between the $Mo_2(SO_4)_4{}^{4-}$ ion and glycine in 2 *M* H_2SO_4. This result suggests that the driving force for reaction 1 is not due solely to the chelating nature of the carboxyl group but that electronic factors may also be involved.

The substance first precipitated from the solutions of glycine and $Mo_2Cl_8{}^{4-}$ in hydrochloric acid has a composition approximating to $Mo_2(O_2CCH_2NH_3)_4Cl_4\cdot xH_2O$ where x is approximately 2. However, the analyses, for several different preparations, never agreed precisely with any such formula and, in addition, the tetrachloride could never be obtained in crystalline (i.e., macrocrystalline as opposed to powder) form. It was for these reasons the conversion of the chloride to the sulfate was undertaken.

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Registry No. $Mo_2(gly)_4(SO_4)_2\cdot 4H_2O$, 57214-97-8; $Mo_2(gly)_4Cl_4$, 57214-98-9; $Mo_2(O_2CH)_4$, 51329-49-8; $K_4Mo_2Cl_8$, 25448-39-9; glycylglycine, 556-50-3; Mo, 7439-98-7.

Supplementary Material Available: A listing of structure factor amplitudes (Table II), thermal parameters (Table IV), and root-mean-square amplitudes of vibration (Table V) (8 pages). Ordering information is given on any current masthead page.

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Preparation, Properties, and Crystal and Molecular Structure of Diaquosulfato(*N*,*N*,*N*',*N*'-tetramethylethylenediamine)copper(II) Hydrate

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The compound diaquosulfato(*N*,*N*,*N*',*N*'-tetramethylethylenediamine)copper(II) hydrate, $[Cu(tmen)SO_4(OH_2)_2]\cdot H_2O$, has been prepared and its structure determined crystallographically. This substance crystallizes in space group *Pbca* with eight molecules per unit cell of dimensions $a = 12.543$ (1), $b = 15.782$ (1), and $c = 13.862$ (1) Å. The observed and calculated densities are 1.59 (2) and 1.597 g/cm³, respectively. From a total of 2189 independent reflections measured with Ni-filtered copper x radiation, 1869 statistically significant reflections ($|F_o| > 3\sigma(F_o)$) were used to determine the structure and resulted in final values of $R = 0.067$ and $R_w = 0.061$ (154 parameters were least-squares refined). Hydrogen atoms were located but not refined. The molecular structure consists of monomeric $[Cu(tmen)SO_4(OH_2)_2]$ units in which the coordination polyhedron about copper is a tetragonal pyramid. The Cu–OH_2 apical bond length of 2.205 (5) Å is 10% longer than the four remaining bonds to water, 1.974 (5) Å, monodentate sulfate oxygen, 1.986 (5) Å, and chelated diamine nitrogens, 2.024 (5) and 2.025 (5) Å. Copper is situated 0.25 Å above the basal plane, and chelate ring conformation is gauche. All water molecules participate in an extensive hydrogen-bonding network to noncoordinated sulfate oxygens with an average O–O separation of 2.68 Å. The room-temperature magnetic moment is 1.87 BM.

Introduction

Reported complexes of copper(II) and the highly substituted ligand *N*,*N*,*N*',*N*'-tetramethylethylenediamine (tmen) may be grouped in two classes depending on formula type: (A) $Cu(tmen)X_2$, $X^- = Cl^-$,[2] Br^-,[3] SCN^-, picrate;[4] (B) $Cu(tmen)(OH)X$, $X^- = ClO_4{}^-$,[3] $NO_3{}^-$,[4] Cl^-,[5] Br^-.[6] Many of these are known or assumed to be dimeric-bridged structures with room-temperature magnetic moments less than that expected for the spin-only case. For example, $[Cu(tmen)OH]_2(ClO_4)_2$ has a four-coordinate hydroxy-bridged structure with noncoordinated perchlorate anions ($\mu_{eff} = 1.20$ BM),[7] and $[Cu(tmen)Cl_2]_2$ has a five-coordinate chloride-bridged structure.[2] The fact that only monovalent anions are present in the above complexes prompted us to attempt preparations incorporating divalent sulfate anion. We were particularly interested in comparing the sulfate and perchlorate copper(II) complexes of tmen because both anions are of similar size, geometry, and coordinating ability. The preparation and isolation of the reaction product between copper sulfate and tmen and its molecular structure and properties are reported here.

Experimental Section

Preparation of Complex. A 5.8-ml (0.04-mol) amount of ligand in 20 ml of methanol was mixed with 20 ml of an aqueous solution containing 4.98 g (0.02 mol) of copper sulfate. Repeated partial evaporation at the boiling temperature and subsequent addition of methanol to maintain volume decreased the aqueous content of the reaction mixture. Further slow evaporation at room temperature afforded a light blue powder which contained many larger hard and irregularly shaped crystal fragments. The solid was separated by filtration, washed with ether, and air-dried (yield 5.8 g, 88% based on copper). Elemental analyses, ir and electronic spectra, and room-temperature magnetic susceptibility measurements were made on finely ground samples of the isolated bulk solid using methods previously described.[8] The spectral and magnetic information is included in the Discussion. Anal. Calcd for $CuC_6H_{22}N_2O_7S$: Cu, 19.26; C, 21.85; H, 6.72. Found: Cu, 19.3; C, 21.6; H, 6.65.

Unit Cell and Space Group. A crystal fragment, trimmed to an effective size of 0.3 × 0.2 × 0.2 mm, was temporarily mounted on a glass fiber with a thin film of grease and orientated by precession techniques. After location of a reciprocal lattice plane with twofold symmetry, the crystal was remounted with epoxy glue along one of the major reciprocal axes. Further precession (complete set of zero and first levels) and Weissenberg photos (levels 0–7) indicated the

Table I. Final Heavy-Atom Parameters[a]

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu	0.0260 (1)	0.2242 (1)	0.1057 (1)	41 (1)	28 (0)	27 (0)	−2 (1)	3 (1)	0 (1)
S	−0.1345 (1)	0.1005 (1)	0.2076 (1)	26 (1)	19 (1)	32 (1)	−1 (1)	10 (2)	2 (1)
O1	−0.0786 (4)	0.1305 (3)	0.1184 (3)	41 (3)	28 (2)	26 (3)	−7 (5)	7 (5)	−4 (4)
O2	−0.1891 (4)	0.1748 (3)	0.2502 (4)	47 (4)	29 (2)	54 (3)	3 (5)	31 (6)	−2 (5)
O3	−0.0552 (4)	0.0688 (4)	0.2770 (4)	51 (4)	45 (3)	51 (4)	0 (5)	−1 (6)	21 (6)
O4	−0.2112 (4)	0.0363 (3)	0.1798 (4)	50 (4)	38 (3)	65 (4)	−24 (5)	20 (7)	−7 (5)
O5	−0.0828 (4)	0.2989 (3)	0.1637 (4)	57 (4)	16 (2)	62 (4)	2 (5)	22 (7)	−1 (5)
O6	0.0986 (4)	0.1914 (3)	0.2456 (4)	41 (3)	36 (2)	26 (2)	−4 (5)	−15 (5)	8 (5)
O7	0.1048 (5)	−0.0477 (3)	0.2723 (6)	57 (4)	23 (2)	153 (7)	−5 (5)	−7 (10)	20 (7)
N1	0.1065 (5)	0.1538 (4)	0.0079 (4)	56 (5)	27 (3)	27 (3)	0 (6)	20 (7)	−2 (5)
N2	0.1234 (5)	0.3213 (4)	0.0689 (4)	52 (5)	27 (3)	37 (4)	−12 (6)	7 (7)	3 (5)
C1	0.0313 (9)	0.1260 (6)	−0.0711 (6)	121 (10)	60 (5)	28 (5)	18 (13)	3 (12)	−14 (8)
C2	0.1518 (7)	0.0772 (5)	0.0524 (6)	74 (7)	32 (4)	42 (5)	20 (9)	0 (10)	−8 (7)
C3	0.1895 (8)	0.2080 (6)	−0.0360 (8)	91 (8)	48 (5)	84 (8)	−1 (11)	51 (14)	6 (10)
C4	0.2137 (8)	0.2793 (6)	0.0160 (9)	87 (9)	64 (6)	114 (10)	−39 (12)	63 (16)	−35 (13)
C5	0.1669 (7)	0.3658 (5)	0.1547 (7)	70 (7)	33 (4)	59 (6)	−21 (9)	0 (11)	−3 (8)
C6	0.0706 (9)	0.3819 (7)	0.0079 (7)	133 (11)	53 (5)	57 (7)	−27 (13)	−7 (15)	27 (10)

[a] Estimated standard deviations are enclosed in parentheses. Anisotropic thermal parameters are $\times 10^4$ and are of the form $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + \beta_{23}kl)]$.

crystal belonged to the orthorhombic system, with systematic absences noted for $0kl$ (k odd), $h0l$ (l odd), and $hk0$ (h odd) reflections, uniquely characterizing the space group as *Pbca* (D_{2h}^{15}; No. 61). The crystal was then transferred to a Picker four-circle automated diffractometer (a^* axis coincident with the φ axis) and lattice constants were determined by a least-squares fit of carefully measured $\pm 2\theta$ values of the copper $K\alpha_1$–$K\alpha_2$ doublet (λ(Cu $K\alpha_1$) 1.54050 Å, λ(Cu $K\alpha_2$) 1.54434 Å) for 12 strong reflections having $2\theta > 65°$. The resultant unit cell dimensions were $a = 12.543$ (1), $b = 15.782$ (1), $c = 13.862$ (1) Å. The density calculated with $Z = 8$ is 1.597 g/cm^3; the observed density is 1.59 (2) g/cm^3, determined by flotation in a mixture of organic liquids.

Collection and Reduction of X-Ray Diffraction Data. Intensity data were collected on a Picker FACS-I fully automated diffractometer using Ni-filtered copper $K\alpha$ radiation and nickel-foil attenuators. A θ–2θ scan rate of 2°/min with a variable-scan width (2.3° + 0.4° tan θ) and 10-sec background measurements at both extremities of the scan was used to measure 2189 unique reflections to a 2θ maximum of 125° ($d = 0.87$ Å). The intensities of three standard reflections, measured after every block of 50 intensity determinations, remained essentially constant throughout 5 days of data collection, indicating crystal and electronic stability. Structure amplitudes and their estimated errors were calculated from the expressions $|F_o| = (QI_n)^{1/2}$ and $\sigma^2(F_o) = (Q/4I_n)[I_s + (t_s/t_b)^2 I_b + (0.02I_n)^2]$, where Q contains corrections for Lorentz–polarization, absorption, and attenuation, I_s and I_b are the scan and background intensities, t_s and t_b are the scan and background times, and I_n is the net integrated intensity. Absorption was corrected for as a function of φ, with a transmission factor of 1.32:1.00 (linear $\mu = 39.0$ cm^{-1} for copper $K\alpha$ radiation). A total of 1869 reflections had $|F_o| > 3\sigma(F_o)$ and were used in the structure determination.

Structure Determination and Refinement. The asymmetric unit consists of 17 nonhydrogen and 22 hydrogen atoms. An initial position for the copper atom was obtained from a three-dimensional Patterson map. A structure factor calculation[9] in which copper coordinates, isotropic temperature factor, and overall scale were varied in three cycles of least-squares treatment with unit weights, resulted in a conventional $R = 0.51$. Block-diagonal least-squares calculations were employed throughout, and the function minimized was $\sum w(|F_o| - |F_c|)^2$; one overall scale factor was always varied. A subsequent Fourier synthesis afforded the positions of all sulfate group atoms plus three other atoms bonded to copper and assigned as nitrogen at this stage. Five cycles of least-squares adjustment of these nine atoms reduced R to 0.27. The next Fourier synthesis clearly revealed all 17 nonhydrogen atoms and permitted unambiguous atom identification. Five cycles of least-squares adjustment on these positions with isotropic temperature factors and individually weighted reflections gave an R of 0.135 and $R_w = 0.132$. The residuals cited are $R = \sum(||F_o| - |F_c||)/\sum|F_o|$ and $R_w = \sum w(||F_o| - |F_c||)/\sum w|F_o|$ where $w = 1/\sigma^2$. Five additional cycles with anisotropic temperature factors resulted in $R = 0.091$ and $R_w = 0.090$. Several sequential difference Fourier maps led to positions of all hydrogens bonded to water oxygen atoms but revealed only one hydrogen on each methyl group. All missing hydrogen positions were calculated assuming sp^3 hybridization and a C–H bond of 1.0 Å. Hydrogen atoms were assigned isotropic temperature factors of $B = 4.0$ Å^2 and included in subsequent calculations but not varied. Least-squares refinement of 154 parameters was continued until the maximum shift in a parameter was one-tenth of its estimated error. Final values of the residuals were $R = 0.067$ and $R_w = 0.061$, and the "goodness of fit" was 2.28. There was no indication that extinction corrections were necessary. A final difference Fourier map contained a maximum peak of 0.5 e/Å^3. Final atomic positional coordinates and anisotropic temperature factors for nonhydrogen atoms are listed in Table I. Table II contains hydrogen atom coordinates and labels of carbon and oxygen atoms to which they are bonded. A listing of observed and calculated structure factors (×10) is available as supplementary material.

Table II. Hydrogen Coordinates and Origin-Atom Labels

Atom	x	y	z	Origin
H1	0.0031	0.1829	−0.0980	C1
H2	−0.0340	0.0984	−0.0452	C1
H3	0.0657	0.0897	−0.1203	C1
H4	0.0914	0.0478	0.0862	C2
H5	0.2027	0.0926	0.1069	C2
H6	0.1930	0.0418	0.0046	C2
H7	0.1594	0.2280	−0.1022	C3
H8	0.2529	0.1721	−0.0504	C3
H9	0.2523	0.3216	−0.0236	C4
H10	0.2677	0.2597	0.0697	C4
H11	0.1903	0.3202	0.2028	C5
H12	0.1086	0.3964	0.1889	C5
H13	0.2231	0.4071	0.1342	C5
H14	0.0413	0.4261	0.0495	C6
H15	0.0045	0.3538	−0.0232	C6
H16	0.1182	0.3994	−0.0474	C6
H17	−0.1260	0.2670	0.1960	O5
H18	−0.0857	0.3493	0.1808	O5
H19	0.0641	0.1430	0.2600	O6
H20	0.1553	0.1827	0.2739	O6
H21	0.0603	0.0	0.2781	O7
H22	0.1739	−0.0122	0.2879	O7

Description and Discussion of the Structure

The crystal structure of $[Cu(tmen)SO_4(OH_2)_2]\cdot H_2O$ is composed of discrete monomeric molecules. The tetragonal-pyramidal coordination polyhedron [4 + 1] about copper consists of a water molecule at the apex and four base sites occupied by two nitrogens from the chelated diamine and an oxygen atom each from monodentate sulfate and a second water molecule. A third water is not coordinated but plays an important role in intermolecular hydrogen bonding. The bulk of the sulfate anion is above the base of the coordination pyramid, and chelate ring conformation is gauche with a torsional angle of −35.1°. The molecular structure is illustrated

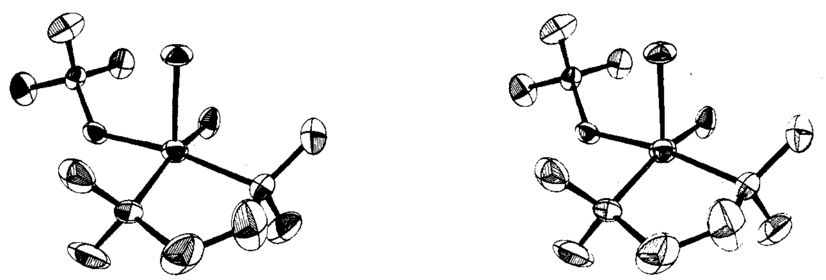

Figure 1. ORTEP stereodrawing of $[Cu(tmen)SO_4(OH_2)_2]$.

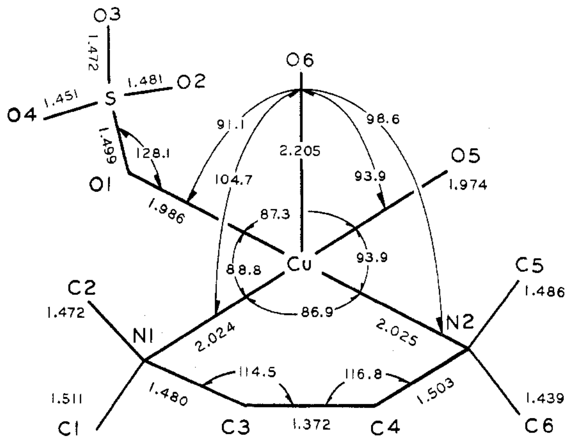

Figure 2. Coordination about the copper ion; distances and angles are indicated.

Table III. Remaining Interatomic Angles (deg)

Atoms	Angle	Atoms	Angle	Atoms	Angle
O1-S-O2	107.2 (3)	Cu-N1-C1	109.5 (5)	C4-N2-C5	108.8 (6)
O1-S-O3	109.3 (3)	Cu-N1-C2	111.3 (5)	C4-N2-C6	110.7 (7)
O1-S-O4	108.1 (3)	Cu-N1-C3	108.0 (5)	C4-N2-Cu	104.2 (5)
O2-S-O3	108.7 (3)	C1-N1-C2	107.9 (6)	Cu-N2-C5	112.2 (5)
O2-S-O4	110.7 (3)	C1-N1-C3	108.0 (7)	Cu-N2-C6	111.9 (6)
O3-S-O4	112.7 (3)	C2-N1-C3	112.1 (6)	C5-N2-C6	109.0 (7)

as an ORTEP[10] stereodrawing in Figure 1, and intramolecular bond lengths and angles are shown in Figure 2. Remaining angles are listed in Table III.

The apical Cu–O6 bond at 2.205 (5) Å is only 10% longer than basal Cu–O bonds as is also the case for copper complexes of hippurate anion,[11] phenoxyacetate,[12] and $[Cu_2(bpy)_2(OH)_2SO_4(OH_2)]\cdot 4H_2O$ with a sulfate oxygen coordinated at the apex.[13] The two $Cu-O_{base}$ bonds are remarkably similar considering that one is to a sulfate oxygen (1.986 Å) and the other to a water molecule (1.974 Å). The four basal donor atoms (O1, O5, N1, N2) lie within one standard deviation (±0.08 Å) of the least-squares plane they generate, the plane being defined by the equation $0.040x - 0.0155y + 0.0594z = 0.259$. Copper is situated 0.25 Å above this plane, which is a larger than usual displacement but is also found in copper complexes of dimethylamine (0.23 Å)[14] and trien (0.37 Å).[15] The two Cu–N bonds are identical at 2.025 Å and with the 86.9° angle between them, their environment duplicates the comparable bonds and angles found in the square-planar complex $[Cu(tmen)OH]_2Br_2$.[6] The nearest Cu–Cu approach is 6.97 Å, the closest potential Cu–O interaction outside the primary coordination sphere is to a sulfate oxygen at 4.17 Å, and the noncoordinated water molecule is 4.30 Å away. Access to the sixth coordination position seems guarded by methyl groups C1 and C6, both of which are below the basal plane and 2.89 Å from copper. In particular, both contain hydrogens (H1 and H15) which span and block this site in a symmetrical manner as described by Hoskins and Whillans.[16] In this regard it is noted that thermal parameters for C1 and C6 are the largest of the thermal parameters for all carbon atoms in the structure.

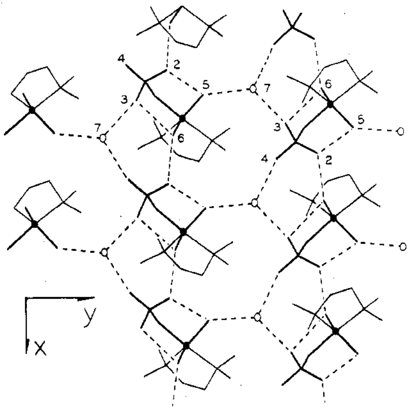

Figure 3. Projection of $[Cu(tmen)SO_4(OH_2)_2]\cdot H_2O$ along z showing hydrogen bonding. Closed circles are copper, open circles are O7, and remaining hydrogen-bonded oxygens are numbered.

Spatial relationships about the chelated diamine are quite different from that found in two related complexes, $[Cu(tmen)OH]_2Br_2$[6] and $[Cu(teen)OH]_2(ClO_4)_2$.[17] In these square-planar dimeric complexes, the angles about the N–C–C–N ligand backbone are within ±1° of 109° and the C–C distances are 1.433 and 1.514 Å, respectively. In contrast here, the backbone angles are larger at 114.5 and 116.8°, and the C–C separation at 1.372 (14) Å is shorter. Furthermore, the four $N-C_{methyl}$ bonds are less equivalent, ranging from 1.439 (12) to 1.511 (11) Å. It seems likely that these distortions are due to steric interactions present in this five-coordinate example which are either absent or reduced in the two companion four-coordinate square-planar complexes.

The internal geometry of the sulfate anion is quite regular in spite of its coordination. As expected, the oxygen joined to copper has the longest S–O bond of 1.499 (6) Å, but the shortest S–O bond of 1.456 (6) Å is not too different and both are within the range for ionic sulfate.[14] The six O–S–O angles (Table III) vary from 107.2 to 112.6° and have an average value of 109.4°. The plane defined by atoms S–O1–Cu makes an angle of 38° with that of atoms $O1-Cu-O6_{apex}$, so that the sulfate group is twisted away from methyl carbon C2. The S–O1–Cu angle of 128.1 (2)° clearly reduces local anion symmetry below C_{3v}.

The individual molecules are joined together by a hydrogen-bonding network involving all water molecules and noncoordinated sulfate oxygen atoms. Thus sulfate O2 is hydrogen bonded to waters O5 and O6, sulfate O3 to waters O6 and O7, and sulfate O4 to water O7. Distances between these oxygens average 2.68 Å with a maximum value of 2.77 Å separating O6 and O3. Noncoordinated water O7 is a crucial center in the hydrogen-bonding scheme, for it joins together three different independent complex molecules through atoms O3, O4, and O5. The network operates in the xy plane and results in stacked layers of joined molecules normal to z. Note that the z component of the thermal parameter for O7 has the largest value of any refined atom and that there are no hydrogen-bonding contacts to O7 in this direction which would constrain its motion along *z*. The hydrogen-bonding network is illustrated in Figure 3.

Physical Properties of the Complex

The blue complex exhibits one broad d–d absorption at 14800 cm^{-1} either as a mulled solid or in nitromethane solution (ϵ 100). Its nitromethane solution is nonconducting and upon evaporation yields crystals with the same ir spectrum as the original solute. After heating of the compound at 150° for 5 hr, it suffered no mass loss or ir spectral changes. The ir spectrum shows broad O–H absorptions with maxima at 3400 and 1650 cm^{-1} and three bands at 1170, 1095, and 1030 cm^{-1} attributed to the coordinated sulfate group. At room temperature the magnetic moment is 1.87 BM.

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Registry No. $[Cu(tmen)SO_4(OH_2)_2]\cdot H_2O$, 57196-94-8.

Supplementary Material Available: Listing of structure factor amplitudes (9 pages). Ordering information is given on any current masthead page.

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Crystal and Molecular Structure by Neutron Diffraction of Potassium Tetracyanoplatinate(II) Trihydrate, the Starting Product for Partially Oxidized Conducting Cyanoplatinate Salts[1a]

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Potassium tetracyanoplatinate(II) trihydrate, $K_2Pt(CN)_4\cdot 3H_2O$, crystallizes in the orthorhombic space group *Pbcn*, with $a = 13.426$ (5), $b = 11.848$ (4), and $c = 6.956$ (2) Å with $Z = 4$. The strongly efflorescent crystals grown from aqueous solution were sealed in capillaries for three-dimensional neutron data collection. The structure was deduced from the neutron Patterson map and was refined by Fourier and full-matrix least-squares techniques to $R_{F^2} = 0.061$ ($R_F = 0.056$) for 587 reflections with $F^2 > \sigma(F^2)$. The structure consists of planar $Pt(CN)_4^{2-}$ groups stacked parallel to *c* forming linear Pt chains with a Pt–Pt separation of 3.478 (1) Å. Alternate $Pt(CN)_4^{2-}$ groups are rotated giving an eclipsed configuration with C–Pt–Pt–C torsion angles of 15.7 (1) and 16.7 (1)°. The $Pt(CN)_4^{2-}$ plane is also tilted with respect to *c* by ~3°. The two types of water molecules serve to link CN^- groups within a $Pt(CN)_4^{2-}$ stack and to cross-link adjacent $Pt(CN)_4^{2-}$ stacks. Comparisons are made with the structure of the mixed-valence compound $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$, KCP(Br).

Introduction

Square-planar platinum complexes with electron-rich ligands are the basic starting materials for the preparation of the novel mixed-valence, highly conducting, one-dimensional metallic salts such as $K_2Pt(CN)_4X_{0.3}\cdot 3H_2O$, KCP(X) where X^- is Br^- or Cl^-. The preparation involves partial oxidation of a Pt^{II} compound such as $K_2Pt(CN)_4\cdot 3H_2O$, KTCP hereafter, with a strong oxidizing agent such as Cl_2, Br_2, or H_2O_2. Although the highly conducting compounds have been the subject of much experimental and theoretical investigation,[2,3] there are few reliable physical and structural data available for the starting material, KTCP, and related complexes.[4] The cyanoplatinate family displays many interesting chemical, optical, and spectroscopic properties.[5] Insofar as electrical conductivity is concerned KTCP is an insulator; its conductivity is $\sim 10^{-9}$ that of KCP(Br). We have chosen to investigate the structure of KTCP by neutron diffraction in order to have accurate data for structural comparisons between the precursor, KTCP, and the partially oxidized products.

Experimental Section

Crystal Preparation. Single crystals of KTCP were prepared by evaporation from an aqueous solution of a sample purchased from K & K Laboratories. Single crystals of a size suitable for neutron diffraction grew within a few hours. The crystals are transparent, have a yellow-green tint when viewed perpendicular to *c*, give intense blue fluorescence when viewed down the *c* axis, and lose water very quickly when exposed to air. The crystal density was not measured because of the rapidity of water loss. The x-ray density is 2.589 g/cm^3.

Space Group. Preliminary x-ray precession and Weissenberg photographs gave the conditions for diffraction as $hk0$ ($h + k = 2n$, $h0l$ ($h + l = 2n$), and $0kl$ ($k + l = 2n$) which would indicate space group P_{nnn}. However, neutron observations gave the corrected conditions as $hk0$ ($h + k = 2n$), $h0l$ ($l = 2n$), and $0kl$, ($k = 2n$) leading to the unique space group P_{bcn}. The apparent discrepancy is due to the dominance of Pt scattering in the x-ray case and the locations of Pt atoms $c/2$ apart in the cell.

Neutron Data. The crystal selected for data collection was a rectangular parallelepiped 1.0 × 1.7 × 6.8 mm. It was quickly sealed in a lead glass capillary and mounted for data collection on the Chemistry Division four-circle neutron diffractometer at the CP-5