Salesite, CuIO₃(OH), and Cu(IO₃)₂·2H₂O: a comparison of the crystal structures and their magnetic behavior[1]

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Abstract

The structurally closely-related compounds $Cu(IO_3)_2 \cdot 2H_2O$ and salesite, $Cu(IO_3)(OH)$, are monoclinic and orthorhombic respectively, with cell dimensions $a = 6.728(1)$, $b = 4.813(1)$, $c = 11.165(2)$A, $\beta = 103.34(1)°$; space group $P2_1/c$, $Z = 2$; and $a = 10.794(2)$, $b = 6.708(1)$, $c = 4.781(1)$A, space group $Pnma$, $Z = 4$. The crystal structure of $Cu(IO_3)_2 \cdot 2H_2O$ has been determined by the heavy-atom method. The crystal structures of both compounds have been refined by the method of least squares to R factors of 0.026 and 0.031, based on 1284 and 715 reflections measured on an automatic single-crystal diffractometer. The hydrogen positions have been determined for both phases.

The $[CuO_4(H_2O)_2]$ octahedron in $Cu(IO_3)_2 \cdot 2H_2O$ and the $[CuO_4(OH)_2]$ octahedron in salesite are tetragonally distorted, with the water molecules and the (OH) ions in each structure occurring in a *trans*-configuration within the square plane. The four square planar Cu–O bonds average 1.953 and 1.968A, and two axial Cu–O bonds average 2.457 and 2.538A in $Cu(IO_3)_2 \cdot 2H_2O$ and salesite respectively. The $[IO_3]$ groups in both structures are trigonal pyramids, deviating significantly from the highest possible point-group symmetry $3m$. The three short I–O bonds average 1.811 and 1.824A, and the O–I–O angles 99.7 and 97.9°; three additional long I–O bonds average 2.815 and 2.637A within the distorted octahedral $[IO_3(H_2O)]$ and $[IO_3(OH)]$ groups in the structures of $Cu(IO_3)_2 \cdot 2H_2O$ and salesite respectively. Both structures consist of corner-sharing I-octahedra forming an open sheet structure, which are cross-linked by Cu-octahedra. In $Cu(IO_3)_2 \cdot 2H_2O$, the Cu-octahedra are isolated, whereas in salesite they share edges to form infinite chains parallel to the b axis. The hydrogen atoms in both structures are involved in hydrogen bonding.

$Cu(IO_3)_2 \cdot 2H_2O$ is paramagnetic down to 1.4 K, whereas salesite may be anti-ferromagnetic below 162 K. The different magnetic behavior in these two phases is explained by the fact that the Cu–Cu separation is 6.508A in $Cu(IO_3)_2 \cdot 2H_2O$ and 3.354A within the octahedral chain in salesite. A model is proposed of the magnetic structure of salesite with the magnetic spins alternately up and down, either parallel or normal to the b axis.

Introduction

Of the two known mineral iodates of copper, salesite, $CuIO_3(OH)$, was described by Palache and Jarrell (1939), and bellingerite, $3Cu(IO_3)_2 \cdot 2H_2O$, by Berman and Wolfe (1940). The crystal structure of salesite was determined by Ghose (1962) and of bellingerite by Ghose and Wan (1974). Both these minerals were synthesized by Granger and de Schulten (1904). Salesite, bellingerite, and four new copper iodates have been synthesized by Nassau *et al.* (1973) by the gel-growth technique. Their crystallographic, mag-

netic, and optical properties were determined by Abrahams *et al.* (1973b). Of these four new copper iodate phases, three are anhydrous $Cu(IO_3)_2$ and the fourth is hydrated, namely $Cu(IO_3)_2 \cdot 2H_2O$. This hydrated phase is monoclinic, with cell dimensions very similar to those of salesite, which is orthorhombic. This fact suggested that these two structures may be closely comparable. This is indeed the case, as shown by the structure determination of $Cu(IO_3)_2 \cdot 2H_2O$ reported in this paper. In this connection, the structure of salesite (Ghose, 1962) has been refined using three-dimensional intensity data. In spite of the structural similarity, the magnetic properties of these two

phases are quite different. While $Cu(IO_3)_2 \cdot 2H_2O$ remains paramagnetic down to 1.4K, $CuIO_3(OH)$ shows possible antiferromagnetic ordering at 162K (Abrahams et al., 1973b). This difference in magnetic behavior is discussed in terms of the structures of these two phases.

Crystal data

Unit-cell dimensions of salesite and $Cu(IO_3)_2 \cdot 2H_2O$ were determined by the least-squares refinement of 15 reflections each, with 2θ values between 35 and 45° measured with MoKα radiation on an automatic single-crystal diffractometer (Table 1). They are in good agreement, within error limits, with those reported by Abrahams et al. (1973b).

Collection of intensity data

Small spheres of $CuIO_3(OH)$ and $Cu(IO_3)_2 \cdot 2H_2O$ with diameters 0.22 and 0.20 mm respectively were prepared. All reflections within $2\theta = 65°$ were measured on a single-crystal automatic diffractometer (Syntex PĪ), using MoKα radiation, monochromatized by reflection from a graphite "single" crystal and a scintillation counter. A variable scan rate was used in both cases, the minimum being 1°/min., and the maximum 24°/min. (50 kV, 12.5 mA). For reflections with intensities less than $0.7\sigma(i)$, where $\sigma(I)$ is the standard error of measurement de-

Table 1. Crystal data: $Cu(IO_3)_2 \cdot 2H_2O$ and salesite, $CuIO_3(OH)$ (standard deviations in parentheses)

	$Cu(IO_3)_2 \cdot 2H_2O$		Salesite $CuIO_3(OH)$ (Chuquicamata, Chile)
a (Å)	6.7280(12)	a (Å)	10.7935(17)Å
b (Å)	4.8132(9)	b (Å)	6.7075(13)
c (Å)	11.1646(16)	c (Å)	4.7813(9)
β (°)	103.34(1)	β (°)	90.0
Cell volume (Å³):	351.79(11)	Cell volume (Å³):	346.15(12)
Space group:	$P2_1/c$	Space group:	Pnra
Cell content:	$2[Cu(IO_3)_2 \cdot 2H_2O]$	Cell content:	$4[CuIO_3(OH)]$
D_m (g.cm⁻³):		D_m (g.cm⁻³):	4.77
D_c (g.cm⁻³):	4.289	D_c (g.cm⁻³):	4.900
μ(MoKα) (cm⁻¹):	121.26	μ(MoKα) (cm⁻¹):	155.44

rived from the counting statistics, I was set equal to $0.7\sigma(I)$, regardless of whether measured I was positive or negative. A total of 1284 reflections were measured for $Cu(IO_3)_2 \cdot 2H_2O$ and 715 for $CuIO_3(OH)$. The measured intensities were corrected for Lorentz, polarization, and absorption factors. No corrections were made for extinction effects.

Determination and refinement of the structures

$Cu(IO_3)_2 \cdot 2H_2O$

The cell content and the space group of $Cu(IO_3)_2 \cdot 2H_2O$, $P2_1/c$ require that the Cu atoms be

Table 2. $Cu(IO_3)_2 \cdot 2H_2O$ and salesite, $CuIO_3(OH)$: atomic positional and thermal parameters (standard deviations in parentheses)

	x	y	z	B eq.*	β_{11}†	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
				$Cu(IO_3)_2 \cdot 2H_2O$						
Cu	0	0	0	0.94(1)	40(1)	136(3)	18(1)	0(1)	5(1)	13(1)
I	0.26058(3)	0.36380(5)	0.26659(2)	0.72(1)	32(1)	113(1)	12(1)	-4(1)	4(1)	3(1)
O(1)	0.4765(4)	0.1552(7)	0.3407(3)	1.47(5)	51(5)	209(13)	31(2)	28(6)	-2(3)	9(4)
O(2)	0.0705(4)	0.1995(6)	0.3364(3)	1.20(4)	55(5)	171(11)	25(2)	-21(6)	15(3)	6(4)
O(3)	0.2101(5)	0.2078(7)	0.1151(3)	1.37(4)	71(5)	233(13)	15(2)	-31(7)	5(3)	-27(4)
O(W)	0.7791(4)	0.2329(6)	0.0311(3)	1.23(4)	70(5)	148(11)	22(2)	25(7)	4(3)	-7(4)
H(1)	0.821(8)	0.383(11)	0.073(5)	0.8(9)						
H(2)	0.655(13)	0.279(18)	-0.041(8)	2.0(1.7)						
				Salesite, $CuIO_3(OH)$						
Cu	0	0	0	1.06(1)	21(1)	52(1)	142(2)	-8(1)	-12(1)	20(2)
I	0.24486(2)	0.25	-0.00005(11)	0.79(1)	15(1)	40(1)	102(1)	0	-1(1)	0
O(1)	0.3866(4)	0.25	0.1947(11)	1.54(7)	21(3)	106(9)	187(18)	0	-19(6)	0
O(2)	0.1624(3)	0.0482(4)	0.1829(7)	1.15(4)	24(2)	54(4)	150(10)	-8(3)	-14(4)	30(7)
(OH)	0.0295(4)	0.25	-0.1967(10)	0.98(5)	24(2)	42(6)	119(13)	0	2(1)	0
H	0.026(11)	0.25	-0.394(31)	6.0(3.3)						

*Equivalent isotropic temperature factor, calculated from anisotropic temperature factors.

†Form of the anisotropic temperature factor (×10⁴): $-exp\{\sum_{i=1}^{3} \sum_{j=1}^{3} h_i h_j \beta_{ij}\}$

Table 4. Cu(IO₃)₂·2H₂O and salesite, CuIO₃(OH): interatomic distances (A) and angles (°) (standard deviations in parentheses)

$Cu(IO_3)_2 \cdot 2H_2O$

The Cu-Octahedron

Cu-O(2)	2.457(3) (x2)	O(2)-Cu-O(3)	87.2(1) (x2)
Cu-O(3)	1.951(3) (x2)	O(2)-Cu-O(W)	94.5(1) (x2)
Cu-O(W)	1.955(3) (x2)	O(2)-Cu-O(3')	92.8(1) (x2)
Mean of		O(2)-Cu-O(W')	85.5(1) (x2)
nearest 4	1.953	O(3)-Cu-O(W)	93.1(1) (x2)
Mean of 6	2.121	O(4)-Cu-O(3')	86.9(1) (x2)
O(2)-O(3)	3.063(4) (x2)		
O(2)-O(W)	3.259(4) (x2)		
O(2)-O(3')	3.211(4) (x2)		
O(2)-O(4')	3.017(4) (x2)		
O(3)-O(W)	2.837(4) (x2)		
O(4)-O(3')	2.686(4) (x2)		
Mean	3.012		

The I-Polyhedron

I-O(1)	1.802(3)	O(1)-I-O(2)	97.7(1)
I-O(2)	1.824(3)	O(2)-I-O(3)	102.7(1)
I-O(3)	1.807(3)	O(3)-I-O(1)	98.9(2)
Mean of 3	1.811	Mean	99.7
I-O(1')	2.739(3)		
I-O(2')	2.777(3)		
I-O(W')	2.930(3)		
I-O (mean of 6)	2.313		

Hydrogen bonds

H(1)-O(W)	0.87(6)	H(1)-O(W)-H(2)	110(6)
H(1)-O(2")	1.88(6)	O(4)-H(1)-O(2')	176(5)
O(W)-O(2")	2.749(4)	H(1)-O(4)-Cu	114(4)
H(2)-O(W)	1.04(9)	H(1)-O(4)-I	99(4)
H(2)-O(1')	1.60(9)	O(4)-H(2)-O(1")	176(8)
O(W)-O(1')	2.635(4)	H(2)-O(4)-Cu	119(5)
		H(2)-O(4)-I	122(5)

Salesite, CuIO₃(OH)

The Cu-Octahedron

Cu-O(1)	2.538(3) (x2)	O(1)-Cu-O(2)	86.3(1) (x2)
Cu-O(2)	1.986(3) (x2)	O(1)-Cu-O(2')	93.7(1) (x2)
Cu-(OH)	1.949(2) (x2)	O(1)-Cu-(OH)	102.3(1) (x2)
Mean of		O(1)-Cu-(OH)'	77.8(1) (x2)
nearest 4	1.968	O(2)-Cu-(OH)	85.9(2) (x2)
Mean of 6	2.158	O(2)-Cu-(OH)'	94.1(2) (x2)
		Mean	90.0
O(1)-O(2)	2.773(4) (x2)		
O(1)-O(2')	3.120(5) (x2)		
O(1)-(OH)	3.514(7) (x2)		
O(1)-(OH)'	2.853(7) (x2)		
O(2)-(OH)	2.680(5) (x2)		
O(2)-(OH)'	2.880(4) (x2)		
Mean	2.970		
Cu-Cu	3.354(1)		
Cu-I	3.130(1)		

The I-Polyhedron

I-O(1)	1.791(4)	O(1)-I-O(2)	99.6(2) (x2)
I-O(2)	1.840(3) (x2)	O(2)-I-O(2')	94.7(2)
Mean	1.824	Mean	97.9
O(1)-O(2)	2.773(4) (x2)		
O(2)-O(2")	2.707(6)		
Mean	2.751		
I-(OH)	2.507(4)		
I-O(2)	2.702(3) (x2)		
I-O(mean of 6)	2.231		

Hydrogen bond

H-(OH)	0.94(2)	(OH)-H...O(1)	135.7(10.0)
H-O(1)	2.08(1)	H-(OH)-Cu	118.5(1.5)
(OH)-O(1)	2.837(7)		

in a two-fold special position, which were assigned to (0,0,0) and (0,1/2,1/2). The positions of four equivalent iodine atoms were determined from the three-dimensional Patterson synthesis. A refinement of the structure with contributions from Cu and I atoms yielded an R factor of 0.15. A difference Fourier synthesis indicated the positions of four different oxygen atoms. Inclusion of these oxygen positions in the refinement of the structure, using isotropic temperature factors, reduced the R factor to 0.069.

Two cycles of least-squares refinement of the structure, using anisotropic temperature factors based on all non-hydrogen atoms, yielded an R factor of 0.026. A difference Fourier synthesis calculated at this stage clearly showed the positions of the two different hydrogen atoms. Two cycles of refinement using anisotropic temperature factors for all atoms, except hydrogens for which isotropic temperature factors were used, yielded an R factor of 0.025 for 1284 reflections.

CuIO₃(OH)

A structure factor calculation for $CuIO_3(OH)$ based on the atomic coordinates of Ghose (1962) yielded an R factor of 0.091 for 715 reflections. Eight lower-angle reflections showed large differences between observed and calculated structure factors. These reflections were believed to be affected by extinction and were excluded from the refinement. Three cycles of refinement using anisotropic temperature factors for Cu, I, and O yielded an R factor of 0.028. A difference Fourier synthesis calculated at this stage showed the hydrogen position clearly. However, attempts to refine the hydrogen position using isotropic temperature factors failed because of an interaction of the temperature factor with the z parameter. The refinement was terminated when the R factor for 707 unrejected reflections showed a minimum value of 0.026. The R factor for all reflections at this stage was 0.031. The hydrogen position is tentative in view of the lack of refinement.

For the refinement of both structures, scattering factors for Cu, I, O, and H were taken from Cromer and Mann (1968). Anomalous dispersion corrections were made according to Cromer and Liberman (1970). The full-matrix least-squares program RFINE (Finger, 1969) was used for the refinement of both structures. The observed structure factors (F_o's) were weighted according to the formula $F_o/\sigma^2(F_o)$, where $\sigma(F_o)$ is the standard deviation in the measurement of F_o, as derived from the counting statistics. The atomic parameters for both phases are listed in Table

2, and the observed and calculated structure factors in Table 3.[2] Table 4 lists the bond lengths and angles, and Table 5 lists the ellipsoids of thermal vibration. The average standard deviations in Cu–O, I–O, and O–H bond lengths in both structures are 0.003, 0.003, and 0.06A and in O–Cu–O, O–I–O, and H–O–H angles 0.1, 0.1, and 6.0° respectively.

Description of the structures

$Cu(IO_3)_2 \cdot 2H_2O$

The structure of $Cu(IO_3)_2 \cdot 2H_2O$ consists of corner-sharing $[CuO_4(H_2O)_2]$ octahedra and trigonal pyramidal $[IO_3]$ groups.

Stereochemistry of the cupric ion. The isolated $[CuO_4(H_2O)_2]$ octahedron is in fact a tetragonal bipyramid and shows the usual Jahn-Teller type distortion (Fig. 1). Two oxygen atoms and two water molecules form a square plane around the copper atom [Cu–O 1.951 and Cu–O(W) 1.955A], while two further oxygen atoms (Cu–O 2.457A) complete the octahedron. The Cu octahedron has the point-group symmetry $\bar{1}$. The water molecules occur in *trans*-configuration within the square plane. The Cu–O–H angles are 114 and 119°.

Stereochemistry of the iodine (V) ion. The iodine atom is closely bonded to three oxygen atoms at distances of 1.802, 1.824, and 1.807A (Fig. 1). The $[IO_3]$ group is a trigonal pyramid, with O–I–O angles of 97.7, 102.7, and 98.9°. It deviates slightly but significantly from the highest possible point-group symmetry $3m$. The iodine atom is further bonded to two oxygen atoms and a water molecule at distances of 2.739, 2.777, and 2.930A respectively. The $[IO_6(H_2O)]$ polyhedron can be described as a highly distorted octahedron or a trigonal anti-prism (Fig. 3a).

Configuration of the H_2O molecule and hydrogen bonding. The water molecule forms a common corner of both the Cu- and I-octahedra. The O–H distances are 0.87 and 1.04A, and the H–O–H angle is 110°, which is well within the limit of 102.5–115.5° found in crystalline hydrates (Falk and Knop, 1973): H(1) is hydrogen bonded to O(2″), which is bridging the Cu- and I-octahedra. The H(1)···O(2″) distance is 1.88A, and the O(W)–H(1)···O(2″) angle is 176° (Fig. 1). H(2) is hydrogen bonded to O(1″), which is a non-bridging corner of the iodine-polyhedron. The

Table 5. $Cu(IO_3)_2 \cdot 2H_2O$ and salesite, $CuIO_3(OH)$: ellipsoids of thermal vibration (standard deviations in parentheses)

Atom	Axis, r_i	Root mean square displacement (Å)	Angle (°) with respect to +a	+b	+c
		$Cu(IO_3)_2 \cdot 2H_2O$			
Cu	1	0.093	168(18)	81(9)	69(18)
	2	0.096	116(16)	112(7)	134(12)
	3	0.133	97(1)	31(2)	117(2)
I	1	0.082	148(36)	80(10)	47(33)
	2	0.084	54(36)	88(4)	49(36)
	3	0.116	86(1)	7(1)	97(1)
O(1)	1	0.093	160(6)	109(6)	71(6)
	2	0.146	115(14)	91(12)	142(14)
	3	0.161	105(12)	15(12)	86(14)
O(2)	1	0.092	135(10)	74(6)	118(8)
	2	0.125	61(24)	90(16)	164(24)
	3	0.147	72(8)	24(10)	79(7)
O(3)	1	0.078	98(6)	69(3)	22(4)
	2	0.124	35(7)	98(5)	69(7)
	3	0.175	77(4)	18(4)	105(3)
O(4)	1	0.110	142(195)	126(198)	87(158)
	2	0.112	91(124)	111(101)	154(12)
	3	0.148	124(10)	49(8)	111(8)
		$CuIO_3(OH)$			
Cu	1	0.095	129(9)	40(9)	94(5)
	2	0.105	51(7)	63(5)	130(6)
	3	0.142	63(3)	63(3)	40(2)
I	1	0.095	176(19)	90	86(19)
	2	0.095	90	180	90
	3	0.109	86(4)	90	4(4)
O(1)	1	0.101	156(17)	90	66(17)
	2	0.155	114(273)	90	156(273)
	3	0.156	90	0	90
O(2)	1	0.096	100(20)	29(16)	117(10)
	2	0.108	30(33)	95(30)	119(34)
	3	0.151	62(7)	61(7)	42(4)
(OH)	1	0.098	90	0	90
	2	0.115	131(99)	90	138(99)
	3	0.120	138(101)	90	49(101)

H(2)···O(1″) distance is 2.04A, and the O(W)–H(2)–O(1″) angle is 176°. Hence, both hydrogen bonds are nearly straight bonds, deviating very slightly from O(W)–O(2″) and O(W)–O(1″) directions. Although the H–O–H angle is close to the ideal tetrahedral angle, other bonds around O(W), namely O(W)–Cu and O(W)···I deviate considerably from an ideal tetrahedral configuration with respect to the O(W)–H(1) and O(W)–H(2) bonds (Table 3). In fact the H(2)–O(W)–Cu and H(2)–O(W)–I angles are close to being trigonal rather than tetrahedral.

The three-dimensional framework. The $[IO_6(H_2O)]$ polyhedron shares four corners with adjacent I polyhedra. An open polyhedral sheet parallel to the (001) plane is thereby formed (Fig. 3a). Isolated $[CuO_4(H_2O)_2]$ octahedra bind these sheets together in a three-dimensional framework by sharing two sets of octahedral edges with two iodine-polyhedral sheets
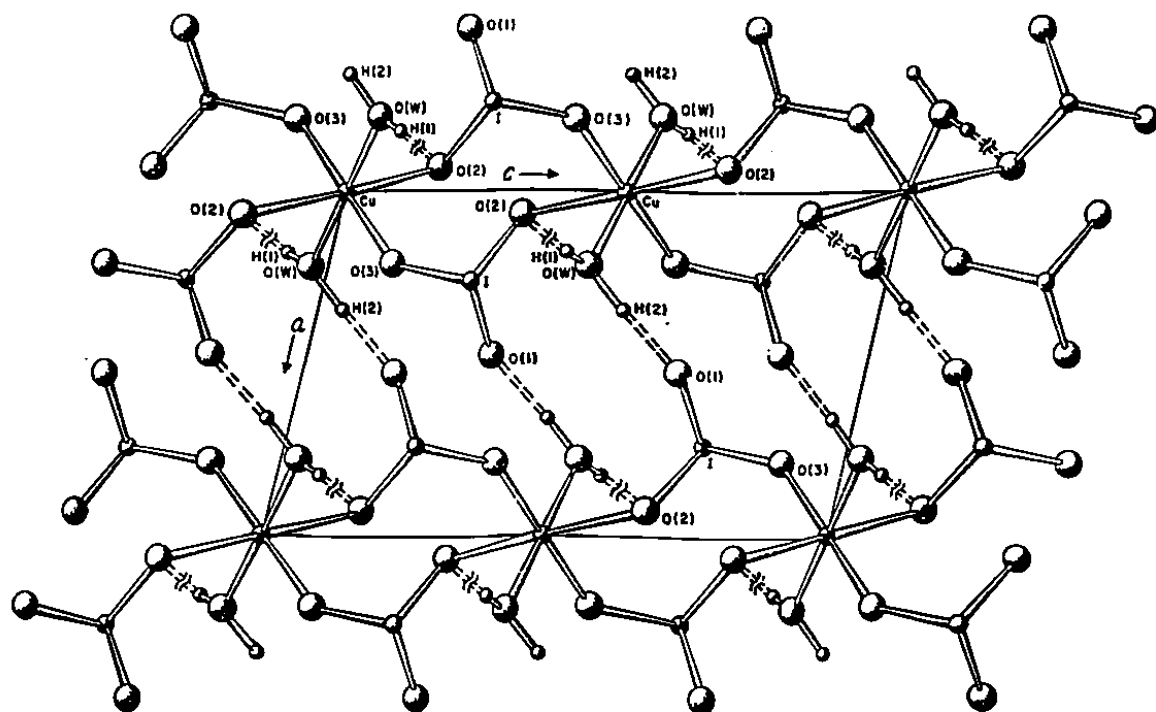
Fig. 1. A view of the $Cu(IO_3)_2 \cdot 2H_2O$ structure down the b axis. Note the hydrogen bonds (shown by broken lines).
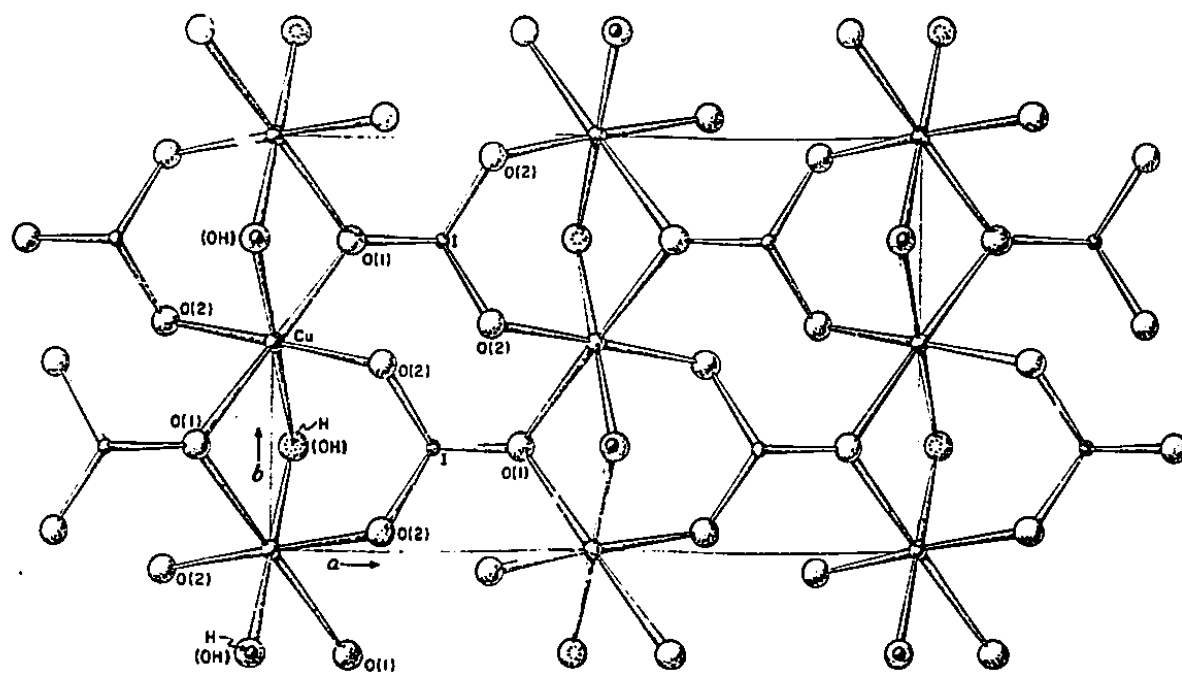
Fig. 2. A view of salesite, $CuIO_3(OH)$ structure, down the c axis.

on either side. One of the hydrogen bonds [O(W)–H(1)···O(2″)] binds two isolated Cu octahedra together, whereas the other [O(W)–H(2)–O(1″)] binds a Cu octahedron to an I polyhedron.

Salesite, CuIO$_3$(OH)

The structure of salesite consists of chains of edge-sharing [CuO$_4$(OH)$_2$] octahedra and corner-sharing trigonal pyramidal [IO$_3$] groups (Ghose, 1962).

Stereochemistry of the cupric ion. The [CuO$_4$(OH)$_2$] polyhedron is a tetragonal bipyramid with the point group symmetry $\bar{1}$. Two oxygen atoms and two (OH) ions form a square plane around the Cu atom [Cu–O 1.986A, Cu–(OH) 1.949A]; two further oxygen atoms (Cu–O 2.538A) complete the bipyramid. The (OH) ions occur in a *trans*-configuration within the square plane.

Stereochemistry of the iodine (V) ion. The iodine atom is closely bonded to three oxygen atoms in the form of a trigonal pyramid. The [IO$_3$] group, with the point group symmetry *m*, deviates significantly from the highest possible symmetry *3m*. Thus, the I–O(1)

bond (1.791A) is significantly shorter than the two I–O(2) bonds (1.804A), and one of the O–I–O angles [O(2)–I–O(2′) 94.7°] is significantly smaller than the other two [O(1)–I–O(2) 99.6°]. The iodine atom is further bonded to the (OH) ion at 2.507A and two oxygen atoms at 2.702A. The [IO$_3$(OH)] polyhedron can be described as a highly distorted octahedron or a trigonal antiprism (Fig. 3b).

The weak I–(OH) bond (2.507A) is the shortest extra-pyramidal bond recorded so far, the only other analogous case being Ce(IO$_3$)$_4$·H$_2$O (Ibers, 1956), where an I–O contact of 2.51A has been reported. The (OH) group is charge-deficient, because it is bonded to two Cu atoms at 2.539A in addition to the H atom at 0.94A. Hence the I–(OH) bond must be significant, albeit weak.

Hydrogen bond. The (OH) group is hydrogen-bonded to O(1″), an oxygen corner belonging to an adjacent Cu-octahedral chain (see below) separated by the *c* dimension. The O–H and H···O distances are 0.94 and 2.08A. The O–H···O angle is 136°. Hence, the hydrogen bond is a strongly-bent bond.
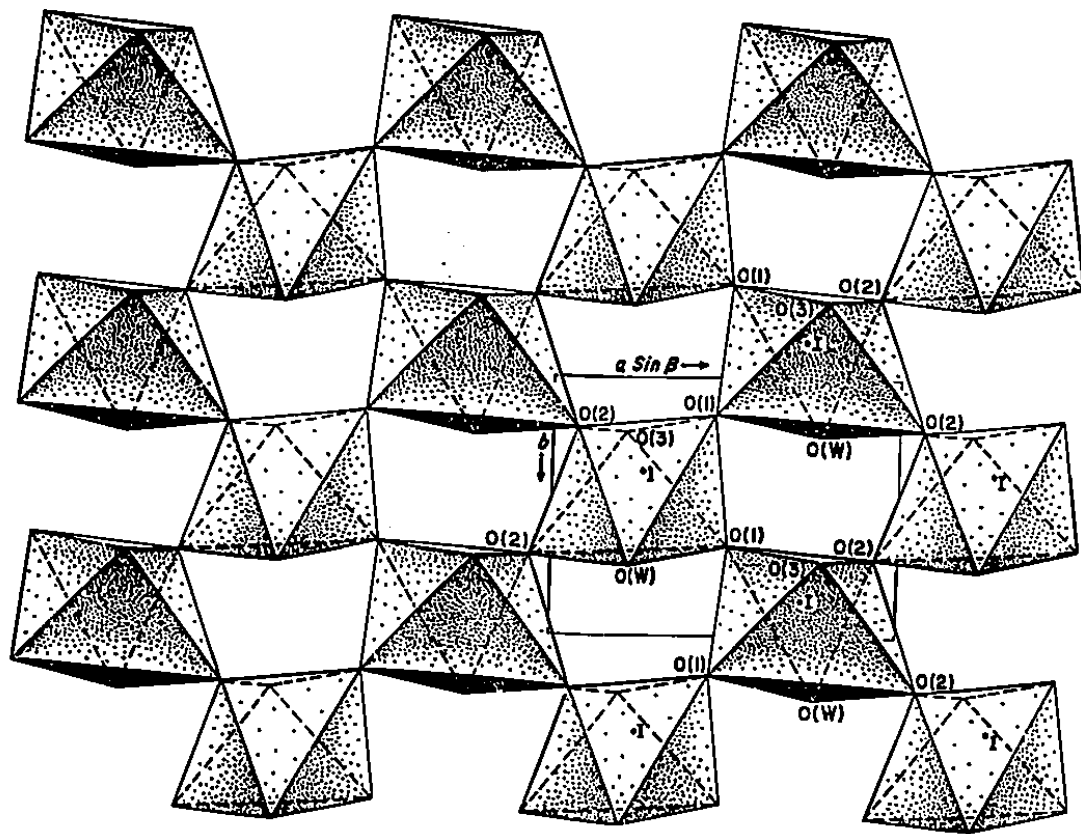
Fig. 3a. Linkage of the I-octahedra in Cu(IO$_3$)$_2$·2H$_2$O, viewed down the *c* axis.

The three-dimensional framework. The $[IO_5(OH)]$ octahedron shares four oxygen corners with four adjacent I octahedra to form an open octahedral sheet parallel to the (100) plane (Fig. 3b). The $[CuO_4(OH)_2]$ octahedron shares two opposite edges with two adjacent Cu octahedra to form octahedral chains parallel to the *b* axis (Fig. 2). Adjacent Cu-octahedral chains are separated from each other by $1/2a + 1/2c$. Each Cu octahedron shares a set of two edges with two sets of I octahedra belonging to the two I-polyhedral sheets occurring on either side of the octahedron. In this fashion, the Cu-octahedral chains and the I-polyhedral sheets are connected together in a three-dimensional framework.

A comparison of the structural schemes of $CuIO_3(OH)$ and $Cu(IO_3)_2 \cdot 2H_2O$

In both structures, the I octahedra share corners to form an open sheet structure (Figs. 3a, b), which are connected by Cu octahedra. In $Cu(IO_3)_2 \cdot 2H_2O$ with the Cu:I ratio 1:2, the $[CuO_4(H_2O)_2]$ octahedron is isolated; in $CuIO_3(OH)$, on the other hand, with

Cu:I ratio 1:1, the $[CuO_4(OH)_2]$ octahedra form infinite chains. Topologically, the $Cu(IO_3)_2 \cdot 2H_2O$ structure can be derived from that of $Cu(IO_3)(OH)$, by removing half of the Cu octahedra, specifically those which occur on either side of the Cu octahedron occurring at (0,0,0) (Figs. 1 and 2).

The reason for the deviation from orthorhombic symmetry in $Cu(IO_3)_2 \cdot 2H_2O$ probably lies in the Cu-octahedral edges shared with the I polyhedra; in $CuIO_3(OH)$, the edges of the Cu square plane are shared, whereas in $Cu(IO_3)_2 \cdot 2H_2O$ the bipyramidal edges are shared.

Models of magnetic structures for $Cu(IO_3)_2 \cdot 2H_2O$ and $CuIO_3(OH)$

$Cu(IO_3)_2 \cdot 2H_2O$ is a simple paramagnet down to 1.4 K; its paramagnetic moment of $1.72\mu_B$ is exactly that predicted for spin-only Cu^{2+}. The inverse magnetic susceptibility of salesite shows an inflection at 162 K, which may indicate antiferromagnetic ordering. Its high-temperature paramagnetism, with a Curie constant of 0.62 cm^3 K mole^{-1}, corresponds to a
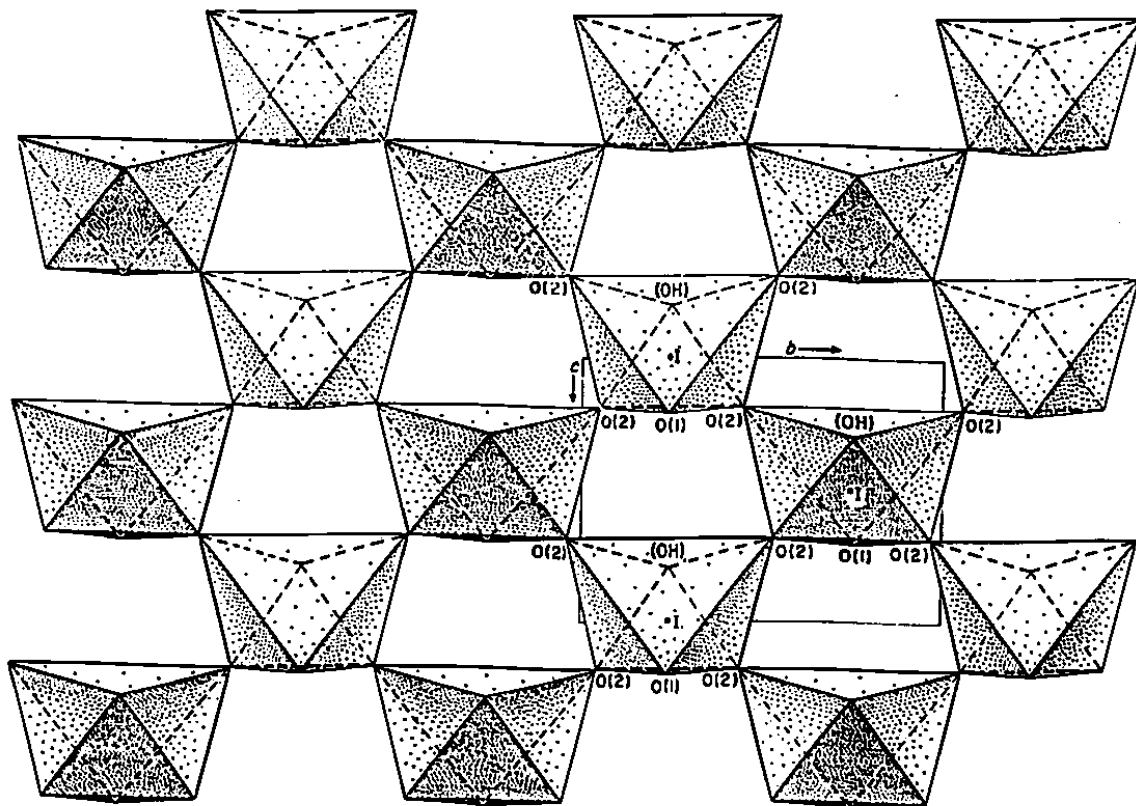
Fig. 3b. Linkage of the I-octahedra in salesite, $CuIO_3(OH)$, viewed down the *a* axis.

moment of $2.23\mu_B$; extrapolation gives a Curie temperature of -340 K, corresponding to very strong antiferromagnetic Cu–Cu interactions (Abrahams *et al.*, 1973b).

In $Cu(IO_3)_2 \cdot 2H_2O$, the Cu atoms occur in isolated octahedra, the nearest Cu–Cu distance being 6.508A. A possible magnetic interaction between two neighboring Cu atoms involves a long super-exchange path: Cu–O(3)–I–O(2)–Cu along [011]. Cu–O(2) is the long (2.46A) bond, where the covalency factor is very small. A larger Cu–Cu separation, along with the long Cu–O bond involved in the exchange path, may account for a lack of magnetic ordering in $Cu(IO_3)_2 \cdot 2H_2O$ down to 1.4 K. It is quite possible, however, that a transition to a magnetically-ordered state exists below this temperature.

$Ni(IO_3)_2 \cdot 2H_2O$, on the other hand, is weakly ferromagnetic below 3 K, which involves interaction between two closest Ni atoms, 5.636A apart, through an exchange path of the type Ni–O–I–O–Ni (Abrahams *et al.*, 1973a).

The situation in $Cu(IO_3)OH$ is quite different, where the Cu atoms occur in octahedral chains parallel to the *b* axis, the Cu–Cu separation within the chain being 3.354A. Of the two short exchange paths, Cu–(OH)–Cu is the shortest, with Cu–(OH) distance 1.949A; the next shortest path is Cu–O(1)–Cu, with Cu–O(1) distance 2.538A. A longer path involves O(2) and I, namely Cu–O(2)–I–O(2)–Cu. The interaction between the neighboring chains of Cu-atoms involves a long exchange path Cu–O(2)–I–O(1)–Cu.

We may conceive of two possible models for antiferromagnetic ordering in $Cu IO_3(OH)$: (1) within any single chain the spins are alternately up and down either parallel or normal to the *b* axis; (2) the spins are collinear in each chain, but antiparallel with respect to neighboring chains. In view of the long exchange path involved in terms of two neighboring Cu chains, the first model is to be preferred.

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The following material did not appear in the original publication.

Table 3a. Cu(IO₃)₂.2H₂O : Observed and Calculated structure Factors

(Ghose & Wan, 1977)

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	0	2	117.338	125.776	-125.694	-4.544	-8.438	-22.0651	1.0000
0	0	4	153.884	167.028	166.787	8.964	-13.144	-24.1879	1.0000 *
0	0	6	46.554	45.601	-45.485	-3.259	.952	2.2532	1.0000
0	0	8	114.404	117.196	117.000	6.773	-2.792	-3.4369	1.0000
0	0	10	36.957	36.263	-36.246	-1.132	.694	2.3397	1.0000
0	0	12	48.343	47.855	47.698	3.876	.488	1.2525	1.0000
0	0	14	2.499*	2.015	-1.660	1.143	.484	.2710	1.0000 **
0	0	16	3.072*	1.212	-.567	1.071	1.860	1.1295	1.0000 **
0	1	1	60.579	58.644	58.568	2.978	1.934	4.4050	1.0000
0	1	2	37.991	34.895	34.877	1.134	3.095	8.3336	1.0000
0	1	3	33.579	32.093	32.076	1.037	1.486	4.2305	1.0000
0	1	4	100.037	96.267	-96.243	-2.138	3.769	6.4179	1.0000
0	1	5	82.702	81.514	81.382	4.646	1.188	1.0130	1.0000
0	1	6	59.989	56.903	56.819	3.090	3.086	5.9394	1.0000
0	1	7	27.612	26.140	-26.132	-.654	1.472	7.2496	1.0000
0	1	8	54.253	52.510	-52.381	-3.689	1.743	3.4386	1.0000
0	1	9	91.960	93.817	93.651	5.590	-1.857	-2.0756	1.0000
0	1	10	43.833	43.966	43.763	4.227	-.133	-.3735	1.0000
0	1	11	35.407	35.058	-35.017	-1.694	.349	1.5514	1.0000
0	1	12	69.530	71.873	-71.745	-4.291	-2.343	-3.7670	1.0000
0	1	13	58.897	60.831	60.573	5.603	-1.934	-4.0818	1.0000
0	1	14	59.691	62.274	62.123	4.344	-2.583	-5.2287	1.0000
0	1	15	25.589	26.879	-26.808	-1.944	-1.290	-4.2213	1.0000
0	1	16	41.570	43.740	-43.563	-3.922	-2.170	-7.6515	1.0000
0	2	0	39.028	40.286	-40.261	1.427	-1.258	-2.0654	1.0000
0	2	1	117.532	120.621	120.428	6.826	-3.089	-5.2425	1.0000
0	2	2	53.840	52.861	52.756	3.324	.979	2.1923	1.0000
0	2	3	143.061	147.451	-147.311	-6.422	-4.390	-6.8556	1.0000
0	2	4	34.188	33.613	33.581	1.473	.575	1.7854	1.0000
0	2	5	130.375	134.823	134.696	5.829	-4.447	-6.1072	1.0000
0	2	6	32.646	32.235	32.098	2.974	.411	1.4863	1.0000
0	2	7	91.675	93.011	-92.889	-4.752	-1.336	-1.6011	1.0000
0	2	8	13.814	13.790	13.699	1.583	.024	.0804	1.0000
0	2	9	52.853	52.656	52.519	3.792	.198	.4526	1.0000
0	2	10	32.049	31.774	31.686	2.372	.275	1.2132	1.0000
0	2	11	28.917	29.885	-29.792	-2.348	-.968	-3.8892	1.0000
0	2	12	16.912	17.081	16.998	1.684	-.169	-.5213	1.0000
0	2	13	11.983	12.877	12.807	1.333	-.894	-2.1052	1.0000
0	2	14	21.287	21.527	21.462	1.675	-.240	-.7411	1.0000
0	2	15	8.056	.491	.485	.077	7.565	11.7125	1.0000
0	3	1	25.792	25.848	25.795	1.659	-.056	-.3224	1.0000
0	3	2	22.915	22.121	22.108	.747	.795	4.2162	1.0000
0	3	3	45.758	45.523	45.356	3.900	.235	.6447	1.0000
0	3	4	12.764	11.805	-11.733	-1.307	.959	3.5894	1.0000
0	3	5	8.148	7.917	-7.898	-.545	.231	.5588	1.0000
0	3	6	37.473	36.719	36.662	2.045	.754	2.7093	1.0000
0	3	7	85.714	87.679	87.503	5.552	-1.966	-2.1445	1.0000
0	3	8	34.214	34.033	-33.958	-2.266	.181	.7592	1.0000
0	3	9	52.630	53.254	-53.212	-2.126	-.624	-1.3322	1.0000
0	3	10	47.628	48.860	48.778	2.831	-1.232	-3.3173	1.0000
0	3	11	76.658	78.858	78.615	6.187	-2.200	-3.4452	1.0000
0	3	12	27.389	27.660	-27.532	-2.657	-.271	-.9741	1.0000
0	3	13	28.052	29.975	-29.848	-2.762	-1.924	-5.6122	1.0000

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	3	14	31.094	32.505	32.369	2.970	-1.411	-4.8181	1.0000
0	4	0	62.653	63.505	-63.393	-3.772	-.851	-1.6441	1.0000
0	4	1	10.748	10.628	-10.500	-1.646	.119	.3605	1.0000
0	4	2	125.995	129.311	129.083	7.684	-3.316	-3.7604	1.0000
0	4	3	35.561	35.158	35.120	1.630	.403	1.5193	1.0000
0	4	4	56.729	55.886	-55.792	-3.239	.843	1.7794	1.0000
0	4	5	31.347	30.867	-30.840	-1.276	.480	2.2057	1.0000
0	4	6	87.653	88.282	88.047	6.444	-.629	-.9049	1.0000
0	4	7	23.181	22.671	22.636	-1.251	.510	2.0055	1.0000
0	4	8	29.790	30.232	-30.177	-1.823	-.442	-1.8035	1.0000
0	4	9	6.364	3.544	-3.486	-.637	2.820	4.3532	1.0000
0	4	10	51.210	51.212	51.027	4.350	-.002	-.0048	1.0000
0	4	11	6.671	6.289	6.254	.654	.383	.5533	1.0000
0	4	12	11.536	10.434	-10.434	.001	1.102	2.4588	1.0000
0	4	13	4.368*	3.267	3.267	.070	1.100	.9777	1.0000
0	5	1	20.028	19.214	19.149	1.579	.814	3.0682	1.0000
0	5	2	23.302	22.137	-22.115	-.990	1.164	4.6783	1.0000
0	5	3	33.830	33.729	33.641	2.429	.101	.4345	1.0000
0	5	4	29.316	28.907	28.831	2.090	.409	1.6812	1.0000
0	5	5	2.283*	2.172	-2.061	-.687	.111	.0684	1.0000
0	5	6	38.042	38.834	-38.741	-2.688	-.793	-3.2566	1.0000
0	5	7	31.168	31.324	31.178	3.024	-.156	-.5981	1.0000
0	5	8	38.891	38.963	38.795	3.614	-.072	-.2843	1.0000
0	5	9	3.431*	.432	-.430	-.036	2.999	2.3185	1.0000
0	5	10	44.852	45.431	-45.284	-3.650	-.579	-2.1981	1.0000
0	5	11	28.353	29.053	28.874	3.219	-.699	-2.3168	1.0000
0	6	0	40.419	40.374	40.219	3.531	.045	.1796	1.0000
0	6	1	59.730	60.653	60.497	-4.348	-.924	-2.0863	1.0000
0	6	2	16.458	16.177	-16.173	-.374	.282	.8141	1.0000
0	6	3	48.563	48.633	48.449	4.222	-.070	-.2167	1.0000
0	6	4	29.570	29.700	29.521	3.259	-.130	-.4704	1.0000
0	6	5	43.432	43.566	-43.416	-3.609	-.133	-.5167	1.0000
0	6	6	2.534*	2.783	-2.783	-.015	-.249	-.1375	1.0000
0	6	7	36.179	37.048	36.902	3.287	-.869	-3.1257	1.0000
0	6	8	23.781	23.354	23.216	2.532	.427	1.3405	1.0000
0	6	9	28.302	28.340	-28.253	-2.229	-.038	-.1232	1.0000
0	7	1	11.383	11.256	11.124	1.721	.127	.2605	1.0000
0	7	2	3.480**	.898	.883	-.165	2.582	1.8892	1.0000
0	7	3	4.807*	5.079	-5.079	.054	-.273	-.2643	1.0000
0	7	1	5.057*	4.827	4.800	.504	.231	.2302	1.0000
1	0	-16	75.026	72.561	72.219	7.043	2.465	3.8932	1.0000
1	0	-14	68.946	68.308	-68.195	-3.929	.637	1.0853	1.0000
1	0	-12	103.542	102.372	102.084	7.685	1.170	1.1218	1.0000
1	0	-10	57.336	55.498	-55.403	-3.246	1.839	3.3385	1.0000
1	0	-8	99.543	95.649	95.396	6.954	3.894	4.8587	1.0000
1	0	-6	72.373	66.207	-66.193	-1.318	6.166	8.9869	1.0000
1	0	-4	104.964	104.224	104.109	4.904	.740	1.3566	1.0000
1	0	-2	35.330	32.600	32.566	1.488	2.730	8.2443	1.0000
1	0	0	52.191	52.630	52.591	2.042	-.439	-1.1829	1.0000
1	0	2	103.583	104.939	104.845	4.449	-1.357	-2.9422	1.0000
1	0	4	32.439	28.681	-28.669	-.845	3.758	12.7565	1.0000
1	0	6	146.493	147.835	147.681	6.749	-1.342	-1.8709	1.0000
1	0	8	42.495	40.157	-40.046	-2.987	2.339	6.8347	1.0000

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	0	10	111.011	111.014	110.740	7.792	-.002	-.0026	1.0000
1	0	12	63.493	63.842	-63.721	-3.924	-.349	-.6330	1.0000
1	0	14	87.148	88.281	87.969	7.418	-1.133	-1.6561	1.0000
1	1	-16	5.163 *	2.589	-2.587	.096	2.574	2.6799 **	1.0000
1	1	-15	16.797	16.066	15.943	1.987	.731	1.9771	1.0000
1	1	-14	8.000	7.671	7.642	.669	.329	.5530	1.0000
1	1	-13	5.048	3.475	3.394	.746	1.573	1.9275	1.0000
1	1	-12	27.484	26.423	-26.364	-1.767	1.061	4.2654	1.0000
1	1	-11	51.913	50.320	50.163	3.981	1.593	3.7842	1.0000
1	1	-10	44.040	41.945	41.862	2.635	2.095	5.9325	1.0000
1	1	-9	21.276	20.114	-20.105	-.612	1.162	5.0011	1.0000
1	1	-8	74.488	73.190	-73.099	-3.659	1.298	2.1960	1.0000
1	1	-7	104.388	102.530	102.366	5.811	1.857	2.4169	1.0000
1	1	-6	89.801	88.579	88.472	4.362	1.222	1.7343	1.0000
1	1	-5	57.710	52.981	-52.953	-1.720	4.729	10.0959	1.0000
1	1	-4	66.225	65.858	-65.667	-5.012	.367	.6128	1.0000
1	1	-3	148.760	153.545	153.387	6.963	-4.784	-9.0165	1.0000
1	1	-2	161.499	169.066	168.983	5.311	-7.567	-15.6068	1.0000
1	1	-1	53.832	52.915	-52.870	-2.193	.917	1.9136	1.0000
1	1	0	139.526	146.283	-146.184	-5.382	-6.757	-14.9513	1.0000
1	1	1	151.834	161.636	161.481	7.089	-9.802	-20.6036	1.0000
1	1	2	138.684	143.000	142.906	5.168	-4.316	-8.3048	1.0000
1	1	3	67.268	63.155	-63.127	-1.858	4.113	7.0035	1.0000
1	1	4	71.899	70.580	-70.427	-4.638	1.319	2.0716	1.0000
1	1	5	121.931	123.157	123.004	6.148	-1.226	-1.7966	1.0000
1	1	6	83.415	81.177	81.079	3.982	2.238	2.9690	1.0000
1	1	7	19.649	18.531	-18.513	-.830	1.118	5.0495	1.0000
1	1	8	60.388	59.740	-59.664	-3.020	.648	1.2609	1.0000
1	1	9	62.447	61.249	61.089	4.426	1.197	2.1885	1.0000
1	1	10	23.711	23.491	23.393	2.143	.220	.8981	1.0000
1	1	11	2.827 *	.539	-.664	.539	1.972	1.4966 **	1.0000
1	1	12	16.918	17.003	-16.972	-1.036	-.086	-.2641 **	1.0000
1	1	13	25.400	24.596	24.477	2.417	.805	2.8192	1.0000
1	1	14	4.316 *	3.234	3.227	.212	1.082	.9955	1.0000
1	1	15	15.838	15.138	15.030	1.807	.700	1.7795	1.0000
1	2	-16	7.678	6.916	6.868	.810	.762	1.0845	1.0000
1	2	-15	55.499	56.655	56.418	5.184	-1.156	-2.8463	1.0000
1	2	-14	33.872	32.211	32.114	2.489	1.661	6.0939	1.0000
1	2	-13	67.189	68.241	-68.013	-5.570	-1.051	-1.8066	1.0000
1	2	-12	8.781	5.841	5.742	1.070	2.940	5.8649	1.0000
1	2	-11	78.643	78.244	78.073	5.171	.399	.5429	1.0000
1	2	-10	35.716	34.384	34.272	2.777	1.332	4.7908	1.0000
1	2	-9	86.213	86.556	-86.417	-4.893	-.343	-.3637	1.0000
1	2	-8	33.731	32.959	32.926	1.477	.772	2.7031	1.0000
1	2	-7	69.301	68.853	68.741	3.915	.448	.7510	1.0000
1	2	-6	58.736	57.927	57.860	2.783	.809	1.4175	1.0000
1	2	-5	44.826	44.264	-44.163	-2.987	.562	1.4560	1.0000
1	2	-4	38.838	37.421	37.369	1.979	1.417	4.2084	1.0000
1	2	-3	36.851	34.608	34.570	1.615	2.243	7.1259	1.0000
1	2	-2	42.973	43.762	43.690	2.520	-.789	-2.0739	1.0000
1	2	-1	13.203	11.253	-11.250	-.272	1.950	10.0562	1.0000
1	2	0	31.083	31.144	31.046	2.464	-.060	-.2377	1.0000
1	2	1	21.205	21.010	-20.979	-1.145	.194	1.2078	1.0000

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	2	2	38.448	38.029	37.972	2.078	.419	1.3551	1.0000	
1	2	3	55.982	53.375	53.315	2.530	2.607	5.3164	1.0000	
1	2	4	49.714	48.773	48.693	2.794	.941	2.1970	1.0000	
1	2	5	66.139	63.316	-63.214	-3.602	2.823	5.1596	1.0000	
1	2	6	3.817*	2.450	-1.864	1.590	1.367	1.7137	1.0000	**
1	2	7	81.913	82.962	82.831	4.659	-1.150	-1.3199	1.0000	
1	2	8	23.958	23.239	23.062	2.862	-.719	3.1195	1.0000	
1	2	9	83.845	84.208	-84.053	-5.108	-.363	-.5307	1.0000	
1	2	10	10.783	10.006	9.937	1.174	.777	1.9566	1.0000	
1	2	11	72.576	74.478	74.267	5.611	-1.902	-3.0760	1.0000	
1	2	12	27.375	27.060	26.931	2.635	.315	1.1617	1.0000	
1	2	13	62.840	64.241	-64.017	-5.367	-1.401	-2.5951	1.0000	
1	2	14	4.669*	1.719	1.466	.896	2.951	2.8850	1.0000	**
1	2	15	56.321	58.854	58.615	5.301	-2.533	-5.7690	1.0000	
1	3	-15	11.482	10.795	10.718	1.285	.686	1.3642	1.0000	
1	3	-14	10.517	9.159	9.149	.438	1.358	2.6604	1.0000	
1	3	-13	28.734	28.752	28.609	2.873	-.018	-.0643	1.0000	
1	3	-12	18.001	17.606	-17.550	-1.395	.395	1.2064	1.0000	
1	3	-11	9.650	10.613	-10.606	-.386	-.963	-2.0173	1.0000	
1	3	-10	24.484	23.994	23.933	1.704	.490	1.8841	1.0000	
1	3	-9	68.080	67.967	67.772	5.143	.114	.1929	1.0000	
1	3	-8	32.028	31.747	-31.644	-2.557	.281	1.2899	1.0000	
1	3	-7	39.959	39.030	-38.978	-2.017	.930	2.8227	1.0000	
1	3	-6	43.480	42.450	42.356	2.823	1.030	2.9013	1.0000	
1	3	-5	121.227	126.199	126.008	6.935	-4.972	-5.9071	1.0000	
1	3	-4	85.628	85.406	-85.339	-3.358	.222	.2745	1.0000	
1	3	-3	67.625	67.907	-67.838	-3.066	-.282	-.5021	1.0000	
1	3	-2	58.893	60.347	60.247	3.465	-1.453	-2.6131	1.0000	
1	3	-1	120.301	125.209	124.972	7.704	-4.908	-6.5749	1.0000	
1	3	0	70.327	69.446	-69.355	-3.539	.882	1.6558	1.0000	
1	3	1	61.521	62.326	-62.246	-3.159	-.805	-1.4669	1.0000	
1	3	2	49.293	48.743	48.622	3.433	.550	1.3657	1.0000	
1	3	3	127.329	130.745	130.547	7.203	-3.416	-4.3221	1.0000	
1	3	4	61.590	61.040	-60.965	-3.029	.550	1.1096	1.0000	
1	3	5	57.355	56.002	-55.956	-2.259	1.353	2.6599	1.0000	
1	3	6	41.641	41.303	41.211	2.747	.338	.9997	1.0000	
1	3	7	71.956	72.718	72.503	5.590	-.762	-1.1316	1.0000	
1	3	8	31.283	31.148	-31.085	-1.978	.135	.5899	1.0000	
1	3	9	16.894	17.478	-17.465	-.678	-.584	-1.9112	1.0000	
1	3	10	30.123	30.219	30.175	1.632	-.097	-.3857	1.0000	
1	3	11	37.623	38.332	38.185	3.361	-.709	-2.8301	1.0000	
1	3	12	5.484	5.200	-5.153	-.699	.283	.3331	1.0000	
1	3	13	8.726	6.224	6.134	1.058	2.502	4.2858	1.0000	
1	3	14	4.959*	2.261	2.221	.421	2.697	2.6952	1.0000	**
1	4	-14	57.155	59.111	58.801	6.045	-1.956	-4.3636	1.0000	
1	4	-13	10.693	9.751	9.680	1.171	.942	1.8453	1.0000	
1	4	-12	39.879	40.332	-40.222	-2.972	-.453	-1.6953	1.0000	
1	4	-11	18.930	18.891	-18.828	-1.547	.039	.1195	1.0000	
1	4	-10	64.688	65.817	65.542	6.009	-1.128	-1.9579	1.0000	
1	4	-9	22.906	22.490	22.464	1.079	.416	1.4970	1.0000	
1	4	-8	41.043	41.829	-41.785	-1.911	-.786	-2.5126	1.0000	
1	4	-7	18.658	18.027	-17.988	-1.184	.631	2.2673	1.0000	
1	4	-6	63.839	64.348	64.164	4.862	-.508	-.8767	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	4	-5	5.270	4.803	4.757	.666	.467	.7286	1.0000	
1	4	-4	15.512	14.984	-14.984	.033	.528	1.9235	1.0000	
1	4	-3	12.008	11.288	-11.277	-.495	.720	2.3154	1.0000	
1	4	-2	36.840 *	37.910	37.804	2.834	-1.070	-3.8224	1.0000	**
1	4	-1	2.904	2.978	-2.978	.037	-.075	-.0700	1.0000	
1	4	0	41.560	42.521	42.452	2.409	-.960	-2.8839	1.0000	
1	4	1	6.829	7.529	7.522	.338	-.701	-1.4235	1.0000	
1	4	2	5.284	3.611	-3.581	.463	1.673	2.7137	1.0000	
1	4	3	12.153	11.522	-11.505	-.611	.631	1.9831	1.0000	
1	4	4	63.645	62.879	62.711	4.581	.767	1.6052	1.0000	
1	4	5	8.301	7.317	7.238	1.075	.984	2.1690	1.0000	
1	4	6	18.511	18.113	-18.042	-1.607	.398	1.4512	1.0000	
1	4	7	15.900	15.003	-14.965	-1.073	.897	2.9018	1.0000	
1	4	8	79.994	81.001	80.782	5.963	-1.008	-1.3174	1.0000	
1	4	9	25.567	25.810	25.766	1.514	-.243	-.8812	1.0000	
1	4	10	42.494	42.884	-42.788	-2.867	-.390	-1.4118	1.0000	
1	4	11	15.994	15.459	-15.411	-1.221	.535	1.4613	1.0000	
1	4	12	66.725	69.803	69.523	6.240	-3.078	-5.4267	1.0000	
1	4	13	14.973	15.268	15.187	1.571	-.295	-.6926	1.0000	
1	5	-12	16.980 *	16.027	15.974	1.303	.953	2.4797	1.0000	**
1	5	-11	2.589	1.991	-1.949	.408	.598	.3233	1.0000	
1	5	-10	30.824	31.098	-30.986	-2.634	-.274	-.9539	1.0000	
1	5	-9	34.853	34.297	34.164	3.015	.556	2.0800	1.0000	
1	5	-8	37.433	36.955	36.823	3.120	.477	1.8762	1.0000	
1	5	-7	15.703	13.927	-13.926	-.104	1.776	5.2257	1.0000	
1	5	-6	50.158	50.194	-50.022	-4.153	-.036	-.0943	1.0000	
1	5	-5	36.712	35.932	35.735	3.760	.779	3.3023	1.0000	
1	5	-4	71.334	71.544	71.404	4.472	-.210	-.3431	1.0000	
1	5	-3	8.364	7.557	-7.545	-.434	.807	1.7704	1.0000	
1	5	-2	69.175	71.043	-70.872	-4.925	-1.869	-3.1232	1.0000	
1	5	-1	55.364	55.908	55.758	4.081	-.544	-1.2754	1.0000	
1	5	0	77.427	76.699	76.541	4.929	.727	1.2422	1.0000	
1	5	1	19.399	18.999	-18.994	-.464	.399	1.4745	1.0000	
1	5	2	59.605	59.831	-59.648	-4.674	-.226	-.4784	1.0000	
1	5	3	50.175	49.994	49.842	3.887	.181	.4969	1.0000	
1	5	4	59.847	59.603	59.445	4.351	.243	.5015	1.0000	
1	5	5	5.676	5.450	-5.447	-.182	.226	.3221	1.0000	
1	5	6	44.675	44.579	-44.444	-3.466	.096	.3158	1.0000	
1	5	7	37.846	38.080	37.943	3.233	-.234	-.9278	1.0000	
1	5	8	37.908	38.590	38.477	2.942	-.682	-2.6048	1.0000	
1	5	9	5.464 *	2.054	2.030	.316	3.409	3.8184	1.0000	**
1	5	10	24.893	25.084	-25.028	-1.681	-.191	-.6066	1.0000	
1	5	11	17.924	18.712	18.571	2.293	-.788	-2.0899	1.0000	
1	6	-9	30.472	29.961	29.825	2.854	.511	1.7024	1.0000	
1	6	-8	29.733	28.858	28.725	2.759	.876	2.9906	1.0000	
1	6	-7	28.897	28.516	-28.388	-2.691	.381	1.3022	1.0000	
1	6	-6	2.487 *	.391	-.033	.390	2.095	1.1805	1.0000	
1	6	-5	22.282	21.898	21.829	1.738	.384	1.2568	1.0000	
1	6	-4	26.714	25.588	25.491	2.224	1.126	3.9963	1.0000	
1	6	-3	10.605	10.142	-10.080	-1.121	.663	1.5090	1.0000	
1	6	-2	10.967	10.369	10.294	1.249	.598	1.3590	1.0000	
1	6	-1	7.769	7.675	7.674	.142	.094	.1638	1.0000	
1	6	0	8.170	9.051	8.943	1.395	-.882	-1.5491	1.0000	

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
1	6	1	6.349	5.669	5.619	.750	.680	1.0154	1.0000	
1	6	2	21.507	20.431	20.320	2.120	1.076	3.5640	1.0000	
1	6	3	18.039	17.772	-17.709	-1.503	.267	.8101	1.0000	
1	6	4	2.450 *	1.067	-.928	.526	1.383	.7899	1.0000	**
1	5	5	37.731	36.995	36.915	2.428	.736	2.7541	1.0000	
1	6	6	23.730	23.011	22.848	2.741	.718	2.2956	1.0000	
1	6	7	35.122	35.211	-35.103	-2.750	-.089	-.3120	1.0000	
1	6	8	9.782	9.252	-9.251	-.136	.530	.9591	1.0000	
1	7	-4	11.128	11.451	11.404	1.032	-.322	-.6222	1.0000	
1	7	-3	48.671	48.569	48.300	5.104	.102	.3708	1.0000	
1	7	-2	15.659	15.835	-15.786	-1.233	-.176	-.4406	1.0000	
1	7	-1	35.550	35.172	-35.071	-2.674	.377	1.3223	1.0000	
1	7	0	10.226	9.789	9.716	1.196	.437	.8384	1.0000	
1	7	1	58.654	57.018	56.780	5.201	1.636	4.3405	1.0000	
1	7	2	15.015	14.085	-14.040	-1.116	.930	2.3107	1.0000	
1	7	3	35.515	34.632	-34.552	-2.361	.883	3.0348	1.0000	
2	0	-16	7.873	7.157	7.013	1.429	.715	1.0440	1.0000	
2	0	-14	37.784	36.599	36.458	3.204	1.185	4.6271	1.0000	
2	0	-12	2.933 *	.827	-.386	-.731	2.106	1.6445	1.0000	**
2	0	-10	85.858	83.410	83.187	6.097	2.448	2.6390	1.0000	
2	0	-8	90.138	86.606	-86.558	-2.890	3.531	4.3666	1.0000	
2	0	-6	168.692	173.385	173.178	8.471	-4.694	-6.8226	1.0000	
2	0	-4	122.850	120.433	-120.354	-4.350	2.417	4.1274	1.0000	
2	0	-2	158.467	176.436	176.174	9.611	-17.969	-35.5818	1.0000	*
2	0	0	126.591	132.403	-132.323	-4.601	-5.812	-11.7643	1.0000	
2	0	2	157.153	166.814	166.563	9.153	-9.661	-17.1989	1.0000	
2	0	4	103.325	99.101	-99.037	-3.542	4.224	6.3246	1.0000	
2	0	6	152.471	155.339	155.170	7.236	-2.868	-3.7051	1.0000	
2	0	8	36.745	35.242	-35.208	-1.528	1.503	5.3339	1.0000	
2	0	10	46.978	44.651	44.429	4.449	2.327	6.2342	1.0000	
2	0	12	17.432	16.350	16.332	.784	1.081	3.3017	1.0000	
2	1	-16	22.764	22.822	22.767	1.582	-.058	-.1837	1.0000	
2	1	-15	42.766	42.931	-42.731	-4.139	-.165	-.5971	1.0000	
2	1	-14	59.984	59.380	59.142	5.309	.604	1.2851	1.0000	
2	1	-13	50.111	49.941	49.767	4.167	.170	.4219	1.0000	
2	1	-12	32.017	31.692	-31.641	-1.792	.325	1.2765	1.0000	
2	1	-11	66.758	66.566	-66.432	-4.220	.192	.3119	1.0000	
2	1	-10	76.986	74.500	74.297	5.492	2.486	3.5291	1.0000	
2	1	-9	55.316	53.765	53.632	3.777	1.552	3.1761	1.0000	
2	1	-8	22.251	20.393	-20.373	-.916	1.858	8.1233	1.0000	
2	1	-7	81.415	79.677	-79.608	-3.304	1.739	2.0749	1.0000	
2	1	-6	75.290	71.824	71.666	4.762	3.466	4.3844	1.0000	
2	1	-5	49.624	47.848	47.786	2.422	1.776	4.0452	1.0000	
2	1	-4	4.035	.948	.682	.659	3.087	5.3215	1.0000	
2	1	-3	11.749	11.258	-11.156	-1.511	.490	2.1440	1.0000	
2	1	-2	82.786	82.682	82.618	3.257	.104	.1759	1.0000	
2	1	-1	36.691	34.585	-34.583	-.388	2.106	5.9037	1.0000	
2	1	0	40.247	40.510	40.427	2.586	-.263	-.7735	1.0000	
2	1	1	4.856	2.529	2.426	.715	2.327	5.2550	1.0000	
2	1	2	3.683	4.873	4.676	1.374	-1.190	-2.0388	1.0000	
2	1	3	22.972	19.162	19.079	-1.776	3.810	19.6461	1.0000	
2	1	4	96.750	95.211	95.112	4.357	1.539	2.3759	1.0000	
2	1	5	69.998	67.074	67.017	2.753	2.924	4.1828	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	1	5	17.957	16.252	-16.248	-.370	1.705	8.1720	1.0000
2	1	6	69.959	68.522	-68.435	-3.470	1.417	2.4584	1.0000
2	1	7	81.293	79.725	79.536	5.489	1.568	1.8080	1.0000
2	1	8	82.286	80.085	79.980	4.086	2.202	3.4089	1.0000
2	1	9	32.117	28.577	-28.535	-1.540	3.541	16.1255	1.0000
2	1	10	59.053	58.375	-58.218	-4.272	.678	1.3000	1.0000
2	1	11	70.426	70.990	70.760	5.710	-.564	-.8989	1.0000
2	1	12	58.238	59.374	59.210	4.406	-1.136	-2.3879	1.0000
2	1	13	31.168	31.606	-31.547	-1.934	-.439	-1.5873	1.0000
2	1	14	42.182	42.875	-42.680	-4.082	-.692	-2.5740	1.0000
2	1	15	52.160	53.530	53.292	5.046	-1.370	-3.5485	1.0000
2	2	-16	11.644	11.636	11.543	1.473	.008	.0162	1.0000
2	2	-15	7.699	7.328	-7.275	-.882	.371	.5576	1.0000
2	2	-14	12.277	10.840	10.721	1.600	1.438	3.2604	1.0000
2	2	-13	28.809	28.428	28.370	1.827	.381	1.3961	1.0000
2	2	-12	11.331	10.468	10.242	2.162	.863	2.1547	1.0000
2	2	-11	57.580	56.660	-56.565	-3.286	.919	1.9322	1.0000
2	2	-10	18.394	17.546	17.479	1.527	.848	3.1117	1.0000
2	2	-9	65.654	64.082	63.942	4.242	1.572	2.8736	1.0000
2	2	-8	57.832	56.609	56.540	2.797	1.223	2.3286	1.0000
2	2	-7	85.483	84.337	-84.162	-5.438	1.146	1.3673	1.0000
2	2	-6	17.897	16.705	16.643	1.434	1.192	5.2954	1.0000
2	2	-5	107.936	108.232	108.061	6.081	-.297	-.3974	1.0000
2	2	-4	58.763	58.240	58.151	3.218	.523	1.0109	1.0000
2	2	-3	138.552	141.538	-141.381	-6.666	-2.986	-4.3983	1.0000
2	2	-2	46.389	46.413	46.392	1.397	-.024	-.0601	1.0000
2	2	-1	148.349	154.336	154.187	6.760	-5.987	-9.2170	1.0000
2	2	0	72.955	73.855	73.781	3.309	-.900	-1.3520	1.0000
2	2	1	145.443	148.546	-148.401	-6.553	-3.103	-4.6456	1.0000
2	2	2	38.179	37.815	37.787	1.451	.364	.9653	1.0000
2	2	3	122.286	122.446	122.296	6.052	-.160	-.2195	1.0000
2	2	4	58.694	57.844	57.764	3.044	.850	1.5335	1.0000
2	2	5	80.660	76.403	-76.231	-5.121	4.257	5.2521	1.0000
2	2	6	8.673	4.028	3.707	1.577	4.644	11.3519	1.0000
2	2	7	59.318	59.170	59.021	4.192	.148	.2771	1.0000
2	2	8	29.453	28.885	28.777	2.502	.568	2.5433	1.0000
2	2	9	44.336	44.536	-44.446	-2.821	-.199	-.5293	1.0000
2	2	10	23.130	23.123	23.060	1.705	.007	.0254	1.0000
2	2	11	33.144	33.430	33.383	1.826	-.286	-1.1246	1.0000
2	2	12	8.397	7.922	7.709	1.771	.475	.8342	1.0000
2	2	13	6.322	6.186	-6.177	-.346	.135	.1705	1.0000
2	2	14	3.561 *	4.995	4.678	1.751	-1.434	-1.0129	1.0000
2	3	-15	38.647	39.720	-39.626	-2.728	-1.072	-3.7563	1.0000
2	3	-14	31.120	31.673	31.568	2.578	-.553	-1.9023	1.0000
2	3	-13	66.600	66.220	65.949	5.981	.380	.7043	1.0000
2	3	-12	29.321	28.430	-28.286	-2.852	.892	3.2927	1.0000
2	3	-11	38.946	38.466	-38.398	-2.288	.480	1.9580	1.0000
2	3	-10	39.917	39.998	39.930	2.317	-.080	-.2925	1.0000
2	3	-9	70.035	70.180	69.957	5.591	-.146	-.2488	1.0000
2	3	-8	29.431	27.863	-27.775	-2.216	1.568	6.9663	1.0000
2	3	-7	12.442	12.336	-12.303	-.893	.106	.3302	1.0000
2	3	-6	29.682	29.080	29.042	1.478	.602	2.8871	1.0000
2	3	-5	70.745	70.003	69.879	4.160	.741	1.2061	1.0000

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CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	3	-4	21.047	21.011	-20.986	-1.027	.036	.1653	1.0000	
2	3	-3	6.430	6.168	-6.047	1.213	.262	.5723	1.0000	
2	3	-2	11.708	11.266	11.264	.234	.442	1.6001	1.0000	
2	3	-1	39.646	40.341	40.289	2.040	-.694	-2.1809	1.0000	
2	3	0	15.798	15.122	15.116	.437	.675	2.9534	1.0000	
2	3	1	77.214	78.309	78.231	3.493	-1.095	-1.3753	1.0000	
2	3	2	36.659	36.050	-36.033	-1.089	.609	2.2789	1.0000	
2	3	3	25.173	24.927	-24.926	-.179	.246	1.1916	1.0000	
2	3	4	17.624	16.321	16.221	1.795	1.303	5.2765	1.0000	
2	3	5	75.657	75.484	75.297	5.311	.173	.2695	1.0000	
2	3	6	35.014	34.699	-34.640	-2.135	-.315	1.3647	1.0000	
2	3	7	28.476	27.904	-27.840	-1.891	-.572	2.4596	1.0000	
2	3	8	35.226	34.788	34.683	2.706	.438	1.9140	1.0000	
2	3	9	71.943	73.791	73.531	6.180	-1.848	-2.9613	1.0000	
2	3	10	40.801	41.260	-41.175	-2.649	-.459	-1.4404	1.0000	
2	3	11	31.541	32.570	32.432	2.987	-1.029	-3.5309	1.0000	
2	3	12	61.471	63.476	63.198	5.943	-2.005	-3.6272	1.0000	
2	3	13	2.642 *	.297	-.036	.295	2.345	-3.8179	1.0000	**
2	4	-14	10.711	10.082	-10.066	-.557	.629	1.2430	1.0000	
2	4	-13	42.980	42.178	42.007	3.792	.803	1.2695	1.0000	
2	4	-12	15.075	15.089	15.081	.488	-.014	2.7762	1.0000	
2	4	-11	30.899	24.838	-24.793	-1.495	6.060	-.0362	1.0000	
2	4	-10	8.550	8.434	-8.353	-1.163	.117	23.4902	1.0000	
2	4	-9	69.588	69.680	69.425	5.960	-.092	.2312	1.0000	
2	4	-8	9.646	9.464	9.395	1.137	.183	-.1502	1.0000	
2	4	-7	59.481	59.029	-58.953	-2.999	.452	.4265	1.0000	
2	4	-6	21.613	20.804	-20.743	-1.593	.809	.6879	1.0000	
2	4	-5	107.910	110.369	110.120	7.410	-2.459	3.2739	1.0000	
2	4	-4	32.494	32.609	32.572	1.558	-.115	-2.6304	1.0000	
2	4	-3	73.628	75.796	-75.705	-3.714	-2.168	-.5341	1.0000	
2	4	-2	33.208	32.579	-32.536	-1.682	.628	-3.3091	1.0000	
2	4	-1	101.006	104.170	103.886	7.694	-3.164	3.0386	1.0000	
2	4	0	28.703	28.351	28.305	-1.614	.352	-3.4722	1.0000	
2	4	1	65.592	65.069	-64.981	-3.384	.523	1.6318	1.0000	
2	4	2	25.373	24.944	-24.906	-1.379	.429	.9597	1.0000	
2	4	3	91.466	92.930	92.686	6.717	-1.463	1.8612	1.0000	
2	4	4	8.124	7.640	7.529	1.297	.484	-2.1271	1.0000	
2	4	5	38.272	38.360	-38.302	-2.112	-.088	1.0252	1.0000	
2	4	6	7.489	6.099	-6.050	-.774	1.390	-.3335	1.0000	
2	4	7	58.742	60.110	59.919	4.781	-1.368	2.5242	1.0000	
2	4	8	11.249	11.907	11.884	.732	-.658	-2.9442	1.0000	
2	4	9	9.401	9.404	-9.399	-.321	-.003	-1.4851	1.0000	
2	4	10	11.423	10.771	-10.771	-.059	.652	-.0061	1.0000	
2	4	11	23.408	23.104	22.973	2.456	.304	1.3492	1.0000	
2	5	-12	36.721	36.164	35.983	3.607	.557	.9378	1.0000	
2	5	-11	11.436	7.691	-7.689	-.166	3.745	1.9389	1.0000	
2	5	-10	48.702	48.644	-48.501	-3.730	.058	7.8711	1.0000	
2	5	-9	32.697	32.135	31.994	3.015	.562	.1693	1.0000	
2	5	-8	36.977	36.868	36.759	2.833	.109	2.0607	1.0000	
2	5	-7	3.085 *	3.422	-3.386	.494	-.337	.4220	1.0000	**
2	5	-6	35.266	35.167	-35.085	-2.400	.099	-.2519	1.0000	
2	5	-5	22.992	23.136	22.998	2.521	-.143	.3995	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
2	5	-4	14.497	14.205	14.148	1.275	.292	.9063	1.0000	
2	5	-3	17.392	17.705	17.652	1.363	-.313	-1.0503	1.0000	
2	5	-2	3.001*	2.219	-2.180	-.414	.782	.6456	1.0000	**
2	5	-1	14.898	14.388	14.283	1.735	.509	1.6182	1.0000	
2	5	0	10.514	9.882	-9.859	-.670	.632	1.5917	1.0000	
2	5	1	13.858	12.058	11.847	2.246	1.800	5.3468	1.0000	
2	5	2	23.582	23.858	23.798	1.701	-.277	-1.0433	1.0000	
2	5	3	8.386	7.618	7.570	.855	.768	1.5652	1.0000	
2	5	4	24.101	24.316	-24.192	-2.448	-.215	-.7982	1.0000	
2	5	5	37.337	37.386	37.272	2.921	-.049	-.1973	1.0000	
2	5	6	46.541	46.731	46.609	3.366	-.190	-.5673	1.0000	
2	5	7	9.460	8.910	-8.910	-.097	.549	1.0646	1.0000	
2	5	8	43.943	44.835	-44.693	-3.570	-.892	-3.3174	1.0000	**
2	5	9	32.055	31.991	31.829	3.222	.064	.2221	1.0000	
2	5	10	49.329	50.732	50.561	4.172	-1.403	-4.8225	1.0000	
2	6	-9	39.758	39.102	-38.986	-3.007	.656	2.3296	1.0000	
2	6	-8	4.993*	4.275	-4.275	-.049	.718	.7517	1.0000	**
2	6	-7	42.193	41.688	41.557	3.296	.506	1.8676	1.0000	
2	6	-6	36.406	36.204	36.071	3.095	.202	.7414	1.0000	
2	6	-5	47.681	48.093	-47.920	-4.064	-.412	-1.3977	1.0000	
2	6	-4	9.999	8.713	-8.706	-.344	1.266	2.6230	1.0000	
2	6	-3	46.742	46.922	46.735	4.179	-.180	-.6175	1.0000	
2	6	-2	38.646	39.311	39.157	3.470	-.665	-2.5602	1.0000	
2	6	-1	54.023	54.848	-54.674	-4.372	-.826	-2.1592	1.0000	**
2	6	0	3.608*	4.379	-4.361	-.400	-.771	-.6345	1.0000	
2	6	1	55.576	55.883	55.722	4.238	-.307	-.8019	1.0000	
2	6	2	37.153	36.561	36.411	3.312	.592	2.2615	1.0000	
2	6	3	45.383	45.233	-45.072	-3.810	.150	.5808	1.0000	
2	6	4	7.829	7.491	-7.490	-.088	.339	.5460	1.0000	
2	6	5	45.072	44.870	44.736	3.464	.202	.7457	1.0000	
2	6	6	28.547	28.434	28.308	2.673	.113	.3789	1.0000	
2	6	7	29.124	29.077	-28.966	-2.539	.047	.1556	1.0000	
2	7	8	4.774*	1.848	-1.787	.475	2.925	2.7565	1.0000	**
2	7	-4	4.918*	5.837	5.833	.209	-.919	-.8568	1.0000	**
2	7	-3	17.503	17.829	17.719	1.975	-.326	-.8560	1.0000	
2	7	-2	2.627*	3.453	-3.450	-.147	-.826	-.4402	1.0000	**
2	7	-1	11.961	11.673	11.588	1.404	.288	.6078	1.0000	
2	7	0	5.980	3.607	-3.605	-.115	2.373	2.9013	1.0000	
2	7	1	6.464	4.552	4.539	.337	1.913	2.4595	1.0000	
2	7	2	5.703	5.327	5.315	.362	.376	.4250	1.0000	
3	0	-16	41.910	42.233	-42.061	-3.806	-.323	-1.1770	1.0000	
3	0	-14	89.571	88.229	87.925	7.320	1.342	1.6403	1.0000	
3	0	-12	50.502	50.116	-50.002	-3.385	.386	.8645	1.0000	
3	0	-10	114.526	111.485	111.271	6.905	3.041	3.2465	1.0000	
3	0	-8	49.706	46.505	-46.473	-1.732	3.202	7.3211	1.0000	
3	0	-6	109.324	108.357	108.234	5.166	.967	1.3021	1.0000	
3	0	-4	54.229	50.351	50.343	.891	3.878	8.0292	1.0000	
3	0	-2	7.174	8.183	7.791	2.504	-1.009	-3.1866	1.0000	**
3	0	0	37.476	38.130	37.937	3.838	-.654	-1.9319	1.0000	
3	0	2	7.291	6.144	6.134	-.355	1.148	3.3905	1.0000	
3	0	4	103.696	101.120	100.924	6.303	2.576	3.4252	1.0000	
3	0	6	81.165	77.942	-77.897	-2.632	3.223	3.7722	1.0000	
3	0	8	107.555	106.283	106.009	7.627	1.272	1.3397	1.0000	

CU(IO3)2.2H2O FINAL

T	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DFLTA F	DELTA/SIGMA	EXT. FACTOR
3	0	10	64.878	65.064	-64.954	-3.793	-.186	-.3443	1.0000
3	0	12	85.362	87.100	86.773	7.547	-1.738	-2.1107	1.0000
3	0	14	42.397	43.743	-43.584	-3.725	-1.347	-4.8740	1.0000
3	1	-16	14.764	14.556	14.553	.316	.208	.5046	1.0000
3	1	-15	6.569	5.398	5.322	.902	1.171	1.5680	1.0000
3	1	-14	12.704	12.483	-12.408	-1.364	.221	.5367	1.0000
3	1	-13	44.395	43.497	43.361	3.431	.898	2.4177	1.0000
3	1	-12	18.026	17.530	17.392	2.194	.496	1.6442	1.0000
3	1	-11	17.523	17.554	-17.549	-.398	-.030	-.1043	1.0000
3	1	-10	49.207	46.781	-46.669	-3.235	2.425	5.9710	1.0000
3	1	-9	77.983	75.039	74.852	5.292	2.944	4.5456	1.0000
3	1	-8	83.860	81.262	81.166	3.958	2.598	3.0083	1.0000
3	1	-7	28.278	26.906	-26.862	-1.543	1.372	6.4649	1.0000
3	1	-6	116.669	113.698	-113.601	-6.698	2.970	3.9118	1.0000
3	1	-5	119.499	119.128	118.945	6.601	.372	.5140	1.0000
3	1	-4	82.365	79.699	79.538	5.067	2.666	3.8643	1.0000
3	1	-3	63.841	61.204	-61.167	-2.133	2.637	3.9054	1.0000
3	1	-2	119.860	122.192	-122.078	-5.275	-2.332	-3.6309	1.0000
3	1	-1	144.299	148.079	147.915	6.965	-3.780	-5.9363	1.0000
3	1	0	83.908	83.937	83.779	5.151	-.029	-.0443	1.0000
3	1	1	56.743	53.812	-53.776	-1.946	2.932	6.0012	1.0000
3	1	2	93.204	91.397	-91.273	-4.761	1.807	2.5854	1.0000
3	1	3	108.636	108.771	108.590	6.270	-.135	-.1829	1.0000
3	1	4	86.197	83.950	83.846	4.176	2.246	2.8816	1.0000
3	1	5	22.610	21.505	-21.480	-1.035	1.105	5.2530	1.0000
3	1	6	76.012	73.239	-73.164	-3.312	2.774	4.4848	1.0000
3	1	7	65.769	63.447	63.271	4.724	2.322	4.3023	1.0000
3	1	8	43.271	42.428	42.357	2.459	.843	2.3150	1.0000
3	1	10	* 3.423	2.664	-2.275	-1.385	.759	.6475	1.0000
3	1	11	33.338	32.800	32.682	2.777	.538	2.0700	1.0000
3	1	12	6.938	7.046	7.026	.531	-.108	-.1565	1.0000
3	1	13	14.003	13.514	13.418	1.613	.489	1.1612	1.0000
3	1	14	8.300	3.288	3.256	.457	5.011	7.9852	1.0000 **
3	2	-16	16.076	14.685	14.509	2.267	1.391	3.4399	1.0000
3	2	-15	63.468	64.084	-63.861	-5.343	-.617	-1.1950	1.0000
3	2	-14	5.339	1.927	1.687	.931	3.412	3.9589	1.0000
3	2	-13	66.898	66.738	66.546	5.057	.160	.2762	1.0000
3	2	-12	21.772	21.684	21.528	2.598	.088	.3086	1.0000
3	2	-11	66.382	67.360	-67.178	-4.944	-.977	-1.5994	1.0000
3	2	-10	6.313	6.139	5.997	1.313	.173	.2753	1.0000
3	2	-9	57.190	56.433	56.285	4.081	.757	1.5561	1.0000
3	2	-8	39.026	37.864	37.769	2.671	1.163	3.9470	1.0000
3	2	-7	52.158	50.995	-50.886	-3.322	1.163	2.5954	1.0000
3	2	-6	9.260	8.477	8.282	1.809	.783	2.1615	1.0000
3	2	-5	47.284	46.006	45.962	2.015	1.278	3.4408	1.0000
3	2	-4	18.835	19.027	18.865	2.479	-.192	-.9380	1.0000
3	2	-3	39.628	38.223	-38.215	-.791	1.405	4.3393	1.0000
3	2	-2	58.434	58.397	58.351	2.317	.037	.0699	1.0000
3	2	-1	15.408	14.978	-14.964	-.645	.430	1.3950	1.0000
3	2	0	49.099	48.481	48.436	2.095	.618	1.9576	1.0000
3	2	1	59.257	57.169	57.134	1.990	2.088	3.8823	1.0000
3	2	2	34.600	34.199	34.092	2.701	.401	1.4245	1.0000
3	2	3	69.952	69.925	-69.853	-3.167	.028	.0481	1.0000

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
3	2	4	29.151	28.483	28.436	1.639	.668	3.0951	1.0000	
3	2	5	64.584	63.146	63.002	4.264	1.438	2.2709	1.0000	
3	2	6	51.796	50.561	50.501	2.843	1.215	2.8370	1.0000	
3	2	7	67.594	67.713	-67.538	-4.871	-.120	-.2116	1.0000	
3	2	8	16.629	16.273	16.226	1.233	.355	1.1913	1.0000	
3	2	9	75.346	76.361	76.166	5.459	-1.015	-1.3597	1.0000	
3	2	10	33.385	33.307	33.198	2.690	.078	.3090	1.0000	
3	2	11	68.957	68.625	-68.414	-5.375	.332	.5690	1.0000	
3	2	12	5.019 *	3.340	3.203	-.948	1.679	1.7544	1.0000	**
3	2	13	62.384	64.393	64.166	5.395	-2.008	-3.8377	1.0000	
3	3	-15	17.787	17.844	17.692	2.327	-.057	-.1496	1.0000	
3	3	-14	15.232	12.924	-12.875	-1.130	2.308	6.0364	1.0000	
3	3	-13	16.839	16.648	-16.648	-.114	.191	.5317	1.0000	
3	3	-12	23.865	22.709	22.666	1.397	1.157	4.0006	1.0000	
3	3	-11	58.976	59.969	59.796	4.549	-.993	-1.9520	1.0000	
3	3	-10	32.851	33.102	-33.023	-2.291	-.251	-1.0323	1.0000	
3	3	-9	29.450	29.399	-29.399	-1.732	.376	1.5811	1.0000	
3	3	-8	39.482	39.341	39.259	2.537	.141	.4818	1.0000	
3	3	-7	79.046	78.773	78.509	6.443	.273	.4027	1.0000	
3	3	-6	44.442	43.178	-43.061	-3.174	1.265	3.9050	1.0000	
3	3	-5	55.344	55.414	-55.339	-2.885	-.070	-.1524	1.0000	
3	3	-4	65.899	65.583	65.501	3.279	.316	.6242	1.0000	
3	3	-3	124.044	127.756	127.539	7.440	-3.711	-4.4192	1.0000	
3	3	-2	47.031	47.116	-46.987	-3.494	-.085	-.2144	1.0000	
3	3	-1	71.116	71.303	-71.233	-3.159	-.187	-.3116	1.0000	
3	3	0	68.236	67.364	67.279	3.393	.872	1.4437	1.0000	
3	3	1	121.838	124.420	124.210	7.220	-2.582	-3.0611	1.0000	
3	3	2	57.294	57.893	-57.808	-3.134	-.599	-1.3364	1.0000	
3	3	3	45.754	45.663	-45.598	-2.439	.091	.2564	1.0000	
3	3	4	50.969	50.229	50.148	2.847	.740	1.8897	1.0000	
3	3	5	76.603	75.205	74.978	5.848	1.398	2.0539	1.0000	
3	3	6	26.796	26.746	-26.656	-2.193	.051	.2100	1.0000	
3	3	7	13.825	13.315	-13.281	-.964	.510	1.5146	1.0000	
3	3	8	18.663	18.632	18.543	1.819	.031	.1068	1.0000	
3	3	9	49.130	49.162	49.019	3.746	-.032	-.0826	1.0000	
3	3	10	20.438	19.772	-19.749	-.950	.666	2.1294	1.0000	
3	3	11	2.565 *	3.903	-3.826	.774	-1.338	-.7306	1.0000	**
3	3	12	7.826	4.182	4.135	.623	3.644	5.5627	1.0000	
3	3	13	9.515	10.026	9.910	1.520	-.511	-.8366	1.0000	
3	4	-14	33.535	34.348	-34.219	-2.974	-.813	-2.7248	1.0000	
3	4	-13	18.861	18.576	-18.513	-1.524	.285	.7795	1.0000	
3	4	-12	68.922	68.896	68.648	5.845	.026	.0464	1.0000	
3	4	-11	13.427	13.631	13.590	1.052	-.204	-.5050	1.0000	
3	4	-10	34.662	34.467	-34.400	-2.138	.196	.7580	1.0000	
3	4	-9	10.836	11.189	-11.119	-1.245	-.353	-.8182	1.0000	
3	4	-8	64.126	64.234	64.042	4.959	-.107	-.1970	1.0000	
3	4	-7	4.752 *	4.220	4.161	-.698	.532	.6701	1.0000	**
3	4	-6	5.429	3.766	-3.746	-.388	1.663	2.4836	1.0000	
3	4	-5	10.929	10.437	-10.418	-.629	.492	1.3505	1.0000	
3	4	-4	38.499	39.609	39.484	3.143	-1.110	-4.2421	1.0000	
3	4	-3	19.111	19.101	19.101	1.109	.010	.0394	1.0000	
3	4	-2	16.801	16.618	16.508	1.905	.183	.6658	1.0000	
3	4	-1	4.629	3.085	3.080	.172	1.545	2.1372	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	4	0	7.129	5.211	5.139	.864	1.918	3.8818	1.0000
3	4	1	17.975	17.901	-17.893	-.536	.074	.2786	1.0000
3	4	2	49.020	49.250	49.076	4.138	-.230	-.6793	1.0000
3	4	3	21.730	21.468	21.447	.928	.262	1.0238	1.0000
3	4	4	31.286	31.043	-31.017	-1.255	.244	1.0494	1.0000
3	4	5	10.647	10.289	-10.237	-1.034	.358	.8508	1.0000
3	4	6	69.003	69.205	68.970	5.705	-.202	-.3700	1.0000
3	4	7	14.559	14.306	14.235	1.428	.253	.7056	1.0000
3	4	8	47.229	47.747	-47.673	-2.667	-.518	-1.4834	1.0000
3	4	9	16.041	16.838	-16.792	-1.235	-.797	-2.1340	1.0000
3	4	10	61.073	62.739	62.739	6.222	-1.666	-3.5154	1.0000
3	4	11	14.592	14.756	14.673	1.558	-.164	-.3908	1.0000
3	5	-12	21.858	22.528	-22.414	-2.258	-.670	-1.9161	1.0000
3	5	-11	23.603	21.880	21.712	2.706	1.723	5.3202	1.0000
3	5	-10	32.979	32.841	32.730	2.696	.138	.4860	1.0000
3	5	-9	5.458	5.806	-5.806	-.024	-.348	-.4050	1.0000
3	5	-8	51.285	52.097	-51.956	-3.827	-.811	-2.2971	1.0000
3	5	-7	45.593	45.569	45.434	3.508	.024	.0699	1.0000
3	5	-6	54.454	54.095	53.937	4.133	.359	.8809	1.0000
3	5	-5	10.933	11.352	-11.345	-.397	-.419	-.9917	1.0000
3	5	-4	66.390	67.393	-67.224	-4.758	-1.003	-2.0299	1.0000
3	5	-3	46.616	47.485	47.322	3.937	-.869	-2.7616	1.0000
3	5	-2	55.982	56.052	55.849	4.772	-.070	-.1704	1.0000
3	5	-1	14.228	14.560	-14.552	-.485	-.332	-.9708	1.0000
3	5	0	64.910	66.131	-65.962	-4.721	-1.221	-2.7358	1.0000
3	5	1	39.769	40.072	39.884	3.875	-.303	-1.2734	1.0000
3	5	2	60.579	60.906	60.746	4.404	-.327	-.7742	1.0000
3	5	3	8.753	8.496	-8.492	-.261	.257	.5147	1.0000
3	5	4	53.256	53.487	-53.359	-3.703	-.231	-.5967	1.0000
3	5	5	37.820	37.989	37.841	3.338	-.168	-.6593	1.0000
3	5	6	38.979	38.884	38.755	3.158	.095	.3620	1.0000
3	5	7	12.177	11.204	-11.202	.204	.973	2.1707	1.0000
3	5	8	20.583	20.580	-20.481	-2.018	.003	.0064	1.0000
3	5	9	19.545	19.740	19.585	2.471	-.195	-.5475	1.0000
3	6	-9	32.198	31.622	-31.494	-2.847	.576	1.9303	1.0000
3	6	-8	6.199	6.433	-6.428	.243	-.233	-.2866	1.0000
3	6	-7	26.996	26.697	26.629	1.904	.299	.9841	1.0000
3	6	-6	18.012	17.705	17.562	2.244	.307	.8550	1.0000
3	6	-5	20.061	20.332	-20.281	-1.440	-.271	-.8181	1.0000
3	6	-4	10.129	10.346	10.292	1.060	-.217	-.4370	1.0000
3	6	-3	2.437	2.358	-2.321	.415	.079	.0726	1.0000
3	6	-2	11.944	12.101	12.010	1.486	-.157	-.3598	1.0000
3	6	-1	5.595	5.397	5.385	.359	.198	.2373	1.0000
3	6	0	18.026	17.443	17.335	1.942	.583	1.7046	1.0000
3	6	1	14.667	14.386	-14.334	-1.221	.281	.7328	1.0000
3	6	2	7.379	8.135	8.110	.638	-.756	-1.1352	1.0000
3	6	3	21.688	21.559	21.459	2.080	.128	.3988	1.0000
3	6	4	29.373	27.833	27.709	2.626	1.539	5.3239	1.0000
3	6	5	30.373	30.093	-29.984	-2.552	.454	1.5423	1.0000
3	6	6	6.995	6.299	-6.299	-.051	.696	.9363	1.0000
4	0	-16	24.945	24.922	24.797	2.494	.023	.0715	1.0000
4	0	-14	13.935	14.468	-14.464	-.356	-.533	-1.3478	1.0000
4	0	-12	63.466	60.977	60.749	5.271	2.489	5.1135	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	0	-10	47.533	46.223	-46.157	-2.465	1.310	3.3607	1.0000
4	0	-8	130.745	130.703	130.475	7.722	.042	.0478	1.0000
4	0	-6	62.223	58.461	-58.321	-4.036	3.763	7.9401	1.0000
4	0	-4	167.048	171.750	171.507	9.122	-4.701	-6.4076	1.0000
4	0	-2	106.748	105.323	-105.226	-4.517	1.425	1.9973	1.0000
4	0	0	182.350	194.989	194.780	9.022	-12.638	-17.6203 *	1.0000
4	0	2	65.363	62.279	-62.168	-3.715	3.084	5.5264	1.0000
4	0	4	112.120	108.840	108.585	7.444	3.280	3.9140	1.0000
4	0	6	46.546	44.583	-44.544	-1.884	1.963	4.9440	1.0000
4	0	8	61.299	60.160	59.963	4.871	1.139	2.1769	1.0000
4	0	10	5.293	6.435	-6.424	-.380	-1.142	-1.3895	1.0000
4	0	12	17.728	16.958	16.833	2.050	.771	2.1598	1.0000
4	0	-16	47.915	48.424	48.266	3.914	-.509	-1.6094	1.0000
4	1	-15	25.922	26.688	-26.625	-1.822	-.766	-2.5068	1.0000
4	1	-14	51.620	51.443	-51.282	-4.067	.177	.4572	1.0000
4	1	-13	59.530	59.025	58.795	5.207	.505	1.0575	1.0000
4	1	-12	53.368	52.786	52.654	3.729	.582	1.3713	1.0000
4	1	-11	25.735	25.716	-25.691	-1.132	.019	.0741	1.0000
4	1	-10	35.508	34.304	-34.137	-3.387	1.203	5.2196	1.0000
4	1	-9	68.064	68.369	68.207	4.699	-.305	-.5501	1.0000
4	1	-8	53.966	52.649	52.585	2.604	1.317	2.8114	1.0000
4	1	-7	5.317	3.110	-3.098	-.275	2.207	3.5581	1.0000
4	1	-6	41.495	39.806	-39.764	-1.813	1.689	5.0996	1.0000
4	1	-5	54.674	52.944	52.834	3.399	1.730	4.2219	1.0000
4	1	-4	14.049	14.880	14.862	.743	-.832	-3.3172	1.0000
4	1	-3	33.844	33.460	33.393	2.116	.384	1.3899	1.0000
4	1	-2	2.902	6.784	6.778	.290	-3.882	-3.5779 **	1.0000
4	1	-1	20.530	20.647	20.581	1.642	-.117	-.5930	1.0000
4	1	0	31.671	30.998	-30.968	-1.367	.672	2.8932	1.0000
4	1	1	68.342	67.143	67.028	3.920	1.199	2.1851	1.0000
4	1	2	36.673	36.273	36.196	2.351	.401	1.3857	1.0000
4	1	3	6.603	4.285	-4.284	-.089	2.319	4.8185	1.0000
4	1	4	76.080	74.568	-74.502	-3.139	1.512	2.4513	1.0000
4	1	5	74.797	73.118	72.934	5.196	1.679	2.5994	1.0000
4	1	6	49.598	48.796	48.647	3.808	.802	1.8039	1.0000
4	1	7	31.947	31.924	-31.895	-1.342	.023	.1033	1.0000
4	1	8	52.164	52.281	-52.119	-4.110	-.117	-.2661	1.0000
4	1	9	71.138	71.996	71.776	5.618	-.858	-1.3469	1.0000
4	1	10	52.791	53.618	53.443	4.324	-.827	-1.8594	1.0000
4	1	11	30.533	30.086	-30.028	-1.866	.447	1.6275	1.0000
4	1	12	56.118	56.625	-56.475	-4.109	-.507	-1.1991	1.0000
4	1	13	48.343	49.256	48.986	5.146	-.913	-2.6396	1.0000
4	1	-15	14.760	15.131	15.075	1.304	-.371	-.9049	1.0000
4	1	-14	20.945	20.273	20.185	1.895	.671	2.0732	1.0000
4	2	-13	33.893	34.191	-34.083	-2.717	-.308	-1.1546	1.0000
4	2	-12	15.920	15.136	15.069	1.415	.785	2.2815	1.0000
4	2	-11	50.396	51.207	51.077	3.636	-.810	-2.0504	1.0000
4	2	-10	26.474	25.843	25.719	2.533	.631	2.5167	1.0000
4	2	-9	68.607	68.171	-67.996	-4.886	.436	.7571	1.0000
4	2	-8	6.631	6.314	6.170	1.339	.317	.5852	1.0000
4	2	-7	95.367	94.132	93.968	5.563	1.235	1.3580	1.0000
4	2	-6	27.667	27.378	27.213	3.002	.290	1.3649	1.0000
4	2	-5	115.972	117.695	-117.526	-6.293	-1.723	-2.0382	1.0000

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	2	-4	11.158	6.184	6.044	1.310	4.973	15.7118	1.0000
4	2	-3	115.900	117.156	116.977	6.474	-1.256	-1.5493	1.0000
4	2	-2	51.969	53.019	52.924	3.174	-1.051	-2.4876	1.0000
4	2	-1	106.087	105.983	-105.786	-6.464	.104	.1295	1.0000
4	2	0	9.436	1.808	1.179	1.370	7.628	20.3372	1.0000
4	2	1	100.554	101.611	101.430	6.061	-1.056	-1.2828	1.0000
4	2	2	26.760	26.882	26.713	3.002	-.122	-.5847	1.0000
4	2	3	95.777	97.172	-97.027	-5.317	-1.395	-1.5922	1.0000
4	2	4	23.569	23.153	23.104	1.508	.416	1.7337	1.0000
4	2	5	71.612	71.567	71.428	4.451	.045	.0665	1.0000
4	2	6	39.008	37.301	37.215	2.539	1.706	6.0561	1.0000
4	2	7	48.438	47.955	-47.848	-3.206	.484	1.1904	1.0000
4	2	8	16.424	15.878	15.791	1.660	.545	1.7035	1.0000
4	2	9	27.446	26.995	26.909	2.157	.451	1.6990	1.0000
4	2	10	20.914	20.061	19.969	1.911	.853	2.7265	1.0000
4	2	11	7.981	8.499	-8.464	-.773	-.518	-.8022	1.0000
4	2	12	17.690	16.438	16.346	1.741	1.251	3.4544	1.0000
4	3	-15	53.953	54.663	54.377	5.586	-.710	-1.9904	1.0000
4	3	-14	33.005	32.957	-32.841	-2.770	.047	.1619	1.0000
4	3	-13	31.903	32.661	-32.576	-2.363	-.758	-2.6909	1.0000
4	3	-12	28.862	28.874	28.783	2.286	-.011	-.0406	1.0000
4	3	-11	67.907	68.627	68.412	5.430	-.720	-1.2535	1.0000
4	3	-10	40.651	40.591	-40.526	-2.295	.061	.2313	1.0000
4	3	-9	28.385	28.098	-28.073	-1.191	.287	1.1516	1.0000
4	3	-8	14.967	15.132	15.049	1.588	-.165	-.5242	1.0000
4	3	-7	51.101	50.978	50.800	4.255	.122	.2961	1.0000
4	3	-6	12.664	12.082	-12.017	-1.254	.581	1.7456	1.0000
4	3	-5	5.623	5.217	5.163	.745	.406	.6766	1.0000
4	3	-4	9.725	8.610	8.598	.449	1.115	2.9583	1.0000
4	3	-3	28.379	28.345	28.250	2.325	.034	.1600	1.0000
4	3	-2	3.899 *	3.412	-3.410	-.127	.487	.5777 **	1.0000
4	3	-1	39.793	39.344	39.232	2.976	.449	1.8024	1.0000
4	3	0	8.580	7.386	-7.338	-.842	1.193	2.8604	1.0000
4	3	1	9.745	8.550	-8.548	.173	1.195	3.2182	1.0000
4	3	2	30.781	30.738	30.702	1.492	.044	-.2025	1.0000
4	3	3	59.607	60.095	59.896	4.888	-.488	-.9956	1.0000
4	3	4	22.954	22.286	-22.201	-1.936	.668	2.6855	1.0000
4	3	5	27.945	27.496	-27.449	-1.603	.449	1.8604	1.0000
4	3	6	43.943	44.195	44.125	2.490	-.253	-.8174	1.0000
4	3	7	79.009	79.746	79.523	5.958	-.736	-1.1629	1.0000
4	3	8	33.925	33.511	-33.414	-2.553	.414	1.6271	1.0000
4	3	9	42.717	43.458	-43.382	-2.568	-.741	-2.7009	1.0000
4	3	10	31.810	32.461	32.331	2.900	-.651	-2.2956	1.0000
4	3	11	60.677	61.158	60.868	5.953	-.481	-1.0642	1.0000
4	3	12	24.835	24.569	-24.432	-2.585	.266	.8131	1.0000
4	3	-13	4.860 *	4.510	4.498	.341	.349	.3385 **	1.0000
4	4	-12	22.833	21.395	-21.364	-1.154	1.438	4.5164	1.0000
4	4	-11	18.264	15.214	-15.178	-1.043	3.050	8.8208	1.0000
4	4	-10	65.083	65.139	64.923	5.310	-.056	-.1159	1.0000
4	4	-9	10.232	10.144	10.097	.974	.088	.1872	1.0000
4	4	-8	40.374	40.284	-40.097	-2.685	-.096	-.3969	1.0000
4	4	-7	25.634	23.876	-23.829	-1.504	1.758	6.7200	1.0000
4	4	-6	92.752	94.077	93.823	6.899	-1.324	-1.7868	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
4	4	-5	24.842	24.360	24.318	1.426	.482	1.9241	1.0000	
4	4	-4	49.602	50.479	-50.354	-3.545	-.877	-2.4693	1.0000	
4	4	-3	21.404	20.642	-20.575	-1.660	.762	2.9337	1.0000	
4	4	-2	100.807	102.867	102.597	7.440	-2.060	-2.9164	1.0000	
4	4	-1	16.323	15.377	15.299	1.546	.946	3.2314	1.0000	
4	4	0	55.726	56.321	-56.217	-3.421	-.594	-1.5182	1.0000	
4	4	1	20.762	20.063	-20.012	-1.435	.698	2.6145	1.0000	
4	4	2	97.244	99.779	99.550	6.754	-2.534	-3.4715	1.0000	
4	4	3	28.862	28.432	28.402	1.301	.431	1.7429	1.0000	
4	4	4	40.058	40.269	-40.201	-2.337	-.211	-.7959	1.0000	
4	4	5	13.331	11.894	-11.861	-.888	1.437	3.8700	1.0000	
4	4	6	51.329	51.440	51.192	5.046	-.111	-.3137	1.0000	
4	4	7	7.981	7.525	7.484	.786	.457	.7750	1.0000	
4	4	8	15.600	14.310	-14.296	-.644	1.290	3.4563	1.0000	
4	4	9	2.563 *	.625	-.595	-.190	1.939	1.0585	1.0000	**
4	4	10	24.714	24.909	24.748	2.828	-.195	-.6162	1.0000	
4	5	-11	22.524	21.805	21.612	2.899	.719	2.1704	1.0000	
4	5	-10	37.703	38.062	37.954	2.873	-.359	-1.2817	1.0000	
4	5	-9	3.195 *	.705	-.640	.294	2.490	1.7426	1.0000	**
4	5	-8	26.110	26.483	-26.354	-2.605	-.373	-1.2573	1.0000	
4	5	-7	33.356	33.154	33.058	2.516	.202	.7514	1.0000	
4	5	-6	18.769	17.363	17.298	1.500	1.407	4.3930	1.0000	
4	5	-5	5.879	6.097	5.995	1.108	-.218	-.2858	1.0000	
4	5	-4	11.714	11.281	-11.253	-.792	.433	1.0609	1.0000	
4	5	-3	16.367	16.386	16.285	1.819	-.020	-.0597	1.0000	
4	5	-2	2.369 *	1.765	-1.732	-.341	.604	.3570	1.0000	**
4	5	-1	25.797	25.570	25.493	1.987	.227	.8437	1.0000	
4	5	0	13.776	12.588	12.524	1.268	1.188	3.2462	1.0000	
4	5	1	7.156	7.793	7.731	.984	-.637	-1.0486	1.0000	
4	5	2	32.423	32.857	-32.787	-2.134	-.434	-1.6464	1.0000	
4	5	3	30.644	29.845	29.721	2.715	.799	2.9523	1.0000	
4	5	4	35.656	35.928	35.802	3.007	-.273	-1.0347	1.0000	
4	5	5	4.481 *	2.980	-2.972	.220	1.501	1.4674	1.0000	**
4	5	6	45.503	45.580	-45.455	-3.374	-.077	-.2911	1.0000	
4	5	7	24.877	25.121	-24.927	-3.110	-.244	-.7652	1.0000	
4	5	8	40.142	40.863	40.669	3.978	-.721	-2.5427	1.0000	
4	6	-8	24.974	24.937	24.776	2.835	.037	.1119	1.0000	
4	6	-7	40.126	39.804	-39.624	-3.780	.322	1.1416	1.0000	
4	6	-6	11.611	10.268	-10.264	-.312	1.343	2.8014	1.0000	
4	6	-5	48.069	46.922	46.761	3.884	1.147	4.0434	1.0000	
4	6	-4	29.799	29.186	29.000	3.292	.613	2.0940	1.0000	
4	6	-3	53.697	54.465	-54.299	-4.250	-.768	-2.1643	1.0000	
4	6	-2	13.655	13.418	-13.412	-.418	.237	.5737	1.0000	
4	6	-1	51.940	51.769	51.606	4.115	.171	.5700	1.0000	
4	6	0	33.210	33.236	33.077	3.250	-.027	-.0945	1.0000	
4	6	1	43.551	43.330	-43.155	-3.880	.222	.8239	1.0000	
4	6	2	9.006	9.566	-9.163	-.163	-.560	-.9451	1.0000	
4	6	3	31.912	32.248	32.055	3.523	-.336	-1.1337	1.0000	
5	0	-16	25.556	24.004	23.849	2.718	1.552	4.8746	1.0000	
5	0	5	34.492	34.023	-33.910	-2.766	.469	1.5834	1.0000	
5	0	-14	74.543	74.350	74.044	-5.737	.193	.3641	1.0000	
5	0	-12	61.687	61.629	-61.536	-3.394	.058	.1262	1.0000	
5	0		70.472	69.635	69.321	6.613	.837	1.4989	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	0	-10	26.540	25.613	-25.531	-2.052	.927	3.7531	1.0000
5	0	-8	67.863	65.653	65.445	5.217	2.210	3.9991	1.0000
5	0	-6	23.752	22.446	-22.444	.304	1.306	5.8496	1.0000
5	0	-4	56.125	54.921	54.848	2.836	1.204	2.4366	1.0000
5	0	-2	50.614	49.158	49.058	3.127	1.456	3.4308	1.0000
5	0	0	3.112	3.146	-3.144	.108	-.033	-.0347	1.0000
5	0	2	114.239	113.214	113.072	5.656	1.025	1.1770	1.0000
5	0	4	48.254	47.088	-47.036	-2.213	1.165	2.6763	1.0000
5	0	6	91.658	91.730	91.447	7.203	-.072	-.0712	1.0000
5	0	8	37.396	36.727	-36.556	-3.546	-.669	-2.7689	1.0000
5	0	10	87.080	87.188	86.872	7.417	-.108	-.1288	1.0000
5	0	12	57.104	58.352	-58.235	-3.693	-1.248	-2.8421	1.0000
5	1	-16	15.189	14.547	-14.515	-.966	.641	1.5504	1.0000
5	1	-15	24.851	25.205	25.046	2.826	-.354	-1.1049	1.0000
5	1	-14	23.303	23.652	23.589	1.731	-.349	-1.1029	1.0000
5	1	-13	7.560	7.731	-7.729	-.204	-.171	-.2734	1.0000
5	1	-12	38.973	38.907	-38.810	-2.747	.066	.2689	1.0000
5	1	-11	53.521	53.135	52.932	4.638	.386	.9132	1.0000
5	1	-10	59.124	57.772	57.668	3.462	1.352	3.1310	1.0000
5	1	-9	30.055	29.422	-29.392	-1.340	.633	2.7442	1.0000
5	1	-8	59.810	54.130	-53.962	-4.253	5.680	11.6710	1.0000
5	1	-7	96.481	95.425	95.234	6.037	1.057	1.1505	1.0000
5	1	-6	67.147	66.063	65.897	4.674	1.084	2.0577	1.0000
5	1	-5	51.071	49.521	-49.480	-2.017	1.550	3.8335	1.0000
5	1	-4	74.799	72.954	-72.782	-5.000	1.845	3.0287	1.0000
5	1	-3	99.129	100.308	100.090	6.607	-1.179	-1.3975	1.0000
5	1	-2	119.739	122.825	122.725	4.965	-3.086	-3.7067	1.0000
5	1	-1	33.376	31.920	-31.858	-1.977	1.456	6.4187	1.0000
5	1	0	93.289	93.085	-92.965	-4.720	.204	.2390	1.0000
5	1	1	96.708	95.657	95.458	6.167	1.051	1.2195	1.0000
5	1	2	60.778	58.957	58.805	4.225	1.821	3.4438	1.0000
5	1	3	35.466	35.185	-35.164	-1.210	.280	1.0350	1.0000
5	1	4	42.530	41.840	-41.694	-3.488	.690	1.9451	1.0000
5	1	5	71.544	70.344	70.176	4.847	1.200	2.1027	1.0000
5	1	6	35.482	35.202	35.100	2.687	.280	1.1160	1.0000
5	1	7	12.349	5.752	-5.752	.035	6.597	18.0267	1.0000
5	1	8	30.803	29.871	-29.823	-1.687	.933	3.6152	1.0000
5	1	9	29.449	28.856	28.696	3.036	.594	2.1775	1.0000
5	1	10	10.235	8.836	8.796	.833	1.400	2.7919	1.0000
5	1	11	11.637	11.275	11.193	1.355	.362	.7525	1.0000
5	1	12	8.126	6.446	-6.444	.145	1.680	2.5360	1.0000
5	2	-15	46.252	47.627	47.387	4.779	-1.376	-4.9791	1.0000
5	2	-14	31.438	31.511	31.424	2.343	-.073	-.2493	1.0000
5	2	-13	56.085	57.356	-57.153	-4.814	-1.271	-3.0867	1.0000
5	2	-12	16.081	15.432	15.392	1.114	.650	1.8393	1.0000
5	2	-11	63.179	63.392	63.260	4.088	-.214	-.4200	1.0000
5	2	-10	20.910	20.508	20.358	2.470	-.403	-1.4285	1.0000
5	2	-9	57.567	57.431	-57.324	-3.508	.135	.2837	1.0000
5	2	-8	20.497	19.867	19.804	1.583	.629	2.3562	1.0000
5	2	-7	33.306	33.006	32.925	2.311	.301	1.3585	1.0000
5	2	-6	39.892	39.471	39.401	2.348	.421	1.4468	1.0000
5	2	-5	8.578	8.013	-7.916	-1.242	.565	1.3359	1.0000
5	2	-4	21.208	20.570	20.564	2.093	.638	2.7242	1.0000

CU(D3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	2	-3	7.381	7.295	-7.293	-.157	.087	.1820	1.0000
5	2	-2	22.634	21.963	21.869	2.030	.671	2.9553	1.0000
5	2	-1	24.860	24.019	23.977	1.417	.842	3.8340	1.0000
5	2	0	26.412	25.927	25.805	2.513	.485	2.2289	1.0000
5	2	1	33.175	32.490	-32.382	-2.649	.684	3.2811	1.0000
5	2	2	2.198 *	2.166	1.437	1.621	.031	.0198	1.0000 **
5	2	3	50.089	49.314	49.172	3.742	.775	1.8987	1.0000
5	2	4	33.746	32.858	32.746	2.721	.887	3.9744	1.0000
5	2	5	65.746	66.299	-66.148	-4.479	-.554	-.9199	1.0000
5	2	6	10.415	10.203	10.127	1.239	.212	.4909	1.0000
5	2	7	76.126	77.426	77.256	5.128	-1.301	-2.0310	1.0000
5	2	8	15.412	14.784	14.545	2.646	.628	1.7152	1.0000
5	2	9	70.651	70.442	-70.249	-5.206	.209	.3517	1.0000
5	2	10	2.585 *	2.342	2.136	-.960	.244	.1321	1.0000 **
5	3	-14	53.143	54.509	54.250	5.309	-1.367	-3.6257	1.0000
5	3	-13	13.064	12.935	12.890	1.081	.129	.2872	1.0000
5	3	-12	36.276	37.150	36.949	3.862	-.874	-3.1013	1.0000
5	3	-11	25.371	25.056	-24.978	-1.974	.315	1.0573	1.0000
5	3	-10	19.267	19.282	-19.229	-1.427	-.015	-.0458	1.0000
5	3	-9	24.527	24.488	24.390	2.195	.039	.1396	1.0000
5	3	-8	70.565	72.602	72.372	5.772	-2.036	-3.6611	1.0000
5	3	-7	42.528	43.248	-43.151	-2.897	-.720	-2.6236	1.0000
5	3	-6	54.515	54.887	-54.824	-2.633	-.372	-.8470	1.0000
5	3	-5	43.934	44.376	44.275	2.999	-.442	-1.4834	1.0000
5	3	-4	104.611	105.790	105.562	6.939	-1.179	-1.1841	1.0000
5	3	-3	58.516	58.776	-58.681	-3.334	-.259	-.5779	1.0000
5	3	-2	46.916	46.217	-46.115	-3.063	.699	2.0663	1.0000
5	3	-1	37.548	37.797	37.658	3.242	-.249	-1.1361	1.0000
5	3	0	81.110	81.251	80.950	6.988	-.141	-.2044	1.0000
5	3	1	48.404	48.449	-48.347	-3.130	-.045	-.1393	1.0000
5	3	2	46.814	46.860	-46.791	-2.539	-.046	-.1542	1.0000
5	3	3	44.625	44.758	44.667	2.847	-.132	-.4331	1.0000
5	3	4	85.767	86.967	86.767	5.895	-1.200	-1.6520	1.0000
5	3	5	33.226	33.518	-33.437	-2.330	-.292	-1.2092	1.0000
5	3	6	32.298	32.413	-32.390	-1.222	-.115	-.4611	1.0000
5	3	7	24.518	25.412	25.338	1.941	-.894	-3.1711	1.0000
5	3	8	40.177	40.049	39.849	3.994	.129	.5018	1.0000
5	3	9	12.896	12.154	-12.097	-1.170	.742	1.8032	1.0000
5	3	10	3.539 *	2.180	2.132	.457	1.359	1.0117	1.0000
5	4	-14	13.330	13.509	13.485	.802	-.180	-.4055	1.0000
5	4	-13	11.238	10.965	10.920	.995	.273	.5257	1.0000
5	4	-12	34.033	34.662	-34.587	-2.270	-.629	-2.1744	1.0000
5	4	-11	22.094	21.932	-21.896	-1.255	.162	.4976	1.0000
5	4	-10	49.492	50.762	50.528	4.868	-1.270	-4.1561	1.0000
5	4	-9	15.077	14.898	14.881	.707	.179	.4780	1.0000
5	4	-8	16.914	16.939	-16.922	-.762	-.025	-.0731	1.0000
5	4	-7	6.688	6.600	-6.560	-.727	.087	.1359	1.0000
5	4	-6	35.387	36.408	36.258	3.311	-1.022	-4.1358	1.0000
5	4	-5	5.431	6.517	-6.515	.174	-1.087	-1.4451	1.0000
5	4	-4	8.989	8.486	-8.376	1.365	.503	1.0657	1.0000
5	4	-3	4.891 *	.815	.815	.013	4.076	5.1683	1.0000 **
5	4	-2	13.044	12.862	12.805	1.202	.183	.5040	1.0000
5	4	-1	8.199	7.737	-7.724	-.449	.462	.9352	1.0000

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
5	4	0	49.545	50.281	50.153	3.572	-.735	-2.3093	1.0000	
5	4	1	3.919*	4.350	4.284	.759	-.431	-.4246	1.0000	**
5	4	2	16.705	16.181	-16.157	-.884	.524	1.6470	1.0000	
5	4	3	6.891	6.508	-6.437	-.963	.382	.6130	1.0000	
5	4	4	62.747	63.190	62.971	5.258	-.443	-1.0045	1.0000	
5	4	5	15.897	16.302	16.251	1.296	-.406	-1.1145	1.0000	
5	4	6	30.661	31.362	-31.270	-2.391	-.701	-2.5200	1.0000	
5	4	7	22.621	22.096	-22.063	-1.211	.525	1.6570	1.0000	
5	4	8	65.199	65.440	65.165	5.991	-.241	-.5015	1.0000	
5	4	9	21.388	21.632	21.581	1.492	-.245	-.7039	1.0000	
5	5	-10	35.356	35.709	-35.546	-3.402	-.353	-1.2130	1.0000	
5	5	-9	30.009	30.075	29.909	3.154	-.066	-.2201	1.0000	
5	5	-8	43.500	43.461	43.305	3.689	.038	.1440	1.0000	
5	5	-7	7.299	7.016	-7.007	-.355	.283	.4173	1.0000	
5	5	-6	48.210	48.618	-48.415	-4.443	-.409	-1.5295	1.0000	
5	5	-5	32.959	33.508	33.307	3.665	-.549	-2.0288	1.0000	
5	5	-4	60.926	60.976	60.813	4.469	-.050	-.1260	1.0000	
5	5	-3	16.660	16.133	-16.125	-.495	.527	1.4837	1.0000	
5	5	-2	57.267	57.921	-57.738	-4.607	-.655	-1.7283	1.0000	
5	5	-1	49.231	49.727	49.587	4.309	-.496	-1.5150	1.0000	
5	5	0	58.701	58.715	58.556	-.334	-.013	-.0354	1.0000	
5	5	1	7.291	8.130	-8.123	-.839	-.839	-1.2696	1.0000	
5	5	2	45.496	45.309	-45.148	-3.808	.187	.7313	1.0000	
5	5	3	30.328	30.162	29.978	3.322	.166	.5810	1.0000	
5	5	4	33.495	33.476	33.317	3.262	.019	.0681	1.0000	
5	5	5	4.183*	1.566	-1.564	.083	2.616	2.2697	1.0000	**
5	5	6	25.922	25.905	-25.805	-2.284	.016	.0521	1.0000	
5	6	-6	4.695*	2.633	2.494	.846	2.062	1.9262	1.0000	**
5	6	-5	12.325	12.129	11.110	.654	1.196	2.5228	1.0000	
5	6	-4	15.756	14.773	14.696	1.515	.982	2.4626	1.0000	
5	6	-3	5.650*	2.971	2.971	-.016	2.679	3.0503	1.0000	**
5	6	-2	12.795	12.308	12.190	1.705	.487	1.0862	1.0000	
5	6	-1	7.460	7.854	-7.801	-.913	-.394	-.5626	1.0000	
5	6	0	4.796*	2.522	-2.418	.716	2.274	2.1801	1.0000	**
5	6	1	20.143	19.551	19.479	1.679	.592	1.6938	1.0000	
5	6	2	22.160	22.065	21.932	2.424	.095	.2780	1.0000	
6	0	-14	45.165	44.488	44.273	4.367	.677	2.4337	1.0000	
6	0	-12	35.250	33.867	-33.807	-2.017	1.383	5.3603	1.0000	
6	0	-10	89.320	87.823	87.560	6.786	1.497	1.9760	1.0000	
6	0	-8	67.769	67.816	-67.718	-3.627	-.046	-.0780	1.0000	
6	0	-6	103.380	103.115	102.775	8.360	.265	.803	1.0000	
6	0	-4	86.063	83.384	-83.273	-4.298	2.679	4.0902	1.0000	
6	0	-2	134.582	136.333	136.062	8.588	-1.751	-1.9216	1.0000	
6	0	0	76.256	74.427	-74.332	-3.763	1.829	2.7610	1.0000	
6	0	2	97.213	95.512	95.227	7.381	1.701	1.7574	1.0000	
6	0	4	37.321	36.862	-36.798	-2.171	.459	1.7549	1.0000	
6	0	6	71.017	69.496	69.308	5.106	1.522	2.3827	1.0000	
6	0	8	4.913*	2.689	-2.688	-.035	2.224	2.4214	1.0000	**
6	0	-10	22.978	22.299	22.166	2.433	.679	2.0834	1.0000	
6	1	-15	46.023	46.061	45.814	4.768	-.038	-.1387	1.0000	
6	1	-14	43.434	44.220	44.077	3.553	-.786	-.9231	1.0000	
6	1	-13	21.708	22.453	-22.416	-1.283	-.745	-2.3275	1.0000	
6	1	-12	43.257	43.045	-42.916	-3.336	.212	.7865	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
6	1	-11	53.862	54.210	54.025	4.469	-.348	-.8488	1.0000
6	1	-10	26.504	25.861	25.722	2.672	.643	2.4575	1.0000
6	1	-9	10.133	10.041	-10.040	-.082	.092	.2197	1.0000
6	1	-8	34.657	34.300	-34.241	-2.016	.357	1.5483	1.0000
6	1	-7	39.308	38.928	38.780	3.399	.380	1.5486	1.0000
6	1	-6	18.925	19.129	19.101	1.036	-.204	-.7483	1.0000
6	1	-5	18.601	17.805	17.732	1.610	.796	2.9991	1.0000
6	1	-4	6.627	4.277	4.276	-.103	2.350	4.3397	1.0000
6	1	-3	22.264	21.048	20.969	1.819	1.216	5.1121	1.0000
6	1	-2	9.337	9.162	-9.113	-.946	.175	.4223	1.0000
6	1	-1	43.597	42.373	42.239	3.375	1.224	3.6949	1.0000
6	1	0	31.310	30.924	30.866	1.891	.386	1.7430	1.0000
6	1	1	7.405	6.544	-6.542	.164	.861	1.7365	1.0000
6	1	2	37.204	36.748	-36.647	-2.725	.455	1.8999	1.0000
6	1	3	60.868	60.644	60.459	4.735	.224	.4332	1.0000
6	1	4	61.219	60.642	60.546	3.419	.577	1.0905	1.0000
6	1	5	24.441	24.084	-24.058	-1.120	.357	1.3375	1.0000
6	1	6	44.528	44.368	-44.203	-3.820	.160	.5475	1.0000
6	1	7	63.504	63.125	62.899	5.335	.380	.7255	1.0000
6	1	8	47.820	47.966	47.790	4.100	-.146	-.4373	1.0000
6	1	9	26.101	26.655	-26.597	-1.747	-.553	-1.8333	1.0000
6	2	-14	47.853	47.803	-47.636	-4.001	.050	.1504	1.0000
6	2	-13	11.267	10.365	10.287	1.262	.903	1.8344	1.0000
6	2	-12	33.446	34.698	34.569	2.987	-1.252	-4.3880	1.0000
6	2	-11	21.702	21.513	21.399	2.208	.190	.5962	1.0000
6	2	-10	52.153	53.072	-52.903	-4.231	-.920	-2.8558	1.0000
6	2	-9	7.996	5.808	5.683	1.201	2.188	3.9076	1.0000
6	2	-8	65.561	65.953	65.770	4.914	-.392	-.7907	1.0000
6	2	-7	37.081	37.173	37.075	2.698	-.091	-.3844	1.0000
6	2	-6	85.121	86.366	-86.175	-5.743	-1.245	-1.6971	1.0000
6	2	-5	23.766	23.374	23.344	1.178	.393	1.5330	1.0000
6	2	-4	92.262	91.775	91.579	5.997	.487	.6932	1.0000
6	2	-3	36.309	37.549	37.434	2.935	.760	3.0311	1.0000
6	2	-2	86.930	88.460	-88.245	-6.163	-1.530	-2.2006	1.0000
6	2	-1	9.665	9.142	9.057	1.239	.523	1.2759	1.0000
6	2	0	84.422	84.764	84.561	5.866	-.342	-.4919	1.0000
6	2	1	40.957	40.368	40.267	2.853	.589	2.2192	1.0000
6	2	2	83.739	81.437	-81.263	5.322	2.302	3.2239	1.0000
6	2	3	15.344	15.379	15.317	1.382	-.035	-.1064	1.0000
6	2	4	70.406	70.707	70.561	4.547	-.301	-.4911	1.0000
6	2	5	26.403	25.344	25.223	2.480	1.059	4.1031	1.0000
6	2	6	43.762	43.247	-43.108	1.552	.515	1.7691	1.0000
6	2	7	7.871	7.343	7.178	2.458	.528	.8641	1.0000
6	2	8	27.155	27.621	27.512	1.922	-.466	-1.6440	1.0000
6	2	9	9.745	9.645	9.451	-1.165	.100	.1855	1.0000
6	2	10	12.993	13.961	-13.912	1.667	-.968	-2.1082	1.0000
6	3	-13	12.384	11.604	11.484	5.090	.780	1.6778	1.0000
6	3	-12	49.575	51.253	51.000	-2.279	-1.679	-5.4932	1.0000
6	3	-11	21.604	22.042	-21.924	-1.415	-.439	-1.3393	1.0000
6	3	-10	27.386	28.146	-28.111	1.629	-.761	-2.5660	1.0000
6	3	-9	25.717	25.830	25.779	4.182	-.113	-.3843	1.0000
6	3	-8	48.830	49.345	49.167	-1.408	-.515	-1.5552	1.0000
6	3	-7	16.952	17.148	-17.090		-.196	-.6008	1.0000

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
6	3	-7	2.346*	1.699	1.674	.293	.647	.3862	1.0000	**
6	3	-6	11.544	11.213	11.196	.627	.330	.8245	1.0000	
6	3	-5	27.084	27.433	27.319	2.494	-.349	-1.3640	1.0000	
6	3	-4	7.226	6.372	-6.370	-.157	.854	1.4952	1.0000	
6	3	-3	26.445	26.222	26.112	2.395	.223	.8905	1.0000	
6	3	-2	15.796	15.745	-15.734	-.586	.051	.1618	1.0000	
6	3	-1	2.287*	.536	.235	-.482	1.751	1.0719	1.0000	**
6	3	0	18.151	18.416	18.380	1.160	-.266	-.8848	1.0000	
6	3	1	52.832	54.101	53.928	4.323	-1.270	-3.4358	1.0000	
6	3	2	25.795	26.274	-26.220	-1.684	-.479	-1.7928	1.0000	
6	3	3	22.249	21.903	-21.865	-1.288	.346	1.2205	1.0000	
6	3	4	16.753	16.972	16.829	2.200	-.219	-.6509	1.0000	
6	3	5	61.578	61.855	61.607	5.542	-.278	-.5730	1.0000	
6	3	6	31.760	32.051	-31.962	-2.377	-.290	-1.0373	1.0000	
6	3	7	37.605	38.442	-38.369	-2.358	-.837	-3.0500	1.0000	
6	3	8	32.196	32.609	32.496	2.718	-.413	-1.4114	1.0000	
6	3	9	56.081	57.897	57.610	5.759	-1.816	-4.9377	1.0000	
6	4	-12	43.577	44.711	44.478	4.552	-1.134	-3.9977	1.0000	
6	4	-11	8.792	8.722	8.685	.801	.070	.1126	1.0000	
6	4	-10	30.450	31.025	-30.938	-2.322	-.575	-1.9647	1.0000	
6	4	-9	10.031	11.194	-11.110	-1.372	-1.164	-2.1928	1.0000	
6	4	-8	61.753	62.884	62.578	6.201	-1.131	-2.7974	1.0000	
6	4	-7	20.381	20.392	20.353	1.262	-.010	-.0322	1.0000	
6	4	-6	56.341	55.589	-55.492	-3.279	.752	2.0980	1.0000	
6	4	-5	25.053	25.047	-24.997	-1.583	.005	.0189	1.0000	
6	4	-4	83.064	84.820	84.535	6.950	-1.756	-2.6806	1.0000	
6	4	-3	16.548	16.678	16.616	1.435	-.130	-.3785	1.0000	
6	4	-2	53.362	54.078	-53.974	-3.349	-.716	-1.9373	1.0000	
6	4	-1	15.556	15.151	-15.082	-1.439	.405	1.1540	1.0000	
6	4	0	73.268	73.644	73.352	6.553	-.377	-.7350	1.0000	
6	4	1	15.787	15.351	15.299	1.261	.436	1.2222	1.0000	
6	4	2	35.387	35.553	-35.466	-2.479	-.166	-.6294	1.0000	
6	4	3	16.499	16.354	-16.325	-.967	.145	.4019	1.0000	
6	4	4	54.019	54.726	54.485	5.124	-.707	-1.8839	1.0000	
6	4	5	8.892	6.092	6.038	.810	2.801	4.9058	1.0000	
6	4	6	15.026	15.987	-15.959	-.941	-.961	-2.3239	1.0000	
6	4	7	7.010	4.022	-4.010	-.313	2.988	4.1027	1.0000	
6	5	-9	18.746	18.899	18.744	2.417	-.153	-.4168	1.0000	
6	5	-8	19.692	19.698	19.629	1.651	-.007	-.0193	1.0000	
6	5	-7	2.627*	2.753	2.623	-.837	-.126	-.0671	1.0000	**
6	5	-6	15.064	15.267	-15.227	-1.100	-.202	-.5053	1.0000	
6	5	-5	12.724	12.419	12.284	1.826	.305	.6995	1.0000	
6	5	-4	5.734	2.679	-2.679	-.029	3.055	3.7610	1.0000	
6	5	-3	11.650	12.110	11.994	1.677	-.460	-.9868	1.0000	
6	5	-2	15.485	15.566	15.544	.830	-.081	-.2099	1.0000	
6	5	-1	10.665	9.675	9.617	1.063	.990	2.0497	1.0000	
6	5	0	21.232	21.882	-21.810	-1.771	-.650	-1.9412	1.0000	
6	5	1	19.604	19.483	19.331	2.425	.121	.3501	1.0000	
6	5	2	31.041	31.791	31.687	2.572	-.750	-2.5302	1.0000	
6	5	3	7.198	6.410	-6.402	-.323	.788	1.1021	1.0000	
6	5	4	28.421	28.589	-28.423	-3.077	-.168	-.5496	1.0000	
7	0	-14	66.126	67.466	67.189	6.114	-1.340	-3.0904	1.0000	
7	0	-12	31.685	31.310	-31.229	-2.254	.375	1.3413	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
7	0	-10	67.722	66.753	66.560	5.063	.969	1.8850	1.0000	
7	0	-8	17.269	16.276	-16.274	-.224	.993	3.2117	1.0000	
7	0	-6	28.672	27.177	27.009	3.017	1.495	6.1422	1.0000	
7	0	-4	41.452	40.050	39.979	2.378	1.403	5.3230	1.0000	
7	0	-2	7.747	6.766	-6.747	.509	.981	1.9705	1.0000	
7	0	0	40.863	39.650	39.350	4.866	1.213	3.9949	1.0000	
7	0	2	31.259	30.558	30.507	-1.764	.701	2.8576	1.0000	
7	0	4	80.685	79.785	79.515	6.559	.900	1.3939	1.0000	
7	0	6	55.686	55.421	55.328	-3.207	.265	.5761	1.0000	
7	0	8	75.279	76.118	75.792	7.039	-.840	-1.3342	1.0000	
7	1	-14	16.861	17.815	-17.675	-2.235	-.954	-2.4491	1.0000	
7	1	-13	42.980	42.892	42.714	3.910	.088	.3255	1.0000	
7	1	-12	26.871	27.218	27.061	2.915	-.346	-1.1616	1.0000	
7	1	-11	21.086	21.201	-21.201	-1.125	-.115	-.3608	1.0000	
7	1	-10	57.258	57.192	-57.071	-3.718	.065	.1470	1.0000	
7	1	-9	59.644	59.764	59.526	5.326	-.120	-.2551	1.0000	
7	1	-8	61.735	61.152	61.010	4.168	.583	1.2799	1.0000	
7	1	-7	30.406	29.988	-29.930	-1.854	.419	1.6820	1.0000	
7	1	-6	70.111	70.065	-69.915	-4.582	.047	.0883	1.0000	
7	1	-5	77.057	78.327	78.093	6.051	-1.270	-2.1040	1.0000	
7	1	-4	57.340	56.897	56.709	4.629	.443	1.0204	1.0000	
7	1	-3	39.511	38.786	-38.737	-1.946	.725	2.7903	1.0000	
7	1	-2	65.557	64.341	-64.182	-4.521	1.216	2.3483	1.0000	
7	1	-1	78.691	78.981	78.763	5.854	-.290	-.4839	1.0000	
7	1	0	51.306	51.222	51.056	4.126	.083	.2169	1.0000	
7	1	1	29.206	29.378	-29.347	-1.339	-.172	-.6903	1.0000	
7	1	2	48.733	48.108	-47.978	-3.531	.625	1.7518	1.0000	
7	1	3	53.413	52.776	52.559	4.789	.637	1.5828	1.0000	
7	1	4	50.226	49.437	49.357	2.810	.789	2.0063	1.0000	
7	1	5	6.730	6.106	-6.102	-.219	.624	.8951	1.0000	
7	1	6	27.960	26.336	-26.267	-1.915	1.624	5.6881	1.0000	
7	1	7	30.046	30.153	29.985	3.171	-.107	-.3666	1.0000	
7	1	8	8.093	8.964	8.897	1.092	-.871	-1.3118	1.0000	
7	1	9	5.440 *	2.047	1.754	1.055	3.393	3.6150	1.0000	**
7	2	-13	43.868	45.224	45.052	3.944	-1.357	-4.8785	1.0000	
7	2	-12	16.813	17.246	17.105	2.203	-.433	-1.1434	1.0000	
7	2	-11	39.363	40.306	-40.150	-3.536	-.943	-3.5049	1.0000	
7	2	-10	4.527 *	4.680	4.489	1.325	-.153	-.1490	1.0000	**
7	2	-9	26.816	26.248	26.294	2.484	.406	1.4400	1.0000	
7	2	-8	23.351	23.303	23.204	2.143	.048	.1693	1.0000	
7	2	-7	20.672	20.927	-20.866	-1.589	-.254	-.8632	1.0000	
7	2	-6	22.850	22.208	22.134	1.813	.641	2.2763	1.0000	
7	2	-5	11.718	11.269	11.265	.280	.449	1.1413	1.0000	
7	2	-4	11.566	11.221	11.061	1.892	.344	.8874	1.0000	
7	2	-3	6.404	3.743	3.644	.857	2.661	4.2026	1.0000	
7	2	-2	26.176	26.248	26.151	2.249	-.072	-.2782	1.0000	
7	2	-1	34.454	34.656	-34.593	-2.090	-.203	-.8390	1.0000	
7	2	0	28.793	28.931	28.890	1.540	-.138	-.5424	1.0000	
7	2	1	49.977	50.750	50.653	3.140	-.773	-2.3336	1.0000	
7	2	2	28.714	27.909	27.796	2.508	.805	3.0553	1.0000	
7	2	3	53.406	53.192	-53.044	-3.968	.214	.5467	1.0000	
7	2	4	7.033	6.815	6.710	1.193	.219	.3339	1.0000	
7	2	5	52.832	53.054	52.850	4.648	-.223	-.5995	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
7	2	6	28.866	28.332	28.220	2.509	.534	1.8358	1.0000	
7	2	7	51.357	52.221	-51.993	-4.875	-.864	-2.5665	1.0000	
7	2	8	5.200*	5.214	5.130	.931	-.014	-.0146	1.0000	**
7	3	-12	23.835	23.630	24.562	1.827	-.794	-2.3982	1.0000	
7	3	-11	50.107	50.967	50.723	4.984	-.860	-2.7013	1.0000	
7	3	-10	21.047	22.676	-22.532	-2.552	-1.629	-4.8128	1.0000	
7	3	-9	28.392	28.997	-28.904	-2.328	-.605	-2.0805	1.0000	
7	3	-8	33.416	33.619	33.514	2.651	-.203	-.7483	1.0000	
7	3	-7	65.993	66.827	66.534	6.249	-.834	-1.7328	1.0000	
7	3	-6	37.511	38.048	-37.924	-3.074	-.537	-2.0955	1.0000	
7	3	-5	45.986	46.199	-46.109	-2.881	-.213	-.7968	1.0000	
7	3	-4	46.453	45.981	45.883	2.997	.472	1.7793	1.0000	
7	3	-3	81.994	83.084	82.826	6.532	-1.090	-1.6731	1.0000	
7	3	-2	35.089	35.886	-35.759	-3.017	-.797	-3.1346	1.0000	
7	3	-1	43.304	44.181	-44.107	-2.553	-.877	-3.4967	1.0000	
7	3	0	37.504	37.076	36.974	2.751	.428	1.6813	1.0000	
7	3	1	68.821	69.791	69.555	5.730	-.970	-1.8659	1.0000	
7	3	2	30.251	30.415	-30.322	-2.377	-.164	-.6010	1.0000	
7	3	3	18.222	18.134	-18.077	-1.427	.089	.2563	1.0000	
7	3	4	19.514	18.774	16.668	1.988	.740	2.1992	1.0000	
7	3	5	34.371	35.244	35.006	4.085	-.872	-3.0952	1.0000	
7	3	6	17.723	17.585	-17.534	-1.337	.138	.3671	1.0000	
7	3	7	5.427*	3.842	-3.839	.134	1.585	1.6473	1.0000	**
7	4	-10	16.096	17.096	-17.063	-1.060	-1.000	-2.4727	1.0000	
7	4	-9	2.642*	2.642	-3.756	-.784	-1.195	-1.6328	1.0000	**
7	4	-8	33.693	33.705	33.540	3.332	-.013	-.0445	1.0000	
7	4	-7	6.179	4.885	4.880	.226	1.294	1.6186	1.0000	**
7	4	-6	3.074*	2.758	2.628	.838	.315	.2033	1.0000	
7	4	-5	6.757	6.935	-6.934	-.125	-.178	-.2460	1.0000	
7	4	-4	10.171	9.831	9.723	1.452	.340	.6836	1.0000	
7	4	-3	3.522*	2.459	2.433	-.354	1.063	.8196	1.0000	
7	4	-2	29.190	29.038	28.890	2.935	.151	.5295	1.0000	
7	4	-1	14.841	14.428	14.416	.581	.413	1.0701	1.0000	
7	4	0	17.748	17.934	-17.927	-.525	-.186	-.5325	1.0000	
7	4	1	17.867	17.440	-17.418	-.866	.428	1.2303	1.0000	
7	4	2	42.159	42.251	-41.993	-4.664	-.092	-.3409	1.0000	
7	4	3	12.431	11.974	11.921	1.131	.457	1.0024	1.0000	
7	4	4	29.695	29.542	-29.470	-2.062	.153	.5090	1.0000	
7	4	5	8.596	8.751	-8.675	-1.149	-.155	-.2395	1.0000	
7	5	-6	45.749	45.687	45.507	4.049	.061	.195	1.0000	
7	5	-5	8.062	7.670	-7.654	-.491	.392	.5847	1.0000	
7	5	-4	51.183	51.088	-50.903	-4.346	.095	.3490	1.0000	
7	5	-3	30.701	30.669	30.473	3.460	.032	.1077	1.0000	
7	5	-2	42.314	42.024	41.825	4.078	.291	1.0448	1.0000	
7	5	-1	10.869	10.560	10.553	-.393	.308	.5894	1.0000	
7	5	0	41.785	41.415	-41.242	-3.775	.371	1.3247	1.0000	
7	5	1	28.026	28.298	28.118	3.187	-.272	-.8656	1.0000	
8	0	-12	56.065	55.982	55.686	5.746	.083	.2610	1.0000	
8	0	-10	47.342	47.057	-46.951	-3.155	.286	1.1000	1.0000	
8	0	-8	98.717	98.535	-98.257	7.398	.183	.2237	1.0000	
8	0	-6	55.882	54.868	-54.725	-3.964	1.014	2.4625	1.0000	
8	0	-4	99.749	98.057	97.739	7.895	1.692	2.1759	1.0000	
8	0	-2	52.098	51.116	-50.984	-3.682	.981	2.5788	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
8	0	0	80.673	79.969	79.657	7.059	.704	1.0805	1.0000	
8	0	2	40.267	39.577	-39.507	-2.365	.690	2.6539	1.0000	
8	0	4	61.431	60.955	60.738	5.137	.476	1.0212	1.0000	
8	0	6	17.415	17.744	-17.739	-.424	-.329	-.8679	1.0000	
8	1	-13	38.576	39.456	39.242	4.101	-.880	-3.0626	1.0000	
8	1	-12	31.641	32.385	32.279	2.627	-.744	-2.5252	1.0000	
8	1	-11	9.637	8.753	-8.745	-.381	.884	1.6317	1.0000	
8	1	-10	28.368	28.426	-28.347	-2.109	-.057	-.1951	1.0000	
8	1	-9	31.228	31.195	31.024	3.264	.033	-.1178	1.0000	
8	1	-8	22.595	22.221	22.186	1.247	.374	1.2244	1.0000	
8	1	-7	7.108	6.263	6.163	1.111	.846	1.3244	1.0000	
8	1	-6	3.365 *	1.433	-1.365	-.436	1.932	1.5017	1.0000	**
8	1	-5	22.668	22.394	23.313	1.897	.275	.9501	1.0000	
8	1	-4	21.309	21.343	-21.336	-.547	-.034	-.1178	1.0000	
8	1	-3	27.506	27.671	27.532	2.770	-.165	-.6142	1.0000	
8	1	-2	13.121	12.943	12.865	1.422	.178	.4607	1.0000	
8	1	-1	7.035	6.242	-6.231	.372	.743	1.2531	1.0000	
8	1	0	24.855	23.944	-23.837	-2.263	.911	3.2114	1.0000	
8	1	1	49.371	49.402	49.227	4.152	-.030	-.0834	1.0000	
8	1	2	29.951	30.486	30.343	2.953	-.536	-1.9383	1.0000	
8	1	3	16.502	17.061	-17.038	-.890	-.559	-1.5343	1.0000	
8	1	4	49.335	48.590	-48.469	-3.427	.745	2.1995	1.0000	
8	1	5	46.583	47.084	46.830	4.886	-.501	-1.6712	1.0000	
8	1	6	42.552	42.565	42.399	3.756	-.013	-.0458	1.0000	
8	2	-12	8.519	7.993	7.926	1.034	.526	.7968	1.0000	
8	2	-11	47.480	48.567	48.386	4.189	-1.087	-3.9881	1.0000	**
8	2	-10	20.312	20.836	20.704	2.336	-.524	-1.5226	1.0000	
8	2	-9	52.383	53.980	-53.742	-5.064	-1.597	-4.7170	1.0000	**
8	2	-8	2.790 *	2.254	-2.013	1.014	.536	.3203	1.0000	
8	2	-7	63.455	63.878	63.651	5.372	-.423	-.9319	1.0000	
8	2	-6	21.285	21.850	21.693	2.616	-.409	-1.3000	1.0000	
8	2	-5	73.537	73.837	-73.618	-5.681	-.301	-.5150	1.0000	
8	2	-4	4.679 *	3.141	2.952	1.072	1.538	1.6071	1.0000	
8	2	-3	73.328	73.715	73.510	5.489	-.387	-.7445	1.0000	
8	2	-2	24.204	23.554	23.409	2.614	.650	2.2326	1.0000	
8	2	-1	67.568	68.504	-68.311	-5.140	-.936	-1.7830	1.0000	
8	2	0	11.802	11.915	11.853	1.213	-.113	-.2559	1.0000	
8	2	1	53.874	54.011	53.825	4.477	-.136	-.3881	1.0000	
8	2	2	21.118	21.118	20.989	2.334	.167	.5126	1.0000	
8	2	3	39.321	39.615	-39.453	-3.586	-.294	-1.0870	1.0000	
8	2	4	7.321	6.926	6.784	1.392	.395	.5564	1.0000	
8	2	5	24.945	25.595	25.457	2.649	-.650	-2.0310	1.0000	
8	2	6	20.567	20.567	20.482	1.860	.113	.3148	1.0000	
8	3	-10	15.739	16.376	-16.309	-1.482	-.637	-1.5742	1.0000	
8	3	-9	7.584	3.379	-3.378	.757	4.205	6.3311	1.0000	**
8	3	-8	8.475	4.515	4.452	2.539	3.960	6.4796	1.0000	**
8	3	-7	23.018 *	23.242	23.102	-.393	-.224	-.7146	1.0000	
8	3	-6	2.715 *	3.018	-2.992	1.801	-.303	-.1742	1.0000	
8	3	-5	5.469 *	6.299	6.036	-.342	-.830	-.9165	1.0000	
8	3	-4	3.797 *	2.792	-2.771	.725	1.005	.8232	1.0000	
8	3	-3	6.646	4.732	4.676	.830	1.914	2.6953	1.0000	
8	3	-2	12.898	12.403	12.375	3.665	.495	1.1453	1.0000	
8	3	-1	42.512	42.750	42.592		-.238	-.9020	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
8	3	0	14.706	14.683	-14.616	-1.401	.023	.0557	1.0000	
8	3	1	24.244	24.472	-24.453	-.972	-.228	-.7333	1.0000	
8	3	2	24.537	25.037	24.968	1.865	-.501	-1.5544	1.0000	
8	3	3	48.321	49.131	48.880	4.969	-.810	-2.8755	1.0000	
8	3	4	21.183	21.903	-21.799	-2.137	-.721	-2.1065	1.0000	
8	4	-7	13.253	13.925	-13.848	-1.458	-.672	-1.4579	1.0000	
8	4	-6	67.268	68.098	67.808	6.271	-.830	-2.0153	1.0000	
8	4	-5	15.884	16.171	16.120	1.290	-.287	-.7075	1.0000	
8	4	-4	36.505	36.535	-36.397	-3.173	-.030	-.1051	1.0000	
8	4	-3	15.714	15.357	-16.298	-1.390	-.643	-1.5841	1.0000	
8	4	-2	61.797	63.011	62.711	6.140	-1.214	-2.8113	1.0000	
8	4	-1	17.845	16.978	16.937	1.185	.967	2.3462	1.0000	
8	4	0	37.409	36.968	-36.882	-2.525	.441	1.5442	1.0000	
8	4	1	12.501	11.826	-11.783	-1.004	.675	1.4075	1.0000	
9	0	-10	14.224	13.147	-13.131	-.653	1.077	2.5707	1.0000	
9	0	-8	34.454	34.264	34.128	3.045	.190	.6789	1.0000	
9	0	-6	13.350	12.725	12.617	1.654	.625	1.4846	1.0000	
9	0	-4	7.903	5.287	5.223	.821	2.615	4.2670	1.0000	
9	0	-2	45.309	44.296	44.115	4.004	1.014	3.5510	1.0000	
9	0	0	19.724	19.896	-19.852	-1.321	-.171	-.5086	1.0000	
9	0	2	70.375	68.886	68.645	5.754	1.489	2.6597	1.0000	
9	0	4	35.592	36.331	-36.223	-2.803	-.739	-2.5094	1.0000	
9	1	-10	43.352	44.674	44.530	3.592	-1.323	-4.6941	1.0000	
9	1	-9	24.828	25.457	-25.403	-1.654	-.629	-1.9650	1.0000	
9	1	-8	39.529	40.316	-40.111	-4.060	-.787	-2.8864	1.0000	
9	1	-7	57.993	58.480	58.234	5.350	-.486	-1.2139	1.0000	
9	1	-6	49.672	49.434	49.258	4.174	.237	.7495	1.0000	
9	1	-5	30.084	30.280	-30.223	-1.855	-.196	-.6861	1.0000	
9	1	-4	52.469	52.514	-52.346	-6.186	-.044	-.1323	1.0000	
9	1	-3	56.187	56.140	55.883	5.364	.047	.1251	1.0000	
9	1	-2	54.723	54.642	54.503	3.892	.082	.2271	1.0000	
9	1	-1	21.411	21.255	-21.208	-1.411	.157	.4843	1.0000	
9	1	0	39.270	39.279	-39.128	-3.443	-.009	-.0337	1.0000	
9	1	1	47.511	47.487	47.268	4.559	.024	.0808	1.0000	
9	1	2	25.117	25.508	25.352	2.819	-.392	-1.2376	1.0000	
9	1	3	12.590	12.502	-12.494	-.445	.088	.1883	1.0000	
9	2	-9	17.794	19.216	19.131	-1.811	-1.422	-3.7553	1.0000	**
9	2	-8	*4.503	5.881	5.684	1.506	-1.378	-1.2222	1.0000	**
9	2	-7	8.640	6.776	6.746	.634	1.864	3.1638	1.0000	
9	2	-6	*13.599	13.745	13.639	1.698	-.146	-.3454	1.0000	
9	2	-5	4.962	5.796	5.785	.355	-.834	-.8302	1.0000	
9	2	-4	15.728	15.331	15.209	1.934	.397	1.0243	1.0000	
9	2	-3	17.951	18.132	-18.066	-1.536	-.180	-.5047	1.0000	
9	2	-2	6.792	5.944	5.776	1.406	.847	1.1550	1.0000	
9	2	-1	30.862	30.624	30.521	2.508	.238	.8240	1.0000	
9	2	0	16.422	16.541	16.391	-2.225	-.120	-.3081	1.0000	
9	2	1	35.925	36.115	-35.956	-3.381	-.190	-.6607	1.0000	
9	2	2	*2.649	1.124	.219	-1.102	1.526	.8058	1.0000	
9	3	-7	38.197	38.098	-38.007	-2.627	-.100	.3449	1.0000	
9	3	-6	27.451	27.891	27.762	2.680	-.439	-1.3961	1.0000	
9	3	-5	59.869	60.970	60.684	5.898	-1.102	-3.1361	1.0000	**
9	3	-4	30.353	29.386	-29.251	-2.807	.968	3.2442	1.0000	
9	3	-3	29.947	30.283	-30.182	-2.479	-.336	-1.1131	1.0000	

CU(IO3)2.2H2O FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR	
9	3	-2	24.970	25.752	25.623	2.570	-.781	-2.3722	1.0000	
9	3	-1	49.862	50.398	50.111	5.374	-.536	-1.8786	1.0000	
9	3	-0	29.365	29.410	-29.317	-2.331	-.045	-.1434	1.0000	
10	0	-6	63.583	64.813	64.433	7.013	-1.230	-2.8138	1.0000	
10	0	-4	55.089	54.762	-54.651	-3.482	.327	.8562	1.0000	
10	0	-2	74.825	75.739	75.458	6.516	-.914	-1.5757	1.0000	
10	1	-6	4.190 *	4.485	4.481	-.198	-.295	-.2395	1.0000	**
10	1	-5	19.717	19.767	19.649	2.157	-.050	-.1393	1.0000	
10	1	-4	12.230	11.558	11.517	.980	.672	1.3799	1.0000	
10	1	-3	2.649 *	1.227	-1.110	.524	1.422	.7509	1.0000	**
10	1	-2	16.689	16.815	-16.719	-1.790	-.126	-.3153	1.0000	
10	1	-2	36.009	16.815	-16.719	-1.790	19.194	22.3197	1.0000	*

CU(IO3)2.2H2O FINAL

ALL REFLECTIONS

	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	15347.33	1543418.50	1284	.032
UNWEIGHTED R	1257.55	50476.74	1284	.025

RANGES OF F(OBS)

4387.16	998336.63	472	.066
3851.77	5758187.83	362	.026
1772.00	4317335.12	237	.020
779.79	1698594.97	121	.021
208.97	558534.03	39	.019
434.58	716270.07	29	.025
469.51	479358.74	11	.031
3443.56	907501.10	13	.062

RANGES OF (SIN(THETA)/LAMBDA)**2

5000.36	1754559.52	61	.053
2100.32	1558640.47	101	.037
1315.32	1692618.36	135	.028
1154.52	2033414.09	154	.024
1047.21	1884744.74	173	.024
1143.28	2306113.30	199	.022
1023.81	2061668.30	218	.022
2562.52	2142359.71	243	.035

UNREJECTED REFLECTIONS

	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	12687.57	15189077.36	1280	.029
UNWEIGHTED R	1194.61	49946.03	1280	.024

RANGES OF F(OBS)

4387.16	998336.63	472	.066
3353.60	5756434.54	361	.024
1772.00	4317335.12	237	.020
779.79	1698594.97	121	.021
208.97	558534.03	39	.019
434.58	716270.07	29	.025
469.51	479358.74	11	.031
1281.97	664213.25	10	.044

RANGES OF (SIN(THETA)/LAMBDA)**2

3734.30	1656093.18	60	.047
1789.84	1494005.19	100	.035
1315.32	1692618.36	135	.028
1154.52	2033414.09	154	.024
1047.21	1884744.74	173	.024
1143.28	2306113.30	199	.022
1023.81	2061668.30	218	.022
1479.29	2060420.19	241	.027

SUM FCAL   50174.81
STANDARD DEV OF UNIT WEIGHT OBS   3.15

SALESITE,FINAL

RECIPROCAL CELL PARAMETERS .092648 .149087 .209148 .000000 .000000 .000000

Table 3b. Solesite, $Cu(IO_3)(OH)$: Observed and calculated structure factors

(Ghose & Wan, 1977)

SALESITE, FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
0	0	2	169.531	186.524	186.154	11.742	-16.993	-32.9657	1.0000 *
0	0	4	148.633	156.733	156.401	10.191	-8.100	-10.7891	1.0000
0	0	6	97.901	102.374	102.057	8.057	-4.474	-6.6825	1.0000
0	0	8	44.398	44.036	43.651	5.813	.362	1.5671	1.0000
0	0	10	14.267	12.538	-12.538	-.018	1.729	13.8169	1.0000
0	1	0	78.864	87.363	-87.336	-2.174	-8.499	-19.4319	1.0000
0	2	0	57.772	55.446	-55.404	-2.162	2.325	3.9748	1.0000
0	2	2	56.621	55.322	-55.282	-2.106	1.298	2.8500	1.0000
0	2	4	33.784	34.045	-33.988	-1.964	-.261	-1.2635	1.0000
0	2	6	23.901	23.946	-23.884	-1.712	-.045	-.1714	1.0000
0	2	8	30.473	29.472	-29.472	-.060	1.001	4.4366	1.0000
0	3	1	6.227	4.208	4.205	-.161	2.019	6.2943	1.0000
0	3	3	6.617	6.746	-6.743	-.214	-.129	-.2563	1.0000
0	3	5	156.710	158.853	158.476	10.938	-2.143	-3.0926	1.0000
0	3	7	125.103	126.447	126.089	9.501	-1.344	-1.5990	1.0000
0	4	2	83.606	84.434	84.098	7.521	-.828	-1.1733	1.0000
0	4	4	17.765	18.818	-18.818	-.087	-1.052	-6.0377	1.0000
0	4	6	6.926	6.519	-6.511	-.306	.407	.8012	1.0000
0	5	1	64.971	71.377	-71.347	-2.079	-6.405	-11.5415	1.0000
0	5	3	35.219	33.428	-33.365	-2.056	1.792	7.5804	1.0000
0	5	5	43.017	41.854	-41.807	-1.973	1.163	3.8157	1.0000
0	5	7	32.184	32.215	-32.165	-1.805	-.031	-.1340	1.0000
0	6	2	11.672	13.236	-13.235	-.112	-1.564	-6.3863	1.0000
0	6	4	104.773	110.532	110.143	9.265	-5.759	-6.2989	1.0000
0	6	6	92.982	97.768	97.367	8.846	-4.786	-5.0508	1.0000
0	8	0	78.509	78.276	77.896	7.702	.233	.3950	1.0000
0	8	2	45.134	46.138	-46.100	-1.855	-1.003	-3.4120	1.0000
0	10	0	20.963	20.864	-20.785	-1.818	.099	.3915	1.0000
1	0	0	118.317	123.496	123.385	5.214	-5.178	-13.6787	1.0000
1	0	1	32.031	31.034	-31.034	.027	.998	3.9866	1.0000
1	0	2	55.531	57.097	56.907	4.660	-1.566	-3.3671	1.0000
1	0	3	18.508	19.374	19.374	-.047	-.867	-4.6309	1.0000
1	0	4	47.650	47.941	47.796	3.724	-.290	-.9390	1.0000
1	0	5	5.451	5.081	-5.081	.053	.370	.7082	1.0000
1	0	6	19.244	18.877	18.689	2.661	.367	1.4366	1.0000
1	0	7	184.895	192.915	-192.784	-7.124	-8.020	-19.4282	1.0000
1	1	1	16.571	14.799	14.799	-.041	1.772	12.8453	1.0000
1	1	2	109.919	110.092	-109.896	-6.566	-.173	-.2639	1.0000
1	1	3	13.311	12.907	-12.907	-.069	.404	1.8906	1.0000
1	1	4	86.202	88.200	-88.023	-5.578	-1.997	-3.3000	1.0000
1	1	5	5.349	5.086	5.085	-.079	.263	.4952	1.0000
1	1	6	46.853	47.367	-47.166	-4.368	-.515	-1.9973	1.0000
1	1	7	95.786	95.775	95.662	4.653	.012	.0236	1.0000
1	2	1	14.674	13.191	-13.191	.018	1.483	9.7633	1.0000
1	2	2	52.668	52.133	51.968	4.148	.535	1.3278	1.0000
1	2	3	7.820	8.366	8.366	.030	-.547	-1.7811	1.0000
1	2	4	34.801	34.773	34.617	3.295	.028	.1488	1.0000
1	2	5	18.441	17.917	17.764	2.352	.525	2.0187	1.0000
1	3	1	140.204	142.384	142.216	6.932	-2.180	-3.8468	1.0000
1	3	2	25.982	24.889	-24.888	-.108	1.093	6.2705	1.0000
1	3	3	118.731	117.995	117.822	6.587	.736	1.0229	1.0000
1	3	4	16.626	16.440	16.439	-.182	.187	.9101	1.0000
1	3	5	72.085	72.088	71.884	5.423	-.003	-.0049	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
1	3	6	10.027	9.984	-9.982	-.205	.042	.1253	1.0000
1	3	7	46.104	46.250	46.055	4.243	-.145	-.5693	1.0000
1	4	0	203.216	250.068	249.805	11.466	-46.853	-75.5361	1.0000 *
1	4	1	73.954	77.957	77.809	4.805	-4.003	-6.1764	1.0000
1	4	2	8.626	8.270	-8.270	.024	.356	1.4740	1.0000
1	4	3	50.622	48.810	48.620	4.300	1.813	4.6440	1.0000
1	4	4	6.589	6.635	6.635	.042	-.046	-.1260	1.0000
1	4	5	35.707	35.984	35.819	3.443	-.277	-1.3059	1.0000
1	5	1	17.295	17.050	16.870	2.468	.245	.8776	1.0000
1	5	2	116.318	123.132	-122.963	-6.450	-6.813	-9.4526	1.0000
1	5	3	75.372	74.537	-74.300	-5.947	.835	1.4378	1.0000
1	5	4	5.939	6.299	-6.292	-.290	-.360	-.8507	1.0000
1	5	5	74.133	73.149	-72.975	-5.056	.983	1.7716	1.0000
1	5	6	39.221	39.344	-39.144	-3.962	-.123	-.5296	1.0000
1	6	1	43.423	44.290	44.115	3.938	-.867	-2.5901	1.0000
1	6	2	37.753	38.486	38.325	3.518	-.733	-2.6683	1.0000
1	6	3	19.107	18.867	18.657	2.807	.240	.9897	1.0000
1	7	1	80.027	82.761	82.547	5.940	-2.733	-4.4685	1.0000
1	7	2	11.617	12.158	-12.156	-1.207	-.541	-2.0903	1.0000
1	7	3	74.500	75.637	75.439	5.472	-1.138	-1.7353	1.0000
1	7	4	7.967	7.729	7.721	-.350	.238	.6329	1.0000
1	7	5	51.298	50.569	50.355	4.643	.730	2.0861	1.0000
1	7	6	7.944	8.030	-8.020	-.396	-.086	-.1918	1.0000
1	8	1	33.609	34.627	34.422	3.763	-1.018	-5.1193	1.0000
1	8	2	29.665	29.857	29.666	3.377	-.195	-.9104	1.0000
1	8	3	19.458	19.440	19.249	2.720	.018	.0702	1.0000
1	9	1	62.537	64.665	-64.460	-5.148	-2.128	-4.2796	1.0000
1	9	2	49.016	48.931	-48.700	-4.748	.085	.2695	1.0000
1	9	3	6.158	6.560	-6.548	-.390	-.402	-.7717	1.0000
1	9	4	44.546	43.896	-43.709	-4.038	.650	2.8550	1.0000
1	9	5	19.226	18.196	17.976	2.821	1.031	4.1006	1.0000
1	10	1	5.349	4.824	4.824	-.007	.526	.9018	1.0000
1	10	2	21.790	22.153	22.008	2.531	-.364	-1.4352	1.0000
1	10	3	4.790	5.107	-5.107	.012	-.317	-.4558	1.0000
1	10	4	47.925	47.082	46.868	4.481	.844	3.0581	1.0000
1	11	1	75.421	76.125	-76.094	-2.167	-.703	-2.0426	1.0000
1	11	2	12.445	9.291	-9.291	-.021	3.154	22.5125	1.0000
2	0	0	74.049	71.046	-71.013	-2.156	3.004	5.4964	1.0000
2	0	1	3.367	.942	-.940	-.056	2.425	4.6278	1.0000
2	0	2	47.965	48.114	-48.068	-2.105	-.149	-.4280	1.0000
2	0	3	5.095	4.922	4.921	-.074	.173	.3621	1.0000
2	0	4	37.242	37.650	-37.599	-1.967	-.409	-1.9905	1.0000
2	0	5	25.486	25.390	-25.332	-1.718	.095	.3724	1.0000
2	1	0	12.448	8.646	-8.634	-.447	3.802	30.6517	1.0000
2	1	1	27.470	25.630	-25.630	-.022	1.840	7.3536	1.0000
2	1	2	11.757	10.958	-10.949	-.430	.799	4.9840	1.0000
2	1	3	7.539	7.548	-7.548	-.060	-.009	-.0339	1.0000
2	1	4	5.745	5.522	-5.509	-.382	.223	.5884	1.0000
2	1	5	5.371	4.631	-4.620	-.313	.740	1.4090	1.0000
2	2	0	187.065	219.726	219.398	11.996	-32.661	-69.5679	1.0000 *
2	2	1	58.327	53.990	-53.990	.026	4.337	8.3442	1.0000
2	2	2	229.344	238.971	238.697	11.442	-9.627	-16.2497	1.0000
2	2	3	14.413	13.593	13.593	.069	.820	4.4050	1.0000

SALESITE, FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
2	2	4	140.363	143.095	142.750	9.933	-2.732	-3.4993	1.0000
2	2	5	6.860	6.419	6.418	.092	.442	1.1975	1.0000
2	2	6	81.411	81.439	81.059	7.856	-.028	-.0497	1.0000
2	2	7	6.535	6.442	-6.441	.093	.094	.1830	1.0000
2	2	8	54.427	54.793	54.498	5.671	-.365	-1.2107	1.0000
2	3	0	27.188	26.847	-26.842	-.495	.341	1.6035	1.0000
2	3	1	5.357	3.716	-3.716	-.055	1.640	5.8770	1.0000
2	3	2	29.177	28.057	28.053	.473	1.120	4.8266	1.0000
2	3	4	7.990	6.208	6.194	.414	1.782	6.0360	1.0000
2	4	0	46.753	48.003	-47.956	-2.123	-1.250	-3.3009	1.0000
2	4	1	10.124	8.931	8.931	.018	1.193	5.7507	1.0000
2	4	2	64.204	62.228	-62.192	-2.106	1.977	3.9075	1.0000
2	4	3	4.843	4.309	-4.309	-.049	.535	1.2528	1.0000
2	4	4	42.917	42.458	-42.409	-2.039	.459	1.5660	1.0000
2	4	5	32.534	32.043	-31.987	-1.887	.491	2.2199	1.0000
2	5	0	18.961	20.356	-20.353	-.351	-1.395	-8.1040	1.0000
2	5	1	14.728	15.643	15.643	-.090	-.915	-4.7791	1.0000
2	5	2	7.812	1.586	1.549	-.339	6.226	22.0525	1.0000
2	5	3	7.609	7.877	-7.873	-.241	-.269	-.8517	1.0000
2	5	5	5.475	5.223	-5.213	-.321	.252	.5001	1.0000
2	5	6	7.313	7.273	-7.269	-.258	.040	.0895	1.0000
2	6	0	131.424	141.645	141.262	10.406	-10.221	-12.9852	1.0000
2	6	1	6.359	5.270	-5.270	.020	1.089	3.1628	1.0000
2	6	2	134.951	138.206	137.849	9.931	-3.255	-3.9429	1.0000
2	6	4	97.123	97.949	97.568	8.635	-.826	-.8868	1.0000
2	6	6	63.800	64.017	63.650	6.847	-.217	-.5402	1.0000
2	7	0	5.819	6.210	-6.193	.470	-.392	-.9488	1.0000
2	7	2	13.002	13.035	13.028	.448	-.033	-.1350	1.0000
2	7	4	6.155	5.616	5.603	.389	.538	1.1708	1.0000
2	8	0	29.543	30.508	-30.445	-1.969	-.965	-4.7758	1.0000
2	8	1	11.645	12.213	12.213	.012	-.568	-1.9965	1.0000
2	8	2	44.811	44.209	-44.166	-1.938	.602	1.9623	1.0000
2	8	3	4.854	4.666	-4.666	.032	.188	.3305	1.0000
2	8	4	30.790	30.733	-30.678	-1.838	.057	.2521	1.0000
2	9	0	6.164	5.267	-5.261	-.242	.897	1.9741	1.0000
2	10	0	5.141	4.474	4.472	-.120	.667	1.2176	1.0000
2	10	2	75.153	75.587	75.179	7.838	-.434	-.7246	1.0000
2	11	0	72.732	72.056	71.666	7.488	.676	1.2900	1.0000
2	11	2	4.618	4.478	4.462	.383	.140	.2012	1.0000
3	0	0	6.194	2.380	2.351	.364	3.815	7.2499	1.0000
3	0	1	69.843	69.880	69.752	4.216	-.036	-.0767	1.0000
3	0	2	5.424	3.994	-3.994	.063	1.430	4.9165	1.0000
3	0	3	61.149	61.998	61.884	3.744	-.849	-1.7521	1.0000
3	0	5	5.297	4.672	4.671	.105	.624	1.4932	1.0000
3	0	7	26.338	26.464	26.299	2.951	-.127	-.6469	1.0000
3	1	1	13.000	11.973	11.794	2.061	1.027	3.3342	1.0000
3	1	2	153.934	152.693	152.531	7.039	1.241	2.5393	1.0000
3	1	3	132.691	134.139	133.982	6.486	-1.448	-2.1286	1.0000
3	1	4	8.621	8.386	-8.386	-.049	.235	.8377	1.0000
3	1	5	69.232	70.160	69.943	5.507	-.928	-1.8387	1.0000
3	1	7	50.693	50.978	50.795	4.308	-.285	-1.0278	1.0000
3	2	1	79.626	79.964	79.776	5.475	-.338	-.6204	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
3	2	2	3.282	2.767	2.767	.071	.515	1.0461	1.0000
3	2	3	99.307	100.163	100.043	4.908	-.856	-1.2144	1.0000
3	2	4	3.955	.683	.672	.119	3.272	6.1315	1.0000
3	2	5	26.828	26.238	25.940	3.946	.589	2.9787	1.0000
3	2	7	26.524	26.340	26.186	2.847	.184	.7719	1.0000
3	3	1	127.543	129.975	-129.801	-6.730	-2.432	-4.0175	1.0000
3	3	2	11.601	10.478	10.478	-.115	1.123	5.7061	1.0000
3	3	3	116.373	115.825	-115.658	-6.208	.548	.7396	1.0000
3	3	4	9.973	10.374	-10.372	-.195	-.400	-1.5037	1.0000
3	3	5	64.982	65.551	-65.338	-5.280	-.570	-1.2443	1.0000
3	3	7	47.325	47.210	-47.028	-4.142	.116	.4849	1.0000
3	4	1	54.723	55.459	55.324	3.871	-.737	-1.8565	1.0000
3	4	3	36.158	35.490	35.323	3.442	.668	2.8276	1.0000
3	4	4	27.481	26.817	26.679	2.718	.664	3.1839	1.0000
3	4	5	8.861	8.838	8.631	1.905	.023	.0566	1.0000
3	5	1	101.808	104.921	104.720	6.483	-3.113	-4.1877	1.0000
3	5	2	11.900	12.751	12.750	-.158	-.851	-3.7722	1.0000
3	5	3	97.223	97.357	97.174	5.967	-.135	-.1609	1.0000
3	5	4	15.077	15.820	-15.818	-.267	-.744	-3.1460	1.0000
3	5	5	56.098	56.240	56.012	5.057	-.142	-.3555	1.0000
3	5	7	42.639	43.133	42.952	3.947	-.494	-2.1190	1.0000
3	6	1	51.566	53.613	53.410	4.667	-2.048	-5.5178	1.0000
3	6	3	47.094	47.783	47.599	4.192	-.688	-2.1388	1.0000
3	6	5	27.012	25.936	25.715	3.383	1.075	4.8114	1.0000
3	7	1	75.483	78.157	-77.951	-5.674	-2.673	-4.3102	1.0000
3	7	2	5.828	3.812	3.806	-.211	2.017	4.7986	1.0000
3	7	3	71.396	72.366	-72.176	-5.238	-.970	-1.7894	1.0000
3	7	4	7.497	7.733	-7.725	-.357	-.237	-.5901	1.0000
3	8	1	46.391	46.536	-46.322	-4.464	-.146	-.5675	1.0000
3	8	3	29.411	29.928	29.778	2.996	-.517	-2.5030	1.0000
3	8	5	11.084	9.678	9.302	2.672	1.406	4.5487	1.0000
3	9	1	22.052	21.798	21.694	2.124	.254	1.0045	1.0000
3	9	3	60.419	60.133	59.903	5.250	.286	.6974	1.0000
3	10	1	56.899	56.851	56.646	4.829	.048	.1363	1.0000
3	10	3	6.214	6.918	-6.909	-.368	-.704	-1.3271	1.0000
3	11	1	28.199	28.040	27.834	3.392	.159	.6808	1.0000
3	11	2	20.548	20.172	19.938	3.058	.376	1.4482	1.0000
3	11	3	44.282	42.788	-42.579	-4.224	1.493	6.5560	1.0000
4	0	0	4.539	3.108	-3.100	-.227	1.431	2.0058	1.0000
4	0	1	209.528	228.731	228.421	11.915	-19.204	-39.9047 **	1.0000
4	0	2	215.455	228.770	228.488	11.364	-13.315	-22.1937	1.0000
4	0	3	53.219	49.156	49.156	-.052	4.063	7.5826	1.0000
4	0	4	9.252	8.439	-8.438	.139	.813	3.3178	1.0000
4	0	5	138.837	142.064	141.721	9.865	-3.227	-4.0993	1.0000
4	0	6	4.680	4.013	-4.009	.186	.666	1.2902	1.0000
4	0	7	79.454	81.569	81.195	7.802	-2.115	-3.7810	1.0000
4	0	8	7.387	8.693	8.691	.187	-1.307	-2.7458	1.0000
4	1	0	52.463	52.640	52.338	5.631	-.177	-.6495	1.0000
4	1	1	24.243	23.982	23.964	-.939	.260	1.2956	1.0000
4	1	1	42.394	38.529	38.529	-.016	3.866	12.0890	1.0000
4	1	2	25.049	18.102	18.080	-.900	6.947	38.6661	1.0000
4	1	3	12.288	11.638	-11.638	-.043	.650	3.1471	1.0000
4	1	4	15.693	10.900	10.871	.793	4.793	23.4644	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
4	1	6	8.930	8.831	8.808	.643	.098	.2689	1.0000
4	1	7	4.662	4.165	4.165	-.055	.497	.7212	1.0000
4	2	0	81.666	79.664	-79.636	-2.105	2.002	3.5994	1.0000
4	2	1	7.897	6.313	6.313	-.040	1.584	7.2594	1.0000
4	2	2	54.623	50.887	-50.844	-2.092	3.737	8.0321	1.0000
4	2	3	5.104	2.763	2.761	.106	2.341	5.8062	1.0000
4	2	4	47.092	46.252	-46.207	-2.036	.840	2.4472	1.0000
4	2	6	36.759	36.898	-36.850	-1.897	-.139	-.6628	1.0000
4	3	0	13.368	9.295	9.261	-.790	4.073	24.2604	1.0000
4	3	1	11.931	11.290	-11.290	-.058	.641	3.5031	1.0000
4	3	2	28.516	28.308	-28.298	-.761	.208	1.1879	1.0000
4	3	4	10.815	10.049	-10.026	-.682	.766	2.9846	1.0000
4	3	5	4.989	2.785	-2.777	-.207	2.204	4.2931	1.0000
4	3	6	4.639	2.627	-2.565	-.567	2.012	3.2782	1.0000
4	4	0	166.745	181.232	180.892	11.097	-14.487	-21.2329	1.0000 *
4	4	1	17.747	16.947	16.947	.046	.800	4.6753	1.0000
4	4	2	160.903	166.367	166.030	10.588	-5.464	-7.3840	1.0000
4	4	3	3.715	2.680	-2.677	.123	1.035	1.8791	1.0000
4	4	4	114.058	116.817	116.454	9.198	-2.759	-3.1656	1.0000
4	4	6	73.053	72.500	72.133	7.283	.552	1.2068	1.0000
4	4	7	4.682	4.976	4.973	.167	-.294	-.4280	1.0000
4	5	0	25.601	27.097	27.080	.963	-1.496	-8.9111	1.0000
4	5	1	22.657	22.995	22.995	-.082	-.338	-1.9300	1.0000
4	5	2	8.821	8.524	8.475	.920	.296	1.0819	1.0000
4	5	3	10.656	10.482	-10.480	-.219	.174	.6498	1.0000
4	5	4	8.375	8.282	8.243	.801	.093	.2775	1.0000
4	5	5	5.303	5.362	-5.354	-.291	-.059	-.1104	1.0000
4	5	6	10.412	10.707	10.688	.637	-.295	-.8293	1.0000
4	6	0	45.069	44.638	-44.592	-2.011	.431	1.2681	1.0000
4	6	1	8.630	8.712	-8.712	-.030	-.082	-.2867	1.0000
4	6	2	46.702	46.236	-46.194	-1.987	.465	1.4958	1.0000
4	6	3	4.649	4.830	4.830	.081	-.182	-.3402	1.0000
4	6	4	37.244	36.171	-36.121	-1.906	1.073	5.2537	1.0000
4	6	6	27.128	27.365	-27.309	-1.743	-.237	-.9833	1.0000
4	7	0	10.908	2.987	2.930	-.580	7.921	29.8677	1.0000
4	7	2	15.840	15.155	-15.145	-.563	.685	2.9384	1.0000
4	7	4	7.507	7.237	-7.219	-.514	.270	.6798	1.0000
4	8	0	102.550	106.888	106.511	8.971	-4.338	-4.6683	1.0000
4	8	2	88.829	89.163	88.751	8.566	-.334	-.4922	1.0000
4	8	4	73.342	73.366	72.985	7.459	-.023	-.0448	1.0000
4	9	0	11.235	9.998	9.962	.847	1.238	3.9907	1.0000
4	9	1	7.383	6.221	6.220	.112	1.163	2.8309	1.0000
4	9	2	9.064	9.009	8.973	.807	.055	.1513	1.0000
4	9	3	4.933	4.765	-4.755	-.300	.168	.2718	1.0000
4	10	0	5.501	5.080	5.032	-.697	.421	.7169	1.0000
4	10	1	26.491	27.061	-27.002	-1.790	-.571	-2.3824	1.0000
4	10	2	8.985	8.148	-8.148	-.017	.838	2.2445	1.0000
4	11	0	32.471	30.748	-30.698	-1.754	1.723	7.3555	1.0000
4	11	1	4.855	3.341	-3.319	-.379	1.515	2.2918	1.0000
5	0	1	5.100	5.634	-5.632	-.115	-.534	-.8165	1.0000
5	0	2	119.738	119.648	119.504	5.853	.091	.1591	1.0000
5	0	3	31.961	31.531	31.531	.115	.430	1.8884	1.0000
5	0	4	55.339	54.596	54.342	5.259	.742	1.7483	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
5	0	4	19.979	19.816	-19.815	.195	.163	.8357	1.0000
5	0	5	55.359	55.710	55.548	4.247	-.351	-.9487	1.0000
5	0	6	10.077	10.793	10.791	.221	-.716	-2.1112	1.0000
5	0	7	21.454	22.419	22.205	3.086	-.965	-3.7748	1.0000
5	1	1	140.394	139.752	-139.589	-6.753	.642	1.0975	1.0000
5	1	1	8.489	6.394	-6.394	-.048	2.095	8.9040	1.0000
5	1	2	109.707	109.267	-109.090	-6.226	.440	.6024	1.0000
5	1	3	71.513	72.010	-71.815	-5.293	-.497	-.9493	1.0000
5	1	5	44.226	45.023	-44.831	-4.148	-.797	-3.5647	1.0000
5	1	7	50.854	49.988	49.862	3.553	.866	1.9380	1.0000
5	2	1	7.225	6.087	6.088	.100	1.137	4.1543	1.0000
5	2	2	43.350	42.101	41.984	3.143	1.249	3.9332	1.0000
5	2	3	4.646	.400	-.363	.167	4.246	8.6310	1.0000
5	2	4	14.929	15.037	14.835	2.456	-.108	-.4468	1.0000
5	2	5	13.498	12.672	12.559	1.691	.826	2.6645	1.0000
5	2	7	131.849	134.547	134.381	6.686	-2.699	-4.0441	1.0000
5	3	1	8.148	3.636	-3.635	-.091	4.512	17.3608	1.0000
5	3	2	86.265	84.208	83.983	6.155	2.057	2.6210	1.0000
5	3	3	74.818	76.215	76.036	5.216	-1.397	-2.6019	1.0000
5	3	5	40.594	40.974	40.771	4.071	-.379	-1.6580	1.0000
5	3	7	82.179	83.633	83.458	5.412	-1.454	-1.9961	1.0000
5	4	1	12.197	12.606	12.605	.102	-.409	-1.8830	1.0000
5	4	2	48.151	47.341	47.091	4.867	.809	2.3580	1.0000
5	4	3	8.498	8.301	-8.300	.173	.196	.6080	1.0000
5	4	4	44.582	44.328	44.153	3.937	.254	.9623	1.0000
5	4	5	4.982	6.016	6.013	.197	-1.033	-1.6269	1.0000
5	4	6	19.611	19.939	19.732	2.869	-.328	-1.2025	1.0000
5	4	7	88.474	92.563	-92.367	-6.009	-4.089	-5.1948	1.0000
5	5	1	7.222	7.520	-7.518	-.169	-.299	-.9243	1.0000
5	5	2	86.538	88.067	-87.892	-5.550	-1.529	-2.4991	1.0000
5	5	3	52.733	52.873	-52.661	-4.732	-.140	-.4170	1.0000
5	5	5	38.775	38.178	-37.996	-3.724	.598	2.5399	1.0000
5	5	7	24.940	24.921	24.742	2.981	.019	.0989	1.0000
5	6	1	4.417	5.497	-5.496	.077	-1.080	-2.0406	1.0000
5	6	2	28.087	28.118	27.994	2.643	-.031	-.1519	1.0000
5	6	3	8.193	8.450	8.449	.129	-.257	-.6876	1.0000
5	6	4	8.168	7.976	7.702	2.074	.192	.4815	1.0000
5	6	5	5.303	3.958	-3.955	-.146	1.345	2.1915	1.0000
5	7	1	80.389	83.001	82.797	5.820	-2.612	-4.1124	1.0000
5	7	2	56.150	56.652	56.399	5.350	-.502	-1.3641	1.0000
5	7	3	54.568	54.947	54.761	4.522	-.380	-1.2825	1.0000
5	7	5	41.215	41.431	41.209	4.279	-.216	-.9274	1.0000
5	8	1	30.237	30.879	30.637	3.858	-.642	-2.8987	1.0000
5	8	2	26.806	26.228	26.040	3.138	.578	2.3721	1.0000
5	8	3	54.885	54.823	-54.620	-4.723	.062	.1808	1.0000
5	8	5	50.315	48.972	-48.777	-4.368	1.343	4.7036	1.0000
5	9	1	9.960	9.924	9.700	2.095	.036	.0991	1.0000
5	9	3	6.217	6.379	-6.379	.044	-.162	-.3039	1.0000
5	10	1	15.641	15.359	15.245	1.865	.283	.9514	1.0000
5	10	2	45.243	44.754	44.533	4.445	.489	2.1286	1.0000
6	0	0	29.545	26.946	-26.869	-2.032	2.599	11.3034	1.0000
6	0	1	6.523	4.955	4.954	-.059	1.568	5.7040	1.0000
6	0	2	73.562	71.487	-71.458	-2.020	2.075	3.0177	1.0000

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
6	0	3	4.014	.182	-.090	.158	3.832	7.2531	1.0000
6	0	4	46.387	45.618	-45.575	-1.968	.770	2.5531	1.0000
6	0	6	26.747	26.882	-26.819	-1.835	-.134	-.5898	1.0000
6	1	0	52.784	51.553	-51.537	-1.271	1.231	2.7796	1.0000
6	1	1	5.077	4.003	4.003	-.022	1.074	3.1481	1.0000
6	1	2	8.621	7.142	-7.036	-1.222	1.479	5.8850	1.0000
6	1	4	19.204	18.814	-18.783	-1.086	.390	1.8976	1.0000
6	1	6	12.737	13.386	-13.356	-.891	-.649	-2.1442	1.0000
6	2	0	206.282	221.682	221.398	11.235	-15.401	-24.0014	1.0000 *
6	2	1	4.531	4.220	4.219	.072	.311	.7700	1.0000
6	2	2	158.466	162.540	162.186	10.717	-4.074	-5.7546	1.0000
6	2	4	116.971	118.827	118.462	9.308	-1.856	-2.1781	1.0000
6	2	5	5.215	2.439	2.426	.260	2.775	5.3066	1.0000
6	2	6	80.690	81.388	81.054	7.366	-.698	-1.1995	1.0000
6	3	0	48.146	49.564	49.544	1.404	-1.418	-3.4537	1.0000
6	3	1	26.545	25.898	-25.898	-.048	.647	3.7598	1.0000
6	3	2	7.637	6.945	6.814	1.343	.692	2.4508	1.0000
6	3	3	6.091	5.451	5.450	-.129	.640	1.7399	1.0000
6	3	4	19.103	19.048	19.012	1.176	.055	.2586	1.0000
6	3	6	13.258	13.704	13.672	.944	-.447	-1.5184	1.0000
6	3	7	6.591	6.875	-6.873	-.169	-.284	-.5349	1.0000
6	4	0	43.588	43.564	-43.519	-1.988	.023	.0680	1.0000
6	4	2	52.209	51.973	-51.936	-1.971	.236	.5878	1.0000
6	4	4	40.953	40.150	-40.105	-1.905	.802	3.3348	1.0000
6	4	6	27.021	27.186	-27.129	-1.759	-.165	-.6984	1.0000
6	5	0	28.867	27.840	-27.822	-.998	1.027	5.8572	1.0000
6	5	1	8.217	8.808	-8.808	-.083	-.591	-2.0387	1.0000
6	5	2	7.950	7.624	-7.562	-.966	.327	1.0566	1.0000
6	5	4	14.075	13.190	-13.161	-.873	.885	3.3914	1.0000
6	5	6	9.222	10.078	-10.052	-.735	-.857	-2.1829	1.0000
6	6	0	117.675	122.262	121.873	9.750	-4.586	-5.4082	1.0000
6	6	2	115.922	116.915	116.544	9.306	-.993	-1.1204	1.0000
6	6	4	84.748	84.948	84.561	8.095	-.200	-.3544	1.0000
6	6	6	58.203	58.469	58.115	6.422	-.267	-.7741	1.0000
6	7	0	26.978	27.167	27.134	1.334	-.188	-.9371	1.0000
6	7	1	13.047	13.202	-13.202	-.096	-.155	-.6017	1.0000
6	7	2	7.317	8.199	8.100	1.272	-.882	-2.2409	1.0000
6	7	4	13.302	13.530	13.485	1.103	-.229	-.7757	1.0000
6	8	0	40.726	41.738	-41.698	-1.837	-1.012	-4.1510	1.0000
6	8	2	29.497	29.848	-29.793	-1.807	-.351	-1.6012	1.0000
6	9	0	28.736	28.289	-28.237	-1.713	.446	1.9060	1.0000
6	9	2	15.600	15.280	-15.264	-.691	.320	1.1819	1.0000
6	10	0	9.098	8.146	-8.123	-.619	.951	2.3915	1.0000
6	10	1	62.379	61.167	60.724	7.351	1.211	2.7765	1.0000
6	10	2	69.354	68.676	68.316	7.024	.679	1.5442	1.0000
7	0	0	46.565	45.220	45.119	3.021	1.345	3.3263	1.0000
7	0	1	17.846	16.503	16.288	2.658	1.342	6.8974	1.0000
7	0	3	20.687	19.794	19.688	2.052	.893	4.0136	1.0000
7	0	5	5.721	5.345	5.339	.260	.376	.6938	1.0000
7	0	7	6.130	5.407	5.228	1.383	.722	1.2992	1.0000
7	1	1	120.304	118.201	118.021	6.514	2.104	3.1073	1.0000
7	1	3	100.253	99.192	99.010	6.000	1.062	1.3487	1.0000
7	1	5	63.590	63.151	62.946	5.091	.439	1.0390	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
7	1	7	43.447	43.217	43.033	3.980	.230	1.0134	1.0000
7	2	1	91.554	92.769	92.582	5.892	-1.215	-1.7242	1.0000
7	2	2	18.678	19.185	-19.184	.149	-.507	-2.7571	1.0000
7	2	3	60.039	59.544	59.307	5.307	.495	1.0472	1.0000
7	2	4	20.399	20.742	20.740	.252	-.343	-1.6261	1.0000
7	2	5	46.358	46.619	46.419	4.308	-.261	-.9289	1.0000
7	2	6	6.494	5.463	-5.456	.286	1.030	2.0673	1.0000
7	2	7	24.333	24.330	24.125	3.155	.003	.0108	1.0000
7	3	1	107.647	109.709	-109.538	-6.119	-2.062	-2.7818	1.0000
7	3	2	9.636	10.068	-10.067	-.112	-.432	-1.6635	1.0000
7	3	3	78.860	77.983	-77.778	-5.650	.876	1.4816	1.0000
7	3	4	6.877	6.546	6.544	-.190	.331	.8818	1.0000
7	3	5	64.858	63.390	-63.207	-4.815	1.467	3.6985	1.0000
7	3	6	6.016	6.151	-6.148	-.218	-.136	-.2605	1.0000
7	3	7	39.485	39.717	-39.536	-3.786	-.231	-.9914	1.0000
7	4	1	29.911	29.178	29.047	2.760	.733	4.2566	1.0000
7	4	2	5.780	6.614	6.613	.121	-.834	-2.0569	1.0000
7	4	3	17.757	17.124	16.951	2.430	.633	2.9742	1.0000
7	4	4	4.050	4.557	-4.553	.203	-.507	-.7752	1.0000
7	4	5	13.735	12.689	12.549	1.880	1.046	3.7331	1.0000
7	4	6	6.393	6.327	6.322	.229	.066	.1266	1.0000
7	4	7	4.910	5.643	5.498	1.271	-.733	-1.0263	1.0000
7	5	1	84.363	85.638	85.420	6.099	-1.275	-2.1678	1.0000
7	5	2	7.058	5.502	-5.501	-.132	1.556	4.4222	1.0000
7	5	3	81.905	83.512	83.324	5.606	-1.607	-2.4957	1.0000
7	5	4	48.243	48.577	48.345	4.737	-.334	-1.1510	1.0000
7	5	5	53.660	54.322	54.086	5.052	-.662	-1.7994	1.0000
7	6	1	47.090	46.770	46.547	4.558	.320	1.1885	1.0000
7	6	2	7.151	7.461	7.458	.198	-.310	-.6997	1.0000
7	6	3	29.209	29.398	29.163	3.712	-.189	-.8131	1.0000
7	6	4	67.758	68.915	-68.728	-5.072	-1.157	-2.4376	1.0000
7	6	5	6.337	6.751	-6.748	-.196	-.414	-.9255	1.0000
7	7	1	52.591	52.287	-52.076	-4.693	.304	1.0451	1.0000
7	7	2	46.015	44.991	-44.812	-4.016	1.024	4.5604	1.0000
7	7	3	12.001	11.329	11.133	2.100	.672	2.2199	1.0000
7	7	4	8.094	8.128	8.127	.081	-.033	-.0855	1.0000
7	7	5	13.126	13.150	13.019	1.855	-.024	-.0801	1.0000
7	8	1	7.539	7.883	-7.882	-.137	-.344	-.7654	1.0000
7	8	2	7.303	4.114	3.852	1.444	3.189	6.7159	1.0000
7	8	3	53.758	52.912	52.675	5.008	.846	2.6714	1.0000
7	8	4	52.476	51.276	51.069	4.595	1.200	4.2673	1.0000
7	8	5	28.508	27.525	27.273	3.718	.983	4.0661	1.0000
8	0	0	175.102	180.294	179.970	10.796	-5.192	-7.4123	1.0000
8	0	1	13.427	12.869	-12.869	.094	.557	2.7138	1.0000
8	0	2	149.283	151.236	150.885	10.300	-1.952	-2.5821	1.0000
8	0	3	5.913	4.892	4.885	.251	1.021	2.6669	1.0000
8	0	4	112.511	113.332	112.979	8.947	-.821	-.9329	1.0000
8	0	5	7.344	7.476	7.468	.337	-.132	-.3293	1.0000
8	0	6	69.081	69.852	69.492	7.083	-.772	-1.6663	1.0000
8	1	0	11.156	7.668	7.470	1.730	3.488	15.6820	1.0000
8	1	1	5.502	5.882	-5.882	-.012	-.379	-1.0023	1.0000
8	1	2	43.152	41.202	41.169	1.659	1.950	6.0378	1.0000
8	1	4	23.803	18.779	18.722	1.462	5.025	25.1258	1.0000

SALESITE, FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
8	1	6	9.286	9.260	9.183	1.186	.026	.0691	1.0000
8	2	0	63.892	65.194	-65.166	-1.909	-1.302	-2.4691	1.0000
8	2	1	17.008	16.810	-16.810	.072	.198	1.0473	1.0000
8	2	2	39.744	38.656	-38.609	-1.895	1.089	4.0232	1.0000
8	2	3	6.880	7.515	7.512	.192	-.635	-1.7566	1.0000
8	2	4	39.480	38.856	-38.813	-1.839	.624	2.9758	1.0000
8	2	5	5.288	5.001	4.995	.253	.287	.5258	1.0000
8	2	6	31.589	31.718	-31.672	-1.707	-.129	-.5648	1.0000
8	3	0	23.411	24.686	-24.643	-1.459	-1.275	-7.2246	1.0000
8	3	1	7.850	8.389	8.389	-.052	-.540	-1.7894	1.0000
8	3	2	24.160	23.219	-23.177	-1.406	.941	5.0879	1.0000
8	3	4	14.652	15.596	-15.545	-1.260	-.944	-3.7392	1.0000
8	3	6	12.924	12.828	-12.785	-1.046	-.096	-.3117	1.0000
8	4	0	137.554	144.624	144.274	10.060	-7.070	-8.7446	1.0000
8	4	4	119.959	121.903	121.524	9.600	-1.944	-2.2924	1.0000
8	4	5	95.624	95.019	94.652	8.345	.605	.9067	1.0000
8	4	6	5.477	4.594	4.584	.300	.883	1.6344	1.0000
8	5	0	63.402	62.284	61.932	6.614	1.118	2.9532	1.0000
8	5	2	36.700	36.691	36.652	1.692	.009	.0416	1.0000
8	5	4	16.808	16.843	16.779	1.474	-.035	-.1391	1.0000
8	5	5	6.150	5.587	5.462	1.173	.563	1.0352	1.0000
8	6	0	42.620	43.712	-43.674	-1.816	-1.092	-4.2023	1.0000
8	6	2	33.185	33.845	-33.798	-1.794	-.660	-3.2654	1.0000
8	6	4	31.578	31.614	-31.568	-1.717	-.036	-.1645	1.0000
8	6	6	24.573	24.398	-24.348	-1.567	.175	.6878	1.0000
8	7	0	15.415	15.284	-15.246	-1.075	.131	.5171	1.0000
8	7	1	4.782	4.213	4.212	-.094	.569	1.0212	1.0000
8	7	2	14.471	14.254	-14.216	-1.043	.217	.8098	1.0000
8	7	4	9.921	9.428	-9.379	-.951	.494	1.3943	1.0000
8	8	0	88.472	87.901	87.523	8.141	.571	.8149	1.0000
8	8	2	8.236	8.712	8.712	.058	-.476	-1.1842	1.0000
8	8	4	73.223	74.294	73.886	7.775	-1.071	-2.3290	1.0000
8	9	0	62.791	62.244	61.874	6.773	.547	1.5146	1.0000
8	9	2	8.838	8.223	8.074	1.557	.615	1.5892	1.0000
8	10	0	18.947	19.582	19.526	1.482	-.635	-2.3944	1.0000
8	10	2	27.175	26.151	-26.101	-1.608	1.025	4.1293	1.0000
8	0	0	25.001	24.430	-24.379	-1.575	.571	2.2812	1.0000
8	0	1	74.181	72.424	72.171	6.044	1.757	2.2945	1.0000
8	0	2	5.155	4.740	4.736	.185	.415	.9596	1.0000
8	0	3	83.091	82.813	82.633	5.455	.278	.4594	1.0000
8	0	5	31.710	31.995	31.685	4.445	-.285	-1.3412	1.0000
8	0	6	4.778	3.662	3.644	.356	1.117	1.7145	1.0000
8	0	7	28.589	28.186	27.996	3.275	.403	1.6367	1.0000
9	1	1	103.316	102.278	-102.103	-5.993	1.038	1.3424	1.0000
9	1	2	6.965	6.908	6.907	-.050	.058	.1672	1.0000
9	1	3	75.481	73.757	-73.550	-5.528	1.724	2.8434	1.0000
9	1	5	8.412	8.117	-8.116	-.086	.296	.8745	1.0000
9	1	6	62.125	62.755	-62.579	-4.702	-.630	-1.5538	1.0000
9	1	7	4.294	2.377	2.375	-.101	1.916	2.7110	1.0000
9	2	1	34.598	34.972	-34.777	-3.688	-.374	-1.5628	1.0000
9	2	2	19.181	18.604	18.455	2.352	.577	2.9820	1.0000
9	2	3	4.494	4.322	-4.319	.160	.172	.3457	1.0000
9	2	4	19.461	18.222	16.106	2.055	1.239	5.9129	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
9	2	4	9.012	8.772	8.768	.269	.240	.7075	1.0000
9	2	5	7.423	6.288	6.091	1.562	1.135	2.6470	1.0000
9	2	6	4.751	1.599	-1.570	.303	3.152	4.8722	1.0000
9	2	7	5.178	2.158	1.900	1.023	3.020	4.8355	1.0000
9	3	1	91.263	93.831	93.636	6.038	-2.568	-3.1349	1.0000
9	3	3	73.293	72.757	72.544	5.553	.537	1.0345	1.0000
9	3	5	57.187	57.368	57.176	4.697	-.182	-.5031	1.0000
9	4	1	61.959	61.693	61.438	5.605	.266	.5341	1.0000
9	4	2	4.674	5.143	5.140	.164	-.468	-.8968	1.0000
9	4	4	61.362	61.434	61.225	5.062	-.072	-.1746	1.0000
9	4	5	31.941	31.712	31.442	4.131	.229	1.0234	1.0000
9	5	1	4.537	4.361	4.350	.317	.175	.2446	1.0000
9	5	2	73.369	76.106	-75.926	-5.238	-2.737	-5.2666	1.0000
9	5	3	9.694	8.903	8.902	-.151	.791	2.6151	1.0000
9	5	4	56.289	55.584	-55.373	-4.846	.705	1.7771	1.0000
9	5	5	11.851	12.592	-12.589	-.258	-.740	-2.3954	1.0000
9	6	1	52.069	51.873	-51.707	-4.146	.196	.7143	1.0000
9	6	3	14.720	13.724	13.585	1.947	.996	3.9801	1.0000
9	6	4	5.350	3.840	3.441	1.704	1.510	2.8246	1.0000
9	6	5	4.446	4.029	4.024	.208	.416	.6168	1.0000
9	7	1	9.282	8.868	8.772	1.300	.414	1.0487	1.0000
9	7	3	63.233	64.383	64.161	5.335	-1.150	-2.8518	1.0000
9	7	4	52.523	51.872	51.641	4.894	.650	1.9621	1.0000
9	7	5	4.562	4.994	-4.988	-.251	-.432	-.6330	1.0000
9	8	1	43.368	43.724	43.529	4.122	-.356	-1.5400	1.0000
9	8	2	40.455	40.369	40.121	4.470	.086	.3962	1.0000
9	8	3	5.566	4.337	4.336	.113	1.229	2.2451	1.0000
9	9	1	32.412	31.544	31.283	4.046	.869	3.7775	1.0000
9	9	2	46.170	45.783	-45.603	-4.050	.388	1.7428	1.0000
10	0	1	37.683	36.650	-36.457	-3.757	1.034	4.4345	1.0000
10	0	2	51.636	52.931	-52.901	-1.783	-1.295	-3.1700	1.0000
10	0	3	23.970	23.136	23.136	.086	.834	4.5072	1.0000
10	1	1	38.560	37.044	-37.001	-1.770	1.517	5.7891	1.0000
10	1	2	5.875	5.232	-5.227	.231	.643	1.5151	1.0000
10	1	3	35.332	35.056	-35.014	-1.717	.276	1.3571	1.0000
10	1	4	28.094	28.606	-28.561	-1.593	-.512	-2.1559	1.0000
10	1	6	29.099	28.466	-28.402	-1.903	.633	3.5659	1.0000
10	2	0	27.887	28.013	-27.953	-1.829	-.125	-.6697	1.0000
10	2	1	23.152	21.311	-21.249	-1.624	1.841	8.4392	1.0000
10	2	2	14.359	14.183	-14.120	-1.332	.177	.5916	1.0000
10	2	0	119.561	123.459	123.065	9.850	-3.898	-4.7586	1.0000
10	2	1	3.940	2.722	-2.720	.105	1.218	2.1610	1.0000
10	2	2	126.166	127.575	127.228	9.400	-1.409	-1.6449	1.0000
10	2	3	6.957	6.815	6.809	.284	.142	.3647	1.0000
10	2	4	91.336	90.687	90.318	8.170	.648	.9622	1.0000
10	2	6	57.043	57.354	56.988	6.475	-.311	-.9535	1.0000
10	3	0	38.408	39.029	38.973	2.096	-.620	-2.3394	1.0000
10	3	1	12.511	12.390	12.390	-.037	.121	.4950	1.0000
10	3	2	22.290	22.218	22.127	2.005	.072	.3544	1.0000
10	3	3	5.572	5.312	-5.311	-.099	.260	.5329	1.0000
10	3	4	19.860	20.354	20.278	1.756	-.493	-2.0322	1.0000
10	3	6	17.017	17.828	17.772	1.411	-.811	-2.8296	1.0000
10	4	0	38.573	40.053	-40.015	-1.739	-1.480	-6.0699	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
10	4	1	12.878	13.106	13.106	.076	-.228	-.9031	1.0000
10	4	2	37.827	37.112	-37.072	-1.722	.715	3.7119	1.0000
10	4	3	5.151	3.038	-3.031	.202	2.114	4.0336	1.0000
10	4	4	30.699	30.965	-30.920	-1.659	-.266	-1.2192	1.0000
10	4	6	24.155	24.428	-24.380	-1.526	-.273	-1.0709	1.0000
10	5	0	15.339	15.250	-15.176	-1.500	.089	.3694	1.0000
10	5	2	22.618	22.597	-22.551	-1.450	.021	.0966	1.0000
10	5	4	17.027	17.026	-16.976	-1.310	-.001	.0039	1.0000
10	6	0	92.412	95.086	94.700	8.558	-2.674	-3.9746	1.0000
10	6	1	7.782	7.396	-7.395	.083	.387	1.0184	1.0000
10	6	2	84.409	85.358	84.966	8.170	-.949	-1.6688	1.0000
10	6	3	5.629	6.046	6.042	.224	-.416	-.7588	1.0000
10	6	4	69.750	68.749	68.380	7.111	1.002	2.3299	1.0000
10	7	0	28.824	29.194	29.126	1.987	-.370	-1.6538	1.0000
10	7	1	7.009	6.740	6.739	-.077	.269	.6185	1.0000
10	7	2	16.398	16.233	16.122	1.894	.165	.6130	1.0000
10	7	3	4.809	3.844	-3.839	-.205	.965	1.5112	1.0000
10	7	4	15.649	15.485	15.397	1.644	.164	.5643	1.0000
10	8	0	23.114	23.715	-23.661	-1.596	-.602	-2.4778	1.0000
10	8	2	30.561	30.605	-30.565	-1.570	-.044	-.1893	1.0000
10	9	0	11.732	11.714	-11.668	-1.042	.017	.0515	1.0000
10	9	2	12.153	11.534	-11.490	-1.014	.618	1.8244	1.0000
11	0	1	13.819	11.327	11.181	1.816	2.492	10.6876	1.0000
11	0	2	10.056	9.890	9.888	.185	.166	.5723	1.0000
11	0	3	9.648	7.177	7.003	1.570	2.472	7.8882	1.0000
11	0	4	5.318	5.506	-5.498	.311	-.188	-.3423	1.0000
11	0	5	4.517	2.375	2.070	1.165	2.142	3.1202	1.0000
11	0	6	5.990	5.894	5.884	.350	.095	.1686	1.0000
11	1	1	79.246	79.172	78.971	5.642	.074	.1217	1.0000
11	1	3	74.211	73.764	73.581	5.195	.447	.8324	1.0000
11	1	5	44.728	45.325	45.110	4.406	-.597	-2.6466	1.0000
11	2	1	70.753	70.969	70.726	5.859	-.215	-.4275	1.0000
11	2	3	9.047	9.129	9.127	.203	-.082	-.2574	1.0000
11	2	4	50.799	50.938	50.661	5.299	-.139	-.4106	1.0000
11	2	5	40.764	40.912	40.681	4.337	-.147	-.6685	1.0000
11	2	6	4.788	4.935	4.920	.392	-.147	-.2159	1.0000
11	3	1	64.457	65.497	-65.290	-5.205	-1.041	-2.0103	1.0000
11	3	3	74.008	75.462	-75.308	-4.811	-1.454	-2.6407	1.0000
11	3	5	35.994	35.340	-35.101	-4.108	.653	2.8822	1.0000
11	4	1	7.976	7.464	7.281	1.644	.512	1.4115	1.0000
11	4	3	6.907	5.941	5.769	1.423	.966	2.2472	1.0000
11	4	5	5.882	1.444	.984	1.057	4.438	8.0111	1.0000
11	5	1	66.542	67.344	67.130	5.369	-.802	-1.6781	1.0000
11	5	3	55.012	55.587	55.368	4.927	-.575	-1.6900	1.0000
11	5	5	41.864	42.648	42.445	4.153	-.784	-3.4100	1.0000
11	6	1	47.873	49.099	48.839	5.052	-1.226	-4.2002	1.0000
11	6	3	38.735	38.637	38.366	4.575	.097	.4455	1.0000
11	6	5	4.754	4.123	4.114	.271	.630	.9552	1.0000
11	7	1	31.291	31.248	31.022	3.753	.043	.1781	1.0000
11	7	2	43.921	44.617	-44.416	-4.238	-.696	-2.9319	1.0000
11	7	3	4.316	2.007	-2.000	-.165	2.310	3.2973	1.0000
11	8	3	53.090	53.068	-52.922	-3.931	.021	.0715	1.0000
11	8		5.338	3.871	3.725	1.053	1.466	2.3242	1.0000

SALESITE,FINAL   STRUCTURE FACTORS   PAGE 12

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
11	9	1	44.394	43.672	43.443	4.466	.722	3.1559	1.0000
12	0	0	116.217	116.898	116.539	9.155	-.681	-.7767	1.0000
12	0	1	14.085	13.205	13.205	.119	.880	3.5637	1.0000
12	0	2	101.939	101.438	101.061	8.738	.501	.5516	1.0000
12	0	4	75.884	75.911	75.530	7.598	-.026	-.0456	1.0000
12	0	6	56.387	57.074	56.755	6.025	-.688	-1.9484	1.0000
12	1	0	31.916	32.551	32.472	2.264	-.635	-3.2815	1.0000
12	1	2	27.421	27.942	27.858	2.171	-.521	-2.5386	1.0000
12	1	4	22.745	21.895	21.811	1.914	.249	3.5941	1.0000
12	1	6	17.020	16.421	16.348	1.553	.599	2.0805	1.0000
12	2	0	20.791	20.771	20.708	-1.617	.019	.0901	1.0000
12	2	1	5.869	4.729	-4.728	.092	1.140	2.6058	1.0000
12	2	2	44.804	44.643	44.614	-1.602	.161	.5561	1.0000
12	2	3	4.837	4.056	4.049	.245	.781	1.3349	1.0000
12	2	4	28.992	28.824	28.782	-1.548	.168	.7419	1.0000
12	2	6	18.465	17.884	17.826	-1.429	.581	2.0660	1.0000
12	3	0	23.465	23.058	22.979	-1.917	.407	1.9316	1.0000
12	3	2	7.684	7.469	-7.468	-.044	.215	.5786	1.0000
12	3	4	26.789	26.795	-26.731	-1.847	-.005	-.0255	1.0000
12	4	0	18.649	18.205	-18.130	-1.654	.443	1.7341	1.0000
12	4	1	91.346	92.833	92.440	8.536	-1.487	-2.2359	1.0000
12	4	2	8.439	8.165	8.164	.106	.274	.7448	1.0000
12	4	4	87.200	89.605	89.435	8.149	-2.605	-3.7712	1.0000
12	5	0	66.219	66.438	66.059	7.090	-.219	-.5540	1.0000
12	5	1	29.374	29.261	29.169	2.311	.113	.5216	1.0000
12	5	2	7.092	7.959	-7.959	-.051	-.867	-1.9678	1.0000
12	5	4	22.359	23.421	23.317	2.208	-1.063	-4.5176	1.0000
12	6	0	19.368	19.799	19.706	1.924	-.431	-1.6445	1.0000
12	6	1	26.454	26.429	-26.385	-1.528	.025	.1109	1.0000
12	6	2	6.479	6.233	-6.232	.070	.246	.5035	1.0000
12	6	4	30.875	30.171	-30.133	-1.508	.704	3.0919	1.0000
12	7	0	4.879	4.280	-4.276	.188	.599	.9149	1.0000
12	7	2	23.547	23.477	-23.433	-1.439	.070	.2756	1.0000
12	7	3	15.321	14.902	-14.834	-1.418	.419	1.4843	1.0000
12	7	4	5.478	5.369	-5.569	-.077	.108	.1911	1.0000
12	8	0	17.743	17.911	-17.859	-1.376	-.169	-.6255	1.0000
12	8	1	56.782	55.261	54.826	6.922	1.521	4.6483	1.0000
12	8	2	64.412	64.246	63.905	6.612	.165	.4265	1.0000
13	0	0	64.752	65.173	64.916	5.708	-.422	-.7761	1.0000
13	0	2	44.114	44.575	44.266	5.245	-.461	-1.6985	1.0000
13	1	1	5.610	5.749	5.737	.382	-.139	-.2484	1.0000
13	1	3	40.634	41.568	41.344	4.308	-.934	-4.1002	1.0000
13	1	4	67.026	67.239	-67.055	-4.975	-.213	-.3904	1.0000
13	1	5	8.502	7.139	-7.139	-.047	1.363	3.8510	1.0000
13	2	1	52.054	50.665	-50.456	-4.590	1.390	3.9379	1.0000
13	2	2	7.731	6.906	6.906	-.081	.825	1.9388	1.0000
13	2	3	45.882	44.996	-44.826	-3.907	.885	3.7625	1.0000
13	2	4	5.831	4.287	4.107	1.231	1.543	3.2286	1.0000
13	2	5	4.979	3.377	-3.211	1.047	1.602	2.7091	1.0000
13	3	1	7.082	7.570	7.563	.321	-.488	-1.0413	1.0000
13	3	3	61.726	62.217	62.008	5.099	-.491	-1.1274	1.0000
13	3	4	53.688	54.248	54.045	4.685	-.559	-1.7152	1.0000
13	3	5	40.947	40.844	40.652	3.957	.103	.4469	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
13	4	1	52.467	53.486	53.214	5.382	-1.019	-3.1853	1.0000
13	4	3	41.559	42.238	41.956	4.879	-.679	-3.0991	1.0000
13	4	4	4.481	2.587	2.564	.340	1.894	2.6477	1.0000
13	4	5	33.787	33.788	33.549	4.011	-.000	-.0019	1.0000
13	5	1	55.333	54.065	-53.897	-4.269	1.268	3.5076	1.0000
13	5	2	8.766	8.811	-8.810	-.123	-.045	-.1167	1.0000
13	5	3	37.595	37.467	-37.257	-3.956	.128	.5695	1.0000
13	5	4	7.435	7.532	7.529	-.211	-.098	-.2077	1.0000
13	7	1	45.775	46.360	46.134	4.571	-.585	-2.5933	1.0000
13	7	3	41.939	42.508	42.301	4.187	-.569	-2.4526	1.0000
13	8	0	33.870	33.650	33.371	4.326	.219	.9204	1.0000
14	0	1	40.419	40.588	-40.562	-1.458	-.169	-.6764	1.0000
14	0	2	7.775	7.432	-7.432	.099	.343	.8799	1.0000
14	0	4	25.573	23.739	-23.695	-1.444	1.834	8.2058	1.0000
14	0	5	26.510	24.830	-24.790	-1.393	1.680	6.9529	1.0000
14	1	0	4.523	4.373	4.359	.350	.150	.2041	1.0000
14	1	2	35.183	35.891	-35.819	-2.266	-.708	-2.9412	1.0000
14	1	4	21.662	20.983	-20.870	-2.178	.679	2.8874	1.0000
14	2	0	22.101	22.567	-22.484	-1.934	-.466	-1.8400	1.0000
14	2	2	92.454	92.503	92.150	8.080	-.049	-.0719	1.0000
14	2	4	5.835	5.149	-5.147	.121	.686	1.3446	1.0000
14	3	0	74.409	74.470	74.069	7.714	-.061	-.1225	1.0000
14	3	2	65.395	64.475	64.125	6.713	.920	2.1252	1.0000
14	3	4	25.833	26.707	26.591	2.486	-.874	-3.8719	1.0000
14	4	0	27.421	27.559	27.456	2.378	-.138	-.6020	1.0000
14	4	2	4.699	.403	-.398	-.063	4.296	6.7288	1.0000
14	4	4	22.288	23.002	22.908	2.085	-.714	-2.7838	1.0000
14	5	0	34.664	35.807	-35.779	-1.417	-1.142	-5.2105	1.0000
14	5	2	21.740	21.683	-21.637	-1.400	.058	.2344	1.0000
14	5	4	23.341	23.116	-23.077	-1.343	.225	.8796	1.0000
14	6	0	32.360	32.084	-32.034	-1.796	.276	1.2223	1.0000
14	6	2	13.115	12.824	-12.706	-1.736	.292	.9310	1.0000
14	7	0	17.015	17.279	-17.208	-1.566	-.264	-.9180	1.0000
15	0	1	69.260	70.290	69.937	7.031	-1.029	-2.1633	1.0000
15	0	3	57.553	57.713	57.321	6.714	-.160	-.4648	1.0000
15	1	1	21.121	20.812	20.679	2.350	.309	1.1849	1.0000
15	1	2	21.463	22.091	21.977	2.241	-.628	-2.3488	1.0000
15	2	1	11.248	6.576	-6.530	.769	4.673	14.7610	1.0000
15	2	2	7.846	4.106	4.058	.632	3.740	8.8760	1.0000
15	2	3	53.015	53.602	53.407	4.567	-.587	-1.6246	1.0000
15	2	4	45.065	45.094	44.897	4.204	-.029	-.1161	1.0000
15	3	2	48.156	49.149	48.850	5.418	-.993	-3.3284	1.0000
15	3	3	46.924	46.848	46.589	4.919	.076	.3052	1.0000
15	3	4	7.872	8.054	8.045	.385	-.182	-.4035	1.0000
15	4	1	49.127	49.171	-48.997	-4.137	-.044	-.1438	1.0000
15	4	3	5.806	5.987	5.987	-.079	-.182	-.3215	1.0000
15	5	1	38.703	38.332	-38.140	-3.826	.371	1.6192	1.0000
15	5	2	9.144	8.374	-8.373	-.136	.769	1.9084	1.0000
15	5	3	4.740	4.967	-4.920	-.680	-.227	-.3496	1.0000
15	5	4	45.240	45.795	45.582	4.415	-.560	-2.5066	1.0000
15	6	1	41.312	41.093	40.894	4.047	.219	.9460	1.0000
15	6	3	40.050	40.139	39.864	4.696	-.089	-.3861	1.0000
16	0	0	67.802	63.032	62.613	7.259	4.770	9.3112	1.0000

SALESITE,FINAL

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	EXT. FACTOR
16	0	2	71.087	70.755	70.414	6.931	.332	.6314	1.0000
16	0	4	53.717	53.230	52.887	6.037	.487	1.5865	1.0000
16	1	0	24.112	24.754	24.628	2.493	-.642	-2.6788	1.0000
16	1	2	28.390	28.072	27.970	2.391	.318	1.3514	1.0000
15	1	4	20.606	20.599	20.491	2.109	.007	.0256	1.0000
16	2	0	26.714	27.405	-27.375	-1.272	-.691	-2.9352	1.0000
16	2	1	6.818	6.141	6.140	.097	.677	1.3909	1.0000
16	2	2	21.661	22.009	-21.973	-1.258	-.348	-1.3726	1.0000
16	3	0	17.033	17.525	-17.396	-2.122	-.492	-1.8050	1.0000
16	3	1	8.552	8.115	8.115	-.035	.437	1.0996	1.0000
16	3	2	27.034	26.541	-26.462	-2.045	.493	2.0383	1.0000
16	4	0	58.123	58.985	58.595	6.774	-.861	-2.3975	1.0000
16	5	0	60.677	60.195	59.846	6.470	.482	1.3257	1.0000
16	5	2	24.626	24.456	25.329	2.535	-.830	-3.2757	1.0000
16	0	2	23.693	23.786	23.662	2.422	-1.093	-.3621	1.0000
17	0	1	43.549	43.959	43.654	5.168	-.410	-1.6160	1.0000
17	0	2	7.106	7.161	7.157	.234	-.055	-.1115	1.0000
17	0	3	43.306	43.148	42.891	4.699	.159	.6864	1.0000
17	1	1	40.099	40.006	-39.820	-3.855	.093	.4100	1.0000
17	1	3	39.887	39.322	-39.161	-3.558	.566	2.4372	1.0000
17	1	1	41.506	42.311	42.120	4.020	-.806	-3.5049	1.0000
18	0	0	38.983	38.971	38.672	4.817	.011	.0491	1.0000
18	1	1	15.495	15.399	-15.360	-1.104	.096	.3204	1.0000
18	1	0	22.931	22.264	-22.140	-2.348	.667	2.6091	1.0000
18	1	0	7.601	6.666	-6.666	-.017	.935	2.0055	1.0000
18	2	0	57.726	58.357	58.027	6.193	-.631	-1.6169	1.0000

RESULTS OF STRUCTURE FACTOR CALCULATIONS

SALESITE,FINAL

ALL REFLECTIONS

	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	29866.68	10885290.79	715	.052
UNWEIGHTED R	862.03	27523.18	715	.031

RANGES OF F(OBS)

	NUMERATOR	DENOMINATOR	NUMBER	R
	10694.36	1890366.62	395	.075
	1535.00	4464329.26	169	.019
	1033.02	1660047.89	84	.025
	239.55	514162.84	29	.022
	697.59	761646.23	22	.030
	1764.30	493792.99	8	.060
	5272.09	421873.27	3	.112
	8630.77	679071.69	5	.113

RANGES OF (SIN(THETA)/LAMBDA)**2

	NUMERATOR	DENOMINATOR	NUMBER	R
	20377.43	2076850.68	52	.099
	2448.77	1200248.43	75	.045
	2325.16	1084884.14	90	.046
	2162.58	994802.14	87	.047
	586.85	1312084.29	98	.021
	778.02	1201901.60	97	.025
	692.17	1569026.72	116	.021
	495.70	1445492.79	100	.019

UNREJECTED REFLECTIONS

	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	14954.08	10001528.28	707	.039
UNWEIGHTED R	692.90	26033.93	707	.027

RANGES OF F(OBS)

	NUMERATOR	DENOMINATOR	NUMBER	R
	10694.36	1890366.62	395	.075
	1535.00	4464329.26	169	.019
	1033.02	1660047.89	84	.025
	239.55	514162.84	29	.022
	528.98	733766.30	21	.027
	226.72	325898.49	6	.026
	432.40	263108.23	2	.041
	264.05	149848.65	1	.042

RANGES OF (SIN(THETA)/LAMBDA)**2

	NUMERATOR	DENOMINATOR	NUMBER	R
	6084.28	1280693.94	46	.069
	1997.94	1140522.58	74	.042
	2156.54	1057004.22	89	.045
	2162.58	994802.14	87	.047
	586.85	1312084.29	98	.021
	778.02	1201901.60	97	.025
	692.17	1569026.72	116	.021
	495.70	1445492.79	100	.019

SUM FCAL   27621.33
STANDARD DEV OF UNIT WEIGHT OBS   4.60

End of supplemental material.