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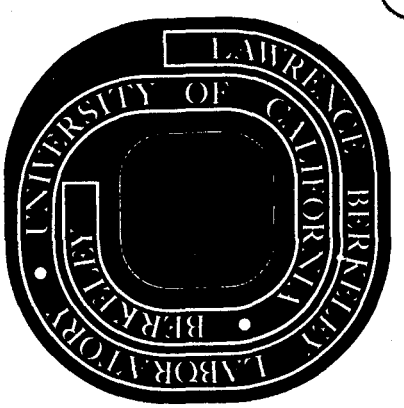

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The Crystal Structure of *l*-Ferrous-tris(1,10-phenanthroline) Bis(antimonous d-tartrate) Octahydrate[1]

By Allan Zalkin,* David H. Templeton, and Tatzuo Ueki

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[1]Work done under the auspices of the U.S. Atomic Energy Commission.

The compound ℓ-ferrous-tris (1,10-phenanthroline) bis(antimonous d-tartrate) octahydrate, $Fe(C_{12}N_2H_8)_3(C_4O_6H_2Sb)_2 \cdot 8H_2O$, crystallizes in the trigonal space group $P3_221$. Three formula units occupy a unit cell of dimensions a = 18.58(2) and c = 12.04(2) Å. Intensities were measured by the stationary-crystal stationary-counter technique using a scintillation counter and MoKα X-rays. The structure was refined by full-matrix least-squares to a conventional R factor of 0.048 for 1600 reflections whose intensities were observed to be greater than their estimated standard deviations. The structure consists of a ferrous tris(1,10-phenanthroline) cation and a bis(antimonous d-tartrate) anion. The iron atom lies on a two-fold axis and is octahedrally coordinated to the nitrogen atoms of the three phenanthroline groups at an average distance of 1.97(1) Å. The antimony tartrate complex is a dimer in which each of the two antimony atoms is coordinated to four oxygen atoms of the tartrate; Sb-O distances average 1.94(1) and 2.13(2) Å respectively for alcohol and carboxyl oxygen atoms. The absolute configurations of the complex ions were determined by the anomalous dispersion effect. The cation, $\Lambda(-)_{589}Fe\ phen_3^{2+}$, phen = phenanthroline, has a pseudo three-fold axis and resembles a three-bladed left-handed propeller, the blades being the planar phenanthroline ligands. The configuration of the d-tartrate in the $[Sb(+)tartrate]_2^{2-}$ ion is in agreement with previous determinations.

Introduction

Ferrous ion and 1,10-phenanthroline make octahedral complexes which exist in enantiomers that can be resolved by precipitation of the *l*-isomer with antimony d-tartrate as shown by Dwyer and Gyarfas.[2] Professor R. E. Powell

(2) F. P. Dwyer and E. C. Gyarfas, J. Proc. Roy. Soc. N. S. Wales, 83, 263 (1950).

of this University provided us crystals of this precipitate and suggested that we determine the structure and absolute configuration by X-ray diffraction to permit a check of methods of configuration determination by theoretical analysis of the optical properties. This paper reports such a study.[3]

(3) For a preliminary account, see D. H. Templeton, A. Zalkin and T. Ueki, Acta Crystallogr., 21, A154 (1966).

We show that the (--)-$[Fe\ phen_3]^{2+}$ which precipitates with d-tartrate is in the conformation of a left-handed propeller, in agreement with the assignment of McCaffery, Mason and Norman[1] on the basis of analysis of circular dichroism,

(1) A. J. McCaffery, S. F. Mason, and B. J. Norman, J. Chem. Soc. (A), 1969, 1428.

thus providing a confirmation of the validity of that method.

Another result of this study is that the antimony tartrate, which has been formulated classically in tartar emetic and similar salts as "antimonyl tartrate," $SbO(C_4H_4O_6)^-$, or sometimes[5] as $H_2O\ Sb(C_4H_2O_6)^-$, exists

(5) H. Reihlen and E. Hezel, Leib. Annalen, 486, 213 (1931).

in this crystal as a cyclic dimer of composition $((C_4H_2O_6)Sb)_2^{2-}$. In this complex Sb(III) has displaced hydrogen from the alcohol groups as well as the carboxyl groups and is complexed only by tartrate. The same complex anion has been found by Kiosse, Golovastikov, and Belov[6] in d,ℓ-$(NH_4)_2Sb_2(C_4H_2O_6)_2\cdot 4H_2O$,

(6) G. A. Kiosse, N. I. Golovastikov, and N. V. Belov, Dokl. Akad. Nauk SSSR, 155, 545 (1964).

by Kiosse, Golovastikov, Ablov, and Belov[7] in d-$(NH_4)_2Sb_2(C_4H_2O_6)_2\cdot 3H_2O$, and by Kamenar, Grdenic, and Prout[8] in d,ℓ-$K_2Sb_2(C_4H_2O_6)_2\cdot 3H_2O$.

(7) G. A. Kiosse, N. I. Golovastikov, A. V. Ablov, and N. V. Belov, Dokl. Akad. Nauk SSSR, 177, 329 (1967).

(8) B. Kamenar, D. Grdenic, and C. K. Prout, Acta Crystallogr., Sect. B, 26, 181 (1970).

Earlier conflicting reports[9] concerning the d,ℓ-K salt

(9) D. Grdenic and B. Kamenar, Acta Crystallogr., 16, A40 (1963); 19, 197 (1965).

have been withdrawn,[8] and the dimer structure is the only one known in crystals.

Experimental

The sample of ℓ-ferrous tris(1,10-phenanthroline) bis(antimonous d-tartrate) octahydrate consisted of crystals of small deep-red needles. A fragment ~0.1 mm in diameter and ~0.3 mm long was glued to a pyrex fiber, and subsequent Weissenberg photography showed the needle axis to be c of a trigonal unit cell. Cell dimensions and intensities were measured with a manual General Electric XRD-5 X-ray diffraction apparatus equipped with a quarter-circle Eulerian-cradle goniostat, and a scintillation counter with pulse height discrimination. MoKα X-rays, λ = 0.70926 Å for $K\alpha_1$, filtered by a 0.003-in thick Zr filter on the receiving slit were used for the measurements. The X-ray tube was operated at 40 kv and 20 ma. The crystal was so oriented that the c axis was parallel to the ϕ axis of the instrument.

Counts for ten sec each were made of 1748 independent reflections using a stationary-counter stationary-crystal technique; these include all the reflections whose indices

are positive and whose Bragg angles are less than 22.5°. The diffractometer was set at a 4° takeoff angle to the tube. Background was plotted as a function of 2θ and these values were used for most of the intensities; in cases where background was affected by streaking, individual backgrounds were measured. Typical backgrounds between 20° and 45° of 2θ were from 2 to 4 counts per sec. The 0,3,2 reflection was the largest intensity registering a counting rate of 7856 cps. 80 reflections were observed to be equal to or below background, and an additional 64 had intensities less than an estimated standard deviation; in the least-squares refinements these data were assigned zero weights. The data were corrected for the Lorentz-polarization factors, and no correction was made for absorption. The absorption coefficient μ is estimated to be 15 cm^{-1}. No extinction correction was found necessary.

In the course of some experiments using CuKα radiation, the cell dimensions were observed to be very much affected by relative humidity. When the relative humidity, as read from a simple Abbeon Relative Humidity Indicator, read 30% the trigonal cell dimensions were calculated to be $\underline{a}$ = 18.55 and $\underline{c}$ = 12.00 Å; at 46% they swelled to 18.61 and 12.04 Å. This behavior is somewhat similar to that we observed in collecting data for ferrichrome-A.[10] Had we

(10) A. Zalkin, J. D. Forrester, and D. H. Templeton, J. Amer. Chem. Soc., 88, 1810 (1966).

had fluctuations to the limits of the two extremes in humidity reported above, the error in the 2θ angle at 45° with Mo X-rays is about 0.15°; this does not produce a serious setting error, and in fact no problem was noticed during the manual collection of the data. With copper radiation, setting errors are serious; for at a comparable $\sin\theta/\lambda$ value the error amounts to about 0.6°. We collected some 8000 scanned intensities on a second crystal using CuKα radiation with an automatic diffractometer, but we abandoned the set for two reasons. We lacked confidence in the settings due to humidity changes that occurred during the two weeks required to collect the data, even though we attempted daily modifications of the cell dimensions. Secondly, Cu data suffer much more from absorption. We made some refinements using the Cu data, and the resulting coordinates were within two standard deviations of the results from the manually collected Mo data we report here.

Fourier, least-squares, and distance calculations were performed using our own unpublished programs on a Control Data Corporation 6600 computer. The full-matrix least-squares program minimizes the function $\Sigma w(|F_o| -$

$|F_c|)^2/\Sigma wF_o^2$; F_o and F_c are the observed and calculated structure factors, and w is the weighting factor. Atomic scattering factors for Sb^{3+}, Fe^{2+}, neutral O, N, C and H were used,[11,12] and both the real and imaginary parts of

(11) D. T. Cromer and J. T. Waber, Acta Crystallogr., 18, 104 (1965).

(12) R. F. Stewart, E. R. Davidson, and W. T. Simpson, J. Chem. Phys., 42, 3175 (1965).

the anomalous dispersion correction[13] for Sb and Fe were

(13) D. T. Cromer, Acta Crystallogr., 18, 17 (1965).

included in the least-squares calculations. Anisotropic temperature factors used have the form $\exp-(h^2\beta_{11} + k^2\beta_{22} + \ell^2\beta_{33} + 2hk\beta_{12} + 2h\ell\beta_{13} + 2k\ell\beta_{23})$; for convenience the thermal parameters are reported here as B_{ij}, in units $Å^2$, where $B_{ij} = 4\beta_{ij}/a_i^* a_j^*$ and a_i^* is the ith reciprocal cell length. The weighting on each reflection, w, was set to $(\sigma(F_o))^{-2}$ with the exception that w = 0 when I(net count) $\leq \sigma(I)$. The standard deviation of the observed structure factor was calculated as $\sigma(F_o) = F_o - (F_o^2 - s\sigma(I)/Lp)^{1/2}$, where s is a scaling

factor, $F_o = (sI/Lp)^{1/2}$, and Lp is the Lorentz-polarization correction. $\sigma(I) = (I + p^2I^2 + 2B)^{1/2}$, where p is an estimated fractional uncertainty in I, and B is the background. A value of p = 0.07 was found necessary to reduce the weights of the intense reflections so that their weighted residuals were comparable to those of lesser intensity.

Results

Unit Cell and Space Group.—The cell dimensions are a = 18.58 ± 0.02 and c = 12.04 ± 0.02 Å at ~24°; the accuracy is limited by the humidity effect and these reported values are estimated to have been measured when the relative humidity was between 35 and 40%. The observed Laue symmetry of the reflections is $\bar{3}$m1. The observed setting of the symmetry, $I(hk\ell) = I(kh\bar{\ell})$, the known asymmetry of the molecules, and the observed absences where $00\ell \neq 3n$, indicate the enantiomorphic pair of space groups $P3_121$ and $P3_221$ as the sole choices; anomalous dispersion effects established the space group to be $P3_221$, (D_3^6). Allowing for three formula units per unit cell, the calculated X-ray density is 1.77 g/cc.

Structure Determination.—The positions of the iron and antimony atoms were readily determined from a three-dimensional Patterson map. The iron occupies a

special position on a two-fold axis, and all of the other atoms occupy the general six-fold set. A Fourier phased on the Fe and Sb atoms resulted in the location of 19 of the 35 non-hydrogen atoms. The partial structure was refined to an R factor, $R = \Sigma |\Delta F| / \Sigma |F_o|$, of 0.20. A second Fourier revealed the remaining atoms with the exception of the hydrogen and the water oxygen atoms. Further refinement of the structure followed by a difference Fourier revealed four water oxygen atoms. Hydrogen atoms did not show up very well on the difference Fourier maps, and eventually the parameters of all but the water hydrogens were included but constrained to their estimated positions with a fixed isotropic thermal parameter of 5.0 $Å^2$. From the humidity effect it is evident that water is loosely bound in this crystal and most probably occurs in its sites with partial occupancy. This conclusion is supported by the large temperature parameters of the water oxygen atoms. Since there is no clear-cut ordered hydrogen bond pattern in the water substructure, we could not estimate the hydrogen positions of the water molecules.

The results of the least-squares refinement are shown in Tables I and II. Figures 1 and 2 serve as guides to the numbering system. The refinement was arbitrarily started in space group $P3_121$, but this was changed to $P3_221$ in

order that the configuration of the d-tartrate would be the same as that reported by Bommel and Bijvoet.[14]

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(14) A. J. van Bommel and J. M. Bijvoet, Acta Crystallogr., 11, 61 (1958).

The final R factor on 1600 non-zero weighted data is 0.048; the weighted R_2 factor, $\Sigma(\Delta F)^2/\Sigma w|F_o|^2$, is 0.056; the standard deviation of an observation of unit weight is 1.07; and the R factor for all 1748 data, including the zero-weighted ones, is 0.057. A table of observed and calculated structure factors is available upon request.[15]

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(15) A listing of structure factor amplitudes will appear immediately following this article in the microfilm edition of this volume of the journal. Single copies may be obtained from the Business Operations Office, Books and Journals Division, American Chemical Society, 1155 Sixteenth St., N.W., Washington, D. C. 20036, by referring to author, title of article, volume and page number. Remit $\_\_\_\_$ for photocopy or $\_\_\_\_$ for microfiche.

A difference function based on the final set of parameters was calculated. The maximum peak height on this map was 0.8e/Å^3. The largest peaks appear near the

antimony atom, but no attempt was made to associate them with any electron pair structure. From the size of these peaks and their locations, it is evident that there is no antimonyl type oxygen in this compound.

A series of refinements made with the anomalous dispersion reversed, resulted in R increasing from 0.048 to 0.052 and R_2 went from 0.056 to 0.062. This is in agreement with the configuration for the d-tartrate determined by Bommel and Bijvoet.[14] An additional experiment to check the absolute configuration was performed using CuKα radiation to measure some 528 data representing about 120 independent reflections. The Δf" for Fe and Sb, respectively, is 3.5 and 5.8 electrons with CuKα radiation. The Fe and Sb were refined anisotropically, carbon, oxygen and nitrogen were included with isotropic thermal parameters but were not refined; hydrogen atoms were omitted. The set of 120 reflections refined to R = 0.06 with the correct configuration; when the anomalous dispersion effect was reversed the R factor went to 0.10.

Description of the Structure

The cation consists of an iron atom complexed by three planar phenanthroline ligands to form a left-handed propeller-type structure, see Figure 3. In keeping with recent nomenclature proposals[16] this ion would be described as $\Lambda\,(--)_{589}$Fe $phen_3^{2+}$, phen = phenanthroline.

(16) Tentative Proposals for Nomenclature of Absolute Configurations Concerned with Six-Coordinated Complexes Based on the Octahedron, Inorg. Chem., 9, 1 (1970).

The ion itself lies on a crystallographic two-fold axis, but its molecular symmetry is also very nearly three-fold. The iron atom is coordinated to all six nitrogen atoms of the three phananthroline groups at an average distance of 1.97 $\pm$ 0.01 Å. A list of distances and angles in the cation is presented in Table III.

The anion consists of a dimer of antimony tartrate on a crystallographic two-fold axis. Figure 4 shows a stereoscopic view of this ion. A list of distances and angles of this anion is shown in Table IV. Each antimony is coordinated to four oxygen atoms from the tartrate ligands, and there is no evidence in this study of any further coordination to the antimony, i.e., an antimonyl oxygen. The same complex has been reported with very similar shape in the studies cited above.[6-8] Average distances are 2.13 Å for Sb-O (carbonyl) and 1.94 Å for Sb-O (alcohol), somewhat shorter than the corresponding average values reported for the other crystals: (2.15, 2.04),[6] (2.18, 2.02),[7] and (2.20, 2.01).[8]

The anion and cation pack in a way which is not simple to describe. A stereographic view of the structure looking down the three-fold axis is shown in Figure 5. The closest approach of the cation to the anion occurs between O(6) in the anion and H(12) in the cation at a distance of 2.35 Å; the closest non-hydrogen approach is between O(5) in the anion and C(13) in the cation at a distance of 3.16 Å.

The water structure in this crystal is indicated in Figure 6; in this figure all contact distances less than 3.04 Å are indicated with a connection. The O(7) water molecules form a spiral in the direction of the c axis, and waters O(8), O(9), and O(10) form a structure with hydrogen bonding to O(1) and O(4) of the tartrate groups. The temperature factors of the water molecules are large, which probably represents incomplete occupancy and disorder. The observation that the cell dimensions change reversibly and radically with humidity is indicative that water can readily enter and leave the crystal, and that these sites were partially occupied under the conditions of the experiment. Disorder in the water structure is evident in the close approach across two-fold axes of O(7) to another O(7) and similarly O(10) to O(10); for if the close approaches are due to hydrogen bonding one must invoke disorder to describe the hydrogen atom positions.

One can identify three hydrogen bonds in Table V which must be ordered, since they are between water and carbonyl oxygen atoms. The other distances in the table provide only four and one-half bonds for the other five hydrogen atoms in the asymmetric unit, and all of these bonds have the possibility of alternate configurations for the hydrogen. The lack of a satisfactory unique hydrogen bond configuration may contribute to the ease with which water can escape from the structure.

Acknowledgment.—We thank Professor Richard E. Powell for bringing this problem to our attention and providing us with crystals.

TABLE I

ATOMIC COORDINATES[a]

[a]Numbers in parentheses here and in subsequent tables indicate estimated standard deviations of the least significant digits.

(Table to be reproduced photographically)

ATOM	X	Y	Z
FE	-.3985(1)	0	-1/3
SB	-.48029(7)	-.34732(6)	-.39066(7)
O(1)	-.2399(9)	-.2714(8)	-.3044(9)
O(2)	-.3769(9)	-.3256(7)	-.2931(8)
O(3)	-.3931(6)	-.3003(7)	-.5013(7)
O(4)	-.6430(7)	-.5199(8)	-.6147(8)
O(5)	-.5627(6)	-.3996(7)	-.5308(7)
O(6)	-.5023(6)	-.4609(6)	-.3872(6)
O(7)	.110(1)	.069(1)	-.399(1)
O(8)	.277(1)	.079(1)	-.421(1)
O(9)	.155(2)	.229(1)	-.298(2)
O(10)	-.066(2)	-.317(2)	-.099(2)
N(1)	-.3499(6)	-.0604(6)	-.2624(7)
N(2)	-.3582(6)	.0845(6)	-.2140(8)
N(3)	-.4396(6)	.0705(6)	-.3976(7)
C(1)	-.307(1)	-.291(1)	-.344(1)
C(2)	-.310(1)	-.272(1)	-.464(1)
C(3)	-.589(1)	-.476(1)	-.544(1)
C(4)	-.559(1)	-.5182(9)	-.465(1)
C(5)	-.3820(9)	-.1206(9)	-.191(1)
C(6)	-.339(1)	-.156(1)	-.145(1)
C(7)	-.262(2)	-.132(1)	-.176(1)
C(8)	-.139(1)	-.029(1)	-.298(1)
C(9)	-.222(1)	-.065(1)	-.255(1)
C(10)	-.2703(8)	-.0325(9)	-.296(1)
C(11)	-.3121(8)	.0927(8)	-.125(1)
C(12)	-.2835(8)	.1602(9)	-.056(1)
C(13)	-.3052(8)	.2193(8)	-.0698(9)
C(14)	-.3784(9)	.2716(9)	-.190(1)
C(15)	-.4249(8)	.2618(8)	-.279(1)
C(16)	-.4924(8)	.1826(8)	-.453(1)
C(17)	-.5072(9)	.117(1)	-.522(1)
C(18)	-.4803(7)	.0623(8)	-.4919(9)
C(19)	-.3547(8)	.2125(8)	-.161(1)
C(20)	-.4488(7)	.1931(7)	-.3564(9)
C(21)	-.4245(7)	.1355(8)	-.3308(9)
C(22)	-.3774(8)	.1448(8)	-.2329(9)
H(1)	-.443	-.142	-.167
H(2)	-.368	-.206	-.089
H(3)	-.231	-.158	-.143
H(4)	-.103	-.051	-.271
H(5)	-.298	.048	-.110
H(6)	-.247	.166	.012
H(7)	-.284	.268	-.015
H(8)	-.363	.321	-.141
H(9)	-.443	.304	-.295
H(10)	-.512	.222	-.475
H(11)	-.537	.111	-.594
H(12)	-.492	.013	-.542
H(13)	-.271	-.212	-.490
H(14)	-.610	-.566	-.424

TABLE II

ANISOTROPIC THERMAL PARAMETERS, $Å^2$

(Table to be reproduced photographically)

ATOM	B11	B22	B33	B12	B13	B23
FE	3.24(8)	2.7642	2.12(8)	1.38(6)	-.07(4)	-.1402
SR	7.16(7)	4.92(5)	3.54(4)	4.12(5)	1.03(4)	.31(4)
O(1)	8.3(8)	8.0(7)	5.7(5)	4.1(6)	-2.9(6)	-1.9(5)
O(2)	8.6(8)	5.0(6)	3.7(5)	2.8(5)	.1(5)	.2(4)
O(3)	5.9(5)	6.5(6)	3.9(4)	3.6(5)	.4(4)	1.7(4)
O(4)	6.2(6)	8.5(7)	5.6(5)	5.1(6)	-1.7(5)	.4(5)
O(5)	6.0(5)	5.5(6)	4.8(5)	4.2(5)	-.4(4)	.6(4)
O(6)	5.7(5)	4.7(5)	2.2(4)	3.1(4)	-.4(3)	.2(3)
O(7)	12.9(13)	10.0(11)	9.1(8)	5.1(9)	.1(8)	-.2(8)
O(8)	15.0(14)	14.6(15)	8.5(9)	3.1(12)	1.1(9)	-5.7(9)
O(9)	17.7(18)	15.4(17)	17.8(16)	10.0(15)	-6.1(15)	-5.1(14)
O(10)	27.3(27)	18.8(20)	20.1(19)	17.5(19)	11.1(19)	5.9(16)
N(1)	3.6(6)	2.7(5)	3.1(4)	1.4(4)	.2(4)	.1(4)
N(2)	3.5(5)	3.5(5)	2.6(4)	1.9(4)	-.4(4)	.1(4)
N(3)	3.8(5)	3.5(5)	2.0(4)	1.9(4)	.2(4)	-.0(4)
C(1)	7.6(11)	5.4(9)	4.3(8)	3.9(9)	-2.1(9)	-1.5(7)
C(2)	7.4(10)	5.5(8)	3.8(7)	3.5(8)	-.4(6)	.4(6)
C(3)	5.7(8)	6.0(9)	2.2(5)	4.3(8)	-.4(6)	.3(6)
C(4)	4.2(7)	6.2(8)	3.2(6)	3.1(7)	.7(6)	.1(6)
C(5)	4.8(8)	3.9(7)	3.8(6)	2.8(6)	-.8(6)	-.9(5)
C(6)	7.1(11)	6.2(9)	3.4(7)	4.1(8)	.1(7)	.3(6)
C(7)	9.6(13)	7.9(11)	6.1(9)	7.2(10)	-2.8(10)	-2.4(9)
C(8)	7.3(11)	11.9(18)	5.8(10)	7.0(12)	-.3(8)	.0(9)
C(9)	5.5(9)	7.4(10)	4.7(7)	4.0(8)	-.4(7)	.0(8)
C(10)	3.8(7)	4.6(8)	3.3(6)	1.9(6)	-1.0(5)	-1.0(5)
C(11)	2.9(6)	3.5(7)	3.7(6)	1.4(5)	-.4(5)	.5(5)
C(12)	3.8(7)	4.0(7)	3.2(6)	1.4(6)	-.4(5)	-.8(5)
C(13)	3.6(6)	3.7(7)	2.7(5)	.9(5)	-.6(5)	-1.6(5)
C(14)	4.7(8)	4.6(8)	3.4(6)	2.3(6)	.4(6)	-.2(5)
C(15)	4.6(7)	2.7(6)	5.0(7)	2.7(6)	1.5(6)	1.1(5)
C(16)	4.3(7)	3.8(6)	4.2(6)	2.3(6)	-.3(5)	.9(5)
C(17)	3.8(7)	5.8(8)	2.9(5)	2.4(6)	-1.0(5)	.0(5)
C(18)	3.3(6)	3.6(6)	2.5(5)	1.2(5)	-.2(5)	.5(4)
C(19)	3.9(6)	2.3(5)	3.1(5)	1.5(5)	.5(5)	-.6(5)
C(20)	3.2(5)	2.8(6)	3.2(5)	1.6(5)	.3(4)	.2(5)
C(21)	3.2(6)	3.7(6)	2.2(5)	1.5(5)	.5(4)	.3(5)
C(22)	2.9(6)	3.5(6)	2.1(5)	1.3(5)	.6(4)	1.1(5)

TABLE III

DISTANCES AND ANGLES IN THE Fe $phen_3$ CATION

Distances, Å

Fe	- N(1)	1.96(1)	C(5)	- C(6)	1.39(2)	C(13)	- C(19)	1.39(2)
Fe	- N(2)	1.98(1)	C(6)	- C(7)	1.32(3)	C(14)	- C(15)	1.33(2)
Fe	- N(3)	1.97(1)	C(7)	- C(9)	1.44(3)	C(15)	- C(20)	1.46(2)
N(1)	- C(5)	1.30(2)	C(8)	- C(8)	1.26(4)	C(16)	- C(17)	1.38(2)
N(1)	- C(10)	1.36(2)	C(8)	- C(9)	1.44(3)	C(16)	- C(20)	1.37(2)
N(2)	- C(11)	1.33(2)	C(9)	- C(10)	1.39(2)	C(17)	- C(18)	1.39(2)
N(2)	- C(22)	1.35(2)	C(10)	- C(10)	1.38(3)	C(19)	- C(22)	1.41(2)
N(3)	- C(18)	1.33(2)	C(11)	- C(12)	1.38(2)	C(20)	- C(21)	1.39(2)
N(3)	- C(21)	1.36(2)	C(12)	- C(13)	1.36(2)	C(21)	- C(22)	1.43(2)

Angles, deg.

N(1)	-Fe -N(1)	82.9(3)	C(6)	-C(7) -C(9)	119(2)	C(16)	-C(17)-C(18)	120(2)
N(1)	-Fe -N(2)	92.2(5)	C(8)	-C(8) -C(9)	123(2)	N(3)	-C(18)-C(17)	122(2)
N(1)	-Fe -N(2)	89.4(5)	C(7)	-C(9) -C(8)	128(2)	C(13)	-C(19)-C(14)	125(2)
N(1)	-Fe -N(3)	94.7(6)	C(7)	-C(9) -C(10)	116(2)	C(13)	-C(19)-C(22)	117(2)
N(1)	-Fe -N(3)	174.6(7)	C(8)	-C(9) -C(10)	116(2)	C(14)	-C(19)-C(22)	118(2)
N(2)	-Fe -N(2)	177.9(3)	N(1)	-C(10)-C(9)	123(2)	C(15)	-C(20)-C(16)	124(2)
N(2)	-Fe -N(3)	82.9(5)	N(1)	-C(10)-C(10)	116(2)	C(15)	-C(20)-C(21)	117(2)
N(2)	-Fe -N(3)	95.6(5)	C(9)	-C(10)-C(10)	121(2)	C(16)	-C(20)-C(21)	118(2)
N(3)	-Fe -N(3)	88.1(3)	N(2)	-C(11)-C(12)	122(2)	N(3)	-C(21)-C(20)	123(1)
C(5)	-N(1) -C(10)	118(2)	C(11)	-C(12)-C(13)	122(2)	N(3)	-C(21)-C(22)	116(1)
C(11)	-N(2) -C(22)	117(2)	C(12)	-C(13)-C(19)	118(2)	C(20)	-C(21)-C(22)	120(2)
C(18)	-N(3) -C(21)	117(2)	C(15)	-C(14)-C(19)	122(2)	N(2)	-C(22)-C(19)	123(2)
N(1)	-C(5) -C(6)	123(2)	C(14)	-C(15)-C(20)	122(2)	N(2)	-C(22)-C(21)	116(1)
C(5)	-C(6) -C(7)	120(2)	C(17)	-C(16)-C(20)	119(2)	C(19)	-C(22)-C(21)	121(2)

TABLE IV

DISTANCES AND ANGLES IN THE BIS(ANTIMONY TARTRATE) ANION

Distances, Å

Sb - O(3)	1.94(1)	O(5) - C(3)	1.27(2)
Sb - O(6)	1.94(1)	O(3) - C(2)	1.44(2)
Sb - O(2)	2.11(2)	O(6) - C(4)	1.41(2)
Sb - O(5)	2.16(2)	C(1) - C(2)	1.50(2)
O(1) - C(1)	1.21(2)	C(3) - C(4)	1.50(2)
O(4) - C(3)	1.26(2)	C(2) - C(2)	1.49(4)
O(2) - C(1)	1.28(2)	C(4) - C(4)	1.56(3)

Angles, Deg.

O(2)-Sb -O(3)	79.7(6)	O(1)-C(1)-C(2)	117(2)
O(2)-Sb -O(5)	153.5(7)	O(2)-C(1)-C(2)	116(2)
O(2)-Sb -O(6)	82.7(5)	O(3)-C(2)-C(1)	111(2)
O(3)-Sb -O(5)	84.9(5)	O(3)-C(2)-C(2)	109(2)
O(3)-Sb -O(6)	100.3(6)	C(1)-C(2)-C(2)	112(2)
O(5)-Sb -O(6)	79.1(5)	O(4)-C(3)-O(5)	123(2)
Sb -O(2)-C(1)	115.3(8)	O(4)-C(3)-C(4)	119(2)
Sb -O(3)-C(2)	117.3(7)	O(5)-C(3)-C(4)	118(2).
Sb -O(5)-C(3)	113.0(7)	O(6)-C(4)-C(3)	111(2)
Sb -O(6)-C(4)	118.6(7)	O(6)-C(4)-C(4)	112(2)
O(1)-C(1)-O(2)	127(2)	C(3)-C(4)-C(4)	108(2)

TABLE V

DISTANCES AND ANGLES INVOLVING WATER OXYGEN ATOMS

Distances, Å

O(7)	-O(7)	2.73(4)
O(7)	-O(7)	2.77(3)
O(7)	-O(9)	2.93(3)
O(7)	-O(8)	3.03(3)
O(8)	-O(1)	2.74(2)
O(8)	-O(10)	2.90(4)
O(9)	-O(1)	2.88(3)
O(10)	-O(10)	2.69(5)
O(10)	-O(4)	2.73(3)

Angles, Deg.

O(7)	-O(7)	-O(7)	135(1)
O(7)	-O(7)	-O(8)	109(1)
O(7)	-O(7)	-O(9)	94(1)
O(7)	-O(7)	-O(8)	95(1)
O(7)	-O(7)	-O(9)	119(1)
O(8)	-O(7)	-O(9)	103(1)
O(1)	-O(8)	-O(7)	101(1)
O(1)	-O(8)	-O(10)	105(1)
O(7)	-O(8)	-O(10)	76(1)
O(1)	-O(9)	-O(7)	109(1)
O(4)	-O(10)	-O(8)	112(1)
O(4)	-O(10)	-O(10)	113(1)
O(8)	-O(10)	-O(10)	128(1)

LEGEND CAPTIONS

Figure 1.—Diagram of the ferrous tris(1,10-phenathroline) cation indicating the numbering system used.

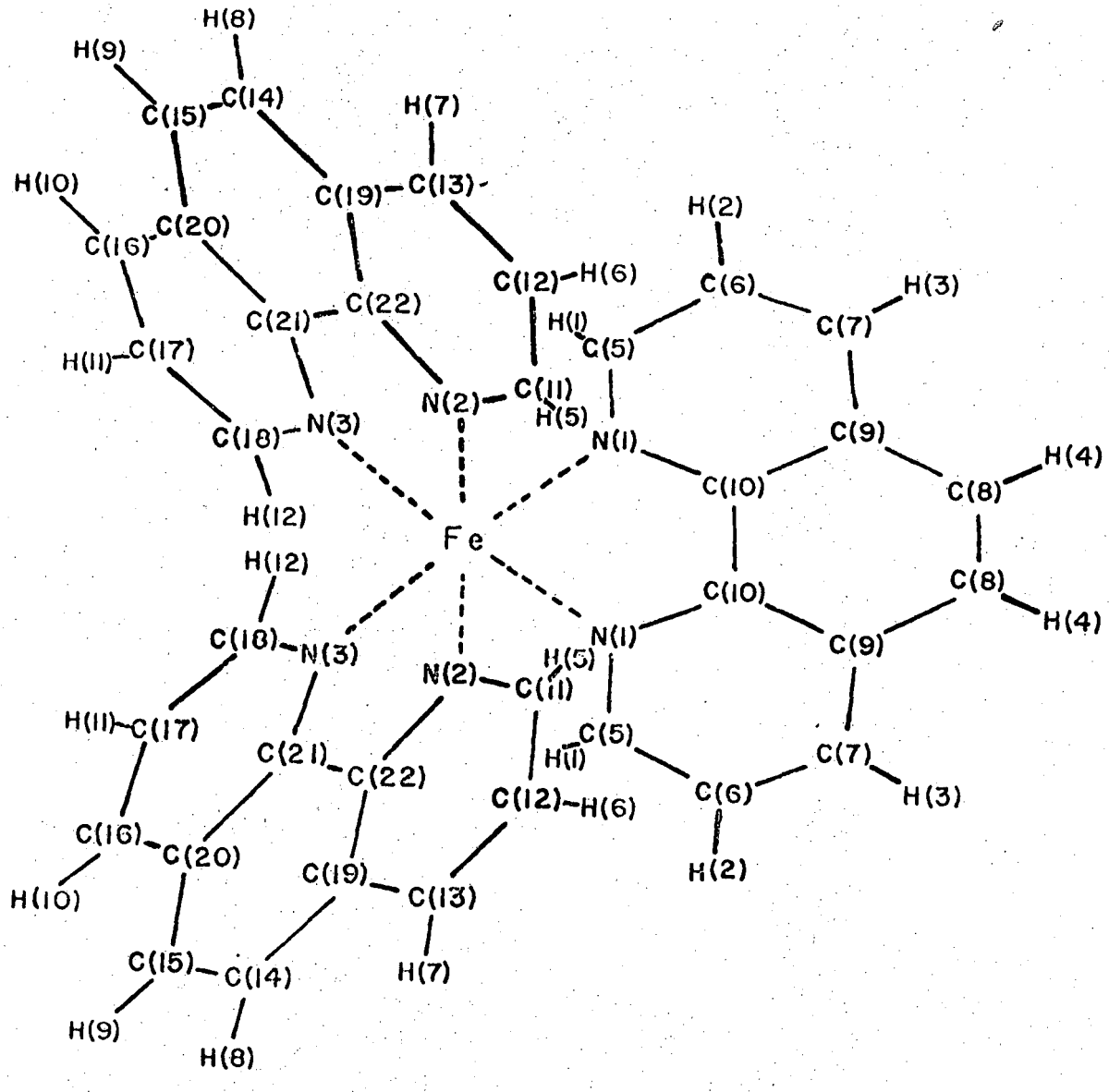
Figure 2.—Diagram of the bis(antimony tartrate) anion indicating the numbering system used.

Figure 3.—Stereoscopic view of the $(-)_{589}Fe\ phen_3^{2+}$ ion.

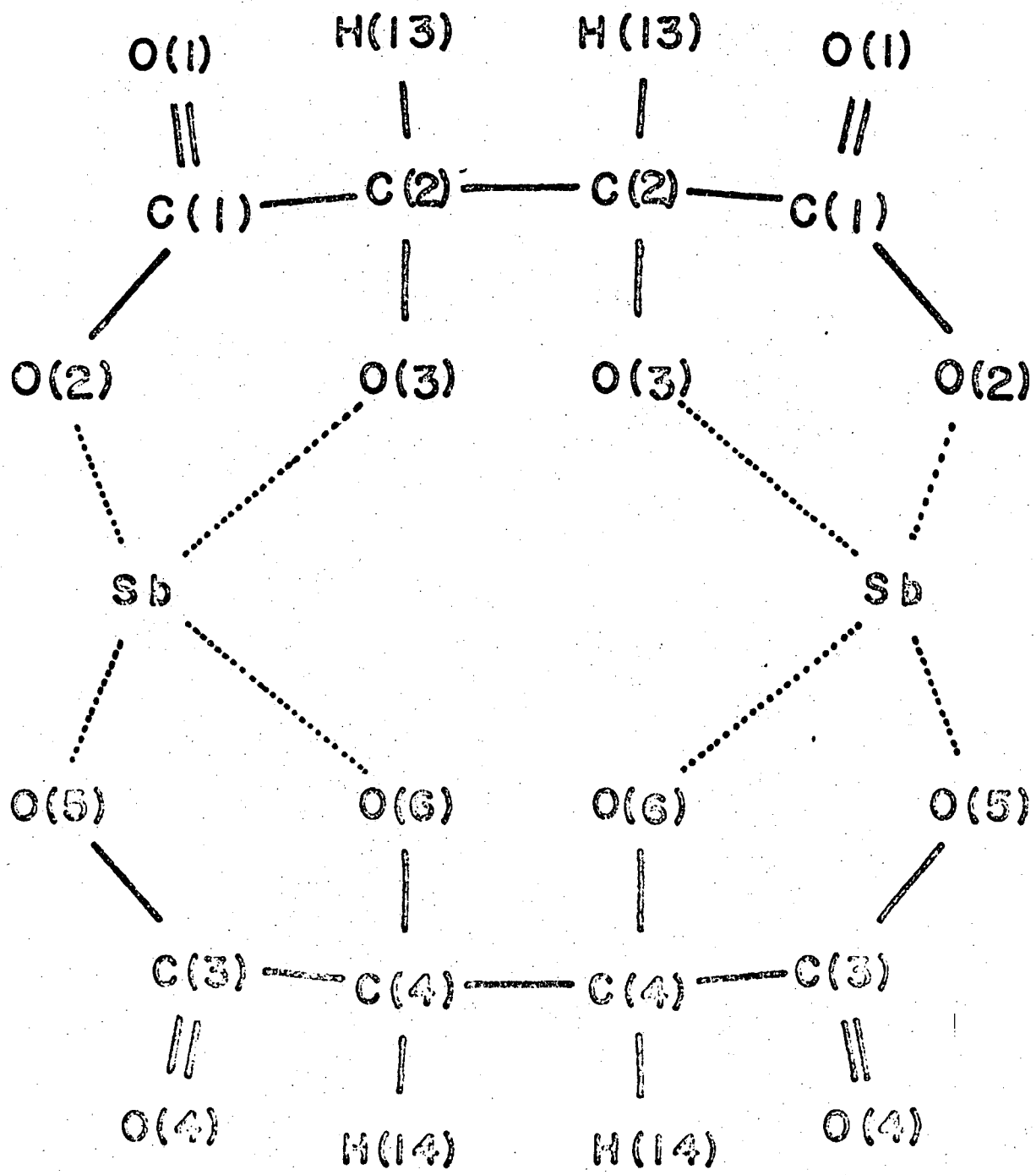
Figure 4.—Stereoscopic view of the bis(antimony d-tartrate)$^{2-}$ ion.

Figure 5.—Stereoscopic packing diagram as viewed down the c axis.

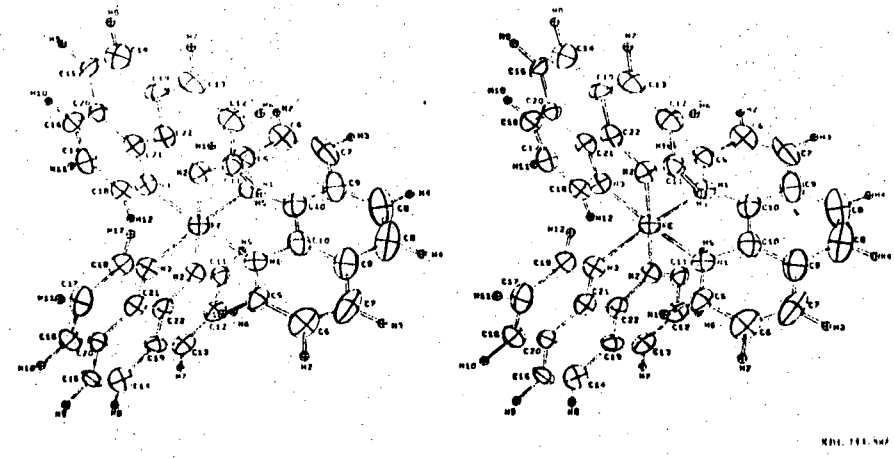
Figure 6.—Stereoscopic view showing the water oxygen structure. Atoms O(7) through O(10) represent water oxygen atoms; O(1) and O(4) represent tartrate oxygen atoms.

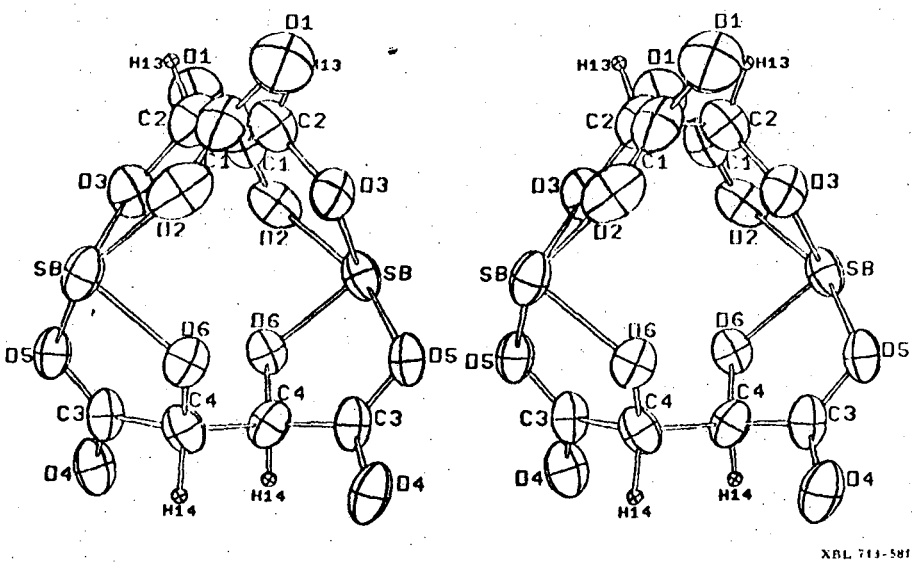

H(8)
H(9)
C(15)
C(14)
H(7)
H(10)
C(19)
C(13)
C(16)
C(20)
H(2)
C(12)
H(6)
C(6)
H(3)
C(21)
C(22)
H(1)
C(5)
C(7)
H(11)
C(17)
N(2)
C(11)
H(5)
C(18)
N(3)
N(1)
C(9)
H(4)
C(10)
C(8)
H(12)
Fe
H(12)
C(10)
C(8)
C(18)
N(3)
N(1)
H(4)
N(2)
C(11)
H(5)
C(9)
H(11)
C(17)
C(5)
C(7)
C(21)
C(22)
H(1)
C(12)
H(6)
C(6)
H(3)
C(16)
C(20)
H(2)
H(10)
C(19)
C(13)
C(15)
C(14)
H(7)
H(9)
H(8)

XBL 713-578

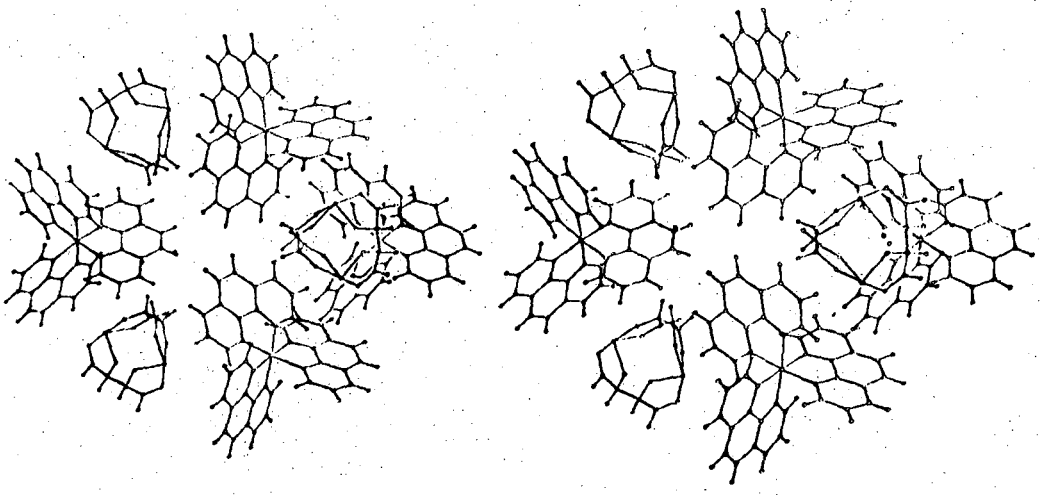

O(1)
H(13)
H(13)
O(1)
C(1)
C(2)
C(2)
C(1)
O(2)
O(3)
O(3)
O(2)
Sb
Sb
O(5)
O(6)
O(6)
O(5)
C(3)
C(4)
C(4)
C(3)
O(4)
H(14)
H(14)
O(4)

XBL 713-577

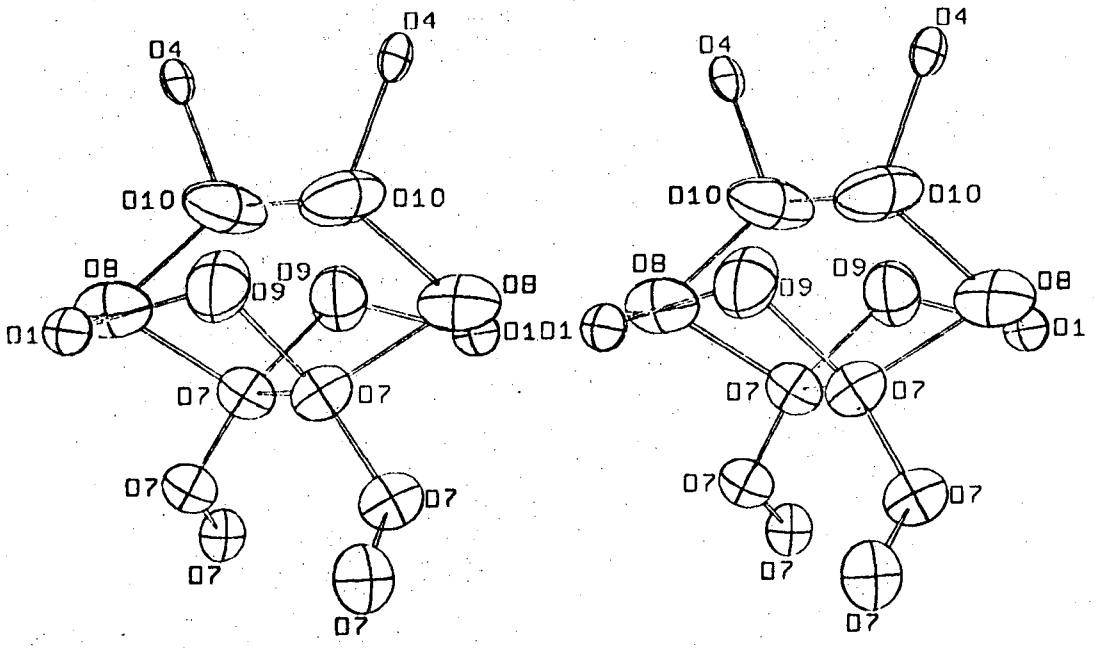



O1
H13
O1
H13
C2
C2
C1
C1
O3
O3
O2
O2
SB
SB
O6
O6
O5
O5
C4
C4
C3
C3
O4
O4
H14
H14
O1
H13
O1
H13
C2
C2
C1
C1
O3
O3
O2
O2
SB
SB
O6
O6
O5
O5
C4
C4
C3
C3
O4
O4
H14
H14

XBL 713-581



XBL 718-1267


O4
O4
O10
O10
O8
O9
O9
O8
O1
O101
O7
O7
O7
O7
O7
O7
O4
O4
O10
O10
O8
O9
O9
O8
O1
O7
O7
O7
O7
O7

XBL 718-1268

APPENDIX

TABLE OF OBSERVED STRUCTURE FACTORS FOR FERROUS TRIS (1,10-PHENANTHROLINE) BIS(ANTIMONY TARTRATE) OCTAHYDRATE

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 3.0) FOR FE++(1,10-PHENANTHROLINE) BIS(SB TARTRATE) OCTAHYDRATE. F(0,0,0) = 5516

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	0,	0		9	0	27	-5*	11	33	26	-8	8	57	10	6	H,K=	1,	2	
3	332	12	32	10	21	29	1*	H,K=	0,	9		H,K=	0,	14		0	151	6	6
6	65	6	-8	11	115	7	11	1	81	6	5	1	149	8	-3	1	430	15	-15
9	436	16	9	12	0	29	-40*	2	301	11	-7	2	0	26	-3*	2	577	21	46
12	86	8	12	H,K=	0,	5		3	160	7	-1	3	94	7	10	3	641	23	25
H,K=	0,	1		1	58	13	-1	4	0	27	-24*	4	0	27	-5*	4	290	11	22
1	629	22	7	2	398	14	41	5	102	6	13	5	93	7	4	5	278	10	4
2	765	27	84	3	619	22	17	6	59	8	-2	6	0	30	-17*	6	185	8	0
3	49	5	-7	4	0	21	-4*	7	44	9	4	7	0	29	-6*	7	94	6	2
4	446	16	-11	5	91	9	-14	8	170	8	9	H,K=	0,	15		8	40	9	19
5	417	15	5	6	586	21	-3	9	0	32	-14*	1	0	29	-19*	9	232	9	-5
6	202	8	22	7	152	7	-4	10	169	8	3	2	0	27	-1*	10	76	8	-6
7	40	8	-2	8	26	28	5*	11	82	8	5	3	73	8	2	11	114	7	-3
8	66	7	-4	9	212	9	-13	H,K=	0,	10		4	123	8	-1	12	190	9	-13
9	105	7	-9	10	59	8	8	1	24	19	15	5	0	32	-5*	H,K=	1,	3	
10	239	10	-12	11	88	8	-3	2	124	7	1	6	0	29	-23*	0	480	17	-6
11	60	9	10	12	40	12	2	3	232	9	8	H,K=	0,	16		1	279	10	18
12	90	8	-2	H,K=	0,	6		4	51	8	6	1	60	9	-15	2	277	10	31
H,K=	0,	2		1	106	5	-8	5	0	27	-32*	2	45	12	-2	3	24	10	6
1	252	9	16	2	96	5	6	6	48	14	4	3	61	9	-4	4	90	5	-1
2	62	4	-14	3	40	12	1	7	224	9	-14	4	0	29	-5*	5	441	16	-4
3	389	14	37	4	370	14	-2	8	120	7	-1	5	154	8	2	6	181	8	-2
4	460	17	7	5	98	6	-2	9	203	9	9	H,K=	0,	17		7	209	8	-4
5	31	9	-3	6	83	7	-8	10	23	29	4*	1	57	10	-4	8	164	7	-11
6	26	11	7	7	95	10	6	H,K=	0,	11		2	78	9	-4	9	111	7	1
7	485	18	-15	8	178	8	1	1	88	6	-2	H,K=	1,	0		10	20	26	15*
8	71	11	-10	9	231	10	-6	2	213	9	6	0	491	18	-1	11	43	11	20
9	80	6	25	10	60	9	0	3	41	10	16	1	437	16	15	12	131	8	-4
10	64	8	2	11	158	8	5	4	226	9	-13	2	353	13	64	H,K=	1,	4	
11	121	7	3	12	0	26	-14*	5	0	24	-3*	3	221	8	9	0	326	12	-11
12	23	29	17*	H,K=	0,	7		6	154	8	8	4	139	6	1	1	665	24	2
H,K=	0,	3		1	59	5	-8	7	103	7	15	5	242	9	15	2	506	18	31
1	19	19	-0*	2	274	10	7	8	22	28	14*	6	178	7	-3	3	165	7	-7
2	1298	46	-9	3	303	11	3	9	68	9	26	7	33	14	21	4	177	7	-0
3	177	7	23	4	354	13	17	10	0	32	-28*	8	257	10	-4	5	294	11	-4
4	48	8	-4	5	140	7	-2	H,K=	0,	12		9	53	11	0	6	194	8	-6
5	49	8	2	6	259	10	-2	1	307	12	-3	10	85	8	-1	7	162	7	-6
6	133	6	4	7	138	7	-7	2	150	7	3	11	0	28	-18*	8	200	8	-7
7	243	10	6	8	87	8	2	3	106	7	-10	12	55	10	0	9	85	7	-6
8	236	9	-8	9	156	8	0	4	59	8	-3	H,K=	1,	1		10	168	8	1
9	135	7	-9	10	220	9	6	5	204	9	-5	0	357	13	49	11	66	9	-3
10	149	8	2	11	23	29	7*	6	0	26	-23*	1	513	18	47	12	77	8	2
11	146	8	-7	H,K=	0,	8		7	38	13	8	2	144	6	1	H,K=	1,	5	
12	51	12	-5	1	218	9	-2	8	0	28	-3*	3	115	5	23	0	210	8	4
H,K=	0,	4		2	177	7	5	9	66	9	-9	4	138	6	8	1	305	11	-28
1	645	23	64	3	100	6	-1	H,K=	0,	13		5	253	10	13	2	95	5	4
2	626	22	7	4	104	6	-3	1	84	7	10	6	85	5	9	3	347	13	-14
3	85	8	3	5	450	17	12	2	109	7	-4	7	283	11	-13	4	451	16	9
4	623	22	29	6	0	24	-14*	3	128	7	12	8	289	11	-48	5	351	13	-5
5	36	8	6	7	85	7	3	4	29	23	6	9	236	10	8	6	179	8	-4
6	15	21	-5*	8	261	11	-12	5	0	28	-27*	10	194	9	-2	7	50	8	-2
7	292	11	1	9	130	7	0	6	102	7	7	11	95	7	0	8	77	7	-1
8	131	7	-14	10	0	27	-5*	7	22	31	-1*	12	68	9	3	9	111	7	-2

OBSERVED STRUCTURES FACTORS (CONT) FOR
FE++(1,10-PHENANTHROLINE) BIS(SB TARTRATE) OCTAHYDRATE.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
10	76	7	6	1	89	6	-11	H,K=	1,	16		10	266	11	-13	H,K=	2,	8	
11	109	7	4	2	171	8	-9	0	32	19	-11	11	49	10	-1	0	169	7	-7
12	91	9	-8	3	209	9	-12	1	40	14	-2	12	65	9	9	1	421	15	-8
H,K=	1,	6		4	247	10	2	2	83	8	-8	H,K=	2,	4		2	154	7	-2
0	190	8	3	5	69	7	-9	3	97	8	4	0	278	10	-19	3	104	6	2
1	143	6	-2	6	82	7	-1	H,K=	2,	0		1	111	5	6	4	110	6	-1
2	125	6	1	7	117	7	-1	0	459	16	32	2	135	6	-1	5	154	7	-0
3	145	6	1	8	86	7	1	1	243	9	10	3	333	12	1	6	98	7	1
4	212	8	-7	9	119	8	8	2	686	25	22	4	527	19	-3	7	149	7	0
5	323	12	-6	10	107	8	4	3	27	8	-0	5	256	10	-2	8	88	7	5
6	73	6	1	H,K=	1,	11		4	61	5	-10	6	96	6	4	9	31	24	-11
7	154	7	-5	0	99	6	-0	5	462	17	-2	7	223	9	-2	10	60	9	4
8	197	8	-3	1	125	7	-10	6	43	9	-3	8	101	6	1	11	109	8	5
9	61	8	-3	2	107	6	-8	7	233	9	-7	9	114	7	-3	H,K=	2,	9	
10	83	7	4	3	105	7	-2	8	132	7	-2	10	47	10	2	0	36	11	3
11	50	11	10	4	127	7	-13	9	0	27	-5*	11	49	10	3	1	184	8	-10
12	82	8	-1	5	178	8	-5	10	53	9	-7	12	57	10	4	2	168	7	-1
H,K=	1,	7		6	124	7	5	11	255	11	-2	H,K=	2,	5		3	224	9	-2
0	436	16	5	7	77	8	-4	12	39	18	39	0	126	6	7	4	205	9	-5
1	291	11	-3	8	54	10	3	H,K=	2,	1		1	249	9	5	5	57	8	9
2	245	9	1	9	40	14	-4	1	263	10	27	2	525	19	-2	6	219	9	2
3	314	12	-8	H,K=	1,	12		2	308	11	-8	3	188	8	0	7	50	9	8
4	289	11	-11	0	143	7	-6	3	511	18	22	4	93	5	2	8	95	7	-7
5	254	10	-5	1	124	7	-2	4	211	8	9	5	82	6	-10	9	118	7	8
6	178	8	3	2	75	7	-0	5	363	13	3	6	107	6	-2	10	96	8	4
7	218	9	-4	3	71	7	-11	6	500	18	-7	7	18	24	-14*	H,K=	2,	10	
8	144	7	2	4	0	27	-8*	7	243	10	7	8	156	7	-4	0	148	7	-4
9	147	8	6	5	0	26	-6*	8	76	6	5	9	119	7	-6	1	105	6	-1
10	161	8	6	6	86	7	1	9	173	8	-12	10	120	7	-4	2	85	6	-12
11	40	14	8	7	121	7	10	10	50	10	10	11	78	8	-5	3	83	7	-4
H,K=	1,	8		8	32	19	3	11	121	7	5	12	62	10	-2	4	19	25	10*
0	247	10	-7	H,K=	1,	13		12	95	8	-8	H,K=	2,	6		5	277	11	-3
1	186	8	-12	0	78	7	-11	H,K=	2,	2		0	227	9	2	6	120	7	5
2	180	8	-6	1	61	8	2	0	594	21	2	1	160	7	-6	7	73	8	-6
3	349	13	-10	2	112	7	-4	1	209	8	20	2	511	19	-9	8	167	8	2
4	0	23	-24*	3	117	7	5	2	545	20	20	3	445	16	-0	9	76	8	5
5	242	10	1	4	63	8	-4	3	409	15	20	4	382	14	-5	H,K=	2,	11	
6	125	7	5	5	37	13	-10	4	105	5	-4	5	143	7	3	0	169	8	3
7	93	7	3	6	122	8	6	5	76	5	1	6	111	6	-1	1	112	7	-12
8	35	14	-9	7	79	8	6	6	183	8	5	7	213	9	-4	2	63	8	3
9	85	8	13	8	63	10	5	7	254	10	4	8	48	9	-5	3	58	8	-2
10	45	12	-6	H,K=	1,	14		8	215	9	-7	9	65	8	6	4	107	7	13
11	81	8	2	0	99	7	5	9	179	8	6	10	31	18	-5	5	77	7	-1
H,K=	1,	9		1	52	9	5	10	141	7	-0	11	119	8	4	6	79	7	2
0	110	6	-3	2	52	9	5	11	137	8	-4	H,K=	2,	7		7	82	8	-4
1	134	6	4	3	61	9	-2	12	51	11	12	0	126	6	-5	8	96	8	4
2	82	6	-6	4	82	8	-7	H,K=	2,	3		1	57	6	-7	9	47	12	-2
3	133	7	9	5	110	8	9	0	292	11	-4	2	198	8	-10	H,K=	2,	12	
4	191	8	-1	6	56	10	-1	1	467	17	-8	3	327	12	-1	0	54	8	4
5	32	13	-10	7	53	11	-3	2	444	15	4	4	23	18	-3	1	136	7	-6
6	19	26	-13*	H,K=	1,	15		3	142	6	2	5	65	6	-1	2	69	8	-3
7	184	8	-10	0	96	7	-0	4	254	10	14	6	351	13	-5	3	117	7	-2
8	86	7	10	1	22	26	-21*	5	229	9	2	7	38	11	-2	4	62	8	-4
9	65	8	-17	2	22	28	-5*	6	82	6	-1	8	0	27	-20*	5	131	7	1
10	86	8	12	3	50	11	-14	7	84	6	-1	9	79	7	-3	6	22	28	-2*
H,K=	1,	10		4	0	28	-2*	8	66	7	-3	10	104	7	-1	7	39	14	-10
0	183	8	-5	5	81	8	1	9	34	14	-3	11	23	30	-4*	8	107	8	2

OBSERVED STRUCTURES FACTORS (CONT) FOR
FE++(1,10-PHENANTHROLINE) BIS(SB TARTRATE) OCTAHYDRATE.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	2,	13		3	121	5	-2	5	97	5	-4	1	20	26	-10*	6	265	10	9
0	36	13	-3	4	172	7	6	6	120	7	-2	2	62	8	-6	7	198	8	4
1	36	13	0	5	381	14	-17	7	175	8	4	3	131	7	-1	8	240	10	13
2	115	7	0	6	88	6	-5	8	77	7	-2	4	82	7	4	9	208	9	-4
3	30	18	-5	7	97	6	-7	9	111	7	3	5	103	7	11	10	173	8	7
4	118	7	9	8	338	13	5	10	112	7	-2	6	53	9	4	11	58	9	-1
5	0	28	-27*	9	75	7	1	11	57	10	-17	7	80	8	0	12	95	7	1
6	32	19	13	10	97	7	5	H,K=	3,	7		8	57	10	-2	H,K=	4,	2	
7	117	8	0	11	53	10	2	0	242	9	-4	H,K=	3,	12		1	246	9	4
H,K=	2,	14		12	52	11	6	1	190	8	-3	0	50	9	-3	2	443	16	13
0	37	13	10	H,K=	3,	3		2	262	10	5	1	0	25	-19*	3	310	11	1
1	57	9	9	0	514	19	-12	3	137	6	2	2	157	8	-8	4	277	10	-1
2	31	19	-7	1	94	5	-1	4	156	7	3	3	107	7	-0	5	306	11	0
3	70	8	-15	2	290	11	18	5	95	6	-3	4	67	8	-3	6	221	9	5
4	32	19	-18	3	168	7	-10	6	104	7	-7	5	65	8	-7	7	165	7	2
5	95	8	-1	4	61	5	7	7	150	7	-6	6	105	8	1	8	32	13	-7
6	33	20	-2	5	297	11	-10	8	100	7	-4	7	86	8	5	9	71	7	-4
H,K=	2,	15		6	101	6	-1	9	101	7	6	H,K=	3,	13		10	115	7	-2
0	102	8	2	7	190	8	-14	10	71	8	-3	0	0	26	-26*	11	136	8	0
1	0	28	-24*	8	166	8	-4	11	187	9	-6	1	60	8	-15	12	47	12	3
2	0	28	-24*	9	210	9	-6	H,K=	3,	8		2	61	8	5	H,K=	4,	3	
3	51	11	-3	10	162	8	4	0	58	6	1	3	53	9	0	1	277	10	13
4	23	30	-18*	11	88	8	3	1	257	10	-10	4	109	7	-2	2	130	6	-2
H,K=	2,	16		12	52	11	3	2	34	10	0	5	82	8	-2	3	408	15	3
0	53	11	3	H,K=	3,	4		3	164	7	-4	6	40	14	-7	4	225	9	13
1	147	8	3	0	197	8	-1	4	197	8	1	H,K=	3,	14		5	53	6	5
2	24	30	-10*	1	365	13	21	5	87	7	-4	0	77	8	-6	6	414	15	2
H,K=	3,	0		2	258	10	3	6	210	9	-4	1	39	14	-5	7	88	6	-12
0	38	7	-35	3	389	14	1	7	97	7	-12	2	63	9	-0	8	0	25	-16*
1	462	17	31	4	169	7	18	8	116	7	7	3	64	9	0	9	144	7	-3
2	223	8	17	5	263	10	-4	9	0	27	-8*	4	0	29	-22*	10	100	7	7
3	98	6	12	6	63	6	-7	10	40	14	12	5	41	14	-6	11	50	11	-7
4	197	8	-3	7	101	6	-4	H,K=	3,	9		H,K=	3,	15		12	58	10	-1
5	57	5	12	8	141	7	-13	0	285	11	-13	0	40	14	5	H,K=	4,	4	
6	220	9	-6	9	67	8	-13	1	40	9	6	1	77	8	-2	0	216	9	-21
7	321	12	20	10	42	11	1	2	113	6	4	2	74	9	6	1	187	7	1
8	257	10	3	11	32	19	20	3	220	9	5	3	47	12	-5	2	385	14	5
9	108	7	-5	12	147	8	-4	4	167	8	-6	H,K=	4,	0		3	135	6	4
10	146	7	-12	H,K=	3,	5		5	166	8	-11	0	282	10	17	4	189	8	-3
11	37	15	27	0	55	6	-4	6	126	7	-1	1	30	9	-9	5	62	6	4
12	32	19	17	1	203	8	-3	7	81	7	8	2	197	8	-17	6	191	8	-14
H,K=	3,	1		2	285	11	-17	8	87	7	-0	3	177	7	-1	7	217	9	7
1	294	11	26	3	58	6	-1	9	72	8	-4	4	290	11	-2	8	152	7	6
2	578	21	20	4	473	17	8	10	47	12	0	5	248	9	-10	9	161	8	-2
3	380	14	17	5	164	7	3	H,K=	3,	10		6	47	7	11	10	92	7	-7
4	401	15	13	6	30	12	-2	0	194	8	-4	7	358	13	-5	11	128	8	-7
5	183	7	-5	7	313	12	-2	1	62	7	-1	8	51	9	2	H,K=	4,	5	
6	339	13	8	8	70	7	1	2	98	7	-10	9	70	7	14	0	25	12	-11
7	45	8	-9	9	46	10	-3	3	83	7	-9	10	77	8	-3	1	264	10	2
8	0	24	-25*	10	97	7	-14	4	71	7	-5	11	115	7	-5	2	349	13	-5
9	67	7	-1	11	39	14	-2	5	188	8	-11	12	46	14	13	3	271	10	1
10	152	8	1	H,K=	3,	6		6	59	8	-6	H,K=	4,	1		4	268	10	3
11	139	8	8	0	173	7	-19	7	53	9	4	1	128	5	6	5	87	6	4
12	82	8	-0	1	319	12	-21	8	45	12	-5	2	205	8	-5	6	119	6	-3
H,K=	3,	2		2	128	6	2	9	0	29	-23*	3	157	6	14	7	112	7	-6
1	222	8	5	3	132	6	1	H,K=	3,	11		4	57	5	-6	8	40	12	-4
2	104	5	-12	4	93	6	-0	0	216	9	-1	5	143	6	0	9	59	8	5

OBSERVED STRUCTURES FACTORS (CONT) FOR
FE++(1,10-PHENANTHROLINE) BIS(SB TARTRATE) OCTAHYDRATE.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
10	98	7	2	6	57	9	-4	4	459	17	24	10	90	8	18	8	0	29	-15*
11	46	12	-6	7	58	9	0	5	119	6	8	11	52	11	17	H,K=	5,	11	
H,K=	4,	6		8	107	8	1	6	194	8	9	H,K=	5,	6		0	104	7	9
0	289	11	-17	9	67	9	-2	7	285	11	8	0	126	6	-12	1	55	9	-8
1	74	5	-8	H,K=	4,	11		8	19	26	7*	1	251	10	13	2	63	8	-3
2	134	6	-8	0	72	8	-5	9	28	22	-43	2	152	7	-8	3	109	7	5
3	62	6	-10	1	145	7	1	10	36	13	8	3	248	10	1	4	43	11	2
4	116	6	2	2	122	7	-4	11	86	8	-16	4	191	8	4	5	38	14	8
5	292	11	-8	3	97	7	-6	12	91	8	7	5	233	9	-7	6	39	14	3
5	113	7	-5	4	103	7	7	H,K=	5,	2		6	131	7	-7	7	23	30	-19*
7	44	10	-2	5	53	9	-14	1	502	18	-4	7	0	27	-12*	H,K=	5,	12	
8	95	7	-12	6	137	8	-2	2	27	10	-11	8	125	7	2	0	41	12	-4
9	168	8	1	7	32	19	-17	3	228	9	3	9	85	8	1	1	78	8	1
10	45	12	-1	8	0	29	-47*	4	148	7	6	10	79	8	7	2	31	19	-2
11	66	9	-8	H,K=	4,	12		5	161	7	11	H,K=	5,	7		3	0	28	-13*
H,K=	4,	7		0	66	8	14	6	24	19	-7	0	302	11	-21	4	0	28	-19*
0	82	6	-2	1	56	9	2	7	130	7	5	1	110	6	-2	5	40	14	11
1	195	8	-9	2	21	27	13*	8	156	7	-13	2	134	7	-8	6	74	9	-8
2	206	8	-12	3	74	8	-5	9	121	7	-11	3	200	8	-8	H,K=	5,	13	
3	131	7	-7	4	49	10	10	10	133	7	8	4	292	11	3	0	141	8	-4
4	161	7	-7	5	63	9	3	11	0	28	-39*	5	47	9	-8	1	45	12	-8
5	127	7	-7	6	32	19	3	12	97	8	3	6	56	9	0	2	99	8	8
6	225	9	4	7	75	9	2	H,K=	5,	3		7	216	9	-1	3	100	8	6
7	72	8	6	H,K=	4,	13		1	229	9	8	8	96	7	4	4	0	29	-16*
8	183	8	4	0	108	7	-4	2	300	11	5	9	95	8	2	H,K=	5,	14	
9	88	8	-3	1	88	8	-6	3	275	10	1	10	40	14	-12	0	23	30	-4*
10	132	8	5	2	44	12	-5	4	216	9	-9	H,K=	5,	8		1	0	29	-21*
H,K=	4,	8		3	45	12	6	5	175	7	-1	0	51	8	-8	2	75	8	11
0	161	7	-7	4	82	8	-7	6	148	7	-7	1	112	6	-9	H,K=	6,	0	
1	173	8	-7	5	73	9	1	7	61	7	1	2	187	8	11	0	282	11	6
2	144	7	4	6	0	30	-24*	8	125	7	-0	3	82	7	-6	1	26	10	-6
3	201	8	-6	H,K=	4,	14		9	89	7	-2	4	61	8	-9	2	141	6	-2
4	163	8	8	0	55	10	1	10	65	8	4	5	20	27	-11*	3	210	8	7
5	88	7	-5	1	69	9	-1	11	183	9	-9	5	50	9	-4	4	161	7	-4
6	49	10	-9	2	73	9	7	H,K=	5,	4		7	95	7	-7	5	114	6	4
7	88	7	9	3	87	8	4	1	277	11	-10	8	22	28	-8*	6	310	12	-6
8	61	9	-4	4	33	20	3	2	174	7	-3	9	132	8	10	7	306	12	5
9	115	8	0	H,K=	4,	15		3	173	7	12	H,K=	5,	9		8	162	8	-8
10	47	12	3	0	47	12	5	4	16	22	-3*	0	95	7	-11	9	132	7	1
H,K=	4,	9		H,K=	5,	0		5	347	13	-2	1	128	7	-3	10	85	7	18
0	68	7	-3	0	527	19	5	6	80	6	-4	2	114	7	-2	11	0	28	-50*
1	86	6	-4	1	33	7	12	7	46	9	-8	3	62	8	-10	12	74	9	1
2	191	8	-2	2	115	5	-4	8	118	7	-2	4	131	7	8	H,K=	6,	1	
3	73	7	2	3	465	17	-11	9	21	27	-4*	5	133	7	-3	1	359	13	-20
4	124	7	-4	4	227	9	-13	10	38	13	6	6	79	7	1	2	307	11	-6
5	77	7	1	5	53	9	4	11	46	12	11	7	161	8	-3	3	175	7	4
5	124	7	3	6	69	6	15	H,K=	5,	5		8	45	12	7	4	523	19	-4
7	52	9	2	7	39	9	9	0	474	17	-29	9	33	20	2	5	132	6	3
8	54	10	5	8	105	6	-5	1	77	5	-5	H,K=	5,	10		6	194	8	-10
9	57	10	-2	9	338	13	3	2	23	18	3	0	42	10	4	7	185	8	-1
H,K=	4,	10		10	42	12	-2	3	265	10	-2	1	161	8	-8	8	33	14	4
0	19	26	-9*	11	22	28	8*	4	76	6	-4	2	144	7	-5	9	76	8	0
1	167	8	-22	12	226	10	-17	5	183	8	2	3	168	8	-2	10	152	8	8
2	128	7	-3	H,K=	5,	1		6	72	7	-4	4	78	7	-4	11	87	8	-3
3	91	7	2	1	158	6	1	7	93	7	-5	5	37	15	2	12	41	12	25
4	99	7	2	2	163	7	-18	8	108	7	-10	6	139	8	5	H,K=	6,	2	
5	110	7	7	3	141	6	-0	9	196	9	11	7	68	9	-7	1	225	9	9

OBSERVED STRUCTURES FACTORS (CONT) FOR
FE++(1,10-PHENANTHROLINE) BIS(SB TARTRATE) OCTAHYDRATE.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	154	7	9	H,K=	6,	7		0	82	8	3	4	40	9	-8	7	87	8	11
3	295	11	3	0	42	9	-2	1	57	10	2	5	120	7	3	H,K=		7,	10
4	153	7	5	1	209	9	-17	2	41	14	-8	6	72	7	-1	0	43	11	7
5	152	7	8	2	252	10	1	3	85	8	1	7	140	7	4	1	57	9	-4
6	353	13	1	3	117	7	-8	H,K=		7,	0	8	162	8	3	2	136	8	16
7	56	8	3	4	145	7	-2	0	48	6	5	9	98	7	0	3	138	8	14
8	104	7	-4	5	20	27	-14*	1	284	11	-5	10	72	9	7	4	54	10	3
9	156	8	-5	6	84	7	-3	2	57	5	-1	H,K=		7,	5	5	0	28	-37*
10	53	9	2	7	76	7	5	3	143	6	2	1	30	12	3	6	66	9	4
11	112	8	1	8	58	9	7	4	142	6	11	2	108	6	3	H,K=		7,	11
H,K=		6,	3	9	56	10	-10	5	509	19	3	3	178	8	1	0	61	9	-6
1	207	8	4	H,K=		6,	8	6	121	6	5	4	101	6	3	1	50	10	6
2	354	13	1	0	124	7	-3	7	37	18	-1	5	69	7	-12	2	100	8	-7
3	294	11	-7	1	73	7	-7	8	310	12	6	6	56	9	-2	3	60	9	8
4	164	7	-1	2	139	7	-15	9	105	7	12	7	105	7	6	4	124	8	6
5	0	23	-13*	3	65	9	-3	10	68	8	1	8	64	8	2	5	78	9	7
6	218	9	6	4	49	10	4	11	0	28	-12*	9	90	8	-14	H,K=		7,	12
7	115	7	-3	5	61	8	-4	H,K=		7,	1	10	52	11	4	0	23	29	-7*
8	197	9	8	6	99	7	-9	1	131	6	-3	H,K=		7,	6	1	77	8	-4
9	151	8	-3	7	98	7	4	2	222	9	-4	1	255	10	-10	2	101	8	4
10	54	10	2	8	85	8	-11	3	256	10	11	2	69	7	-8	3	74	9	7
11	69	9	-3	9	97	8	-2	4	160	7	12	3	176	8	-1	H,K=		8,	0
H,K=		6,	4	H,K=		6,	9	5	180	8	-5	4	69	7	-8	0	322	12	-14
1	109	6	2	0	99	7	6	6	138	7	4	5	120	7	6	1	176	7	2
2	257	10	-4	1	223	9	-7	7	146	7	-3	6	119	7	-4	2	142	6	-12
3	151	7	-2	2	92	7	2	8	157	8	-5	7	104	7	-8	3	183	8	-4
4	257	10	-0	3	84	7	-7	9	99	7	-6	8	22	28	16*	4	221	9	-7
5	237	9	1	4	78	7	-4	10	141	8	5	9	32	19	14	5	94	6	-8
6	113	7	-2	5	67	8	-0	11	108	8	-1	H,K=		7,	7	6	0	24	-35*
7	131	7	2	6	127	7	-5	H,K=		7,	2	0	241	10	-9	7	33	14	24
8	74	7	7	7	45	12	7	1	243	9	-13	1	127	7	-1	8	40	13	21
9	154	8	4	8	81	8	2	2	149	7	5	2	27	21	-0	9	51	10	10
10	78	8	-2	H,K=		6,	10	3	304	11	-5	3	67	7	-2	10	125	7	-5
11	23	30	-8*	0	46	10	5	4	120	6	1	4	114	7	2	11	61	10	3
H,K=		6,	5	1	131	7	3	5	201	8	-7	5	58	8	-1	H,K=		8,	1
1	62	6	2	2	51	9	-3	6	103	6	-2	6	79	7	2	1	97	5	-1
2	100	6	9	3	84	7	1	7	19	26	15*	7	111	8	-1	2	125	6	-1
3	81	6	-7	4	96	7	3	8	121	7	-1	8	32	19	-2	3	205	8	-15
4	125	6	-6	5	76	8	-2	9	192	9	9	9	66	9	5	4	181	8	-1
5	219	9	1	6	75	8	3	10	0	28	-16*	H,K=		7,	8	5	185	8	9
6	195	8	9	7	23	30	3*	11	52	11	10	0	116	7	2	6	186	8	8
7	0	27	-12*	H,K=		6,	11	H,K=		7,	3	1	120	7	-1	7	182	8	-0
8	198	9	-10	0	21	27	-3*	1	96	6	-7	2	87	7	-1	8	54	8	-5
9	31	19	2	1	140	8	1	2	180	8	-0	3	67	8	-2	9	21	27	17*
10	135	8	12	2	53	9	-3	3	169	7	-6	4	36	13	0	10	120	8	3
H,K=		6,	6	3	66	8	-6	4	244	10	8	5	115	7	2	11	23	30	-7*
0	88	11	-14	4	100	8	6	5	18	24	-4*	6	102	7	-7	H,K=		8,	2
1	134	7	-11	5	79	8	3	6	37	11	-5	7	39	14	-3	1	60	6	-7
2	225	9	7	6	40	14	6	7	283	11	-10	8	81	8	-12	2	356	13	-7
3	124	7	2	H,K=		6,	12	8	105	7	7	H,K=		7,	9	3	0	23	-18*
4	103	6	-2	0	89	8	1	9	57	9	6	0	224	9	-3	4	202	8	5
5	144	7	6	1	74	8	-6	10	71	8	2	1	82	7	5	5	120	7	-4
6	48	11	-10	2	86	8	-6	11	47	12	0	2	78	7	2	6	42	10	2
7	118	7	5	3	99	8	-1	H,K=		7,	4	3	56	9	-9	7	259	10	4
8	91	7	7	4	91	10	2	1	189	8	-3	4	101	7	7	8	140	7	2
9	89	8	-0	5	113	8	3	2	154	7	-1	5	85	8	-4	9	92	7	1
10	90	8	1	H,K=		6,	13	3	81	6	-6	6	32	19	-6	10	68	9	4

OBSERVED STRUCTURES FACTORS (CONT) FOR
FE++(1,10-PHENANTHROLINE) BIS(SB TARTRATE) OCTAHYDRATE.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
11	82	8	-6	4	148	8	2	9	77	8	8	H,K=	9,	9		9	40	14	8
H,K=	8,	3		5	112	7	1	10	70	9	7	0	77	10	-5	H,K=	10,	4	
1	256	10	-5	6	22	29	-4*	H,K=	9,	3		1	38	14	14	1	58	8	-1
2	282	11	-4	7	65	9	5	1	152	7	-5	2	50	10	14	2	159	8	-7
3	174	8	-5	H,K=	8,	9		2	62	7	-2	3	50	11	1	3	59	8	-4
4	185	8	8	0	69	8	10	3	156	7	-12	4	110	8	1	4	64	8	-1
5	79	7	2	1	77	8	6	4	168	8	13	5	47	12	-2	5	62	8	6
5	110	7	-8	2	96	7	7	5	144	7	-10	H,K=	9,	10		6	80	7	-7
7	103	7	-3	3	138	8	6	6	0	27	-10*	0	23	29	-9*	7	73	8	14
8	135	7	4	4	54	10	1	7	142	7	-9	1	51	11	-1	8	69	9	-11
9	82	8	7	5	39	14	-3	8	49	10	12	2	83	8	-9	9	24	30	-5*
10	23	29	-6*	6	0	29	-26*	9	106	8	1	3	23	30	-6*	H,K=	10,	5	
H,K=	8,	4		H,K=	8,	10		10	111	8	8	4	24	27	8*	1	0	27	-32*
1	89	6	-4	0	59	9	3	H,K=	9,	4		H,K=	9,	11		2	132	7	-9
2	212	9	-7	1	44	12	3	1	204	9	-2	0	86	8	15	3	108	7	6
3	102	6	-1	2	71	8	2	2	133	7	-4	H,K=	10,	0		4	42	11	-3
4	104	6	-1	3	23	29	14*	3	159	7	-2	0	155	7	9	5	21	27	-18*
5	96	7	-6	4	100	8	11	4	141	7	5	1	107	6	18	6	22	28	-16*
6	188	8	9	5	23	30	-12*	5	205	9	3	2	321	12	-13	7	51	11	-5
7	46	10	-6	H,K=	8,	11		6	92	7	-1	3	165	7	-3	8	78	9	-7
8	68	8	-3	0	76	8	11	7	77	8	4	4	72	7	2	H,K=	10,	6	
9	123	8	-0	1	95	8	7	8	99	7	2	5	59	8	2	1	55	9	-2
10	41	14	-5	2	57	10	3	9	98	8	17	6	356	13	-2	2	167	8	4
H,K=	8,	5		3	0	29	-10*	H,K=	9,	5		7	70	8	10	3	70	8	-4
1	282	11	-3	H,K=	9,	0		1	71	7	2	8	95	7	7	4	30	18	-7
2	150	7	-6	0	45	12	15	2	33	14	-15	9	125	8	-3	5	0	27	-20*
3	142	7	-10	1	283	11	-11	3	140	7	-4	10	0	29	-14*	6	78	8	5
4	123	7	-4	2	56	6	11	4	143	7	2	H,K=	10,	1		7	66	9	9
5	44	10	-7	3	310	12	5	5	50	9	6	1	170	7	-1	H,K=	10,	7	
6	167	8	7	4	77	6	0	6	85	7	-6	2	92	6	-3	1	142	8	5
7	82	7	16	5	332	13	3	7	128	7	-0	3	188	8	7	2	31	18	-1
8	49	10	3	6	59	8	8	8	127	8	19	4	118	7	-3	3	82	8	2
9	124	8	-1	7	165	8	4	9	82	8	7	5	83	7	7	4	38	14	5
H,K=	8,	6		8	109	7	6	H,K=	9,	6		6	193	8	9	5	56	10	3
1	217	9	2	9	43	13	-1	1	77	7	-6	7	103	7	-4	6	66	9	2
2	57	8	-1	10	128	8	9	2	96	7	0	8	82	7	2	H,K=	10,	8	
3	211	9	1	11	41	14	2	3	142	7	-0	9	125	8	-4	1	77	8	5
4	72	8	-7	H,K=	9,	1		4	55	9	-4	10	78	9	4	2	45	12	2
5	79	7	-2	1	132	6	1	5	56	9	3	H,K=	10,	2		3	0	28	-34*
6	164	8	3	2	291	11	-1	6	87	7	9	1	132	7	6	4	40	14	-7
7	69	8	6	3	199	8	-2	7	90	8	-12	2	32	13	12	5	23	30	-8*
8	51	11	6	4	229	9	-6	8	74	9	-2	3	91	6	2	H,K=	10,	9	
9	108	8	-7	5	153	7	2	H,K=	9,	7		4	121	7	4	1	115	8	-10
H,K=	8,	7		6	145	7	3	1	36	13	10	5	20	27	-16*	2	46	12	4
1	106	7	-8	7	179	8	10	2	117	7	12	6	124	7	12	3	84	8	5
2	139	7	-8	8	172	8	8	3	21	27	-11*	7	42	11	-5	4	92	8	3
3	50	10	0	9	31	19	-2	4	64	8	-1	8	54	10	18	H,K=	10,	10	
4	117	7	-1	10	86	8	14	5	82	8	8	9	129	8	12	0	134	8	-1
5	99	7	-4	H,K=	9,	2		6	32	19	5	H,K=	10,	3		H,K=	11,	0	
6	0	27	-33*	1	257	10	-11	7	101	8	-6	1	105	6	-2	0	118	7	-6
7	0	28	-15*	2	115	6	-11	H,K=	9,	8		2	100	7	4	1	311	12	-6
8	125	8	4	3	132	7	2	1	148	8	-1	3	112	7	-3	2	105	6	8
H,K=	8,	8		4	87	6	-2	2	43	11	-4	4	171	8	15	3	169	8	-1
0	116	8	-1	5	171	8	6	3	97	7	-4	5	211	9	2	4	105	7	4
1	109	7	6	6	39	12	-5	4	31	19	-3	6	29	18	-5	5	194	8	-1
2	93	7	-3	7	117	7	0	5	55	10	3	7	43	11	6	6	64	8	33
3	47	10	-8	8	119	7	2	6	90	8	2	8	125	8	-9	7	21	29	12*

OBSERVED STRUCTURES FACTORS (CONT) FOR
FE++(1,10-PHENANTHROLINE) BIS(SB TARTRATE) OCTAHYDRATE.

L	FOB	SG	DEL
8	72	9	11
9	64	9	12
10	98	8	12
H,K=	11,		1
1	139	7	4
2	121	7	0
3	171	8	0
4	146	7	6
5	138	7	-0
6	65	8	-2
7	74	8	-2
8	54	10	-4
9	57	10	3
H,K=	11,		2
1	104	7	3
2	81	7	4
3	205	9	1
4	93	7	2
5	272	11	17
6	37	13	12
7	72	8	-2
8	115	8	-2
9	41	14	-10
H,K=	11,		3
1	39	12	-2
2	145	7	2
3	169	8	4
4	123	7	1
5	157	8	12
6	61	9	0
7	107	7	11
8	61	10	-5
H,K=	11,		4
1	132	7	1
2	61	8	-5
3	157	8	5
4	125	7	9
5	37	13	-11
6	73	8	4
7	121	8	0
8	33	20	-4
H,K=	11,		5
1	55	9	7
2	94	7	0
3	43	11	1
4	97	7	0
5	66	8	16
6	56	10	4
7	153	8	-4
H,K=	11,		6
1	155	8	7
2	69	8	3
3	44	11	3
4	59	9	1
5	88	8	7
6	52	11	4
H,K=	11,		7

L	FOB	SG	DEL
1	22	28	-5*
2	84	8	-7
3	0	28	-12*
4	0	29	-24*
5	23	30	-21*
H,K=	11,		8
1	33	20	-17
2	33	20	-7
3	84	19	10
H,K=	12,		0
0	53	9	3
1	38	11	-13
2	171	8	3
3	114	12	6
4	136	7	5
5	0	27	-33*
6	66	8	-5
7	58	9	38
8	50	11	-0
9	70	9	3
H,K=	12,		1
1	43	10	-2
2	134	7	-10
3	103	7	0
4	175	8	-7
5	144	7	-9
6	37	13	15
7	59	9	-10
8	94	8	9
H,K=	12,		2
1	56	9	4
2	181	8	13
3	124	7	9
4	36	13	10
5	105	7	2
6	154	8	11
7	32	19	13
8	57	9	5
H,K=	12,		3
1	233	10	10
2	29	17	11
3	135	7	3
4	102	7	5
5	62	9	14
6	129	8	14
7	96	10	-3
H,K=	12,		4
1	105	7	-0
2	144	8	7
3	91	7	1
4	58	9	4
5	22	28	-9*
6	154	8	10
7	58	9	8
H,K=	12,		5
1	136	8	6
2	82	8	3

L	FOB	SG	DEL
3	70	8	-1
4	23	29	-17*
5	145	8	6
6	33	20	-2
H,K=	12,		6
1	39	14	-1
2	0	28	-17*
3	46	12	-20
4	90	8	7
5	75	8	9
H,K=	12,		7
1	77	8	2
2	40	14	-5
3	58	10	-12
H,K=	13,		0
0	83	7	7
1	52	9	25
2	45	11	16
3	139	7	4
4	155	8	8
5	76	7	2
6	44	11	37
7	146	8	7
8	57	10	22
H,K=	13,		1
1	78	8	-5
2	82	7	-9
3	21	26	-3*
4	161	8	-0
5	92	7	11
6	104	7	-1
7	123	8	0
8	24	30	-1*
H,K=	13,		2
1	179	8	0
2	55	9	3
3	37	13	9
4	31	18	18
5	66	8	4
6	75	8	3
7	132	8	20
H,K=	13,		3
1	77	8	9
2	83	7	-5
3	49	10	-2
4	89	8	-2
5	32	19	6
6	80	8	9
H,K=	13,		4
1	31	19	-3
2	44	12	-2
3	95	8	6
4	0	28	-16*
5	127	8	20
6	63	9	9
H,K=	13,		5
1	0	29	-13*

L	FOB	SG	DEL
2	32	19	-5
3	86	8	4
4	57	10	-4
H,K=	13,		6
1	47	12	-2
2	0	29	-22*
3	95	8	11
H,K=	14,		0
0	105	7	-4
1	41	11	23
2	132	7	2
3	47	10	29
4	81	8	5
5	88	8	-11
6	143	8	12
7	23	30	4*
H,K=	14,		1
1	150	8	-5
2	104	7	5
3	65	8	4
4	120	7	5
5	119	8	2
6	40	14	-12
7	24	30	-2*
H,K=	14,		2
1	61	9	4
2	93	10	5
3	80	8	12
4	75	8	1
5	0	29	-18*
6	107	8	10
H,K=	14,		3
1	107	7	8
2	0	28	-22*
3	79	8	-4
4	56	10	0
5	53	11	2
H,K=	14,		4
1	23	29	3*
2	83	8	13
3	96	8	7
4	118	8	15
H,K=	14,		5
1	53	11	-3
2	53	11	3
H,K=	15,		0
0	126	8	5
1	101	7	-8
2	102	7	9
3	117	7	-4
4	0	28	-24*
5	135	8	8
6	0	29	-2*
H,K=	15,		1
1	0	27	-18*
2	94	8	3
3	95	8	-4

L	FOB	SG	DEL
4	69	9	5
5	66	9	10
H,K=	15,		2
1	51	11	-2
2	60	9	8
3	150	8	23
4	91	8	0
H,K=	15,		3
1	23	29	10*
2	109	8	-2
3	33	15	20
H,K=	16,		0
0	0	30	-14*
1	23	29	11*
2	0	28	-24*
3	65	9	2
4	74	9	12
5	24	30	21*
H,K=	16,		1
1	61	9	2
2	46	12	-1
3	70	9	7
H,K=	15,		2
1	58	10	2
2	128	8	1
H,K=	17,		0
0	23	32	-14*
1	33	20	3
2	24	30	-4*

TECHNICAL INFORMATION DIVISION
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UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720