2	58	48	5	15	2	57	46	15	1	3	31	28	12	4	3	68	67
9	8	2	98	-94	10	11	2	152	-156	8	15	2	191	-193	17	1	3	52	-45	13	4	3	171	169
10	8	2	46	46	11	11	2	24	-11	9	15	2	58	-72	14	1	3	30	30	14	4	3	24	-10
12	8	2	78	76	12	11	2	103	94	8	15	2	70	69	0	2	3	185	187	15	4	3	44	-41
13	8	2	27	27	13	11	2	84	-67	11	15	2	71	-70	1	2	3	215	-224	16	4	3	74	-68
14	8	2	51	-55	14	11	2	45	41	10	15	2	103	105	2	2	3	171	-166	17	4	3	25	14
16	8	2	47	-32	15	11	2	66	80	11	15	2	98	86	4	2	3	706	707	18	4	3	57	42
17	8	2	43	-52	0	12	2	109	-110	0	16	2	202	202	5	2	3	269	-210	1	5	3	89	84
1	9	2	76	-81	1	12	2	90	93	1	16	2	84	-84	6	2	3	607	-615	2	5	3	43	31

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
3	4	3	226	-230	3	4	3	122	-117	2	12	3	88	-66	4	16	3	114	-102	13	1	4	43	34
4	4	3	41	-68	4	4	3	219	-227	3	12	3	73	57	5	16	3	47	-5	14	1	4	28	26
5	4	3	215	226	5	4	3	28	-20	4	12	3	141	108	6	16	3	43	-38	15	1	4	71	74
6	4	3	151	102	6	4	3	107	88	5	12	3	38	43	7	16	3	91	-40	16	1	4	31	-25
7	4	3	241	-252	7	4	3	225	-208	6	12	3	73	-63	8	16	3	73	74	17	1	4	49	54
8	4	3	70	-77	8	4	3	129	134	7	12	3	172	169	9	16	3	102	98	0	2	4	178	180
9	4	3	135	122	9	4	3	177	189	8	12	3	92	-98	10	16	3	33	-29	1	2	4	255	-249
10	4	3	96	88	10	4	3	51	-53	9	12	3	132	-140	1	17	3	104	108	2	2	4	43	39
11	4	3	269	-281	11	4	3	132	134	10	12	3	82	84	2	17	3	120	-107	3	2	4	88	84
12	4	3	95	-91	12	4	3	80	-73	11	12	3	95	-93	3	17	3	144	-138	4	2	4	42	50
13	4	3	171	161	13	4	3	291	-291	12	12	3	72	67	5	17	3	51	-44	5	2	4	44	-43
14	4	3	45	41	14	4	3	93	92	13	12	3	241	270	6	17	3	45	44	7	2	4	44	47
15	4	3	79	-78	15	4	3	73	74	1	13	3	115	-116	7	17	3	56	45	8	2	4	42	-42
17	4	3	41	29	1	5	3	50	55	2	13	3	151	145	8	17	3	34	-39	9	2	4	77	-74
0	5	3	182	-174	2	5	3	141	-142	3	13	3	134	126	9	17	3	115	102	11	2	4	75	-77
2	5	3	30	40	4	5	3	56	51	4	13	3	122	119	0	18	3	114	-115	12	2	4	39	35
3	5	3	250	-252	5	5	3	102	-104	5	13	3	117	-109	1	18	3	54	53	13	2	4	102	97
4	5	3	61	65	6	5	3	77	76	7	13	3	145	-142	2	18	3	195	-187	15	2	4	30	-32
5	5	3	248	248	7	5	3	244	249	8	13	3	44	43	4	18	3	50	54	1	3	4	155	162
7	5	3	69	71	8	5	3	80	79	9	13	3	37	-34	5	18	3	160	162	2	3	4	157	-149
8	5	3	130	-122	9	5	3	172	-173	10	13	3	76	77	7	18	3	28	14	3	3	4	241	-246
9	5	3	151	-145	10	5	3	91	-92	11	13	3	72	68	9	18	3	48	-53	4	3	4	247	250
10	5	3	43	47	11	5	3	48	55	12	13	3	39	42	2	19	3	28	19	5	3	4	236	241
11	5	3	97	94	12	5	3	96	94	13	13	3	47	46	3	19	3	62	64	6	3	4	19	0
12	5	3	95	98	13	5	3	122	-121	0	14	3	104	-97	4	19	3	47	50	7	3	4	205	-207
13	5	3	80	82	14	5	3	112	110	1	14	3	60	60	1	0	4	155	154	8	3	4	71	71
14	5	3	55	-58	0	10	3	50	48	2	14	3	64	62	2	0	4	76	79	9	3	4	365	369
15	5	3	46	41	1	10	3	37	37	3	14	3	127	-122	3	0	4	827	693	10	3	4	75	-76
16	5	3	30	-45	5	10	3	32	-36	4	14	3	25	-11	4	0	4	229	-210	11	3	4	339	-331
1	7	3	127	121	6	10	3	34	-32	5	14	3	140	-136	5	0	4	447	-402	12	3	4	68	69
2	7	3	75	-81	7	10	3	41	41	6	14	3	25	15	6	0	4	64	61	13	3	4	134	135
3	7	3	34	-	8	10	3	28	28	8	14	3	55	58	7	0	4	58	-51	15	3	4	48	-38
3	7	3	441	441	13	10	3	43	-50	9	14	3	62	60	8	0	4	29	48	17	3	4	32	36
4	7	3	25	-23	12	11	3	145	134	10	14	3	58	-7	9	0	4	242	236	1	4	4	160	173
5	7	3	229	242	2	11	3	157	-150	1	15	3	36	-3	10	0	4	40	-69	3	4	4	527	-535
6	7	3	168	-178	3	11	3	46	-50	2	15	3	48	45	13	0	4	88	-75	4	4	4	122	116
7	7	3	267	-263	5	11	3	284	-295	3	15	3	96	-98	14	0	4	145	-141	5	4	4	481	486
9	7	3	28	-16	6	11	3	58	54	5	15	3	158	158	15	0	4	60	65	6	4	4	101	-100
10	7	3	132	131	7	11	3	290	307	6	15	3	28	0	17	0	4	262	260	7	4	4	28	38
11	7	3	89	89	9	11	3	0	20	9	15	3	164	-167	1	1	4	262	262	8	4	4	58	-64
12	7	3	76	-77	0	12	3	178	-180	8	15	3	27	-12	3	1	4	166	-154	9	4	4	206	-211
13	7	3	112	108	10	11	3	103	-108	9	15	3	113	104	3	1	4	414	-390	10	4	4	35	23
14	7	3	106	-110	11	11	3	84	90	10	15	3	48	48	4	1	4	88	97	11	4	4	42	-37
15	7	3	44	-47	12	11	3	84	84	11	15	3	71	71	5	1	4	84	84	12	4	4	52	52
16	7	3	57	46	13	11	3	124	-121	0	16	3	75	70	6	1	4	274	263	13	4	4	93	85
0	8	3	197	198	14	11	3	136	131	1	16	3	166	163	10	1	4	129	-131	14	4	4	129	130
1	8	3	475	467	0	12	3	149	-149	2	16	3	99	-96	11	1	4	130	-124	16	4	4	47	-45
2	8	3	73	76	1	12	3	404	-418	3	16	3	27	19	12	1	4	71	66	17	4	4	197	-186

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR BKCO

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
1	E	A	242	-237	8	E	A	41	35	5	17	A	101	-101	1	18	A	90	-46	9	3	E	82	-64
2	E	A	164	105	0	E	A	78	83	9	17	A	27	15	3	18	A	28	-40	8	3	E	166	-184
3	E	A	348	338	12	E	A	97	-95	1	13	E	43	-50	4	18	A	90	93	10	3	E	90	83
4	E	A	748	748	11	E	A	40	46	2	13	A	45	39	5	18	A	61	57	11	3	E	271	265
6	E	A	304	-316	10	E	A	31	-42	4	13	A	96	96	1	19	A	113	-103	12	3	E	51	-51
7	E	A	297	-293	1	0	A	144	146	5	13	A	206	206	2	19	A	58	58	13	3	E	36	19
8	E	A	71	71	2	0	A	82	86	6	13	A	59	53	1	1	E	920	964	14	3	E	40	23
9	E	A	121	-126	3	0	A	122	-114	7	13	A	222	-224	2	1	E	124	-122	15	3	E	132	-128
10	E	A	74	78	4	0	A	46	-33	8	13	A	57	59	3	1	E	246	-304	17	3	E	49	-38
11	E	A	214	220	5	0	A	283	-285	9	13	A	88	86	4	1	E	132	128	0	4	E	93	97
13	E	A	42	53	6	0	A	228	227	10	13	A	99	-4	5	1	E	28	28	1	4	E	272	265
14	E	A	66	-67	7	0	A	370	392	11	13	A	53	-46	6	1	E	197	-197	2	4	E	142	-140
15	E	A	154	-154	8	0	A	74	-77	12	13	A	31	10	7	1	E	78	-42	3	4	E	46	-44
16	E	A	25	27	9	0	A	54	-44	13	13	A	105	103	8	1	E	130	122	4	4	E	182	187
17	E	A	40	-28	10	0	A	28	-14	0	14	A	105	102	9	1	E	304	296	5	4	E	31	-27
0	E	A	126	129	11	0	A	38	-27	1	14	A	279	281	10	1	E	112	-117	6	4	E	45	-42
1	E	A	414	424	12	0	A	126	-134	2	14	A	28	-32	11	1	E	272	-287	7	4	E	148	-137
2	E	A	88	-87	14	0	A	47	40	3	14	A	44	-39	12	1	E	119	110	8	4	E	184	182
3	E	A	61	-80	15	0	A	150	153	5	14	A	78	-81	13	1	E	58	57	11	4	E	44	53
4	E	A	47	-44	1	10	A	379	-387	7	14	A	131	-127	14	1	E	61	52	12	4	E	48	-43
5	E	A	77	-68	1	10	A	599	-644	8	14	A	56	57	15	1	E	57	44	13	4	E	177	-178
7	E	A	194	-201	2	10	A	52	50	9	14	A	137	138	16	1	E	30	21	14	4	E	80	83
8	E	A	82	79	3	10	A	84	87	10	14	A	30	-29	17	1	E	30	38	15	4	E	42	38
9	E	A	195	209	4	10	A	53	56	11	14	A	43	43	0	2	E	315	312	16	4	E	45	-42
10	E	A	38	-39	5	10	A	55	58	12	14	A	43	-43	1	2	E	20	-25	1	5	E	87	84
11	E	A	107	108	7	10	A	216	220	1	15	A	137	130	2	2	E	158	-158	2	5	E	61	60
12	E	A	58	-54	8	10	A	67	70	2	15	A	24	24	3	2	E	494	-482	3	5	E	154	167
13	E	A	212	-214	9	10	A	192	-195	3	15	A	182	-184	4	2	E	170	170	4	5	E	140	-132
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17	E	A	38	-42	13	10	A	219	208	6	15	A	45	41	7	2	E	46	42	7	5	E	78	71
1	F	A	91	-90	14	10	A	57	-61	7	15	A	113	110	8	2	E	50	59	8	5	E	148	144
3	F	A	77	79	15	10	A	78	82	8	15	A	102	94	9	2	E	237	-222	9	5	E	249	254
4	F	A	218	-227	1	11	A	159	-156	10	15	A	55	-53	10	2	E	28	19	10	5	E	140	157
5	F	A	212	218	2	11	A	81	70	11	15	A	137	-130	11	2	E	64	46	11	5	E	117	102
6	F	A	256	278	3	11	A	74	74	0	16	A	38	-25	12	2	E	80	81	12	5	E	82	91
7	F	A	71	76	4	11	A	151	151	1	16	A	57	52	13	2	E	100	107	13	5	E	122	118
8	F	A	207	-213	5	11	A	74	80	2	16	A	32	-22	14	2	E	51	51	14	5	E	82	84
11	F	A	132	140	7	11	A	238	-238	3	16	A	145	-138	15	2	E	126	118	15	5	E	85	83
12	F	A	142	-141	8	11	A	66	64	4	16	A	66	60	16	2	E	84	71	16	5	E	58	46
15	F	A	49	50	9	11	A	30	32	5	16	A	187	186	17	2	E	205	-204	0	6	E	141	-139
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1	G	A	22	16	11	11	A	37	35	9	16	A	70	-66	2	3	E	31	26	2	6	E	176	179
2	G	A	77	77	13	11	A	84	84	10	16	A	29	19	3	3	E	144	140	3	6	E	239	231
3	G	A	141	147	14	11	A	61	-60	2	17	A	66	66	4	3	E	48	-47	4	6	E	94	96
4	G	A	29	-27	0	12	A	36	-4	6	17	A	74	-77	5	3	E	174	181	5	6	E	297	-298
5	G	A	174	-177	1	12	A	103	-97	7	17	A	57	51	6	3	E	22	28	6	6	E	84	84
7	G	A	35	-38	3	12	A	53	54	0	18	A	42	-28	7	3	E	237	-211	7	6	E	80	-82

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2	0	R	126	-128
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3	0	R	250	-254
3	0	R	58	52
3	0	R	126	133
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5	0	R	95	-95
6	0	R	158	166
6	0	R	205	-209
7	0	R	419	-422
7	0	R	147	151
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8	0	R	145	-149
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13	5	R	127	-125
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14	18	R	147	-144
15	18	R	166	167
16	18	R	133	-135
17	18	R	142	-142
18	18	R	174	-166

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 0KCO

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
0	A	R	93	82	1	12	E	78	92	E	1	7	102	124	E	4	7	80	73	C	8	7	88	98
1	A	R	71	-85	2	12	E	61	-63	7	1	7	134	-142	8	4	7	56	47	1	8	7	152	158
2	A	R	34	-24	3	12	E	40	-45	8	1	7	231	-237	9	4	7	70	-70	2	8	7	222	-231
3	A	R	124	-131	4	12	E	28	29	9	1	7	42	-36	10	4	7	42	-37	3	8	7	110	117
4	A	R	129	126	5	12	E	46	53	10	1	7	82	86	11	4	7	28	-20	4	8	7	210	217
5	A	R	26	31	6	12	E	27	-30	11	1	7	76	76	12	4	7	28	8	5	8	7	162	-163
6	A	R	47	-48	7	12	E	54	58	12	1	7	112	-107	13	4	7	69	76	6	8	7	145	-140
7	A	R	41	41	8	12	E	68	86	13	1	7	74	79	14	4	7	55	-47	7	8	7	4	-17
8	A	R	27	28	9	12	E	36	-32	14	1	7	123	130	0	5	7	90	-88	8	8	7	40	-51
1	B	R	186	-184	A	13	E	168	-186	15	1	7	37	-50	1	5	7	23	-14	0	A	7	134	128
2	B	R	128	-124	B	13	E	121	-113	16	1	7	58	-44	2	5	7	186	197	1	A	7	4	34
3	B	R	167	166	C	13	E	72	74	0	2	7	472	-464	3	5	7	239	-237	11	A	7	49	35
4	B	R	101	101	1	13	E	195	187	1	2	7	177	190	4	5	7	29	33	12	A	7	77	-86
5	B	R	172	172	2	13	E	49	-108	2	2	7	277	278	5	5	7	227	223	13	A	7	58	43
6	B	R	42	-46	3	13	E	64	-58	3	2	7	152	150	10	5	7	206	-202	1	B	7	76	78
7	B	R	218	-206	10	13	E	143	141	4	2	7	37	-32	12	5	7	145	141	2	B	7	133	130
8	B	R	111	107	0	14	E	61	-64	5	2	7	277	-274	13	5	7	39	-5	3	B	7	72	-76
9	B	R	44	-49	1	14	E	194	-198	6	2	7	119	111	14	5	7	113	-116	4	B	7	176	-184
10	B	R	124	-131	2	14	E	98	90	7	2	7	87	-92	15	5	7	28	5	5	B	7	4	-84
11	B	R	48	50	3	14	E	57	-54	8	2	7	174	-176	0	6	7	293	298	6	B	7	79	68
12	B	R	41	100	4	14	E	127	-123	9	2	7	168	165	1	6	7	122	-129	7	B	7	74	78
13	B	R	67	69	5	14	E	90	97	11	2	7	45	36	2	6	7	186	-184	8	C	7	117	-123
0	10	R	118	123	6	14	E	81	94	12	2	7	150	151	3	6	7	115	-111	9	C	7	42	31
1	10	R	240	234	7	14	E	47	46	13	2	7	100	-113	4	6	7	49	46	10	C	7	163	166
2	10	R	226	-229	8	14	E	134	-134	14	2	7	122	-117	5	6	7	114	111	11	C	7	30	-50
3	10	R	55	56	1	15	E	120	-111	15	2	7	35	30	6	6	7	66	-61	12	C	7	97	-117
4	10	R	223	229	2	15	E	49	-48	1	3	7	152	153	7	6	7	27	17	0	D	7	32	-36
5	10	R	126	-123	3	15	E	110	122	2	3	7	163	168	8	6	7	124	124	1	D	7	50	38
6	10	R	110	-118	4	15	E	27	-17	3	3	7	208	-204	9	6	7	104	-110	2	D	7	35	-15
7	10	R	119	-118	5	15	E	20	4	4	3	7	70	74	10	6	7	26	-19	4	D	7	57	57
8	10	R	28	-22	6	15	E	48	52	5	3	7	115	-110	11	6	7	37	-33	5	D	7	50	-47
9	10	R	188	178	7	15	E	130	-121	6	3	7	214	-213	12	6	7	58	-65	6	D	7	27	-29
10	10	R	66	67	8	15	E	78	-68	7	3	7	398	397	13	6	7	58	60	8	D	7	28	-7
11	10	R	71	77	0	16	E	144	-152	8	3	7	77	72	14	6	7	56	52	9	D	7	29	32
12	10	R	28	-21	2	16	E	117	120	9	3	7	110	114	15	6	7	30	20	10	D	7	31	10
13	10	R	138	-140	4	16	E	103	104	10	3	7	48	38	1	7	7	184	-185	13	D	7	31	-18
14	10	R	79	71	5	16	E	53	-54	11	3	7	145	-143	2	7	7	110	-101	1	E	7	108	107
1	11	R	111	111	6	16	E	101	-98	12	3	7	47	24	3	7	7	174	176	2	E	7	149	150
2	11	R	79	77	8	16	E	40	40	13	3	7	36	-43	4	7	7	83	83	3	E	7	100	-97
3	11	R	101	-102	2	17	E	46	-41	14	3	7	94	-101	5	7	7	116	117	4	E	7	110	-112
4	11	R	87	-82	3	17	E	28	-26	15	3	7	105	100	6	7	7	48	49	5	E	7	71	-70
5	11	R	120	-119	4	17	E	40	46	0	4	7	122	-123	7	7	7	136	-141	6	E	7	61	54
7	11	R	144	140	5	17	E	74	67	1	4	7	114	-119	8	7	7	67	70	7	E	7	89	84
8	11	R	46	-50	1	18	E	67	65	2	4	7	144	154	9	7	7	78	-74	8	E	7	54	-44
10	11	R	88	88	1	1	7	148	-144	3	4	7	21	-33	10	7	7	175	-178	9	E	7	42	36
11	11	R	89	-87	2	1	7	238	242	4	4	7	254	-247	11	7	7	139	136	10	E	7	137	140
12	11	R	68	-64	4	1	7	102	-100	5	4	7	308	303	12	7	7	48	46	11	E	7	78	-87
0	12	R	96	88	6	1	7	124	128	8	4	7	85	88	13	7	7	35	38	12	E	7	93	-103

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR OCCO

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
0	12	7	KO	-67	2	0	A	409	-406	12	3	A	218	212	2	7	A	81	91	10	10	A	36	-53
1	12	7	132	-127	3	0	A	291	258	14	3	A	120	-124	3	7	A	76	-75	12	10	A	49	-52
2	12	7	192	130	2	0	A	297	295	15	3	A	43	46	4	7	A	125	-127	1	11	A	57	-52
3	12	7	116	-112	5	0	A	48	-48	0	4	A	368	378	5	7	A	26	32	2	11	A	134	-127
4	12	7	216	-214	6	0	A	53	53	1	4	A	200	-204	6	7	A	113	114	3	11	A	75	82
5	12	7	116	122	7	0	A	121	-116	2	4	A	187	-180	7	7	A	28	-27	4	11	A	58	58
6	12	7	107	99	8	0	A	107	-102	3	4	A	19	6	8	7	A	156	-159	5	11	A	26	32
7	12	7	52	55	9	0	A	96	109	4	4	A	42	-44	9	7	A	89	76	6	11	A	44	50
8	12	7	78	69	12	0	A	141	163	5	4	A	65	60	10	7	A	16	178	7	11	A	46	-32
9	12	7	197	-193	13	0	A	101	-115	6	4	A	55	-57	11	7	A	7	-61	8	11	A	37	32
11	12	7	29	-44	14	0	A	119	-121	7	4	A	45	38	12	7	A	123	-124	9	11	A	42	-44
1	13	7	79	-79	1	1	A	107	107	8	4	A	170	170	13	7	A	94	88	10	11	A	124	-125
2	13	7	101	-102	2	1	A	157	159	9	4	A	89	-101	0	8	A	139	-144	11	11	A	74	76
3	13	7	84	88	3	1	A	78	-79	10	4	A	44	-48	1	8	A	78	78	0	12	A	54	-57
4	13	7	82	78	4	1	A	58	60	11	4	A	77	-85	2	8	A	63	61	1	12	A	40	44
5	13	7	72	69	5	1	A	113	-120	12	4	A	134	-132	4	8	A	55	53	2	12	A	57	58
7	13	7	114	-108	6	1	A	226	-225	13	4	A	100	101	5	8	A	34	-37	3	12	A	42	-34
8	13	7	28	4	7	1	A	140	142	14	4	A	104	98	6	8	A	71	-72	4	12	A	39	-39
9	13	7	32	-27	8	1	A	138	141	1	5	A	109	-106	8	8	A	80	82	5	12	A	32	-17
10	13	7	88	-80	11	1	A	52	-42	2	5	A	223	-231	10	8	A	32	16	7	12	A	44	44
0	14	7	182	-184	12	1	A	42	46	3	5	A	124	127	11	8	A	27	20	9	13	A	106	-108
1	14	7	45	42	13	1	A	58	-60	4	5	A	32	28	12	8	A	67	61	0	13	A	53	53
2	14	7	88	88	14	1	A	120	-115	5	5	A	79	77	13	8	A	58	-64	4	13	A	42	40
3	14	7	40	37	15	1	A	63	73	6	5	A	147	141	1	9	A	80	80	6	13	A	28	-12
4	14	7	41	-44	0	2	A	36	28	7	5	A	84	-88	2	9	A	148	138	8	13	A	44	-41
5	14	7	46	44	1	2	A	22	6	8	5	A	33	-35	3	9	A	121	-120	9	13	A	28	-3
8	14	7	36	-38	2	2	A	67	62	9	5	A	67	-61	4	9	A	84	89	7	14	A	37	33
0	15	7	50	44	3	2	A	57	-52	10	5	A	150	-148	5	9	A	28	-23	9	13	A	74	-58
1	15	7	94	-90	4	2	A	120	-124	11	5	A	108	98	6	9	A	54	-46	3	14	A	24	28
2	15	7	76	-69	5	2	A	58	47	12	5	A	51	44	7	9	A	41	42	4	14	A	29	-25
4	15	7	68	74	6	2	A	50	46	13	5	A	24	22	8	9	A	60	-59	5	14	A	72	73
5	15	7	28	32	7	2	A	95	-93	14	5	A	72	66	9	9	A	74	74	6	14	A	144	133
6	15	7	67	-78	10	2	A	37	37	0	6	A	78	84	10	9	A	156	163	8	14	A	84	-86
7	15	7	40	-32	11	2	A	38	40	2	6	A	140	-148	11	9	A	104	-112	9	14	A	61	-68
8	15	7	66	104	2	3	A	30	-11	3	6	A	158	160	12	9	A	96	92	7	14	A	29	-34
0	16	7	96	-90	4	3	A	139	139	4	6	A	282	292	0	10	A	38	36	8	14	A	51	51
1	16	7	80	77	5	3	A	108	-109	5	6	A	164	-162	2	10	A	137	132	2	15	A	108	113
2	16	7	61	-69	6	3	A	282	-298	6	6	A	118	-117	3	10	A	183	-180	3	15	A	54	-57
3	16	7	45	45	7	3	A	124	127	8	6	A	88	-87	4	10	A	284	-284	4	15	A	29	16
4	16	7	100	104	8	3	A	214	208	9	6	A	61	60	5	10	A	144	141	5	15	A	43	-42
5	16	7	66	-71	9	3	A	82	-74	10	6	A	49	41	8	10	A	102	98	6	15	A	142	144
6	16	7	28	-29	10	3	A	92	-96	13	6	A	41	-30	9	10	A	93	94	3	16	A	44	-47
1	17	7	76	77	11	3	A	29	29	1	7	A	44	48	0	11	A	78	-84	2	16	A	84	-72
2	17	7	60	63																				

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 8EX2

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
3	0	0	60	51	9	1	0	74	73	12	7	0	20	-22	-12	4	0	12	-13	0	5	0	64	61
4	0	0	288	-289	10	1	0	46	-85	13	7	0	30	28	-11	4	0	13	14	1	5	0	124	121
5	0	0	91	41	11	1	0	55	-65	14	7	0	7	-7	-10	4	0	97	-100	2	5	0	118	-120
6	0	0	149	144	12	1	0	89	84	15	7	0	48	44	-9	4	0	11	-14	3	5	0	43	-41
7	0	0	81	-86	14	1	0	28	25	-15	8	0	49	44	-8	4	0	88	97	5	5	0	30	-30
8	0	0	20	21	15	1	0	19	18	-14	9	0	45	45	-7	4	0	15	16	6	5	0	114	115
9	0	0	86	-87	-15	2	0	25	25	-13	9	0	32	-30	-6	4	0	53	50	7	5	0	32	33
10	0	0	117	-111	-14	2	0	53	51	-12	9	0	8	10	-5	4	0	86	-84	8	5	0	85	-86
11	0	0	47	40	-13	2	0	36	-34	-11	9	0	41	-41	-4	4	0	721	-717	9	5	0	8	-8
12	0	0	98	97	-12	2	0	22	-23	-10	9	0	38	-37	-3	4	0	37	37	10	5	0	42	-38
13	0	0	8	8	-10	2	0	20	-19	-9	9	0	146	146	-2	4	0	69	60	11	5	0	9	6
15	0	0	67	-62	-11	2	0	43	-43	-8	9	0	31	-8	-1	4	0	32	33	12	5	0	57	57
-15	1	0	62	62	-10	2	0	228	233	-7	9	0	37	-36	0	4	0	137	135	-14	6	0	58	-56
-14	1	0	37	-38	-9	2	0	51	50	-6	9	0	11	14	1	4	0	136	-134	-13	6	0	11	9
-13	1	0	48	-47	-8	2	0	26	-24	-5	9	0	160	-159	2	4	0	46	-45	-12	6	0	27	29
-12	1	0	6	8	-7	2	0	27	21	-3	9	0	140	144	3	4	0	51	53	-11	6	0	7	8
-11	1	0	26	-27	-6	2	0	128	-129	-2	9	0	63	60	4	4	0	29	-28	-10	6	0	58	60
-10	1	0	62	62	-5	2	0	25	21	-1	9	0	22	20	5	4	0	93	93	-9	6	0	20	-20
-10	1	0	46	48	-4	2	0	209	204	0	9	0	103	-105	6	4	0	62	62	-8	6	0	103	-104
-9	1	0	87	-83	-3	2	0	8	9	1	9	0	202	-208	7	4	0	100	-104	-7	6	0	14	13
-8	1	0	47	-46	-2	2	0	10	-13	2	9	0	84	84	8	4	0	58	-60	-6	6	0	81	81
-7	1	0	84	-81	-1	2	0	90	-87	3	9	0	25	24	11	4	0	45	41	-4	6	0	132	132
-6	1	0	88	-88	0	2	0	283	-284	4	9	0	59	53	13	4	0	94	-93	-3	6	0	81	-80
-5	1	0	232	244	1	2	0	49	39	5	9	0	59	58	14	4	0	27	-23	-2	6	0	65	-64
-4	1	0	110	112	2	2	0	41	39	6	9	0	113	-116	15	4	0	51	51	-1	6	0	10	-1
-3	1	0	122	-124	3	2	0	61	-61	7	9	0	44	-42	-11	5	0	25	27	0	6	0	43	-43
-2	1	0	15	-16	4	2	0	67	68	8	9	0	34	35	-10	5	0	122	-124	1	6	0	123	116
-1	1	0	28	-26	6	2	0	92	-95	9	9	0	10	-11	-9	5	0	42	43	2	6	0	79	79
0	1	0	24	22	8	2	0	146	-147	10	9	0	76	74	-8	5	0	23	25	3	6	0	84	-81
1	1	0	15	-17	9	2	0	208	207	11	9	0	29	30	-6	5	0	121	119	4	6	0	7	4
2	1	0	177	-183	0	2	0	10	21	12	9	0	77	-74	-4	5	0	83	-74	6	6	0	45	-42
3	1	0	80	80	2	2	0	37	35	-15	6	0	33	-33	-3	5	0	157	-156	8	6	0	17	-16
4	1	0	57	60	10	2	0	60	59	-14	6	0	84	83	-2	5	0	51	48	7	7	0	56	60
5	1	0	27	-28	11	2	0	104	-101	-13	6	0	7	9	-1	5	0	7	5	9	6	0	13	-13

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REV2

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
10	8	0	8	-4	5	5	0	74	71	7	-6	1	30	41	5	-7	1	43	-42	-10	-5	1	41	-40
11	8	0	49	-48	6	5	0	8	8	8	-6	1	61	60	7	-7	1	69	-67	-9	-5	1	67	-65
-11	9	0	49	-48	7	5	0	61	-63	9	-6	1	31	-30	8	-7	1	51	-50	-7	-5	1	13	12
-12	9	0	5	-9	8	5	0	14	14	-7	-6	1	78	-80	9	-7	1	80	77	-6	-5	1	107	104
-10	7	0	15	15	-8	6	0	29	-30	-6	-6	1	11	-6	10	-7	1	94	94	-5	-5	1	16	-16
-9	7	0	41	44	-7	6	0	43	42	-5	-6	1	8	9	11	-7	1	8	9	-4	-5	1	9	6
-8	7	0	37	-38	-7	6	0	42	40	-3	-6	1	79	80	12	-7	1	69	-68	-3	-5	1	37	-38
-7	7	0	84	-88	-8	6	0	95	-95	-2	-6	1	8	-6	-11	-8	1	48	-45	-2	-5	1	118	-115
-5	7	0	7	-7	-5	6	0	5	5	-1	-6	1	58	-54	-10	-8	1	7	8	-1	-5	1	80	89
-5	7	0	42	-42	-4	6	0	42	-46	0	-6	1	9	-9	-9	-8	1	14	-15	0	-5	1	-8	8
-4	7	0	76	77	-3	6	0	91	-93	1	-6	1	32	-26	-7	-8	1	43	42	1	-5	1	9	-9
-3	7	0	87	84	-2	6	0	98	95	2	-6	1	24	20	-6	-8	1	7	2	2	-5	1	36	37
-2	7	0	60	-60	-1	6	0	17	14	3	-6	1	77	77	-5	-8	1	46	-43	3	-5	1	103	-100
-1	7	0	8	-5	0	6	0	71	-65	4	-6	1	44	-44	-4	-8	1	11	-10	4	-5	1	92	-93
0	7	0	29	-28	1	6	0	9	0	5	-6	1	21	-23	-3	-8	1	44	-44	5	-5	1	106	104
1	7	0	42	-42	2	6	0	43	41	6	-6	1	14	-13	-2	-8	1	51	50	6	-5	1	27	24
2	7	0	90	87	-4	10	0	11	7	7	-6	1	40	-47	-1	-8	1	121	122	7	-5	1	46	45
3	7	0	14	11	-3	10	0	44	-42	8	-6	1	78	80	0	-8	1	32	-35	8	-5	1	14	13
4	7	0	20	-17	-2	10	0	16	-16	9	-6	1	42	44	1	-8	1	12	9	10	-5	1	32	-30
6	7	0	62	-62	-1	10	0	36	34	10	-6	1	23	-23	2	-8	1	47	-44	11	-5	1	28	26
8	7	0	58	58	0	10	0	8	-1	11	-6	1	8	-2	3	-8	1	88	-80	12	-5	1	9	6
-10	8	0	29	-28	1	10	1	41	39	12	-6	1	40	-34	4	-8	1	104	105	13	-5	1	89	85
-9	8	0	31	31	-10	10	1	12	-11	-9	-7	1	8	-7	5	-8	1	42	45	14	-5	1	27	-27
-8	8	0	70	71	-9	10	1	56	-53	-8	-7	1	59	58	6	-8	1	6	0	15	-5	1	52	-48
-7	8	0	42	-40	-8	10	1	7	8	-6	-7	1	83	-83	7	-8	1	30	34	-13	-4	1	32	-29
-6	8	0	20	-20	-7	10	1	7	9	-5	-7	1	8	-2	8	-8	1	119	-117	-11	-4	1	42	39
-5	8	0	20	-20	-6	-5	1	41	41	-4	-7	1	20	-21	9	-8	1	36	-35	-8	-4	1	14	-13
-4	8	0	44	-44	-7	-5	1	77	-77	-3	-7	1	30	34	10	-8	1	66	62	-7	-4	1	124	-122
-3	8	0	76	74	1	-5	1	8	7	-2	-7	1	102	99	11	-8	1	6	8	-6	-4	1	85	87
-2	8	0	93	94	2	-5	1	83	84	-1	-7	1	24	-25	12	-8	1	92	94	-5	-4	1	87	85
-1	8	0	27	-26	3	-5	1	25	-25	0	-7	1	1	-26	13	-8	1	7	-7	-4	-4	1	15	-15
0	8	0	8	20	4	-5	1	30	-32	2	-7	1	1	-24	14	-8	1	44	45	-3	-4	1	40	38
1	8	0	57	-61	5	-5	1	7	13	3	-7	1	1	24	-12	-8	1	88	85	-2	-4	1	46	-46
2	8	0	21	-23	6	-5	1	29	-28	4	-7	1	1	42	-11	-8	1	8	12	-1	-4	1	108	-108

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEX2

H	K	L	FO	FC
0	-4	1	91	92
1	-4	1	30	31
2	-4	1	50	50
3	-4	1	40	42
4	-4	1	184	-184
5	-4	1	47	-47
6	-4	1	48	48
7	-4	1	31	30
8	-4	1	138	137
9	-4	1	15	-15
10	-4	1	102	-100
11	-4	1	8	10
12	-4	1	11	12
13	-4	1	91	96
14	-4	1	27	-25
15	-4	1	11	-8
-16	-3	1	77	-75
-15	-3	1	21	22
-14	-3	1	74	77
-13	-3	1	20	-17
-12	-3	1	61	59
-11	-3	1	56	-57
-10	-3	1	140	-148
-9	-3	1	93	99
-8	-3	1	44	43
-7	-3	1	20	19
-6	-3	1	31	31
-5	-3	1	237	-236
-4	-3	1	89	-93
-3	-3	1	68	70
-2	-3	1	20	-27
-1	-3	1	110	114
0	-3	1	34	39
1	-3	1	171	-168
2	-3	1	91	92
3	-3	1	31	31
4	-3	1	50	50
5	-3	1	40	42
6	-3	1	169	169
7	-3	1	15	-15
8	-3	1	137	137
9	-3	1	15	-15
10	-3	1	19	-22
11	-3	1	64	-61
12	-3	1	98	-98
13	-3	1	41	41
14	-3	1	98	-98
15	-3	1	67	69
16	-3	1	28	-26
-13	-2	1	27	26
-12	-2	1	16	-15
-11	-2	1	104	-107
-10	-2	1	49	49
-9	-2	1	41	41
-8	-2	1	14	13
-7	-2	1	117	115
-6	-2	1	139	-136
-5	-2	1	123	-122
-4	-2	1	107	106
-3	-2	1	57	-54
-2	-2	1	88	86
-1	-2	1	148	144
0	-2	1	144	-107
1	-2	1	16	4
2	-2	1	27	-27
3	-2	1	31	-34
4	-2	1	244	244
5	-2	1	22	-23
6	-2	1	220	-225
7	-2	1	104	-103
8	-2	1	72	68
9	-2	1	144	143
10	-2	1	41	-39
11	-2	1	41	-37
12	-2	1	44	-35
13	-2	1	33	-31
14	-2	1	24	24
15	-2	1	169	169
16	-2	1	19	-22
-11	-1	1	84	-81
-10	-1	1	98	-88
-9	-1	1	41	41
-8	-1	1	67	69
-7	-1	1	28	-26
-6	-1	1	27	26
-5	-1	1	14	-15
-4	-1	1	104	-107
-3	-1	1	49	49
-2	-1	1	104	-107
-1	-1	1	47	46
0	-1	1	14	-17
1	-1	1	60	60
2	-1	1	121	120
3	-1	1	164	-164
4	-1	1	73	-73
5	-1	1	44	47
6	-1	1	44	43
7	-1	1	228	224
8	-1	1	115	117
9	-1	1	19	20
10	-1	1	49	-52
11	-1	1	410	418
12	-1	1	49	-50
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REV2

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0	2	1	160	-171	2	3	1	131	-131	-14	4	1	28	-26	1	5	1	124	116	-2	5	1	77	78
1	2	1	67	69	1	3	1	71	-76	-13	5	1	50	49	2	5	1	94	92	-1	5	1	47	45
2	2	1	206	199	0	3	1	36	34	-11	5	1	20	20	3	5	1	76	-79	0	5	1	34	-31
3	2	1	134	128	0	3	1	73	-74	-10	5	1	12	15	4	5	1	12	11	1	5	1	9	0
4	2	1	66	64	10	3	1	84	82	-9	5	1	113	-110	5	5	1	30	-26	2	5	1	64	-60
5	2	1	114	-113	11	3	1	49	38	-7	5	1	42	42	6	5	1	31	-32	3	5	1	32	-27
6	2	1	164	-168	12	3	1	73	-69	-6	5	1	8	8	7	5	1	41	48	4	5	1	74	69
7	2	1	78	76	-13	4	1	35	-32	-5	5	1	106	106	8	5	1	16	-19	5	5	1	8	8
8	2	1	6	6	-12	4	1	59	56	-4	5	1	54	-56	11	5	1	46	-53	8	5	1	9	8
9	2	1	35	42	-11	4	1	23	23	-3	5	1	105	-104	-10	7	1	8	6	-4	6	1	38	37
10	2	1	44	47	-10	4	1	7	-7	-2	5	1	92	92	-9	7	1	80	78	-3	6	1	45	43
11	2	1	103	-100	-9	4	1	17	18	-1	5	1	140	134	-8	7	1	23	-25	-2	6	1	20	-20
12	2	1	24	-22	-8	4	1	100	-98	0	5	1	120	-120	-7	7	1	84	-84	-1	6	1	45	47
13	2	1	22	18	-7	4	1	28	-25	1	5	1	43	-47	-6	7	1	44	-44	0	6	1	44	-43
14	2	1	48	48	-6	4	1	84	83	2	5	1	34	-35	-4	7	1	68	68	-2	6	1	61	61
-15	3	1	48	49	-5	4	1	7	-7	3	5	1	117	108	-3	7	1	95	88	-1	6	1	22	21
-14	3	1	46	47	-4	4	1	73	72	4	5	1	44	45	-2	7	1	63	-61	0	6	1	13	7
-13	3	1	28	-27	-3	4	1	8	0	5	5	1	72	-67	-1	7	1	21	-20	2	6	1	74	-69
-12	3	1	44	-42	-2	4	1	172	-168	6	5	1	7	6	0	7	1	31	-31	4	6	1	39	36
-10	3	1	47	46	-1	4	1	26	25	10	5	1	41	-39	1	7	1	55	-50	-4	10	1	8	9
-9	3	1	131	130	-2	4	1	65	67	12	5	1	50	48	2	7	1	102	94	-3	10	1	49	-51
-8	3	1	8	-4	-1	4	1	34	34	-13	6	1	18	-17	3	7	1	28	25	-2	10	1	20	-21
-7	3	1	16	-17	0	4	1	140	147	-12	6	1	26	24	4	7	1	26	-24	-1	10	1	33	33
-6	3	1	34	34	1	4	1	134	-132	-10	6	1	50	47	5	7	1	12	9	0	10	1	9	5
-5	3	1	140	-137	2	4	1	179	-174	-9	6	1	10	-9	6	7	1	42	-45	1-10		2	42	41
-3	3	1	111	110	3	4	1	15	14	-8	6	1	96	-94	7	7	1	9	-8	3-10		2	51	-50
-2	3	1	48	47	4	4	1	96	-94	-7	6	1	31	31	8	7	1	50	50	-4	-9	2	36	34
-1	3	1	72	72	5	4	1	59	57	-6	6	1	11	-11	-10	8	1	20	-19	-3	-9	2	13	14
0	3	1	119	-118	6	4	1	74	76	-5	6	1	34	34	-9	8	1	22	23	-2	-9	2	89	-87
1	3	1	265	-268	7	4	1	105	-103	-4	6	1	129	126	-8	8	1	66	70	-1	-9	2	8	-2
2	3	1	66	66	8	4	1	97	-99	-3	6	1	82	-83	-7	8	1	90	-90	2	-9	2	61	60

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR BPY2

H	K	L	FO	FC
3	-8	2	17	-15
4	-8	2	46	-46
5	-8	2	30	-30
7	-8	2	28	24
8	-8	2	40	44
9	-8	2	26	-27
10	-8	2	7	-10
-7	-8	2	41	-44
-5	-8	2	10	-11
-4	-8	2	0	0
-3	-8	2	9	-10
-2	-8	2	70	69
1	-8	2	31	-33
2	-8	2	27	25
3	-8	2	26	25
4	-8	2	29	-32
5	-8	2	23	-20
6	-8	2	8	-8
7	-8	2	51	48
8	-8	2	57	51
9	-8	2	43	41
12	-8	2	40	-37
-8	-7	2	44	40
-7	-7	2	9	10
-6	-7	2	56	-54
-4	-7	2	24	-23
-3	-7	2	12	8
-2	-7	2	93	81
-1	-7	2	18	-17
0	-7	2	40	-40
1	-7	2	23	-23
2	-7	2	71	-74
3	-7	2	56	54
4	-7	2	85	87
5	-7	2	14	-12
6	-7	2	16	16
7	-7	2	47	-46
8	-7	2	77	77
9	-7	2	28	28
10	-7	2	22	-18
11	-7	2	6	6
13	-7	2	56	-54
-8	-6	2	91	-94
-7	-6	2	8	-12
-6	-6	2	7	-5
-5	-6	2	74	-74
-3	-6	2	24	-24
-2	-6	2	122	121
-1	-6	2	22	-23
0	-6	2	6	7
1	-6	2	15	-14
2	-6	2	59	-60
3	-6	2	46	46
4	-6	2	25	-23
5	-6	2	109	106
-3	-5	2	10	-22
-2	-5	2	147	-147
-1	-5	2	100	98
0	-5	2	86	86
2	-5	2	67	69
3	-5	2	104	-103
4	-5	2	72	-70
5	-5	2	88	88
6	-5	2	13	13
7	-5	2	44	47
8	-5	2	10	15
9	-5	2	125	-130
10	-5	2	16	-20
11	-5	2	16	16
12	-5	2	7	11
13	-5	2	64	64
14	-5	2	14	-15
15	-5	2	53	-52
-11	-4	2	76	73
-7	-4	2	238	-238
-6	-4	2	52	52
-5	-4	2	93	96
-4	-4	2	29	-27
-3	-4	2	177	-177
-2	-4	2	97	-97
-1	-4	2	177	-177
0	-4	2	103	104
1	-4	2	23	24
2	-4	2	97	97
3	-4	2	174	-178
4	-4	2	46	-46
5	-4	2	47	48
6	-4	2	16	-13
7	-4	2	109	112
8	-4	2	8	10
10	-4	2	101	-98
11	-4	2	17	-16
12	-4	2	19	17
13	-4	2	77	77
14	-4	2	28	-25
15	-4	2	28	-26
-13	-3	2	14	13
-12	-3	2	82	-81
-11	-3	2	7	8
-10	-3	2	74	75
-9	-3	2	18	-17
-8	-3	2	54	53
-7	-3	2	77	-78
-6	-3	2	141	-140
-5	-3	2	54	52
-4	-3	2	93	96
-3	-3	2	11	14
-2	-3	2	139	139
-1	-3	2	204	-208
0	-3	2	115	-114
1	-3	2	97	96
2	-3	2	85	-85
3	-3	2	73	73
4	-3	2	80	81
5	-3	2	158	-160
6	-3	2	7	-8
7	-3	2	19	-17
8	-3	2	13	-15
9	-3	2	179	178
10	-3	2	18	-20
11	-3	2	81	-78
12	-3	2	14	12
13	-3	2	46	-44
14	-3	2	43	41
15	-3	2	73	70
16	-3	2	31	-31
-11	-2	2	32	31
-10	-2	2	28	30
-9	-2	2	43	43
-7	-2	2	96	94
-6	-2	2	94	-95
-5	-2	2	127	-124
-4	-2	2	72	73
-3	-2	2	24	-27
-2	-2	2	79	77
-1	-2	2	144	143
0	-2	2	210	-210
1	-2	2	25	21
2	-2	2	63	-60
4	-2	2	177	183
5	-2	2	23	-28
6	-2	2	161	-161
7	-2	2	7	7
8	-2	2	40	-41
9	-2	2	12	14
10	-2	2	186	187
11	-2	2	31	-32
12	-2	2	47	-47
14	-2	2	59	-57
15	-2	2	51	49
16	-2	2	43	40
17	-2	2	24	23
-12	-1	2	46	44

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REV3

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
-11	-1	2	37	-36	-7	0	3	44	-44	-2	1	2	35	34	2	2	2	65	66	10	2	2	72	70
-10	-1	2	104	-100	-6	0	3	140	138	-1	1	2	134	-129	3	2	2	7	6	11	3	2	44	42
-9	-1	2	25	25	-5	0	3	137	135	0	1	2	51	-49	4	2	2	47	44	12	3	2	71	-68
-8	-1	2	8	8	-4	0	3	58	-62	1	1	2	234	224	5	2	2	131	-124	-14	4	2	50	47
-7	-1	2	44	46	-3	0	3	113	-112	2	1	2	38	-34	6	2	2	178	-173	-13	4	2	23	23
-6	-1	2	130	119	-2	0	3	56	-48	3	1	2	42	40	7	2	2	74	74	-12	4	2	7	-7
-5	-1	2	121	-121	-1	0	3	21	-19	4	1	2	31	-31	8	2	2	36	38	-11	4	2	25	24
-4	-1	2	70	-68	0	0	3	300	307	5	1	2	157	-160	9	2	2	47	46	-10	4	2	89	-85
-3	-1	2	44	42	1	0	3	98	94	6	1	2	70	67	10	2	2	40	39	-9	4	2	35	-34
-2	-1	2	32	-32	2	0	3	42	-35	7	1	2	87	84	11	2	2	86	-87	-8	4	2	103	100
-1	-1	2	214	212	3	0	3	44	47	8	1	2	33	35	12	2	2	29	28	-7	4	2	6	-8
0	-1	2	52	52	4	0	3	204	-200	9	1	2	48	50	13	2	2	32	31	-6	4	2	60	60
1	-1	2	139	-136	5	0	3	61	61	10	1	2	97	-96	14	2	2	7	-13	-5	4	2	8	-7
2	-1	2	37	-38	6	0	3	178	176	11	1	2	76	-76	15	2	2	48	46	-4	4	2	176	-174
3	-1	2	110	-110	7	0	3	27	-27	12	1	2	47	48	-14	3	2	48	46	-3	4	2	10	9
4	-1	2	33	33	8	0	3	27	27	13	1	2	26	30	-13	3	2	92	-93	-2	4	2	34	35
5	-1	2	261	272	9	0	3	78	-77	14	1	2	27	28	-11	3	2	44	-40	0	4	2	133	133
6	-1	2	94	-92	10	0	3	126	-128	15	1	2	37	-35	-9	3	2	111	108	1	4	2	57	-56
7	-1	2	72	-75	11	0	3	68	68	-14	2	2	27	-25	-8	3	2	15	14	2	4	2	127	-126
8	-1	2	35	-34	12	0	3	33	32	-13	2	2	107	-98	-7	3	2	28	26	3	4	2	70	68
9	-1	2	118	-122	13	0	3	8	-9	-12	2	2	15	-14	-6	3	2	176	-172	4	4	2	117	117
10	-1	2	83	71	14	0	3	26	27	-11	2	2	87	-85	-5	3	2	107	105	5	4	2	110	108
11	-1	2	61	51	15	0	3	34	-33	-10	2	2	97	93	-4	3	2	13	-13	7	4	2	110	-110
12	-1	2	11	-14	-14	1	3	65	-62	-9	2	2	74	72	-3	3	2	67	62	8	4	2	33	-32
13	-1	2	19	12	-13	1	3	25	-26	-8	2	2	60	-60	0	3	2	69	-69	9	4	2	8	-7
14	-1	2	33	-28	-11	1	3	64	61	-7	2	2	12	11	1	3	2	226	-224	10	4	2	30	-28
15	-1	2	55	-55	-10	1	3	158	156	-6	2	2	86	-85	2	3	2	51	51	11	4	2	81	78
16	-1	2	49	49	-9	1	3	79	-82	-5	2	2	52	-51	3	3	2	30	34	12	4	2	15	13
-14	0	2	9	9	-8	1	3	94	-94	-4	2	2	149	151	4	3	2	37	37	13	4	2	58	-58
-13	0	2	8	-1	-7	1	3	58	-63	-3	2	2	40	-37	5	3	2	117	115	-15	5	2	44	43
-12	0	2	15	17	-6	1	3	64	-62	-2	2	2	31	-28	6	3	2	118	-115	-11	5	2	26	24
-11	0	2	77	76	-5	1	3	172	175	-1	2	2	97	95	7	3	2	102	-99	-10	5	2	23	20
-10	0	2	72	-71	-4	1	3	74	76	0	2	2	244	-240	8	3	2	35	34	-9	5	2	124	-122
-9	0	2	68	-68	-3	1	3	4	-85	1	2	2	8	-1	9	3	2	13	-11	-8	5	2	14	-14

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR RSX2

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
-7	E	2	45	44	4	E	2	14	-13	-7	E	2	44	40	1	-6	1	38	-31	-2	-E	3	38	37
-E	E	2	6	7	E	E	2	E0	-E0	-1	E	2	36	-33	2	-E	3	18	19	-1	-E	3	104	105
-5	E	2	4E	4E	E	E	2	E0	-E0	0	E	2	0	3	3	-6	1	40	37	0	-E	3	13	-4
-4	E	2	36	-33	7	E	2	7A	77	1	E	2	64	-64	4	-6	3	23	-21	1	-E	3	16	15
-3	E	2	11E	-11E	E	E	2	14	-15	2	E	2	42	-41	5	-6	3	29	-26	2	-E	3	37	-36
-2	E	2	23	22	10	E	2	1E	E	3	E	2	70	7E	6	-6	3	20	-18	3	-E	3	112	-115
-1	E	2	3E	-31	11	E	2	E0	-47	4	E	2	17	15	7	-6	3	53	-50	4	-E	3	55	51
0	E	2	4E	4A	-10	7	2	5	4	5	E	2	11	13	8	-6	3	47	44	5	-E	3	57	55
1	E	2	15E	160	-9	7	2	73	71	7	E	2	4E	-47	9	-6	3	45	45	7	-E	3	42	42
2	E	2	114	-112	-8	7	2	14	-13	8	E	2	5	E	10	-6	3	17	-15	8	-E	3	-	-E2
3	E	2	72	-E0	-7	7	2	E6	-A5	-7	E	3	6E	65	12	-6	3	33	-31	9	-E	3	-	-36
4	E	2	1E	-17	-E	7	2	E	0	-E	E	3	1A	-1E	-A	-7	3	4A	47	10	-E	3	41	32
E	E	2	3E	-3E	-5	7	2	A5	-A2	-E	E	3	12	E	-7	-7	3	1A	1A	11	-E	3	E	2
E	E	2	15E	112	-4	7	2	A7	A5	-A	E	3	42	-39	-E	-7	3	E3	-A3	12	-E	3	3A	32
7	E	2	AA	A5	-3	7	2	AA	AA	-3	E	3	47	-AE	-A	-7	3	2E	-24	13	-E	3	E	A
E	E	2	AE	-A7	-2	7	2	44	-42	-2	E	3	EE	E5	-2	-7	3	4E	4E	14	-E	3	AE	-AE
9	E	2	E	2	-1	7	2	1A	-15	-1	E	3	2E	2A	-1	-7	3	7	5	-10	-5	3	33	-33
10	E	2	1E	-1E	0	7	2	5E	-52	0	E	3	A	E	-E	-7	3	3E	-32	-9	-5	3	E	9
11	E	2	1E	-1E	1	7	2	EE	-E7	2	E	3	71	-67	1	-7	3	72	-1A	-E	-5	3	EA	-EE
12	E	2	E0	E0	2	7	2	101	AE	3	E	3	E	-1A	2	-7	3	EE	-E3	-6	-5	3	97	9E
-11	E	3	1E	-1A	3	7	2	A1	9E	4	E	3	9A	9E	3	-7	3	5E	53	-5	-5	3	1A	-1E
-12	E	3	23	21	4	7	2	2E	-27	-3	-E	3	1E	1E	4	-7	3	AE	AE	-4	-5	3	E	E
-1E	E	3	E1	E3	E	7	2	E	1A	-2	-E	3	E1	-E1	E	-7	3	2E	-2A	-3	-5	3	1A	-A
-A	E	3	4E	-4E	E	7	2	E	-E1	-1	-E	3	E2	E0	7	-7	3	4E	-E0	-2	-5	3	1E7	-147
-E	E	3	7	-10	A	7	2	E1	E7	0	-E	3	1E	E0	8	-7	3	5A	-AE	-1	-5	3	7E	7E
-5	E	3	23	20	10	7	2	0	12	1	-E	3	3E	-3E	9	-7	3	E6	E5	0	-5	3	79	77
-A	E	3	1A	1A1	-10	8	2	24	-2E	2	-E	3	27	-24	11	-7	3	1E	1E	1	-5	3	24	-2E
-3	E	3	43	-AA	-9	A	2	1E	1E	3	-E	3	3E	3A	12	-7	3	E	5	2	-5	3	5E	E7
-2	E	3	E0	-E0	-5	E	2	E3	E0	4	-E	3	51	E2	13	-7	3	13	10	3	-5	3	104	-105
-1	E	3	7	0	-7	E	2	32	-32	E	-E	3	21	-21	14	-7	3	37	-E	4	-5	3	11E	-11A
0	E	3	41	-AA	-E	E	2	11	-10	-E	-A	3	1E	-1E	-A	-E	3	2A	-21	5	-5	3	33	32
1	E	3	1A0	9E	-5	E	2	15	-14	-A	-A	3	9	-11	-A	-E	3	12	-1E	6	-5	3	1E	1A
2	E	3	100	97	-4	E	2	EE	-E3	-3	-E	3	E	E5	-5	-E	3	3E	-2A	7	-5	3	3E	3A
3	E	3	7E	-77	-3	E	2	E4	E2	-1	-E	3	5E	-E4	-3	-E	3	71	-E4	A	-E	3	57	60

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR SFX2

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
0	-6	3	104	-106	-5	-3	3	61	58	0	-2	3	164	-165	6	-1	3	13	-12	10	0	3	116	-119
10	-6	3	17	-8	-4	-3	3	68	67	1	-2	3	70	-74	7	-1	3	52	-53	11	0	3	61	60
11	-6	3	33	31	-3	-3	3	25	29	2	-2	3	22	-21	8	-1	3	0	0	12	0	3	37	34
13	-6	3	53	53	-2	-3	3	115	115	3	-2	3	20	-22	9	-1	3	141	-140	13	0	3	12	10
14	-6	3	58	-54	-1	-3	3	148	-146	4	-2	3	134	132	10	-1	3	48	48	14	0	3	27	27
-11	-5	3	77	76	0	-3	3	125	-125	5	-2	3	93	91	11	-1	3	95	93	15	0	3	58	-56
-10	-5	3	12	15	1	-3	3	54	50	6	-2	3	108	-111	12	-1	3	15	-16	16	0	3	35	-32
-9	-5	3	16	-15	2	-3	3	26	-30	8	-2	3	70	-78	13	-1	3	21	20	-14	1	3	41	-40
-8	-5	3	159	-161	3	-3	3	101	101	9	-2	3	0	0	14	-1	3	36	-41	-13	1	3	4	-3
-7	-5	3	20	20	4	-3	3	116	117	10	-2	3	154	161	15	-1	3	54	-54	-12	1	3	-34	-32
-6	-5	3	88	86	5	-3	3	152	-154	11	-2	3	26	-24	16	-1	3	43	41	-11	1	3	38	37
-5	-5	3	54	-51	8	-3	3	4	6	12	-2	3	26	-26	-16	0	3	12	9	-10	1	3	88	86
-3	-5	3	66	64	9	-3	3	20	-20	13	-2	3	17	-17	12	0	3	10	10	-9	1	3	71	-69
-2	-5	3	51	-77	0	-4	3	141	141	14	-2	3	65	-65	-11	0	3	92	89	-8	1	3	38	-38
-1	-5	3	174	-168	10	-2	3	7	-12	15	-2	3	47	45	-10	0	3	47	-47	-7	1	3	48	-48
0	-5	3	41	46	11	-2	3	42	-42	16	-2	3	40	41	-9	0	3	71	-69	-6	1	3	81	-82
1	-5	3	32	32	12	-2	3	8	-8	-13	-1	3	7	7	-8	0	3	16	18	-5	1	3	168	166
2	-5	3	37	38	13	-2	3	32	-34	-12	-1	3	60	58	-7	0	3	72	-70	-4	1	3	79	81
3	-5	3	87	84	14	-2	3	19	24	-11	-1	3	17	-20	-6	0	3	117	115	-3	1	3	50	-51
4	-5	3	160	-171	15	-2	3	41	37	-10	-1	3	79	79	-5	0	3	137	139	-2	1	3	25	25
5	-5	3	72	-72	16	-2	3	18	-19	-9	-1	3	34	33	-4	0	3	114	-113	-1	1	3	111	-113
6	-5	3	77	77	-15	-2	3	44	16	-8	-1	3	11	-9	-3	0	3	51	-53	0	1	3	37	-37
7	-5	3	38	-36	-12	-2	3	7	-7	-7	-1	3	47	42	-2	0	3	76	-77	1	1	3	228	220
8	-5	3	82	87	-11	-2	3	83	-88	-6	-1	3	104	104	-1	0	3	26	-28	2	1	3	55	-51
9	-5	3	31	32	-10	-2	3	13	11	-5	-1	3	138	-135	0	0	3	257	262	3	1	3	6	-5
10	-5	3	0	0	-9	-2	3	40	38	-4	-1	3	73	-74	1	0	3	47	46	4	1	3	34	30
11	-5	3	88	86	-8	-2	3	8	8	-3	-1	3	28	-24	2	0	3	24	-24	5	1	3	178	-175
12	-5	3	99	-98	-7	-2	3	88	85	-2	-1	3	60	56	3	0	3	56	49	6	1	3	50	49
14	-5	3	38	-36	-6	-2	3	61	-60	-1	-1	3	200	201	4	0	3	138	-134	7	1	3	85	85
-12	-4	3	81	-81	-5	-2	3	102	-102	0	-1	3	108	108	5	0	3	15	-12	8	1	3	13	13
-10	-4	3	61	60	-4	-2	3	98	96	1	-1	3	89	-82	6	0	3	153	154	9	1	3	54	54
-8	-4	3	44	46	-3	-2	3	5	5	2	-1	3	67	-69	7	0	3	31	-32	10	1	3	90	-93
-7	-4	3	23	-24	-2	-2	3	72	69	3	-1	3	83	-82	8	0	3	27	28	11	1	3	86	-86
-6	-4	3	190	-198	-1	-2	3	118	120	5	-1	3	163	164	9	0	3	46	-44	12	1	3	48	47

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 0KX2

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
13	1	3	10	11	-11	3	3	32	-30	-2	4	1	65	68	6	5	1	62	61	0	7	3	16	-17
14	1	3	27	28	-10	3	3	58	-59	-1	4	1	21	20	7	5	1	62	65	1	7	3	68	-66
15	1	3	28	30	-9	3	3	98	96	0	4	1	107	104	8	5	1	62	-62	2	7	3	28	28
16	1	3	66	-65	-8	3	3	44	41	1	4	1	52	-50	10	5	1	58	-57	3	7	3	42	40
-14	2	3	24	-20	-6	3	3	48	46	2	4	1	117	-117	11	5	1	26	-25	4	7	3	29	-27
-13	2	3	21	-18	-5	3	3	178	-177	3	4	1	13	14	12	5	1	61	60	5	7	3	9	8
-12	2	3	16	-15	-4	3	3	40	-39	4	4	1	45	-42	-12	6	1	20	20	6	7	3	62	-62
-11	2	3	45	-48	-3	3	3	141	138	5	4	1	50	48	-11	6	1	52	51	7	7	3	23	-21
-10	2	3	78	75	-2	3	3	14	-17	6	4	1	100	100	-10	6	1	15	11	8	7	3	64	63
-9	2	3	89	87	-1	3	3	74	75	7	4	1	107	-108	-9	6	1	87	-87	9	7	3	6	6
-8	2	3	49	-47	0	3	3	25	-24	8	4	1	44	-41	-8	6	1	10	20	10	7	3	10	9
-6	2	3	91	-90	1	3	3	302	-303	9	4	1	7	-6	-6	6	1	119	112	-9	8	3	13	8
-5	2	3	49	-51	2	3	3	94	96	10	4	1	27	-27	-5	6	1	49	-45	-8	8	3	60	59
-4	2	3	149	151	3	3	3	13	14	11	4	1	17	17	-2	6	1	81	-80	-7	8	3	16	-11
-3	2	3	6	-2	4	3	3	75	71	12	4	1	25	27	-1	6	1	7	-4	-6	8	3	27	-24
-2	2	3	13	9	5	3	3	129	125	13	4	1	93	-96	0	6	1	57	-54	-5	8	3	13	-6
-1	2	3	19	21	6	3	3	60	-58	14	4	1	8	8	1	6	1	73	73	-4	9	3	46	-47
0	2	3	269	-264	7	3	3	102	-100	-13	5	1	34	36	2	6	1	82	82	-3	9	3	34	30
1	2	3	64	64	8	3	3	38	38	-11	5	1	30	30	3	6	1	48	-46	-2	9	3	51	52
2	2	3	107	103	9	3	3	14	-14	-10	5	1	22	22	4	6	1	4	6	-1	9	3	17	-15
3	2	3	91	90	10	3	3	74	71	-9	5	1	106	-104	5	6	1	27	-27	0	9	3	8	9
4	2	3	75	-75	11	3	3	57	58	-8	5	1	4	-10	6	6	1	31	-33	1	9	3	56	-49
5	2	3	150	-150	12	3	3	72	-72	-7	5	1	56	54	7	6	1	99	91	2	9	3	45	-45
7	2	3	60	60	13	3	3	8	-5	-6	5	1	6	-1	8	6	1	27	27	3	9	3	70	67
8	2	3	28	29	-13	4	3	27	26	-5	5	1	101	100	9	6	1	15	-20	4	9	3	21	20
9	2	3	37	37	-11	4	3	15	20	-4	5	1	22	-22	11	6	1	46	-51	5	9	3	9	7
10	2	3	75	77	-10	4	3	72	-72	-3	5	1	114	-111	-11	7	1	41	41	7	9	3	61	-64
11	2	3	89	-89	-9	4	3	48	44	-2	5	1	22	21	-9	7	1	56	63	-6	0	3	8	-4
12	2	3	47	-47	-8	4	3	79	80	-1	5	1	12	-11	-8	7	1	9	-5	-5	9	3	9	7
13	2	3	15	15	-7	4	3	13	10	0	5	1	39	41	-7	7	1	55	-54	-4	0	3	31	-33
14	2	3	7	-8	-6	4	3	88	85	1	5	1	140	143	-6	7	1	44	-48	-3	0	3	45	-43
15	2	3	46	48	-5	4	3	21	21	2	5	1	78	-74	-5	7	1	36	38	-2	0	3	41	40
-16	3	3	48	46	-4	4	3	164	-160	3	5	1	55	-58	-3	7	1	46	44	-1	0	3	28	25
-13	3	3	10	-10	-3	4	3	7	-3	4	5	1	41	-40	-2	7	1	60	-63	1	0	3	11	8

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR DEV2

H	K	L	FO	FC
2	9	9	50	-57
3	8	9	17	-10
4	0	9	32	29
-0	0	9	47	-47
-1	0	9	31	-30
1	-9	9	8	-8
2	-9	9	83	80
3	-9	9	20	-7
4	-9	9	42	-41
5	-9	9	31	-28
7	-9	9	20	22
8	-9	9	41	40
0	-9	9	14	-15
-4	-8	9	17	-17
-3	-8	9	51	57
-2	-8	9	8	10
-1	-8	9	57	-54
0	-8	9	13	3
1	-8	9	33	-30
2	-8	9	15	10
3	-8	9	76	73
4	-8	9	8	-10
5	-8	9	21	-24
6	-8	9	21	-20
7	-8	9	47	-47
8	-8	9	47	44
9	-8	9	48	46
10	-8	9	13	-13
-7	-7	9	21	20
-6	-7	9	44	-47
-5	-7	9	8	8
-4	-7	9	26	-27
-3	-7	9	12	-10
-2	-7	9	98	98
-1	-7	9	0	-7
0	-7	9	1	-7
1	-7	9	20	-20
2	-7	9	70	-70
3	-7	9	47	48
4	-7	9	76	75
5	-7	9	20	-18
6	-7	9	15	-14
7	-7	9	49	-48
8	-7	9	67	-63
9	-7	9	69	69
10	-7	9	29	30
11	-7	9	20	19
12	-7	9	56	-56
-6	-6	9	24	-25
-5	-6	9	78	75
-4	-6	9	10	11
-3	-6	9	41	-43
-2	-6	9	0	0
-1	-6	9	79	-79
0	-6	9	15	15
1	-6	9	112	117
2	-6	9	22	-23
3	-6	9	14	13
4	-6	9	10	-10
5	-6	9	110	-123
6	-6	9	75	77
7	-6	9	44	44
8	-6	9	84	-86
9	-6	9	56	-58
10	-6	9	53	53
11	-6	9	23	21
-5	-5	9	11	-11
-4	-5	9	44	44
-3	-5	9	84	-86
-2	-5	9	55	-58
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0	-5	9	14	-6
1	-5	9	24	-27
2	-5	9	18	-16
3	-5	9	84	86
4	-5	9	10	-17
5	-5	9	112	-115
6	-5	9	66	67
7	-5	9	85	84
8	-5	9	6	-10
9	-5	9	72	72
10	-5	9	77	-74
11	-5	9	117	-118
-4	-4	9	83	86
-3	-4	9	11	20
-2	-4	9	35	33
-1	-4	9	25	-24
0	-4	9	24	-27
1	-4	9	32	32
2	-4	9	16	17
3	-4	9	83	86
4	-4	9	175	-177
5	-4	9	82	-85
6	-4	9	46	47
7	-4	9	27	-26
8	-4	9	86	87
9	-4	9	84	83
10	-4	9	91	-90
11	-4	9	74	75
12	-4	9	8	-11
13	-4	9	44	-43
-3	-3	9	66	61
-2	-3	9	38	39
-1	-3	9	17	-17
0	-3	9	126	-128
1	-3	9	29	24
2	-3	9	43	41
3	-3	9	81	80
4	-3	9	100	-99
5	-3	9	91	-88
6	-3	9	11	8
7	-3	9	79	-85
8	-3	9	86	80
9	-3	9	66	65
10	-3	9	143	-138
11	-3	9	62	-63
12	-3	9	17	-17
13	-3	9	8	-5
14	-3	9	116	119
-2	-2	9	11	-9
-1	-2	9	14	-6
0	-2	9	152	-150
1	-2	9	72	70
2	-2	9	32	32
3	-2	9	96	97
4	-2	9	83	86
5	-2	9	126	-127
6	-2	9	82	-85
7	-2	9	46	47
8	-2	9	27	-26
9	-2	9	86	87
10	-2	9	84	83
11	-2	9	91	-90
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13	-2	9	8	-11
14	-2	9	44	-43
-1	-1	9	48	-48
0	-1	9	10	13
1	-1	9	34	-32
2	-1	9	25	23
3	-1	9	74	75
4	-1	9	20	-19
5	-1	9	8	9
6	-1	9	67	-66
7	-1	9	11	11
8	-1	9	124	124
9	-1	9	17	-19
10	-1	9	22	-22
11	-1	9	66	-67
12	-1	9	36	36
13	-1	9	43	43

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 0EX2

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
-17	-1	4	38	40	-6	0	4	108	108	1	1	4	194	186	7	2	4	45	43	-10	4	4	69	-67
-11	-1	4	17	-19	-5	0	4	128	125	2	1	4	28	-29	8	2	4	11	11	-9	4	4	52	-48
-10	-1	4	51	-47	-4	0	4	84	-84	3	1	4	32	32	9	2	4	28	24	-8	4	4	67	58
-9	-1	4	19	21	-3	0	4	21	-23	4	1	4	26	22	10	2	4	41	43	-7	4	4	7	-5
-7	-1	4	32	32	-2	0	4	58	-57	5	1	4	229	-232	11	2	4	70	-72	-6	4	4	46	55
-6	-1	4	123	124	-1	0	4	78	-78	6	1	4	49	46	12	2	4	47	-46	-5	4	4	28	25
-5	-1	4	74	-76	0	0	4	224	221	7	1	4	71	69	13	2	4	29	28	-4	4	4	161	-163
-4	-1	4	78	-77	1	0	4	60	54	8	1	4	16	-15	15	2	4	44	48	-3	4	4	10	10
-3	-1	4	44	40	2	0	4	38	-36	9	1	4	58	71	-13	3	4	17	-18	-2	4	4	49	49
-2	-1	4	52	-52	3	0	4	12	10	10	1	4	98	-98	-12	3	4	7	5	0	4	4	125	128
-1	-1	4	178	178	4	0	4	164	-163	11	1	4	40	-39	-11	3	4	37	-33	1	4	4	55	-54
0	-1	4	158	158	5	0	4	21	-19	13	1	4	40	39	-10	3	4	56	-60	2	4	4	124	-124
1	-1	4	191	-192	7	0	4	21	-19	13	1	4	17	10	-9	3	4	71	70	3	4	4	25	25
2	-1	4	59	-61	8	0	4	17	14	14	1	4	24	27	-8	3	4	29	23	4	4	4	19	-22
3	-1	4	85	-89	9	0	4	12	-12	15	1	4	34	37	-7	3	4	7	-6	5	4	4	50	49
4	-1	4	15	10	10	0	4	134	-134	-13	2	4	38	-38	-6	3	4	10	22	6	4	4	110	106
6	-1	4	227	217	11	0	4	44	44	-11	2	4	40	-40	-5	3	4	126	-128	7	4	4	76	-74
8	-1	4	29	26	12	0	4	35	32	-10	2	4	72	66	-4	3	4	43	-44	8	4	4	43	-44
9	-1	4	28	-29	14	0	4	29	30	-9	2	4	76	73	-3	3	4	101	106	10	4	4	28	-27
10	-1	4	17	17	15	0	4	44	-45	-8	2	4	33	-32	-2	3	4	17	17	11	4	4	74	72
0	-1	5	118	-117	16	0	4	37	-38	-7	2	4	10	11	-1	3	4	74	72	12	4	4	28	30
10	-1	4	17	17	-12	1	4	28	-30	-6	2	4	64	-62	1	3	4	176	-173	13	4	4	37	-38
11	-1	4	47	46	-11	1	4	40	37	-5	2	4	56	-55	2	3	4	24	24	-12	5	4	13	12
12	-1	4	21	-20	-10	1	4	106	100	-4	2	4	107	106	3	3	4	13	11	-11	5	4	19	21
13	-1	4	10	10	-9	1	4	40	-41	-3	2	4	30	30	4	3	4	25	27	-10	5	4	28	27
14	-1	4	37	-37	-8	1	4	34	-34	-2	2	4	12	-12	5	3	4	90	95	-9	5	4	85	-86
15	-1	4	83	-82	-7	1	4	27	-27	-1	2	4	44	41	6	3	4	75	-73	-8	5	4	21	-19
16	-1	4	98	97	-6	1	4	83	-82	0	2	4	237	-235	7	3	4	80	-80	-7	5	4	42	41
-13	0	4	41	-41	-5	1	4	126	126	1	2	4	18	-15	8	3	4	28	28	-6	5	4	98	98
-11	0	4	77	72	-4	1	4	61	61	2	2	4	155	152	10	3	4	61	69	-5	5	4	112	-112
-10	0	4	49	-48	-3	1	4	65	-60	3	2	4	14	-14	11	3	4	82	84	-4	5	4	12	-10
-9	0	4	71	-70	-2	1	4	7	-6	4	2	4	87	84	12	3	4	57	-59	0	5	4	99	97
-8	0	4	12	-12	-1	1	4	144	-142	5	2	4	31	-31	13	3	4	13	-14	1	5	4	137	137
-7	0	4	54	-54	0	1	4	71	-68	6	2	4	144	-143	-11	4	4	14	21	2	5	4	70	-69

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR DFX2 PAGE 12

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
3	5	4	52	-50	-4	7	4	19	22	1	-9	5	13	-11	12	-7	5	22	21	8	-5	5	59	61
4	5	4	7	-3	-3	7	4	71	68	3	-9	5	59	55	13	-7	5	51	-50	9	-5	5	88	-87
5	5	4	55	-55	-2	7	4	20	-19	4	-9	5	41	-43	-7	-6	5	57	55	10	-5	5	33	-32
6	5	4	81	82	-1	7	4	20	-20	6	-9	5	27	-26	-5	-6	5	33	-31	11	-5	5	24	26
7	5	4	58	56	0	7	4	10	-12	7	-9	5	20	18	-3	-6	5	62	-63	12	-5	5	7	-5
8	5	4	45	-46	1	7	4	52	-49	8	-9	5	51	47	-2	-6	5	8	-1	13	-5	5	52	52
9	5	4	15	5	2	7	4	58	52	-3	-8	5	40	51	-1	-6	5	80	77	14	-5	5	14	14
10	5	4	38	-38	3	7	4	44	43	-1	-8	5	49	-48	1	-6	5	7	3	15	-5	5	48	-47
11	5	4	25	-25	4	7	4	13	-15	0	-8	5	9	8	2	-6	5	26	-28	-10	-4	5	8	6
12	5	4	63	61	5	7	4	8	8	1	-8	5	37	-33	3	-6	5	91	-89	-9	-4	5	6	-5
-10	6	4	44	43	6	7	4	52	-51	2	-8	5	8	-9	4	-6	5	49	45	-8	-4	5	14	11
-9	6	4	19	18	7	7	4	25	-26	3	-8	5	83	80	5	-6	5	65	65	-7	-4	5	70	-69
-8	6	4	72	-70	8	7	4	56	57	4	-8	5	15	-18	6	-6	5	6	-5	-5	-4	5	64	62
-7	6	4	13	-15	9	7	4	10	11	5	-8	5	23	-22	7	-6	5	48	45	-3	-4	5	46	45
-6	6	4	10	-10	-8	8	4	52	51	6	-8	5	18	-15	8	-6	5	67	-68	-2	-4	5	42	-39
-5	6	4	17	17	-6	8	4	13	-24	7	-8	5	58	-58	9	-6	5	63	-64	-1	-4	5	137	-139
-4	6	4	105	101	-5	8	4	10	-14	8	-8	5	46	45	10	-6	5	48	46	0	-4	5	50	50
-3	6	4	18	-18	-4	8	4	48	-46	9	-8	5	45	45	12	-6	5	27	21	1	-4	5	35	35
-2	6	4	57	-51	-3	8	4	38	38	10	-8	5	13	-12	13	-6	5	24	25	2	-4	5	28	28
0	6	4	51	-54	-2	8	4	42	40	11	-8	5	17	8	14	-6	5	59	-59	3	-4	5	76	75
1	6	4	53	49	-1	8	4	12	-11	-5	-7	5	37	-38	-9	-5	5	8	10	4	-4	5	102	-100
2	6	4	96	96	1	8	4	51	-51	-4	-7	5	19	-16	-8	-5	5	40	-41	5	-4	5	58	-58
3	6	4	56	-57	2	8	4	46	-44	-3	-7	5	20	-22	-7	-5	5	8	-15	6	-4	5	24	24
4	6	4	9	9	3	8	4	55	53	-2	-7	5	91	91	-6	-5	5	73	68	7	-4	5	21	-20
5	6	4	26	-25	4	8	4	16	17	0	-7	5	35	-37	-5	-5	5	8	1	8	-4	5	91	93
6	6	4	60	-63	5	8	4	9	13	2	-7	5	70	-68	-3	-5	5	15	-13	9	-4	5	37	38
7	6	4	71	72	7	8	4	50	-49	3	-7	5	24	21	-2	-5	5	97	-101	10	-4	5	84	-82
8	6	4	23	24	-4	9	4	28	-28	4	-7	5	87	91	-1	-5	5	33	24	11	-4	5	13	-10
9	6	4	25	-24	-3	9	4	48	-49	5	-7	5	20	-19	2	-5	5	54	57	12	-4	5	11	-13
11	6	4	48	-50	-2	9	4	39	38	6	-7	5	12	8	3	-5	5	66	-67	14	-4	5	72	71
-9	7	4	54	54	-1	9	4	23	22	7	-7	5	29	-26	4	-5	5	107	-109	-10	-3	5	44	44
-7	7	4	45	-46	1	9	4	19	16	8	-7	5	80	-80	5	-5	5	65	64	-8	-3	5	27	28
-6	7	4	9	-12	2	9	4	45	-50	9	-7	5	48	49	6	-5	5	17	18	-6	-3	5	97	-99
-5	7	4	33	-31	3	9	4	24	-21	10	-7	5	32	33	7	-5	5	33	33	-5	-3	5	22	21

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR OFYP

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-4	-9	E	30	38	7	-9	E	31	-32	-10	0	E	14	-20	-4	1	E	77	76	4	2	E	81	77
-2	-9	E	106	106	8	-9	E	71	-72	-9	0	E	65	-64	-3	1	E	38	-40	5	2	E	43	-38
-1	-9	E	48	-48	10	-9	E	125	128	-8	0	E	7	5	-2	1	E	22	20	6	2	E	145	-142
0	-9	E	104	-104	22	-9	E	19	-19	-7	0	E	44	-42	-1	1	E	79	-81	7	2	E	31	31
1	-9	E	36	34	14	-9	E	52	-52	-6	0	E	74	75	0	1	E	38	-34	8	2	E	11	9
2	-9	E	27	-27	16	-9	E	24	23	-5	0	E	123	122	1	1	E	146	136	9	2	E	31	31
3	-9	E	82	78	18	-9	E	42	41	-4	0	E	74	-75	2	1	E	24	29	10	2	E	79	81
4	-9	E	104	104	-12	-1	E	96	96	-3	0	E	33	-31	3	1	E	20	19	11	2	E	82	-82
5	-9	E	128	-125	-10	-1	E	87	-88	-2	0	E	41	-39	4	1	E	19	12	12	2	E	41	-40
6	-9	E	35	-34	-9	-1	E	27	20	-1	0	E	84	-82	5	1	E	178	-176	13	2	E	17	17
7	-9	E	6	3	-8	-1	E	7	-9	0	0	E	194	192	6	1	E	22	20	14	2	E	11	-10
8	-9	E	23	-23	-7	-1	E	19	18	1	0	E	48	46	7	1	E	116	116	15	2	E	41	40
9	-9	E	122	123	-6	-1	E	111	112	2	0	E	98	-98	8	1	E	6	-3	-11	3	E	22	-22
11	-9	E	46	-41	-5	-1	E	88	-87	3	0	E	17	19	9	1	E	65	67	-10	3	E	57	-51
13	-9	E	47	-47	-4	-1	E	74	-78	4	0	E	134	-132	10	1	E	41	-41	-9	3	E	67	65
16	-9	E	38	38	-3	-1	E	30	-28	5	0	E	28	-28	11	1	E	46	-46	-8	3	E	47	46
17	-9	E	85	84	-2	-1	E	58	-57	6	0	E	158	151	12	1	E	37	36	-7	3	E	16	11
18	-9	E	11	-13	-1	-1	E	154	155	7	0	E	22	-24	14	1	E	14	15	-6	3	E	40	39
-11	-8	E	66	-66	0	-1	E	113	118	8	0	E	18	18	15	1	E	33	34	-5	3	E	112	-112
-10	-8	E	28	27	1	-1	E	105	-105	10	0	E	190	-193	-19	2	E	9	-4	-4	3	E	48	-50
-8	-8	E	7	5	2	-1	E	17	-17	11	0	E	39	40	-11	2	E	45	-45	-3	3	E	93	92
-7	-8	E	77	78	3	-1	E	80	-82	12	0	E	34	33	-10	2	E	42	44	-2	3	E	20	-19
-6	-8	E	46	-45	4	-1	E	64	-67	13	0	E	8	-8	-8	2	E	58	58	-1	3	E	60	59
-5	-8	E	102	-103	6	-1	E	170	167	14	0	E	32	32	-7	2	E	43	-38	0	3	E	15	18
-4	-8	E	38	35	8	-1	E	11	13	15	0	E	48	-46	-6	2	E	11	8	1	3	E	219	-208
-3	-8	E	8	-8	9	-1	E	41	-41	16	0	E	39	-41	-5	2	E	86	-88	2	3	E	11	9
-2	-8	E	68	67	10	-1	E	117	-114	-12	1	E	27	-28	-4	2	E	77	-76	3	3	E	25	23
-1	-8	E	132	135	11	-1	E	10	11	-11	1	E	13	15	-3	2	E	112	113	4	3	E	8	8
0	-8	E	104	-107	13	-1	E	47	47	-10	1	E	77	75	-2	2	E	31	31	5	3	E	116	114
1	-8	E	77	-75	15	-1	E	25	25	-9	1	E	46	-42	-1	2	E	6	8	6	3	E	62	-59
2	-8	E	46	-43	16	-1	E	14	-14	-8	1	E	32	-30	0	2	E	20	10	7	3	E	46	-43
4	-8	E	153	148	18	-1	E	26	-26	-7	1	E	24	-24	0	2	E	198	-197	8	3	E	19	20
5	-8	E	31	29	6	0	E	31	31	-6	1	E	53	-52	1	2	E	14	-19	9	3	E	26	-28
6	-8	E	107	-108	-11	0	E	87	84	-5	1	E	111	111	2	2	E	107	108	10	3	E	44	46

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REV2

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
11	9	6	51	51	-3	5	6	96	-93	-6	7	6	24	-24	8	-6	6	22	24	-5	-5	6	61	61
12	9	6	61	-62	-9	5	6	12	-11	-8	7	6	19	20	8	-5	6	51	49	-2	-5	6	82	-81
13	9	6	17	-16	-1	5	6	72	-72	-3	7	6	76	72	-4	-7	6	15	-16	-1	-5	6	16	13
-11	10	6	16	16	0	5	6	78	82	-9	7	6	19	-19	-3	-7	6	20	-20	0	-5	6	58	60
-10	10	6	45	-46	1	5	6	178	182	-7	7	6	19	-12	-2	-7	6	66	67	2	-5	6	51	49
-9	10	6	46	-46	2	5	6	42	-36	0	7	6	19	-18	0	-7	6	25	-25	3	-5	6	47	-49
-8	10	6	54	53	3	5	6	46	-49	1	7	6	68	-67	2	-7	6	50	-44	4	-5	6	106	-104
-7	10	6	18	18	4	5	6	7	4	2	7	6	65	66	4	-7	6	9	17	5	-5	6	44	47
-6	10	6	48	48	5	5	6	48	-48	3	7	6	41	37	6	-7	6	54	53	6	-5	6	19	21
-5	10	6	35	35	6	5	6	51	47	4	7	6	13	-12	8	-7	6	7	8	7	-5	6	30	32
-4	10	6	134	-135	7	5	6	84	81	5	7	6	13	12	9	-7	6	37	-35	8	-5	6	58	58
-3	10	6	15	-11	8	5	6	43	-45	6	7	6	46	-52	10	-7	6	60	-60	9	-5	6	80	-79
-2	10	6	40	38	10	5	6	26	-21	7	7	6	26	-27	9	-7	6	31	36	10	-5	6	53	-52
-1	10	6	7	-10	11	5	6	35	-37	8	7	6	43	40	10	-7	6	34	30	12	-5	6	7	-11
0	10	6	113	113	12	5	6	29	29	9	7	6	8	9	12	-7	6	20	15	13	-5	6	56	54
1	10	6	72	-69	13	5	6	21	21	-8	8	6	15	-13	13	-7	6	19	19	14	-5	6	16	13
2	10	6	114	-117	-9	6	6	64	-64	-6	8	6	64	-61	-8	-6	6	26	-24	15	-4	6	17	16
3	10	6	7	-7	-7	6	6	16	-17	-5	8	6	24	24	-4	-6	6	14	14	-7	-4	6	51	-52
4	10	6	19	-17	-6	6	6	8	-9	-2	8	6	54	52	-3	-6	6	48	-48	-8	-4	6	8	9
5	10	6	46	46	-5	6	6	11	11	-1	8	6	12	-12	-2	-6	6	9	-11	-5	-4	6	46	46
6	10	6	104	107	-2	6	6	49	-47	0	8	6	12	8	-1	-6	6	72	69	-3	-4	6	35	35
7	10	6	61	-63	0	6	6	35	-37	1	8	6	35	-39	1	-6	6	16	18	-2	-4	6	20	-23
8	10	6	32	-32	1	6	6	42	45	2	8	6	51	-51	2	-6	6	24	-21	-1	-4	6	115	-120
10	10	6	42	-44	2	6	6	71	71	3	8	6	48	47	3	-6	6	56	-59	0	-4	6	27	24
11	10	6	24	25	3	6	6	24	-26	4	8	6	16	17	4	-6	6	43	39	1	-4	6	21	17
12	10	6	10	10	4	6	6	7	-4	5	8	6	9	7	5	-6	6	40	44	2	-4	6	16	11
13	10	6	30	-30	5	6	6	97	-96	6	8	6	18	19	7	-6	6	42	40	3	-4	6	88	90
-10	11	6	35	33	6	6	6	38	-34	-1	-8	6	29	-29	8	-6	6	23	-22	4	-4	6	86	-83
-9	11	6	66	-67	7	6	6	57	59	0	-8	6	17	4	9	-6	6	48	-48	5	-4	6	71	-70
-8	11	6	34	-33	8	6	6	22	26	1	-8	6	26	-22	10	-6	6	40	39	6	-4	6	30	31
-7	11	6	19	22	9	6	6	10	-12	2	-8	6	9	-11	11	-6	6	7	7	7	-4	6	23	-21
-6	11	6	7	-10	11	6	6	44	-43	3	-8	6	74	73	12	-6	6	22	22	8	-4	6	75	74
-5	11	6	72	70	-7	7	6	58	-59	5	-8	6	23	-24	13	-6	6	23	25	9	-4	6	58	57
-4	11	6	7	9	-6	7	6	7	-1	7	-8	6	50	-47	-7	-5	6	16	-21	-10	-4	6	76	-76

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REF2

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
11	-4	E	15	-17	-1	-2	E	135	127	11	-1	E	81	81	-7	1	E	14	-14	1	2	E	43	-40
12	-4	E	8	-9	0	-2	E	98	-95	12	-1	E	15	-15	-6	1	E	69	-70	2	2	E	94	93
13	-4	E	7	-7	1	-2	E	51	-53	13	-1	E	9	8	-5	1	E	74	75	3	2	E	18	-20
14	-4	E	79	78	2	-2	E	11	-11	14	-1	E	16	-17	-4	1	E	59	55	4	2	E	70	67
15	-4	E	7	-3	3	-2	E	42	-40	15	-1	E	68	-69	-3	1	E	42	-42	5	2	E	11	7
8	-3	E	77	78	4	-2	E	139	144	-11	0	E	49	50	-2	1	E	11	12	6	2	E	157	-148
9	-3	E	78	-72	5	-2	E	72	70	-10	0	E	19	-14	-1	1	E	84	-98	7	2	E	23	24
10	-3	E	16	14	6	-2	E	100	-96	-9	0	E	46	-47	0	1	E	81	76	8	2	E	73	70
11	-3	E	28	25	8	-2	E	84	-83	-8	0	E	10	7	1	1	E	139	134	9	2	E	15	14
12	-3	E	13	-11	9	-2	E	17	15	-7	0	E	51	-52	2	1	E	15	16	10	2	E	42	42
13	-3	E	86	86	10	-2	E	112	113	-6	0	E	41	44	3	1	E	68	73	11	2	E	49	49
-1	-3	E	59	-58	12	-2	E	18	-15	-5	0	E	103	104	4	1	E	21	22	12	2	E	43	-44
0	-3	E	102	-103	13	-2	E	8	5	-4	0	E	84	-83	5	1	E	177	-183	13	2	E	15	14
1	-3	E	33	32	14	-2	E	52	-52	-3	0	E	25	-25	6	1	E	11	-1	14	2	E	12	-15
2	-3	E	28	-27	15	-2	E	18	16	-1	0	E	88	-87	7	1	E	78	76	-10	3	E	51	-49
3	-3	E	85	84	-10	-1	E	84	-87	0	0	E	141	140	8	1	E	12	-11	-9	3	E	38	37
4	-3	E	91	87	-9	-1	E	8	10	1	0	E	72	69	9	1	E	64	64	-8	3	E	90	92
5	-3	E	48	-46	-8	-1	E	6	-4	2	0	E	7	-28	10	1	E	44	-41	-7	3	E	23	23
7	-3	E	6	-6	-7	-1	E	7	6	3	0	E	14	21	11	1	E	43	-46	-6	3	E	88	-87
8	-3	E	72	-72	-6	-1	E	95	96	4	0	E	117	-104	12	1	E	29	29	-4	3	E	49	-49
9	-3	E	100	100	-5	-1	E	42	-42	5	0	E	22	-24	14	1	E	22	23	-3	3	E	67	67
10	-3	E	30	30	-4	-1	E	88	-88	6	0	E	114	112	15	1	E	43	44	-2	3	E	14	15
11	-3	E	44	47	-2	-1	E	46	46	7	0	E	10	9	-11	2	E	43	-42	-1	3	E	52	52
13	-3	E	37	-36	-1	-1	E	113	110	8	0	E	21	22	-10	2	E	33	32	0	3	E	34	30
14	-3	E	8	12	0	-1	E	129	129	9	0	E	7	-8	-9	2	E	44	47	1	3	E	143	-146
15	-3	E	57	54	1	-1	E	98	-99	10	0	E	118	-117	-8	2	E	25	-27	2	3	E	8	11
16	-3	E	29	28	2	-1	E	22	-20	11	0	E	20	20	-7	2	E	27	27	3	3	E	30	30
-8	-2	E	12	-8	3	-1	E	64	-61	12	0	E	44	44	-6	2	E	49	-48	5	3	E	106	103
-7	-2	E	84	80	4	-1	E	80	-82	14	0	E	94	95	-5	2	E	88	-90	6	3	E	40	-39
-6	-2	E	19	-19	5	-1	E	184	140	15	0	E	39	-40	-4	2	E	38	40	7	3	E	46	-44
-5	-2	E	91	-92	6	-1	E	96	99	-11	1	E	11	11	-3	2	E	27	27	8	3	E	20	18
-4	-2	E	24	23	7	-1	E	92	-92	-10	1	E	67	68	-2	2	E	8	6	9	3	E	7	-11
-3	-2	E	13	-16	8	-1	E	12	11	-9	1	E	24	-24	-1	2	E	24	26	10	3	E	47	45
-2	-2	E	32	32	9	-1	E	107	-104	-8	1	E	14	-12	0	2	E	162	-151	11	3	E	66	66

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEY2

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
12	3	6	38	-42	1	5	6	92	95	4	7	6	11	-11	-2	-6	7	9	-18	4	-4	7	61	-59
13	3	6	15	-13	2	5	6	31	-31	5	7	6	14	13	-1	-6	7	53	53	5	-4	7	78	-76
-10	4	6	32	-31	3	5	6	44	-46	6	7	6	38	-39	3	-6	7	70	-69	6	-4	7	27	26
-9	4	6	43	-42	4	5	6	18	-15	7	7	6	33	-33	4	-6	7	24	23	7	-4	7	20	-25
-8	4	6	31	34	5	5	6	43	-47	8	7	6	40	42	5	-6	7	45	46	8	-4	7	53	59
-7	4	6	16	15	6	5	6	48	49	-3	8	6	12	10	7	-6	7	42	42	9	-4	7	51	49
-6	4	6	30	31	7	5	6	54	53	-2	8	6	43	45	8	-6	7	45	-42	10	-4	7	69	-69
-5	4	6	22	22	8	5	6	30	-27	-1	8	6	9	-9	9	-6	7	58	-56	11	-4	7	18	-17
-4	4	6	101	-102	10	5	6	34	-32	0	8	6	10	8	10	-6	7	27	28	12	-4	7	7	-6
-3	4	6	26	-26	11	5	6	27	-30	1	8	6	29	-31	12	-6	7	21	21	13	-4	7	7	-5
-2	4	6	35	36	-8	6	6	51	-54	2	8	6	48	-49	-6	-5	7	58	55	14	-4	7	62	52
-1	4	6	8	1	-7	6	6	7	-6	3	8	6	40	41	-3	-5	7	8	10	-8	-3	7	23	23
0	4	6	100	99	-4	6	6	83	82	4	8	6	10	15	-2	-5	7	78	-78	-7	-3	7	8	8
1	4	6	9	-9	-2	6	6	41	-42	1	-8	7	21	-21	-1	-5	7	8	2	-5	-3	7	72	-74
2	4	6	99	-99	0	6	6	42	-40	2	-8	7	9	-11	0	-5	7	42	42	-4	-3	7	25	26
4	4	6	19	-23	1	6	6	27	25	3	-8	7	57	56	2	-5	7	42	41	-3	-3	7	11	-10
5	4	6	43	46	2	6	6	75	76	5	-8	7	19	-21	3	-5	7	29	-27	-2	-3	7	74	77
6	4	6	92	89	3	6	6	25	-25	7	-8	7	45	-48	4	-5	7	83	-83	-1	-3	7	33	-31
7	4	6	49	-48	4	6	6	17	-2	8	-8	7	21	20	5	-5	7	35	34	0	-3	7	81	-82
8	4	6	37	-38	5	6	6	23	-22	-2	-7	7	60	60	6	-5	7	14	16	1	-3	7	28	31
10	4	6	35	-35	6	6	6	47	-47	-1	-7	7	11	13	7	-5	7	22	19	2	-3	7	21	-23
11	4	6	45	45	7	6	6	53	55	0	-7	7	16	-19	8	-5	7	50	58	3	-3	7	50	47
12	4	6	35	37	8	6	6	29	26	1	-7	7	9	8	9	-5	7	64	-64	4	-3	7	97	95
13	4	6	22	-23	9	6	6	9	-11	2	-7	7	48	-50	11	-5	7	17	12	5	-3	7	92	-90
-9	5	6	47	-49	10	6	6	9	12	3	-7	7	10	2	12	-5	7	10	-12	6	-3	7	47	-47
-8	5	6	24	-26	-5	7	6	36	-35	4	-7	7	61	58	13	-5	7	44	44	8	-3	7	35	-32
-7	5	6	24	24	-4	7	6	9	5	5	-7	7	8	-4	-7	-4	7	61	-61	9	-3	7	107	105
-6	5	6	11	5	-3	7	6	60	58	6	-7	7	14	13	-6	-4	7	15	-15	10	-3	7	31	32
-5	5	6	74	73	-2	7	6	17	-18	7	-7	7	24	-24	-5	-4	7	40	47	11	-3	7	49	-50
-4	5	6	23	23	-1	7	6	14	-14	8	-7	7	59	-60	-2	-4	7	38	38	12	-3	7	6	-2
-3	5	6	79	-79	0	7	6	9	-9	9	-7	7	30	31	-1	-4	7	74	-77	13	-3	7	37	-37
-2	5	6	15	-15	1	7	6	58	-57	10	-7	7	26	28	0	-4	7	31	35	15	-3	7	60	60
-1	5	6	8	-11	2	7	6	46	44	-4	-6	7	10	5	1	-4	7	17	20	-9	-2	7	24	22
0	5	6	18	17	3	7	6	51	51	-3	-6	7	52	-52	3	-4	7	88	88	-8	-2	7	7	3

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PBY2

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-7	-2	7	50	53	5	-1	7	41	38	-4	1	7	52	51	11	2	7	41	-38	2	4	7	87	-87
-6	-2	7	58	-67	7	-1	7	25	-25	-3	1	7	46	-45	12	2	7	44	-44	3	4	7	18	-20
-4	-2	7	14	15	8	-1	7	14	13	-2	1	7	37	35	13	2	7	7	10	4	4	7	23	-23
-3	-2	7	10	-15	9	-1	7	24	-24	-1	1	7	74	-72	14	2	7	8	-9	5	4	7	28	29
-2	-2	7	13	15	11	-1	7	17	17	0	1	7	78	-74	-6	3	7	20	20	6	4	7	77	77
-1	-2	7	102	104	13	-1	7	14	18	1	1	7	123	119	-8	3	7	26	26	7	4	7	34	-32
0	-2	7	70	-72	14	-1	7	7	17	2	1	7	22	24	-7	3	7	11	6	8	4	7	28	-28
2	-2	7	21	-25	15	-1	7	8	-17	3	1	7	15	16	-5	3	7	25	27	9	4	7	13	-14
3	-2	7	69	-70	-5	0	7	45	-45	4	1	7	16	15	-4	3	7	6	-9	10	4	7	38	-38
4	-2	7	114	107	-3	0	7	47	-46	5	1	7	139	-128	-3	3	7	41	-43	11	4	7	43	42
5	-2	7	45	48	-2	0	7	24	27	6	1	7	17	18	-2	3	7	42	41	12	4	7	29	30
6	-2	7	42	-40	-1	0	7	78	78	7	1	7	80	80	-1	3	7	17	16	-7	5	7	13	15
7	-2	7	7	-7	0	0	7	44	-42	8	1	7	55	56	0	3	7	40	44	-6	5	7	18	-16
8	-2	7	50	-48	1	0	7	7	-6	10	1	7	14	-19	1	3	7	37	35	-5	5	7	45	46
9	-2	7	28	-28	2	0	7	23	-21	11	1	7	84	-78	2	3	7	124	-122	-4	5	7	23	21
10	-2	7	106	100	3	0	7	72	-72	12	1	7	14	10	3	3	7	8	-15	-3	5	7	77	-75
11	-2	7	12	11	4	0	7	104	106	14	1	7	7	10	4	3	7	10	11	-2	5	7	5	-2
12	-2	7	11	-10	5	0	7	60	60	15	1	7	40	40	5	3	7	6	4	-1	5	7	13	-10
14	-2	7	17	-14	6	0	7	27	-26	-8	2	7	12	-13	6	3	7	40	40	1	5	7	15	15
15	-2	7	7	7	7	0	7	21	22	-7	2	7	25	-24	8	3	7	25	-24	2	5	7	13	-14
-8	-1	7	14	-15	8	0	7	64	-66	-6	2	7	56	-54	7	3	7	79	-79	3	5	7	33	-32
-7	-1	7	6	-7	9	0	7	37	-33	-4	2	7	51	53	8	3	7	27	-23	5	5	7	37	-40
-6	-1	7	88	91	8	1	7	100	106	-3	2	7	43	43	10	3	7	34	38	6	5	7	34	33
-5	-1	7	20	-20	9	1	7	15	17	-2	2	7	22	22	11	3	7	53	55	7	5	7	53	55
-4	-1	7	51	-50	10	1	7	100	-104	-1	2	7	117	-114	12	3	7	32	-34	8	5	7	23	-23
-3	-1	7	12	14	11	1	7	15	14	0	2	7	35	-34	13	3	7	7	-13	10	5	7	22	-20
-2	-1	7	60	-62	12	1	7	40	40	1	2	7	73	71	-8	4	7	20	20	-5	6	7	17	-15
-1	-1	7	71	69	13	1	7	8	-8	2	2	7	68	64	-6	4	7	26	26	-4	6	7	67	67
0	-1	7	108	104	14	1	7	37	36	5	2	7	12	7	-5	4	7	34	34	-3	6	7	10	-1
1	-1	7	61	-62	15	1	7	27	-27	6	2	7	127	-129	-4	4	7	79	-79	-2	6	7	47	-48
2	-1	7	14	-14	-8	1	7	18	-17	7	2	7	19	19	-3	4	7	23	-24	-1	6	7	13	4
3	-1	7	46	-41	-6	1	7	15	-17	8	2	7	24	21	-2	4	7	29	24	0	6	7	38	-36
4	-1	7	70	-68	-5	1	7	57	-58	9	2	7	7	11	0	4	7	44	44	1	6	7	18	19
5	-1	7	124	118	-4	1	7	45	48	10	2	7	77	76	1	4	7	4	1	2	6	7	73	70

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 0EY2

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	6	7	18	-20	1	-5	A	0	2	3	-1	A	25	26	-2	-1	A	51	-49
5	6	7	45	-48	2	-5	A	43	49	4	-1	A	53	50	-1	-1	A	52	50
7	6	7	42	44	3	-5	A	34	-38	5	-1	A	25	-23	0	-1	A	27	26
8	6	7	32	33	4	-5	A	60	-58	6	-1	A	35	-32	1	-1	A	51	-48
0	6	7	10	-14	5	-5	A	27	27	7	-1	A	7	-8	2	-1	A	9	10
-3	7	7	50	50	7	-5	A	12	11	8	-1	A	30	-32	3	-1	A	35	-33
-1	7	7	10	-10	8	-5	A	51	50	10	-1	A	25	25	4	-1	A	64	-63
0	7	7	15	-10	0	-6	A	49	-46	10	-3	A	27	28	5	-1	A	104	98
1	7	7	50	-50	10	-6	A	38	-38	11	-3	A	45	-46	6	-1	A	34	31
2	7	7	34	31	11	-6	A	16	16	12	-3	A	20	-21	7	-1	A	21	-22
3	7	7	14	11	12	-6	A	11	-11	14	-3	A	7	-8	8	-1	A	32	31
4	7	7	13	-11	0	-8	A	43	43	-7	-2	A	42	46	9	-1	A	41	-41
8	7	7	6	6	-3	-8	A	27	28	-6	-2	A	4	-6	10	-1	A	8	-9
6	7	7	30	-30	-2	-8	A	8	-9	-5	-2	A	65	-66	11	-1	A	60	61
2	-7	8	45	-46	-1	-8	A	42	-44	-3	-2	A	8	-10	13	-1	A	8	13
3	-7	8	13	-14	0	-8	A	10	9	-2	-2	A	18	18	-4	-2	A	7	-8
5	-7	8	53	54	4	-8	A	8	-9	-1	-2	A	104	104	-3	-2	A	27	-32
6	-7	8	17	11	5	-8	A	54	56	0	-2	A	47	-46	-2	-2	A	21	22
7	-7	8	9	-12	6	-8	A	38	-34	1	-2	A	36	-37	-1	-2	A	78	78
8	-7	8	51	-49	5	-8	A	52	-51	2	-2	A	14	17	-3	-2	A	35	-34
9	-7	8	17	21	8	-8	A	28	28	3	-2	A	70	-69	-4	-2	A	8	-4
-2	-6	8	17	-18	9	-8	A	51	51	4	-2	A	86	78	-1	-2	A	79	-76
-1	-6	8	58	61	0	-9	A	8	8	5	-2	A	76	72	0	-2	A	73	71
0	-6	8	7	7	10	-8	A	47	-49	6	-2	A	31	-35	1	-2	A	54	49
2	-6	8	13	3	11	-8	A	16	-17	7	-2	A	9	-12	2	-2	A	44	-46
3	-6	8	64	-67	12	-8	A	18	-17	8	-2	A	44	-44	3	-2	A	28	28
4	-6	8	33	32	13	-8	A	46	-48	9	-2	A	37	-37	4	-2	A	47	-47
7	-6	8	34	-33	4	-9	A	20	20	10	-2	A	75	75	5	-2	A	66	-68
8	-6	8	26	-26	-3	-9	A	7	4	11	-2	A	7	12	6	-2	A	47	51
9	-6	8	48	-50	-2	-9	A	44	41	12	-2	A	11	-10	7	-2	A	9	10
10	-6	8	21	20	-1	-9	A	22	-26	14	-2	A	51	-51	8	-2	A	15	15
-4	-5	8	8	8	0	-9	A	73	-71	-8	-1	A	73	74	9	-2	A	14	8
-2	-5	8	76	-72	1	-9	A	12	12	-7	-1	A	27	-27	10	-2	A	50	-48
0	-5	8	41	40	2	-9	A	27	-29	-6	-1	A	58	-57	12	-2	A	36	40

H	K	L	FO	FC
13	0	A	10	-1
14	0	A	26	32
-6	1	A	13	-16
-7	1	A	16	-17
-6	1	A	13	-17
-5	1	A	32	33
-4	1	A	53	51
-3	1	A	36	-37
-1	1	A	63	-60
0	1	A	64	60
1	1	A	31	28
2	1	A	21	19
4	1	A	23	12
5	1	A	103	-100
6	1	A	18	-16
7	1	A	57	54
8	1	A	55	54
10	1	A	12	9
11	1	A	73	-75
12	1	A	9	11
-4	2	A	10	-11
-7	2	A	14	13
-6	2	A	35	-32
-5	2	A	53	-54
-4	2	A	45	44
-3	2	A	17	17
-2	2	A	7	7
-1	2	A	27	28
0	2	A	47	-43
1	2	A	24	-19
2	2	A	41	42
3	2	A	9	7
4	2	A	58	60
5	2	A	30	8

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REV2

H	K	L	FO	FC
6	2	8	93	-84
7	2	8	21	17
8	2	8	7	5
10	2	8	88	85
11	2	8	96	-97
12	2	8	98	-60
-5	3	8	39	33
-4	3	8	47	-47
-3	3	8	48	-45
-2	3	8	46	40
-1	3	8	79	79
0	3	8	33	29
1	3	8	69	-69
2	3	8	11	-15
3	3	8	18	17
4	3	8	79	78
5	3	8	17	-16
6	3	8	88	-85
8	3	8	12	8
9	3	8	12	-13
10	3	8	93	93
11	3	8	61	62
12	3	8	28	-29
-5	4	8	29	22
-4	4	8	24	24
-3	4	8	58	-58
-2	4	8	27	-25
-1	4	8	21	20
0	4	8	18	-14
1	4	8	75	74
2	4	8	14	12
3	4	8	82	-82
4	4	8	8	8
5	4	8	16	-16

H	K	L	FO	FC
6	4	8	77	77
7	4	8	36	-35
8	4	8	26	-27
10	4	8	36	-35
11	4	8	33	33
-5	5	8	41	44
-4	5	8	24	25
-3	5	8	56	-55
-2	5	8	12	-6
-1	5	8	16	-11
0	5	8	77	78
1	5	8	30	-30
2	5	8	32	-32
3	5	8	21	21
4	5	8	55	54
5	5	8	19	-21
6	5	8	4	5
-2	6	8	26	-28
0	6	8	35	-36
1	6	8	11	11
2	6	8	50	51
3	6	8	9	-14
4	6	8	43	-45
7	6	8	11	14
8	6	8	6	5
1	-6	8	86	-87
2	-6	8	17	16
3	-6	8	38	38
4	-6	8	20	-20
5	-6	8	44	-43
-1	-5	8	15	-8
0	-5	8	34	36
1	-5	8	34	32

H	K	L	FO	FC
-	-4	8	15	-11
0	-4	8	84	-82
4	-4	8	14	15
7	-3	8	8	8
-4	-3	8	53	50
9	-3	8	32	-30
10	-3	8	30	-32
0	-2	8	74	-73
1	-2	8	64	-55
2	-2	8	8	-5
3	-2	8	66	-62
5	-2	8	44	-45
6	-2	8	9	8
7	-2	8	33	-30
8	-2	8	41	-39
10	-2	8	73	72
11	-2	8	12	14
12	-2	8	7	-7
-4	-1	8	38	-40
-3	-1	8	37	-39
-1	-1	8	37	38
0	-1	8	78	78
1	-1	8	78	-83
2	-1	8	14	-9
3	-1	8	18	-19
4	-1	8	72	-69
6	-1	8	84	84
9	-1	8	38	37
10	-1	8	98	-95
11	-1	8	22	23
12	-1	8	58	-58
0	0	8	28	-28
1	0	8	83	83

H	K	L	FO	FC
10	-3	9	34	35
11	-3	9	32	-32
-8	-2	9	40	-47
-4	-2	9	9	-4
-3	-2	9	12	14
-1	-2	9	83	84
0	-2	9	74	-83
1	-2	9	64	-56
2	-2	9	8	-5
4	-2	9	66	-62
5	-2	9	44	-45
6	-2	9	7	8
9	-2	9	33	-30
10	-2	9	79	72
12	-2	9	7	-7
-4	-1	9	39	-40
-3	-1	9	37	-39
-1	-1	9	37	38
0	-1	9	78	78
1	-1	9	78	-83
2	-1	9	14	-9
3	-1	9	18	-19
4	-1	9	72	-69
6	-1	9	84	84
9	-1	9	38	37
10	-1	9	98	-95
11	-1	9	22	23
12	-1	9	58	-58
0	0	9	28	-28
1	0	9	83	83

H	K	L	FO	FC
-5	0	9	46	48
-4	0	9	20	-17
-3	0	9	16	-17
-2	0	9	22	-16
-1	0	9	52	-54
0	0	9	56	54
1	0	9	43	41
2	0	9	24	25
4	0	9	41	-41
5	0	9	26	-27
6	0	9	20	17
7	0	9	14	15
8	0	9	7	7
10	0	9	71	-73
12	0	9	25	25
-4	1	9	44	-47
-3	1	9	25	27
-2	1	9	40	44
-1	1	9	21	-18
0	1	9	17	15
1	1	9	48	-46
2	1	9	61	-58
3	1	9	68	62
4	1	9	8	11
6	1	9	13	10
7	1	9	26	27
8	1	9	82	-78
9	1	9	13	-11
10	1	9	30	30
11	1	9	6	0
12	1	9	47	48
0	2	9	8	-7
1	2	9	62	-63

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR DEY2

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
-5	2	9	58	-58	1	4	9	24	19	6	-3	10	37	-36	2	0	10	20	-17	0	3	10	32	28
-4	2	9	41	41	2	4	9	58	-61	8	-3	10	33	-33	3	0	10	16	15	1	3	10	60	-61
-3	2	9	35	33	6	4	9	52	57	9	-3	10	40	43	4	0	10	52	-52	2	3	10	18	-15
-2	2	9	8	-1	7	4	9	9	-9	10	-3	10	34	35	5	0	10	51	-48	3	3	10	10	10
-1	2	9	30	25	8	4	9	27	-26	-2	-2	10	10	7	6	0	10	56	50	5	3	10	45	53
0	2	9	52	-52	9	4	9	9	1	-1	-2	10	50	51	7	0	10	9	5	6	3	10	10	9
1	2	9	43	-42	-2	5	9	9	-4	0	-2	10	20	-16	8	0	10	19	15	7	3	10	44	-48
2	2	9	38	37	-1	5	9	8	-9	1	-2	10	24	-25	9	0	10	21	17	0	4	10	43	44
4	2	9	31	35	0	5	9	9	-14	3	-2	10	34	-34	10	0	10	60	-59	1	4	10	22	19
5	2	9	18	10	1	5	9	53	59	4	-2	10	45	43	11	0	10	8	0	2	4	10	41	-44
6	2	9	25	-24	3	5	9	21	-26	5	-2	10	55	55	-3	1	10	14	-13	4	4	10	17	-15
8	2	9	10	11	4	5	9	9	5	6	-2	10	29	-30	-2	1	10	14	14	5	-3	11	21	-21
9	2	9	9	5	5	5	9	36	-36	8	-2	10	22	-23	-1	1	10	27	-30	3	-2	11	34	-32
10	2	9	59	61	6	5	9	10	17	9	-2	10	35	-36	0	1	10	60	-58	4	-2	11	29	27
11	2	9	20	-19	7	5	9	44	47	10	-2	10	40	42	1	1	10	50	49	5	-2	11	50	48
-5	3	9	37	-40	3	-5	10	9	-1	11	-2	10	19	15	2	1	10	28	24	6	-2	11	23	-22
-4	3	9	42	-44	4	-5	10	57	-57	-2	-1	10	35	-32	4	1	10	24	27	1	-1	11	13	-15
-3	3	9	25	24	5	-5	10	13	10	-1	-1	10	22	23	5	1	10	57	-58	4	-1	11	43	-44
-2	3	9	13	5	6	-5	10	7	6	0	-1	10	64	64	6	1	10	31	-28	5	-1	11	40	38
-1	3	9	32	30	7	-5	10	13	11	1	-1	10	23	-22	7	1	10	31	30	6	-1	11	33	31
0	3	9	33	35	0	-4	10	10	0	2	-1	10	9	-7	8	1	10	9	-4	7	-1	11	10	-13
1	3	9	72	-71	1	-4	10	8	11	3	-1	10	25	-23	9	1	10	34	37	8	-1	11	10	14
2	3	9	15	-14	3	-4	10	49	53	4	-1	10	44	-44	10	1	10	7	4	1	0	11	37	37
3	3	9	15	12	4	-4	10	23	-19	5	-1	10	63	56	-3	2	10	21	23	2	0	11	11	-12
4	3	9	14	-12	5	-4	10	15	11	6	-1	10	29	28	-1	2	10	30	28	3	0	11	15	17
5	3	9	57	55	7	-4	10	18	-15	8	-1	10	15	17	0	2	10	55	-55	4	0	11	27	-32
7	3	9	55	-57	8	-4	10	26	25	9	-1	10	51	-49	1	2	10	45	-41	5	0	11	40	-40
9	3	9	15	-16	9	-4	10	50	49	10	-1	10	17	-15	2	2	10	37	36	6	0	11	43	45
10	3	9	9	13	0	-3	10	48	-48	11	-1	10	31	33	4	2	10	32	37	7	0	11	20	14
-4	4	9	45	-47	1	-3	10	9	0	-3	0	10	8	-9	5	2	10	31	27	1	1	11	36	35
-3	4	9	28	-26	2	-3	10	13	-13	-2	0	10	8	-5	6	2	10	54	-56	2	1	11	20	18
-2	4	9	10	12	3	-3	10	10	19	-1	0	10	53	-53	8	2	10	15	12	4	1	11	28	24
-1	4	9	10	-15	4	-3	10	55	54	0	0	10	41	41	-2	3	10	13	6	5	1	11	45	-49
0	4	9	51	54	5	-3	10	32	-33	1	0	10	50	47	-1	3	10	21	24	6	1	11	26	-24
7	1	11	30	31	4	2	11	25	28															

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REM3

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	78	-52	4	4	0	119	115	3	4	0	67	64	10	12	0	46	-45	9	19	0	37	-40
4	0	0	921	-929	8	4	0	80	78	4	4	0	154	157	1	13	0	16	27	4	19	0	31	-29
6	0	0	74	72	5	4	0	108	-110	5	4	0	177	-173	2	13	0	154	147	-13	0	1	43	38
8	0	0	78	79	7	4	0	232	-219	6	4	0	65	69	3	13	0	83	-81	-11	0	1	9	1
10	0	0	14	-9	8	4	0	35	9	7	4	0	81	84	4	13	0	15	8	-9	0	1	60	35
12	0	0	52	51	9	4	0	79	-87	8	4	0	68	-65	5	13	0	34	37	-7	0	1	84	-88
2	1	0	114	90	10	4	0	55	53	0	5	0	59	59	6	13	0	72	-72	-6	0	1	204	-193
3	1	0	58	-53	11	4	0	117	120	10	5	0	61	-61	7	13	0	75	75	-3	0	1	253	254
4	1	0	224	-221	12	4	0	17	-20	11	5	0	32	-27	8	13	0	15	-14	2	0	1	268	-258
5	1	0	187	190	13	4	0	35	31	1	6	0	35	38	9	13	0	42	-44	5	0	1	194	196
6	1	0	60	-66	1	5	0	80	88	2	6	0	113	131	0	14	0	82	83	7	0	1	61	63
7	1	0	82	86	2	5	0	439	-445	3	6	0	108	114	1	14	0	44	46	9	0	1	33	-35
8	1	0	177	169	3	5	0	47	-47	4	6	0	45	-47	2	14	0	58	-59	13	0	1	44	-40
9	1	0	146	-152	4	5	0	76	78	5	6	0	138	-135	3	14	0	68	-65	-13	1	1	56	59
10	1	0	42	-40	5	5	0	86	-85	6	6	0	80	-87	5	14	0	72	-79	-12	1	1	92	-87
11	1	0	46	-47	7	5	0	225	222	7	6	0	94	-92	6	14	0	29	-22	-11	1	1	24	-31
12	1	0	57	-57	7	5	0	35	34	8	6	0	71	17	7	14	0	78	82	-10	1	1	44	-38
13	1	0	70	68	8	5	0	38	-34	0	7	0	149	152	8	14	0	32	25	-9	1	1	102	-87
1	2	0	592	594	9	5	0	15	9	11	7	0	40	35	8	14	0	16	46	-8	1	1	178	178
2	2	0	68	62	10	5	0	19	-4	0	10	0	242	-277	1	15	0	114	-111	-7	1	1	109	109
3	2	0	911	912	11	5	0	12	6	1	10	0	148	-148	2	15	0	107	108	-6	1	1	70	73
4	2	0	86	-87	0	6	0	172	169	2	10	0	94	98	3	15	0	161	58	-5	1	1	72	75
5	2	0	222	-221	2	6	0	76	-75	3	10	0	36	-30	4	15	0	26	-33	-4	1	1	124	-139
6	2	0	158	-161	3	6	0	136	140	4	10	0	185	192	5	15	0	52	49	-3	1	1	152	-148
7	2	0	16	-21	4	6	0	37	-33	5	10	0	53	55	6	15	0	46	-47	-2	1	1	102	-90
8	2	0	37	35	5	6	0	22	27	7	10	0	31	29	7	15	0	25	-31	2	1	1	42	37
9	2	0	54	52	6	6	0	241	246	8	10	0	80	-87	8	15	0	19	17	3	1	1	142	-148
10	2	0	94	94	7	6	0	123	-120	9	10	0	32	-4	0	16	0	13	8	4	1	1	135	135
11	2	0	27	-26	8	6	0	41	-40	10	10	0	17	15	1	16	0	13	-23	5	1	1	77	77
12	2	0	28	-30	9	6	0	48	-48	11	10	0	10	-5	2	16	0	30	45	6	1	1	74	-73
13	2	0	25	24	10	6	0	197	-194	1	11	0	13	42	3	16	0	31	26	7	1	1	108	113
1	3	0	961	-958	11	6	0	69	66	2	11	0	30	-32	4	16	0	26	-28	8	1	1	174	-180
2	3	0	181	-183	12	6	0	35	37	3	11	0	32	-36	5	16	0	16	-12	9	1	1	67	-69
3	3	0	449	449	1	7	0	207	224	4	11	0	134	148	8	16	0	13	21	10	1	1	41	38
4	3	0	154	-151	2	7	0	70	68	5	11	0	44	-46	1	17	0	66	-67	11	1	1	26	-30
5	3	0	21	14	3	7	0	230	-229	6	11	0	21	-29	2	17	0	84	89	12	1	1	57	59
6	3	0	105	108	4	7	0	141	-140	8	11	0	174	-167	3	17	0	45	45	13	1	1	56	54
7	3	0	143	-143	5	7	0	124	-120	0	12	0	23	24	4	17	0	20	27	-13	2	1	39	27
8	3	0	102	105	6	7	0	11	14	10	11	0	32	33	5	17	0	57	54	-12	2	1	57	51
9	3	0	42	44	7	7	0	84	83	11	11	0	10	10	6	17	0	38	32	-11	2	1	81	77
10	3	0	37	-36	8	7	0	58	61	0	12	0	120	116	7	17	0	15	-13	-10	2	1	16	-13
11	3	0	16	2	9	7	0	57	54	1	12	0	161	-160	0	18	0	85	81	-9	2	1	52	54
12	3	0	57	-57	10	7	0	35	-35	2	12	0	46	-48	1	18	0	21	-24	-8	2	1	81	86
13	3	0	41	-34	11	7	0	19	8	3	12	0	137	-137	3	18	0	20	21	-7	2	1	132	-138
1	4	0	112	-123	0	8	0	75	-44	4	12	0	57	-57	4	18	0	24	-40	-6	2	1	43	44
2	4	0	49	-79	1	8	0	219	-212	5	12	0	79	82	5	18	0	41	34	-5	2	1	83	83
3	4	0	80	79	2	8	0	147	149	6	12	0	84	87	1	19	0	10	18	-4	2	1	252	-252
4	4	0	148	143	3	8	0	22	-26	7	12	0	57	58	2	19	0	28	-35	-3	2	1	173	160

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR BEN3

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
-9	2	1	17	14	-7	4	1	44	-35	-7	6	1	153	159	-6	8	1	65	61	4	10	1	131	131
-1	2	1	98	20	-6	4	1	266	-229	-5	6	1	108	-107	-4	8	1	113	-119	5	10	1	101	-103
0	2	1	417	443	-5	4	1	337	339	-4	6	1	132	-134	-3	8	1	156	-166	7	10	1	40	-47
1	2	1	34	-20	-4	4	1	44	-64	-3	6	1	64	-70	-2	8	1	92	-89	8	10	1	70	-80
2	2	1	16	12	-3	4	1	84	-84	-2	6	1	80	-85	-1	8	1	154	-166	9	10	1	26	31
3	2	1	142	-128	-2	4	1	93	96	-1	6	1	48	49	0	8	1	154	157	10	10	1	9	-10
4	2	1	254	-264	-1	4	1	94	-110	0	6	1	46	47	1	8	1	139	146	-13	11	1	30	34
5	2	1	87	-88	0	4	1	48	46	0	6	1	48	48	2	8	1	57	-66	-10	11	1	10	8
6	2	1	44	48	1	4	1	107	111	1	6	1	91	-91	3	8	1	154	170	-9	11	1	106	107
7	2	1	141	148	2	4	1	99	98	2	6	1	88	84	4	8	1	124	-124	-8	11	1	35	-32
8	2	1	53	56	3	4	1	82	86	3	6	1	64	69	5	8	1	53	-51	-7	11	1	71	-76
9	2	1	86	88	4	4	1	97	-89	4	6	1	71	-71	6	8	1	86	94	-6	11	1	12	-19
10	2	1	16	-24	5	4	1	122	-122	5	6	1	130	134	7	8	1	109	-107	-5	11	1	100	-106
11	2	1	78	-78	6	4	1	218	-227	6	6	1	136	-139	8	8	1	12	8	-4	11	1	25	24
12	2	1	22	22	7	4	1	36	37	7	6	1	158	-161	9	8	1	26	-27	-3	11	1	71	68
13	2	1	28	-27	8	4	1	42	44	8	6	1	46	49	10	8	1	66	-65	-2	11	1	82	86
-13	3	1	43	42	9	4	1	48	47	9	6	1	47	-48	11	8	1	41	44	-1	11	1	11	9
-12	3	1	8	18	10	4	1	142	144	10	6	1	48	46	12	8	1	21	25	0	11	1	50	-57
-11	3	1	43	-45	11	4	1	42	-44	11	6	1	42	44	-10	9	1	47	44	1	11	1	68	66
-10	3	1	14	14	12	4	1	29	-31	12	6	1	31	-8	-9	9	1	13	9	2	11	1	74	69
-9	3	1	90	-109	-10	5	1	8	5	-9	7	1	13	18	-8	9	1	141	-144	3	11	1	107	-108
-8	3	1	87	-85	-9	5	1	22	-24	-11	7	1	26	-26	-7	9	1	44	46	4	11	1	43	-78
-7	3	1	27	24	-8	5	1	8	5	-10	7	1	27	27	-6	9	1	33	-34	5	11	1	22	22
-6	3	1	125	131	-7	5	1	104	-104	-9	7	1	79	-73	-5	9	1	44	46	6	11	1	104	108
-5	3	1	178	187	-6	5	1	60	-1	-8	7	1	10	-2	-4	9	1	152	163	11	11	1	61	56
-4	3	1	163	167	-5	5	1	124	127	-7	7	1	19	17	-3	9	1	114	-113	-10	12	1	24	-22
-3	3	1	11	14	-4	5	1	0	12	-6	7	1	161	-162	-2	9	1	16	11	-9	12	1	44	41
-2	3	1	270	-304	-3	5	1	261	263	-5	7	1	74	74	-1	9	1	93	98	-8	12	1	44	-50
-1	3	1	179	-182	-2	5	1	164	164	-4	7	1	30	-33	1	9	1	90	97	-7	12	1	38	37
0	3	1	8	-12	-1	5	1	274	-279	-3	7	1	103	101	2	9	1	57	-51	-6	12	1	83	-91
1	3	1	175	-182	0	5	1	0	2	-2	7	1	13	-11	3	9	1	112	-112	-5	12	1	157	153
2	3	1	273	283	1	5	1	270	-295	-1	7	1	102	-102	4	9	1	166	-166	-3	12	1	15	-13
3	3	1	12	12	2	5	1	177	-187	0	7	1	86	-93	5	9	1	52	46	-2	12	1	87	92
4	3	1	169	-182	3	5	1	269	265	1	7	1	11	3	6	9	1	38	35	-1	12	1	234	-234
5	3	1	158	167	4	5	1	13	-11	2	7	1	81	76	7	9	1	52	45	1	12	1	83	-83
6	3	1	154	-153	5	5	1	137	134	3	7	1	146	142	8	9	1	144	146	2	12	1	11	-12
7	3	1	27	24	6	5	1	49	44	4	7	1	65	62	9	9	1	11	7	3	12	1	153	153
8	3	1	88	88	7	5	1	110	-110	5	7	1	42	-41	10	9	1	43	-45	5	12	1	83	84
9	3	1	174	-180	8	5	1	10	8	10	7	1	31	-28	-9	10	1	24	-30	7	12	1	46	-40
10	3	1	17	-18	9	5	1	90	-94	11	7	1	27	-25	-8	10	1	29	-30	8	12	1	51	-49
11	3	1	47	-45	10	5	1	11	-5	12	7	1	30	-28	-7	10	1	40	45	9	12	1	30	-30
12	3	1	10	-15	11	5	1	0	-7	-12	8	1	26	24	-6	10	1	95	102	10	12	1	10	-23
13	3	1	46	42	12	5	1	11	-7	-11	8	1	10	-8	-4	10	1	124	132	-9	13	1	27	29
-12	4	1	20	-20	-12	6	1	19	-7	-10	8	1	69	-66	-3	10	1	130	-127	-8	13	1	68	73
-11	4	1	44	47	-11	6	1	96	-93	-9	8	1	32	28	-1	10	1	148	-179	-7	13	1	10	17
-10	4	1	130	141	-10	6	1	87	85	-8	8	1	12	10	0	10	1	183	-187	-6	13	1	10	-12
-9	4	1	47	-47	-9	6	1	54	55	-7	8	1	104	107	1	10	1	154	161	-5	13	1	78	-74
-8	4	1	49	53	-8	6	1	46	49	-6	8	1	89	90	3	10	1	123	126	-4	13	1	71	-65

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEN3

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
-9	19	1	84	-81	4	18	1	18	17	-5	1	2	143	146	-11	2	2	11	-13	13	4	2	107	-107
-9	19	1	88	82	5	18	1	39	-45	-7	1	2	80	-84	-10	2	2	38	-38	12	4	2	23	17
-1	19	1	118	108	7	18	1	76	74	-4	1	2	206	-194	-9	2	2	33	-29	-12	5	2	11	-9
1	19	1	117	108	-8	17	1	68	62	-4	1	2	133	-134	-8	2	2	98	98	-11	5	2	13	-13
2	19	1	44	-46	-1	17	1	12	-15	-3	1	2	30	-19	-7	2	2	134	134	-10	6	2	26	-27
3	19	1	86	-86	-3	17	1	43	41	-2	1	2	60	62	-5	2	2	102	101	-9	6	2	23	-16
4	19	1	88	84	-2	17	1	84	-82	-1	1	2	108	93	-3	2	2	54	-52	-8	5	2	9	-6
5	19	1	74	-78	-1	17	1	84	-89	1	1	2	98	95	-4	2	2	109	-100	-7	6	2	31	-28
6	19	1	12	23	0	17	1	1	0	2	1	2	84	-86	-5	2	2	211	-217	-6	6	2	165	169
7	19	1	34	17	1	17	1	61	-68	3	1	2	28	-18	-2	2	2	174	-187	-4	6	2	28	22
8	19	1	79	-98	2	17	1	84	82	4	1	2	118	124	-1	2	2	242	241	-3	6	2	22	24
9	19	1	30	30	3	17	1	64	60	5	1	2	206	-194	0	2	2	17	3	-2	6	2	76	76
-8	18	1	18	-17	4	17	1	15	18	7	1	2	61	-68	1	2	2	241	244	-1	6	2	240	-240
-7	18	1	46	-48	5	17	1	46	0	8	1	2	146	-143	2	2	2	159	160	-3	6	2	141	-138
-6	18	1	88	103	6	17	1	42	-42	9	1	2	129	134	3	2	2	209	-214	0	6	2	4	-1
-5	18	1	28	-26	-5	18	1	44	-38	10	1	2	28	24	4	2	2	97	96	1	6	2	144	-144
-3	18	1	74	71	-3	18	1	62	68	11	1	2	68	61	5	2	2	53	-50	2	6	2	371	400
-2	18	1	68	-68	-2	18	1	73	74	12	1	2	63	62	6	2	2	98	-103	3	6	2	77	74
-1	18	1	88	86	-1	18	1	68	67	13	1	2	67	-71	7	2	2	196	197	4	6	2	27	-22
1	18	1	56	-54	0	18	1	16	-12	-13	2	2	14	18	8	2	2	100	-84	5	6	2	23	20
2	18	1	91	87	1	18	1	77	-77	-12	2	2	30	28	9	2	2	33	-29	6	6	2	164	-161
3	18	1	67	-70	2	18	1	28	27	-11	2	2	70	68	10	2	2	28	28	7	6	2	30	-29
4	18	1	11	-2	3	18	1	46	-48	-10	2	2	85	-89	11	2	2	11	-12	8	6	2	14	-16
5	18	1	27	28	4	18	1	69	68	-9	2	2	36	36	12	2	2	56	62	10	6	2	28	28
6	18	1	98	103	-3	19	1	29	26	-8	2	2	38	-40	13	2	2	30	26	11	6	2	9	-13
7	18	1	46	44	-2	19	1	20	21	-7	2	2	87	-87	-13	3	2	19	16	-12	6	2	30	-25
8	18	1	14	-11	-1	20	1	30	-33	-6	2	2	120	119	-11	3	2	109	104	-11	6	2	56	51
-7	17	1	34	40	0	20	1	18	12	-5	2	2	183	-177	-10	3	2	46	-52	-10	6	2	129	124
-6	17	1	67	62	2	19	1	21	-22	-4	2	2	74	74	-9	3	2	74	-74	-9	6	2	41	-38
-5	17	1	28	-25	3	19	1	16	9	-3	2	2	172	173	-8	3	2	11	12	-8	6	2	36	34
-4	17	1	74	-74	-12	0	2	29	-27	-2	2	2	101	-100	-7	3	2	142	-145	-7	6	2	116	-116
-2	17	1	142	-138	-10	0	2	9	-1	-1	2	2	307	320	-6	3	2	83	82	-6	6	2	145	-146
-1	17	1	46	47	-8	0	2	96	-97	0	2	2	84	-86	-5	3	2	100	101	-5	6	2	12	21
1	17	1	38	37	-6	0	2	14	14	1	2	2	298	-314	-4	3	2	97	-101	-4	6	2	23	12
2	17	1	146	136	-4	0	2	401	392	2	2	2	157	-164	-3	3	2	157	156	-3	6	2	113	112
3	17	1	70	-76	-2	0	2	61	-51	3	2	2	164	-170	-2	3	2	85	-70	-2	6	2	109	114
4	17	1	36	-36	0	0	2	408	-424	4	2	2	66	66	-1	3	2	100	96	-1	6	2	66	63
5	17	1	28	27	2	0	2	97	-94	5	2	2	175	171	0	3	2	20	20	0	6	2	39	-45
6	17	1	56	-62	4	0	2	374	392	6	2	2	193	190	1	3	2	66	-65	1	6	2	65	64
7	17	1	40	38	6	0	2	23	-23	7	2	2	76	68	2	3	2	64	-64	2	6	2	114	114
-7	16	1	64	-79	8	0	2	93	-95	8	2	2	42	-40	3	3	2	157	-156	3	6	2	114	-112
-6	16	1	14	-16	10	0	2	9	-9	9	2	2	38	-38	4	3	2	98	-104	4	6	2	0	13
-5	16	1	51	45	12	0	2	36	-21	10	2	2	46	-48	5	3	2	46	-46	5	6	2	20	-22
-4	16	1	16	4	-11	1	2	46	47	11	2	2	0	0	6	3	2	71	72	6	6	2	138	-138
-3	16	1	64	69	-10	1	2	67	-69	12	2	2	27	26	7	3	2	119	114	7	6	2	116	114
-1	16	1	13	-6	-12	1	2	71	50	13	2	2	26	-19	8	3	2	14	14	8	6	2	41	38
0	16	1	34	-32	-10	1	2	67	-64	14	2	2	24	27	9	3	2	73	75	9	6	2	40	38
3	16	1	48	-49	-8	1	2	134	132	-13	3	2	63	-62	10	3	2	53	-52	10	6	2	124	122

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR DEMO

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
11	5	2	54	[illegible]	-7	0	2	190	-121	4	11	2	120	-115	-8	14	2	21	25	0	17	2	11	-1
12	5	2	24	[illegible]	-6	0	2	33	6	5	11	2	40	37	-5	14	2	72	-67	1	17	2	64	60
-12	7	2	44	-7	-5	0	2	80	80	6	11	2	15	17	-4	14	2	54	52	2	17	2	80	78
-11	7	2	19	[illegible]	-4	0	2	58	-58	7	11	2	13	7	-3	14	2	46	-41	3	17	2	28	-25
-10	7	2	38	-34	-3	0	2	130	140	8	11	2	141	136	-1	14	2	35	25	4	17	2	24	-27
-9	7	2	95	-96	-2	0	2	37	-30	9	11	2	19	-14	0	14	2	88	-78	5	17	2	60	-56
-8	7	2	93	98	-1	0	2	74	-73	10	11	2	27	-29	1	14	2	26	-24	6	17	2	17	20
-7	7	2	71	-70	-2	0	2	67	66	-10	12	2	39	44	2	14	2	18	-26	-6	17	2	24	24
-6	7	2	139	141	-1	0	2	30	-30	-9	12	2	14	-6	3	14	2	33	44	-4	18	2	61	59
-5	7	2	64	-67	1	0	2	24	-30	-7	12	2	63	67	4	14	2	52	-63	-3	18	2	15	20
-3	7	2	171	173	2	0	2	90	-97	-6	12	2	57	-60	5	14	2	79	57	0	18	2	53	-79
-2	7	2	19	22	3	0	2	77	-73	-5	12	2	69	67	6	14	2	23	25	1	18	2	15	11
-1	7	2	192	-190	4	0	2	52	55	-4	12	2	52	64	7	14	2	85	-79	2	18	2	26	-20
0	7	2	12	-2	5	0	2	146	143	-3	12	2	141	-129	8	14	2	34	30	3	18	2	60	64
1	7	2	203	-202	6	0	2	88	88	-2	12	2	83	85	9	14	2	45	-40	5	18	2	17	-25
2	7	2	15	-18	7	0	2	86	84	-1	12	2	141	-131	-9	15	2	10	7	-8	19	2	41	30
3	7	2	171	178	8	0	2	192	-118	0	12	2	98	-89	-7	15	2	34	34	-7	19	2	40	-38
4	7	2	87	88	10	0	2	8	-8	1	12	2	125	126	-6	15	2	47	-49	-6	19	2	42	36
5	7	2	142	147	-11	1	2	43	-44	2	12	2	49	45	-5	15	2	84	-86	-5	19	2	26	30
6	7	2	7	-3	-10	1	2	11	2	3	12	2	139	136	-4	15	2	10	-14	-4	19	2	40	-37
7	7	2	71	-71	-9	1	2	67	60	4	12	2	47	47	-3	15	2	84	-91	-3	0	3	15	6
8	7	2	54	54	-8	1	2	34	49	5	12	2	82	-88	-2	15	2	67	65	-2	0	3	34	-38
9	7	2	30	-34	-7	1	2	33	4	6	12	2	77	-81	-1	15	2	107	96	-1	0	3	84	81
10	7	2	29	28	-6	1	2	67	72	7	12	2	64	-68	0	15	2	108	98	0	0	3	207	220
12	7	2	44	46	-5	1	2	180	-179	8	12	2	32	-1	1	15	2	90	-86	-9	0	3	212	-224
-12	8	2	44	-46	-4	1	2	161	-48	9	12	2	10	4	2	15	2	79	-75	-8	0	3	334	-327
-10	8	2	63	64	-3	1	2	110	-117	10	12	2	47	49	4	15	2	15	11	-7	0	3	230	220
-9	8	2	67	67	0	1	2	202	230	-9	13	2	46	43	5	15	2	80	-84	-6	0	3	217	225
-8	8	2	46	43	1	1	2	131	127	-8	13	2	24	-24	6	15	2	47	48	-5	0	3	232	-222
-7	8	2	32	27	2	1	2	300	47	-7	13	2	81	-80	7	15	2	32	32	-4	0	3	45	41
-6	8	2	86	-84	4	1	2	181	-178	-6	13	2	80	-87	8	15	2	12	-5	-3	0	3	38	34
-5	8	2	139	-137	5	1	2	75	-80	-5	13	2	36	-36	-11	16	2	81	11	-2	0	3	3	-1
-4	8	2	181	-180	6	1	2	37	37	-4	13	2	50	71	-6	16	2	16	15	-1	0	3	37	36
-3	8	2	48	48	7	1	2	37	-42	-2	13	2	148	136	-4	16	2	19	16	-13	1	3	51	-52
-1	8	2	141	146	8	1	2	80	8	-1	13	2	11	-27	-2	16	2	34	-37	-12	1	3	57	60
0	8	2	168	176	10	1	2	10	0	0	13	2	13	-1	-1	16	2	14	-26	-11	1	3	47	48
2	8	2	146	-147	-10	1	2	22	10	1	13	2	21	-20	1	16	2	26	20	-10	1	3	40	38
3	8	2	9	9	-9	1	2	11	11	2	13	2	193	-134	2	16	2	24	-26	-9	1	3	101	102
4	8	2	44	-44	-8	1	2	124	-134	3	13	2	71	68	4	16	2	21	14	-8	1	3	163	-158
6	8	2	164	-170	-7	1	2	13	-1	4	13	2	15	-7	5	16	2	15	-14	-7	1	3	114	-116
7	8	2	146	140	-6	1	2	34	-17	5	13	2	35	-32	6	16	2	78	80	-6	1	3	112	-109
8	8	2	90	-95	-5	1	2	95	98	6	13	2	86	85	7	16	2	16	8	-5	1	3	70	-72
9	8	2	27	-28	-4	1	2	129	118	7	13	2	64	-66	-8	17	2	24	24	-4	1	3	172	168
10	8	2	65	61	-3	1	2	26	30	8	13	2	27	26	-7	17	2	44	-47	-3	1	3	83	79
11	8	2	46	-47	-2	1	2	11	1	9	13	2	44	41	-6	17	2	26	28	-2	1	3	20	13
12	8	2	60	53	-1	1	2	51	-54	-9	14	2	33	33	-5	17	2	46	-37	-1	1	3	114	-111
11	9	2	50	46	1	1	2	46	-51	-8	14	2	20	-30	-3	17	2	26	-26	0	1	3	7	1
-11	9	2	49	-46	2	1	2	76	74	-7	14	2	84	80	-1	17	2	60	60	1	1	3	108	-108

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEN3

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	1	3	A	-11	2	3	3	266	-268	1	5	3	268	268	2	7	3	288	288	7	8	3	35	-35
3	1	3	94	96	3	3	3	65	-65	2	5	3	152	154	3	7	3	68	67	8	8	3	134	-137
4	1	3	180	-189	4	3	3	85	85	3	5	3	238	-237	4	7	3	78	-74	10	8	3	38	37
5	1	3	79	-78	5	3	3	156	-158	4	5	3	77	77	5	7	3	131	-130	11	8	3	10	3
6	1	3	110	107	6	3	3	214	216	5	5	3	106	-100	6	7	3	68	67	-10	10	3	10	3
7	1	3	111	-116	7	3	3	31	-29	6	5	3	42	-42	8	7	3	67	73	-9	10	3	28	26
8	1	3	162	160	8	3	3	76	76	7	5	3	91	90	10	7	3	11	12	-8	10	3	29	28
9	1	3	100	102	9	3	3	109	107	8	5	3	18	13	11	7	3	21	25	-7	10	3	38	-33
10	1	3	30	-30	11	3	3	47	41	9	5	3	26	18	12	7	3	22	17	-6	10	3	12	-8
11	1	3	50	51	12	3	3	72	71	10	5	3	12	-7	-11	8	3	32	40	-5	10	3	110	-113
12	1	3	46	-42	-12	4	3	29	21	11	5	3	8	9	-10	8	3	57	59	-4	10	3	124	-126
13	1	3	60	-59	-11	4	3	38	-37	12	5	3	8	13	-9	8	3	29	31	-3	10	3	123	123
-12	2	3	21	-27	-10	4	3	134	-134	-12	6	3	12	12	-8	8	3	11	-8	-2	10	3	142	134
-11	2	3	75	-72	-9	4	3	38	34	-11	6	3	82	84	-7	8	3	42	-44	0	10	3	157	174
-10	2	3	19	16	-8	4	3	46	-53	-10	6	3	78	-77	-6	8	3	94	-96	1	10	3	156	-157
-9	2	3	182	181	-7	4	3	28	29	-9	6	3	73	-73	-5	8	3	50	48	2	10	3	12	-8
-8	2	3	72	-68	-6	4	3	203	203	-8	6	3	36	-33	-4	8	3	114	114	3	10	3	122	-122
-7	2	3	137	131	-5	4	3	114	-109	-7	6	3	124	-125	-3	8	3	162	170	4	10	3	120	-121
-6	2	3	63	-61	-4	4	3	41	40	-6	6	3	111	107	-2	8	3	78	84	5	10	3	110	114
-5	2	3	49	-49	-3	4	3	97	97	-5	6	3	132	130	-1	8	3	124	127	6	10	3	17	4
-4	2	3	288	284	-2	4	3	100	-101	-4	6	3	55	52	0	8	3	175	-177	7	10	3	34	33
-3	2	3	191	-178	-1	4	3	156	156	-3	6	3	64	66	1	8	3	131	-128	8	10	3	28	27
-2	2	3	6	6	0	4	3	139	-139	-2	6	3	33	32	2	8	3	39	44	9	10	3	20	-26
-1	2	3	46	46	1	4	3	246	-246	-1	6	3	98	-96	3	8	3	178	-172	10	10	3	20	4
0	2	3	119	-128	2	4	3	104	-101	0	6	3	108	-113	4	8	3	131	117	-9	11	3	100	-108
1	2	3	94	94	3	4	3	93	93	1	6	3	83	85	5	8	3	81	98	-8	11	3	11	25
2	2	3	46	46	4	4	3	61	64	2	6	3	54	52	6	8	3	65	64	-7	11	3	72	73
3	2	3	175	176	5	4	3	129	129	3	6	3	68	66	7	8	3	87	84	-6	11	3	23	21
4	2	3	257	251	6	4	3	202	202	4	6	3	64	64	8	8	3	31	29	-5	11	3	108	108
5	2	3	87	86	7	4	3	47	47	5	6	3	129	-130	9	8	3	45	44	-4	11	3	34	34
6	2	3	46	-46	8	4	3	61	61	6	6	3	119	119	10	8	3	66	69	-3	11	3	40	-39
7	2	3	134	-129	9	4	3	37	38	7	6	3	124	120	11	8	3	35	38	-2	11	3	56	52
8	2	3	72	72	10	4	3	140	137	8	6	3	32	30	12	8	3	30	30	-1	11	3	20	22
9	2	3	62	62	11	4	3	38	34	9	6	3	70	72	-11	9	3	38	39	0	11	3	54	52
10	2	3	74	76	12	4	3	99	90	10	6	3	77	78	-10	9	3	130	128	2	11	3	56	55
11	2	3	28	27	-12	5	3	52	54	-11	7	3	91	92	-9	9	3	28	29	3	11	3	54	49
-12	3	3	21	-24	-11	5	3	11	3	-12	7	3	15	17	-8	9	3	27	25	4	11	3	101	107
-11	3	3	46	41	-10	5	3	10	1	-11	7	3	22	24	-7	9	3	47	46	5	11	3	22	23
-10	3	3	119	107	-9	5	3	59	58	-10	7	3	23	23	-6	9	3	141	-140	7	11	3	74	73
-9	3	3	72	76	-8	5	3	32	-12	-9	7	3	73	74	-5	9	3	93	91	8	11	3	76	76
-8	3	3	31	-31	-7	5	3	91	86	-8	7	3	10	-9	-4	9	3	17	-15	9	11	3	104	-107
-7	3	3	193	-197	-6	5	3	49	51	-7	7	3	85	89	-3	9	3	80	-87	-10	12	3	14	19
-6	3	3	134	-136	-5	5	3	108	-108	-6	7	3	192	192	2	9	3	87	-86	-8	12	3	33	-32
-5	3	3	90	-93	-4	5	3	10	2	-5	7	3	78	-75	3	9	3	18	15	-6	12	3	57	56
-4	3	3	49	49	-3	5	3	249	-239	-4	7	3	9	6	4	9	3	89	89	-5	12	3	34	-34
-3	3	3	270	271	-2	5	3	157	-152	-3	7	3	64	64	5	9	3	140	142	-4	12	3	23	16
-2	3	3	170	166	-1	5	3	263	267	-2	7	3	267	-266	6	9	3	56	56	-3	12	3	74	72
1	3	3	167	164	0	5	3	10	-3	-1	7	3	19	-12	8	9	3	28	-28	-2	12	3	138	-132

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REM3

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-1	12	9	70	-72	-2	15	9	331	124	2	0	4	21	-21	5	2	4	134	-136	6	4	4	95	94
0	12	9	144	144	-1	15	9	81	-83	4	0	4	286	-290	7	2	4	43	-39	8	4	4	70	72
1	12	9	73	79	1	15	9	58	-60	6	0	4	32	31	8	2	4	48	47	9	4	4	102	-102
2	12	9	132	-130	2	15	9	117	-123	8	0	4	98	95	9	2	4	38	36	7	4	4	168	-166
5	12	9	64	-70	3	15	9	58	58	10	0	4	28	27	10	2	4	78	78	8	4	4	10	-2
6	12	9	114	-114	5	15	9	27	26	12	0	4	64	64	11	2	4	18	-14	9	4	4	76	-73
7	12	9	41	46	6	15	9	82	83	-11	1	4	97	-97	10	2	4	24	-25	10	4	4	41	40
A	12	9	57	56	7	15	9	37	-35	-10	1	4	28	30	-12	3	4	67	60	11	4	4	99	99
9	12	9	35	34	A	15	9	23	9	-9	1	4	196	-192	-11	3	4	21	15	12	4	4	20	-18
10	12	9	22	20	-7	16	9	84	72	-8	1	4	195	-194	-10	3	4	29	29	-12	5	4	23	17
-C	13	9	31	-32	-6	16	9	14	8	-7	1	4	60	-57	-9	3	4	35	33	-10	5	4	12	4
-B	13	9	84	-79	-5	16	9	62	-66	-6	1	4	15	15	-8	3	4	61	-62	-9	5	4	23	11
-A	13	9	46	-43	-4	16	9	16	-15	-5	1	4	177	177	-7	3	4	107	-115	-8	5	4	32	29
-E	13	9	10	14	-3	16	9	44	-46	-4	1	4	129	130	-6	3	4	88	-89	-7	5	4	30	28
-9	13	9	69	70	-2	16	9	12	12	-3	1	4	47	-48	-5	3	4	50	44	-6	5	4	156	-154
-8	13	9	84	86	-1	16	9	31	27	-2	1	4	81	-80	-4	3	4	77	73	-5	5	4	26	-26
-7	13	9	68	78	3	16	9	30	24	-1	1	4	80	83	-3	3	4	242	225	-4	5	4	32	-34
-6	13	9	74	-63	4	16	9	16	-14	0	1	4	F	1	-2	3	4	131	132	-3	5	4	84	-83
-5	13	9	100	-99	5	16	9	42	40	1	1	4	61	-64	-1	3	4	207	-199	-2	5	4	157	162
-4	13	9	81	-82	6	16	9	12	9	2	1	4	87	78	0	3	4	2	2	-1	5	4	84	83
-3	13	9	52	49	7	16	9	74	-72	3	1	4	47	-48	1	3	4	209	-200	0	5	4	7	1
-2	13	9	80	78	-8	17	9	58	-60	4	1	4	127	-126	2	3	4	132	-130	1	5	4	84	84
-1	13	9	60	-62	-7	17	9	15	18	5	1	4	170	172	3	3	4	256	250	2	5	4	161	-162
0	13	9	40	36	-6	17	9	71	-64	6	1	4	18	-16	4	3	4	73	71	3	5	4	44	-41
1	13	9	17	-16	-5	17	9	26	27	7	1	4	82	80	5	3	4	43	44	4	5	4	31	33
2	13	9	30	-27	-4	17	9	69	64	A	1	4	136	137	6	3	4	98	92	5	5	4	32	-35
3	13	9	80	72	0	17	9	14	6	9	1	4	135	-133	7	3	4	114	-113	6	5	4	156	159
4	13	9	40	-33	1	17	9	66	66	10	1	4	29	-30	8	3	4	94	92	7	5	4	33	30
5	13	9	16	22	2	17	9	76	-78	11	1	4	43	-42	9	3	4	34	34	8	5	4	21	-24
-7	14	9	44	45	3	17	9	56	-54	12	1	4	62	-60	10	3	4	38	-39	9	5	4	111	10
-6	14	9	100	-104	4	17	9	25	-27	-12	2	4	28	-29	11	3	4	21	15	11	5	4	13	17
-5	14	9	88	94	5	17	9	67	66	-11	2	4	21	16	-12	4	4	64	-60	-12	6	4	32	29
-4	14	9	11	8	-9	18	9	55	-57	-10	2	4	50	46	-11	4	4	28	28	-11	6	4	52	-53
-3	14	9	61	-66	-1	18	9	68	-66	-9	2	4	41	-37	-10	4	4	104	-100	-10	6	4	115	-114
-2	14	9	51	50	0	18	9	17	10	-8	2	4	47	44	-9	4	4	39	40	-9	6	4	39	42
-1	14	9	37	-40	1	18	9	57	56	-7	2	4	93	91	-8	4	4	77	76	-8	6	4	29	-27
0	14	9	16	-25	2	18	9	44	47	-6	2	4	220	-226	-7	4	4	19	-5	-7	6	4	84	83
1	14	9	55	48	-7	19	9	14	-22	-5	2	4	188	187	-6	4	4	168	167	-6	6	4	140	138
2	14	9	42	48	-1	19	9	19	19	-4	2	4	62	-64	-5	4	4	49	-50	-5	6	4	26	-29
3	14	9	60	63	0	19	9	15	1	-3	2	4	178	-178	-4	4	4	73	-72	-4	6	4	21	-21
4	14	9	28	-28	1	19	9	37	35	-2	2	4	86	84	-3	4	4	102	97	-3	6	4	116	-120
5	14	9	104	-104	2	19	9	24	27	-1	2	4	297	-284	-2	4	4	152	-147	-2	6	4	72	-67
7	14	9	40	-46	-12	0	4	22	22	0	2	4	37	41	-1	4	4	94	94	-1	6	4	46	-46
A	14	9	23	21	-11	0	4	68	68	1	2	4	261	264	-1	4	4	7	-1	0	6	4	41	44
-7	15	9	57	-55	-10	0	4	31	28	2	2	4	52	52	0	4	4	98	-98	1	6	4	48	48
-6	15	9	88	-86	-9	0	4	378	-380	3	2	4	174	177	1	4	4	10	6	2	6	4	58	-64
-5	15	9	30	27	-8	0	4	24	-23	4	2	4	61	-60	2	4	4	93	92	3	6	4	117	117
-4	15	9	68	68	-7	0	4	494	496	5	2	4	140	-138	3	4	4	144	147	4	6	4	17	-29

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEM3

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
5	6	A	26	30	6	A	A	30	-26	-6	11	A	27	25	8	13	A	14	-21	3	17	A	35	36
6	6	A	178	186	7	A	A	61	66	-5	11	A	24	-30	9	13	A	41	-45	4	17	A	31	33
7	6	A	47	-36	8	A	A	84	-83	-4	11	A	126	-132	-8	14	A	44	44	5	17	A	49	44
8	6	A	26	-27	11	A	A	40	44	-3	11	A	39	-38	-7	14	A	74	-77	-4	18	A	46	-49
9	6	A	61	-61	-11	B	A	46	37	-2	11	A	21	24	-6	14	A	15	-17	0	18	A	87	80
10	6	A	143	-134	-10	B	A	12	7	-1	11	A	28	24	-5	14	A	63	62	1	18	A	14	-12
11	6	A	55	52	-9	B	A	134	117	0	11	A	24	29	-4	14	A	54	-54	2	18	A	13	2
12	6	A	26	28	-8	B	A	10	-16	2	11	A	26	-23	-3	14	A	41	43	3	18	A	14	18
-10	7	A	29	25	-7	B	A	77	-77	3	11	A	38	40	-2	14	A	23	19	4	18	A	44	-50
-9	7	A	17	10	-6	B	A	48	44	4	11	A	124	119	-1	14	A	54	-43	-9	0	R	39	36
-8	7	A	74	-78	-5	B	A	304	-304	5	11	A	29	-30	0	14	A	64	61	-7	0	R	26	-21
-7	7	A	64	64	-4	B	A	32	3	6	11	A	29	-24	1	14	A	39	42	-5	0	R	154	-166
-6	7	A	105	-103	-3	B	A	85	84	7	11	A	19	14	2	14	A	49	-42	-3	0	R	190	184
-5	7	A	42	41	-2	B	A	91	-102	8	11	A	122	-123	3	14	A	58	-52	-1	0	R	304	307
-4	7	A	141	-143	-1	B	A	40	36	9	11	A	24	22	5	14	A	80	-84	1	0	R	201	-201
-3	7	A	21	-20	0	B	A	19	-17	10	11	A	28	32	6	14	A	18	-19	2	0	R	190	-184
-2	7	A	208	206	1	B	A	10	18	-7	12	A	26	-27	7	14	A	75	78	3	0	R	152	157
-1	7	A	10	-2	2	B	A	104	104	-6	12	A	57	57	8	14	A	33	30	7	0	R	70	79
0	7	A	206	203	3	B	A	77	82	-5	12	A	66	-68	-7	15	A	32	-28	8	0	R	46	-42
1	7	A	21	21	4	B	A	177	-176	-4	12	A	56	-58	-6	15	A	66	63	-11	1	R	12	6
2	7	A	133	-136	5	B	A	67	-67	-3	12	A	110	110	-5	15	A	69	64	-10	1	R	77	-67
3	7	A	74	74	7	B	A	73	-77	-2	12	A	29	-29	-4	15	A	12	12	-11	1	R	33	-30
4	7	A	145	-150	8	B	A	74	71	-1	12	A	108	114	-3	15	A	85	82	-10	1	R	37	37
5	7	A	10	6	-8	B	A	111	118	0	12	A	90	91	-2	15	A	86	-88	-9	1	R	82	-86
6	7	A	58	57	-11	B	A	96	97	1	12	A	111	-113	-1	15	A	87	-83	-8	1	R	132	144
7	7	A	78	77	-10	B	A	17	9	2	12	A	20	-19	0	15	A	74	-74	-7	1	R	82	81
8	7	A	24	20	-9	B	A	11	10	3	12	A	113	-111	1	15	A	78	81	-6	1	R	77	79
10	7	A	97	-96	-8	B	A	88	-87	4	12	A	60	-60	2	15	A	74	80	-5	1	R	80	84
11	7	A	11	0	-7	B	A	70	71	5	12	A	79	80	3	15	A	15	-17	-4	1	R	104	-100
-11	8	A	45	44	-6	B	A	12	-18	6	12	A	68	66	4	15	A	47	47	-3	1	R	129	-134
-10	8	A	68	-63	-5	B	A	147	-155	7	12	A	51	50	5	15	A	43	-43	-2	1	R	53	-46
-9	8	A	84	-84	-4	B	A	167	168	8	12	A	16	7	7	15	A	30	-30	-1	1	R	47	50
-8	8	A	40	-38	-3	B	A	85	86	-9	13	A	49	-47	-6	15	A	51	49	0	1	R	7	3
-7	8	A	42	-44	-2	B	A	32	35	-8	13	A	21	21	-5	15	A	15	-11	1	1	R	46	44
-6	8	A	54	54	-1	B	A	101	108	-7	13	A	60	64	-3	15	A	35	37	2	1	R	50	41
-5	8	A	134	142	0	B	A	217	-223	-6	13	A	77	77	-2	15	A	11	14	3	1	R	126	-133
-4	8	A	121	132	1	B	A	111	-106	-5	13	A	31	33	0	16	A	30	30	4	1	R	101	111
-3	8	A	7	-16	2	B	A	34	34	-4	13	A	14	-8	1	16	A	14	-15	5	1	R	56	53
-2	8	A	36	38	3	B	A	98	-98	-3	13	A	70	-70	2	16	A	11	7	6	1	R	55	-57
-1	8	A	146	-142	4	B	A	166	166	-2	13	A	108	-108	3	16	A	19	11	7	1	R	47	53
0	8	A	109	-107	5	B	A	58	57	-1	13	A	93	98	4	16	A	72	-81	8	1	R	100	-106
1	8	A	186	174	6	B	A	24	-19	0	13	A	18	21	5	16	A	44	44	-11	2	R	48	-48
2	8	A	30	-33	7	B	A	31	32	1	13	A	105	111	-4	17	A	33	-33	10	2	R	40	40
3	8	A	34	36	8	B	A	44	-46	2	13	A	76	-73	-3	17	A	36	36	11	2	R	29	-33
4	8	A	135	135	-10	B	A	11	4	3	13	A	14	11	-2	17	A	52	56	12	2	R	50	55
5	8	A	162	-162	-10	B	A	35	-32	4	13	A	50	52	-1	17	A	50	-50	-12	3	R	35	34
6	8	A	72	71	-9	B	A	25	29	5	13	A	67	-70	1	17	A	81	-80	-11	3	R	63	59
7	8	A	61	63	-8	B	A	126	121	7	13	A	50	50	2	17	A	77	-76	-10	3	R	45	48

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR BEN3

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-15	2	5	68	66	-8	4	5	39	-36	-2	8	5	82	83	1	8	5	130	136	-8	11	5	98	97
-14	2	5	117	-122	-7	4	5	38	34	-1	8	5	66	60	2	8	5	69	-68	-7	11	5	15	-20
-13	2	5	58	60	-6	4	5	32	-35	0	8	5	61	65	3	8	5	124	124	-6	11	5	84	-89
-12	2	5	90	83	-5	4	5	172	-171	1	8	5	97	-99	4	8	5	108	-108	-5	11	5	20	-22
-11	2	5	202	-210	-4	4	5	114	114	2	8	5	43	42	5	8	5	32	-26	-4	11	5	85	-87
-10	2	5	97	98	-3	4	5	74	-75	3	8	5	46	44	6	8	5	85	87	-3	11	5	89	85
-9	2	5	16	-20	-2	4	5	47	-41	4	8	5	58	-61	7	8	5	70	-71	-2	11	5	43	42
-8	2	5	0	4	-1	4	5	83	82	5	8	5	117	117	8	8	5	10	10	-1	11	5	14	0
-7	2	5	93	92	0	4	5	87	-87	6	8	5	74	-76	9	8	5	19	-21	0	11	5	50	-46
-6	2	5	0	-4	1	4	5	15	9	7	8	5	117	-117	10	8	5	52	-56	1	11	5	71	64
-5	2	5	16	-16	2	4	5	86	80	8	8	5	29	27	11	8	5	28	35	2	11	5	89	-86
-4	2	5	68	-71	3	4	5	11	22	9	8	5	62	-61	-10	9	5	41	36	3	11	5	20	21
-3	2	5	206	-211	4	4	5	44	40	10	8	5	67	64	-9	9	5	133	-134	4	11	5	63	-64
-2	2	5	66	-67	5	4	5	73	-71	11	8	5	80	78	-7	9	5	39	32	5	11	5	20	20
-1	2	5	97	97	6	4	5	110	-111	-11	7	5	14	-23	-6	9	5	95	-92	6	11	5	86	87
0	2	5	125	122	7	4	5	168	-170	-10	7	5	15	19	-5	9	5	59	-60	7	11	5	36	36
1	2	5	58	56	8	4	5	32	35	-9	7	5	72	-84	-4	9	5	119	122	8	12	5	42	-46
2	2	5	47	49	9	4	5	96	93	-8	7	5	12	2	-3	9	5	64	-66	-7	12	5	36	32
3	2	5	64	-66	10	4	5	34	34	-7	7	5	66	64	-1	9	5	82	82	-6	12	5	20	14
4	2	5	21	17	-10	5	5	118	118	-6	7	5	64	-103	0	9	5	14	-1	-5	12	5	84	-87
-12	3	5	36	37	-9	5	5	36	-32	-5	7	5	50	48	1	9	5	47	46	-4	12	5	121	124
-11	3	5	44	-48	-8	5	5	17	-26	-4	7	5	10	-10	2	9	5	13	-3	-3	12	5	14	-12
-10	3	5	15	8	-7	5	5	11	1	-3	7	5	78	-75	3	9	5	66	-62	-2	12	5	66	61
-9	3	5	76	-78	-6	5	5	10	-2	-2	7	5	240	252	4	9	5	122	-122	-1	12	5	147	-143
-8	3	5	46	-50	-5	5	5	58	-58	-1	7	5	11	-12	5	9	5	42	-38	0	12	5	71	-65
-7	3	5	20	7	-4	5	5	34	31	0	7	5	10	-10	6	9	5	11	9	1	12	5	13	-13
-6	3	5	112	108	-3	5	5	111	107	2	7	5	254	-252	7	9	5	33	33	4	12	5	124	124
-5	3	5	148	143	-2	5	5	30	-28	3	7	5	74	-76	8	9	5	129	116	5	13	5	64	66
-4	3	5	41	42	-1	5	5	213	211	4	7	5	9	8	9	9	5	17	4	6	13	5	17	-35
-3	3	5	29	25	0	5	5	130	123	5	7	5	80	82	10	9	5	32	-34	7	13	5	43	-44
-2	3	5	277	-279	1	5	5	202	-207	6	7	5	104	103	-8	10	5	33	-23	8	13	5	29	-28
-1	3	5	131	-135	2	5	5	7	1	7	7	5	64	64	-7	10	5	20	-21	-7	13	5	69	70
0	3	5	5	-4	3	5	5	202	-208	8	7	5	10	-9	-6	10	5	29	27	-6	13	5	21	19
1	3	5	111	-106	4	5	5	130	-128	9	7	5	66	64	-5	10	5	12	-3	-5	13	5	12	-8
2	3	5	233	234	5	5	5	207	210	10	7	5	12	-19	-4	10	5	44	44	-4	13	5	58	56
3	3	5	24	22	6	5	5	21	26	11	7	5	28	26	-3	10	5	84	102	-3	13	5	54	-54
4	3	5	87	-90	8	5	5	108	106	-11	8	5	33	-35	-2	10	5	92	-83	-2	14	5	71	-72
5	3	5	145	142	9	5	5	34	34	-10	8	5	58	-60	-1	10	5	154	-156	-1	13	5	47	48
6	3	5	102	-104	-11	6	5	28	-28	-9	8	5	16	19	0	10	5	154	156	0	13	5	73	76
7	3	5	12	8	-10	6	5	78	-76	-8	8	5	13	10	1	10	5	154	158	1	13	5	71	77
8	3	5	84	81	-9	6	5	68	63	-7	8	5	76	73	2	10	5	8	-10	2	13	5	61	-60
9	3	5	81	-78	-8	6	5	82	80	-6	8	5	90	89	3	10	5	88	84	3	13	5	74	-72
10	3	5	10	-5	-7	6	5	98	96	-5	8	5	28	27	4	10	5	105	103	4	13	5	56	56
11	3	5	30	-29	-6	6	5	116	117	-4	8	5	102	-101	5	10	5	91	88	5	13	5	61	61
-13	4	5	29	-29	-5	6	5	77	78	-3	8	5	124	-124	6	10	5	13	-12	6	13	5	14	9
-12	4	5	35	-28	-4	6	5	130	-131	-2	8	5	47	-48	7	10	5	52	-56	7	13	5	16	20
-11	4	5	38	32	-3	6	5	60	-60	-1	8	5	134	-136	8	10	5	20	-27	8	13	5	59	-58
-10	4	5	115	114	-2	6	5	68	-68	0	8	5	143	140	9	10	5	15	22	-6	14	5	17	-14

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REM1

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
-7	14	R	46	-40	0	14	R	10	-4	7	2	E	88	-87	7	4	E	136	135	10	6	R	93	92
-6	14	R	50	51	1	14	R	40	-48	8	2	E	141	-136	8	4	E	54	57	11	6	R	44	-44
-5	14	R	27	-21	2	14	R	26	27	9	2	E	90	84	10	4	E	44	-40	-10	7	R	28	-22
-4	14	R	16	-2	3	14	R	67	-63	10	2	E	143	125	11	4	E	46	-41	-9	7	R	16	-20
-3	14	R	46	48	-8	0	E	33	-36	6	3	E	103	101	-11	5	E	17	-7	-8	7	R	70	70
-2	14	R	45	-40	-7	0	E	239	227	7	3	E	28	30	-10	5	E	35	-4	-7	7	R	51	-57
-1	14	R	38	38	-6	0	E	22	17	8	3	E	32	-29	-9	5	E	13	4	-6	7	R	15	8
0	14	R	27	28	-5	0	E	429	-418	9	3	E	29	-31	-8	5	E	20	-20	-5	7	R	49	49
1	14	R	40	-38	-4	0	E	10	11	10	3	E	68	-68	-7	5	E	14	-11	-4	7	R	75	-73
2	14	R	28	28	-3	0	E	295	294	11	3	E	12	13	-6	5	E	131	127	-3	7	R	142	144
3	14	R	41	-38	-2	0	E	26	-24	-11	4	E	12	-7	-5	5	E	35	35	-2	7	R	34	33
4	14	R	17	20	-1	0	E	59	-63	-10	4	E	24	-26	-4	5	E	33	30	-1	7	R	150	-148
5	14	R	17	-7	0	0	E	36	35	-9	4	E	75	-80	-3	5	E	10	11	0	7	R	11	-1
7	14	R	41	40	-10	1	E	23	-25	-8	4	E	73	72	-2	5	E	774	-272	1	7	R	153	-152
9	14	R	13	-15	-9	1	E	91	103	-7	4	E	98	98	-1	5	E	64	-63	2	7	R	37	-33
-7	15	R	34	32	-8	1	E	112	108	-6	4	E	89	91	0	5	E	9	-1	3	7	R	144	142
-6	15	R	47	44	-7	1	E	66	-65	-5	4	E	11	-24	1	5	E	64	-65	4	7	R	70	69
-5	15	R	23	-25	-6	1	E	18	-11	-4	4	E	71	-69	2	5	E	277	272	5	7	R	65	67
-4	15	R	52	-49	-5	1	E	120	-122	-3	4	E	188	-187	3	5	E	60	61	7	7	R	58	-56
-3	15	R	109	-107	-4	1	E	100	-107	-2	4	E	105	-106	4	5	E	35	-30	8	7	R	64	-65
-2	15	R	46	44	-3	1	E	27	22	-1	4	E	147	149	5	5	E	33	32	9	7	R	23	-22
-1	15	R	54	52	-2	1	E	77	80	1	4	E	365	374	6	5	E	125	-126	10	7	R	28	22
0	15	R	104	101	-1	1	E	67	69	2	4	E	107	103	7	5	E	23	-19	-10	8	R	49	45
1	15	R	50	-48	0	1	E	15	-2	3	4	E	194	-183	8	5	E	14	-9	-9	8	R	48	41
2	15	R	15	-8	1	1	E	69	68	4	4	E	71	71	9	5	E	10	-8	-8	8	R	43	36
3	15	R	19	-22	2	1	E	72	-68	6	4	E	27	-27	10	5	E	11	11	-7	8	R	32	30
4	15	R	54	-54	3	1	E	24	23	7	4	E	70	-71	11	5	E	14	-9	-6	8	R	37	-43
7	15	R	31	33	4	1	E	107	105	8	4	E	93	92	-11	6	E	41	42	-5	8	R	115	-107
-8	15	R	27	-27	5	1	E	124	-124	9	4	E	75	-74	-10	6	E	94	90	-4	8	R	110	-109
-6	15	R	60	59	8	1	E	11	14	10	4	E	29	-29	-9	6	E	24	-29	-3	8	R	34	32
-5	15	R	22	14	7	3	E	47	-44	10	3	E	28	23	-8	6	E	24	24	-2	8	R	22	22
-4	15	R	22	18	8	1	E	112	-107	11	3	E	16	-7	-7	6	E	77	-74	-1	8	R	118	113
-3	15	R	16	-26	-8	2	E	107	100	-11	4	E	77	71	-6	6	E	152	-146	0	8	R	134	135
1	15	R	12	5	10	3	E	24	23	-10	4	E	41	-42	-5	6	E	22	23	1	8	R	123	-115
2	15	R	34	-36	11	1	E	48	45	-9	4	E	63	-66	-4	6	E	20	17	2	8	R	23	21
3	15	R	17	19	11	2	E	15	-11	-8	4	E	146	-139	-3	6	E	77	77	3	8	R	31	-34
5	15	R	42	-38	-10	2	E	60	-60	-6	4	E	70	68	-2	6	E	71	69	4	8	R	104	-101
6	15	R	16	-13	-9	2	E	34	32	-5	4	E	74	72	-1	6	E	25	26	5	8	R	105	107
7	15	R	26	-15	-8	2	E	23	-23	-4	4	E	76	77	0	6	E	52	-46	6	8	R	38	-43
-8	17	E	51	55	-7	2	E	32	-29	-3	4	E	110	111	1	6	E	24	-24	7	8	R	30	-31
-7	17	E	20	-16	-6	2	E	100	98	-2	4	E	47	-47	2	6	E	71	68	8	8	R	32	38
-6	17	E	52	-45	-5	2	E	141	-140	-1	4	E	77	72	3	6	E	77	-78	9	8	R	49	-40
1	17	E	47	-47	-4	2	E	46	49	0	4	E	77	75	4	6	E	23	20	10	8	R	43	44
2	17	E	71	64	-3	2	E	138	137	2	4	E	46	-46	5	6	E	25	-31	-10	9	R	15	3
3	17	E	77	69	-2	2	E	77	78	3	4	E	114	-116	6	6	E	144	-145	-9	9	R	105	-97
4	17	E	19	15	-1	2	E	208	201	4	4	E	78	-78	7	6	E	69	77	-8	9	R	17	11
-2	18	R	18	17	0	2	E	46	-44	5	4	E	71	-69	8	6	R	30	28	-7	9	R	58	58
-1	18	R	54	49	1	2	E	268	-260	6	4	E	67	68	9	6	R	31	31	-6	9	R	42	-40

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR OPW3

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-5	0	5	97	98	1	11	5	100	100	-4	14	5	12	-17	1	3	7	84	-86	4	3	7	91	86
-4	0	5	12	-19	2	11	5	16	-18	-3	14	5	84	-84	2	3	7	31	-34	5	3	7	92	-91
-3	0	5	82	-86	-7	12	5	47	43	-2	14	5	64	69	3	3	7	97	95	6	3	7	74	80
-2	0	5	84	87	-6	12	5	51	-52	-1	14	5	72	73	4	3	7	104	-99	7	3	7	20	-21
-1	0	5	98	100	-5	12	5	98	96	1	14	5	72	76	5	3	7	59	-59	8	3	7	60	-62
1	0	5	92	-19	-4	12	5	44	41	2	14	5	76	-71	6	3	7	44	42	9	3	7	57	58
2	0	5	92	-85	-3	12	5	78	-80	3	14	5	51	-54	7	3	7	88	-86	10	3	7	12	12
3	0	5	97	96	-2	12	5	61	64	4	14	5	16	17	8	3	7	100	100	11	3	7	24	24
4	0	5	29	19	-1	12	5	100	-102	5	14	5	32	-36	9	3	7	71	72	-11	4	7	28	-32
5	0	5	95	96	0	12	5	76	-74	6	14	5	36	36	10	3	7	22	-22	-10	4	7	81	-82
6	0	5	47	44	1	12	5	100	100	-5	15	5	12	12	11	3	7	18	18	-9	4	7	32	35
7	0	5	87	86	2	12	5	32	33	-4	15	5	12	-5	12	3	7	44	-44	-8	4	7	43	-41
8	0	5	18	-19	3	12	5	97	93	-3	15	5	30	-31	-10	3	7	21	22	-7	4	7	25	28
9	0	5	84	-85	4	12	5	61	62	-1	15	5	31	-16	-9	3	7	48	44	-6	4	7	144	144
-10	1	5	17	13	5	12	5	51	-44	0	15	5	17	-5	-8	3	7	45	-43	-5	4	7	73	-72
-9	1	5	39	38	6	12	5	66	-61	1	15	5	16	17	-7	3	7	76	75	-4	4	7	17	20
-7	1	5	28	25	7	12	5	44	-44	2	15	5	32	-31	-6	3	7	25	-27	-3	4	7	24	31
-6	1	5	13	14	-7	13	5	23	-25	3	15	5	14	7	-5	3	7	24	-20	-2	4	7	71	-64
-5	1	5	44	47	-6	13	5	47	46	4	15	5	16	15	-4	3	7	169	170	-1	4	7	91	90
-4	1	5	126	-130	-5	13	5	60	-64	-3	17	5	36	-32	-3	3	7	26	-25	0	4	7	27	-33
-3	1	5	27	-27	-4	13	5	39	-36	-2	17	5	62	-60	-2	3	7	34	34	1	4	7	84	-83
-2	1	5	22	-20	-3	13	5	14	7	-1	17	5	47	47	-1	3	7	15	-2	2	4	7	70	69
-1	1	5	88	-81	-2	13	5	64	68	1	17	5	48	47	0	3	7	280	-287	3	4	7	37	-31
0	1	5	177	177	-1	13	5	69	68	2	17	5	16	10	1	3	7	15	1	4	4	7	20	20
1	1	5	47	46	0	13	5	26	-25	3	17	5	36	-32	2	3	7	17	17	5	4	7	7	7
2	1	5	22	-20	1	13	5	96	-92	-6	0	7	13	-21	3	3	7	91	86	6	4	7	144	144
3	1	5	76	68	2	13	5	103	-98	-5	0	7	33	34	4	3	7	174	168	7	4	7	20	-20
4	1	5	114	-112	3	13	5	66	-67	-4	0	7	150	154	5	3	7	34	31	8	4	7	39	40
5	1	5	56	-55	4	13	5	98	-97	-3	0	7	150	-153	6	3	7	37	-35	9	4	7	34	-33
6	1	5	12	13	5	13	5	46	48	-1	0	7	253	-250	7	3	7	74	-77	10	4	7	93	-93
7	1	5	22	-20	6	13	5	72	-68	1	0	7	253	256	8	3	7	44	-42	11	4	7	35	31
8	1	5	33	37	8	13	5	13	10	3	0	7	150	156	9	3	7	43	-42	-10	5	7	11	11
9	1	5	11	4	-7	14	5	65	60	5	0	7	161	-167	10	3	7	19	22	-8	5	7	20	-13
-10	1	5	18	-15	-6	14	5	32	35	7	0	7	34	-37	11	3	7	55	55	-7	5	7	77	77
-9	1	5	170	-171	-5	14	5	22	23	9	0	7	25	23	-11	3	7	27	24	-6	5	7	39	38
-7	1	5	11	8	-4	14	5	44	44	11	0	7	11	-8	-9	3	7	65	66	-5	5	7	76	-75
-6	1	5	30	31	-3	14	5	34	-31	-11	1	7	18	20	-8	3	7	60	60	-4	5	7	11	-13
-4	1	5	91	93	-2	14	5	27	27	-10	1	7	25	22	-7	3	7	20	23	-3	5	7	172	-170
-3	1	5	96	98	-1	14	5	52	-51	-9	1	7	69	72	-6	3	7	81	-78	-2	5	7	61	61
-2	1	5	19	-19	0	14	5	32	-36	-8	1	7	103	-104	-5	3	7	92	-96	-1	5	7	164	163
-1	1	5	27	-27	1	14	5	12	-17	-7	1	7	85	86	-4	3	7	88	-85	0	5	7	166	164
0	1	5	14	0	2	14	5	17	22	-6	1	7	47	-46	-3	3	7	27	25	1	5	7	4	4
1	1	5	34	-29	4	14	5	66	67	-5	1	7	54	-52	-2	3	7	104	108	2	5	7	170	-171
2	1	5	27	31	5	14	5	72	69	-4	1	7	139	140	-1	3	7	97	97	3	5	7	17	11
3	1	5	23	19	6	14	5	19	15	-3	1	7	68	68	0	3	7	14	7	4	5	7	7	-9
4	1	5	92	-84	7	14	5	60	-56	-2	1	7	32	37	1	3	7	89	88	5	5	7	37	-34
5	1	5	31	28	-8	15	5	31	-34	-1	1	7	67	-68	2	3	7	203	-196	6	5	7	71	76
7	1	5	13	8	-6	15	5	40	-38	0	1	7	14	9	3	3	7	28	-23	8	5	7	13	8

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
0	6	7	19	22	-1	6	7	67	65	-6	11	7	15	14	4	14	7	23	10	-8	2	8	22	-9
-10	6	7	49	-42	0	6	7	192	-198	-5	11	7	53	54	5	14	7	14	-11	-7	2	8	34	31
-9	6	7	45	-48	1	6	7	57	-55	-4	11	7	13	-17	6	14	7	54	-71	-6	2	8	26	23
-8	6	7	27	-30	2	6	7	51	47	-3	11	7	51	-54	-5	15	7	12	13	-5	2	8	51	-53
-7	6	7	56	-55	3	6	7	305	-304	-2	11	7	37	-35	-4	15	7	47	52	-4	2	8	44	44
-6	6	7	74	71	4	6	7	66	71	-1	11	7	21	-25	-3	15	7	53	52	-3	2	8	43	-39
-5	6	7	109	98	5	6	7	30	39	0	11	7	17	-15	-2	15	7	30	-43	-2	2	8	98	98
-4	6	7	37	33	6	6	7	61	-67	1	11	7	35	36	-1	15	7	53	5	-1	2	8	45	45
-3	6	7	49	43	7	6	7	63	62	2	11	7	60	-56	0	15	7	45	-46	0	2	8	143	-145
-2	6	7	28	-21	8	6	7	13	-7	3	11	7	24	18	1	15	7	55	-52	1	2	8	39	38
-1	6	7	60	-55	9	6	7	22	16	4	11	7	60	64	2	15	7	55	55	2	2	8	142	140
0	6	7	60	52	10	6	7	44	44	5	11	7	23	-14	3	15	7	29	10	3	2	8	43	44
1	6	7	73	68	-8	7	7	61	100	7	11	7	27	24	-4	16	7	27	-24	4	2	8	100	101
2	6	7	20	-21	-7	7	7	38	-37	-6	12	7	27	30	0	16	7	21	22	6	2	8	41	-39
3	6	7	43	-47	-6	7	7	20	21	-5	12	7	12	-25	1	16	7	17	-10	8	2	8	44	-44
4	6	7	36	34	-5	7	7	31	24	-4	12	7	16	-6	2	16	7	25	29	9	2	8	64	-64
5	6	7	86	-100	-4	7	7	102	-102	-3	12	7	54	54	-10	0	8	15	-3	7	2	8	28	-25
6	6	7	68	71	-3	7	7	64	64	-2	12	7	31	-27	-9	0	8	44	43	8	2	8	19	16
7	6	7	91	97	-2	7	7	11	10	-1	12	7	15	-2	-8	0	8	15	14	9	2	8	23	22
8	6	7	28	-30	-1	7	7	59	-62	0	12	7	82	-84	-7	0	8	172	-178	10	2	8	48	54
9	6	7	48	48	0	7	7	14	6	1	12	7	146	148	-6	0	8	31	26	-8	3	8	23	17
10	6	7	55	-54	1	7	7	60	-60	2	12	7	63	62	-5	0	8	294	284	-7	3	8	31	-35
-10	7	7	14	-10	2	7	7	88	86	4	12	7	82	-80	-4	0	8	11	-3	-6	3	8	72	-72
-9	7	7	34	37	4	7	7	98	103	5	12	7	37	-48	-3	0	8	181	-180	-5	3	8	48	-48
-8	7	7	19	-19	5	7	7	31	25	6	12	7	21	-8	-2	0	8	13	10	-4	3	8	21	16
-7	7	7	45	-45	7	7	7	30	-29	7	12	7	26	28	-1	0	8	27	42	-3	3	8	52	54
-6	7	7	105	102	8	7	7	92	-101	8	12	7	26	20	-10	1	8	14	16	-2	3	8	135	124
-5	7	7	57	-56	9	7	7	14	1	-11	13	7	37	41	-9	1	8	44	-50	-1	3	8	71	72
-4	7	7	12	10	-8	10	7	10	24	-4	13	7	44	47	-8	1	8	75	-77	0	3	8	102	-104
-3	7	7	63	61	-6	10	7	37	35	-3	13	7	56	56	-7	1	8	63	63	1	3	8	15	1
-2	7	7	160	-171	-5	10	7	17	-1	-2	13	7	7	7	-6	1	8	29	11	2	3	8	102	-108
-1	7	7	24	-22	-4	10	7	16	4	-1	13	7	77	-74	-5	1	8	45	46	3	3	8	84	-78
1	7	7	24	-20	-3	10	7	74	-77	0	13	7	4	1	-4	1	8	75	78	4	3	8	126	125
2	7	7	179	176	-2	10	7	24	-26	1	13	7	71	-73	-3	1	8	34	-36	5	3	8	57	-54
3	7	7	41	40	-1	10	7	60	57	2	13	7	37	40	-2	1	8	60	62	6	3	8	13	18
4	7	7	20	-19	-2	10	7	24	-22	3	13	7	60	64	-1	1	8	57	-55	8	3	8	49	49
5	7	7	55	-54	-1	10	7	104	105	4	13	7	47	-47	0	1	8	10	-1	9	3	8	70	-73
6	7	7	97	101	0	10	7	121	120	5	13	7	37	43	1	1	8	54	-55	10	3	8	52	55
7	7	7	43	-45	1	10	7	111	-107	6	13	7	21	-16	2	1	8	41	44	0	4	8	14	18
8	7	7	63	67	2	10	7	26	-20	-6	14	7	66	-72	4	1	8	11	-10	10	4	8	24	-17
-10	8	7	32	31	3	10	7	41	40	-4	14	7	17	12	5	1	8	78	-75	-10	5	8	38	35
-8	8	7	16	-9	4	10	7	33	-28	-3	14	7	47	-48	6	1	8	46	46	-9	5	8	58	62
-7	8	7	82	-82	5	10	7	72	75	-2	14	7	25	31	8	1	8	12	-15	-8	5	8	14	-8
-6	8	7	85	-85	7	10	7	71	70	-1	14	7	33	-32	9	1	8	47	46	-7	5	8	104	101
-5	8	7	46	-46	8	10	7	26	17	0	14	7	14	7	10	1	8	72	-77	-6	5	8	40	-42
-4	8	7	88	82	9	10	7	40	-33	1	14	7	26	30	-9	1	8	57	-58	-5	5	8	44	-51
-3	8	7	108	104	-8	11	7	17	12	2	14	7	29	32	-10	2	8	21	-15	-4	5	8	48	53
-2	8	7	47	47	-7	11	7	40	40	3	14	7	51	44	-10	2	8	21	14	-3	5	8	74	-72

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REMS

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
-9	4	A	35	15	7	E	A	60	-62	1	9	A	18	12	4	12	A	20	24	-3	1	9	28	26
-8	4	A	16	-7	8	E	A	24	-23	2	9	A	66	61	5	12	A	31	34	0	1	9	12	-1
-7	4	A	66	-66	9	E	A	22	-22	3	9	A	42	44	-6	13	A	20	19	1	1	9	32	28
-6	4	A	31	8	-8	7	A	22	-20	4	9	A	22	24	-5	13	A	15	17	2	1	9	34	30
-5	4	A	20	18	-7	7	A	66	-66	5	9	A	70	-75	-4	13	A	15	-2	3	1	9	70	-73
-4	4	A	72	71	-6	7	A	46	46	6	9	A	33	-34	-3	13	A	43	-42	4	1	9	66	65
-3	4	A	63	62	-5	7	A	14	16	7	9	A	16	-15	-2	13	A	72	-73	5	1	9	33	33
-2	4	A	28	-3	-4	7	A	75	-76	8	9	A	12	9	-1	13	A	13	0	6	1	9	32	-24
-1	4	A	62	-62	-3	7	A	69	71	-9	10	A	32	-30	0	13	A	13	13	7	1	9	58	57
0	4	A	101	-101	-2	7	A	101	-102	-8	10	A	26	-24	1	13	A	61	70	8	1	9	75	-78
1	4	A	12	-8	-1	7	A	23	-21	-7	10	A	39	-44	2	13	A	43	-43	9	1	9	45	-46
2	4	A	30	-33	0	7	A	66	66	-6	10	A	63	62	3	13	A	24	17	-9	2	9	28	-27
3	4	A	10	14	1	7	A	66	67	-5	10	A	50	47	4	13	A	24	-24	-8	2	9	30	28
4	4	A	14	12	2	7	A	19	24	-4	10	A	11	7	-5	14	A	35	38	-7	2	9	64	-63
5	4	A	12	8	3	7	A	103	-100	-3	10	A	73	71	-4	14	A	30	-32	-6	2	9	33	33
6	4	A	12	6	4	7	A	52	-50	0	10	A	104	-104	-3	14	A	17	21	-5	2	9	21	24
-7	5	A	20	17	5	7	A	74	-76	1	10	A	73	-71	-2	14	A	22	12	-4	2	9	119	-120
-6	5	A	100	-97	6	7	A	16	3	2	10	A	12	7	-1	14	A	18	-14	-3	2	9	47	48
-5	5	A	27	-24	-7	8	A	66	66	3	10	A	47	-49	0	14	A	46	47	-2	2	9	20	-12
-4	5	A	37	-36	-6	8	A	5	5	4	10	A	90	91	1	14	A	19	13	-1	2	9	19	9
-3	5	A	38	-36	-5	8	A	15	20	-8	10	A	39	43	2	14	A	17	12	0	2	9	178	181
-2	5	A	141	141	-4	8	A	20	-36	-7	10	A	18	-8	3	14	A	29	-21	1	2	9	11	-5
-1	5	A	17	21	-3	8	A	30	-27	-6	10	A	18	16	4	14	A	17	-12	2	2	9	11	11
0	5	A	62	64	-2	8	A	20	-20	-5	10	A	30	-31	5	14	A	33	-32	3	2	9	20	-17
1	5	A	133	-136	-1	8	A	24	26	-4	11	A	14	-9	-9	15	A	37	44	4	2	9	119	-120
2	5	A	13	-13	0	8	A	72	68	-3	11	A	27	22	-8	15	A	44	-51	5	2	9	23	-24
3	5	A	25	26	1	8	A	57	55	-2	11	A	66	-62	-7	15	A	57	55	6	2	9	27	31
4	5	A	31	-26	-9	9	A	30	-31	-1	11	A	11	-9	-6	15	A	57	-57	7	2	9	58	59
5	5	A	94	96	-8	9	A	20	19	0	11	A	14	9	-5	15	A	54	52	8	2	9	31	29
6	5	A	26	18	-7	9	A	71	-76	1	11	A	71	71	-4	15	A	54	49	9	2	9	74	74
-7	6	A	14	-7	-6	9	A	73	-77	2	11	A	13	-7	-9	0	9	27	28	-8	3	9	46	-45
-6	6	A	10	9	-5	9	A	77	77	3	11	A	73	74	-8	0	9	33	-31	-7	3	9	42	-41
-5	6	A	14	-13	-4	9	A	12	-17	4	11	A	13	-4	-7	0	9	48	-47	-6	3	9	17	8
-4	6	A	27	-23	-3	9	A	34	31	5	11	A	68	69	-6	0	9	110	108	-5	3	9	62	63
-3	6	A	21	20	-2	9	A	58	57	6	11	A	22	-23	-5	0	9	154	150	-4	3	9	72	71
-2	6	A	104	100	-1	9	A	58	-57	7	11	A	11	-4	-4	0	9	154	-154	-3	3	9	73	68
-1	6	A	11	-12	0	9	A	32	34	8	11	A	12	-1	-3	0	9	104	-104	-2	3	9	19	14
0	6	A	11	-11	1	9	A	20	20	-9	12	A	33	32	-2	0	9	97	97	-1	3	9	131	-133
1	6	A	51	-52	2	9	A	32	-28	-8	12	A	36	-37	-1	0	9	99	99	0	3	9	61	-61
-3	7	A	56	-56	3	9	A	46	46	-7	12	A	11	-10	0	0	9	24	-23	1	3	9	20	2
-2	7	A	14	-10	-9	0	A	47	-41	-6	12	A	68	66	-8	1	9	48	-49	2	3	9	80	-81
-1	7	A	39	40	-8	0	A	36	34	-5	12	A	25	-27	-7	1	9	79	77	3	3	9	130	132
0	7	A	22	19	-7	0	A	73	-76	-4	12	A	75	75	-6	1	9	54	54	4	3	9	20	12
1	7	A	9	-10	-6	0	A	13	14	-3	12	A	53	56	-5	1	9	25	25	5	3	9	65	-59
2	7	A	69	69	-5	0	A	44	44	-2	12	A	62	-64	-4	1	9	60	60	6	3	9	73	71
3	7	A	14	-14	-4	0	A	55	-50	-1	12	A	30	-25	-3	1	9	54	-56	7	3	9	61	-62
4	7	A	19	12	-3	0	A	14	14	0	12	A	67	-68	-2	1	9	70	-75	8	3	9	11	8
5	7	A	98	101	-2	0	A	14	6	1	12	A	27	-31	-1	1	9	37	-31	9	3	9	38	39

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR BEN3

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
0	3	0	47	-48	2	8	0	32	30	9	0	0	63	-62	-7	14	0	31	-27	-5	3	10	23	24
-0	4	0	29	-24	3	8	0	39	25	4	9	0	73	-73	-1	14	0	17	22	-4	3	10	18	-12
-1	4	0	26	24	4	8	0	27	-29	5	9	0	29	-30	0	14	0	17	16	-3	3	10	34	-35
-7	4	0	28	-24	5	8	0	28	29	7	9	0	22	19	1	14	0	27	-22	-2	3	10	104	-105
-6	4	0	95	-97	6	8	0	44	-45	-7	10	0	15	18	2	14	0	20	-25	-7	3	10	49	-51
-5	4	0	54	55	7	8	0	26	-31	-6	10	0	61	61	-6	0	10	37	-36	-1	3	10	82	82
-4	4	0	29	-28	8	8	0	11	17	-4	10	0	42	41	-4	0	10	24	-24	0	3	10	54	-1
-3	4	0	27	-25	-7	9	0	34	34	-3	10	0	88	-84	-6	0	10	123	121	1	3	10	46	47
-2	4	0	49	50	-6	9	0	68	-68	-2	10	0	10	7	-2	0	10	28	21	2	3	10	44	50
-1	4	0	48	-48	-5	9	0	28	33	-1	10	0	93	-89	0	0	10	911	-919	3	3	10	103	-107
0	4	0	10	4	-4	9	0	20	-19	0	10	0	84	-85	2	0	10	21	21	4	3	10	32	35
1	4	0	46	50	-3	9	0	41	-44	1	10	0	87	87	4	0	10	122	120	5	3	10	29	-31
2	4	0	47	48	-2	9	0	128	131	2	10	0	93	94	6	0	10	24	-27	6	3	10	24	-26
3	4	0	27	27	-1	9	0	10	8	3	10	0	60	60	8	0	10	14	-16	7	3	10	58	54
4	4	0	25	-26	0	9	0	11	-1	5	10	0	51	-52	-8	1	10	60	65	8	3	10	27	-41
5	4	0	55	-53	1	9	0	13	7	6	10	0	12	8	-7	1	10	17	-33	-6	4	10	12	-1
6	4	0	92	-87	2	9	0	121	-137	7	10	0	15	-10	-6	1	10	14	-12	-5	4	10	71	-75
7	4	0	16	21	3	9	0	43	-45	-8	11	0	13	-11	-5	1	10	55	-56	-4	4	10	44	47
8	4	0	28	24	4	9	0	11	7	-7	11	0	69	-68	-4	1	10	64	-65	-3	4	10	48	44
9	4	0	29	27	5	9	0	95	94	-6	11	0	12	8	-3	1	10	27	27	-2	4	10	48	-46
-8	5	0	19	-8	6	9	0	57	-58	-5	11	0	41	42	-2	1	10	53	52	-1	4	10	75	74
-7	5	0	58	-57	7	9	0	34	32	-4	11	0	31	33	-1	1	10	23	25	0	4	10	30	-30
-6	5	0	32	-29	8	9	0	24	23	-3	11	0	17	8	0	1	10	11	1	1	4	10	21	-23
-5	5	0	69	68	-8	A	0	12	8	0	11	0	11	5	1	1	10	25	24	2	4	10	66	63
-4	5	0	13	-7	-7	A	0	41	44	1	11	0	32	-34	2	1	10	66	-61	3	4	10	24	20
-3	5	0	120	122	-6	A	0	51	53	2	11	0	44	40	3	1	10	25	21	4	4	10	41	-38
-2	5	0	81	80	-5	A	0	18	10	3	11	0	12	-7	4	1	10	54	52	5	4	10	31	-28
-1	5	0	112	-112	-4	A	0	62	-62	4	11	0	42	-44	5	1	10	56	-57	6	4	10	49	-45
0	5	0	18	1	-3	A	0	24	23	-6	12	0	49	-49	6	1	10	20	13	8	4	10	44	-46
1	5	0	107	-113	-2	A	0	20	-24	-4	12	0	68	68	7	1	10	31	-36	-8	5	10	58	57
2	5	0	57	-58	-1	A	0	56	-60	-3	12	0	21	8	8	1	10	60	-65	-7	5	10	75	75
3	5	0	122	126	0	A	0	89	89	-2	12	0	12	-8	-8	2	10	22	-14	-6	5	10	27	-22
4	5	0	14	4	1	A	0	56	61	-1	12	0	39	42	-7	2	10	58	61	-5	5	10	31	-32
5	5	0	59	60	2	A	0	32	-24	0	12	0	60	-61	-6	2	10	60	-67	-4	5	10	71	70
6	5	0	24	24	3	A	0	68	68	1	12	0	46	-41	-5	2	10	16	18	-3	5	10	14	15
7	5	0	28	-26	4	A	0	28	-29	2	12	0	12	-6	-4	2	10	72	74	-2	5	10	27	34
8	5	0	11	-1	-8	B	0	35	-19	3	12	0	14	-8	-3	2	10	25	-29	-1	5	10	34	38
9	5	0	19	1	-7	B	0	48	51	4	12	0	70	69	-2	2	10	106	110	-7	6	10	143	-148
-8	6	0	28	16	-6	B	0	7	-49	5	12	0	49	52	-1	2	10	107	-109	-6	6	10	98	-92
-7	6	0	72	71	-5	B	0	17	21	-4	13	0	33	-34	0	2	10	28	-26	-5	6	10	10	0
-6	6	0	64	-64	-4	B	0	21	-11	-3	13	0	46	-49	1	2	10	72	-73	-4	6	10	32	-34
-5	6	0	64	-68	-3	B	0	27	-21	-2	13	0	27	31	2	2	10	23	19	-3	6	10	146	144
-4	6	0	37	-33	-2	B	0	74	75	-1	13	0	27	28	3	2	10	27	27	-2	6	10	34	38
-3	6	0	27	-25	-1	B	0	41	-41	0	13	0	13	1	4	2	10	50	52	-1	6	10	20	-19
-2	6	0	71	71	0	B	0	14	-6	1	13	0	52	49	7	2	10	14	5	0	6	10	21	17
-1	6	0	49	42	-1	B	0	40	37	2	13	0	37	-33	-7	3	10	15	-17	1	6	10	84	-89
0	6	0	33	28	1	B	0	40	40	3	13	0	48	-42	-6	3	10	40	41	2	6	10	18	-14
1	6	0	37	-43	2	B	0	12	8	4	13	0	40	38	-7	3	10	54	56	3	6	10	20	22

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEM3

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-7	6	10	38	-47	4	9	10	49	49	-4	1	11	44	FC	-4	5	11	37	-47
-6	6	10	88	-88	5	9	10	35	32	0	1	11	68	-68	-3	5	11	39	-41
-5	6	10	15	14	-5	10	10	29	34	1	1	11	20	23	1	5	11	42	46
-4	6	10	20	21	-4	10	10	77	-71	2	1	11	40	-37	2	5	11	41	43
-3	6	10	40	41	-3	10	10	40	-37	3	1	11	41	-40	3	5	11	41	43
-2	6	10	13	13	-2	10	10	15	-18	4	1	11	38	44	4	5	11	44	-48
0	6	10	32	32	-1	10	10	46	-52	5	1	11	33	-37	5	5	11	32	34
1	6	10	17	-8	0	10	10	97	105	-5	2	11	24	-19	6	5	11	16	-14
2	6	10	34	36	1	10	10	50	49	-4	2	11	42	43	6	6	11	33	32
3	6	10	40	-41	2	10	10	17	-19	-3	2	11	39	34	-6	6	11	46	42
4	6	10	28	31	3	10	10	45	34	-2	2	11	23	19	-4	6	11	16	16
5	6	10	26	-14	4	10	10	28	-32	0	2	11	110	-110	-3	6	11	15	17
6	6	10	22	-25	5	10	10	28	-34	1	2	11	32	31	-2	6	11	20	-19
7	6	10	34	34	-4	11	10	29	30	2	2	11	27	26	-1	6	11	30	-27
-7	7	10	16	-16	-3	11	10	16	12	3	2	11	40	38	0	6	11	31	30
-6	7	10	24	28	-2	11	10	22	21	4	2	11	11	16	1	6	11	31	-26
-5	7	10	46	-45	-1	11	10	26	-30	5	2	11	29	31	2	6	11	17	-18
-4	7	10	24	26	0	11	10	14	0	6	2	11	26	-27	3	6	11	33	1
-3	7	10	28	26	1	11	10	27	-13	7	2	11	46	-46	4	6	11	16	16
-2	7	10	23	-24	2	11	10	17	20	-5	3	11	42	-43	5	6	11	33	-29
0	7	10	10	1	3	11	10	18	19	-4	3	11	44	-46	6	6	11	26	32
1	7	10	42	-42	4	11	10	29	-20	-3	3	11	3	-32	-5	7	11	24	-22
2	7	10	37	-37	5	11	10	40	-40	-2	3	11	10	13	-4	7	11	14	11
3	7	10	11	11	-2	12	10	22	19	-2	3	11	38	34	-3	7	11	33	30
4	7	10	44	47	-1	12	10	47	-44	-1	3	11	40	37	-2	7	11	35	-35
5	7	10	40	40	0	12	10	27	-28	0	3	11	11	8	-1	7	11	13	-7
7	7	10	36	-36	1	12	10	27	24	1	3	11	39	37	0	7	11	31	-1
-6	8	10	29	-22	2	12	10	15	18	2	3	11	33	33	1	7	11	34	34
-5	8	10	31	28	3	12	10	14	10	3	3	11	14	-12	2	7	11	24	26
-4	8	10	40	-42	4	12	10	17	0	4	3	11	37	31	4	7	11	21	-10
-3	8	10	20	10	-7	0	11	20	34	5	3	11	40	-45	5	7	11	16	-21
-2	8	10	15	6	-6	0	11	31	37	6	3	11	29	29	-6	8	11	47	46
-1	8	10	57	51	-5	0	11	73	-72	7	3	11	15	-7	-5	8	11	24	24
0	8	10	73	77	-4	0	11	104	-107	-6	4	11	71	70	-2	8	11	32	27
1	8	10	72	-72	1	0	11	107	106	-5	4	11	46	-46	-1	8	11	33	33
2	8	10	19	10	2	0	11	66	70	-4	4	11	23	11	0	8	11	51	-47
3	8	10	22	-10	3	0	11	78	-77	-3	4	11	12	5	1	8	11	34	-40
4	8	10	46	-43	7	0	11	27	-24	-2	4	11	33	-39	2	8	11	32	26
5	8	10	27	27	-7	1	11	25	-40	-1	4	11	61	7	3	8	11	25	-27
6	8	10	24	-22	-6	1	11	24	-24	0	4	11	12	-6	4	8	11	44	46
-6	9	10	16	-20	-4	1	11	24	-26	1	4	11	42	-43	5	8	11	16	15
-5	9	10	47	47	-3	1	11	54	50	2	4	11	37	-32	-4	9	11	44	-47
-4	9	10	40	-40	-2	1	11	76	80	3	4	11	17	-10	-3	9	11	22	26
-2	9	10	57	60	-1	1	11	10	10	4	4	11	21	11	-1	9	11	35	-30
0	9	10	11	7	0	1	11	10	-9	5	4	11	47	47	1	9	11	29	-29
1	9	10	23	-6	1	1	11	16	0	6	4	11	37	36	3	9	11	51	54
2	9	10	48	-50	3	1	11	31	-26	-6	5	11	24	16	4	9	11	47	47
3	9	10	38	-40	4	1	11	14	-7	-5	5	11	31	-38	-5	10	11	37	38

H	K	L	FO	FC
-1	10	11	62	61
0	10	11	55	58
1	10	11	58	-52
2	10	11	37	-32
3	10	11	35	-33
-4	5	12	45	-46
-2	0	12	11	6
0	0	12	105	105
2	0	12	10	-4
4	0	12	44	-48
-4	1	12	44	42
-3	1	12	36	35
-2	1	12	20	-15
-1	1	12	33	-33
1	1	12	15	-14
2	1	12	12	6
3	1	12	34	32
-2	2	12	20	-15
-1	2	12	38	-35
0	2	12	42	42
1	2	12	46	-46
-4	2	12	14	-14
-3	2	12	32	-32
-2	2	12	21	21
-1	2	12	72	-73
1	2	12	72	72
2	2	12	24	24
3	2	12	40	40
-4	3	12	12	-14
-3	3	12	18	18
-2	3	12	12	-12
-1	3	12	23	20
0	3	12	29	29
-3	3	12	28	30
-2	3	12	19	19
-1	3	12	42	42
1	3	12	49	-46
2	3	12	22	22
3	3	12	24	24
-3	4	12	24	24
-2	4	12	24	24
-1	4	12	24	24
1	4	12	40	-36
2	4	12	11	24
3	4	12	34	29
-4	4	12	14	-15

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [illegible]

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
-3	5	12	25	-25	-3	6	12	24	-23	-2	7	12	11	-16	0	8	12	41	-44	2	1	13	13	5
-2	5	12	47	46	-2	6	12	20	-18	-1	7	12	46	49	1	8	12	40	42	-1	1	13	11	-3
-1	5	12	26	23	-1	6	12	46	-45	0	7	12	23	0	-1	0	13	64	72	0	1	13	75	79
1	5	12	25	28	0	6	12	24	20	1	7	12	46	46	1	0	13	66	-71	-1	3	13	23	-22
2	5	12	44	-45	2	6	12	23	-20	2	7	12	17	15	-1	1	13	16	17	0	3	13	13	-1
3	5	12	22	-21	3	6	12	24	24	3	7	12	43	-41	0	1	13	19	-1	1	3	13	21	-23
4	5	12	16	-16	-3	7	12	20	-21	-1	8	12	42	-42	1	1	13	22	17					

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	1196	-1196	8	8	0	133	-101	2	2	1	66	20	0	6	1	13	-2	5	9	1	44	-34
4	0	0	973	-1000	9	8	0	119	-93	3	2	1	156	-173	10	6	1	87	63	7	9	1	84	-59
6	0	0	962	908	10	8	0	101	87	4	2	1	62	-66	11	6	1	34	28	8	9	1	43	32
8	0	0	446	467	12	8	0	92	28	5	2	1	28	-28	12	6	1	20	-27	9	9	1	9	-2
10	0	0	156	-147	1	9	0	195	182	6	2	1	13	-19	13	6	1	22	-16	10	9	1	19	16
12	0	0	340	-174	2	9	0	112	88	7	2	1	79	72	14	6	1	58	-13	3	10	1	77	67
14	0	0	139	116	3	9	0	167	-158	8	2	1	28	28	1	7	1	84	78	4	10	1	76	66
1	1	0	177	-187	7	9	0	30	-14	9	2	1	19	-6	3	7	1	41	33	6	10	1	60	-52
3	1	0	681	646	8	9	0	104	95	10	2	1	13	3	5	7	1	74	-62	8	10	1	22	-16
7	1	0	18	-8	11	9	0	30	-22	11	2	1	25	-21	6	7	1	46	-35	9	10	1	31	-23
9	1	0	915	-925	0	A	0	171	151	14	2	1	19	3	8	7	1	42	-34	5	10	1	72	-63
11	1	0	67	72	2	A	0	42	-48	15	2	1	18	12	9	7	1	31	-18	7	10	1	64	63
13	1	0	132	120	4	A	0	162	-124	1	3	1	80	82	7	7	1	83	69	8	10	1	36	28
15	1	0	87	-68	6	A	0	76	71	2	3	1	193	-190	8	7	1	98	88	1	11	1	84	-82
0	2	0	697	-698	8	A	0	67	60	3	3	1	31	24	9	7	1	34	11	2	11	1	67	-66
2	2	0	24	-27	10	A	0	57	-61	4	3	1	61	54	10	7	1	47	45	3	11	1	59	-60
4	2	0	488	418	12	A	0	33	-23	5	3	1	40	-33	11	7	1	46	-37	4	11	1	17	13
6	2	0	161	-129	1	B	0	150	-104	6	3	1	85	83	12	7	1	49	-36	5	11	1	33	-26
8	2	0	787	-761	3	B	0	91	-56	7	3	1	81	86	13	8	1	14	17	6	11	1	56	46
10	2	0	158	136	5	B	0	116	97	8	3	1	48	-42	1	7	1	87	81	7	11	1	74	58
12	2	0	57	55	7	B	0	42	28	9	3	1	14	6	2	7	1	79	-66	3	12	1	40	-32
14	2	0	117	-68	9	B	0	84	-65	10	3	1	38	-35	3	7	1	51	-34	5	12	1	60	-50
1	3	0	280	270	0	C	0	36	-17	11	3	1	18	-18	4	7	1	21	-17	9	12	1	64	40
3	3	0	179	182	2	C	0	17	17	12	3	1	22	18	6	7	1	40	-33	4	13	1	17	19
5	3	0	94	-100	4	C	0	37	25	13	3	1	27	22	8	7	1	51	47	5	13	1	14	13
7	3	0	54	-49	6	C	0	33	-36	14	3	1	10	13	7	7	1	107	90	2	0	2	54	-51
9	3	0	246	217	8	C	0	18	-7	1	4	1	103	-111	9	7	1	96	-79	3	0	2	142	-138
11	3	0	44	30	9	C	0	50	45	2	4	1	42	-34	1	8	1	9	4	4	0	2	158	138
13	3	0	112	-100	1	D	0	26	22	3	4	1	94	84	10	7	1	37	-36	5	0	2	456	449
15	3	0	51	38	3	D	0	86	-64	4	4	1	49	39	11	7	1	59	-47	6	0	2	101	87
0	4	0	941	974	5	D	0	8	2	5	4	1	91	75	12	7	1	28	25	7	0	2	32	28
2	4	0	73	-58	7	D	0	41	30	6	4	1	58	58	1	8	1	108	-84	8	0	2	174	145
4	4	0	935	-975	9	D	0	15	-17	7	4	1	79	-72	2	8	1	101	-121	9	0	2	264	-257
6	4	0	598	549	4	E	0	37	-34	8	4	1	42	-36	3	8	1	102	99	10	0	2	61	-57
8	4	0	192	165	0	F	1	17	16	9	4	1	14	4	4	8	1	57	43	11	0	2	73	71
10	4	0	161	-117	1	F	1	76	-72	10	4	1	44	-42	5	8	1	69	50	13	0	2	115	110
12	4	0	91	-74	4	F	1	124	-117	11	4	1	18	16	6	8	1	84	75	14	0	2	41	38
14	4	0	68	-77	5	F	1	87	-79	12	4	1	25	22	7	8	1	88	-77	15	0	2	46	-39
1	5	0	211	-217	6	F	1	27	28	13	4	1	10	-14	8	8	1	20	-48	3	1	2	181	-206
3	5	0	176	-149	7	F	1	69	66	14	4	1	17	19	9	8	1	79	-25	5	1	2	64	58
5	5	0	217	192	8	F	1	82	68	1	5	1	85	-77	10	8	1	43	-33	7	1	2	199	-185
7	5	0	44	49	9	F	1	36	24	2	5	1	97	110	11	8	1	40	34	9	1	2	237	256
9	5	0	171	-140	10	F	1	24	-21	3	5	1	82	68	12	8	1	41	33	11	1	2	169	148
11	5	0	26	11	11	F	1	39	-34	4	5	1	46	-38	1	9	1	58	-60	13	1	2	270	-237
13	5	0	47	74	12	F	1	20	-19	5	5	1	10	10	2	9	1	51	53	7	1	2	107	91
1	6	0	129	-120	13	F	1	11	-7	6	5	1	44	-43	4	9	1	93	86	8	1	2	132	-133
3	6	0	61	42	15	F	1	15	9	8	5	1	62	-64	6	9	1	34	-26	9	1	2	104	-88
5	6	0	174	151	1	G	1	101	100	9	5	1	47	40	8	9	1	21	12	10	1	2	142	121

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEYA

H	K	L	FO	FC
11	1	2	20	-25
12	1	2	21	21
14	1	2	136	-101
0	2	2	128	-84
1	2	2	304	307
2	2	2	16	-21
3	2	2	203	202
4	2	2	105	90
5	2	2	48	-124
6	2	2	9	-8
7	2	2	46	-43
8	2	2	47	45
9	2	2	278	272
10	2	2	41	40
11	2	2	80	-79
12	2	2	29	27
13	2	2	126	-102
14	2	2	9	-24
15	2	2	50	44
0	3	2	417	401
1	3	2	132	114
2	3	2	29	25
3	3	2	64	64
4	3	2	193	-198
5	3	2	106	-101
6	3	2	147	141
7	3	2	0	-4
8	3	2	146	137
9	3	2	56	56
10	3	2	146	-138
11	3	2	30	-30
12	3	2	42	-47
13	3	2	30	-25
14	3	2	111	98
15	3	2	56	50
0	4	2	101	107
1	4	2	948	-941
2	4	2	37	-41
3	4	2	165	-167
4	4	2	59	-58
5	4	2	249	242
6	4	2	58	57
7	4	2	32	34
8	4	2	28	27
9	4	2	101	-106
10	4	2	33	-32
11	4	2	42	39
12	4	2	0	-7
13	4	2	90	83
14	4	2	31	31
15	4	2	116	-104
0	5	2	66	64
1	5	2	321	-318
2	5	2	34	-30
3	5	2	46	44
4	5	2	0	47
5	5	2	281	258
6	5	2	62	63
7	5	2	126	-125
8	5	2	10	-15
9	5	2	153	-146
10	5	2	30	-25
11	5	2	100	97
12	5	2	13	18
13	5	2	51	47
14	5	2	15	10
15	5	2	77	-50
0	6	2	41	-29
1	6	2	197	178
2	6	2	7	0
3	6	2	116	113
4	6	2	35	37
5	6	2	200	-172
6	6	2	28	-27
7	6	2	56	-55
8	6	2	22	-17
9	6	2	139	137
10	6	2	123	122
11	6	2	36	-34
12	6	2	74	-68
13	6	2	0	0
14	6	2	774	198
15	6	2	0	0
0	7	2	67	-68
1	7	2	19	20
2	7	2	194	-185
3	7	2	26	-30
4	7	2	103	88
5	7	2	35	-8
6	7	2	102	85
7	7	2	20	17
8	7	2	46	-39
9	7	2	12	-6
10	7	2	0	-2
11	7	2	42	-28
12	7	2	0	0
13	7	2	24	12
14	7	2	141	-47
15	7	2	13	-11
0	8	2	90	-90
1	8	2	27	-24
2	8	2	98	83
3	8	2	14	15
4	8	2	138	-97
5	8	2	10	-10
6	8	2	25	-15
7	8	2	0	0
8	8	2	0	0
9	8	2	0	0
10	8	2	0	0
11	8	2	0	0
12	8	2	0	0
13	8	2	0	0
14	8	2	0	0
15	8	2	0	0
0	9	2	0	0
1	9	2	0	0
2	9	2	0	0
3	9	2	0	0
4	9	2	0	0
5	9	2	0	0
6	9	2	0	0
7	9	2	0	0
8	9	2	0	0
9	9	2	0	0
10	9	2	0	0
11	9	2	0	0
12	9	2	0	0
13	9	2	0	0
14	9	2	0	0
15	9	2	0	0
0	10	2	110	93
1	10	2	14	14
2	10	2	15	-17
3	10	2	10	10
4	10	2	78	-82
5	10	2	10	-11
6	10	2	28	21
7	10	2	140	-134
8	10	2	7	7
9	10	2	109	-97
10	10	2	12	-7
11	10	2	61	63
12	10	2	37	-37
13	10	2	26	26
14	10	2	20	26
15	10	2	29	19
0	11	2	24	-14
1	11	2	88	86
2	11	2	78	-80
3	11	2	19	-10
4	11	2	46	-48
5	11	2	24	24
6	11	2	0	1
7	11	2	0	0
8	11	2	0	0
9	11	2	0	0
10	11	2	0	0
11	11	2	0	0
12	11	2	0	0
13	11	2	0	0
14	11	2	0	0
15	11	2	0	0
0	12	2	0	0
1	12	2	0	0
2	12	2	0	0
3	12	2	0	0
4	12	2	0	0
5	12	2	0	0
6	12	2	0	0
7	12	2	0	0
8	12	2	0	0
9	12	2	0	0
10	12	2	0	0
11	12	2	0	0
12	12	2	0	0
13	12	2	0	0
14	12	2	0	0
15	12	2	0	0
0	13	2	0	0
1	13	2	0	0
2	13	2	0	0
3	13	2	0	0
4	13	2	0	0
5	13	2	0	0
6	13	2	0	0
7	13	2	0	0
8	13	2	0	0
9	13	2	0	0
10	13	2	0	0
11	13	2	0	0
12	13	2	0	0
13	13	2	0	0
14	13	2	0	0
15	13	2	0	0
0	14	2	0	0
1	14	2	0	0
2	14	2	0	0
3	14	2	0	0
4	14	2	0	0
5	14	2	0	0
6	14	2	0	0
7	14	2	0	0
8	14	2	0	0
9	14	2	0	0
10	14	2	0	0
11	14	2	0	0
12	14	2	0	0
13	14	2	0	0
14	14	2	0	0
15	14	2	0	0
0	15	2	0	0
1	15	2	0	0
2	15	2	0	0
3	15	2	0	0
4	15	2	0	0
5	15	2	0	0
6	15	2	0	0
7	15	2	0	0
8	15	2	0	0
9	15	2	0	0
10	15	2	0	0
11	15	2	0	0
12	15	2	0	0
13	15	2	0	0
14	15	2	0	0
15	15	2	0	0
1	1	3	83	83
2	1	3	64	-65
3	1	3	29	-34
4	1	3	23	-9
5	1	3	30	32
6	1	3	27	-32
7	1	3	43	38
8	1	3	28	21
9	1	3	60	-74
10	1	3	14	-15
11	1	3	33	-26
12	1	3	13	13
13	1	3	13	32
14	1	3	12	6
15	1	3	29	18
0	2	3	169	-145
1	2	3	87	86
2	2	3	120	142
3	2	3	14	20
4	2	3	26	21
5	2	3	59	60
6	2	3	85	-78
7	2	3	42	-36
8	2	3	0	6
9	2	3	54	-64
10	2	3	30	28
11	2	3	30	25
12	2	3	17	-12
13	2	3	17	-16
14	2	3	11	2
15	2	3	184	-197
0	3	3	102	111
1	3	3	88	102
2	3	3	57	-52
3	3	3	67	50
4	3	3	88	-72
5	3	3	111	-96
6	3	3	64	64
7	3	3	24	-31
8	3	3	34	32
9	3	3	44	-36
10	3	3	59	59
11	3	3	58	-59
12	3	3	18	-8
13	3	3	32	-9
14	3	3	88	80
15	3	3	105	130
0	4	3	75	-75
1	4	3	74	-68
2	4	3	64	-66
3	4	3	98	-87
4	4	3	56	53
5	4	3	33	-33
6	4	3	52	-48
7	4	3	39	36
8	4	3	30	34
9	4	3	42	-44
10	4	3	37	-32
11	4	3	23	-23
12	4	3	24	-26
13	4	3	55	-52
14	4	3	29	24
15	4	3	11	10
0	5	3	44	-44
1	5	3	139	-134
2	5	3	54	46
3	5	3	34	33
4	5	3	15	11
5	5	3	105	97
6	5	3	49	-42
7	5	3	52	-47
8	5	3	48	-43
9	5	3	29	22
10	5	3	51	54
11	5	3	109	-83
12	5	3	58	48
13	5	3	138	84
14	5	3	17	-5
15	5	3	26	14
0	6	3	60	-36
1	6	3	104	-87
2	6	3	15	0
3	6	3	3	1
4	6	3	21	25
5	6	3	70	42
6	6	3	21	15
7	6	3	104	74
8	6	3	29	-19
9	6	3	48	-37
10	6	3	100	-98

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 9EVA

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
7	0	1	29	24	0	1	4	242	227	10	4	4	129	118	1	5	4	41	-34	0	1	5	10	6
8	0	1	82	69	10	1	4	85	84	11	4	4	18	30	2	5	4	38	34	10	1	5	10	-9
9	0	1	9	-7	11	1	4	114	-114	12	4	4	81	67	3	5	4	31	-11	11	1	5	11	-9
10	0	1	61	65	12	1	4	36	30	13	4	4	47	36	4	5	4	147	131	12	1	5	12	10
1	1	1	852	729	13	1	4	118	-68	14	4	4	91	-69	5	5	4	39	28	1	2	5	48	-35
2	1	1	84	-80	14	1	4	96	40	0	5	4	147	-152	6	5	4	82	-67	2	2	5	54	-83
3	1	1	90	-76	15	1	4	45	32	1	5	4	276	261	8	5	4	71	-59	3	2	5	54	16
4	1	1	27	34	0	2	4	458	462	2	5	4	35	36	9	5	4	24	-17	4	2	5	21	16
5	1	1	56	-27	1	2	4	135	101	3	5	4	156	144	10	5	4	75	80	5	2	5	34	19
6	1	1	39	33	2	2	4	29	-23	4	5	4	100	117	11	5	4	33	8	6	2	5	82	79
7	1	1	49	76	3	2	4	80	90	5	5	4	191	-212	0	6	4	17	22	7	2	5	8	-14
8	1	1	37	-19	4	2	4	246	-303	6	5	4	77	-70	1	6	4	84	72	8	2	5	25	-22
1	1	1	48	-39	5	2	4	114	-145	7	5	4	35	-25	2	6	4	43	45	9	2	5	20	11
2	1	1	90	-93	6	2	4	112	128	8	5	4	61	-65	3	6	4	43	45	10	2	5	47	-47
3	1	1	51	40	7	2	4	34	-37	9	5	4	161	167	4	6	4	18	-8	11	2	5	24	18
4	1	1	30	17	8	2	4	179	185	10	5	4	69	43	5	6	4	46	-73	12	2	5	17	14
5	1	1	24	15	9	2	4	126	117	11	5	4	36	-27	6	6	4	8	-5	1	3	5	139	-117
6	1	1	48	54	10	2	4	72	-112	12	5	4	28	12	7	6	4	15	4	2	3	5	77	83
7	1	1	46	-34	11	2	4	0	-52	13	5	4	52	-70	8	6	4	71	82	3	3	5	91	53
1	2	1	56	-46	12	2	4	61	-62	14	5	4	37	-27	10	6	4	27		4	3	5	37	-32
2	2	1	16	21	13	2	4	64	-83	0	6	4	232	214	0	10	4	69		5	3	5	44	58
3	2	1	43	44	14	2	4	107	80	2	6	4	95	86	1	10	4	39	16	6	3	5	23	-29
4	2	1	10	-10	15	2	4	33	17	3	6	4	44	-40	2	10	4	17	5	7	3	5	47	49
0	0	2	550	-588	0	3	4	210	173	4	6	4	66	68	3	10	4	18	16	8	3	5	15	18
1	0	2	27	17	1	3	4	277	-245	5	6	4	159	-178	4	10	4	71	-80	9	3	5	17	-11
2	0	2	17	17	2	3	4	77	-115	6	6	4	71	66	5	10	4	54	-19	10	3	5	9	12
3	0	2	56	77	3	3	4	127	-139	7	6	4	110	101	6	10	4	34	27	11	3	5	50	46
4	0	2	248	197	4	3	4	162	-127	8	6	4	19	-10	7	10	4	14	-9	12	3	5	28	-26
5	0	2	48	51	5	3	4	219	248	9	6	4	111	94	8	10	4	77	69	1	4	5	72	68
6	0	2	125	-150	6	3	4	56	63	10	6	4	67	62	0	11	4	35	15	2	4	5	174	186
7	0	2	44	44	7	3	4	74	27	11	6	4	46	-42	1	11	4	27	10	3	4	5	45	-53
8	0	2	221	-208	8	3	4	77	75	12	6	4	51	-19	2	11	4	46	-37	4	4	5	45	-46
9	0	2	61	-48	9	3	4	142	-175	13	6	4	43	-32	3	11	4	12	-14	5	4	5	27	-29
10	0	2	144	144	10	3	4	82	-66	14	6	4	39	-24	4	11	4	21	-30	6	4	5	120	-147
11	0	2	44	34	11	3	4	39	24	0	7	4	55	44	5	11	4	65	78	7	4	5	35	37
12	0	2	72	55	12	3	4	26	-23	1	7	4	163	-176	6	11	4	14	8	8	4	5	40	39
13	0	2	28	32	13	3	4	103	82	2	7	4	22	-22	0	12	4	28	-26	9	4	5	8	8
14	0	2	120	98	14	3	4	0	40	3	7	4	128	-116	1	12	4	15	-9	10	4	5	90	79
15	0	2	32	-19	0	4	4	436	-390	4	7	4	88	-74	2	12	4	12	12	11	5	5	25	-18
0	1	2	307	-280	1	4	4	223	-181	5	7	4	186	161	3	12	4	38	28	12	4	5	43	-32
1	1	2	151	126	2	4	4	58	50	6	7	4	46	48	1	1	5	565	498	13	4	5	36	-27
2	1	2	17	3	3	4	4	96	-80	7	7	4	56	58	2	1	5	55	65	1	5	5	82	78
3	1	2	152	208	4	4	4	232	287	8	7	4	38	32	3	1	5	11	-15	2	5	5	46	-52
4	1	2	151	170	5	4	4	122	148	9	7	4	114	-104	4	1	5	72	-71	3	5	5	60	-56
5	1	2	249	-265	6	4	4	194	-160	10	7	4	60	-75	5	1	5	19	20	4	5	5	15	17
6	1	2	48	-60	7	4	4	25	8	11	7	4	19	17	6	1	5	5	12	5	5	5	13	-12
7	1	2	66	-68	8	4	4	173	-157	12	7	4	18	-7	7	1	5	32	14	6	5	5	38	43
8	1	2	108	-88	9	4	4	76	-72	0	8	4	127	-123	8	1	5	13	21	7	5	5	82	73

RESERVED AND CALCULATED STRUCTURE FACTORS FOR OFYA

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
4	0	0	21	-28	0	0	8	0	0	12	1	F	55	-44	13	4	6	76	-69	5	8	E	53	-53
6	0	0	58	1	40	0	E	35	-8	13	1	F	78	-77	14	4	6	59	-49	6	8	E	30	-41
10	0	0	14	-14	1	10	E	36	-4	14	1	F	58	57	0	5	6	250	224	7	8	E	14	-17
12	0	0	56	-44	2	10	E	48	-90	15	1	F	23	18	1	5	6	170	154	8	8	E	36	-44
14	0	0	58	16	3	10	E	19	9	0	2	F	332	342	2	5	E	56	-52	9	8	E	54	67
16	0	0	33	39	4	10	E	24	27	1	2	F	276	-262	3	5	E	84	88	10	8	E	44	35
18	0	0	11	1	5	10	E	43	54	2	2	F	7	12	4	5	E	174	-174	11	8	E	18	-15
1	1	E	52	-44	7	10	E	15	-7	3	2	F	104	-106	5	5	E	152	-153	0	9	E	86	101
3	1	E	184	-178	8	10	E	24	-29	4	2	F	211	-220	6	5	E	104	112	1	9	E	40	51
5	1	E	58	60	1	11	E	54	-58	5	2	F	258	268	7	5	E	12	-8	2	9	E	20	-27
6	1	E	44	47	3	11	E	27	27	6	2	F	47	58	8	5	E	30	32	3	9	E	10	37
7	1	E	58	75	4	11	E	54	56	7	2	F	98	96	9	5	E	84	84	4	9	E	40	-39
8	1	E	107	126	6	11	E	7	-8	8	2	F	113	134	10	5	E	73	-66	5	9	E	47	-47
9	1	E	37	-36	8	11	E	44	38	9	2	F	121	-128	11	5	E	27	-28	6	9	E	40	46
10	1	E	74	-72	5	11	E	22	-19	10	2	F	50	-74	12	5	E	30	-26	7	9	E	16	-12
11	1	E	72	-63	7	11	E	22	-22	11	2	F	28	22	13	5	E	54	-45	8	9	E	54	41
12	1	E	28	19	1	12	E	14	6	12	2	F	52	-43	0	6	E	157	143	9	9	E	48	37
13	1	E	56	49	2	12	E	20	17	13	2	F	32	22	1	6	E	175	-171	10	9	E	44	-43
1	2	E	110	-121	3	12	E	13	-13	14	2	F	27	24	2	6	E	39	-30	0	10	E	36	47
3	2	E	47	44	4	12	E	30	-20	15	2	F	40	-25	3	6	E	70	-64	1	10	E	43	-35
5	2	E	107	110	0	0	F	410	-444	0	3	F	277	-291	4	6	E	137	-123	2	10	E	8	-8
6	2	E	82	92	1	0	F	217	191	1	3	F	162	-174	5	6	E	143	137	3	10	E	14	-22
7	2	E	28	32	2	0	F	22	-24	2	3	F	44	44	6	6	E	67	68	4	10	E	40	-48
8	2	E	77	76	3	0	F	188	147	3	3	F	108	-115	7	6	E	10	-2	5	10	E	16	14
9	2	E	151	-119	4	0	F	348	314	4	3	F	102	103	8	6	E	30	26	6	10	E	17	14
A	2	E	25	18	5	0	F	209	-202	5	3	F	170	165	9	6	E	67	-66	7	10	E	7	1
11	2	E	39	21	6	0	F	79	-68	6	3	F	124	-142	10	6	E	70	-67	8	10	E	36	28
12	2	E	74	72	7	0	F	44	-35	7	3	F	32	31	11	6	E	28	23	9	10	E	44	-43
13	2	E	15	-12	8	0	F	69	-80	8	3	F	78	-67	12	6	E	24	-21	0	11	E	26	-30
1	3	E	84	74	9	0	F	160	152	9	3	F	107	-102	13	6	E	61	45	1	11	E	17	-21
2	3	E	104	104	10	0	F	46	44	10	3	F	77	76	0	7	E	1180	-1147	2	11	E	11	11
3	3	E	20	-28	11	0	F	93	-17	11	3	E	16	10	1	7	E	111	-105	3	11	E	40	39
4	3	E	49	-48	12	0	F	24	16	12	3	E	24	18	2	7	E	30	30	5	11	E	31	21
5	3	E	151	-150	13	0	F	156	-16	13	3	E	42	24	3	7	E	47	-48	6	11	E	19	-14
6	3	E	100	-88	14	0	E	67	-48	14	3	E	41	-44	4	7	E	142	132	7	11	E	17	14
7	3	E	37	31	15	0	E	60	30	0	4	F	207	-220	5	7	E	106	97	1	12	E	20	16
8	3	E	74	80	0	1	E	607	592	1	4	F	220	198	6	7	E	67	-62	4	12	E	13	13
9	3	E	10	9	1	1	E	188	182	2	4	F	47	52	7	7	E	10	8	1	1	7	144	124
10	3	E	44	33	2	1	E	24	13	3	4	F	127	120	8	7	E	74	-78	2	1	7	35	30
11	3	E	27	-20	3	1	E	68	64	4	4	F	202	183	9	7	E	53	-58	3	1	7	151	-143
1	4	E	70	73	4	1	E	247	-271	5	4	F	185	-203	10	7	E	75	60	4	1	7	9	1
2	4	E	14	-15	5	1	E	171	-205	6	4	E	89	-108	11	7	E	14	15	5	1	7	13	-10
3	4	E	77	-86	6	1	E	53	52	7	4	E	27	-30	12	7	E	37	29	6	1	7	24	27
4	4	E	7	4	7	1	E	14	-16	8	4	E	91	-101	0	8	E	69	-107	7	1	7	13	35
5	4	E	49	-53	8	1	E	127	141	9	4	E	113	111	1	8	E	85	93	8	1	7	14	-12
6	4	E	32	18	9	1	E	104	137	10	4	E	56	61	2	8	E	21	25	10	1	7	21	-25
7	4	E	139	91	10	1	E	74	-102	11	4	E	27	-22	3	8	E	46	49	12	1	7	9	10
8	4	E	9	-6	11	1	E	8	-14	12	4	E	38	36	4	8	E	85	82	13	1	7	12	-9

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR 0EY4

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
1	2	7	122	-103	1	E	7	154	-156	4	11	7	22	-25	14	2	A	41	-47	8	E	A	81	-84
2	2	7	122	-122	2	E	7	44	36	E	11	7	88	-80	A	3	A	202	-215	6	E	A	136	124
3	2	7	56	45	4	E	7	126	144	1	12	7	53	44	1	3	A	215	194	4	E	A	179	174
4	2	7	38	35	6	E	7	14	-19	3	12	7	22	-24	2	3	A	24	20	6	E	A	72	-72
5	2	7	36	36	8	E	7	72	82	A	0	F	207	242	3	3	A	97	95	7	E	A	17	0
6	2	7	37	38	E	E	7	16	-11	1	0	F	269	258	4	3	A	247	234	8	E	A	85	-85
7	2	7	36	-49	7	E	7	114	-130	3	0	F	51	44	5	3	A	210	-184	A	E	A	51	-52
8	2	7	37	-13	8	E	7	20	-20	5	0	F	91	85	E	3	A	94	-86	10	E	A	48	57
A	2	7	10	-8	11	E	7	14	15	7	0	F	232	-227	7	3	A	12	-7	11	E	A	20	24
10	2	7	6	-6	13	E	7	33	-32	9	0	F	268	-274	9	3	A	174	-140	12	E	A	20	20
11	2	7	16	20	1	F	7	12	6	B	0	F	69	68	A	3	A	114	122	13	E	A	34	44
12	2	7	9	-10	3	F	7	158	164	A	0	F	17	16	10	3	A	78	88	C	7	A	142	-137
13	2	7	10	9	5	F	7	6	-11	2	0	A	128	149	11	3	A	28	-27	1	7	A	27	24
1	3	7	20	-10	A	F	7	52	-53	4	0	A	139	151	12	3	A	35	41	2	7	A	32	34
2	3	7	46	40	8	F	7	10	9	10	0	A	74	-83	13	3	A	42	-50	3	7	A	45	50
3	3	7	31	24	C	F	7	105	-102	12	0	A	30	-32	14	3	A	46	-60	4	7	A	122	114
4	3	7	60	-56	7	F	7	7	-4	13	0	A	32	-41	0	4	A	288	284	5	7	A	98	-94
5	3	7	34	29	A	F	7	82	80	14	0	A	86	-66	1	4	A	113	106	E	7	A	76	-84
6	3	7	47	-47	10	F	7	42	49	16	0	A	46	53	2	4	A	96	-90	7	7	A	16	-9
7	3	7	21	-14	11	F	7	6	4	0	1	A	246	-241	3	4	A	74	72	8	7	A	50	-52
A	3	7	63	59	12	F	7	57	-46	1	1	A	147	-175	4	4	A	208	-198	9	7	A	51	57
B	3	7	12	11	2	F	7	100	119	2	1	A	31	-39	5	4	A	146	-133	10	7	A	33	34
10	3	7	30	36	3	F	7	11	13	3	1	A	93	-91	6	4	A	49	44	11	7	A	11	-14
12	3	7	21	-21	A	F	7	86	-101	4	1	A	260	-248	7	4	A	17	-15	12	7	A	14	14
14	3	7	14	17	A	F	7	7	-12	5	1	A	217	214	A	4	A	108	110	C	F	A	73	74
1	4	7	178	186	B	F	7	47	-40	E	1	A	172	174	B	4	A	107	109	1	F	A	61	67
2	4	7	22	-22	7	A	7	111	110	7	1	A	24	26	10	4	A	56	-74	2	F	A	16	-18
3	4	7	103	-104	7	A	7	8	9	A	1	A	120	128	11	4	A	27	-29	3	F	A	37	37
4	4	7	7	9	8	A	7	8	8	B	1	A	132	-132	12	4	A	24	-22	4	F	A	72	-72
5	4	7	76	-74	12	A	7	52	-55	10	1	A	92	-103	13	4	A	46	-42	5	F	A	74	-70
7	4	7	17	11	3	B	7	8	8	11	1	A	18	16	14	4	A	32	44	8	F	A	40	39
8	4	7	58	54	2	C	7	7	7	12	1	A	24	-24	0	5	A	203	200	9	F	A	34	36
A	4	7	6	2	3	C	7	8	-10	13	1	A	54	71	1	5	A	159	-147	A	F	A	47	56
B	4	7	26	28	4	C	7	33	36	14	1	A	61	70	2	5	A	35	-33	10	F	A	36	-30
10	4	7	54	-52	5	C	7	87	85	0	2	A	270	-264	3	5	A	74	-67	11	F	A	17	-14
11	4	7	16	11	7	C	7	6	7	1	2	A	270	-261	4	5	A	173	-163	C	G	A	41	42
3	5	7	32	28	8	C	7	62	-52	2	2	A	52	52	5	5	A	144	138	1	G	A	45	-44
4	5	7	164	-168	B	C	7	7	7	3	2	A	140	-134	6	5	A	90	86	2	G	A	18	-20
5	5	7	13	-16	10	C	7	57	-46	4	2	A	242	224	7	5	A	13	13	3	G	A	39	-39
7	5	7	46	49	1	D	7	47	-43	5	2	A	244	247	A	5	A	88	84	4	G	A	57	-56
8	5	7	31	-32	2	D	7	4	12	6	2	A	195	-192	8	5	A	86	88	E	G	A	51	44
A	5	7	175	179	3	D	7	A	14	7	2	A	34	40	10	5	A	70	72	6	H	A	37	33
7	E	7	6	9	B	D	7	32	30	A	2	A	104	-108	11	5	A	16	22	7	H	A	8	-8
8	E	7	76	-70	7	D	7	78	-74	A	2	A	150	-153	12	5	A	24	-27	8	H	A	20	25
A	E	7	10	25	8	D	7	7	7	10	2	A	77	72	13	5	A	43	43	9	H	A	29	-37
10	E	7	67	-63	1	E	7	7	10	11	2	A	18	13	0	6	A	169	-183	10	H	A	35	-35
12	E	7	20	22	2	E	7	8	-14	12	2	A	36	30	1	6	A	178	-166	0	10	A	36	-30
13	E	7	16	-12	3	E	7	8	-14	13	2	A	58	58	2	6	A	38	39	1	10	A	41	-44

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	10	A	13	10	8	5	0	23	22	6	7	0	46	-24	8	0	10	119	125	11	9	10	11	-11
3	10	A	16	-24	9	5	0	15	-7	7	7	0	100	88	9	0	10	97	-98	12	9	10	13	-17
4	10	A	31	33	11	5	0	24	-23	8	7	0	35	9	10	0	10	111	-116	13	9	10	17	-16
5	10	A	47	45	12	5	0	6	-12	9	7	0	7	7	11	0	10	10	11	14	9	10	25	33
7	10	A	28	-34	13	5	0	14	16	10	7	0	12	13	12	0	10	24	-2	0	A	10	256	247
7	10	A	5	4	1	A	0	17	16	11	7	0	47	-50	13	0	10	37	43	1	A	10	7	-7
8	10	A	12	-11	2	A	0	21	-20	12	7	0	0	-7	14	0	10	61	60	2	A	10	26	-24
0	11	A	24	-29	3	A	0	14	12	1	A	0	29	24	0	1	10	334	-303	3	A	10	37	-37
1	11	A	17	21	4	A	0	49	49	2	A	0	112	-117	1	1	10	292	-290	4	A	10	224	-208
2	11	A	6	11	5	A	0	12	-9	3	A	0	27	-31	2	1	10	21	20	5	A	10	108	111
3	11	A	5	17	6	A	0	73	69	4	A	0	30	32	3	1	10	148	-149	6	A	10	114	107
4	11	A	94	91	7	A	0	7	7	5	A	0	86	84	4	1	10	290	305	7	A	10	11	-9
5	11	A	94	-99	8	A	0	64	-61	6	A	0	30	24	5	1	10	94	101	8	A	10	143	133
6	11	A	14	-15	9	A	0	10	3	7	A	0	51	-47	6	1	10	45	-37	9	A	10	74	-75
0	12	A	11	12	10	A	0	19	-11	8	A	0	6	-1	7	1	10	36	32	10	A	10	95	-97
1	12	A	19	16	11	A	0	9	-10	10	A	0	36	-40	8	1	10	111	-107	11	A	10	22	20
1	1	B	52	-62	12	A	0	25	31	11	A	0	14	-12	9	1	10	165	-181	12	A	10	36	-38
2	1	B	47	-52	13	A	0	6	8	1	B	0	77	-84	10	1	10	59	64	13	A	10	29	32
3	1	B	47	47	1	B	0	124	-137	2	B	0	39	-43	11	1	10	14	-20	0	B	10	139	-136
4	1	B	36	34	2	B	0	77	-84	3	B	0	86	87	12	1	10	31	32	1	B	10	194	-190
5	1	B	28	28	3	B	0	28	32	4	B	0	8	8	13	1	10	84	86	2	B	10	26	28
6	1	B	11	7	4	B	0	11	7	5	B	0	47	50	14	1	10	39	-46	3	B	10	105	-112
7	1	B	61	-66	5	B	0	77	67	6	B	0	32	30	0	2	10	491	-450	4	B	10	109	102
8	1	B	15	-12	6	B	0	28	23	7	B	0	49	-46	1	2	10	101	108	5	B	10	196	182
9	1	B	34	-38	7	B	0	102	-94	8	B	0	11	7	2	2	10	57	54	6	B	10	64	-61
10	1	B	7	5	8	B	0	12	-13	9	B	0	7	-6	3	2	10	45	44	7	B	10	31	27
11	1	B	29	26	9	B	0	22	-23	1	C	0	8	-16	4	2	10	129	105	8	B	10	63	-57
13	1	B	10	-9	10	B	0	27	24	2	C	0	88	100	5	2	10	181	166	9	B	10	320	-321
1	2	B	72	-81	11	B	0	46	46	3	C	0	7	15	6	2	10	168	-165	10	B	10	44	53
2	2	B	76	81	12	B	0	10	12	4	C	0	30	-34	7	2	10	17	-13	11	B	10	19	20
3	2	B	41	38	13	B	0	13	-17	5	C	0	6	10	8	2	10	160	-158	12	B	10	14	14
4	2	B	62	-66	1	E	0	23	-21	6	C	0	7	-13	9	2	10	95	96	13	B	10	46	59
5	2	B	11	-12	2	E	0	128	136	7	C	0	18	-19	10	2	10	108	112	0	E	10	200	-202
6	2	B	56	-61	3	E	0	19	19	8	C	0	43	44	11	2	10	10	-11	1	E	10	94	91
7	2	B	38	-38	4	E	0	64	66	9	C	0	42	44	12	2	10	40	43	2	E	10	44	47
8	2	B	9	10	5	E	0	10	11	9	C	0	13	10	13	2	10	32	-43	3	E	10	47	57
9	2	B	14	18	6	E	0	100	-103	2	C	0	98	-88	14	2	10	59	-75	4	E	10	161	157
10	2	B	34	35	7	E	0	20	-22	3	C	0	15	-19	0	3	10	161	154	5	E	10	45	-44
11	2	B	5	11	8	E	0	43	46	4	C	0	14	-16	1	3	10	274	261	6	E	10	88	-87
12	2	B	17	-18	9	E	0	7	4	5	C	0	46	-47	2	3	10	17	-15	7	E	10	17	-15
14	2	B	12	-14	10	E	0	64	69	0	D	10	798	903	3	3	10	170	174	8	E	10	88	-85
1	3	A	104	98	11	E	0	13	13	1	D	10	96	-102	4	3	10	126	-121	9	E	10	54	50
2	3	A	16	17	12	E	0	34	-41	2	D	10	20	-19	5	3	10	244	-262	10	E	10	84	85
3	3	A	76	81	1	F	0	101	106	3	D	10	73	-70	6	3	10	64	60	11	E	10	27	35
4	3	A	79	-94	2	F	0	61	61	4	D	10	215	-211	7	3	10	64	-60	0	F	10	49	50
6	3	A	11	6	3	F	0	88	-100	5	D	10	140	130	8	3	10	84	68	1	F	10	122	121
7	3	A	14	-18	4	F	0	8	-6	6	D	10	119	122	9	3	10	170	170	2	F	10	19	-19
7	3	A	58	60	5	F	0	24	-30	7	D	10	33	26	10	3	10	51	-51	3	F	10	58	74

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR BRYA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	2	10	76	-78	7	1	11	50	-50	4	5	11	30	-29	0	0	11	7	-5
1	2	10	126	-114	7	1	11	26	-24	5	5	11	19	13	1	10	11	44	58
2	2	10	39	-37	8	1	11	10	5	6	5	11	111	-102	2	10	11	24	32
3	2	10	19	-16	10	1	11	30	27	7	5	11	42	-38	3	10	11	46	48
4	2	10	43	42	11	1	11	19	11	8	5	11	44	42	4	10	11	8	-6
5	2	10	74	75	14	1	11	7	-10	9	5	11	50	44	5	10	11	21	-20
10	2	10	33	-34	1	2	11	44	48	11	5	11	21	24	6	10	11	28	-25
11	2	10	15	-14	2	2	11	67	67	13	5	11	27	-31	7	10	11	66	63
0	3	10	93	96	3	2	11	13	-14	13	5	11	7	-9	8	10	11	14	20
1	3	10	67	-67	4	2	11	13	-14	1	6	11	57	58	1	11	11	21	19
2	3	10	22	-24	5	2	11	32	-34	2	6	11	59	64	3	11	11	21	-22
3	3	10	97	-96	6	2	11	61	-60	3	6	11	67	-71	4	11	11	22	24
4	3	10	46	-49	7	2	11	14	15	4	6	11	24	-21	5	11	11	22	-22
5	3	10	52	56	8	2	11	22	17	5	6	11	35	-31	6	0	12	22	-23
6	3	10	43	46	9	2	11	10	6	6	6	11	45	-44	7	0	12	273	-264
7	3	10	7	3	12	2	11	27	24	7	6	11	31	32	8	0	12	25	27
8	3	10	47	47	13	2	11	10	-9	8	6	11	31	33	9	0	12	134	-133
9	3	10	36	-34	14	2	11	7	-12	9	6	11	16	10	10	0	12	16	-11
10	3	10	44	48	13	3	11	11	7	10	6	11	12	15	11	0	12	349	305
0	4	10	43	-45	14	3	11	8	-7	11	6	11	40	-43	12	0	12	64	-66
1	4	10	52	-57	1	4	11	63	66	12	6	11	11	-15	13	0	12	60	62
2	4	10	12	16	2	4	11	57	-59	1	7	11	56	58	0	1	12	7	0
3	4	10	36	-37	3	4	11	58	-59	2	7	11	104	-113	1	1	12	324	-319
4	4	10	32	37	4	4	11	53	56	3	7	11	53	-57	2	1	12	41	41
5	4	10	29	27	5	4	11	19	-15	4	7	11	37	40	3	1	12	21	22
6	4	10	27	-25	6	4	11	44	46	5	7	11	17	-14	4	1	12	7	-11
7	4	10	7	1	7	4	11	40	36	6	7	11	57	58	5	1	12	13	7
8	4	10	11	-12	8	4	11	43	-38	7	7	11	47	44	6	1	12	14	-12
9	4	10	46	-45	10	4	11	24	-24	8	7	11	52	-48	7	1	12	463	-482
10	4	10	66	-76	11	4	11	14	-17	10	7	11	41	-40	8	1	12	104	97
1	10	10	26	24	12	4	11	10	14	11	7	11	20	-21	9	1	12	24	31
2	10	10	17	20	13	4	11	6	7	1	8	11	86	-85	10	1	12	64	65
3	10	10	13	19	1	5	11	114	-103	2	8	11	50	-50	11	1	12	260	315
4	10	10	64	65	2	5	11	64	-65	3	8	11	50	50	12	1	12	20	-17
5	10	10	39	-38	3	5	11	79	82	4	8	11	18	15	0	2	12	147	-136
6	10	10	29	-30	4	5	11	25	16	5	8	11	21	21	1	2	12	29	-16
7	10	10	8	-3	6	5	11	33	29	6	8	11	48	42	2	2	12	184	-173
8	10	10	36	-28	7	5	11	52	52	7	8	11	60	76	3	2	12	60	54
0	11	10	10	10	8	5	11	16	-12	8	8	11	27	-25	4	2	12	116	122
1	11	10	24	22	9	5	11	27	-21	10	8	11	27	-22	5	2	12	42	45
2	11	10	19	17	1	6	11	7	7	1	9	11	32	-32	6	2	12	22	-26
3	11	10	11	-13	10	6	11	23	-24	2	9	11	96	104	7	2	12	82	-84
8	11	10	32	-34	11	6	11	23	22	3	9	11	27	26	8	2	12	69	71
1	1	11	14	-21	12	6	11	14	18	4	9	11	27	-28	1	3	12	247	243
2	1	11	42	43	14	6	11	15	-11	5	9	11	22	18	2	3	12	43	41
3	1	11	16	16	1	7	11	33	-27	6	9	11	52	-48	3	3	12	143	139
4	1	11	5	5	2	7	11	109	113	7	9	11	36	-35	4	3	12	45	-43
5	1	11	16	14	3	7	11	39	37	8	9	11	49	39	5	3	12	325	-283

H	K	L	FO	FC
6	2	12	40	38
7	2	12	35	-33
8	2	12	34	33
9	2	12	148	139
10	2	12	36	-35
11	2	12	24	-24
12	2	12	15	-13
0	3	12	343	325
1	3	12	97	-90
2	3	12	47	-43
3	3	12	48	-48
4	3	12	273	-249
5	3	12	102	96
6	3	12	148	127
7	3	12	11	6
8	3	12	192	162
9	3	12	54	-44
10	3	12	104	-106
11	3	12	16	14
12	3	12	34	-42
0	4	12	17	-20
1	4	12	68	-71
2	4	12	14	12
3	4	12	128	-130
4	4	12	54	52
5	4	12	241	215
6	4	12	44	-35
7	4	12	33	32
8	4	12	78	-85
9	4	12	154	-146
10	4	12	28	30
11	4	12	27	30
12	4	12	25	27
0	5	12	236	-225
1	5	12	38	36
2	5	12	57	58
3	5	12	24	26
4	5	12	183	177
5	5	12	45	-46
6	5	12	121	-108
7	5	12	10	-4
8	5	12	111	-98
9	5	12	32	30
10	5	12	48	47
11	5	12	7	-31
12	5	12	30	33
0	6	12	62	60
1	6	12	148	143

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REV4

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	8	12	13	-4	0	11	12	72	31	0	4	13	8	-3	2	9	13	46	51	5	2	14	173	144
3	8	12	70	80	1	11	12	6	-4	10	4	13	24	26	3	9	13	60	-66	7	2	14	17	8
4	8	12	56	-53	0	11	12	31	-32	11	4	13	22	24	4	9	13	13	-10	8	2	14	162	150
5	8	12	152	-138	1	12	12	6	2	12	4	13	7	16	5	9	13	26	-25	9	2	14	18	-20
6	8	12	30	29	0	1	13	67	-63	13	4	13	19	-11	6	9	13	48	-42	10	2	14	121	-118
7	8	12	37	-32	1	1	13	17	-21	1	5	13	67	62	7	9	13	66	62	12	2	14	36	-41
8	8	12	36	32	2	1	13	22	19	2	5	13	57	54	8	10	13	21	20	0	3	14	40	36
9	8	12	64	61	3	1	13	31	-27	3	5	13	75	-72	1	10	13	30	28	1	3	14	287	-286
10	8	12	23	-24	4	1	13	9	-10	4	5	13	23	-19	2	10	13	51	-53	2	3	14	11	6
11	8	12	16	-18	5	1	13	54	50	5	5	13	26	-25	3	10	13	39	-42	3	3	14	156	-155
19	8	12	6	-8	6	1	13	6	5	6	5	13	57	-51	4	10	13	23	23	4	3	14	26	24
0	9	12	121	122	0	2	13	32	32	7	5	13	84	73	5	10	13	15	-15	5	3	14	318	280
1	9	12	47	-49	1	2	13	6	6	8	5	13	36	28	6	10	13	51	46	6	3	14	16	-19
2	9	12	30	-30	11	1	13	14	-21	0	5	13	8	3	7	11	13	35	-38	7	3	14	29	28
3	9	12	22	-22	12	1	13	8	-6	14	5	13	24	27	9	11	13	30	-47	8	3	14	12	-10
4	9	12	151	-156	0	3	13	60	57	15	5	13	33	-34	3	11	13	41	44	9	3	14	186	-176
5	9	12	44	37	2	2	13	57	-53	12	5	13	20	-19	0	0	14	336	-340	10	3	14	10	10
6	9	12	20	21	3	2	13	24	-23	1	6	13	61	56	1	0	14	19	5	11	3	14	23	27
7	9	12	9	7	4	2	13	31	27	3	6	13	100	-96	2	0	14	21	14	12	3	14	8	2
8	9	12	56	51	5	2	13	50	-49	4	6	13	66	-69	4	0	14	26	-21	13	3	14	69	80
9	9	12	29	-26	6	2	13	60	60	5	6	13	35	30	6	0	14	287	253	0	4	14	298	-292
10	9	12	57	-58	7	2	13	34	30	6	6	13	14	-18	8	0	14	10	-4	1	4	14	28	29
11	9	12	8	7	8	2	13	14	-10	7	6	13	78	64	10	0	14	131	-114	2	4	14	45	44
0	10	12	42	-42	0	3	13	34	35	8	6	13	67	58	7	0	14	21	21	3	4	14	5	7
1	10	12	80	-81	1	3	13	33	-34	9	6	13	40	-32	8	0	14	167	-163	4	4	14	249	224
2	10	12	18	14	10	2	13	15	10	10	6	13	22	-22	9	0	14	17	-2	5	4	14	24	17
3	10	12	46	-47	12	2	13	14	20	11	6	13	27	-26	10	0	14	113	117	6	4	14	131	-114
4	10	12	30	32	3	3	13	72	-69	1	7	13	69	-71	12	0	14	40	44	7	4	14	12	3
5	10	12	80	78	5	3	13	79	-78	2	7	13	64	-69	0	1	14	79	68	8	4	14	135	-124
6	10	12	27	-29	9	3	13	44	47	3	7	13	44	44	1	1	14	209	201	9	4	14	10	7
7	10	12	17	10	4	3	13	47	43	4	7	13	35	35	2	1	14	6	3	10	4	14	93	84
8	10	12	14	-11	6	3	13	24	27	5	7	13	32	32	3	1	14	104	106	12	4	14	34	36
9	10	12	62	-63	7	3	13	44	44	6	7	13	66	71	4	1	14	60	63	0	5	14	17	15
10	10	12	17	16	7	3	13	53	-55	7	7	13	70	-66	5	1	14	269	-244	1	5	14	181	186
0	11	12	78	74	8	3	13	34	-37	8	7	13	17	-15	6	1	14	3	3	2	5	14	107	115
1	11	12	17	12	10	3	13	8	-7	9	7	13	37	-34	7	1	14	17	-19	3	5	14	15	-12
2	11	12	21	24	10	3	13	34	-36	10	7	13	28	-31	8	1	14	34	30	4	5	14	195	-179
3	11	12	72	74	11	3	13	23	26	11	7	13	36	34	9	1	14	174	160	8	5	14	12	10
4	11	12	14	-13	12	3	13	14	20	1	8	13	92	-91	10	1	14	9	7	9	5	14	31	-28
5	11	12	40	-40	13	3	13	6	-10	2	8	13	78	68	11	1	14	31	-32	7	5	14	6	8
6	11	12	19	12	1	4	13	71	-69	3	8	13	82	72	12	1	14	14	-11	8	5	14	118	120
7	11	12	30	-34	2	4	13	57	52	4	8	13	21	-21	13	1	14	67	-66	10	5	14	12	-10
8	10	12	14	10	3	4	13	44	42	6	8	13	33	34	0	2	14	197	189	11	5	14	24	20
0	12	12	44	52	4	4	13	33	-26	8	8	13	63	-62	1	2	14	15	-3	0	6	14	193	197
1	12	12	21	22	5	4	13	56	-56	9	8	13	62	-67	2	2	14	72	-71	1	6	14	25	28
4	12	12	17	-16	6	4	13	47	-42	0	9	13	32	31	3	2	14	20	-17	2	6	14	37	38
7	12	12	4	-3	7	4	13	44	-40	2	9	13	13	-17	4	2	14	111	-120	3	6	14	25	-29
9	12	12	5	1	8	4	13	42	1	1	9	13	52	50	5	2	14	20	17	4	6	14	172	-162

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PEKA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	5	14	49	41	0	1	15	0	-3	10	5	15	28	-28	5	0	16	18	-14
6	5	14	80	78	0	1	15	8	4	11	5	15	26	-30	7	0	16	55	-64
7	5	14	39	35	1C	1	15	7	-14	1	6	15	30	-35	8	0	16	43	38
8	5	14	101	94	11	1	15	14	-17	2	6	15	71	77	9	0	16	100	100
9	5	14	23	-24	1	2	15	25	-30	3	6	15	37	33	10	0	16	17	16
10	5	14	84	-89	2	2	15	73	-80	4	6	15	43	38	11	0	16	13	-18
11	5	14	5	-9	3	2	15	30	27	5	6	15	7	-9	12	0	16	13	15
0	7	14	12	-7	4	2	15	35	30	6	6	15	63	60	13	0	16	72	-69
1	7	14	96	-88	5	2	15	29	26	7	6	15	17	-16	0	1	16	444	440
2	7	14	6	7	6	2	15	24	-18	8	6	15	19	-23	1	1	16	66	65
3	7	14	82	-82	7	2	15	32	-29	10	6	15	22	-23	3	1	16	35	-36
4	7	14	111	97	8	2	15	17	-14	11	6	15	16	16	4	1	16	29	20
5	7	14	7	-7	10	2	15	12	-20	1	7	15	53	-53	5	1	16	292	-288
7	7	14	18	12	11	2	15	18	15	2	7	15	47	49	6	1	16	44	-44
8	7	14	37	-31	12	2	15	16	14	4	7	15	56	61	8	1	16	162	174
11	7	14	7	7	13	2	15	6	-4	6	7	15	21	-19	9	1	16	13	-3
0	8	14	61	-61	1	3	15	59	-58	8	7	15	20	21	0	2	16	154	147
1	8	14	12	10	2	3	15	19	21	9	7	15	40	-37	1	2	16	29	27
2	8	14	20	22	3	3	15	84	82	10	7	15	57	-60	2	2	16	104	-112
3	8	14	8	8	4	3	15	7	-8	11	7	15	12	24	12	2	16	37	-39
4	8	14	46	44	5	3	15	18	20	0	7	16	12	-11	13	2	16	11	-14
5	8	14	10	-10	6	3	15	30	-34	11	7	16	11	20	0	3	16	11	14
6	8	14	43	-43	7	3	15	84	-87	1	8	15	42	45	1	3	16	242	-241
8	8	14	40	-45	8	3	15	20	10	2	8	15	87	78	2	3	16	20	-10
9	8	14	10	9	9	3	15	12	-7	3	8	15	51	-48	3	3	16	143	-141
0	9	14	7	-7	10	3	15	20	22	4	8	15	16	-15	4	3	16	70	-73
1	9	14	56	54	11	3	15	21	26	5	8	15	22	-18	6	3	16	249	248
3	9	14	36	37	12	3	15	13	-16	7	8	15	61	-66	8	3	16	36	30
4	9	14	4	1	1	4	15	46	39	8	8	15	42	-37	9	3	16	38	34
5	9	14	30	-27	2	4	15	58	58	9	8	15	27	24	1	4	16	34	31
6	9	14	8	4	3	4	15	40	-39	1	9	15	45	47	0	4	16	170	-166
7	9	14	7	-1	4	4	15	61	-58	2	9	15	58	-54	10	4	16	17	-19
8	9	14	6	-6	5	4	15	54	-52	3	9	15	56	-59	11	5	16	20	23
0	10	14	43	42	7	4	15	41	31	4	9	15	21	19	12	5	16	14	-14
1	10	14	8	-8	8	4	15	43	37	6	9	15	25	-27	0	6	16	125	-126
2	10	14	13	-19	9	4	15	16	-11	8	9	15	46	47	1	6	16	34	33
3	10	14	6	-5	10	4	15	32	27	9	9	15	28	32	2	6	16	44	44
4	10	14	47	-47	11	4	15	11	12	1	10	15	31	-34	3	6	16	24	-26
5	10	14	8	7	12	4	15	22	-22	2	10	15	81	85	4	6	16	77	83
6	10	14	28	28	1	5	15	88	88	3	10	15	48	43	5	6	16	244	247
1	11	14	36	-32	2	5	15	96	94	4	10	15	22	19	6	6	16	116	-123
2	11	14	33	33	3	5	15	80	-83	5	10	15	15	17	7	6	16	16	7
3	11	14	13	-13	4	5	15	46	41	7	0	16	76	-78	8	6	16	151	-138
5	11	14	19	-10	6	5	15	40	-38	1	0	16	261	270	10	6	16	37	-33
6	11	14	7	7	7	5	15	8	5	2	0	16	10	4	11	6	16	40	39
4	12	14	28	-24	7	6	15	76	71	4	0	16	171	162	11	7	16	6	5
7	12	14	19	17	8	6	15	38	-32	6	0	16	68	64	12	7	16	42	42
9	12	14	31	29	9	6	15	31	8	8	0	16	114	-120	0	8	16	34	-42

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR BEXA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	0	1E	42	41	3	4	17	78	-87	2	9	17	77	-80	2	9	18	10	12	5	7	18	103	-88
0	0	2E	82	-76	4	4	17	31	31	3	9	17	34	30	3	J	18	101	93	6	7	18	18	-17
0	0	3E	8	-5	5	4	17	23	-22	4	9	17	27	22	4	9	18	65	62	7	7	18	7	-1
0	0	4E	6	2	6	4	17	10	6	5	9	17	14	6	5	3	1E	195	-173	8	7	18	32	-31
0	0	5E	71	70	7	4	17	64	67	6	9	17	64	67	6	3	1P	44	-36	0	8	18	66	64
0	0	6E	11	7	8	4	17	29	-29	7	10	17	44	-47	7	3	1E	15	-14	1	8	18	28	27
0	0	7E	5	-21	9	4	17	6	4	8	10	17	17	2E	8	3	1E	35	-34	2	8	18	57	-58
0	0	8E	5	2	10	4	17	7	4	9	10	17	72	67	9	3	2E	116	118	3	8	18	18	14
0	0	9E	77	-78	11	4	17	27	-28	0	0	1A	248	321	10	3	2E	37	36	4	8	18	48	-77
0	0	10E	6	4E	1	5	17	71	-75	1	0	1A	98	107	11	3	2E	21	-23	5	8	18	35	-27
0	0	11E	36	18	2	5	17	46	-48	2	0	1A	43	-43	0	4	1E	188	709	6	8	18	49	46
0	0	12E	6	0	3	5	17	72	71	3	0	1P	78	69	1	4	1E	80	84	0	9	18	25	24
0	1P	1E	5	-2	4	5	17	25	25	4	0	1P	744	-277	2	4	1E	34	-35	1	9	18	51	-60
1	1P	1E	36	-41	5	5	17	32	30	5	0	1P	116	-108	3	4	1E	66	63	2	9	18	7	-7
1	1P	1E	94	-91	6	5	17	37	38	6	0	1P	133	126	4	4	1E	171	-168	3	9	18	36	-34
1	1P	1E	7	4	7	5	17	52	-48	7	0	1P	24	-29	5	4	1E	96	-93	4	9	18	29	-20
1	1	17	21	-21	8	5	17	30	-30	8	0	1A	121	123	6	4	1E	89	87	5	9	18	69	60
2	1	17	16	-16	9	5	17	11	-18	0	1	1A	72	74	7	4	1E	27	-25	0	10	18	49	-52
3	1	17	26	18	10	5	17	14	-16	1	1	1A	92	-96	8	4	1E	88	88	1	10	18	8	-7
4	1	17	16	14	11	5	17	20	20	2	1	1A	90	-98	9	4	1E	57	62	2	10	18	19	-21
6	1	17	6	-7	1	6	17	52	-51	0	1	1E	122	130	10	4	1E	71	-72	3	1	19	43	38
7	1	17	12	-8	2	6	17	22	6	1	1	1E	700	704	11	4	1E	F	-1	4	1	19	22	25
8	1	17	6	3	3	6	17	20	20	2	1	1E	15	-15	0	5	1E	5P	55	5	1	19	74	-80
12	1	17	7	2	4	6	17	27	-21	3	1	1A	117	-110	1	5	1E	111	-121	6	1	19	24	-17
1	2	17	47	-44	5	6	17	10	23	4	1	1P	107	-98	2	5	1E	14	-12	7	1	19	14	-14
2	2	17	10	9	6	6	17	29	27	5	1	1P	240	222	3	5	1E	85	-74	8	1	19	17	13
3	2	17	42	40	7	6	17	58	-58	6	1	1P	44	41	4	5	1E	57	-47	10	1	19	10	5
4	2	17	7	2	8	6	17	32	34	7	1	1E	21	16	5	5	1E	133	123	11	1	19	8	5
5	2	17	14	12	9	6	17	8	-7	8	1	1E	54	52	6	5	1E	24	24	1	2	19	29	25
6	2	17	20	-16	10	6	17	11	12	9	1	1A	142	-144	7	5	1E	28	21	2	2	19	19	17
7	2	17	47	-41	0	7	17	45	47	10	1	1A	33	-36	8	5	1P	31	30	3	2	19	32	-24
8	2	17	7	4	2	7	17	9	8	11	1	1A	24	27	9	5	1E	88	-86	4	2	19	18	-18
10	2	17	11	11	3	7	17	56	-46	12	1	1A	17	-20	10	5	1E	48	-44	5	2	19	14	15
11	2	17	16	16	4	7	17	25	-24	0	2	1P	234	-247	0	6	1E	86	-102	7	2	19	28	19
12	2	17	7	-5	5	7	17	32	-25	1	2	1A	71	-77	1	6	1E	19	-14	8	2	19	21	17
1	3	17	57	60	6	7	17	41	-73	2	2	1A	93	91	2	6	1E	14	14	9	2	19	14	-13
2	3	17	91	96	7	7	17	57	48	3	2	1A	45	-46	3	6	1E	?	-6	10	2	19	12	11
3	3	17	30	-28	8	7	17	17	3E	4	2	1A	212	197	4	6	1E	95	92	11	2	19	10	-8
4	3	17	27	-23	9	7	17	12	8	5	2	1A	77	77	5	6	1E	23	23	1	3	19	45	44
5	3	17	27	-26	1	8	17	56	62	6	2	1A	119	-104	6	6	1E	54	-51	2	3	19	37	-47
6	3	17	72	-66	2	8	17	46	-43	7	2	1A	17	15	7	6	1E	?	-6	3	3	19	33	-34
7	3	17	47	46	3	8	17	75	-67	8	2	1A	112	-111	8	6	1E	56	-56	4	3	19	12	12
8	3	17	34	31	4	8	17	31	12	9	2	1A	52	-56	0	7	1E	19	-16	5	3	19	23	-18
10	3	17	30	29	5	8	17	44	-24	10	2	1A	60	62	0	7	1P	42	-44	6	3	19	31	35
11	3	17	11	-12	6	8	17	44	51	11	2	1A	7	7	1	7	1P	14	14	7	3	19	9A	37
12	3	17	15	-14	7	8	17	17	5E	12	2	1A	24	27	2	7	1E	10	8	8	3	19	16	-14
1	4	17	70	72	8	8	17	17	-16	0	3	1A	5E	-53	3	7	1E	46	44	9	3	19	10	6
2	4	17	91	-96	1	9	17	24	-27	1	3	1P	161	155	4	7	1E	46	37	10	3	19	13	-16

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PRY4

H	K	L	FO	FC
11	3	10	16	-20
7	4	10	47	-109
8	4	10	12	11
9	4	10	58	51
6	4	10	17	-11
5	4	10	40	-36
4	4	10	15	12
10	4	10	46	-38
1	5	10	47	-44
2	5	10	49	46
3	5	10	51	50
4	5	10	12	-16
5	5	10	26	-27
6	5	10	26	-28
7	5	10	13	14
8	5	10	11	8
9	5	10	10	-7
10	5	10	12	11
1	6	10	6	A
2	6	10	104	110
3	6	10	7	-5
4	6	10	30	-28
5	6	10	26	-24
6	6	10	19	9
7	6	10	42	42
8	6	10	8	-8
9	6	10	7	10
10	6	10	7	-10
1	7	10	16	-14
2	7	10	72	-70
3	7	10	42	-38
4	7	10	14	16
5	7	10	19	23
6	7	10	26	-24
7	7	10	9	9
8	7	10	51	-50
9	7	10	14	13
10	7	10	25	24
A	7	10	7	3
B	7	10	25	25
1	8	10	57	-62
2	8	10	15	14
3	8	10	44	42
4	8	10	A	5
5	8	10	106	106
6	8	10	29	-29
7	8	10	11	-12
8	8	10	13	-13
9	8	10	117	-114

H	K	L	FO	FC
8	0	20	177	184
9	0	20	44	45
A	0	20	6	3
B	0	20	87	84
C	0	20	94	-102
1	1	20	42	-44
2	1	20	17	21
3	1	20	208	-221
4	1	20	103	-113
5	1	20	24	24
6	1	20	62	-74
7	1	20	94	96
8	1	20	123	119
9	1	20	80	-82
A	1	20	94	90
B	1	20	24	-24
C	1	20	86	-88
D	1	20	26	-28
E	1	20	83	84
F	1	20	47	47
0	2	20	187	-189
1	2	20	134	141
2	2	20	20	17
3	2	20	60	67
4	2	20	144	131
5	2	20	173	-154
6	2	20	52	-58
7	2	20	25	-20
8	2	20	53	60
9	2	20	150	100
A	2	20	48	51
B	2	20	15	18
C	2	20	187	188
D	2	20	86	91
E	2	20	34	-28
F	2	20	50	52
0	3	20	173	-146
1	3	20	104	-89
2	3	20	8	11
3	3	20	92	84
4	3	20	104	121
5	3	20	136	-140
6	3	20	27	-29
7	3	20	101	94
8	3	20	44	45

H	K	L	FO	FC
3	4	20	38	34
4	4	20	46	48
5	4	20	42	-100
6	4	20	31	-34
7	4	20	131	-146
8	4	20	61	-72
9	4	20	22	22
A	4	20	62	-62
B	4	20	136	135
C	4	20	73	71
D	4	20	58	-64
E	4	20	66	-73
F	4	20	71	-78
0	5	20	74	84
1	5	20	26	18
2	5	20	53	52
3	5	20	77	67
4	5	20	67	-81
5	5	20	35	-33
6	5	20	6	-6
7	5	20	40	-39
8	5	20	85	101
9	5	20	46	54
A	5	20	23	-27
B	5	20	35	33
C	5	20	31	44
D	5	20	57	60
E	5	20	44	46
F	5	20	6	-6
0	6	20	40	-39
1	6	20	46	46
2	6	20	20	-20
3	6	20	68	-66
4	6	20	11	-12
5	6	20	34	-35
6	6	20	23	-27
7	6	20	24	-25
8	6	20	18	18
9	6	20	16	-13
A	6	20	18	13
B	6	20	33	28
C	6	20	10	-14
D	6	20	7	-12
E	6	20	20	-19
F	6	20	10	4
0	7	20	11	8
1	7	20	36	33
2	7	20	77	-81
3	7	20	38	-33
4	7	20	44	44
5	7	20	7	-8
6	7	20	40	-44
7	7	20	65	-66
8	7	20	11	-12
9	7	20	34	-35
A	7	20	53	-57
B	7	20	72	66
C	7	20	24	-25
D	7	20	18	15
E	7	20	16	-13
F	7	20	18	13
0	8	20	10	-14
1	8	20	10	-4
2	8	20	104	121
3	8	20	33	28
4	8	20	10	-14
5	8	20	7	-12
6	8	20	20	-19
7	8	20	10	4
8	8	20	11	8
9	8	20	36	33

H	K	L	FO	FC
1	2	21	50	55
2	2	21	28	-23
3	2	21	49	-44
4	2	21	21	14
5	2	21	32	-36
6	2	21	11	3
7	2	21	52	44
8	2	21	12	-12
9	2	21	11	11
A	2	21	37	-39
B	2	21	68	-60
C	2	21	49	42
D	2	21	19	17
E	2	21	22	15
F	2	21	64	57
0	3	21	28	-25
1	3	21	25	-26
2	3	21	33	-33
3	3	21	44	41
4	3	21	16	11
5	3	21	50	48
6	3	21	12	-9
7	3	21	69	-64
8	3	21	14	-14
9	3	21	11	-12
A	3	21	66	66
B	3	21	22	17
C	3	21	37	-43
D	3	21	44	-44
E	3	21	11	-8
F	3	21	41	36
0	4	21	8	0
1	4	21	61	72
2	4	21	11	12
3	4	21	73	-73
4	4	21	38	-32
5	4	21	72	70
6	4	21	5	-4
7	4	21	74	-83
8	4	21	25	23
9	4	21	85	83
A	4	21	44	-10
B	4	21	40	5
C	4	21	8	-5
0	5	22	134	-140
1	5	22	106	-102
2	5	22	23	24

H	K	L	FO	FC
3	0	22	74	-70
4	0	22	117	135
5	0	22	125	117
6	0	22	70	68
7	0	22	24	28
8	0	22	55	-56
9	0	22	84	-87
10	0	22	55	57
1	1	22	114	-135
2	1	22	101	111
3	1	22	14	10
4	1	22	84	85
5	1	22	129	109
6	1	22	173	-116
7	1	22	47	-46
8	1	22	14	-12
9	1	22	71	-72
A	1	22	76	78
B	1	22	43	44
C	1	22	104	128
D	1	22	92	97
E	1	22	19	-16
F	1	22	72	64
0	2	22	102	-108
1	2	22	112	-107
2	2	22	55	55
3	2	22	21	-19
4	2	22	54	54
5	2	22	78	80
6	2	22	47	-51
7	2	22	152	169
8	2	22	74	-84
9	2	22	30	-28
A	2	22	43	-49
B	2	22	140	-127
C	2	22	102	94
D	2	22	71	68
E	2	22	8	5
F	2	22	70	69
0	3	22	70	-71
1	3	22	119	-139
2	3	22	112	-114
3	3	22	24	21
4	3	22	64	-64
5	3	22	114	110
6	3	22	124	112
7	3	22	64	-66
8	3	22	9	2

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REXA

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
A	A	22	88	-88	A	2	22	12	-6	A	2	24	136	-134	A	2	26	11	14	2	2	28	27	32
A	A	22	72	-71	A	2	22	7	-10	A	2	24	93	88	A	2	26	15	-18	2	2	28	23	23
A	K	22	173	-172	A	4	22	29	-25	A	2	24	71	67	A	4	26	13	-19	2	4	28	112	122
A	K	22	76	85	A	4	22	67	70	A	2	24	10	6	A	4	26	26	26	2	4	28	42	-42
A	K	22	22	22	A	4	22	48	31	A	2	24	77	80	A	4	26	12	22	K	4	28	66	-61
A	K	22	47	46	A	6	22	42	-39	A	4	24	85	-107	A	6	26	9	-8	A	6	28	44	40
A	K	22	106	94	A	6	22	58	-55	A	4	24	114	-114	A	6	26	21	-22	A	6	28	41	48
E	K	22	82	-88	A	4	22	24	-23	A	4	24	13	14	A	8	26	12	-10	A	8	28	8	-9
E	K	22	95	-91	A	8	22	28	25	A	4	24	75	-79	A	A	26	10	13	2	A	28	60	66
I	K	22	9	-3	A	8	22	56	60	A	4	24	91	96	A	2	26	35	38	A	A	28	44	-39
A	K	22	56	-56	2	K	22	72	81	A	6	24	127	125	A	4	26	31	-30	K	A	28	99	-88
0	K	22	77	92	3	K	22	25	-40	A	6	24	28	-38	A	6	26	14	-16	A	6	28	101	105
1	K	22	72	78	A	K	23	18	-15	7	3	24	13	14	A	6	26	12	-10	3	6	28	36	-38
2	K	22	22	-20	E	K	23	34	-31	8	3	24	44	-46	E	A	26	22	-23	3	6	28	19	-18
3	K	22	57	58	E	K	23	20	-20	C	A	24	117	-128	1	A	26	20	23	3	6	28	19	-15
A	K	22	76	-72	I	K	23	28	24	1	A	24	84	90	2	A	26	42	-42	A	A	28	97	88
E	K	22	26	-27	1	E	23	15	15	2	A	24	27	27	2	K	26	30	-39	0	6	28	34	-38
I	K	22	47	44	2	E	23	31	-30	2	A	24	49	41	4	E	26	14	16	1	6	28	76	-70
7	K	22	21	-14	3	E	23	18	-20	A	A	24	110	105	5	F	26	8	-12	2	6	28	6	-7
A	K	22	58	78	A	E	23	28	26	E	A	24	71	-73	1	F	26	46	-47	3	1	27	14	-17
1	7	22	54	-48	E	I	23	51	57	E	A	24	61	-61	2	E	26	36	-34	3	1	27	A	5
2	7	22	14	11	I	I	23	16	-15	7	A	24	13	8	3	E	26	29	31	4	1	27	18	-13
3	7	22	31	-31	2	7	23	19	-19	0	E	24	60	55	0	I	26	60	59	2	2	27	27	24
A	7	22	72	-66	3	7	23	72	61	1	E	24	46	41	1	0	26	141	148	3	2	27	12	15
1	A	22	77	77	0	A	24	173	-184	2	E	24	17	17	2	0	26	19	-23	4	2	27	15	-11
0	A	22	58	-60	1	0	24	60	68	3	E	24	49	46	3	0	26	44	46	1	3	27	28	28
1	A	22	45	-48	2	0	24	20	19	4	E	24	61	-60	4	0	26	55	-50	2	3	27	24	25
2	A	22	17	16	3	0	24	43	43	5	E	24	40	-49	5	0	26	150	-150	3	3	27	26	-26
3	A	22	33	-27	A	0	24	148	144	6	E	24	37	36	6	0	26	26	20	4	3	27	15	-12
1	I	22	12	11	E	0	24	77	-77	8	E	24	85	85	7	0	26	22	-23	1	4	27	31	28
2	I	22	14	-8	E	0	24	60	-60	1	E	24	41	-42	0	1	26	174	168	2	4	27	32	-38
E	1	22	E	1	1	7	24	23	-24	2	E	24	15	-15	1	1	26	35	-37	3	4	27	15	14
5	1	22	0	9	E	0	24	40	-40	3	E	24	27	-25	2	1	26	26	-29	4	4	27	9	-10
0	1	22	E	A	E	0	24	68	61	4	E	24	89	-83	3	1	26	21	-22	1	5	27	29	-31
1	1	22	116	114	1	1	24	116	117	5	E	24	48	50	4	1	26	149	-148	2	5	27	169	178
2	1	22	7	-36	1	1	24	115	117	0	7	24	44	-46	5	1	26	47	41	1	0	28	10	-8
3	1	22	15	-15	2	1	24	12	-13	1	7	24	64	-62	E	1	26	74	76	2	0	28	28	-28
A	1	22	15	-17	3	1	24	78	71	2	7	24	14	12	7	1	26	8	A	3	0	28	8	-4
E	1	22	36	37	A	1	24	90	-92	3	7	24	43	-36	0	2	26	77	-71	4	0	28	133	-136
8	1	22	17	16	E	1	24	131	-127	1	1	25	14	14	1	2	26	173	-134	A	0	28	13	11
9	1	22	11	-9	E	1	24	47	43	3	1	25	22	-19	2	2	26	A	10	1	1	28	13	-8
0	2	22	11	9	7	1	24	10	-13	E	1	25	6	6	3	2	26	41	-41	2	1	28	135	-130
1	2	22	38	-38	E	1	24	84	86	7	1	25	16	11	4	2	26	31	36	3	1	28	6	3
2	2	22	29	-29	0	2	24	93	87	1	2	25	10	-6	A	2	26	135	139	1	2	28	73	-74
3	2	22	32	26	C	2	24	149	170	1	2	25	17	-17	5	2	26	37	-34	A	2	28	6	2
E	2	22	24	23	1	2	24	80	-81	2	2	25	17	-21	7	2	26	22	20	C	2	28	156	-161
5	2	22	36	33	2	2	24	26	-22	3	2	25	8	11	0	3	26	134	-133	1	2	28	13	12
7	2	22	40	-37	3	2	24	66	-64	4	2	25	8	9	1	3	26	34	40	2	2	28	23	23

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REV4

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
3	2	3P	4	2	1	3	3A	100	88	0	4	2A	107	108	1	1	2P	4	-8	1	2	2P	16	18
4	2	2P	131	126	2	3	2A	7	-4	1	4	2P	12	-11	2	1	2P	15	14	2	2	2P	23	17
0	3	2A	17	14	3	3	2A	6P	81															

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MKTP

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
4	0	0	110	-102	14	2	0	43	-41	12	6	0	26	23	12	6	0	26	25	14	8	0	21	-18
6	0	0	20	22	16	2	0	44	-51	13	6	0	28	-28	14	6	0	28	28	16	8	0	11	18
8	0	0	166	156	18	2	0	7	-11	14	6	0	33	33	16	6	0	15	16	18	8	0	10	12
10	0	0	24	-26	17	2	0	9	6	15	6	0	24	-24	15	6	0	24	29	17	8	0	10	11
12	0	0	46	-41	18	2	0	16	17	16	6	0	36	-35	16	6	0	12	13	18	8	0	11	10
14	0	0	77	79	19	2	0	14	18	17	6	0	12	11	17	6	0	13	14	19	8	0	10	-17
16	0	0	28	28	20	2	0	14	11	18	6	0	11	-12	18	6	0	11	11	20	8	0	11	-9
18	0	0	22	22	21	2	0	8	8	19	6	0	9	-8	19	6	0	4	4	21	8	0	8	-8
20	0	0	17	-11	22	2	0	19	-19	20	6	0	6	-2	20	6	0	12	10	1	9	0	10	-10
22	0	0	4	3	23	2	0	13	-13	21	6	0	6	-9	21	6	0	4	4	3	9	0	42	40
24	0	0	1	-3	24	2	0	7	7	22	6	0	16	15	22	6	0	6	7	5	9	0	6	-7
1	1	0	93	90	25	2	0	1	1	23	6	0	3	-2	23	6	0	7	6	7	9	0	4	-3
3	1	0	4	-3	1	3	0	74	-77	24	6	0	9	-8	1	7	0	13	-12	9	9	0	36	36
5	1	0	76	82	2	3	0	78	-76	1	7	0	77	76	3	7	0	20	20	7	9	0	20	-20
7	1	0	129	123	3	3	0	36	-33	2	7	0	16	16	4	7	0	58	58	8	9	0	3	1
9	1	0	51	47	4	3	0	25	23	3	7	0	44	-44	5	7	0	15	16	9	9	0	4	2
11	1	0	71	-68	5	3	0	74	-72	4	7	0	7	-6	6	7	0	4	4	10	9	0	30	-30
13	1	0	107	-101	6	3	0	21	19	5	7	0	80	-77	7	7	0	44	-42	11	9	0	19	18
15	1	0	91	-90	7	3	0	34	30	6	7	0	17	-17	8	7	0	29	-26	12	9	0	12	-11
17	1	0	30	-28	8	3	0	38	-36	7	7	0	42	39	9	7	0	5	-3	13	9	0	24	-24
19	1	0	41	41	9	3	0	7	-8	8	7	0	44	-42	10	7	0	25	-24	14	9	0	27	25
21	1	0	24	-23	10	3	0	29	-27	9	7	0	76	68	11	7	0	32	31	15	9	0	20	-20
23	1	0	66	63	11	3	0	32	32	10	7	0	16	16	12	7	0	28	29	16	9	0	7	6
25	1	0	13	8	12	3	0	24	-23	11	7	0	30	-30	13	7	0	34	32	17	9	0	4	2
1	2	0	1	-1	13	3	0	40	-40	12	7	0	3	3	14	7	0	4	4	18	9	0	17	-16
3	2	0	43	-41	14	3	0	8	8	13	7	0	22	-22	15	7	0	14	-13	19	9	0	5	-4
5	2	0	19	-17	15	3	0	25	-26	14	7	0	10	-11	16	7	0	13	14	20	9	0	4	4
7	2	0	7	-8	16	3	0	33	33	15	7	0	28	27	17	7	0	6	6	0	10	0	63	62
9	2	0	19	19	17	3	0	24	23	16	7	0	10	-10	18	7	0	12	11	1	10	0	7	7
11	2	0	20	20	18	3	0	13	-11	17	7	0	16	17	19	7	0	7	8	2	10	0	4	5
13	2	0	4	1	19	3	0	5	-5	18	7	0	2	-1	20	7	0	9	8	3	10	0	4	1
15	2	0	7	9	20	3	0	20	-20	19	7	0	8	-7	21	7	0	15	15	4	10	0	50	-50
17	2	0	2	2	21	3	0	10	-10	20	7	0	4	2	22	7	0	4	5	5	10	0	4	2
19	2	0	9	9	22	3	0	10	9	21	7	0	4	-3	22	7	0	3	-7	6	10	0	6	-5
0	3	0	171	-171	23	3	0	8	8	22	7	0	7	-7	0	8	0	9	6	7	10	0	11	11
2	3	0	31	32	24	3	0	10	10	23	7	0	7	7	1	8	0	12	13	8	10	0	44	42
4	3	0	22	24	0	4	0	10	-9	0	8	0	23	-24	2	8	0	20	-20	9	10	0	8	-11
6	3	0	15	15	1	4	0	9	9	1	8	0	61	-62	3	8	0	2	2	10	10	0	8	-8
8	3	0	74	-72	2	4	0	50	-48	2	8	0	14	-14	4	8	0	14	14	11	10	0	8	8
10	3	0	42	39	3	4	0	46	46	3	8	0	52	-52	5	8	0	28	-27	12	10	0	24	-24
12	3	0	16	16	4	4	0	103	97	4	8	0	29	30	6	8	0	20	-19	13	10	0	6	6
14	3	0	41	-42	5	4	0	44	42	5	8	0	79	77	7	8	0	31	29	14	10	0	6	6
16	3	0	46	-42	6	4	0	24	25	6	8	0	16	15	8	8	0	2	2	15	10	0	8	5
18	3	0	36	-32	7	4	0	12	-12	7	8	0	45	46	9	8	0	7	6	16	10	0	10	12
20	3	0	54	56	8	4	0	29	-29	8	8	0	29	-29	10	8	0	22	21	17	10	0	4	4
22	3	0	78	76	9	4	0	58	58	9	8	0	30	-30	11	8	0	33	-30	18	10	0	12	9
24	3	0	9	8	10	4	0	24	-23	10	8	0	4	4	12	8	0	21	-20	19	10	0	5	7
1	4	0	42	40	11	4	0	9	9	11	8	0	23	-23	13	8	0	6	-8	1	11	0	6	-4

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	11	0	41	-38	8	14	0	5	5	-6	1	1	68	-68	-2	2	1	102	-98	-9	3	1	24	-34
3	11	0	15	13	9	14	0	12	12	-5	1	1	147	142	-1	2	1	17	-16	-8	3	1	58	-61
4	11	0	9	9	2	15	0	5	2	-9	1	1	29	-30	0	2	1	24	24	-7	3	1	73	-73
6	11	0	19	17	3	15	0	11	-11	0	1	1	95	96	1	2	1	29	-26	0	3	1	3	-1
8	11	0	40	40	-3	0	1	20	18	1	1	1	147	146	2	2	1	4	4	1	3	1	23	-23
9	11	0	14	15	-21	0	1	7	4	2	1	1	73	-74	3	2	1	112	111	2	3	1	83	81
A	11	0	7	-6	-18	0	1	9	0	3	1	1	33	30	4	2	1	12	12	3	3	1	70	-70
B	11	0	17	-17	-17	0	1	13	-13	4	1	1	18	16	5	2	1	36	35	4	3	1	79	-76
10	11	0	22	-21	-15	0	1	10	11	5	1	1	72	-71	6	2	1	44	-44	5	3	1	74	-75
11	11	0	12	11	-13	0	1	47	-46	6	1	1	17	17	7	2	1	55	-51	6	3	1	29	27
12	11	0	12	10	-11	0	1	15	15	8	1	1	20	-18	8	2	1	22	20	7	3	1	36	-34
13	12	0	4	6	-9	0	1	32	33	10	1	1	45	45	9	2	1	18	20	8	3	1	94	96
14	11	0	16	14	-7	0	1	94	93	11	1	1	49	49	10	2	1	4	4	9	3	1	4	-2
15	11	0	1	-1	-5	0	1	35	-35	12	1	1	17	17	11	2	1	6	-5	10	3	1	10	9
16	11	0	4	-5	-3	0	1	134	136	13	1	1	7	7	12	2	1	13	-12	11	3	1	4	-6
17	11	0	6	-6	-1	0	1	141	-140	14	1	1	44	-45	13	2	1	24	-28	12	3	1	24	-29
0	12	0	12	-12	0	0	1	178	183	15	1	1	65	-64	14	2	1	9	-10	13	3	1	4	1
1	12	0	6	7	1	0	1	95	82	16	1	1	7	-4	15	2	1	12	12	14	3	1	4	-3
2	12	0	7	-7	2	0	1	174	-113	17	1	1	7	-8	16	2	1	31	30	15	3	1	4	-3
3	12	0	11	11	11	0	1	24	-25	18	1	1	26	25	17	2	1	4	5	16	3	1	4	9
4	12	0	10	10	12	0	1	108	104	19	1	1	18	18	18	2	1	3	1	17	3	1	13	-16
5	12	0	4	4	13	0	1	17	17	0	2	1	7	6	19	2	1	15	-14	18	3	1	2	-3
6	12	0	8	-8	17	0	1	34	-34	21	2	1	8	-8	20	2	1	18	-19	20	3	1	3	-7
7	12	0	18	-18	18	0	1	31	-32	22	2	1	14	-14	21	2	1	9	-9	21	3	1	13	12
8	12	0	12	-12	21	0	1	19	19	23	2	1	17	-18	22	2	1	8	-8	22	3	1	7	6
9	12	0	5	5	22	0	1	6	6	24	2	1	6	-6	23	2	1	7	7	23	3	1	7	-2
10	12	0	8	8	25	0	1	30	-31	25	2	1	3	-5	24	2	1	16	16	24	3	1	14	13
11	12	0	9	9	26	0	1	13	13	26	2	1	2	0	25	2	1	10	-10	25	3	1	7	-5
12	12	0	8	8	27	0	1	6	6	27	2	1	15	-15	26	2	1	13	12	26	3	1	10	10
13	12	0	2	-2	28	0	1	9	-2	28	2	1	19	-19	27	2	1	4	-4	27	3	1	3	4
14	12	0	8	-8	29	0	1	6	0	29	2	1	11	12	28	2	1	12	12	28	3	1	14	-14
15	12	0	9	-9	31	0	1	10	-9	30	2	1	3	-3	29	2	1	16	16	29	3	1	4	7
2	13	0	2	-2	20	1	1	21	-20	31	2	1	11	10	30	2	1	22	-22	30	3	1	9	-9
3	13	0	12	-12	19	1	1	31	-31	32	2	1	44	44	31	2	1	6	7	31	3	1	10	10
4	13	0	2	-2	18	1	1	4	4	33	2	1	14	-14	32	2	1	7	-8	32	3	1	4	3
5	13	0	10	-9	17	1	1	4	4	34	2	1	7	-7	33	2	1	10	-10	33	3	1	13	13
6	13	0	5	-5	16	1	1	20	20	35	2	1	16	-16	34	2	1	31	-30	34	3	1	3	1
7	13	0	6	6	15	1	1	21	-22	36	2	1	12	-12	35	2	1	7	8	35	3	1	23	-22
9	13	0	10	9	14	1	1	12	-12	37	2	1	59	60	36	2	1	43	42	36	3	1	16	16
10	13	0	2	-1	13	1	1	8	-8	38	2	1	8	9	37	2	1	61	62	37	3	1	17	-17
12	13	0	7	-7	12	1	1	58	58	39	2	1	11	12	38	2	1	33	-34	38	3	1	12	14
13	13	0	2	-2	11	1	1	24	24	40	2	1	10	10	39	2	1	23	23	39	3	1	11	11
0	14	0	7	-7	10	1	1	3	2	0	3	1	82	-85	0	3	1	45	48	0	4	1	48	48
1	14	0	5	5	9	1	1	23	-23	1	3	1	1	1	1	3	1	21	21	1	4	1	8	-8
2	14	0	4	-4	8	1	1	50	48	2	3	1	21	23	2	3	1	7	8	2	4	1	9	-9
3	14	0	6	6	7	1	1	141	-140	3	3	1	92	95	3	3	1	22	22	3	4	1	36	-37
4	14	0	2	2	6	1	1	78	-78	4	3	1	22	23	4	3	1	86	85	4	4	1	128	-129
8	14	0	5	-5	5	1	1	38	36	5	3	1	10	-10	5	3	1	14	-14	5	4	1	38	37

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MNTP

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
-1	0	1	11F	114	1	0	1	2F	-2F	3	0	1	24	-25	7	0	1	6	F	12	0	1	11	11
0	1	1	148	148	2	0	1	106	-106	4	0	1	72	73	8	0	1	4	4	14	0	1	5	5
1	1	1	F	F	3	0	1	20	18	5	0	1	28	-27	10	0	1	33	-32	15	0	1	4	1
2	1	1	7F	-7F	4	0	1	27	27	6	0	1	11	-11	11	0	1	30	-28	16	0	1	12	-12
3	1	1	37	-37	5	0	1	17	15	7	0	1	0	1	12	0	1	7	-7	17	0	1	3	3
4	1	1	42	-41	6	0	1	7A	7F	8	0	1	56	-56	13	0	1	7	-7	18	0	1	8	-7
5	1	1	40	-40	7	0	1	10	9	9	0	1	27	27	14	0	1	12	-12	19	0	1	11	9
6	1	1	7F	7G	8	0	1	4	-5	10	0	1	5	-3	15	0	1	8	8	20	0	1	7	7
7	1	1	3	-3	9	0	1	12	12	11	0	1	60	64	16	0	1	16	16	21	0	1	4	1
8	1	1	4F	4F	10	0	1	9A	-9	12	0	1	22	-20	17	0	1	9	10	-20	0	1	15	-14
9	1	1	14	13	11	0	1	1	1	13	0	1	28	-28	18	0	1	3	3	-19	0	1	5	5
10	1	1	37	-36	12	0	1	43	41	15	0	1	17	-17	19	0	1	7	-7	-18	0	1	2	4
11	1	1	30	-31	13	0	1	13	-13	16	0	1	19	-20	20	0	1	8	-9	-17	0	1	10	-10
12	1	1	4A	-4F	14	0	1	8A	8F	17	0	1	2	2	21	0	1	10	-11	-16	0	1	18	18
13	1	1	2	1	15	0	1	6	8	18	0	1	16	17	22	0	1	2	-1	-15	0	1	4	5
14	1	1	33	33	16	0	1	17	-17	19	0	1	8	8	-21	0	1	6	-7	-14	0	1	9	0
15	1	1	2G	-32	17	0	1	21	-21	20	0	1	12	12	-20	0	1	7	-F	-13	0	1	12	-12
16	1	1	22	21	18	0	1	2A	-23	21	0	1	4	-4	-19	0	1	15	-13	-12	0	1	27	-27
17	1	1	11	10	19	0	1	4	1	22	0	1	0	-0	-18	0	1	20	-19	-11	0	1	22	-21
18	1	1	3	-3	20	0	1	1A	18	23	0	1	4	5	-17	0	1	10	-10	-10	0	1	4	2
19	1	1	13	12	21	0	1	9	-4	-21	0	1	8	-8	-16	0	1	2	2	-9	0	1	8	-8
20	1	1	7	-7	22	0	1	12	12	-20	0	1	0	0	-15	0	1	A	-8	-8	0	1	51	51
21	1	1	6	7	23	0	1	6	-7	-19	0	1	14	14	-14	0	1	27	28	-7	0	1	12	11
22	1	1	2A	2G	-22	0	1	9	9	-18	0	1	7	7	-13	0	1	24	24	-6	0	1	7	-7
23	1	1	12	-12	-21	0	1	9	-10	-17	0	1	12	12	-12	0	1	2	1	-5	0	1	16	-17
24	1	1	5	4	-20	0	1	4	-5	-16	0	1	17	-17	-11	0	1	10	10	-4	0	1	45	-45
-22	2	1	2	1	-19	0	1	6	-8	-15	0	1	10	-17	-10	0	1	18	-17	-3	0	1	12	-12
-21	2	1	7	7	-18	0	1	2	2	-14	0	1	6	-7	-9	0	1	22	-22	-2	0	1	12	11
-20	2	1	2	-2	-17	0	1	3	5	-13	0	1	11	-11	-8	0	1	7	7	-1	0	1	36	35
-19	2	1	4	4	-16	0	1	9	9	-12	0	1	26	27	-7	0	1	49	-46	0	0	1	34	34
-18	2	1	2	2	-15	0	1	11	10	-11	0	1	25	24	-6	0	1	47	47	1	0	1	23	23
-17	2	1	10	-11	-14	0	1	6	8	-10	0	1	16	-17	-5	0	1	33	32	2	0	1	7	6
-16	2	1	2	-1	-13	0	1	16	-17	-9	0	1	40	40	-4	0	1	22	-22	3	0	1	19	-19
-15	2	1	3	-4	-12	0	1	22	23	-8	0	1	16	-16	-3	0	1	1A	-1F	4	0	1	27	26
-14	2	1	1F	-1F	-11	0	1	1F	-1F	-7	0	1	41	-41	-2	0	1	29	-29	5	0	1	29	-27
-13	2	1	3	3	-10	0	1	11	12	-6	0	1	37	37	-1	0	1	11	-13	6	0	1	8	8
-12	2	1	E	E	-9	0	1	8	10	-5	0	1	48	-48	0	0	1	3	3	7	0	1	28	28
-11	2	1	9	9	-8	0	1	16	-17	-4	0	1	70	70	1	0	1	22	-22	8	0	1	11	10
-10	2	1	2	-2	-7	0	1	52	52	-3	0	1	7	7	2	0	1	1F	1F	9	0	1	4	2
-9	2	1	7	7	-6	0	1	2A	2A	-2	0	1	4F	-4F	3	0	1	31	31	10	0	1	16	16
-8	2	1	1F	-1F	-5	0	1	3F	-37	-1	0	1	10	10	4	0	1	7	8	11	0	1	21	-20
-7	2	1	1F	-1F	-4	0	1	47	4A	0	0	1	14	-15	5	0	1	12	11	12	0	1	3	-3
-6	2	1	1F	-1F	-3	0	1	1F	-2G	1	0	1	34	-3F	6	0	1	19	-19	13	0	1	8	8
-5	2	1	44	41	-2	0	1	F	-F	2	0	1	3F	3F	7	0	1	2	2	14	0	1	1F	-16
-4	2	1	F	-F	-1	0	1	1F	1G	3	0	1	6F	-6F	8	0	1	2	-1	15	0	1	21	19
-3	2	1	6A	-7	0	0	1	8F	-6F	4	0	1	2G	-2F	9	0	1	2	3	16	0	1	8	-8
-2	2	1	2	1	1	0	1	5A	5A	5	0	1	7	8	10	0	1	8	-9	17	0	1	2	0
0	2	1	F	4	2	0	1	7	-8	6	0	1	3	-3	12	0	1	5	5	18	0	1	9	9

PRESERVED AND CALCULATED STRUCTURE FACTORS FOR MAYP

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
10	9	1	10	-11	-6	11	1	14	-14	14	12	1	2	0	-13	0	2	7	-7	4	1	2	48	-38
20	9	1	4	5	-5	11	1	21	20	15	13	1	3	3	-16	0	2	34	34	5	1	2	165	144
-18	10	1	8	9	-2	11	1	2	-3	-17	13	1	13	13	-14	0	2	20	-20	8	1	2	63	-61
-17	10	1	7	-8	-1	11	1	20	-20	-13	13	1	14	-14	-12	0	2	13	-14	7	1	2	38	35
-16	10	1	2	1	0	11	1	20	20	-10	13	1	2	2	-10	0	2	16	18	6	1	2	48	47
-15	10	1	1	0	1	11	1	17	-15	-8	13	1	9	-10	-8	0	2	13	12	5	1	2	77	-74
-14	10	1	8	-9	2	11	1	8	7	-6	13	1	11	-10	-6	0	2	195	-196	10	1	2	26	29
-13	10	1	6	-7	3	11	1	14	14	-4	13	1	13	12	-4	0	2	27	-27	11	1	2	15	-15
-12	10	1	5	7	4	11	1	12	-13	-3	13	1	1	0	0	0	2	137	-126	12	1	2	41	-42
-11	10	1	13	13	5	11	1	22	20	-1	13	1	4	5	2	0	2	23	23	13	1	2	40	41
-10	10	1	9	10	6	11	1	11	-11	0	13	1	6	-7	4	0	2	153	-152	14	1	2	43	-42
-9	10	1	4	5	7	11	1	20	19	-1	13	1	14	-12	6	0	2	88	-89	15	1	2	27	27
-7	10	1	11	-12	8	11	1	9	-9	-2	15	1	2	3	8	0	2	45	-46	16	1	2	9	11
-6	10	1	7	-8	9	11	1	7	6	-1	15	1	4	-4	10	0	2	32	33	17	1	2	10	-11
-5	10	1	3	-5	10	11	1	10	11	0	15	1	9	-9	12	0	2	36	37	18	1	2	2	1
-4	10	1	1	1	11	11	1	20	19	1	15	1	10	10	14	0	2	74	-78	19	1	2	7	-8
-3	10	1	10	10	12	11	1	4	-5	2	15	1	3	-2	16	0	2	28	-30	20	1	2	10	-10
-2	10	1	12	11	13	11	1	3	4	4	15	1	0	0	18	0	2	26	26	21	1	2	4	2
-1	10	1	12	12	14	11	1	8	-8	5	15	1	3	-2	20	0	2	22	22	22	1	2	14	-14
0	10	1	5	-6	15	11	1	14	-15	6	15	1	12	10	22	0	2	35	-35	23	1	2	15	15
1	10	1	42	-41	16	11	1	3	4	7	15	1	1	3	24	0	2	15	-14	24	1	2	16	15
2	10	1	6	-6	17	11	1	4	-9	8	15	1	3	-4	-25	1	2	7	7	-23	2	2	7	2
3	10	1	27	-24	-15	12	1	2	-1	10	15	1	3	-3	-22	1	2	15	-16	-22	2	2	14	14
4	10	1	7	7	-14	12	1	14	-11	11	15	1	7	7	-21	1	2	4	3	-21	2	2	20	20
5	10	1	52	52	-13	12	1	8	7	-14	16	1	3	4	-20	1	2	24	20	-20	2	2	10	10
6	10	1	8	7	-12	12	1	4	-5	-7	16	1	0	0	-19	1	2	20	20	-19	2	2	3	-3
7	10	1	12	12	-11	12	1	2	2	-6	16	1	1	0	-18	1	2	19	20	-18	2	2	12	-11
8	10	1	6	-6	-10	12	1	18	18	-4	16	1	9	-9	-17	1	2	7	6	-17	2	2	37	-38
9	10	1	46	-45	-9	12	1	15	-14	-4	16	1	12	-12	-16	1	2	7	-7	-16	2	2	4	-5
10	10	1	3	3	-8	12	1	8	7	-3	16	1	2	-2	-15	1	2	35	-34	-15	2	2	12	13
11	10	1	12	-12	-7	12	1	17	-17	-2	16	1	7	-7	-14	1	2	24	-25	-14	2	2	46	44
12	10	1	8	7	-6	12	1	17	18	-1	16	1	10	11	-13	1	2	15	16	-13	2	2	67	68
13	10	1	27	27	-4	13	1	9	-8	0	16	1	6	-6	-12	1	2	18	19	-12	2	2	11	-11
14	10	1	7	-7	-3	13	1	18	-20	1	16	1	9	-8	-11	1	2	31	31	-11	2	2	10	9
15	10	1	3	7	-2	13	1	13	14	2	16	1	7	6	-10	1	2	31	31	-10	2	2	60	-62
16	10	1	4	4	-1	13	1	15	-17	3	16	1	4	-7	-9	1	2	27	-28	-9	2	2	75	-74
17	10	1	21	-21	0	13	1	4	4	4	16	1	6	-6	-7	1	2	28	-28	-8	2	2	49	49
18	10	1	7	5	1	13	1	10	9	5	16	1	10	-9	-6	1	2	29	30	-7	2	2	7	7
-17	11	1	2	3	2	13	1	14	-15	7	16	1	1	1	-5	1	2	15	14	-6	2	2	20	22
-15	11	1	9	9	3	13	1	14	14	8	16	1	2	2	-4	1	2	7	-8	-4	2	2	84	86
-13	11	1	9	-6	4	13	1	11	-11	-9	15	1	13	12	-3	1	2	56	-60	-3	2	2	74	-80
-11	11	1	7	8	5	13	1	15	-15	-8	15	1	3	4	-2	1	2	42	44	-2	2	2	12	-10
-10	11	1	7	-7	6	13	1	10	10	0	15	1	9	-9	-1	1	2	19	19	-1	2	2	60	-63
-9	11	1	8	-8	7	13	1	7	-7	1	15	1	4	-4	0	1	2	7	-5	0	2	2	132	-131
-8	11	1	10	11	8	13	1	14	14	2	15	1	12	-13	1	1	2	60	-59	1	2	2	122	122
-7	11	1	10	-10	9	13	1	12	12	-24	0	2	7	7	2	1	2	76	-73	2	2	2	44	-43
-6	11	1	5	5	10	13	1	9	-8	-22	0	2	16	-16	3	1	2	31	31	3	2	2	7	8
-5	11	1	22	22	11	13	1	1	-2	-20	0	2	30	-30	4	1	2	34	-34	4	2	2	11	13

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR VETO

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
4	2	2	12	-10	4	3	2	30	-12	4	4	2	7	-5	5	5	2	*	4	7	6	2	11	-11
5	2	2	95	95	5	3	2	7	8	5	4	2	57	58	6	5	2	33	-33	8	6	2	54	53
6	2	2	36	-34	6	3	2	83	84	6	4	2	46	50	7	5	2	32	-32	10	6	2	24	-24
7	2	2	72	-71	7	3	2	14	15	7	4	2	18	19	8	5	2	24	-28	11	6	2	14	-14
8	2	2	98	96	8	3	2	43	42	8	4	2	51	-50	9	5	2	15	17	12	6	2	6	-6
9	2	2	5	-5	9	3	2	26	27	9	4	2	32	-33	10	5	2	4	4	13	6	2	57	-58
10	2	2	7	4	10	3	2	7	-2	10	4	2	17	-20	11	5	2	41	41	14	6	2	16	16
11	2	2	31	30	11	3	2	2	1	11	4	2	20	20	12	5	2	24	24	15	6	2	5	2
12	2	2	26	-26	12	3	2	25	-25	12	4	2	20	18	13	5	2	28	-29	16	6	2	11	11
13	2	2	8	8	13	3	2	7	7	13	4	2	51	51	14	5	2	12	-13	17	6	2	37	37
14	2	2	6	6	14	3	2	7	6	14	4	2	14	14	15	5	2	24	-27	18	6	2	7	-5
15	2	2	32	-35	15	3	2	17	17	15	4	2	21	21	16	5	2	7	8	19	6	2	16	-16
16	2	2	10	-11	16	3	2	4	-4	16	4	2	4	4	17	5	2	4	3	20	6	2	12	-12
17	2	2	1	-4	17	3	2	15	14	17	4	2	27	-25	18	5	2	10	11	21	6	2	20	-20
18	2	2	4	-5	18	3	2	8	8	18	4	2	16	-14	19	5	2	30	30	22	6	2	10	8
20	2	2	8	-8	19	3	2	4	-5	19	4	2	12	11	20	5	2	7	9	-22	7	2	8	9
21	2	2	8	8	20	3	2	7	5	20	4	2	4	2	21	5	2	17	-11	-20	7	2	6	8
22	2	2	4	7	22	3	2	7	-5	21	4	2	14	14	22	5	2	5	5	-18	7	2	11	-11
24	2	2	7	-5	23	3	2	7	-6	22	4	2	5	1	23	5	2	15	-16	-17	7	2	11	-12
25	2	2	7	-6	24	3	2	7	7	24	4	2	7	7	-22	6	2	7	0	-16	7	2	16	-16
-24	1	2	5	-1	-24	4	2	5	-7	24	4	2	7	10	-21	6	2	30	-30	-15	7	2	12	12
-23	1	2	9	12	-23	4	2	14	13	-21	5	2	8	8	-20	6	2	5	5	-14	7	2	11	12
-22	1	2	7	-7	-22	4	2	5	-10	-22	5	2	5	-1	-19	6	2	23	20	-13	7	2	33	31
-21	1	2	7	8	-21	4	2	15	14	-20	5	2	20	-19	-18	6	2	11	11	-12	7	2	27	26
-20	1	2	29	-28	-20	4	2	15	14	-20	5	2	7	8	-17	6	2	12	11	-11	7	2	22	-22
-19	1	2	7	-10	-19	4	2	15	-15	-19	5	2	20	-19	-16	6	2	15	-16	-10	7	2	33	-32
-18	1	2	17	16	-18	4	2	8	8	-18	5	2	6	-7	-15	6	2	15	-16	-9	7	2	9	2
-17	1	2	9	4	-17	4	2	3	-5	-17	5	2	8	7	-14	6	2	16	-19	-8	7	2	50	-52
-16	1	2	23	24	-16	4	2	7	-7	-16	5	2	7	7	-13	6	2	5	11	-7	7	2	12	13
-15	1	2	10	10	-15	4	2	11	11	-15	5	2	7	7	-12	6	2	7	7	-6	7	2	32	31
-14	1	2	31	-30	-14	4	2	46	-47	-14	5	2	8	8	-11	6	2	27	27	-5	7	2	15	17
-13	1	2	20	20	-13	4	2	8	-8	-13	5	2	26	-26	-10	6	2	15	17	-4	7	2	52	54
-12	1	2	62	-65	-12	4	2	34	34	-12	5	2	8	-7	-9	6	2	5	5	-3	7	2	30	-30
-11	1	2	52	-56	-11	4	2	28	-27	-10	5	2	3	4	-8	6	2	41	-41	-2	7	2	50	-50
-10	1	2	27	25	-10	4	2	46	46	-9	5	2	2	-3	-7	6	2	2	-1	-1	7	2	4	3
-9	1	2	21	20	-9	4	2	35	36	-8	5	2	9	-9	-6	6	2	31	-32	0	7	2	55	-58
-8	1	2	31	28	-8	4	2	14	-14	-7	5	2	2	2	-5	6	2	10	-11	1	7	2	27	26
-7	1	2	80	84	-7	4	2	24	25	-6	5	2	3	3	-4	6	2	7	-7	2	7	2	17	18
-6	1	2	100	-100	-6	4	2	17	-18	-5	5	2	26	-26	-3	6	2	16	-16	3	7	2	17	-17
-5	1	2	40	102	-5	4	2	15	-17	-4	5	2	15	15	-2	6	2	15	17	4	7	2	41	41
-4	1	2	134	-137	-4	4	2	20	23	-3	5	2	7	7	-1	6	2	1	-2	5	7	2	26	-27
-3	1	2	90	-91	-3	4	2	126	128	-2	5	2	28	-28	0	6	2	1	3	6	7	2	14	-16
-2	1	2	52	54	-2	4	2	15	16	-1	5	2	20	-22	1	6	2	16	17	7	7	2	20	20
-1	1	2	146	148	-1	4	2	76	77	0	5	2	42	-41	2	6	2	60	-62	8	7	2	34	-34
0	1	2	174	174	0	4	2	8	-8	1	5	2	16	-15	3	6	2	12	13	9	7	2	8	8
1	1	2	146	149	1	4	2	124	-128	2	5	2	37	37	4	6	2	10	9	10	7	2	7	6
2	1	2	71	-70	2	4	2	34	-34	3	5	2	10	10	5	6	2	53	-52	11	7	2	41	-40
3	1	2	50	-47	3	4	2	10	-11	4	5	2	2	3	6	6	2	7	-5	12	7	2	10	11

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MATA

H	K	L	FO	FC
13	7	2	1	-1
14	7	2	2	2
15	7	2	16	14
16	7	2	24	-24
17	7	2	4	4
18	7	2		-16
19	7	2		-13
20	7	2	3	6
21	7	2		0
-21	8	2	8	-10
-18	8	2	2	1
-17	8	2	3	3
-16	8	2	5	-7
-15	8	2	2	-2
-14	8	2	9	11
-13	8	2	22	-22
-12	8	2	4	6
-11	8	2	16	14
-10	8	2	28	-25
-9	8	2	61	61
-8	8	2	94	95
-7	8	2	15	15
-6	8	2	145	145
-5	8	2	91	-92
-4	8	2	29	-30
-3	8	2	8	-5
-2	8	2	19	19
-1	8	2	40	41
0	8	2	37	37
1	8	2	39	39
2	8	2	62	63
3	8	2	58	-57
4	8	2	25	-25
5	8	2	4	4
6	8	2	13	-12
7	8	2	29	28
8	8	2	2	2
9	8	2	4	2
10	8	2	17	18
11	8	2	20	-22
12	8	2	11	-11
13	8	2	4	4
14	8	2	13	-14
15	8	2	11	10
16	8	2	5	7
17	8	2	4	4
18	8	2	4	-2

H	K	L	FO	FC
20	8	2	7	8
-19	9	2	17	17
-18	9	2	9	-10
-16	9	2	6	8
-15	9	2	14	-14
-14	9	2	3	1
-13	9	2	1	-2
-12	9	2	2	3
-11	9	2	9E	27
-10	9	2	2	-3
-9	9	2	7	-11
-8	9	2	12	12
-7	9	2	40	-40
-6	9	2	7	7
-5	9	2	16	-10
-4	9	2	16	-15
-3	9	2	57	58
-2	9	2	M	9
-1	9	2	11	9
0	9	2	47	-47
1	9	2	24	-25
2	9	2	10	-9
3	9	2	4	4
4	9	2	47	48
5	9	2	22	23
6	9	2	12	12
7	9	2	14	-15
8	9	2	15	-15
9	9	2	30	-29
10	9	2	18	-20
11	9	2	6	6
12	9	2	11	9
13	9	2	12	12
14	9	2	23	21
15	9	2	11	12
16	9	2	7	-5
17	9	2	7	-4
18	9	2	1	-1
19	9	2	8	-8
-21	10	2	2	-1
-20	10	2	2	-1
-19	10	2	3	3
-18	10	2	7	-6
-17	10	2	7	7
-16	10	2	14	-14
-15	10	2	6	6
-14	10	2	7	-8
-13	10	2	3	-4
-12	10	2	7	-4
-11	10	2	1	-1
-10	10	2	2	-4
-9	10	2	3	2
-8	10	2	3	3
-7	10	2	25	27
-6	10	2	13	13
-5	10	2	2	-2
-4	10	2	12	-19
-3	10	2	12	-11
-2	10	2	3	1
-1	10	2	24	22
0	10	2	11	10
1	10	2	28	27
2	10	2	8	-9
3	10	2	13	13
4	10	2	14	-17
5	10	2	15	-12
6	10	2	10	-11
7	10	2	26	21
8	10	2	3	-2
9	10	2	5	4
10	10	2	4	-2
11	10	2	2	4
12	10	2	1	-2
13	10	2	3	2
14	10	2	15	-13
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR WWTP

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-17	1	0	12	-14	-17	2	3	4	5	-16	3	3	3	6	-16	4	3	3	-1	-14	5	3	17	-17
-17	1	0	33	-32	-16	2	3	27	28	-15	3	3	15	-15	-14	4	3	21	-21	-13	5	3	4	1
-16	1	0	2	2	-15	2	3	10	11	-14	3	3	12	-13	-13	4	3	24	28	-12	5	3	30	32
-15	1	0	4	4	-14	2	3	3	2	-13	3	3	4	-5	-12	4	3	11	-13	-11	5	3	10	-13
-14	1	0	56	56	-13	2	3	22	-23	-12	3	3	24	-26	-11	4	3	7	-6	-10	5	3	22	24
-13	1	0	46	46	-12	2	3	32	-32	-11	3	3	47	48	-10	4	3	50	52	-9	5	3	14	-14
-11	1	0	4	-4	-11	2	3	20	-21	-10	3	3	23	24	-9	4	3	71	-73	-8	5	3	50	-51
-10	1	0	7	-9	-10	2	3	7	-7	-9	3	3	31	-32	-7	4	3	17	16	-7	5	3	44	46
-9	1	0	32	-34	-9	2	3	24	25	-8	3	3	64	64	-6	4	3	11	11	-6	5	3	4	7
-8	1	0	3	-4	-8	2	3	33	35	-7	3	3	76	-80	-5	4	3	69	-72	-5	5	3	22	20
-7	1	0	15	-15	-7	2	3	13	14	-6	3	3	57	-57	-4	4	3	33	36	-4	5	3	4	-6
-6	1	0	77	79	-6	2	3	17	18	-5	3	3	37	37	-3	4	3	20	19	-3	5	3	6	10
-5	1	0	64	67	-5	2	3	37	-36	-4	3	3	51	-53	-2	4	3	9	-10	-2	5	3	14	17
-4	1	0	14	14	-4	2	3	8	-8	-3	3	3	87	90	-1	4	3	21	-20	-1	5	3	21	21
-3	1	0	16	17	-3	2	3	32	-32	-2	3	3	37	37	0	4	3	153	-155	0	5	3	11	11
-2	1	0	27	26	-2	2	3	44	-45	-1	3	3	42	-40	1	4	3	17	-17	1	5	3	21	22
-1	1	0	14	-13	-1	2	3	8	7	0	3	3	66	64	2	4	3	51	51	2	5	3	13	12
0	1	0	5	-3	0	2	3	66	67	1	3	3	104	-101	3	4	3	73	-73	3	5	3	7	7
1	1	0	72	69	1	2	3	46	-46	2	3	3	62	-62	4	4	3	50	50	4	5	3	2	1
2	1	0	29	-29	2	2	3	136	136	3	3	3	32	34	5	4	3	22	23	5	5	3	7	-21
3	1	0	22	21	3	2	3	84	-84	4	3	3	27	-24	6	4	3	4	4	6	5	3	7	-8
4	1	0	64	63	4	2	3	48	-51	5	3	3	80	86	7	4	3	45	-46	7	5	3	27	27
5	1	0	40	40	5	2	3	13	13	6	3	3	55	55	8	4	3	4	-10	8	5	3	29	26
6	1	0	67	-70	6	2	3	54	-54	7	3	3	7	6	9	4	3	19	-12	9	5	3	6	7
7	1	0	15	15	7	2	3	8	11	8	3	3	40	41	10	4	3	7	7	10	5	3	10	-9
8	1	0	42	-44	8	2	3	54	56	9	3	3	54	-56	11	4	3	4	5	11	5	3	32	-33
9	1	0	8	8	9	2	3	28	-28	10	3	3	38	-39	12	4	3	4	5	12	5	3	10	-10
10	1	0	67	68	10	2	3	68	70	11	3	3	31	31	13	4	3	54	56	13	5	3	11	-11
11	1	0	46	-48	11	2	3	32	-32	12	3	3	20	20	14	4	3	9	10	14	5	3	6	6
12	1	0	72	74	12	2	3	44	-46	13	3	3	16	-16	15	4	3	4	-4	15	5	3	28	28
13	1	0	4	4	13	2	3	27	28	14	3	3	30	30	16	4	3	24	-24	17	5	3	2	4
14	1	0	26	-26	14	2	3	21	-22	15	3	3	9	10	17	4	3	20	-22	18	5	3	4	-5
15	1	0	27	28	15	2	3	6	7	16	3	3	6	-7	18	4	3	14	-15	20	5	3	21	-21
16	1	0	10	-11	16	2	3	22	22	17	3	3	11	-10	19	4	3	3	-3	21	5	3	3	-2
17	1	0	3	3	17	2	3	3	-1	18	3	3	7	-8	20	4	3	11	11	22	5	3	6	-6
18	1	0	11	11	18	2	3	10	11	19	3	3	6	6	21	4	3	4	3	-21	6	3	3	-1
19	1	0	27	-28	19	2	3	8	-9	20	3	3	4	-7	22	4	3	14	-14	-19	6	3	19	19
20	1	0	14	13	20	2	3	10	-10	21	3	3	11	10	22	4	3	14	-14	-18	6	3	8	-8

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MNTP

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
-16	6	2	77	-21	-11	7	3	14	-18	-2	8	3	38	40	7	6	3	7	-6	-15	11	3	8	-2
-17	6	2	24	-7	-10	7	3	36	34	3	8	3	6	45	8	6	3	19	-20	-14	11	3	10	8
-18	6	2	26	-26	-9	7	3	14	16	4	8	3	8	-52	9	6	3	6	-6	-13	11	3	24	22
-19	6	2	10	10	-8	7	3	35	35	5	8	3	-9	10	10	6	3	23	24	-12	11	3	8	-7
-14	6	2	25	24	-7	7	3	33	35	6	8	3	5	1	11	6	3	23	23	-11	11	3	5	1
-12	6	3	24	28	-6	7	3	11	-11	8	8	3	4	1	12	6	3	12	12	-10	11	3	5	-4
-13	6	3	8	8	-5	7	3	24	-26	9	8	3	KK	1	13	6	3	4	-2	-8	11	3	27	-26
-12	6	3	12	-12	-4	7	3	44	-49	10	8	3	7	1	14	6	3	20	-21	-7	11	3	7	8
-11	6	3	27	-24	-3	7	3	55	-54	11	8	3	10	10	15	6	3	14	-13	-6	11	3	1	1
-9	6	3	20	22	-2	7	3	11	11	7	8	3	20	22	16	6	3	11	-11	-5	11	3	1	2
-8	6	3	21	21	-1	7	3	43	44	8	8	3	54	58	17	6	3	4	4	-4	11	3	1	-2
-7	6	3	31	32	0	7	3	42	46	9	8	3	21	-25	18	6	3	16	16	-3	11	3	1	-2
-5	6	3	22	23	1	7	3	66	66	10	8	3	14	-14	19	6	3	3	4	-2	11	3	4	-6
-4	6	3	32	32	2	7	3	28	-28	11	8	3	13	-13	-17	10	3	1	2	-1	11	3	7	8
-3	6	3	2	2	3	7	3	12	-13	12	8	3	24	26	-16	10	3	7	5	0	11	3	7	-7
-2	6	3	22	-23	4	7	3	11	-10	13	8	3	14	16	-15	10	3	14	-16	1	11	3	12	-12
-1	6	3	27	-31	6	7	3	22	-20	14	8	3	12	11	-14	10	3	6	6	2	11	3	8	8
0	6	3	17	-18	7	7	3	24	24	15	8	3	22	23	-13	10	3	3	3	3	11	3	1	1
1	6	3	12	13	8	7	3	14	14	16	8	3	20	-20	-12	10	3	14	14	4	11	3	4	4
2	6	3	7	7	9	7	3	14	0	17	8	3	5	-2	-11	10	3	24	24	5	11	3	4	7
3	6	3	7	7	10	7	3	35	35	18	8	3	7	-5	-10	10	3	7	-7	6	11	3	1	-10
4	6	3	37	-38	10	7	3	32	-34	19	8	3	7	-8	-9	10	3	4	7	7	11	3	8	4
5	6	3	15	-16	11	7	3	4	1	20	8	3	10	11	-8	10	3	11	10	8	11	3	2	-3
6	6	3	17	17	12	7	3	6	4	21	8	3	3	-7	-7	10	3	12	-13	10	11	3	2	2
7	6	3	17	-19	13	7	3	20	-19	-14	9	3	7	-7	-6	10	3	4	-1	11	11	3	11	-11
8	6	3	7	-9	14	7	3	23	21	-13	9	3	8	10	-5	10	3	1	4	12	11	3	7	8
10	6	3	26	-27	15	7	3	2	-1	-12	9	3	4	-4	-4	10	3	11	-12	13	11	3	7	6
11	6	3	15	14	16	7	3	15	-15	-11	9	3	3	-4	-3	10	3	14	13	14	11	3	7	-7
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13	6	3	7	7	18	7	3	8	-11	-13	9	3	24	-24	-1	10	3	4	-5	16	11	3	3	-4
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15	6	3	14	-14	20	7	3	6	8	-11	9	3	10	10	1	10	3	14	-15	-15	12	3	8	-8
0	7	3	2	2	21	7	3	5	-4	-10	9	3	15	-20	2	10	3	4	4	-12	12	3	15	-15
1	7	3	4	-4	22	7	3	15	-15	-9	9	3	24	24	3	10	3	4	-4	-11	12	3	13	-12
2	7	3	25	-25	-17	8	3	3	4	-8	9	3	4	-6	4	10	3	8	11	-10	12	3	4	4
3	7	3	11	10	-16	8	3	4	-6	-6	9	3	33	34	5	10	3	8	-8	-9	12	3	4	6
4	7	3	4	4	-15	8	3	2	1	-5	9	3	27	-27	6	10	3	3	3	-8	12	3	17	17
5	7	3	3	2	-14	8	3	19	-19	-4	9	3	15	17	8	10	3	4	4	-7	12	3	8	8
7	7	3	14	-13	-12	8	3	10	11	-3	9	3	18	19	9	10	3	9	8	-6	12	3	8	6
-21	7	3	7	7	-11	8	3	4	-3	-2	9	3	15	-15	10	10	3	7	8	-4	12	3	14	-14
-20	7	3	2	-2	-10	8	3	17	13	-1	9	3	22	22	11	10	3	7	-7	-3	12	3	17	-17
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-18	7	3	15	-16	-8	8	3	15	-17	1	9	3	20	-19	13	10	3	14	-14	-1	12	3	9	-4
-16	7	3	19	19	-7	8	3	17	17	2	9	3	24	24	14	10	3	4	4	0	12	3	7	7
-15	7	3	10	11	-6	8	3	14	-14	3	9	3	11	-12	15	10	3	10	10	1	12	3	22	21
-14	7	3	9	7	-5	8	3	24	-24	4	9	3	11	11	16	10	3	6	6	2	12	3	5	-9
-13	7	3	6	-4	-4	8	3	44	44	5	9	3	17	18	17	10	3	11	10	3	12	3	14	14
-12	7	3	25	-24	-3	8	3	18	18	6	9	3	38	-38	-16	11	3	2	2	4	12	3	4	-1

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MMTB

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
4	12	2	24	-23	-18	0	4	11	-11	5	1	4	19	19	7	2	4	46	47	10	3	4	47	48
5	12	2	7	7	-16	0	4	12	-12	7	1	4	42	42	8	2	4	80	-81	11	3	4	22	22
6	12	2	16	-4	-14	0	4	69	61	8	1	4	37	38	9	2	4	65	-67	12	3	4	6	2
7	12	2	7	4	-12	0	4	17	17	9	1	4	12	11	10	2	4	24	24	13	3	4	29	30
8	12	2	13	12	-10	0	4	44	-44	10	1	4	33	33	11	2	4	34	-35	14	3	4	51	-51
9	12	2	7	10	-8	0	4	29	-29	11	1	4	41	-42	12	2	4	35	38	15	3	4	14	-14
10	12	2	11	10	-6	0	4	67	66	12	1	4	4	7	13	2	4	34	34	16	3	4	8	8
11	12	2	7	-1	-4	0	4	34	34	13	1	4	18	-15	14	2	4	18	18	17	3	4	18	-19
12	12	2	10	-10	-2	0	4	86	-85	14	1	4	36	36	15	2	4	28	28	18	3	4	20	19
-11	13	2	4	4	0	0	4	79	79	15	1	4	7	7	16	2	4	19	-19	19	3	4	12	12
-10	13	2	11	11	2	0	4	47	46	16	1	4	8	-7	17	2	4	9	-10	20	3	4	3	4
-9	13	2	3	-2	4	0	4	15	15	17	1	4	7	7	18	2	4	11	-11	21	3	4	4	4
-8	13	2	7	7	6	0	4	37	-35	18	1	4	7	7	19	2	4	15	-17	22	3	4	18	-18
-7	13	2	11	-12	10	0	4	24	23	19	1	4	18	-17	20	2	4	15	14	23	3	4	14	-13
-6	13	2	12	-11	12	0	4	4	4	20	1	4	8	8	21	2	4	16	15	-22	4	4	5	-4
-5	13	2	4	4	14	0	4	7	7	21	1	4	14	-13	22	2	4	6	-6	-21	4	4	4	4
-4	13	2	16	16	16	0	4	14	14	22	1	4	5	5	23	2	4	15	14	-20	4	4	7	6
-3	13	2	30	30	18	0	4	3	-3	23	1	4	8	8	-23	3	4	9	9	-19	4	4	17	17
-2	13	2	17	17	20	0	4	14	14	-23	2	4	4	-4	-22	3	4	10	-11	-18	4	4	22	21
-1	13	2	4	-4	22	0	4	14	14	-22	2	4	6	-4	-21	3	4	6	-5	-17	4	4	7	-6
0	13	2	6	6	-23	1	4	7	-7	-21	2	4	10	10	-20	3	4	6	-7	-16	4	4	4	-5
1	13	2	19	-19	-22	1	4	12	-12	-20	2	4	13	-12	-19	3	4	4	-6	-15	4	4	24	-25
2	13	2	22	-21	-21	1	4	4	-5	-19	2	4	9	9	-18	3	4	7	7	-14	4	4	4	-5
3	13	2	7	8	-20	1	4	15	-15	-18	2	4	2	-6	-17	3	4	2	2	-13	4	4	7	7
4	13	2	10	-8	-19	1	4	6	6	-17	2	4	13	-11	-16	3	4	8	8	-12	4	4	10	-11
5	13	2	15	-17	-18	1	4	4	-4	-16	2	4	4	-4	-15	3	4	11	11	-11	4	4	39	41
6	13	2	15	14	-17	1	4	15	16	-15	2	4	7	-8	-14	3	4	4	-7	-10	4	4	4	4
7	13	2	5	-5	-16	1	4	4	-4	-14	2	4	27	-28	-13	3	4	22	-24	-9	4	4	47	-46
8	13	2	16	-17	-15	1	4	19	19	-13	2	4	4	4	-12	3	4	6	6	-8	4	4	23	24
9	13	2	7	-8	-14	1	4	7	-7	-12	2	4	2	-2	-11	3	4	27	-27	-7	4	4	33	-32
10	13	2	7	1	-13	1	4	44	-45	-11	2	4	8	8	-10	3	4	28	28	-6	4	4	24	-30
11	13	2	7	4	-12	1	4	7	8	-10	2	4	5	-6	-9	3	4	14	-14	-5	4	4	3	3
-8	14	2	7	-8	-10	1	4	17	-17	-9	2	4	2	2	-8	3	4	42	43	-4	4	4	46	-48
-7	14	2	10	10	-9	1	4	31	31	-8	2	4	18	17	-7	3	4	31	-34	-3	4	4	29	26
-6	14	2	7	7	-8	1	4	93	96	-7	2	4	33	-34	-6	3	4	32	-34	-2	4	4	84	87
-5	14	2	7	-7	-7	1	4	35	35	-6	2	4	23	-24	-5	3	4	19	18	0	4	4	85	87
-4	14	2	7	2	-6	1	4	6	6	-5	2	4	20	22	-4	3	4	8	-9	1	4	4	65	-65
-3	14	2	12	-11	-5	1	4	27	-26	-4	2	4	14	11	-3	3	4	3	-4	2	4	4	34	-35
-2	14	2	7	-9	-4	1	4	58	-60	-3	2	4	35	36	-2	3	4	4	4	3	4	4	17	17
-1	14	2	6	3	-3	1	4	22	-22	-2	2	4	42	43	-1	3	4	77	-78	4	4	4	39	-41
0	14	2	7	-7	-2	1	4	21	19	-1	2	4	26	26	0	3	4	75	76	5	4	4	12	15
1	14	2	28	28	-1	1	4	27	27	0	2	4	17	-17	1	3	4	7	7	6	4	4	2	0
2	14	2	6	7	0	1	4	84	88	1	2	4	41	-41	2	3	4	32	-31	7	4	4	3	-3
3	14	2	7	-6	1	1	4	3	4	2	2	4	34	-36	3	3	4	11	12	8	4	4	47	45
4	14	2	7	-5	2	1	4	20	-22	3	2	4	34	-37	4	3	4	11	-12	9	4	4	10	-11
5	14	2	17	-18	3	1	4	22	-22	4	2	4	20	21	5	3	4	20	-17	10	4	4	8	-9
-22	0	4	24	25	4	1	4	52	-56	5	2	4	44	46	6	3	4	8	10	11	4	4	8	8
-20	0	4	14	14	5	1	4	11	-12	6	2	4	52	57	8	3	4	49	-50	12	4	4	33	-32

PRESERVED AND CALCULATED STRUCTURE FACTORS FOR MATR

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
13	4	4	15	-16	16	4	4	4	-1	-17	7	4	0	0	-6	4	4	34	-35	8	4	4	16	-14
14	4	4	19	19	17	4	4	7	-4	-15	7	4	1	-9	-5	4	4	17	15	8	4	4	17	-16
15	4	4	11	-9	21	4	4	10	8	-14	7	4	2	8	-4	4	4	13	12	8	4	4	18	16
16	4	4	21	22	22	4	4	4	4	-13	7	4	3	27	-28	4	4	23	-24	8	4	4	3	5
17	4	4	6	-7	23	4	4	7	-5	-12	7	4	4	14	11	-3	4	4	21	-20	8	4	4	15	15
18	4	4	5	5	24	4	4	3	3	-11	7	4	5	11	11	-1	4	4	30	-29	10	4	4	0	1
19	4	4	6	-7	25	4	4	29	-31	-10	7	4	6	3	1	0	4	4	20	-22	11	4	4	18	-14
20	4	4	15	-17	26	4	4	11	10	-9	7	4	7	11	10	1	4	4	18	16	12	4	4	5	-5
21	4	4	12	-13	27	4	4	5	11	-8	7	4	8	4	-3	2	4	4	15	-16	13	4	4	13	-14
22	4	4	3	3	28	4	4	4	6	-7	7	4	9	21	-21	3	4	4	22	22	14	4	4	7	-6
-22	5	4	4	4	-15	5	4	24	24	-6	7	4	10	8	-8	4	4	4	21	21	15	4	4	17	15
-21	5	4	21	21	-14	5	4	15	-15	-5	7	4	11	17	-16	5	4	4	7	-7	16	4	4	4	4
-20	5	4	7	-7	-13	5	4	18	-19	-4	7	4	12	24	24	6	4	4	7	-8	17	4	4	12	12
-19	5	4	4	-4	-12	5	4	5	-5	-3	7	4	13	33	33	7	4	4	18	-17	18	4	4	3	-1
-18	5	4	4	5	-11	5	4	42	-44	-2	7	4	14	55	56	8	4	4	25	-24	-14	10	4	7	-7
-17	5	4	37	-37	-10	5	4	17	16	-1	7	4	15	8	9	9	4	4	20	21	-13	10	4	7	-4
-16	5	4	4	-4	-9	5	4	29	30	0	7	4	16	27	-27	10	4	4	18	16	-12	10	4	23	22
-15	5	4	17	19	-8	5	4	23	21	1	7	4	17	40	-41	11	4	4	28	32	-11	10	4	3	2
-14	5	4	17	16	-7	5	4	30	31	2	7	4	18	13	-12	12	4	4	15	14	-10	10	4	5	5
-13	5	4	44	44	-6	5	4	12	-13	3	7	4	19	7	6	13	4	4	21	-20	-9	10	4	8	6
-12	5	4	7	-6	-5	5	4	33	-35	4	7	4	20	18	17	14	4	4	4	-4	-8	10	4	28	-27
-11	5	4	27	-27	-4	5	4	27	-27	5	7	4	21	29	30	15	4	4	17	-16	-7	10	4	3	1
-10	5	4	5	-6	-3	5	4	48	-50	6	7	4	22	47	47	16	4	4	20	-19	-6	10	4	6	-4
-9	5	4	44	-46	-2	5	4	24	22	7	7	4	23	9	8	17	4	4	16	16	-5	10	4	2	1
-8	5	4	10	11	-1	5	4	58	58	8	7	4	24	15	12	18	4	4	5	6	-4	10	4	23	21
-7	5	4	42	42	0	5	4	39	40	9	7	4	25	31	-31	19	4	4	7	7	-3	10	4	2	1
-6	5	4	27	-25	1	5	4	4	5	10	7	4	26	25	-25	-14	5	4	10	12	-2	10	4	7	8
-5	5	4	75	76	2	5	4	4	4	11	7	4	27	15	15	-13	5	4	9	-10	-1	10	4	6	6
-4	5	4	7	-7	3	5	4	34	-34	12	7	4	28	6	7	-12	5	4	5	-4	0	10	4	10	-11
-3	5	4	47	-45	4	5	4	20	-20	13	7	4	29	18	17	-11	5	4	3	-3	1	10	4	2	4
-2	5	4	13	-10	5	5	4	3	2	14	7	4	30	22	22	-10	5	4	11	-10	2	10	4	2	-1
-1	5	4	27	-28	7	5	4	22	21	15	7	4	31	7	-6	-9	5	4	12	12	3	10	4	8	-7
0	5	4	11	12	8	5	4	15	17	16	7	4	32	3	-1	-8	5	4	1	0	4	10	4	2	27
1	5	4	29	28	9	5	4	13	12	17	7	4	33	8	8	-7	5	4	4	-4	5	10	4	21	-21
2	5	4	20	-19	10	5	4	3	3	18	7	4	34	9	-10	-6	5	4	3	3	6	10	4	3	-4
3	5	4	44	47	11	5	4	10	9	19	7	4	35	10	10	-5	5	4	15	-15	7	10	4	9	9
4	5	4	9	-9	12	5	4	19	-20	20	7	4	36	9	9	-4	5	4	12	12	8	10	4	7	-6
5	5	4	13	-12	13	5	4	14	-15	-15	8	4	4	3	2	-3	5	4	6	-7	9	10	4	4	3
6	5	4	12	12	14	5	4	4	0	-14	8	4	5	-4	-5	-2	5	4	5	-7	10	10	4	4	-3
7	5	4	34	-34	15	5	4	4	4	-13	8	4	6	4	-4	-1	5	4	11	12	11	10	4	4	-4
8	5	4	4	4	16	5	4	4	-4	-12	8	4	7	3	2	0	5	4	11	-11	12	10	4	4	-30
9	5	4	17	-17	17	5	4	19	-20	-11	8	4	8	7	7	1	5	4	15	-15	13	10	4	0	0
10	5	4	7	7	18	5	4	4	4	-10	8	4	9	4	-5	2	5	4	31	31	14	10	4	4	1
11	5	4	7	-7	19	5	4	12	12	-9	8	4	10	7	7	3	5	4	13	-13	15	10	4	4	-2
12	5	4	7	7	21	5	4	3	-4	-8	8	4	11	7	8	4	5	4	11	12	16	10	4	4	-5
13	5	4	7	-8	-19	6	4	4	-3	-7	8	4	12	4	-4	5	5	4	7	-7	-14	11	4	4	8
14	5	4	7	-6	-18	6	4	4	4	-6	8	4	13	4	4	6	5	4	21	22	-13	11	4	21	-20

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MLT8

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
-11	11	4	3	1	-8	11	4	-6	-17	1	6	12	12	-13	2	5	1	4	-8	3	5	11	10
-10	11	4	7	-7	-7	11	4	1	-1	1	6	2	-1	-12	2	5	13	-14	-7	3	5	10	-10
-9	11	4	7	-6	-6	11	4	2	-2	1	6	4	-4	-11	2	5	11	12	-6	3	5	11	-11
-8	11	4	20	20	-5	11	4	8	-8	1	6	6	-6	-10	2	5	10	-10	-5	3	5	9	8
-7	11	4	7	7	-4	11	4	4	-5	-13	1	6	16	-16	-9	2	6	7	-7	3	5	13	14
-6	11	4	7	7	-3	11	4	7	-7	-12	1	6	14	13	-8	2	6	22	24	3	5	14	-11
-5	11	4	13	-13	-2	11	4	10	-9	-11	1	6	11	11	-7	2	6	25	27	3	5	14	-14
-4	11	4	21	-21	-1	11	4	14	12	-10	1	6	25	-24	-6	2	6	10	11	0	3	5	23	-22
-3	11	4	7	-7	0	11	4	8	9	-9	1	6	5	5	-5	2	6	11	10	1	3	5	20	20
-2	11	4	14	14	1	11	4	4	4	-8	1	6	34	-33	-4	2	6	31	-30	2	3	5	16	17
-1	11	4	10	10	2	11	4	7	7	-7	1	6	47	-47	-3	2	6	38	-38	3	3	5	23	-24
0	11	4	4	4	3	11	4	17	-17	-6	1	6	30	-30	-2	2	6	15	-16	4	3	5	7	-7
1	11	4	10	10	4	11	4	7	7	-5	1	6	29	-29	-1	2	6	19	-19	5	3	5	17	-16
2	11	4	7	-7	5	11	4	7	-7	-4	1	6	12	13	0	2	6	19	19	7	3	5	50	52
3	11	4	12	-12	6	11	4	7	-7	-3	1	6	27	26	1	2	6	29	28	8	3	5	8	9
5	11	4	7	7	-4	12	4	6	-6	-2	1	6	22	22	2	2	6	12	14	9	3	5	19	20
7	11	4	7	7	-3	12	4	8	8	-1	1	6	44	48	3	2	6	6	6	10	3	5	24	28
8	11	4	7	-7	-2	12	4	4	-5	0	1	6	43	-42	4	2	6	40	-40	11	3	5	42	-44
9	11	4	7	7	-1	12	4	4	4	1	1	6	41	-42	5	2	6	32	-34	12	3	5	5	-4
10	11	4	7	7	0	12	4	7	-9	2	1	6	33	-35	6	2	6	21	-21	13	3	5	7	-6
11	11	4	7	-7	1	12	4	2	2	3	1	6	23	-23	7	2	6	20	20	14	3	5	32	-33
12	11	4	7	7	-11	0	5	10	-11	4	1	6	14	14	8	2	6	15	15	15	3	5	29	30
13	11	4	7	-7	-10	0	5	9	-11	5	1	6	38	38	11	2	6	43	44	16	3	5	6	-4
14	11	4	7	-7	-9	0	5	7	7	6	1	6	18	18	12	2	6	21	22	17	3	5	2	2
-12	12	4	7	-7	-8	0	5	14	13	7	1	6	12	11	13	2	6	21	21	18	3	5	17	17
-11	12	4	11	11	-7	0	5	36	-34	8	1	6	37	-37	14	2	6	13	12	19	3	5	24	-25
-10	12	4	8	-8	-11	0	5	5	-6	9	1	6	27	-29	15	2	6	8	7	20	3	5	8	-8
-9	12	4	8	8	-6	0	5	77	78	10	1	6	24	-30	16	2	6	24	-29	21	3	5	5	-5
-7	12	4	11	-10	-7	0	5	40	39	11	1	6	19	-20	17	2	6	11	11	22	3	5	7	-8
-6	12	4	15	-14	-6	0	5	67	-67	12	1	6	15	16	18	2	6	14	14	-11	4	5	4	4
-5	12	4	9	-9	-5	0	5	43	-40	13	1	6	12	14	19	2	6	6	6	-10	4	5	4	4
-4	12	4	3	3	-4	0	5	109	103	14	1	6	4	3	20	2	6	18	17	-9	4	5	7	-6
-3	12	4	16	16	-3	0	5	84	85	15	1	6	7	-9	21	2	6	14	-14	-8	4	5	7	-7
-2	12	4	17	17	-2	0	5	22	-24	16	1	6	7	-9	22	2	6	10	-9	-7	4	5	22	-22
-1	12	4	19	19	-1	0	5	17	-17	17	1	6	10	-10	-11	3	6	9	9	-6	4	5	7	-7
0	12	4	4	-4	0	0	5	37	37	18	1	6	10	-10	-10	3	6	8	8	-5	4	5	6	7
1	12	4	26	-25	1	0	5	46	46	20	1	6	8	7	-9	3	6	6	-8	-4	4	5	22	21
2	12	4	18	-18	2	0	5	51	-51	21	1	6	9	10	-8	3	6	11	10	-3	4	5	15	16
3	12	4	6	-4	3	0	5	9	4	22	1	6	8	9	-7	3	6	15	16	-2	4	6	9	8
4	12	4	8	8	4	0	5	7	8	-10	2	6	4	6	-6	3	6	8	8	-1	4	6	8	-9
5	12	4	17	15	5	0	5	12	12	-9	2	6	4	4	-5	3	6	4	4	0	4	6	34	-36
7	12	4	7	6	6	0	5	6	-10	-8	2	6	16	-16	-4	3	6	20	-20	1	4	6	15	-15
7	12	4	10	10	7	0	5	6	2	-7	2	6	11	11	-3	3	6	4	-5	2	4	6	21	-22
8	12	4	7	-7	-12	1	5	7	10	-6	2	6	7	7	-2	3	6	7	7	3	4	6	11	-12
9	12	4	12	-12	-11	1	5	11	-10	-5	2	6	6	11	-1	3	6	4	7	4	4	6	49	50
10	12	4	7	-7	-10	1	5	4	5	-4	2	6	13	13	0	3	6	13	14	-5	4	6	35	36
11	12	4	7	-7	-9	1	5	7	8	-3	2	6	2	-1	1	3	6	20	20	-4	4	6	7	-5
12	12	4	8	8	-8	1	5	10	-11	-2	2	6	2	-2	2	3	6	11	-12	-3	4	6	8	10

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR HKTP

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	4	5	43	-46	3	5	5	14	12	11	5	5	7	-4	-14	4	5	1	1	3	9	5	11	-10
-1	4	5	29	32	4	5	5	NO	-4	15	5	5	17	12	-13	4	5	3	-7	4	9	5	11	11
0	4	5	32	32	5	5	5	7	-5	13	5	5	22	23	-12	4	5	15	15	5	9	5	12	-14
1	4	5	48	-49	6	5	5	3	2	14	5	5	19	19	-11	4	5	4	-7	6	9	5	13	13
2	4	5	7	7	7	5	5	11	-11	16	5	5	8	0	-10	4	5	5	-10	7	9	5	14	8
3	4	5	F	2	8	5	5	3F	37	17	5	5	F	-11	-8	4	5	6	0	10	9	5	15	-13
4	4	5	F	-4	9	5	5	7	1	18	5	5	F	-5	-6	4	5	7	-2	11	9	5	F	-4
5	4	5	5F	-5	10	5	5	F	-8	19	5	5	9	9	-4	4	5	8	0	12	9	5	11	13
F	4	5	4C	-41	11	5	5	9	9	20	5	5	5	-4	-4	4	5	19	-7	13	9	5	F	-7
7	4	5	10	-9	12	5	5	11	-11	-16	6	5	11	-10	-3	4	5	11	-11	14	9	5	13	12
8	4	5	23	22	13	5	5	F	-7	-17	6	5	4	7	-2	4	5	4	9	15	9	5	2	-1
9	4	5	3F	-3F	14	5	5	7	7	-18	6	5	7	-4	-1	4	5	10	10	16	9	5	9	-8
10	4	5	2F	2F	15	5	5	F	-F	-15	6	5	14	14	0	4	5	1	-2	-15	10	5	5	5
11	4	5	13	-11	16	5	5	1F	11	-14	6	5	13	-13	1	4	5	13	14	-14	10	5	3	5
12	4	5	1F	-14	17	5	5	F	-8	-13	6	5	3	2	2	4	5	15	-14	-13	10	5	4	-5
13	4	5	2E	-27	18	5	5	4	-4	-12	6	5	22	22	3	4	5	12	12	-12	10	5	16	-15
14	4	5	14	-15	20	5	5	9	-7	-11	6	5	19	-19	4	4	5	7	8	-11	10	5	11	-11
15	4	5	7	3	22	5	5	2	-2	-10	6	5	7	6	5	4	5	12	-11	-10	10	5	1	1
16	4	5	10	10	-18	6	5	2	2	-9	7	5	1	8	6	4	5	8	4	-9	10	5	10	11
17	4	5	33	-32	-17	6	5	22	19	-8	7	5	10	-9	7	4	5	4	-9	-8	10	5	7	7
18	4	5	8	8	-17	6	5	11	-11	-7	7	5	6	-1	8	4	5	10	10	-7	10	5	10	11
19	4	5	4	-5	-16	6	5	2	4	-6	7	5	2	3	9	4	5	7	10	-6	10	5	1	3
20	4	5	3	3	-15	6	5	7	7	-5	7	5	15	14	10	4	5	A	-4	-5	10	5	2E	-2E
21	4	5	14	14	-14	6	5	20	-20	-4	7	5	17	-17	11	4	5	2	-2	-4	10	5	11	-11
-21	5	5	5	-5	-13	6	5	21	22	-3	7	5	7	8	12	4	5	12	-12	-3	10	5	2F	-21
-20	5	5	9	-9	-12	6	5	6	-6	-2	7	5	18	-17	13	4	5	17	-16	-2	10	5	9	9
-19	5	5	3	-3	-11	6	5	4	-4	-1	7	5	11	-11	14	4	5	A	A	-1	10	5	22	20
-18	5	5	7	7	-10	6	5	2	2	0	7	5	4	4	15	4	5	5	-4	0	10	5	8	8
-17	5	5	4	-4	-9	6	5	3E	-1E	1	7	5	1E	1E	16	4	5	12	13	1	10	5	A	A
-16	5	5	2C	2C	-8	6	5	1	1	2	7	5	21	22	17	4	5	F	F	2	10	5	2	2
-15	5	5	F	-F	-7	6	5	7	7	3	7	5	21	21	18	4	5	7	-7	3	10	5	2E	-2E
-14	5	5	7	-4	-6	6	5	44	-44	4	7	5	12	-12	-17	5	5	9	-10	4	10	5	16	16
-13	5	5	4	4	-5	6	5	8	8	5	7	5	2	-2	-16	5	5	7	-7	5	10	5	4	-6
-12	5	5	3	-3E	-4	6	5	10	9	6	7	5	2A	-2F	-15	5	5	4	4	6	10	5	11	11
-11	5	5	3	3	-3	6	5	F	F	7	7	5	14	-14	-14	5	5	14	14	7	10	5	11	-11
-10	5	5	7	-E	-2	6	5	5C	5C	8	7	5	1	-2	-13	5	5	C	C	8	10	5	3	4
-9	5	5	11	11	-1	6	5	22	-22	9	7	5	14	14	-12	5	5	9	-9	9	10	5	13	13
-8	5	5	61	F2	0	6	5	1E	-14	11	7	5	2E	27	-11	5	5	8	-8	10	10	5	11	-11
-7	5	5	2	2	1	6	5	13	-14	12	7	5	7	7	-10	5	5	A	-9	11	10	5	F	11
-6	5	5	5	5	2	6	5	FA	-A	13	7	5	7	-8	-9	5	5	6	-8	12	10	5	8	-8
-5	5	5	10	7	3	6	5	11	-10	14	7	5	7	-8	-7	5	5	1E	1F	14	10	5	4	5
-4	5	5	7	-8E	4	6	5	7	7	15	7	5	21	-21	-6	5	5	2	3	15	10	5	3	-6
-3	5	5	1F	F	5	6	5	2E	2F	16	7	5	2	-1	-5	5	5	6	-6	16	10	5	7	-8
-2	5	5	7	8	6	6	5	4F	4F	17	7	5	2	2	-4	5	5	7	-7	-17	11	5	7	8
-1	5	5	2C	-2E	7	6	5	7	-1	18	7	5	10	11	-2	5	5	9	-9	-13	11	5	8	8
0	5	5	44	44	8	6	5	14	-12	-14	7	5	5	5	0	5	5	12	-13	-10	11	5	4	-4
1	5	5	7	7	9	6	5	2E	-27	-17	7	5	7	6	1	5	5	13	14	-9	11	5	12	13
2	5	5	24	-24	10	6	5	1E	-1F	-16	8	5	9	-10	2	5	5	9	-10	-8	11	5	4	5

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MPTO

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
-7	11	E	18	-16	-14	0	E	22	-22	10	1	E	97	91	-20	3	E	4	-5	-8	5	E	20	20
-6	11	E	4	-5	-12	0	E	5	10	11	1	E	17	15	-19	3	E	5	4	-7	5	E	31	30
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-1	11	E	17	16	-2	0	E	65	64	16	1	E	19	-19	-14	3	E	24	25	-4	6	E	6	-7
0	11	E	14	-14	0	0	E	61	-63	17	1	E	11	11	-13	3	E	27	27	-3	6	E	19	19
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-9	12	E	2	1	-17	1	E	2	0	-9	2	E	15	15	1	3	E	11	12	12	6	E	3	3
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7	12	E	14	-14	-1	1	E	6	6	7	2	E	32	32	-20	4	E	7	-8	-6	8	E	24	-24
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9	12	E	14	-14	1	1	E	6	6	9	2	E	17	-18	-18	4	E	4	-4	-4	8	E	19	-18
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-3	13	E	4	-4	10	1	E	4	-4	19	2	E	4	-4	-9	4	E	3	-3	5	8	E	1F	-1F
-2	13	E	4	-4	11	1	E	4	-4	20	2	E	4	-4	-8	4	E	3	-3	6	8	E	1F	-1F
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-5	15	E	4	-4	9	2	E	4	-4	18	3	E	4	-4	-10	5	E	3	-3	4	9	E	1F	-1F

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR VKTB

H	K	L	FO	FC
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6	5	6	90	92
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8	5	6	11	-10
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1	6	6	4	-7
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3	6	6	6	-6
4	6	6	97	98
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6	6	6	5	-5
7	6	6	2	0
8	6	6	11	-2
9	6	6	3	-3
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MKT2

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13	4	7	17	15	4	8	7	7	6	-7	13	8	7	7	-9	3	8	11	12	7	3	8	8	-7
14	4	7	7	7	5	8	7	7	11	-11	14	8	7	7	-8	3	8	12	-12	8	3	8	4	1
15	4	7	7	4	6	8	7	7	13	12	15	8	7	7	-7	4	8	13	14	9	3	8	21	-22
16	4	7	7	4	7	8	7	7	12	-12	16	8	7	7	-6	4	8	7	-8	10	3	8	7	7
-16	5	7	7	-4	8	8	7	7	7	-7	17	8	7	7	-5	4	8	12	-11	11	3	8	7	-6
-15	5	7	7	7	9	8	7	7	10	10	18	8	7	7	-4	4	8	14	-13	12	3	8	7	-6
-12	5	7	7	-4	10	8	7	7	7	-7	19	8	7	7	-3	4	8	17	17	13	3	8	20	20
-11	5	7	7	3	11	8	7	7	24	-24	20	8	7	7	-2	4	8	6	6	-13	4	8	2	3
-10	5	7	6	-9	12	8	7	7	8	7	21	8	7	15	-1	4	8	21	21	-11	4	8	2	2

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MKTB

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-10	4	4	19	-12	-7	5	4	7	9	-8	8	0	16	-12	1	2	0	13	-11	7	4	8	13	17
-9	4	4	F	F	-6	5	4	4	3	-7	8	0	11	8	2	2	0	29	25	6	4	8	4	4
-8	4	4	9	-6	-5	5	4	5	4	-5	8	0	10	17	3	2	0	7	6	-6	5	8	17	16
-7	4	4	F	F	-4	5	4	7	-2	-3	8	0	16	-17	4	2	0	7	8	-5	5	8	5	-4
-6	4	4	7	6	-3	5	4	6	4	-1	8	0	17	-15	5	2	0	16	16	-4	5	8	3	-1
-5	4	4	7	-6	-1	5	4	7	7	1	8	0	6	6	8	2	0	11	10	-3	5	8	7	7
-4	4	4	16	-14	0	5	4	7	-9	3	8	0	20	20	7	2	0	12	-10	-2	6	8	14	-13
-3	4	4	3	3	1	5	4	7	8	5	8	0	9	-4	8	2	0	4	-4	-1	6	8	1	3
0	4	4	16	-16	2	5	4	7	6	7	8	0	3	-3	9	2	0	4	-3	0	6	8	5	7
1	4	4	11	-11	3	5	4	6	-6	9	8	0	1	1	-5	3	0	5	6	1	6	8	7	-6
2	4	4	22	25	4	5	4	4	3	-10	1	0	4	5	-4	3	0	8	10	2	6	8	7	7
3	4	4	7	6	5	5	4	3	-3	-9	1	0	10	10	-3	3	0	6	4	3	6	8	4	1
4	4	4	13	13	6	5	4	3	-12	-8	1	0	4	F	-2	3	0	4	-5	4	6	8	8	6
5	4	4	7	6	7	5	4	10	-9	-7	1	0	F	F	-1	3	0	11	1	5	6	8	4	-9
6	4	4	15	-15	8	5	4	8	-7	-6	1	0	F	-F	0	3	0	11	-10	-7	8	8	4	4
7	4	4	13	-12	9	5	4	F	-7	-5	1	0	13	-12	1	3	0	18	-17	-6	8	8	2	3
8	4	4	7	-7	-7	6	4	6	1	-4	1	0	11	-11	2	3	0	22	21	-5	8	8	4	4
9	4	4	4	3	-6	6	4	7	4	-3	1	0	20	-19	3	3	0	F	3	-4	8	8	4	4
10	4	4	22	23	-5	6	4	14	-11	-2	1	0	13	11	4	3	0	16	13	-3	8	8	4	4
11	4	4	11	11	-4	6	4	16	-15	-1	1	0	12	12	5	3	0	11	11	-2	8	8	6	-8
12	4	4	7	8	-3	6	4	11	10	0	1	0	17	15	6	3	0	15	-16	-1	8	8	17	-15
-11	5	4	13	12	-2	6	4	5	-3	1	1	0	F	7	8	3	0	3	6	-0	0	10	1	4
-10	5	4	7	8	-1	6	4	16	13	2	1	0	10	-10	9	3	0	3	-0	0	0	10	36	22
-9	5	4	4	0	0	6	4	17	15	3	1	0	14	-14	10	3	0	14	-17	2	0	10	4	-8
-7	5	4	15	-14	1	6	4	12	-11	4	1	0	10	-11	0	4	0	15	14	4	0	10	9	-10
-6	5	4	7	7	2	6	4	15	14	5	1	0	4	-7	-4	4	0	12	-12	-3	1	10	4	4
-5	5	4	3	F	3	6	4	14	-12	6	1	0	11	11	-7	4	0	F	1	-2	1	10	16	15
-3	5	4	6	-6	4	6	4	14	-15	7	1	0	3	0	-6	4	0	4	4	-1	1	10	1	-3
-2	5	4	10	-7	5	6	4	14	13	8	1	0	4	-4	-5	4	0	4	-7	0	1	10	10	-9
-1	5	4	10	10	6	6	4	4	2	-10	2	0	4	5	-4	4	0	12	12	1	1	10	4	-8
1	5	4	F	-8	7	6	4	4	2	-9	2	0	4	F	-3	4	0	13	-9	2	1	10	14	-14
2	5	4	F	6	-6	7	4	8	-7	-8	2	0	9	-9	-2	4	0	4	-3	3	1	10	3	0
3	5	4	7	-7	-5	7	4	11	11	-7	2	0	7	-6	-1	4	0	14	13	4	1	10	5	-5
4	5	4	7	-1	-4	7	4	11	11	-6	2	0	8	-9	0	4	0	9	7	-3	2	10	5	-1
7	5	4	7	F	-3	7	4	13	-10	-5	3	0	2	-1	2	4	0	13	11	-2	2	10	6	-6
8	5	4	6	F	-2	7	4	4	4	-4	3	0	4	3	4	4	0	16	-14	-1	2	10	8	-5
9	5	4	4	F	-1	7	4	20	-19	-3	4	0	23	21	6	4	0	4	4	0	2	10	9	-9
11	5	4	13	-12	2	7	4	11	-12	-2	4	0	20	17	5	4	0	4	-5	1	2	10	4	0
-8	6	4	12	-11	3	7	4	4	-7	-1	4	0	8	-7	8	4	0	4	-9	2	2	10	11	10
-8	6	4	12	9	4	7	4	4	-4	0	4	0	14	-13										

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR YRYY

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	0	0	700	-775	E	8	0	27	48	6	4	1	13	-3	3	0	1	21	-25	4	2	2	14	13
F	0	0	175	151	8	8	0	24	21	5	4	1	15	-7	4	0	1	21	9	5	2	2	32	-36
F	0	0	102	214	10	8	0	26	-19	7	4	1	21	17	F	0	1	21	14	6	2	2	74	80
10	0	0	72	-46	1	9	0	24	-27	8	4	1	13	4	6	0	1	23	-16	10	2	2	14	42
12	0	0	41	-20	2	9	0	52	-53	9	4	1	14	-10	7	0	1	20	12	11	2	2	18	-17
14	0	0	26	18	3	9	0	58	58	10	4	1	13	14	8	0	1	27	-17	1	3	2	124	118
2	1	0	53	-39	4	9	0	27	20	1	5	1	16	21	9	0	1	19	-7	2	3	2	60	48
3	1	0	915	922	5	9	0	34	29	2	5	1	12	-31	10	0	1	22	7	3	3	2	14	12
4	1	0	51	-55	0	10	0	22	21	3	5	1	17	16	1	10	1	15	-16	4	3	2	24	27
5	1	0	44	-42	1	10	0	27	3	4	5	1	23	10	2	10	1	24	-21	5	3	2	58	-58
11	1	0	24	25	2	11	0	27	27	5	5	1	30	31	3	10	1	19	14	6	3	2	38	-41
13	1	0	19	-25	3	11	0	21	14	7	5	1	24	24	4	10	1	17	8	7	3	2	44	50
0	2	0	277	-278	F	11	0	25	-19	7	6	1	16	-10	5	10	1	21	8	8	3	2	12	4
2	2	0	74	-80	F	12	0	27	21	8	6	1	22	-13	7	10	1	18	-16	9	3	2	24	28
4	2	0	157	154	2	13	0	25	-19	6	6	1	20	-16	8	10	1	16	-8	10	3	2	18	21
6	2	0	27	-30	3	13	0	14	4	10	6	1	27	-18	2	11	1	20	24	12	3	2	30	-44
8	2	0	72	-77	1	1	1	100	101	11	6	1	21	-2	3	11	1	20	16	14	3	2	20	20
10	2	0	97	99	0	1	1	61	62	1	7	1	27	-26	4	11	1	15	1	0	4	2	50	44
12	2	0	16	-14	2	1	1	80	87	4	7	1	15	15	F	11	1	21	17	1	4	2	79	-82
1	3	0	56	56	3	1	1	77	-82	5	7	1	14	10	9	12	1	23	21	2	4	2	32	-28
3	3	0	78	84	4	1	1	73	-82	7	7	1	20	-15	10	12	1	15	-15	3	4	2	58	-55
5	3	0	71	-75	5	1	1	30	-38	F	8	1	25	-10	9	0	2	49	-48	4	4	2	12	-8
7	3	0	31	34	6	1	1	21	-26	6	8	1	23	-3	1	0	2	27	-27	5	4	2	56	62
9	3	0	128	130	10	1	1	27	27	10	8	1	24	-15	2	0	2	84	74	6	4	2	32	30
2	4	0	21	-22	11	1	1	20	27	11	8	1	23	11	5	0	2	191	202	7	4	2	14	-14
4	4	0	77	-78	14	1	1	15	-13	13	8	1	21	6	6	0	2	52	52	8	4	2	40	-35
6	4	0	53	52	1	2	1	124	-127	13	8	1	23	-1	7	0	2	22	-23	10	4	2	16	-7
8	4	0	33	36	2	2	1	113	28	1	7	1	13	-16	8	0	2	25	-28	12	4	2	18	12
10	4	0	28	-31	3	2	1	104	105	3	7	1	12	11	9	0	2	64	-76	13	4	2	17	10
1	5	0	58	-58	4	2	1	98	96	5	7	1	14	-13	10	0	2	22	-22	14	4	2	16	3
3	5	0	52	-56	5	2	1	15	7	7	7	1	32	-28	2	1	2	27	21	0	5	2	109	-104
5	5	0	44	48	6	2	1	29	-28	8	7	1	19	8	3	1	2	153	-152	2	5	2	21	22
7	5	0	61	-77	7	2	1	33	-36	10	7	1	21	2	4	1	2	44	-30	4	5	2	90	22
11	5	0	14	5	10	2	1	16	-17	11	7	1	22	12	5	1	2	84	94	6	5	2	44	42
4	6	0	24	26	12	2	1	17	-19	12	7	1	22	-2	6	1	2	112	-122	8	5	2	14	1
F	6	0	25	-31	1	3	1	27	-21	1	8	1	16	12	7	1	2	84	74	9	5	2	43	-43
8	6	0	29	-26	2	3	1	7	5	2	8	1	20	6	8	1	2	58	44	7	5	2	24	-25
10	6	0	20	19	3	3	1	56	-60	3	8	1	25	-34	9	1	2	44	-46	8	5	2	40	-40
12	6	0	15	-4	4	3	1	40	-37	4	8	1	18	-18	10	1	2	89	76	0	6	2	22	3
1	7	0	44	49	5	3	1	12	-4	5	8	1	24	-36	11	1	2	17	-27	10	6	2	4	24
3	7	0	42	41	6	3	1	34	-34	6	8	1	24	-24	12	1	2	23	-24	11	6	2	17	10
5	7	0	46	-49	7	3	1	19	17	7	8	1	22	28	14	1	2	25	-24	1	7	2	49	42
7	7	0	27	27	8	3	1	17	8	9	8	1	22	26	0	2	2	47	70	3	7	2	34	34
9	7	0	26	24	9	3	1	15	21	6	9	1	20	21	1	2	2	157	149	5	7	2	46	-46
11	7	0	26	-14	11	3	1	13	6	11	9	1	17	10	2	2	2	44	-42	7	7	2	14	-13
0	8	0	70	62	1	4	1	70	67	1	0	1	24	-5	3	2	2	57	56	7	7	2	17	12
2	8	0	38	-42	2	4	1	40	-33	3	0	1	20	15	4	2	2	58	58	0	8	2	15	5
4	8	0	56	-61	3	4	1	24	-22	5	0	1	13	3	5	2	2	145	-154	6	8	2	30	34

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MMYY

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
10	5	2	15	6	3	1	3	34	-32	4	6	1	23	15	5	0	4	37	-44	5	4	4	57	-71
11	5	2	39	-21	4	1	3	57	54	5	6	1	20	-14	6	0	4	82	-83	6	4	4	49	-48
12	5	2	24	-10	5	1	3	33	-40	10	6	1	12	17	7	0	4	89	-84	7	4	4	23	-21
13	5	2	33	-12	6	1	3	31	34	11	6	1	21	15	8	0	4	42	-42	10	4	4	35	38
0	6	2	77	74	7	1	3	19	11	12	6	1	7	-4	9	0	4	16	15	11	4	4	20	-14
2	6	2	29	-27	8	1	3	20	-25	13	6	1	19	6	10	0	4	4F	53	0	5	4	81	-77
4	6	2	65	-66	9	1	3	24	21	1	7	1	17	10	11	0	4	15	15	1	5	4	139	134
5	6	2	42	40	2	2	3	37	-41	2	7	1	2F	24	14	0	4	18	-17	2	5	4	2A	30
7	6	2	15	9	3	2	3	2	5	4	7	1	16	15	0	1	4	101	-107	3	5	4	7A	74
8	6	2	22	24	4	2	3	25	-22	6	7	1	23	-19	1	1	4	164	157	4	5	4	44	43
9	6	2	20	-21	5	2	3	29	-26	7	7	1	14	9	2	1	4	19	-16	5	5	4	48	-10C
10	7	2	27	-25	6	2	3	15	-17	8	7	1	17	12	3	1	4	81	77	6	5	4	40	-41
11	7	2	15	-1	7	2	3	25	23	9	7	1	21	-6	4	1	4	4F	43	7	5	4	12	4
12	7	2	19	12	8	2	3	122	118	10	7	1	20	10	5	1	4	133	-135	8	5	4	1F	-9
0	8	2	15	15	9	2	3	152	-142	11	7	1	10	-7	6	1	4	19	19	9	5	4	51	52
1	8	2	4F	-50	3	3	3	114	-111	12	7	1	1F	7	7	1	4	16	-17	10	5	4	27	18
3	8	2	15	-11	4	3	3	29	23	1	8	1	1A	20	8	1	4	18	-20	11	5	4	17	-13
4	8	2	15	-6	5	3	3	12	12	5	8	1	1A	-19	9	1	4	1F	14	12	5	4	21	-14
5	8	2	2F	2F	7	3	3	41	45	6	8	1	1A	9	10	1	4	18	15	0	6	4	85	94
6	8	2	16	0	8	3	3	17	-22	8	8	1	23	4	0	2	4	211	147	1	6	4	37	44
7	8	2	20	-21	10	3	3	19	9	7	1	1	21	15	1	2	4	19	7	2	6	4	32	-34
8	8	2	16	-3	11	3	3	15	-13	8	1	2	1A	6	2	2	4	27	27	3	6	4	34	33
9	8	2	23	-12	1	4	3	62	64	9	1	2	20	-8	3	2	4	37	33	4	6	4	70	-77
10	9	2	19	11	2	4	3	44	-45	10	1	2	2A	-9	4	2	4	75	-74	5	6	4	37	-34
11	9	2	2F	18	4	4	3	19	16	11	1	2	1F	3	5	2	4	47	-45	6	6	4	49	44
0	0	3	4F	-47	5	4	3	37	-47	1	2	2	2A	9E	6	2	4	94	97	7	6	4	17	5
1	0	3	17	15	6	4	3	37	38	2	2	2	44	-39	7	2	4	18	-12	8	6	4	3F	33
2	0	3	27	28	7	4	3	2F	22	3	2	2	2F	-2F	8	2	4	2F	2F	9	6	4	2F	2F
3	0	3	13	0	8	4	3	3E	-40	4	2	2	27	1F	9	2	4	40	49	1F	6	4	32	-34
4	0	3	4A	4F	9	4	3	14	15	5	2	2	21	-13	10	2	4	28	-31	11	6	4	19	-14
6	0	3	34	-17	10	4	3	15	-19	6	2	2	27	34	12	2	4	1F	-12	12	6	4	12	4A
7	0	3	1F	1E	11	4	3	17	-21	7	2	2	19	17	0	3	4	40	40	0	7	4	39	40
8	0	3	2A	-2A	12	4	3	1F	1E	8	2	2	19	-16	1	3	4	5F	-62	1	7	4	94	-102
10	0	3	22	13	3	5	3	3E	-44	9	2	2	1A	1	2	3	4	14	10	2	7	4	18	-23
0	1	3	23	-19	4	5	3	24	-27	10	2	2	19	-11	3	3	4	34	-35	3	7	4	59	58
1	1	3	1F	6	5	5	3	22	14	3	3	2	24	2F	4	3	4	2A	-2F	4	7	4	33	-34
2	1	3	2F	2F	6	5	3	30	31	5	3	2	1F	2	5	3	4	53	55	5	7	4	69	77
4	1	3	1F	-22	7	5	3	2F	2F	6	3	2	1F	-2	6	3	4	27	1F	6	7	4	27	33
7	1	3	14	7	8	5	3	24	-22	7	3	2	2A	-2A	7	3	4	18	-13	7	7	4	19	-7
8	1	3	2A	-20	9	5	3	2F	-2F	8	3	2	17	8	8	3	4	1A	14	8	7	4	37	-41
9	1	3	20	3C	10	5	3	20	-19	2	11	2	2A	2E	9	3	4	3A	-41	11	7	4	1E	7
2	11	3	15	-13	11	5	3	19	15	3	11	2	18	-18	10	3	4	21	23	12	7	4	17	6
4	11	3	32	-29	11	5	3	19	14	4	11	2	2F	-24	0	4	4	197	-200	0	8	4	55	-58
6	11	3	17	-8	1	6	3	AA	-43	0	0	4	193	-200	1	4	4	197	-195	1	8	4	29	-28
8	11	3	1F	1E	3	6	3	44	42	1	0	4	104	108	2	4	4	39	31	2	8	4	27	27
1	12	3	2F	-28	4	6	3	2A	29	2	0	4	2E	-27	3	4	4	46	43	4	8	4	52	54
2	1	3	2E	2A	5	6	3	14	-10	3	0	4	194	193	4	4	4	192	195	5	8	4	32	-38
2	1	3	147	-148	7	6	3	24	-30	4	0	4	122	119	5	4	4	62	65	7	8	4	19	-19

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MPYY

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
A	A	A	21	-93	7	A	E	27	-84	2	9	E	16	-8	4	4	E	28	-91	7	7	E	16	-8
0	A	A	19	6	8	A	E	14	-10	3	9	E	31	29	5	4	E	50	49	8	7	E	32	-30
1A	A	A	27	29	1A	A	E	21	-21	4	9	E	17	15	6	4	E	27	-26	9	7	E	24	-17
11	A	A	29	11	11	A	E	18	8	5	9	E	22	-23	8	4	E	39	-41	10	7	E	28	20
0	B	A	37	32	2	A	E	18	17	6	9	E	18	-4	10	4	E	27	25	11	7	E	16	12
1	B	A	34	37	3	A	E	17	-20	7	9	E	15	3	11	4	E	16	13	12	7	E	17	6
2	B	A	27	24	4	A	E	34	-30	10	9	E	16	4	0	4	F	133	-132	0	8	E	83	-85
3	B	A	24	-23	5	A	E	21	-25	2	10	E	17	19	1	4	E	64	68	1	8	E	40	41
4	B	A	19	-19	6	A	E	15	11	3	10	E	14	9	2	4	E	28	29	2	8	E	23	24
5	B	A	17	-4	7	A	E	24	22	4	10	E	18	-7	3	4	E	40	42	3	8	E	34	34
7	B	A	17	-5	8	A	E	26	18	5	10	E	18	2	4	4	E	78	78	4	8	E	44	47
9	B	A	17	13	1C	A	E	17	7	6	10	E	17	-4	5	4	E	61	-60	5	8	E	32	-28
0	C	A	22	17	1	A	E	15	-14	7	10	E	21	16	6	4	E	46	-44	6	8	E	26	26
1C	C	A	27	5	2	A	E	28	33	1	11	E	19	15	8	4	E	31	-32	7	8	E	1E	-6
2	1C	A	15	-11	3	A	E	25	-25	2	11	E	16	0	9	4	E	37	35	8	8	E	17	-15
3	1C	A	1E	10	4	A	E	28	-28	3	11	E	17	-17	10	4	E	26	28	9	8	E	1E	26
4	1C	A	1C	-15	5	A	E	17	-16	4	11	E	15	0	11	4	E	17	-6	1C	8	E	20	9
F	1C	A	15	-7	6	A	E	1E	-25	0	0	E	223	-201	12	4	E	1E	7	11	8	E	23	-10
E	1C	A	17	11	7	A	E	2E	26	1	0	E	48	47	0	5	E	61	64	0	9	E	49	53
1	11	A	2E	-16	8	A	E	2E	16	2	0	E	47	46	1	5	E	79	75	1	9	E	2E	31
E	11	A	1E	-9	9	A	E	1F	-6	4	0	E	51	54	2	5	E	33	-32	2	9	E	23	-17
F	11	A	2A	20	1E	A	E	2E	26	6	0	E	72	-75	3	5	E	32	32	3	9	E	1E	20
F	11	A	2C	-7	11	E	E	2C	-12	7	0	E	27	-28	4	5	E	41	-44	4	9	E	4C	-42
0	12	A	2E	-16	12	E	E	1E	-9	8	0	E	17	-21	5	5	E	27	-31	5	9	E	2E	-28
1	12	A	1E	-15	13	E	E	1C	1	9	0	E	24	24	6	5	E	51	54	6	9	E	2F	25
2	2F	A	1F	20	1	7	E	34	3E	0	1	E	139	140	7	5	E	1F	12	7	9	E	1F	-5
1	1	E	2A	-25	2	7	E	2E	45	1	1	E	32	41	8	5	E	30	33	8	9	E	2E	23
2	1	E	2A	-28	3	7	E	2E	-35	2	1	E	53	52	10	5	E	3C	-37	9	9	E	1E	14
3	1	E	1E	-11	4	7	E	24	22	3	1	E	80	-7E	12	5	E	17	6	0	10	E	22	21
4	1	E	1C	10	5	7	E	1C	14	4	1	E	48	-5F	0	6	E	5E	5A	1	10	E	3E	-3A
5	1	E	1C	-9	6	7	E	1C	2E	5	1	E	51	5E	1	6	E	1E	1E	2	10	E	1E	-1A
7	2	E	41	38	7	7	E	22	-12	6	1	E	24	2C	2	6	E	2C	-2A	3	10	E	33	-2C
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9	2	E	1F	-15	9	7	E	1E	1	8	1	E	2E	-2A	4	6	E	6C	64	7	10	E	1F	-9
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1	3	E	1E	1A	1	8	E	17	-17	0	2	E	71	-7C	8	6	E	2A	21	3	11	E	1E	-14
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4	3	E	1A	-1A	4	8	E	2C	1E	5	2	E	74	72	11	6	E	33	29	6	11	E	3C	2C
5	3	E	1F	-15	5	8	E	1E	7	7	2	E	2C	-23	12	6	E	1E	9	7	11	E	2C	1E
E	3	E	12	11	6	8	E	1E	-9	8	2	E	4C	39	0	7	E	7C	-6E	1	12	E	131	-120
11	3	E	1E	-1E	7	8	E	2C	-1C	9	2	E	1C	-1A	1	7	E	67	-61	0	1	7	53	-47
1	4	E	4F	45	8	8	E	2E	2A	10	2	E	22	-1F	2	7	E	27	2F	1	1	7	1A5	139
2	4	E	1	-2E	9	8	E	21	-4	12	2	E	14	-1C	3	7	E	2C	-31	2	1	7	2E	-2C
3	4	E	1C	17	1C	8	E	17	3	0	3	E	7C	-72	4	7	E	61	6C	3	1	7	64	67
4	4	E	1E	11	11	8	E	22	1C	1	3	E	72	-6E	5	7	E	4E	4E	4	1	7	130	124
5	4	E	22	22	12	8	E	23	-21	2	3	E	2E	22	6	7	E	3E	-34	6	1	7	3A	-3E

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MXXX

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
0	2	7	27	-34	7	0	7	34	-30	1	3	A	77	72	0	7	A	21	-15	0	2	0	14	-14
1	2	7	22	26	8	0	7	16	3	2	3	A	53	54	1	7	A	25	24	1	2	0	23	-24
2	2	7	41	38	10	0	7	15	-3	4	3	A	60	63	10	7	A	25	20	10	2	0	13	-17
3	2	7	14	-16	3	0	7	24	43	5	3	A	51	-44	11	7	A	15	-14	1	3	0	37	-41
4	2	7	21	20	4	0	7	21	21	6	3	A	22	-27	0	8	A	13	17	4	3	0	14	14
5	2	7	27	-25	4	0	7	14	-4	7	3	A	15	14	1	8	A	35	34	4	3	0	34	-32
6	2	7	16	16	5	0	7	15	46	8	3	A	42	-32	4	8	A	31	28	4	3	0	13	15
7	2	7	16	-15	6	0	7	24	22	9	3	A	23	25	5	8	A	32	29	5	3	0	44	13
0	3	7	30	27	8	0	7	28	31	10	3	A	24	26	8	8	A	24	20	7	4	0	29	24
1	3	7	31	34	9	0	7	17	3	13	3	A	15	1	7	9	A	14	19	9	4	0	10	-17
2	3	7	14	-14	1	1	7	21	21	0	4	B	103	105	8	9	A	14	16	2	4	0	22	-26
3	3	7	20	-19	3	1	7	24	-25	1	4	B	20	-18	9	9	A	15	15	4	4	0	21	-25
4	3	7	15	-14	4	1	7	14	2	2	4	B	73	-76	10	9	A	25	-16	6	4	0	13	15
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3	4	7	32	-35	1	0	8	84	82	0	5	B	34	43	9	A	A	15	6	10	5	0	17	13
4	4	7	24	20	2	0	8	66	64	1	5	B	50	-53	0	B	A	19	-9	11	5	0	11	-13
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11	4	7	15	7	5	0	8	44	-48	5	5	B	30	40	2	10	A	19	20	4	6	0	27	-16
12	4	7	17	-9	6	0	8	29	-27	6	5	B	24	30	3	10	A	21	-17	12	6	0	17	9
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7	5	7	45	39	4	1	8	47	-46	2	6	B	28	31	2	11	A	15	10	2	8	0	27	27
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3	7	7	19	27	1	2	8	84	-73	9	6	B	29	-31	5	1	B	37	-38	2	9	0	28	26
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3	8	7	34	34	0	3	8	111	-105	6	7	B	34	-41	7	2	B	23	24	B	10	0	16	-2

H	K	L	FO	FC
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR WXYY

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2	5	13	15	-15	5	4	14	26	-21	6	4	15	15	14	7	4	16	30	28	8	0	18	18	22
3	5	13	37	-35	10	4	14	34	32	7	4	15	26	-25	10	4	16	25	-19	10	0	18	27	-24
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9	3	14	22	-24	2	4	15	21	19	6	4	16	22	20	2	7	17	17	-17	3	6	18	21	18
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1	4	14	14	21	1	5	15	50	-44	6	6	16	17	-12	4	0	18	50	-51	6	1	19	16	14

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MMYY

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2	3	10	17	22	8	1	20	15	-14	8	6	20	15	-10	4	3	22	23	-33	1	5	23	20	-16
4	3	10	14	-20	0	2	20	24	-21	0	7	20	25	26	8	3	22	15	17	3	5	23	10	-20
0	4	10	27	33	0	3	20	44	-47	4	7	20	20	-23	6	3	22	29	31	2	6	23	15	14
4	4	10	14	14	1	3	20	17	17	1	1	21	29	-24	4	4	22	13	11	0	0	24	22	-23
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8	6	10	15	16	0	4	20	25	25	1	3	21	34	35	8	4	22	13	-17	1	2	24	21	-17
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2	8	10	30	-32	4	5	20	41	-38	5	3	21	15	-17	1	5	22	19	23	8	2	24	25	24
8	8	10	29	29	6	5	20	25	25	1	4	21	18	14	3	5	22	37	36	0	3	24	39	-33
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8	7	10	15	-4	0	6	20	21	26	1	4	21	24	25	8	5	22	19	-16	4	3	24	27	24
1	8	10	18	16	1	6	20	34	-32	2	4	21	27	-22	0	6	22	10	22	6	3	24	24	25
0	0	20	40	38	4	6	20	27	-26	6	4	21	15	17	1	6	22	27	24	8	4	24	35	-37
1	0	20	45	-43	6	6	20	15	-15	7	4	21	15	11	3	6	22	22	15	1	4	24	22	21
4	0	20	27	-26	8	6	20	14	14	4	5	21	10	13	4	7	22	17	-19	2	4	24	15	13
5	0	20	34	37	9	6	20	29	-27	6	5	21	15	-13	6	7	22	25	-22	4	4	24	15	-19
8	0	20	15	19	0	8	20	45	-48	1	6	21	17	-19	0	8	22	14	17	6	4	24	23	-24
0	0	22	17	-14	4	8	20	34	32	3	5	21	14	-16	1	7	22	20	-20	0	5	24	20	22
0	1	20	77	-74	6	8	20	15	-12	5	6	22	32	-34	4	7	22	17	-17	1	5	24	24	24
1	1	20	29	-24	8	8	20	25	-18	5	9	22	19	17	2	1	23	19	19	5	5	24	25	-24
3	1	20	10	-17	0	8	20	11	-14	5	0	22	24	-20	1	3	23	14	14	0	6	24	21	24
4	1	20	45	46	1	8	20	15	15	1	1	22	18	23	3	3	23	14	5	1	6	24	17	-15
6	1	20	32	29	4	8	20	15	12	5	1	22	18	-20	5	4	23	14	-20					

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REP2

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
4	0	0	173	229	19	5	0	89	82	18	2	1	113	-113	-8	6	1	46	60	11	1	2	165	166
6	0	0	148	-157	0	6	0	126	128	-13	3	1	99	-110	-6	6	1	32	11	17	1	2	65	-74
8	0	0	198	-205	2	6	0	111	121	-11	3	1	192	-117	-4	6	1	72	-72	-14	2	2	242	-242
10	0	0	313	-323	4	6	0	53	47	-9	3	1	35	-45	-2	6	1	134	-151	-12	2	2	223	-211
12	0	0	365	-399	6	6	0	69	-65	-7	3	1	24	-12	0	6	1	131	-137	-10	2	2	103	-145
14	0	0	124	-119	10	6	0	143	-148	-5	3	1	88	92	2	6	1	61	-54	-8	2	2	43	-48
16	0	0	77	75	12	6	0	102	-105	-3	3	1	137	140	6	6	1	85	88	-6	2	2	148	141
3	1	0	75	62	14	6	0	47	-50	-1	3	1	168	168	8	6	1	111	106	-4	2	2	368	356
5	1	0	22	-22	16	6	0	35	23	1	3	1	113	116	12	6	1	146	158	-2	2	2	353	346
7	1	0	60	-39	1	7	0	88	-78	3	3	1	28	39	12	6	1	85	76	0	2	2	136	124
11	1	0	131	-134	3	7	0	58	-35	5	3	1	79	-76	14	6	1	26	8	2	2	2	63	-65
13	1	0	162	-162	5	7	0	31	-6	7	3	1	115	-111	-9	7	1	78	68	4	2	2	192	-194
17	1	0	58	62	7	7	0	33	26	9	3	1	120	-115	-7	7	1	33	24	6	2	2	276	-274
0	2	0	311	-315	9	7	0	31	33	11	3	1	136	-135	-5	7	1	49	-51	10	2	2	259	-261
2	2	0	300	-302	11	7	0	81	52	15	3	1	31	25	-3	7	1	135	-126	12	2	2	26	-31
4	2	0	234	-224	-15	1	1	183	186	17	3	1	69	66	-1	7	1	165	-152	14	2	2	81	99
6	2	0	24	31	-13	1	1	371	360	19	3	1	62	52	1	7	1	112	-109	16	2	2	139	132
8	2	0	126	123	-11	1	1	376	369	-12	4	1	302	-303	3	7	1	35	-24	18	2	2	124	125
10	2	0	283	275	-9	1	1	242	244	-10	4	1	215	-215	5	7	1	49	48	-13	3	2	254	-253
12	2	0	202	193	-7	1	1	149	147	-8	4	1	108	-106	7	7	1	105	103	-11	3	2	179	-175
14	2	0	104	98	-5	1	1	66	-69	-6	4	1	46	42	9	7	1	121	128	-9	3	2	58	-59
16	2	0	59	-51	-3	1	1	436	-431	-4	4	1	235	221	11	7	1	106	99	-7	3	2	24	28
18	2	0	122	-119	-1	1	1	633	-633	-2	4	1	358	358	-16	0	2	179	178	-5	3	2	317	328
1	3	0	361	-362	1	1	1	379	-360	0	4	1	314	321	-14	0	2	297	295	-3	3	2	462	452
3	3	0	195	-196	3	1	1	21	-15	2	4	1	147	147	-12	0	2	271	267	-1	3	2	441	448
5	3	0	19	-7	5	1	1	69	68	6	4	1	163	-169	-10	0	2	165	164	5	3	2	220	-223
7	3	0	157	160	7	1	1	268	258	8	4	1	293	-290	-8	0	2	49	45	7	3	2	333	-327
9	3	0	265	269	9	1	1	380	381	10	4	1	330	-326	-6	0	2	133	-128	9	3	2	368	-371
11	3	0	281	284	11	1	1	351	345	12	4	1	177	-171	-4	0	2	497	-498	11	3	2	153	-157
13	3	0	178	175	13	1	1	81	88	14	4	1	22	-2	2	0	2	16	-11	13	3	2	30	52
15	3	0	24	17	15	1	1	82	-95	16	4	1	115	103	6	0	2	487	492	15	3	2	132	133
17	3	0	90	-93	17	1	1	187	-180	18	4	1	124	128	8	0	2	502	505	17	3	2	164	168
19	3	0	119	-127	-14	2	1	299	294	20	4	1	125	117	10	0	2	294	298	19	3	2	146	142
4	4	0	31	-25	-12	2	1	226	218	-11	5	1	68	-71	12	0	2	46	45	-12	4	2	36	25
6	4	0	33	22	-10	2	1	156	158	1	5	1	65	-61	14	0	2	169	-159	-10	4	2	28	-7
8	4	0	44	53	-8	2	1	114	122	-5	5	1	43	53	16	0	2	180	-178	-8	4	2	42	-18
12	4	0	31	3	-6	2	1	48	23	-3	5	1	92	96	-15	1	2	128	111	-6	4	2	24	-33
16	4	0	39	21	-4	2	1	175	-171	12	5	1	197	98	-13	1	2	155	143	-4	4	2	22	-11
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7	5	0	97	-95	6	2	1	245	237	9	5	1	71	-80	-3	1	2	121	-119	14	4	2	38	17
9	5	0	176	-173	8	2	1	266	263	11	5	1	86	-78	-1	1	2	291	-293	16	4	2	29	-16
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13	5	0	118	-126	12	2	1	164	161	17	5	1	54	33	3	1	2	226	218	-11	5	2	149	150
15	5	0	24	-13	14	2	1	20	-19	19	5	1	36	35	7	1	2	140	138	-9	5	2	31	20
17	5	0	72	69	16	2	1	104	-106	-18	6	1	87	96	9	1	2	144	146	-7	5	2	23	-16

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
-5	5	2	185	-188	-8	2	3	191	195	-5	5	3	95	-93	-13	1	4	76	-74	-12	4	4	26	-24
-3	5	2	278	-267	-6	2	3	258	258	-3	5	3	78	-85	-11	1	4	23	-37	-10	4	4	23	-23
-1	5	2	231	-238	-4	2	3	344	339	-1	5	3	54	-52	-9	1	4	105	107	-8	4	4	45	-42
1	5	2	95	-108	-2	2	3	314	302	1	5	3	49	35	-7	1	4	198	196	-6	4	4	32	-24
3	5	2	158	156	0	2	3	228	231	3	5	3	48	71	-5	1	4	131	129	-2	4	4	57	-55
5	5	2	202	212	2	2	3	25	-31	5	5	3	81	84	-1	1	4	27	-40	2	4	4	26	-7
0	5	2	222	222	4	2	3	134	-132	7	5	3	96	83	1	1	4	97	-85	4	4	4	51	38
11	5	2	69	89	6	2	3	316	-315	9	5	3	69	60	3	1	4	96	-91	6	4	4	51	-33
13	5	2	26	-3	8	2	3	256	-263	13	5	3	34	-33	5	1	4	206	-206	12	4	4	28	-17
15	5	2	99	-93	10	2	3	73	-75	15	5	3	58	-47	7	1	4	143	-134	14	4	4	23	-17
17	5	2	103	-111	12	2	3	77	87	17	5	3	34	-50	11	1	4	41	42	16	4	4	25	-9
-10	6	2	72	65	14	2	3	137	134	-6	6	3	55	38	13	1	4	63	65	-9	5	4	61	66
-8	6	2	29	-9	16	2	3	100	119	-6	6	3	135	132	15	1	4	29	43	-7	5	4	208	214
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-4	6	2	139	-134	-13	3	3	78	70	-2	6	3	116	121	-14	2	4	155	164	-3	5	4	168	169
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6	6	2	92	94	-5	3	3	169	-163	8	6	3	106	-107	-8	2	4	139	-116	5	5	4	235	-249
8	6	2	127	116	-3	3	3	179	-179	10	6	3	47	-41	-6	2	4	363	-358	7	5	4	240	-210
10	6	2	97	92	-1	3	3	111	-108	12	6	3	49	50	-4	2	4	256	-249	9	5	4	49	-53
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1	7	2	29	-5	9	3	3	136	138	-3	7	3	149	139	6	2	4	262	262	-8	6	4	67	79
5	7	2	27	-25	13	3	3	44	-48	-1	7	3	77	73	8	2	4	214	219	-6	6	4	177	174
7	7	2	37	-69	15	3	3	72	-78	3	7	3	56	-72	10	2	4	19	17	-4	6	4	115	118
9	7	2	66	-55	17	3	3	55	-65	5	7	3	123	-116	12	2	4	105	-105	-2	6	4	38	39
-15	1	3	284	-286	19	3	3	62	-55	7	7	3	128	-126	14	2	4	146	-156	2	6	4	83	-94
-13	1	3	262	-262	-12	4	3	138	134	9	7	3	78	-84	16	2	4	127	-133	4	6	4	111	-102
-11	1	3	116	-124	-10	4	3	45	36	-16	0	4	314	-329	18	2	4	114	-99	6	6	4	115	-126
-9	1	3	18	-5	-8	4	3	85	-80	-14	0	4	195	-192	-13	3	4	134	132	8	6	4	68	-72
-7	1	3	237	235	-6	4	3	360	-296	-12	0	4	93	-79	-11	3	4	16	25	12	6	4	36	46
-5	1	3	432	434	-4	4	3	437	-432	-10	0	4	28	18	-9	3	4	125	-102	16	6	4	54	77
-3	1	3	463	462	-2	4	3	286	-287	-8	0	4	295	295	-7	3	4	257	-262	-9	7	4	47	-34
-1	1	3	190	183	0	4	3	30	-68	-6	0	4	443	448	-5	3	4	361	-360	-7	7	4	38	-56
1	1	3	184	-183	2	4	3	82	-90	-4	0	4	339	346	-3	3	4	258	-253	-5	7	4	67	-56
3	1	3	155	-152	4	4	3	183	180	-2	0	4	151	156	-1	3	4	48	-43	-3	7	4	56	-61
5	1	3	402	-385	6	4	3	275	288	0	0	4	212	-234	1	3	4	157	153	1	7	4	28	31
7	1	3	417	-415	8	4	3	271	264	2	0	4	115	-131	3	3	4	242	234	5	7	4	43	61
9	1	3	248	-245	10	4	3	128	132	4	0	4	857	-862	5	3	4	329	315	7	7	4	34	22
11	1	3	27	39	12	4	3	77	-76	6	0	4	647	-673	7	3	4	254	256	-15	1	5	151	144
13	1	3	180	191	14	4	3	131	-133	8	0	4	340	-356	9	3	4	86	86	-13	1	5	72	61
15	1	3	203	212	16	4	3	187	-185	10	0	4	69	51	11	3	4	89	-98	-11	1	5	82	-84
17	1	3	199	-204	18	4	3	132	-134	12	0	4	235	233	13	3	4	184	-184	-9	1	5	297	-306
-16	2	3	199	-202	20	4	3	77	-79	14	0	4	196	189	15	3	4	149	-174	-7	1	5	498	-501
-12	2	3	138	-142	-11	5	3	26	12	16	0	4	241	231	17	3	4	156	-146	-5	1	5	426	-419
-10	2	3	51	-53	-7	5	3	89	-75	-15	1	4	92	-93	19	3	4	68	-67	-3	1	5	131	-134

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
-1	1	5	28	45	-2	4	5	45	-17	-8	0	5	375	-387	-5	3	6	85	94	10	6	6	62	-76
1	1	5	275	255	0	4	5	150	-150	-6	0	6	279	-281	-3	3	6	30	-28	12	6	6	80	-70
3	1	5	364	369	2	4	5	246	-248	-4	0	6	34	-27	-1	3	6	186	-179	-9	7	6	51	55
5	1	5	473	472	4	4	5	312	-311	-2	0	6	126	118	1	3	6	294	-298	-5	7	6	30	16
7	1	5	155	155	6	4	5	203	-204	0	0	6	267	259	3	3	6	397	-391	-3	7	6	28	-16
9	1	5	30	-42	8	4	5	23	-25	2	0	6	351	363	5	3	6	191	-188	-1	7	6	28	-32
11	1	5	199	-198	10	4	5	122	129	4	0	6	459	469	7	3	6	28	24	1	7	6	31	-39
13	1	5	220	-205	12	4	5	173	173	6	0	6	165	179	9	3	6	163	163	3	7	6	74	51
15	1	5	264	-294	14	4	5	184	185	8	0	6	86	-81	11	3	6	188	188	5	7	6	34	-33
17	1	5	132	-135	16	4	5	139	153	10	0	6	276	-291	13	3	6	260	281	7	7	6	41	4
-14	2	5	64	75	18	4	5	59	53	12	0	6	307	-311	15	3	6	156	163	-13	1	7	108	115
-12	2	5	48	-51	-11	5	5	21	22	14	0	6	229	-215	17	3	6	33	40	-11	1	7	267	265
-10	2	5	180	-173	-9	5	5	72	70	16	0	6	131	-138	19	3	6	74	-68	-9	1	7	374	375
-8	2	5	269	-268	-7	5	5	77	78	-15	1	6	21	25	-12	4	6	35	-4	-7	1	7	217	228
-6	2	5	250	-245	-5	5	5	67	82	-13	1	6	20	-11	-10	4	6	25	4	-5	1	7	33	-20
-4	2	5	172	-151	-3	5	5	23	15	-11	1	6	83	-78	-8	4	6	29	-17	-3	1	7	155	-157
-2	2	5	28	-15	-1	5	5	95	-82	-9	1	6	164	-163	-6	4	6	25	-26	-1	1	7	288	-300
0	2	5	129	127	3	5	5	85	-89	-7	1	6	119	-123	-4	4	6	44	28	1	1	7	361	-369
2	2	5	167	177	5	5	5	84	-79	-5	1	6	146	-138	-2	4	6	24	18	3	1	7	338	-347
4	2	5	291	292	7	5	5	36	-46	-3	1	6	153	144	0	4	6	32	9	5	1	7	62	-46
6	2	5	188	181	11	5	5	32	41	-1	1	6	269	267	10	4	6	33	-20	7	1	7	134	143
8	2	5	26	-2	13	5	5	60	49	1	1	6	114	112	12	4	6	29	8	9	1	7	235	233
10	2	5	156	-155	15	5	5	58	57	3	1	6	183	191	14	4	6	23	-6	11	1	7	233	227
12	2	5	173	-186	-15	6	5	78	-73	5	1	6	50	53	16	4	6	22	-6	13	1	7	197	186
14	2	5	149	-156	-8	6	5	127	-133	7	1	6	40	39	18	4	6	24	-17	15	1	7	98	89
16	2	5	123	-128	-6	6	5	165	-157	9	1	6	102	-112	-11	5	6	113	-107	17	1	7	66	-62
18	2	5	45	-47	-4	6	5	88	-83	11	1	6	123	-124	-9	5	6	158	-161	-14	2	7	27	33
-13	3	5	24	-11	-2	6	5	26	-11	13	1	6	76	-81	-7	5	6	224	-225	-12	2	7	173	166
-11	3	5	41	44	0	6	5	39	42	15	1	6	85	-86	-5	5	6	69	-68	-10	2	7	263	267
-9	3	5	99	95	2	6	5	81	91	-14	2	6	43	-47	-3	5	6	28	11	-8	2	7	237	235
-7	3	5	153	151	4	6	5	116	126	-12	2	6	56	66	-1	5	6	107	113	-6	2	7	71	79
-5	3	5	109	105	6	6	5	88	102	-10	2	6	234	233	1	5	6	183	186	-4	2	7	193	-181
-3	3	5	29	-7	8	6	5	79	-65	-8	2	6	326	318	3	5	6	216	209	-2	2	7	178	-177
-1	3	5	59	-77	12	6	5	72	-73	-6	2	6	215	211	5	5	6	164	169	0	2	7	246	-243
1	3	5	83	-85	14	6	5	67	-78	-4	2	6	71	-73	9	5	6	114	-113	2	2	7	255	-244
3	3	5	137	-125	-9	7	5	87	80	-2	2	6	197	-197	11	5	6	165	-169	4	2	7	265	-264
5	3	5	120	-133	-7	7	5	112	-135	2	2	6	292	-291	13	5	6	141	-134	6	2	7	26	21
7	3	5	89	-91	-5	7	5	113	-105	4	2	6	268	-263	15	5	6	101	-101	8	2	7	91	98
9	3	5	46	35	-3	7	5	27	-35	6	2	6	52	-48	-10	6	6	46	-51	10	2	7	174	175
11	3	5	94	94	-1	7	5	56	30	8	2	6	114	115	-8	6	6	126	-126	12	2	7	153	157
13	3	5	30	45	1	7	5	80	86	10	2	6	131	131	-6	6	6	108	-105	14	2	7	101	106
15	3	5	95	85	3	7	5	129	123	12	2	6	121	119	-4	6	6	26	-21	16	2	7	24	11
17	3	5	43	52	5	7	5	125	121	14	2	6	152	154	-2	6	6	56	56	18	2	7	75	-83
-12	4	5	27	-3	7	7	5	59	55	16	2	6	98	100	0	6	6	101	106	-13	3	7	61	-57
-10	4	5	106	103	-10	8	5	121	126	-13	3	6	23	-6	2	6	6	113	119	-11	3	7	109	-115
-8	4	5	303	295	-14	0	6	22	19	-11	3	6	178	172	4	6	6	103	94	-9	3	7	115	-113
-6	4	5	340	344	-12	0	6	98	-92	-9	3	6	305	304	6	6	6	38	38	-7	3	7	66	-72
-4	4	5	179	172	-10	0	6	256	-260	-7	3	6	311	300	8	6	6	39	-44	-5	3	7	51	41

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REP2

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
-1	3	7	92	94	12	6	7	56	65	2	2	8	202	196	-8	6	8	72	65	-9	3	9	22	28
1	3	7	145	145	-7	7	7	70	76	6	2	8	203	-203	-4	6	8	56	-43	-7	3	9	40	-38
3	3	7	146	138	-3	7	7	49	-47	8	2	8	174	-188	-2	6	8	112	-124	-5	3	9	61	-81
5	3	7	72	-73	-1	7	7	94	-96	10	2	8	145	-146	0	6	8	125	-132	-3	3	9	84	-78
9	3	7	70	-73	1	7	7	114	-124	12	2	8	127	-131	2	6	8	79	-73	-1	3	9	117	-122
11	3	7	44	-53	3	7	7	92	-94	14	2	8	65	-73	6	6	8	75	71	1	3	9	64	-61
13	3	7	53	-51	5	7	7	32	-28	18	2	8	198	96	8	6	8	77	72	5	3	9	68	77
15	3	7	50	-55	-16	0	8	49	42	-13	3	8	159	-162	10	6	8	88	76	7	3	9	60	89
17	3	7	28	18	-14	0	8	110	114	-11	3	8	253	-251	-5	7	8	36	31	9	3	9	52	64
19	3	7	66	64	-12	0	8	376	378	-9	3	8	204	-218	-3	7	8	51	39	11	3	9	75	72
-12	4	7	130	-137	-10	0	8	351	359	-7	3	8	52	-58	-1	7	8	27	43	15	3	9	32	-47
-10	4	7	221	-223	-8	0	8	127	125	-5	3	8	80	88	1	7	8	61	48	17	3	9	44	-37
-8	4	7	240	-245	-6	0	8	67	54	-3	3	8	169	169	3	7	8	28	36	-12	4	9	190	188
-6	4	7	75	-72	-4	0	8	194	-188	-1	3	8	249	256	-15	1	9	115	-119	-10	4	9	110	116
-4	4	7	66	70	-2	0	8	264	-262	1	3	8	269	269	-13	1	9	261	-257	-8	4	9	28	7
-2	4	7	166	156	0	0	8	337	-341	3	3	8	139	150	-11	1	9	248	-252	-6	4	9	87	-82
0	4	7	312	319	2	0	8	275	-278	5	3	8	76	-79	-9	1	9	96	-91	-4	4	9	159	-163
2	4	7	309	313	4	0	8	62	70	7	3	8	183	-176	-7	1	9	65	71	-2	4	9	270	-267
4	4	7	162	166	6	0	8	158	162	9	3	8	196	-190	-5	1	9	186	187	0	4	9	235	-234
6	4	7	33	-49	8	0	8	328	336	11	3	8	160	-162	-3	1	9	324	302	2	4	9	77	-75
8	4	7	156	-156	10	0	8	361	346	13	3	8	118	-108	-1	1	9	399	399	4	4	9	91	96
10	4	7	172	-173	12	0	8	257	271	15	3	8	32	-5	1	1	9	237	235	6	4	9	186	171
12	4	7	75	-56	14	0	8	142	129	17	3	8	93	116	5	1	9	227	-223	8	4	9	114	103
14	4	7	146	-141	16	0	8	98	-95	19	3	8	194	115	7	1	9	203	-200	10	4	9	155	154
18	4	7	77	65	-15	1	8	26	-7	-12	4	8	39	6	9	1	9	256	-253	12	4	9	86	85
-11	5	7	58	-54	-13	1	8	70	74	-8	4	8	28	16	11	1	9	171	-171	14	4	9	33	-40
-9	5	7	65	-62	-11	1	8	133	131	-6	4	8	29	6	13	1	9	55	-65	16	4	9	114	-118
-7	5	7	31	-27	-9	1	8	193	189	-4	4	8	48	56	15	1	9	94	98	-11	5	9	52	53
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-1	5	7	75	78	-5	1	8	52	-42	2	4	8	29	9	-14	2	9	144	-144	-7	5	9	22	-9
1	5	7	89	81	-3	1	8	128	-121	8	4	8	31	-21	-12	2	9	233	-199	-5	5	9	33	-56
3	5	7	56	-56	-1	1	8	136	-141	10	4	8	27	16	-10	2	9	139	-138	-3	5	9	89	-64
5	5	7	36	-16	1	1	8	148	-114	16	4	8	28	2	-8	2	9	34	22	-1	5	9	74	-76
7	5	7	49	-45	3	1	8	38	-36	-11	5	8	182	176	-6	2	9	135	134	1	5	9	37	-32
9	5	7	63	59	5	1	8	78	91	-9	5	8	137	124	-4	2	9	197	197	3	5	9	27	12
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13	5	7	56	-47	9	1	8	103	96	-5	5	8	42	-52	0	2	9	261	193	7	5	9	77	63
15	5	7	26	-23	11	1	8	96	97	-3	5	8	106	-109	2	2	9	69	75	9	5	9	61	56
-18	6	7	124	116	13	1	8	50	48	-1	5	8	213	-215	4	2	9	99	-107	11	5	9	34	38
-6	6	7	96	165	17	1	8	33	-50	1	5	8	189	-197	6	2	9	125	-132	13	5	9	34	3
-4	6	7	49	-53	-14	2	8	143	-148	3	5	8	81	-77	8	2	9	149	-143	-16	6	9	77	-76
-2	6	7	92	-83	-12	2	8	217	-211	5	5	8	38	30	10	2	9	137	-135	-8	6	9	225	-13
0	6	7	111	-115	-10	2	8	225	-229	7	5	8	129	118	12	2	9	61	-71	-6	6	9	53	57
2	6	7	133	-129	-8	2	8	188	-198	9	5	8	137	131	14	2	9	52	35	-4	6	9	99	82
4	6	7	65	-61	-6	2	8	26	22	11	5	8	136	136	16	2	9	116	118	-2	6	9	123	129
6	6	7	30	15	-4	2	8	76	80	13	5	8	85	92	18	2	9	93	99	0	6	9	185	114
8	6	7	66	61	-2	2	8	210	202	15	5	8	34	-9	-13	3	9	34	88	2	6	9	48	45
10	6	7	84	77	0	2	8	243	236	-10	6	8	84	85	-11	3	9	81	73	4	6	9	26	-32

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REP2

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
6	6	9	63	-78	14	2	10	93	-89	-13	1	11	132	137	-4	4	11	174	173	-7	1	12	86	-86
8	6	9	54	-68	16	2	10	141	-93	-9	1	11	81	-91	-2	4	11	138	147	-5	1	12	114	-116
-16	0	10	126	-132	18	2	10	78	-67	-7	1	11	169	-167	2	4	11	115	-109	-3	1	12	50	-59
-14	0	10	253	-260	-13	3	10	194	206	-5	1	11	265	-264	4	4	11	181	-186	1	1	12	23	18
-12	0	10	268	-245	-11	3	10	97	94	-3	1	11	273	-273	6	4	11	187	-185	3	1	12	75	75
-10	0	10	50	-53	-7	3	10	186	-178	-1	1	11	187	-193	8	4	11	148	-143	5	1	12	86	82
-8	0	10	91	94	-5	3	10	198	-195	1	1	11	98	106	10	4	11	58	-47	7	1	12	73	79
-6	0	10	173	176	-3	3	10	268	-269	3	1	11	210	213	12	4	11	78	67	9	1	12	71	66
-4	0	10	272	269	-1	3	10	192	-191	5	1	11	202	200	14	4	11	122	122	9	1	12	29	-14
-2	0	10	306	305	1	3	10	39	-24	7	1	11	243	198	-11	5	11	24	-14	11	1	12	50	-54
0	0	10	171	167	3	3	10	129	122	9	1	11	125	133	-9	5	11	40	27	13	1	12	73	-59
2	0	10	64	-71	5	3	10	182	177	13	1	11	118	-132	-7	5	11	44	46	15	1	12	60	-51
4	0	10	229	-232	7	3	10	243	197	15	1	11	146	-154	-5	5	11	65	56	17	1	12	66	69
6	0	10	206	-195	9	3	10	178	169	17	1	11	99	-97	-3	5	11	26	37	-14	2	12	86	-86
8	0	10	227	-222	11	3	10	64	64	-14	2	11	147	145	1	5	11	30	-38	-12	2	12	21	21
10	0	10	163	-162	13	3	10	67	-61	-12	2	11	83	83	3	5	11	47	-52	-10	2	12	86	85
12	0	10	48	-51	15	3	10	119	-126	-8	2	11	101	-99	5	5	11	63	-57	-8	2	12	141	138
14	0	10	125	122	17	3	10	116	-112	-6	2	11	173	-181	7	5	11	37	-49	-6	2	12	157	162
16	0	10	206	202	-12	4	10	23	-9	-4	2	11	235	227	9	5	11	28	-12	-4	2	12	196	206
-15	1	10	57	-55	-8	4	10	23	12	-2	2	11	139	-151	11	5	11	33	21	-2	3	12	74	76
-13	1	10	117	-123	-4	4	10	24	-16	0	2	11	27	25	-8	6	11	46	-43	0	3	12	78	-74
-11	1	10	52	-64	-2	4	10	26	22	2	2	11	143	140	-6	6	11	74	-77	2	3	12	146	-142
-9	1	10	24	3	2	4	10	26	-23	4	2	11	167	172	-4	6	11	97	-97	4	3	12	126	-133
-7	1	10	40	50	6	4	10	46	-11	6	2	11	127	118	-2	6	11	66	-73	6	3	12	113	-117
-5	1	10	165	174	8	4	10	29	9	8	2	11	153	162	0	6	11	36	9	8	3	12	85	-83
-3	1	10	97	93	10	4	10	34	-11	10	2	11	45	44	2	6	11	82	65	10	3	12	39	48
-1	1	10	127	147	12	4	10	23	-9	12	2	11	44	-49	4	6	11	84	80	12	3	12	109	119
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3	1	10	153	-151	-7	5	10	89	87	16	2	11	90	-94	-14	8	12	128	138	16	3	12	54	59
5	1	10	117	-119	-5	5	10	104	101	18	2	11	44	-49	-12	8	12	49	-42	-13	3	12	26	-47
7	1	10	100	-95	-3	5	10	180	177	-13	3	11	81	-76	-10	8	12	72	-77	-11	3	12	53	59
9	1	10	42	-55	-1	5	10	138	129	-11	3	11	23	-18	-8	8	12	324	-319	-9	3	12	128	112
13	1	10	22	27	1	5	10	35	34	-9	3	11	51	42	-6	8	12	311	-317	-7	3	12	167	189
15	1	10	71	77	3	5	10	59	-75	-7	3	11	91	81	-4	8	12	228	-229	-5	3	12	205	203
17	1	10	58	61	5	5	10	136	-133	-5	3	11	76	76	-2	8	12	54	-56	-3	3	12	138	134
-14	2	10	171	168	7	5	10	124	-117	-3	3	11	94	101	0	8	12	154	151	-1	3	12	41	-28
-12	2	10	135	136	9	5	10	116	-117	-1	3	11	47	38	2	8	12	196	188	1	3	12	148	-143
-10	2	10	48	42	11	5	10	33	-34	1	3	11	46	-38	4	8	12	184	189	3	3	12	164	-162
-8	2	10	22	-45	-14	6	10	34	-28	3	3	11	77	73	6	8	12	177	181	5	3	12	162	-151
-6	2	10	134	-135	-8	6	10	32	34	5	3	11	77	-81	8	8	12	94	85	7	3	12	132	-132
-4	2	10	209	-216	-6	6	10	66	72	7	3	11	67	-73	10	8	12	53	-56	9	3	12	29	-34
-2	2	10	247	-253	-4	6	10	85	90	9	3	11	53	-53	12	8	12	166	-169	11	3	12	89	86
0	2	10	121	-116	-2	6	10	97	103	13	3	11	56	53	14	8	12	182	-182	13	3	12	119	128
2	2	10	37	41	0	6	10	88	-55	15	3	11	58	47	16	8	12	139	-124	15	3	12	100	98
4	2	10	139	139	4	6	10	84	-74	-12	4	11	77	-69	-14	9	12	54	51	-12	4	12	28	12
6	2	10	168	158	6	6	10	95	-89	-10	4	11	26	27	-13	1	12	28	33	-10	4	12	28	2
8	2	10	158	159	8	6	10	71	-69	-8	4	11	88	91	-11	1	12	23	5	-8	4	12	23	-18
10	2	10	101	107	-15	1	11	191	189	-6	4	11	147	152	-9	1	12	28	-29	-6	4	12	23	-23

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
4	4	12	43	-1	-5	3	13	54	-63	3	1	14	66	-73	-7	1	15	77	-78	-4	0	16	145	139
8	4	12	24	4	-1	3	13	60	75	5	1	14	51	-46	-5	1	15	49	49	-2	0	16	177	181
10	4	12	24	-5	3	3	13	56	61	7	1	14	30	32	-3	1	15	137	133	0	0	16	156	148
-11	5	12	43	-31	5	3	13	61	52	9	1	14	84	76	-1	1	15	156	156	2	0	16	109	104
-9	5	12	91	-85	9	3	13	31	-22	11	1	14	54	63	1	1	15	156	148	6	0	16	119	-113
-7	5	12	131	-132	11	3	13	63	-70	13	1	14	47	33	3	1	15	121	118	8	0	16	146	-138
-5	5	12	146	-143	13	3	13	26	-48	-10	2	14	24	-17	5	1	15	44	10	10	0	16	37	-28
-3	5	12	81	-85	-12	4	13	43	-53	-12	2	14	66	-69	7	1	15	103	-103	-13	1	16	64	-53
1	5	12	91	85	-10	4	13	84	-98	-10	2	14	97	-110	9	1	15	144	-144	-11	1	16	50	-47
3	5	12	128	122	-8	4	13	146	-144	-8	2	14	153	-136	11	1	15	98	-101	-9	1	16	23	-9
5	5	12	117	124	-6	4	13	134	-139	-6	2	14	82	-91	13	1	15	39	-65	-5	1	16	28	22
7	5	12	63	87	-4	4	13	66	-68	-4	2	14	27	8	-14	2	15	52	-53	-3	1	16	42	44
-4	6	12	72	-73	-2	4	13	69	55	-2	2	14	108	106	-12	2	15	95	-98	-1	1	16	62	67
0	6	12	27	29	0	4	13	118	122	0	2	14	124	122	-10	2	15	103	-105	1	1	16	35	49
2	6	12	55	69	2	4	13	146	142	2	2	14	114	132	-8	2	15	103	-112	3	1	16	24	20
-15	1	13	75	-66	4	4	13	132	142	4	2	14	113	114	-6	2	15	34	63	5	1	16	28	-31
-13	1	13	32	23	6	4	13	83	98	6	2	14	55	39	-2	2	15	101	111	7	1	16	49	-53
-11	1	13	94	95	10	4	13	84	-93	8	2	14	53	-56	0	2	15	120	130	9	1	16	38	-46
-9	1	13	153	152	-9	5	13	32	-49	10	2	14	145	-139	2	2	15	111	118	11	1	16	36	-35
-7	1	13	214	221	-7	5	13	51	-51	12	2	14	80	-89	4	2	15	48	47	-12	2	16	88	81
-5	1	13	157	168	-5	5	13	46	-36	-13	3	14	73	-74	6	2	15	44	-46	-10	2	16	186	99
-3	1	13	149	-142	-3	5	13	29	36	-11	3	14	145	-112	8	2	15	114	-116	-8	2	16	42	46
1	1	13	169	-185	1	5	13	36	42	-9	3	14	153	-165	10	2	15	61	-79	-6	2	16	68	-59
3	1	13	266	-262	3	5	13	59	57	-7	3	14	136	-136	12	2	15	74	-71	-4	2	16	123	-112
5	1	13	163	161	5	5	13	46	34	-5	3	14	53	44	-11	3	15	23	44	-2	2	16	101	-97
7	1	13	103	-101	7	5	13	36	6	-3	3	14	75	72	-9	3	15	61	72	0	2	16	186	-180
9	1	13	82	81	-16	6	14	67	-57	-1	3	14	140	136	-7	3	15	53	52	2	2	16	85	-89
11	1	13	148	142	-14	6	14	26	36	1	3	14	156	148	-5	3	15	65	-65	4	2	16	36	-18
13	1	13	152	142	-12	6	14	134	143	3	3	14	140	139	-3	3	15	52	-50	6	2	16	77	76
15	1	13	88	65	-10	6	14	143	147	5	3	14	71	74	1	3	15	32	-48	8	2	16	95	100
-14	2	13	26	-28	-8	6	14	220	219	7	3	14	26	-22	3	3	15	47	-49	-11	3	16	111	112
-12	2	13	47	43	-6	6	14	187	192	9	3	14	125	-109	5	3	15	32	16	-9	3	16	90	95
-10	2	13	92	84	-4	6	14	25	-18	11	3	14	108	-115	7	3	15	33	33	-5	3	16	75	-91
-8	2	13	149	133	-2	6	14	145	-146	-8	4	14	29	3	9	3	15	62	58	-3	3	16	113	-116
-6	2	13	164	153	0	6	14	181	-186	-6	4	14	125	-119	11	3	15	130	134	-1	3	16	129	-111
-4	2	13	66	62	2	6	14	162	-165	0	4	14	35	8	-8	4	15	98	113	1	3	16	93	-97
-2	2	13	53	-65	4	6	14	152	-144	2	4	14	25	3	-6	4	15	33	18	3	3	16	43	-65
0	2	13	152	-145	6	6	14	34	51	4	4	14	23	-13	-4	4	15	76	-69	5	3	16	77	56
2	2	13	145	-151	8	6	14	196	192	-7	5	14	113	111	-2	4	15	113	-117	7	3	16	112	112
4	2	13	124	-122	10	6	14	152	158	-5	5	14	54	49	0	4	15	99	-92	9	3	16	25	4
6	2	13	100	-92	12	6	14	122	121	-3	5	14	61	-60	2	4	15	130	-131	-11	4	16	108	106
8	2	13	91	88	14	6	14	90	79	-1	5	14	103	-92	4	4	15	44	-44	-9	4	16	53	49
12	2	13	93	93	-13	7	14	69	51	1	5	14	90	-96	6	4	15	26	31	-7	4	16	79	-76
14	2	13	66	71	-11	7	14	22	32	3	5	14	86	-88	-16	5	15	125	-116	-5	4	16	111	-113
-13	3	13	23	5	-9	7	14	63	72	-15	5	15	47	-38	-12	0	16	144	-125	-3	4	16	124	-123
-11	3	13	26	-23	-7	7	14	65	76	-13	1	15	100	-94	-10	0	16	151	-145	-1	4	16	111	-108
-9	3	13	45	-50	-1	7	14	79	-84	-11	1	15	120	-125	-8	0	16	26	-43	1	4	16	71	-69
-7	3	13	61	-73	1	7	14	63	-57	-9	1	15	149	-153	-6	0	16	68	59	3	4	16	27	28

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR REP2

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
5	1	17	124	113	0	2	17	72	-69	1	3	17	53	43	4	0	18	114	129	5	1	18	60	46
7	1	17	138	127	2	2	17	32	-15	-8	0	18	101	-87	-9	1	18	37	-27	-6	2	18	84	75
-10	2	17	62	55	4	2	17	37	64	-6	0	18	118	-109	-7	1	18	29	-40	-4	2	18	67	79
-8	2	17	23	-15	6	2	17	100	98	-4	0	18	113	-109	-5	1	18	44	-38	-2	2	18	76	67
-6	2	17	73	-67	-7	3	17	31	12	-2	0	18	161	-165	-1	1	18	28	-35	0	2	18	50	35
-4	2	17	85	-81	-5	3	17	45	36	0	0	18	67	-54	3	1	18	30	37	2	2	18	46	-34
-2	2	17	93	-89	-3	3	17	29	41	2	0	18	52	38										



Author Harris Gillian Wendy
Name of thesis Chemical And Structural Studies Of Substituted Transition Metal Carbonyl Complexes. 1984

PUBLISHER:
University of the Witwatersrand, Johannesburg
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