those found in high- and low-spin nickel(II) complexes with four planar nitrogen donors.[16] This effect may be explained by the absence of electrons in the d orbitals which are antibonding with respect to the Ni–N interaction in the case of the diamagnetic nickel(II) complex as compared to their presence in the antibonding orbitals in the paramagnetic complexes. These antibonding electrons produce the lengthening of the Ni–N bond in the tetragonal (and octahedral) complexes which are paramagnetic as proposed by Cotton and Wise.[17]

All intermolecular contacts in the structure of Ni(TAAB)$I_2 \cdot H_2O$ appear to be quite normal with the closest carbon–carbon approaches of 3.4 Å. However, in the Ni(TAAB)$(BF_4)_2$ structure there is one contact which deserves special mention. This is the Ni–F(1) distance of 2.70 Å which seems to be rather short, although not so short as to be bonding. The next shortest nickel–fluorine distance is Ni–F(7) at 4.0 Å on the other side of the ligand plane. The fluorine ligand contacts are greater than 3.1 Å and seem to be normal, with the exception of DC(26)–F(5) at 2.9 Å which is probably due to the badly positioned atom DC(26).[18] The carbon–carbon contacts in Ni(TAAB)$(BF_4)_2$ are all greater than 3.4 Å. The BF_4^- anions are normal within the errors of the determination of Ni(TAAB)$(BF_4)_2$. The average B–F distance is 1.33 ± 0.04 Å and the average F–B–F angle is 109 ± 4°, where the errors are the rms deviations from the mean. The B–F distance seems short as compared to reported values of 1.40 and 1.43 Å,[19] but some of this discrepancy may be due to the large thermal motion of the BF_4^- anions; the data do not permit the analysis required for this correction.

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The Crystal and Molecular Structures of Zinc and Cadmium O,O-Diisopropylphosphorodithioates

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The crystal and molecular structures of zinc O,O-diisopropylphosphorodithioate and isomorphous cadmium O,O-diisopropylphosphorodithioate have been solved by single-crystal X-ray diffraction techniques. Three-dimensional scintillation counter data were used to refine the structures by full-matrix least-squares procedures to final conventional R factors of 0.088 and 0.083, respectively (based on F). The crystals are monoclinic, space group C2/c (no. 15), with $a = 10.934 \pm 0.008$ Å, $b = 17.098 \pm 0.006$ Å, $c = 25.587 \pm 0.012$ Å, $\beta = 99.23 \pm 0.04°$, $d_{obsd} = 1.37 \pm 0.02$ g/cm^3, and $d_{calcd} = 1.384 \pm 0.002$ g/cm^3 for the zinc complex and $a = 10.964 \pm 0.006$ Å, $b = 16.906 \pm 0.008$ Å, $c = 26.490 \pm 0.008$ Å, $\beta = 99.91 \pm 0.02°$, $d_{obsd} = 1.46 \pm 0.02$ g/cm^3, and $d_{calcd} = 1.480 \pm 0.002$ g/cm^3 for the cadmium complex. Both complexes are binuclear. These dimers, four per unit cell of formula $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$, where M = Zn or Cd, lie on the twofold axes of the unit cell. Each metal atom is coordinated with four sulfur atoms in a distorted tetrahedral environment. The metal–sulfur bonds range in length from 2.302 (6) to 2.409 (5) Å in the zinc complex and from 2.486 (7) to 2.590 (8) Å in the cadmium complex. The metal···metal approach within each dimer is 4.108 (5) and 4.059 (4) Å, respectively. Associated with each metal atom are two $(i\text{-}C_3H_7O)_2PS_2$ groups, one which functions as an *intrachelating* group bound wholly to one metal atom and the other which functions as a bridging, or *interchelating*, group linking two monomeric molecules together to form the dimer; the result is a molecule consisting of two four-membered rings joined to a central eight-membered ring through the metal atoms. The inter- and intrachelating groups deviate only slightly from planarity with the metal atoms and the central eight-membered ring possesses the "cradle" configuration. The phosphorus–sulfur bonds average 1.970 (11) and 1.965 (8) Å in length in the zinc and cadmium structures, respectively; the phosphorus–oxygen bonds average 1.58 (2) Å in length. The molecules pack in the crystals to form layers or sheets and, like the molecules within these sheets, are held together by van der Waals forces.

Introduction

Metal derivatives of O,O-dialkylphosphorodithioic acid[1] are important lubricating oil additives and, depending upon the metal atom and alkyl group, have good antioxidant and antiwear properties. One of these, the zinc derivative, is widely used as a lubricant additive to reduce wear under boundary or thin-film lubrication conditions; it is also known to be an oxidation and corrosion inhibitor.

Our present understanding of the metal O,O-dialkylphosphorodithioates has been advanced through a number of investigations, such as association studies, thermal decomposition studies, and infrared analyses.

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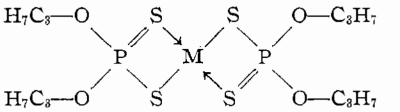
(1) The following names have been used interchangeably in the literature for the $-(RO)_2PS_2$ group: O,O-dialkylphosphorodithioate, O,O-dialkyldithiophosphato, and dialkyldithiophosphate.

Association studies[2] have shown, for example, that in benzene molecules of the zinc, mercury, and lead diisopropyl derivatives are monomers in equilibrium with dimers whereas the cadmium diisopropyl derivative is strictly dimeric in concentrations above 0.005 g/ml. Details regarding bonding and bond orders within these molecules have been obtained from their infrared spectra,[3] and, in accordance with stretching frequencies reported in the literature, these spectra have indicated the presence of both single and double phosphorus–sulfur bonds. Studies of thermal stability[4] have recently been reported to show a dependence of thermal decomposition on both the structure of the alkyl groups and the size of the metal cation. Results of these and related studies[5] have in turn been used to correlate the relation of antiwear activity, *viz.*, in the protection of rubbing metal surfaces, to thermal stability and structure.

Unfortunately, the actual molecular structures of these metal derivatives have not been known and interpretations of some of the results of these and other investigations have been based only on postulated models. A single-crystal X-ray structure determination of the zinc and cadmium chelates of O,O-diisopropylphosphorodithioic acid, having the empirical formula



where M = Zn or Cd, was therefore carried out. Results of these two determinations are reported here.

Experimental Section

Preparation.—Zinc O,O-diisopropylphosphorodithioate, $Zn_2(dtp)_4$, and cadmium O,O-diisopropylphosphorodithioate, $Cd_2(dtp)_4$, where dtp = $(i\text{-}C_3H_7O)_2PS_2$, were each prepared[4] and generously supplied by J. J. Dickert. Soft, colorless, tabular crystals for use in the X-ray investigation were obtained by recrystallization of the compounds from warm absolute ethanol.

Crystal Data.—Zinc O,O-diisopropylphosphorodithioate: $Zn[(i\text{-}C_3H_7O)_2PS_2]_2$; formula weight 491.93; monoclinic, space group C2/c (C_{2h}^6); lattice parameters at 24°, $a = 10.934 \pm 0.008$ Å, $b = 17.098 \pm 0.006$ Å, $c = 25.587 \pm 0.012$ Å, $\beta = 99.23 \pm 0.04°$, $V = 4721 \pm 8$ Å^3; $d_{\text{obsd}} = 1.37 \pm 0.02$ g/cm^3 (by flotation), $d_{\text{calcd}} = 1.384 \pm 0.002$ g/cm^3 using $Z = 8$ monomeric molecules/unit cell; crystal habit, thick tabular (001); linear absorption coefficient for Mo Kα radiation, 15.8 cm^{-1}. Cadmium O,O-diisopropylphosphorodithioate: $Cd[(i\text{-}C_3H_7O)_2PS_2]_2$; formula weight 538.96; monoclinic, space group C2/c (C_{2h}^6); lattice parameters at 24°, $a = 10.964 \pm 0.006$ Å, $b = 16.906 \pm 0.008$ Å; $c = 26.490 \pm 0.008$ Å, $\beta = 99.91 \pm 0.02°$, $V = 4837 \pm 6$ Å^3; $d_{\text{obsd}} = 1.46 \pm 0.02$ g/cm^3 (by flotation), $d_{\text{calcd}} = 1.480 \pm 0.002$ g/cm^3 using $Z = 8$ monomeric molecules/unit cell; crystal habit, tabular (001); linear absorption coefficient for Mo Kα radiation = 17.2 cm^{-1}.

The crystal symmetry was determined from Weissenberg photographs which yielded systematic extinctions (hkl with $h + k = 2n + 1$ and $h0l$ with $l = 2n + 1$) consistent with the space groups Cc and C2/c. The centrosymmetric choice, C2/c, was initially indicated on the basis of intensity statistics[6] and subsequently confirmed for both complexes by the successful refinement of the derived structures. The centrosymmetric space group was also later indicated on the basis of an optical analysis involving second harmonic generation.[7,8] The lattice parameters were determined by a least-squares fit[9] of 150 independent high-angle Kα reflections measured from zero-level Weissenberg zones taken with Cu Kα radiation (λ 1.5418 Å) using crystals mounted in three different orientations; each film was calibrated with superimposed aluminum powder lines ($a_0 = 4.03296$ Å at 24°). The Nelson–Riley extrapolation function was employed in the refinement. The indicated errors in the cell parameters are 2σ. The observed lattice parameters were checked with the computer program TRACER[10] to verify that no symmetry higher than C-centered monoclinic was present.

Collection and Treatment of X-Ray Intensity Data.—Complete three-dimensional X-ray diffraction intensity data were taken at room temperature with zirconium-filtered molybdenum radiation from a crystal of dimensions $0.20 \times 0.20 \times 0.27$ mm for $Zn_2(dtp)_4$ and $0.20 \times 0.20 \times 0.12$ mm for $Cd_2(dtp)_4$; the plate thickness in each case is the third dimension indicated. Each crystal was mounted in a 0.3-mm Lindemann glass capillary with c^* (the normal to the plate face) coincident with the ϕ axis of the diffractometer. A General Electric quarter-circle Eulerian cradle mounted on a Siemens diffractometer equipped with a Siemens air-cooled scintillation counter and a Siemens counter-scaler assembly was used with the moving-crystal, moving-counter measurement technique (θ-2θ coupling) and a 3.0° takeoff angle [3.5° for $Zn_2(dtp)_4$]. The distance from the focal spot of the X-ray tube to the crystal center was 17 cm and from the crystal center to the center of the sodium iodide crystal was 18.5 cm. The receiving aperture size selected to minimize extraneous background was 4.2 mm wide by 2.5 mm high. The counter angle, 2θ, was scanned over 2° at a speed of 1°/min for $Zn_2(dtp)_4$ and 2°/min for $Cd_2(dtp)_4$. Background counts of 24 sec for $Zn_2(dtp)_4$ and 12 sec for $Cd_2(dtp)_4$ were taken at each end of the 2θ scan. All scans were recorded on a chart recorder to provide visual evidence for the existence of observed reflections, proper peak shape, reflection centering in 2θ, and nonoverlap of adjacent reflections. Owing to the rather large thermal motion of the molecules, reflections having 2θ greater than 45° were virtually unobservable and so collection of the data was restricted to the region $2\theta \leq 45°$. Equivalent reflections were not measured. A total of 3083 independent reflections was measured for $Zn_2(dtp)_4$ and 3161 were measured for $Cd_2(dtp)_4$. Typical background counts at 10, 20, 30, and 40° 2θ were 79.3, 30.9, 16.8, and 10.8 counts/sec, respectively, for the zinc crystal and 81.5, 32.5, 18.1, and 12.3 counts/sec, respectively, for the cadmium crystal. Three standard reflections were measured periodically as a check on crystal decomposition. In the case of $Cd_2(dtp)_4$ no apparent decomposition was observed but in the case of $Zn_2(dtp)_4$, whose total irradiation period was twice that

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[10] S. L. Lawton, "TRACER II, a Fortran Lattice Transformation-Cell Reduction Program," Research Department, Paulsboro Laboratory, Mobil Research and Development Corp., Paulsboro, N. J., 1968. This program is an updated and expanded version of TRACER I originally published by S. L. Lawton and R. A. Jacobson in "The Reduced Cell and Its Crystallographic Applications," Report IS-1141, Ames Laboratory, Iowa State University, Ames, Iowa, 1965.

for $Cd_2(dtp)_4$, a 7% decrease in intensities was observed. The alignment of both crystals was checked on a daily basis for ϕ independence at $\chi = 90°$ and adjusted when necessary.

The mosaicity of each crystal was examined by means of a narrow-source (takeoff angle 0.5°) 2θ-scan technique at $2\theta \leq 13°$. In this region the 2θ-scan and ω-scan techniques yield comparable results.[11] The width at half-maximum for three typical strong noncoplanar reflections was found to range from 0.10 to 0.21° θ for $Zn_2(dtp)_4$ and from 0.05 to 0.07° θ for $Cd_2(dtp)_4$. Those for $Cd_2(dtp)_4$ are acceptably low; those for $Zn_2(dtp)_4$ are slightly higher than desired indicating the presence of unusually high thermal motion of the atoms or perhaps some disorder. The largest observed mosaicities for the zinc crystal occurred for the $0k0$ reflections and were about twice as large as for the $h00$ and $00l$ reflections.

The raw intensity of each reflection was corrected for background, crystal decomposition [for $Zn_2(dtp)_4$], Lorentz, and polarization effects. Absorption was not a major problem in either crystal, by virtue of the small linear absorption coefficients and the nearly spherical crystal morphology; therefore no absorption corrections were made. Effects of secondary extinction also proved not to be a major problem and so no such corrections were applied.

The estimated error in each intensity measurement was calculated by the expression[12] $\sigma(I) = [C_T + 0.25(t_c/t_b)^2(B_1 + B_2) + (pI)^2]^{1/2}$, where C_T is the total integrated peak count obtained in a scan time t_c, B_1 and B_2 are the background counts each obtained in time t_b, and $I = C_T - 0.5(t_c/t_b)(B_1 + B_2)$. The value of p was selected as 0.05. Each $\sigma(I)$ was then corrected for crystal decomposition and Lorentz and polarization effects. The estimated standard deviation in each F_o was calculated by the expression $\sigma(F_o) = [(I + \sigma(I)]^{1/2} - |F_o|$, a function based on the finite-difference method. These standard deviations were used during the least-squares refinements to weight the observed structure factors where w, the individual weighting factor, was defined as $1/\sigma^2(F_o)$. For the zinc crystal a total of 1749 reflections were observed above the background level of which 1428 had $F_o > 3\sigma(F_o)$; for the cadmium crystal a total of 1787 reflections were observed above background level of which 1098 had $F_o > 3\sigma(F_o)$. Those with $F_o \leq 3\sigma(F_o)$ were considered as unobserved and thus omitted from the refinements.

Structure Determination of $Cd_2(dtp)_4$.—The unit cell crystal data derived from the X-ray photographs of $Zn_2(dtp)_4$ and $Cd_2(dtp)_4$ indicated that the two complexes were isomorphous in the crystalline state. The structure of $Cd_2(dtp)_4$ was solved first to make use of cadmium as a heavy atom for interpreting the Patterson function. Using all observed reflections an unsharpened three-dimensional Patterson function was calculated from which the cadmium and sulfur atoms were readily located. A series of three-dimensional electron density functions (F_o and $F_o - F_c$) and isotropic least-squares refinements in the space group C2/c led to the location of all remaining nonhydrogen atoms in the structure.

The best fully weighted isotropic refinement of all 23 atoms plus the scale factor resulted in $R = \Sigma||F_o| - |F_c||/\Sigma|F_o| = 0.124$ and $wR = [\Sigma w||F_o| - |F_c||^2/\Sigma w|F_o|^2]^{1/2} = 0.114$ for the reflections above $3\sigma(F_o)$. Further refinement, with ellipsoidal thermal factors introduced for the seven heavy atoms, reduced R and wR to 0.086 and 0.078, respectively.

These refinements produced rather large thermal parameters for the atoms. The average isotropic B values, defined by $-B_i(\sin^2\theta)/\lambda^2$, ranged from 7.4 Å² for cadmium to an average 23.2 Å² for the terminal carbon atoms, the values generally increasing as the distance from cadmium along the bonded directions increased. A three-dimensional difference map at this stage showed evidence for anisotropic motion of the carbon atoms with no evidence for static disorder resulting from possible alternate orientations of the isopropyl groups. Extending anisotropic refinement to the oxygen and carbon atoms, however, resulted in convergence difficulties with thermal quadratic forms of several carbon atoms becoming nonpositive definite. Moreover, the O–C and C–C bond lengths assumed less meaningful values. Since attempts to refine the structure further with anisotropic thermal parameters for the light atoms did not result in an appreciably better description of those parts of the molecule of chemical interest, namely, the inner parts (Cd, S, and P shifts were less than 0.5σ), this phase of the refinement was discontinued.

At this stage of the refinement the existence of the molecule as a dimer with C_2 symmetry (imposed from space group considerations) appeared well established. However, owing to the large thermal parameters, there existed the possibility that the correct space group was Cc, rather than C2/c, in which the dimer would not be restricted to C_2 symmetry. Several iterations of least-squares refinement in the space group Cc were carried out, but no improvement in the parameters or R factors was observed. From this lack of improvement, together with the negative results obtained from the highly sensitive optical analysis utilizing second harmonic generation performed on the zinc analog,[8] the space group was subsequently assumed to be C2/c.

Examination of the reflections $F_o \leq 3\sigma(F_o)$ within the limit of $I_o > \sigma(I_o)$ revealed 35 reflections which satisfied the condition $F_c > 3\sigma(F_o)$. Additional cycles with these included resulted in minor changes in both the positional parameters and the R factors. The reasonableness of the weighting function was also examined. For a proper function the mean value of $[\Delta F/\sigma(F_o)]^2$ for the refined structure should be independent of both $|F_o|$ and $(\sin\theta)/\lambda$.[13] Examination of a smoothed plot of the average values of $[\Delta F/\sigma(F_o)]^2$ for various ranges of $|F_o|$ and of $(\sin\theta)/\lambda$ showed that the condition $[\Delta F/\sigma(F_o)]^2$ equal to a constant was essentially fulfilled. Therefore no modification was made.

Convergence was reached with $R = 0.083$ and $wR = 0.073$ for the 1133 observed reflections. The corresponding values for all 1787 reflections were $R = 0.141$ and $wR = 0.090$. The final standard deviation for an observation of unit weight (*i.e.*, the "error of fit" was 1.28, where the "error of fit" is defined by $[\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - m)]^{1/2}$ with n being the number of observations (1133) and m the number of variables (128). On the final cycle the shift in each positional parameter averaged 0.03 times its own σ. A final difference map calculated on an absolute scale showed no peaks greater than 0.2 e⁻/Å³ in the vicinity of the Cd, S, and P atoms, consistent with good refinement; peaks in the regions of oxygen and carbon ranged from −0.4 to +0.4 e⁻/Å³, or at most 11% of an oxygen atom, 24% of a center carbon atom, and 38% of a terminal carbon atom, and are presumably due to the anisotropy of thermal motion of the isopropyl groups.

Structure Determination of $Zn_2(dtp)_4$.—The final positional parameters determined for $Cd_2(dtp)_4$ were used to initiate the least-squares refinement of $Zn_2(dtp)_4$. The refinement was pursued in the same manner as described for the cadmium complex. No change in the orientations of the four isopropyl groups was detected from difference-Fourier syntheses. The best fully weighted isotropic refinement of all 23 atoms plus the scale factor resulted in $R = 0.129$ and $wR = 0.134$ for the reflections above $3\sigma(F_o)$. Further refinement, with ellipsoidal thermal factors introduced for Zn, S, and P reduced R and wR to 0.091 and 0.097, respectively.

As with $Cd_2(dtp)_4$ rather large thermal parameters for the atoms were observed. A three-dimensional difference map showed anisotropic vibrational patterns for three of the four isopropyl groups which seemed physically reasonable, except those involving C(21) through C(23); no static disorder was found for these three groups. For the isopropyl group consisting of atoms C(21) through C(23) the peaks were indicative of a cer-

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TABLE I

FINAL POSITIONAL AND ISOTROPIC THERMAL PARAMETERS FOR $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$[a]

Zinc O,O-diisopropylphosphorodithioate, $Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$					Cadmium O,O-diisopropylphosphorodithioate, $Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$				
Atom	*x*	*y*	*z*	*B*, Å^2 [b]	Atom	*x*	*y*	*z*	*B*, Å^2 [b]
Zn(1)	0.53294 (18)	0.63383 (11)	0.17319 (8)	...	Cd(1)	0.52606 (19)	0.62578 (12)	0.17599 (8)	...
S(2)	0.4366 (5)	0.7445 (3)	0.1302 (2)	...	S(2)	0.4361 (8)	0.7461 (5)	0.1244 (3)	...
S(3)	0.6353 (5)	0.6218 (3)	0.0969 (2)	...	S(3)	0.6386 (8)	0.6171 (6)	0.0978 (3)	...
S(4)	0.4052 (5)	0.5266 (3)	0.1737 (2)	...	S(4)	0.3867 (8)	0.5091 (4)	0.1718 (3)	...
S(5)	0.3252 (4)	0.6667 (3)	0.2536 (2)	...	S(5)	0.3198 (7)	0.6565 (4)	0.2454 (3)	...
P(6)	0.5231 (5)	0.7088 (3)	0.0720 (2)	...	P(6)	0.5276 (8)	0.7053 (5)	0.0719 (3)	...
P(7)	0.2860 (4)	0.5664 (3)	0.2166 (2)	...	P(7)	0.2781 (7)	0.5509 (4)	0.2168 (3)	...
O(8)	0.4333 (12)	0.6873 (8)	0.0202 (5)	10.5 (3)	O(8)	0.4342 (21)	0.6826 (15)	0.0212 (9)	13.4 (7)
O(9)	0.5884 (12)	0.7769 (8)	0.0462 (5)	11.0 (4)	O(9)	0.5975 (21)	0.7709 (15)	0.0459 (9)	13.3 (7)
O(10)	0.2644 (12)	0.5055 (9)	0.2616 (5)	11.2 (4)	O(10)	0.2715 (16)	0.4934 (11)	0.2639 (7)	9.3 (5)
O(11)	0.1545 (15)	0.5748 (10)	0.1810 (7)	14.5 (5)	O(11)	0.1394 (22)	0.5500 (13)	0.1915 (9)	13.6 (7)
C(12)	0.370 (3)	0.613 (2)	0.012 (1)	15.2 (8)	C(12)	0.386 (5)	0.605 (3)	0.008 (2)	19.0 (15)
C(13)	0.242 (3)	0.628 (2)	0.013 (1)	19.6 (11)	C(13)	0.256 (4)	0.622 (3)	0.013 (2)	20.2 (15)
C(14)	0.385 (4)	0.590 (3)	−0.038 (2)	27.9 (18)	C(14)	0.377 (5)	0.626 (4)	−0.049 (2)	28.9 (24)
C(15)	0.659 (2)	0.831 (1)	0.077 (1)	11.6 (6)	C(15)	0.649 (4)	0.832 (3)	0.074 (2)	16.4 (14)
C(16)	0.795 (3)	0.819 (2)	0.076 (1)	18.9 (10)	C(16)	0.783 (4)	0.820 (2)	0.075 (2)	17.9 (14)
C(17)	0.632 (3)	0.905 (2)	0.044 (2)	24.7 (15)	C(17)	0.665 (4)	0.892 (3)	0.035 (2)	21.6 (17)
C(18)	0.295 (3)	0.411 (2)	0.256 (1)	18.8 (11)	C(18)	0.301 (4)	0.400 (2)	0.260 (2)	16.6 (13)
C(19)	0.182 (5)	0.397 (3)	0.238 (2)	26.7 (17)	C(19)	0.172 (5)	0.390 (3)	0.249 (2)	24.3 (20)
C(20)	0.284 (4)	0.403 (2)	0.315 (2)	25.6 (12)	C(20)	0.306 (4)	0.388 (3)	0.317 (2)	18.4 (9)
C(21)	0.076 (7)	0.639 (4)	0.140 (3)	36.9 (9)	C(21)	0.097 (5)	0.589 (3)	0.142 (2)	22.4 (8)
C(22)	−0.035 (4)	0.543 (3)	0.143 (2)	27.3 (12)	C(22)	−0.021 (6)	0.529 (4)	0.135 (2)	28.3 (7)
C(23)	0.035 (4)	0.672 (3)	0.169 (2)	24.4 (12)	C(23)	0.023 (5)	0.636 (3)	0.166 (2)	23.5 (8)

[a] All atoms are in the general symmetry position (8f). Numbers in parentheses in all tables and in the text are estimated standard deviations occurring in the last digit of the parameter. [b] The final anisotropic thermal parameters for Zn, Cd, S, and P are given in Table II.

tain amount of free rotation of the isopropyl group about the carbon–oxygen bond and to a lesser extent about the phosphorus–oxygen bond. Ellipsoids on the Fourier map were therefore not considered to represent in this case vibrational patterns of individual atoms but rather an extensive librational motion of the isopropyl group with the refined positional parameters representing only the "average" atomic positions in the structure. Static disorder resulting from possible alternate orientations of the group may also explain the peaks if these orientations occur close enough together such that the edges of the thermal ellipsoids overlap to give only the three observed broad peaks. No "ghost" peaks indicative of widely differing orientations of this group were found. It is noteworthy that this particular isopropyl group is directly associated with packing of the molecules along the *b* direction in the unit cell, the direction in which the largest mosaic spreads were observed (*viz.*, the 0*k*0 reflections). Anisotropic refinement was extended to these light atoms and resulted in convergence difficulties in the same manner as occurred for the cadmium complex with only minor effects on the Zn, S, and P positional parameters. The fully anisotropic refinement was therefore discontinued.

Examination of the reflections $F_o \leq 3\sigma(F_o)$ within the limit $I_o > \sigma(I_o)$ revealed 28 reflections which satisfied the condition $F_c > 3\sigma(F_o)$. Additional cycles with these included resulted in small changes in the positional parameters and the *R* factors. The weighting scheme was also examined as functions of $|F_o|$ and of $(\sin \theta)/\lambda$ and found to be reasonably constant; no modification was made.

Convergence was reached with $R = 0.088$ and $wR = 0.084$ for the 1448 observed reflections. The corresponding values for all 1749 reflections were 0.105 and 0.087, respectively. The final "error of fit" was 1.73. On the final cycle the shift in each positional parameter averaged 0.06 times its own σ. A final difference map calculated on an absolute scale showed no peaks greater than 0.2 $e^-/Å^3$ in the vicinity of the Zn, S, and P atoms, consistent with good refinement. Peaks in the regions of the oxygen and carbon atoms [excluding O(11) and C(21) through C(23)] ranged from −0.2 to +0.3 $e^-/Å^3$, or at most 7% of an oxygen atom, 13% of a center carbon atom, and 22% of a terminal carbon atom; peaks in the region of O(11), C(21), C(22), and C(23) ranged from −0.2 to +0.6 $e^-/Å^3$. The maximum residuals may reflect the inadequacy of describing the thermal motion of the isopropyl groups by an isotropic model.

Computations.—Computations were performed on IBM 7040 and CDC 1604 computers. The least-squares refinement was carried out with a locally modified version of ORFLS.[14] Refinement was based on $|F_o|$. The atomic scattering factors for neutral atoms were those tabulated by Hanson, *et al.*[15] Effects of anomalous scattering were included in the structure factor calculations;[16] the values of $\Delta f'$ and $\Delta f''$ for Zn, Cd, S, and P were those given in ref 17. All electron density summations were performed by the Fortran program FOUR.[18]

Final Results.—The final positional and thermal parameters derived from the last cycle of least-squares refinement are presented in Tables I and II, along with the associated standard deviations in these parameters as estimated from the inverse matrix. The root-mean-square amplitudes of vibration of the atoms in the inner coordination sphere are given in Table III. Table IV lists the observed and calculated structure factors, excluding contributions due to hydrogen. The 002 reflection, occurring at 3.22° in 2θ for $Zn_2(dtp)_4$ and 3.12° for $Cd_2(dtp)_4$, was too close to the direct beam to be measured and so only its calculated structure factor is indicated.

Description of the Structure

Molecules of zinc and cadmium diisopropylphosphorodithioates in the crystalline state exist as dimers with C_2 symmetry and may be represented by the for-

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[14] W. R. Busing, K. O. Martin, and H. A. Levy, "ORFLS, a Fortran Crystallographic Least-Squares Program," Report ORNL-TM-305, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1962.

[15] H. P. Hanson, F. Herman, J. D. Lea, and S. Skillman, *Acta Cryst.*, **17**, 1040 (1964).

[16] J. A. Ibers and W. C. Hamilton, *ibid.*, **17**, 781 (1964).

[17] "International Tables for X-ray Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962, pp 215, 216.

[18] L. Guggenberger, "FOUR, an Electron Density Summation Program for the Triclinic Monoclinic, and Orthorhombic Crystal Systems," Experimental Station, E. I. du Pont de Nemours and Co., Wilmington, Del., 1967. (Written entirely in Fortran IV; a modified version of the summation program written by Dr. C. Fritchie.)

TABLE II

FINAL ANISOTROPIC THERMAL PARAMETERS FOR $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$[a]

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B, Å^2 [b]
		A. Zinc O,O-Diisopropylphosphorodithioate, $Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$					
Zn(1)	161.1 (2.5)	49.2 (0.9)	27.8 (0.5)	−3.7 (1.4)	3.0 (0.8)	4.4 (0.6)	6.9
S(2)	207 (7)	57 (2)	35 (1)	22 (3)	13 (2)	9 (1)	8.4
S(3)	217 (7)	82 (3)	30 (1)	33 (4)	21 (2)	5 (2)	9.0
S(4)	210 (7)	52 (2)	32 (1)	−21 (3)	11 (2)	−5 (1)	8.0
S(5)	167 (6)	58 (2)	37 (1)	17 (3)	−6 (2)	−1 (1)	8.2
P(6)	206 (7)	61 (3)	31 (1)	−10 (4)	9 (3)	6 (2)	8.2
P(7)	141 (6)	57 (2)	36 (1)	−3 (3)	−14 (2)	7 (1)	7.8
		B. Cadmium O,O-Diisopropylphosphorodithioate, $Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$					
Cd(1)	192.2 (2.8)	51.4 (1.0)	24.8 (0.4)	−1.6 (1.9)	5.3 (0.8)	6.7 (0.7)	7.7
S(2)	270 (14)	78 (5)	34 (2)	56 (7)	18 (4)	17 (3)	10.2
S(3)	250 (12)	111 (6)	35 (2)	50 (8)	39 (4)	7 (3)	11.0
S(4)	262 (13)	51 (4)	35 (2)	−24 (6)	18 (4)	−15 (2)	9.2
S(5)	173 (10)	51 (4)	32 (2)	16 (5)	4 (3)	−5 (2)	7.7
P(6)	222 (13)	85 (5)	30 (2)	−13 (7)	11 (5)	11 (3)	9.5
P(7)	156 (11)	52 (4)	31 (2)	−7 (6)	−10 (4)	−2 (2)	7.5

[a] The anisotropic thermal parameters and their estimated standard deviations have been multiplied by 10^4. The form of the anisotropic thermal ellipsoid is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$. [b] Calculated from the anisotropic thermal parameters by the equation $B \cong (4/3)(\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + 2\beta_{12}ab \cos \gamma + 2\beta_{13}ac \cos \beta + 2\beta_{23}bc \cos \alpha)$, where β_{ij} are the anisotropic thermal parameters and a, b, c, α, β, and γ are the unit cell parameters: W. C. Hamilton, *Acta Cryst.*, **12,** 609 (1959).

TABLE III

FINAL ROOT-MEAN-SQUARE THERMAL AMPLITUDES OF VIBRATION (Å) IN $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$[a]

Atom	Min	Med	Max
	A. $Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$		
Zn(1)	0.262 (3)	0.291 (2)	0.329 (3)
S(2)	0.264 (6)	0.344 (6)	0.364 (6)
S(3)	0.302 (6)	0.308 (6)	0.396 (6)
S(4)	0.259 (6)	0.326 (6)	0.362 (6)
S(5)	0.270 (6)	0.309 (6)	0.381 (6)
P(6)	0.282 (7)	0.323 (7)	0.360 (7)
P(7)	0.254 (6)	0.286 (6)	0.387 (7)
	B. $Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$		
Cd(1)	0.268 (3)	0.314 (3)	0.347 (3)
S(2)	0.255 (11)	0.355 (11)	0.442 (11)
S(3)	0.296 (11)	0.352 (12)	0.455 (11)
S(4)	0.236 (11)	0.363 (10)	0.402 (10)
S(5)	0.257 (10)	0.310 (9)	0.360 (9)
P(6)	0.294 (12)	0.350 (12)	0.390 (12)
P(7)	0.257 (12)	0.283 (11)	0.373 (11)

[a] An indication of the directions of these principal axes of vibration is given in Figure 4.

mula $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$, M = Zn or Cd. The two species, illustrated[19] in Figures 1–4, are isomorphous in both geometry and molecular packing.

The interatomic distances, angles, and standard deviations for the two structures are given in Tables V and VI. The standard deviations were computed from the final variance–covariance matrix using the program of Busing, Martin, and Levy.[20,21] Correction of the metal–sulfur bond lengths for thermal motion of the atoms may be estimated using the "riding" model of Busing and Levy.[22] From considerations of the molecular geometry each sulfur atom may be assumed to "ride" on the metal atom to which it is bonded. For atoms S(1), S(2), S(3), and S(4) this model gives the following corrected distances: in $Zn_2(dtp)_4$, 2.364 (5), 2.429 (5), 2.315 (5), and 2.313 (6) Å, respectively, and in $Cd_2(dtp)_4$, 2.573 (7), 2.618 (8), 2.499 (7), and 2.499 (7) Å, respectively. The standard deviations cited do not take into consideration uncertainties in the thermal parameters. The simple "riding" model is not

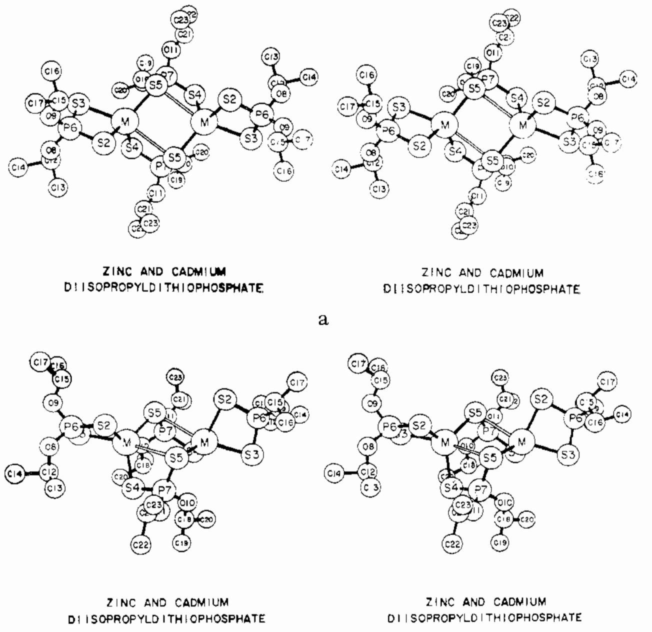

Figure 1.—Stereographic drawings of the zinc and cadmium O,O-diisopropylphosphorodithioate dimers: (a) view along the C_2 symmetry axis of the dimer; (b) view as seen approximately parallel to the a axis of the unit cell.

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[19] C. K. Johnson, "ORTEP, a Fortran Thermal-Ellipsoid Plot Program for Crystal Structure Illustrations," Report ORNL-3794, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1965.

[20] W. R. Busing, K. O. Martin, and H. A. Levy, "ORFFE, a Fortran Crystallographic Function and Error Program," Report ORNL-TM-306, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1964.

[21] The computed standard deviations include the standard deviations of the lattice parameters, which contribute significantly less than those of the atomic coordinates.

[22] W. R. Busing and H. A. Levy, *Acta Cryst.*, **17,** 142 (1964).

TABLE IVA

OBSERVED AND CALCULATED STRUCTURE FACTORS (IN ELECTRONS × 10) FOR ZINC O,O-DIISOPROPYLPHOSPHORODITHIOATE, $Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$[a]

H	L	FO	FC
H 0 L			
0	2		-2582
0	4	414	336
0	6	485	564
0	8	1045	-1006
0	10	742	-801
0	12	2232	2175
0	14	1293	-1233
0	16	393	381
0	18	455	327
0	20	790	-734
0	22	209*	165
0	24	260	252
0	26	475	-375
2	0	1310	1371
2	2	427	165
-2	2	3291	3147
2	4	4613	-4682
-2	4	2607	-2515
2	6	2250	2284
-2	6	4017	4122
2	8	1213	-1274
-2	8	2843	-2675
2	10	829	697
-2	10	1378	-1625
2	12	747	520
-2	12	882	895
2	14	879	-856
2	16	861	843
2	18	469	424
2	20	456	-508
-2	20	876	-916
-2	22	234	280
2	24	262	125
4	0	481	423
4	2	1160	-1195
-4	2	951	-1168
4	4	494	617
4	6	518	-643
-4	6	1458	1472
4	8	432	-521
-4	8	547	-507
4	10	658	642
-4	10	1517	-1515
4	12	237	242
4	14	218	196
-4	14	467	543
4	16	321	271
4	18	326	308
-4	18	218*	90
4	20	684	-609
-4	20	240	-190
-4	22	326	-332
6	0	246	164
6	2	554	-565
6	4	764	798
-6	4	767	-787
6	6	833	-783
-6	6	200	-327
6	8	1095	-963
-6	8	893	647
6	10	980	1006
-6	10	1250	-1226
6	12	384	319
-6	12	674	710
6	14	428	-348
-6	14	188*	151
6	16	530	493
-6	16	400	-400
6	18	417	-456
-6	18	400	427
-6	20	172*	199
-6	22	427	-302
8	0	294	-264
8	2	640	-598
-8	2	1134	1209
8	4	515	485
-8	4	635	-787
8	6	498	-412
-8	6	194*	206
8	8	143*	-217
-8	8	256	-215
8	10	631	557
-8	10	298	-376
-8	12	256	328
-8	14	180*	273
8	16	132*	87
-8	16	362	-411
-8	18	188*	267
-8	20	199*	164
10	2	317	-338
-10	2	243	279
10	4	125*	178
-10	6	184*	-131
10	10	125*	280
-10	10	272	-273
-10	14	218	140
H 1 L			
1	0	2818	3149
1	1	3320	-3566
-1	1	2909	-3007
1	2	186	-271
-1	2	1418	-1383
1	3	2186	-2212
-1	3	1632	-1629
1	4	585	-780
-1	4	815	838
1	5	1095	1049
-1	5	2093	-2219
1	6	2031	2064
1	7	591	540
-1	7	1774	-1900
1	8	623	-609
-1	8	1293	-1365
1	9	355	549
-1	9	388	-539
1	10	242	293
1	11	256	288
-1	11	1048	1085
1	12	1100	1196
-1	12	1399	1361
1	13	710	-860
-1	13	485	-521
1	14	954	-1021
-1	14	679	-710
1	15	652	669
1	16	311	208
-1	16	276	-233
1	17	357	-323
-1	17	237	-231
1	18	343	386
-1	18	468	354
1	19	459	-435
-1	19	408	-428
1	20	162*	-160
-1	20	551	-618
1	21	217	158
-1	21	502	448
1	22	137*	-112
-1	22	293	320
1	23	135*	130
-1	23	139*	33
1	24	196*	183
1	25	142*	-180
3	0	528	-520
3	1	323	-433
-3	1	141*	42
3	2	181	157
-3	2	565	602
3	3	904	-809
-3	3	924	-1050
3	4	809	-904
-3	4	340	-377
3	5	922	878
-3	5	1701	1724
3	6	1574	1309
-3	6	1674	1371
3	7	548	-527
-3	7	3024	-3099
3	8	831	-539
-3	8	1872	-2015
3	9	1323	1346
-3	9	208*	-111
3	10	318	-213
3	11	119*	-193
-3	11	1214	1085
3	12	419	388
-3	12	260	295
3	13	177*	-124
-3	13	299	218
3	14	200	-299
3	15	501	483
-3	15	401	-386
-3	16	246	407
3	18	319	337
3	19	662	-639
-3	19	364	-378
3	20	407	-405
-3	20	251	-285
3	21	279	339
-3	21	181*	275
5	0	510	561
5	1	390	-475
-5	1	749	-805
5	2	1145	-1180
-5	2	412	-374
5	3	1016	1005
-5	3	286	333
5	4	1308	1261
5	5	887	-850
-5	5	559	529
5	6	581	-588
-5	6	322	-223
5	7	96*	190
-5	7	337	-249
5	8	546	-541
-5	8	779	689
5	9	1224	1264
-5	9	975	-910
5	10	457	479
-5	10	841	-928
-5	11	1180	1197
5	12	239	-169
-5	12	170*	-164
5	13	276	-259
-5	14	211	198
5	15	223	205
5	17	362	-318
5	18	196*	-158
-5	18	331	382
5	21	143*	163
-5	21	269	-204
5	22	165*	54
-5	23	238	174
-5	26	197*	23
7	0	366	-350
7	1	323	-253
-7	1	483	402
7	2	132*	-54
-7	2	1007	994
7	3	167*	301
-7	3	666	-624
7	4	318	237
-7	4	940	-922
7	5	437	-446
7	6	177	-235
7	7	237	205
7	8	236	-295
-7	8	813	581
7	9	704	675
-7	9	189*	-67
7	10	321	377
-7	10	493	-454
-7	11	684	698
-7	12	303	265
7	13	360	-379
7	14	255	-274
7	16	255	312
-7	16	232	-317
7	17	234	-222
-7	17	334	333
7	18	205	-241
9	0	178*	145
9	1	225	-122
-9	1	392	485
9	2	485	-473
-9	2	280	304
9	3	371	278
-9	3	369	-357
9	4	253	300
-9	4	240	-239
-9	6	177*	69
9	8	227	-103
9	9	321	308
9	10	356	272
9	11	252	-252
-9	11	223	187
-9	14	245	207
-9	15	183*	-170
-9	16	272	-224
-9	17	188*	174
-11	1	197*	168
-11	5	180*	-114
-11	11	210*	76
H 2 L			
0	0	761	-766
0	1	5454	-4810
0	2	3749	-2953
0	3	294	301
0	4	1356	1207
0	5	2237	1840
0	6	1434	1265
0	7	961	-1109
0	8	539	-482
0	9	602	589
0	10	738	646
0	11	575	549
0	13	2008	-1974
0	14	351	-456
0	15	210	302
0	16	550	-562
0	17	245	243
0	18	443	471
0	19	506	-529
0	25	316	-269
0	27	200	241
2	0	2449	-2588
2	1	1870	-1699
-2	1	2145	-1822
2	2	711	654
-2	2	144*	-102
2	3	824	711
-2	3	3120	-2926
2	4	744	-701
-2	4	218	155
2	5	2634	2587
-2	5	580	597
2	6	1309	1410
-2	6	525	-418
2	7	1912	-1729
-2	7	2132	-2084
-2	8	194	-118
2	9	1044	1030
-2	9	624	577
2	10	769	-765
-2	10	1265	1147
-2	11	1858	2150
2	12	148*	299
-2	12	323	400
2	13	908	-900
-2	13	993	-935
2	14	237	-261
-2	14	738	-750
2	15	852	863
2	16	331	-416
-2	16	311	254
2	19	437	-486
-2	19	559	-583
2	20	288	340
-2	21	395	470
-2	23	151*	114
-2	25	256	-176
4	0	333	-272
4	1	815	-795
-4	1	390	-278
4	2	194	-331
-4	2	624	-659
4	3	1517	1405
-4	3	1042	-1124
4	4	732	798
-4	4	886	890
4	5	506	-483
-4	5	982	936
4	6	126*	-57
-4	6	1280	-1289
4	7	768	-864
-4	7	1546	-1617
4	8	1109	1092
-4	8	600	614
4	9	855	790
-4	9	459	-616
4	10	1164	-1174
-4	10	976	1098
-4	11	906	864
4	12	330	-258
-4	12	582	-643
-4	13	306	428
4	14	185*	201
-4	14	186*	-137
4	15	281	178
4	16	426	-397
-4	16	222	231
-4	17	270	276
4	18	121*	49
4	19	409	-407
-4	19	528	-508
4	21	381	411
-4	23	206	341
6	0	448	-431
6	1	975	-883
-6	1	202	-219
6	2	551	562
-6	2	423	555
6	3	692	709
-6	3	363	-395
6	4	369	-295
-6	4	351	-276
6	5	591	-566
-6	5	447	502
6	6	694	687
6	7	272	-297
-6	7	574	497
-6	8	678	678
6	9	930	962
-6	9	1183	-1095
-6	10	331	317
6	11	202*	-141
-6	11	786	767
6	12	510	-562
-6	12	549	-540
6	13	414	-325
-6	13	297	-232
6	15	424	391
-6	16	185*	-100
6	17	493	-438
-6	17	467	502
6	19	176*	203
-6	19	213	-151
-6	21	251	-253
8	0	238	278
8	1	247	-307
-8	1	570	573
8	3	330	361
-8	3	1048	-1042
8	4	308	271
-8	4	329	-351
8	5	343	-316
-8	5	417	506
8	6	172*	-152
-8	6	242	140
8	7	114*	114
-8	7	163*	-42
8	8	185*	234
-8	8	348	390
8	9	371	386
8	11	342	-259
-8	11	151*	250
8	12	174*	-22
-8	12	148*	22
8	14	208*	-67
8	15	162*	137
-8	15	383	-369
8	16	261	106
-8	17	276	302
-8	18	222	-136
-10	1	237	237
-10	2	237	-211
10	3	241	219
10	6	185*	85
-10	6	185*	66
10	7	215*	-21
-10	9	225	-239
H 3 L			
1	0	2482	-2419
1	1	376	209
-1	1	849	-754
1	2	405	411
-1	2	532	-635
1	3	1111	1191
-1	3	1800	1636
1	4	1363	-1278
-1	4	1334	1348
1	5	2736	2622
-1	5	1391	-1305
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1	2	243	-265
-1	2	747	691
1	3	284	256
-1	3	139*	-15
1	4	642	-648
-1	4	1053	-1059
1	5	1451	1378
-1	5	2038	1928
1	6	155*	-133
-1	6	380	345
1	7	562	-567
-1	7	1261	-1273
-1	8	964	-903
-1	9	413	450
1	10	389	331
1	11	248	247
-1	11	297	325
1	12	311	350
-1	12	297	378
1	13	796	-763
-1	13	657	-710
-1	14	209	237
1	15	704	719
-1	15	272	327
-1	16	159*	43
1	17	135*	206
-1	17	240	141
1	18	187*	215
1	19	294	-354
1	20	250	-256
1	21	355	284
-1	21	344	341
3	0	722	760
3	1	471	-452
-3	1	646	-613
3	2	700	-696
-3	2	651	-587
-3	3	794	764
3	4	242	228
-3	4	569	569
3	5	466	431
-3	5	871	916
-3	6	437	-437
3	7	668	-613
-3	7	468	-468
-3	8	158*	67
3	9	166*	182
-3	9	288	-339
-3	10	904	-876
3	11	337	-334
-3	11	516	545
-3	12	377	412
3	13	124*	-88
-3	13	381	-264
3	14	256	-225
3	15	362	378
5	0	231	-277
5	1	153*	182
5	2	454	400
-5	2	415	426
5	3	391	375
-5	3	137*	-185
-5	4	444	-423
5	5	605	-574
-5	5	887	812
-5	6	357	476
5	8	340	-349
-5	8	241	-254
5	9	228	293
-5	9	401	-440
5	11	219	-199
-5	11	352	315
5	12	252	257
-5	12	231*	-91
5	13	269	-230
-5	13	201*	-200
-5	14	193*	170
5	15	363	374
-5	15	263	-240
-5	17	177*	207
7	0	230	228
7	1	174*	-142
7	2	212	-95
7	3	561	554
-7	3	469	-426
7	4	239*	84
7	5	430	-484
-7	5	286	317
7	8	229	-224
7	9	414	422
-7	9	257	-237
7	11	436	-395
-7	11	253	258
-7	12	176*	-24
7	14	165*	138
-7	15	505	-394
-7	17	280	328
-9	1	221	227
9	3	301	281
-9	3	300	-278
-9	7	181*	73
-9	9	211	-155
-9	11	191*	223
H 10 L			
0	0	580	-674
0	1	836	-830
0	2	957	968
0	3	1040	-1033
0	4	419	445
0	5	1202	1281
0	6	690	-720
0	7	754	-780
0	9	795	793
0	11	396	439
0	13	767	-778
0	15	257	224
0	16	182*	-103
0	18	232*	-84
0	19	301	-348
0	21	262	239
2	0	187	-208
2	1	1382	-1403
-2	1	1104	-1115
-2	2	745	695
2	3	373	360
-2	3	405	427
2	4	301	324
-2	4	608	588
2	5	684	603
2	6	514	-476
-2	6	880	-901
2	7	311	-210
-2	7	812	-735
-2	8	212	-244
-2	9	533	525
-2	10	300	279
2	11	204	211
-2	11	670	634
-2	12	300	-254
2	13	428	-460
2	14	442	415
-2	14	284	221
2	15	238	240
2	17	308	234
2	19	368	-383
-2	19	237	-220
2	20	156*	97
2	21	117*	159
-2	22	176*	-194
4	0	173*	-148
-4	2	314	302
4	3	207	185
4	4	410	-395
-4	4	520	531
4	5	222	-136
-4	5	218	192
-4	6	799	-787
4	7	385	-474
4	9	280	295
-4	9	500	-463
4	10	256	-337
-4	11	706	635
4	12	281	246
-4	12	171*	-251
4	13	186	-226
4	14	236	230
4	15	267	263
-4	16	286	243
4	17	250	-207
-4	19	134*	-166
-6	3	753	-777
6	4	282	-376
6	5	486	-546
-6	5	493	483
6	9	377	445
6	10	231	-242
-6	10	220	252
6	11	211*	-172
6	12	119*	64
-6	12	480	-415
-6	13	228	160
6	14	281	279
-6	14	239*	52
-6	15	186*	-285
-6	17	314	263
8	0	208	190
8	1	304	-329
-8	2	230	-184
8	3	207	277
8	4	236	-243
-8	5	137*	-137
-8	6	231	-192
-8	7	270	218
-8	9	309	-310
-8	11	302	292
-8	15	227	-146
H 11 L			
1	0	1029	-967
1	1	340	-418
1	2	643	625
-1	2	333	372
-1	3	644	-621
1	4	723	745
-1	4	647	658
1	6	715	-732
-1	6	554	-625
1	7	284	-256
-1	7	899	-824
1	8	576	584
-1	8	532	576
-1	9	903	917
1	10	344	-310
1	11	510	522
1	12	253	-305
-1	12	541	-638
1	13	424	-421
-1	13	372	-369
1	14	355	415
-1	14	210	242
1	16	161*	-77
1	17	236	244
1	18	237	-223
-1	18	287	-221
1	19	267	-246
1	20	235	258
-1	20	197	277
-1	21	192*	-16
-1	22	185*	-68
3	0	573	-603
3	1	496	-575
3	2	698	685
3	3	147*	210
-3	3	391	385
3	4	368	-387
-3	4	354	354
3	5	200	108
-3	5	1206	-1137
3	6	164*	-86
-3	6	550	-532
-3	7	200	240
3	8	375	330
-3	10	502	525
3	11	330	375
-3	11	263	244
-3	12	591	-581
3	14	482	411
-3	15	260	98
5	0	208	-203
-5	1	603	616
5	2	228	240
-5	2	314	-268
5	3	197*	-197
-5	3	544	-533
5	4	336	-402
-5	4	561	516
-5	6	400	-401
5	7	134*	-5
5	8	602	595
5	10	356	-397
-5	10	333	319
5	11	301	243
-5	11	232	-177
5	12	155*	6
-5	13	348	345
-5	18	234	-194
7	1	351	-324
7	2	206	270
-7	2	385	-440
-7	3	198	-224
-7	4	214	309
-7	6	177*	-74
-7	7	158*	228
7	8	338	269
-7	8	164*	-93
-7	9	215	-185
7	10	346	-274
-7	10	239	242
7	12	148*	24
-7	12	236	-214
-7	16	154*	210
9	2	226	221
H 12 L			
0	0	320	-430
0	1	409	490
0	2	400	-355
0	3	236	-242
0	4	520	582
0	5	194*	-201
0	6	622	-589
0	8	943	991
0	9	229	-172
0	10	358	-265
0	11	125*	101
0	12	421	-526
0	13	165*	-97
0	16	148*	178
0	18	359	-285
0	19	184*	122
0	20	195*	155
2	0	934	-875
2	1	287	114
2	2	818	851
2	3	190*	-117
-2	3	312	367
2	4	165*	-122
-2	4	187	-277
-2	5	642	-732
-2	6	220	191
2	7	232	333
2	8	375	383
-2	8	538	523
2	9	398	-413
-2	9	266	306
2	10	212	191
-2	10	355	241
-2	11	572	-514
2	12	440	-480
-2	12	700	-634
2	13	165*	226
-2	13	225	247
-2	14	235	195
2	15	324	-352
2	17	219	214
-2	18	249	-137
2	19	199*	-16
-2	20	294	176
4	0	218	-195
4	1	524	596
-4	1	293	345
4	2	490	527
-4	2	400	-441
4	3	454	-492
-4	3	318	267
4	4	263	-187
4	5	319	390
-4	5	517	-595
4	7	188*	173
-4	7	330	350
4	8	478	423
4	9	348	-341
4	10	180*	-16
-4	10	314	330
-4	11	216	-313
4	12	238	-215
4	13	197*	221
-4	14	153*	-18
4	15	162*	-159
4	16	171*	-166
6	1	195	216
6	2	165*	245
-6	2	408	-498
-6	4	449	533
6	6	159*	-9
6	7	394	340
6	8	275	293
-6	8	204*	-162
6	9	285	-302
6	10	325	-269
-6	10	149*	146
-6	11	217	-293
-6	13	191	226
-6	17	162*	-89
8	0	224	-202
-8	1	204*	-145
8	2	234	254
-8	2	230	-187
-8	7	244	124
H 13 L			
1	0	279	-238
1	1	404	474
-1	2	365	-311
-1	3	281	320
1	4	200	131
1	5	255	-178
1	6	200*	-135
1	7	775	714
-1	7	186*	228
-1	8	347	426
1	9	722	-724
-1	9	148*	-218
-1	11	535	-468
1	12	227	-212
-1	13	328	338
-1	16	198*	81
-1	17	192*	-220
3	0	158*	-61
3	1	986	939
3	2	290	261
3	3	760	-724
-3	3	539	530
-3	4	444	-455
3	5	357	284
-3	5	283	-302
-3	6	304	280
3	7	246	324
-3	7	318	271
3	8	185*	-141
3	9	255	-303
3	10	99*	178
3	11	399	-335
-3	11	597	-625
3	13	327	362
-3	13	290	352
3	14	154*	-130
3	15	282	-261
5	0	309	288
5	1	625	661
5	3	277	-323
-5	3	304	-68
-5	4	195	219
-5	5	386	-374
5	7	401	425
-5	7	202	175
-5	8	163*	-80
5	9	524	-518
-5	9	188*	107
7	6	176*	-147
7	1	263	214
-7	3	406	373
-7	5	282	-173
H 14 L			
0	0	270	251
0	1	180*	141
0	2	141*	-165
0	3	302	288
0	4	193*	135
0	7	342	350
0	8	418	-489
0	9	237	-307
0	13	145*	66
0	15	206*	144
0	17	166*	-169
2	1	465	544
2	2	153*	-271
-2	2	434	371
2	3	377	-357
-2	3	236	257
-2	4	274	-276
2	5	135*	-75
2	7	137*	225
2	8	749	-641
2	9	236	-124
-2	9	219	215
-2	11	483	-515
2	12	234	259
-2	12	219	404
-2	13	251	260
2	15	241	-181
-2	17	172*	-107
4	0	562	548
4	1	381	462
4	2	614	-623
4	3	430	-474
-4	3	215	273
4	4	246	251
-4	4	150*	-259
4	5	208*	52
-4	5	351	-363
4	7	215	231
-4	7	247	239
4	8	209	-258
-4	9	165*	175
4	11	179*	-55
-4	11	152*	-214
-4	12	221	208
4	13	215*	55
-6	2	298	233
6	3	154*	23
-6	3	233	255
6	4	172*	-231
-6	4	217	-181
-6	5	257	-262
6	7	212*	191
6	8	167*	-210
-6	9	138*	115
H 15 L			
1	0	307	339
1	2	185	-217
1	6	304	372
1	7	215	-222
-1	7	171*	-138
1	8	528	-567
1	9	211	193
-1	9	250	248
1	11	140*	203
1	12	149*	67
-1	12	165*	301
1	15	167*	-28
3	0	316	411
3	1	272	-111
3	2	625	-643
-3	2	167*	202
3	4	298	302
-3	4	415	-329
-3	6	358	315
3	8	95*	-224
3	9	129*	106
-3	9	162*	237
-3	10	341	-363
3	11	223	166
-3	11	186*	-120
3	12	262	281
-3	12	399	356
3	13	191*	-59
-3	14	188*	-151
5	0	258	333
5	2	317	-321
-5	4	314	-314
5	8	330	-331
H 16 L			
0	0	305	286
0	1	225	-247
0	2	204	-117
0	7	480	-437
0	9	273	287
0	12	171*	-99
0	13	173*	-110
2	1	341	-339
-2	1	155*	-169
2	3	129*	70
-2	4	358	-259
2	5	176*	102
2	6	268	212
-2	6	146*	212
2	7	270	-298
-2	7	253	-197
-2	10	378	-369
-2	11	191*	213
4	1	272	-330
-4	4	273	-236
-4	6	271	380
H 17 L			
1	1	221	-286
-1	1	386	-317
-1	2	171*	16
1	5	410	365
-1	5	188*	277
-1	6	137*	-140
1	7	284	-314
1	8	165*	171
-1	8	240	296
3	0	169*	-186
-3	1	235	-236
H 18 L			
0	0	202	-224
0	1	250	-231
0	2	108*	77
0	3	154*	78
0	4	222	236
0	5	141*	136
2	0	322	-315
-2	2	200	259

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[a] Asterisks denote unobserved reflections.

TABLE IVB

OBSERVED AND CALCULATED STRUCTURE FACTORS (IN ELECTRONS × 10) FOR CADMIUM O,O-DIISOPROPYLPHOSPHORODITHIOATE, $Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$[a]

H	L	FO	FC
H 0 L			
0	2		-3410
0	4	301*	139
0	6	1276	1343
0	8	1845	-1874
0	10	408	-338
0	12	2466	2462
0	14	2075	-2110
0	16	635	925
0	18	719	562
0	20	1226	-1163
0	22	292*	352
0	24	235*	239
0	26	435	-453
0	28	312*	323
2	0	2241	2188
2	2	954	-824
-2	2	2735	2682
2	4	4778	-4638
-2	4	2928	-3104
2	6	2778	2858
-2	6	4694	5148
2	8	2269	-2353
-2	8	3262	-3268
2	10	1440	1394
-2	10	1270	-1409
2	12	799	628
-2	12	1535	1626
2	14	1094	-1178
-2	14	1113	-1133
2	16	962	1002
-2	16	690	640
2	18	499	455
2	20	826	-791
-2	20	1183	-1378
2	22	290*	241
-2	22	461	488
-2	24	312*	248
-2	28	352*	179
4	0	1232	1191
4	2	2048	-2110
-4	2	1046	-1070
4	4	1205	1296
-4	4	674	-807
4	6	328	-378
-4	6	2191	2205
4	8	1023	-1114
-4	8	890	-846
4	10	1165	1144
-4	10	1783	-1800
4	12	561	570
-4	12	336	397
4	14	426	-433
-4	14	227*	302
4	16	688	594
-4	16	205*	44
4	18	258*	32
-4	18	569	634
4	20	585	-586
-4	20	751	-813
4	22	439	357
-4	22	233*	-71
-4	24	297*	219
6	0	671	732
6	2	1147	-1188
6	4	843	883
-6	4	1292	-1378
6	6	352*	-186
-6	6	539	475
6	8	1515	-1365
-6	8	416	427
6	10	1175	1187
-6	10	1680	-1658
6	12	501	329
-6	12	1187	1191
6	14	685	-657
6	16	699	683
-6	16	304*	-340
6	18	592	-499
-6	18	540	668
-6	20	264*	-34
-6	22	219*	-233
-6	26	239*	-225
8	2	932	-852
-8	2	849	936
8	4	568	430
-8	4	837	-897
-8	6	605	673
8	8	364*	-426
-8	8	520	-445
8	10	675	608
-8	10	485	-462
8	12	392*	-107
-8	12	565	587
8	16	442*	84
-8	16	395	-441
-8	18	345*	391
10	2	438	-339
-10	2	259*	238
-10	8	384*	94
-10	10	377*	-372
-10	18	276*	193
H 1 L			
1	0	3368	4026
1	1	3963	-4318
-1	1	3642	-3532
1	2	689	-679
-1	2	1959	-1872
1	3	2052	-2118
-1	3	1521	-1462
1	4	890	-1018
-1	4	641	795
1	5	1390	1419
-1	5	1614	-1625
1	6	2721	2800
-1	6	277*	438
1	7	477	-426
-1	7	2050	-2035
1	8	1453	-1426
-1	8	2030	-2157
1	9	1437	1506
-1	9	511	-430
1	10	445	621
-1	10	300*	19
-1	11	1109	1291
1	12	1422	1495
-1	12	2077	2053
1	13	873	-1100
-1	13	1251	-1338
1	14	1417	-1452
-1	14	1278	-1378
1	15	1108	1045
-1	15	563	767
1	16	488	517
-1	16	272*	12
1	17	244*	-269
-1	17	481	-469
1	18	384	435
-1	18	699	625
1	19	716	-771
-1	19	616	-665
1	20	318*	-427
-1	20	1011	-931
1	21	526	485
-1	21	529	586
-1	22	542	482
1	23	311*	-31
-1	26	316*	-319
-1	27	376*	276
3	0	329*	-83
3	1	1064	-1220
-3	1	689	-701
3	2	435	-316
-3	2	507	552
3	3	405*	-114
-3	3	1118	-1094
3	4	509	-589
-3	4	583	-444
3	5	799	788
-3	5	2432	2451
3	6	1490	1394
-3	6	2404	2188
3	7	1050	-986
-3	7	3455	-3567
3	8	1048	-1075
-3	8	2436	-2518
3	9	1951	1988
-3	9	249*	259
3	10	345	277
3	11	333*	-277
-3	11	1352	1183
3	12	363	322
-3	12	507	514
3	13	457	-554
3	14	460	-560
-3	14	387	-470
3	15	671	762
3	16	411	441
-3	16	419	477
3	17	461	-388
-3	17	330*	-86
3	19	566	-568
-3	19	823	-837
3	20	600	-527
-3	20	549	-512
3	21	479	466
-3	21	613	625
3	22	431	365
-3	22	453*	46
3	25	342*	94
5	0	1228	1286
5	1	1098	-1018
-5	1	1070	-1075
5	2	1900	-1947
-5	2	452	-569
5	3	1277	1350
-5	3	173*	33
5	4	1561	1514
-5	4	705	-613
5	5	689	-658
-5	5	1144	1036
5	6	400	-326
-5	6	511	418
5	7	308*	-111
-5	7	951	-870
5	8	980	-997
-5	8	457	499
5	9	1331	1358
-5	9	947	-921
5	10	856	814
-5	10	1161	-1189
5	11	286*	-80
-5	11	1396	1377
-5	12	475	399
5	13	488	-587
5	14	417	-236
5	15	411	441
5	16	486	483
-5	16	404	-233
5	17	534	-453
5	18	442	-297
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-2	11	458	-587
2	12	359*	118
-2	13	396	442
-2	14	208*	-46
2	15	368*	-513
2	16	219*	-80
4	1	676	801
-4	1	539	436
-4	2	206*	110
4	3	432	-479
-4	5	360	-463
4	6	431*	-46
4	7	357*	280
4	8	414*	15
4	9	429	-263
-4	9	453*	103
4	10	299*	-25
4	11	394*	5
4	13	415*	116
-4	13	298*	285
-6	5	357*	-352
H 15 L			
1	0	434	495
-1	2	365*	-157
1	5	332*	-347
-1	5	374*	-211
1	6	374	418
-1	6	482	416
1	8	411	-447
-1	8	584	-559
1	9	434	-268
1	14	363*	-227
3	0	410	414
3	2	377*	-337
3	3	523	-357
-3	5	428	-460
3	8	419*	-140
-3	11	319*	-367
5	1	327*	97
-5	4	257*	-235
H 16 L			
0	0	510	534
0	2	391	-225
0	4	354*	-305
0	6	452	570
0	7	329*	-210
0	8	419	-425
0	13	400*	-101
2	0	414	458
2	1	338*	-167
2	2	437	-281
-2	2	337*	-262
2	4	246*	-73
2	9	312*	-52
4	4	236*	137
H 17 L			
-1	1	360*	-268
-1	7	426	-446
-1	9	398	232
-3	1	216*	-310
3	2	307*	-129
3	3	278*	105

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[a] Asterisks denote unobserved reflections.

TABLE V

INTERATOMIC DISTANCES (Å) IN $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$

Atoms[a]	$Zn_2(dtp)_4$[b]	$Cd_2(dtp)_4$[b]
M(1)–S(2)	2.351 (5)	2.552 (7)
M(1)–S(3)	2.409 (5)	2.590 (8)
M(1)–S(4)	2.306 (5)	2.486 (7)
M(1)–S(5′)	2.302 (6)	2.499 (7)
M(1)···S(5)	3.347 (6)	3.194 (8)
M(1)···M(1′)	4.108 (5)	4.059 (4)
S(2)···S(3)	3.232 (7)	3.274 (11)
S(4)···S(5)	3.355 (7)	3.323 (10)
S(4)···S(4′)	4.118 (10)	4.449 (16)
S(5)···S(4′)	4.016 (7)	4.352 (10)
S(5)···S(5′)	3.856 (10)	3.917 (15)
P(6)–S(2)	1.984 (7)	1.974 (12)
P(6)–S(3)	1.968 (7)	1.972 (12)
P(7)–S(4)	1.957 (7)	1.957 (11)
P(7)–S(5)	1.971 (7)	1.962 (9)
Av	1.970 (11)	1.965 (8)
P(6)–O(8)	1.56 (1)	1.59 (2)
P(6)–O(9)	1.57 (1)	1.57 (2)
P(7)–O(10)	1.60 (1)	1.59 (2)
P(7)–O(11)	1.58 (2)	1.55 (2)
Av	1.58 (2)	1.58 (2)
O(8)–C(12)	1.44 (3)	1.44 (4)
O(9)–C(15)	1.37 (2)	1.34 (4)
O(10)–C(18)	1.66 (3)	1.62 (4)
O(11)–C(21)	1.66 (7)	1.46 (5)
Av	1.46 (17)	1.47 (11)
C(12)–C(13)	1.43 (3)	1.48 (5)
C(12)–C(14)	1.38 (5)	1.54 (6)
C(15)–C(16)	1.50 (3)	1.48 (5)
C(15)–C(17)	1.51 (4)	1.48 (5)
C(18)–C(19)	1.28 (5)	1.40 (5)
C(18)–C(20)	1.53 (4)	1.52 (5)
C(21)–C(22)	2.04 (7)	1.63 (7)
C(21)–C(23)	1.09 (7)	1.48 (6)
Av	1.45 (10)[c]	1.49 (6)

[a] Bonds signified by – and nonbonds by ···. Primed atoms in all tables, in the figures, and in the text are related to those in Table I by the twofold operation $1 - x, y, {}^1/_2 - z$. [b] Standard deviations for the individual distances were computed from the variance–covariance matrix associated with the final atomic coordinates. Average distances and their corresponding root-mean-square deviations were computed from the expressions

$$\bar{x} = \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \Bigg/ \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \qquad \sigma(\bar{x}) = \left(\frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N - 1} \right)^{1/2}$$

where x_i is an individual observation, σ_i is the corresponding standard deviation, and N is the number of observations. [c] Owing to excessive thermal motion and possible disorder this average does not include the two bonds involving atoms C(21), C(22), and C(23).

TABLE VI

INTERATOMIC ANGLES (DEG) IN $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$

Atoms	$Zn_2(dtp)_4$[a]	$Cd_2(dtp)_4$[a]
Metal Coordination		
S(2)–M(1)–S(3)	85.5 (2)	79.1 (3)
S(2)–M(1)–S(4)	114.6 (2)	115.5 (3)
S(2)–M(1)–S(5′)	112.1 (2)	115.1 (3)
S(3)–M(1)–S(4)	107.2 (2)	107.0 (3)
S(3)–M(1)–S(5′)	109.9 (2)	109.3 (3)
S(4)–M(1)–S(5′)	121.3 (2)	121.6 (2)
S(2)–M(1)···S(5)	81.7 (2)	86.1 (2)
S(3)–M(1)···S(5)	164.0 (2)	162.1 (2)
S(4)–M(1)···S(5)	70.1 (2)	70.3 (2)
S(5′)–M(1)···S(5)	83.9 (2)	86.0 (2)
Sulfur Coordination		
M(1)–S(2)–P(6)	82.6 (2)	84.4 (4)
M(1)–S(3)–P(6)	81.4 (2)	83.4 (4)
M(1)–S(4)–P(7)	100.6 (2)	96.9 (3)
M(1)–S(5′)–P(7′)	104.1 (2)	102.2 (3)
M(1) ··· S(5)–P(7)	71.1 (2)	76.8 (3)
M(1) ··· S(5)–M(1′)	91.4 (2)	90.1 (2)
Phosphorus Coordination		
S(2)–P(6)–S(3)	109.7 (3)	112.2 (5)
S(4)–P(7)–S(5)	117.3 (3)	116.0 (5)
O(8)–P(6)–O(9)	94.9 (8)	95.2 (13)
O(10)–P(7)–O(11)	104.4 (8)	99.2 (12)
S(2)–P(6)–O(8)	113.5 (6)	110.4 (10)
S(2)–P(6)–O(9)	113.0 (6)	114.0 (10)
S(3)–P(6)–O(8)	111.8 (6)	112.4 (11)
S(3)–P(6)–O(9)	113.3 (6)	111.6 (10)
S(4)–P(7)–O(10)	111.5 (6)	111.8 (8)
S(4)–P(7)–O(11)	109.5 (6)	112.7 (10)
S(5)–P(7)–O(10)	105.5 (6)	107.0 (8)
S(5)–P(7)–O(11)	107.8 (7)	108.8 (10)
Oxygen Coordination		
P(6)–O(8)–C(12)	123 (2)	125 (3)
P(6)–O(9)–C(15)	121 (1)	119 (3)
P(7)–O(10)–C(18)	121 (2)	120 (2)
P(7)–O(11)–C(21)	139 (3)	121 (3)
Av	123 (9)	121 (3)
Carbon Coordination		
O(8)–C(12)–C(13)	107 (3)	96 (4)
O(8)–C(12)–C(14)	105 (3)	89 (4)
O(9)–C(15)–C(16)	112 (2)	103 (4)
O(9)–C(15)–C(17)	102 (2)	103 (4)
O(10)–C(18)–C(19)	91 (3)	86 (3)
O(10)–C(18)–C(20)	88 (2)	92 (3)
O(11)–C(21)–C(22)	72 (3)	87 (4)
O(11)–C(21)–C(23)	98 (7)	91 (4)
Av	99 (13)	93 (7)
C(13)–C(12)–C(14)	109 (3)	98 (4)
C(16)–C(15)–C(17)	102 (2)	82 (3)
C(19)–C(18)–C(20)	97 (3)	93 (4)
C(22)–C(21)–C(23)	95 (6)	88 (4)
Av	102 (7)	89 (6)

[a] Standard deviations for the bond angles were computed from the variance–covariance matrix associated with the final atomic coordinates. Average angles and their corresponding root-mean-square deviations were computed from the expressions appearing in footnote *b* of Table V.

entirely applicable for bonds within rings and chains,[23] such as the phosphorus–sulfur bonds in our case. Because of the anticipated complexity of thermal motions within the dtp groups, no attempt was made to correct the lengths of these bonds or those involving the lighter atoms. Little significance should be attached to bond lengths involving atoms in the outer coordination sphere, namely, the carbon atoms, because of the excessive thermal motions which these atoms undergo.

The most interesting feature of these two structures is perhaps the bimolecular nature of the molecules. Each zinc (or cadmium) atom has two dtp groups of which one functions as an *intrachelating* group bound

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(23) G. M. Brown, *Acta Cryst.*, **B24**, 294 (1968).

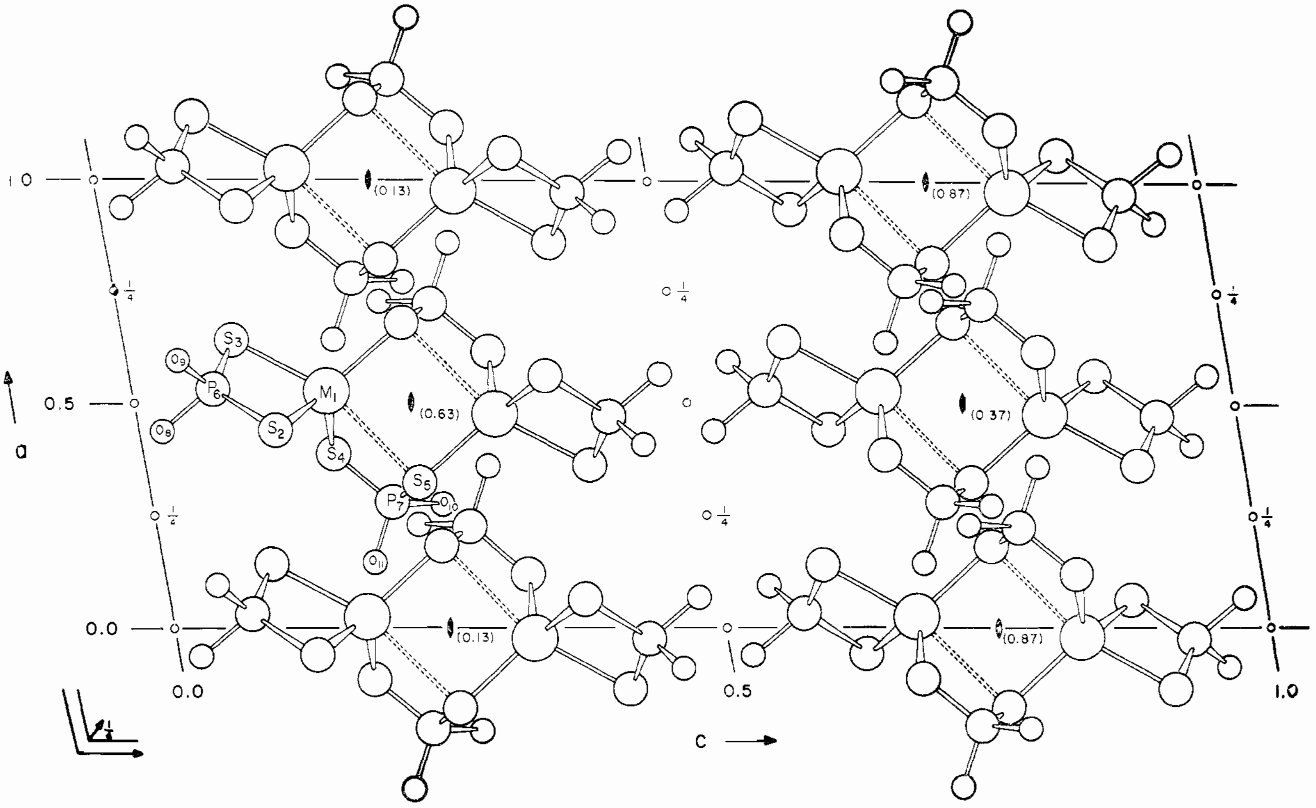
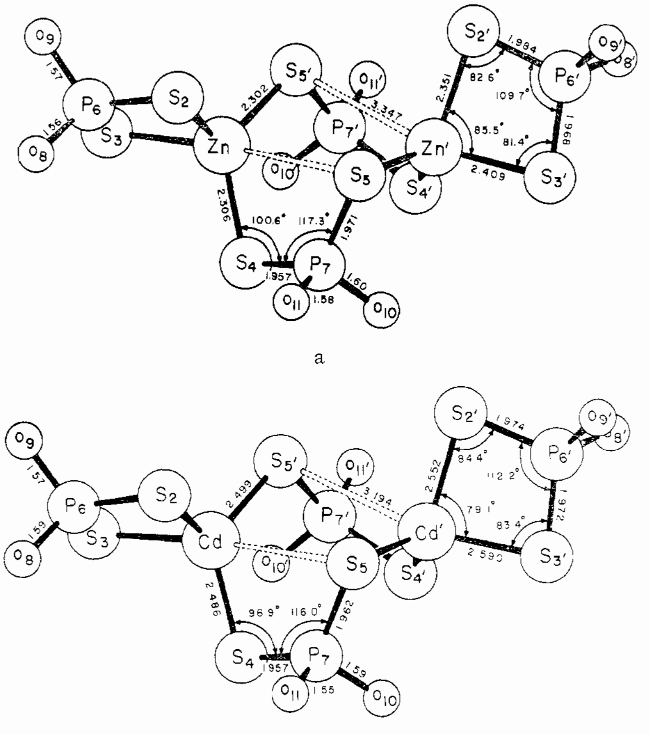


Figure 2.—Molecular arrangement of the zinc and cadmium O,O-diisopropylphosphorodithioate dimers in the unit cell projected along the *b* axis. The *b* axis is normal to the plane of the paper in a right-handed coordinate system. The numbered atoms define the asymmetric unit (Table I). Numbers in parentheses represent the fractional unit cell y coordinate (elevation) of each metal atom pair, where the plane of the paper is $y = 0.0$. For clarity the carbon atoms are not shown.



a

b

Figure 3.—Selected bond distances and angles in the dimers of (a) $Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$ and (b) $Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$. For clarity the carbon atoms are not shown.

wholly to one metal atom and the other functions as a bridging, or *interchelating*, group linking two M(dtp)$_2$ molecules together to form the dimer. The resulting configuration of sulfur about zinc (and cadmium) is a strong distortion from strict tetrahedral symmetry. As a dimer the two monomeric units may be related to each other in either of two ways: by a center of symmetry, C_i, or by twofold rotational symmetry, C_2. The latter linkage of monomeric units was found to be the preferred choice in both Zn$_2$(dtp)$_4$ and Cd$_2$(dtp)$_4$, thereby making them remarkably similar to the structure of dimeric zinc dimethyldithiocarbamate,[24] both from the standpoint of molecular geometry and from packing in the unit cell. The dimeric zinc and cadmium diethyldithiocarbamate complexes, on the other hand, are reported to possess the alternate choice in the crystalline state with C_i symmetry.[25,26] This indicates that apparently the R group, possibly due to packing considerations, determines the final choice of symmetry which the dimer will possess in the crystalline state. It is interesting to note that molecules of the zinc complex in the present study are monomeric in benzene,[2] as was similarly found for zinc diethyldi-

(24) H. P. Klug, *Acta Cryst.*, **21**, 536 (1966).

(25) M. Bonamico, G. Mazzone, A. Vaciago, and L. Zambonelli, *ibid.*, **19**, 898 (1965).

(26) E. A. Shugam and V. M. Agre, *Kristallografiya*, **13**, 253 (1968); *Soviet Phys.-Cryst.*, **13**, 197 (1968).

TABLE VII

COMPARISON OF M–S, M···S, AND M···M DISTANCES IN DIMERS OF ZINC AND CADMIUM DIALKYLDITHIOCARBAMATES AND O,O-DIISOPROPYLPHOSPHORODITHIOATES

Compound	Molecular symmetry	Av M–S dist, Z, in dimer,[a] Å	Long range M···S dist, Z', in dimer, Å	$Z' - Z$, Å	M···M dist in dimer, Å	Ref
			Dithiocarbamates			
$Zn_2[(CH_3)_2CNS_2]_4$	C_2	2.36 (5)	3.036 (6)	+0.68	3.973 (6)	*b*
$Zn_2[(C_2H_5)_2CNS_2]_4$	C_i	2.38 (5)	2.815 (2)	+0.44	3.546 (2)	*c*
$Cd_2[(C_2H_5)_2CNS_2]_4$	C_i	2.57 (6)	2.770 (4)	+0.20	3.58	*d*
			Phosphorodithioates			
$Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$	C_2	2.35 (5)	3.347 (6)	+1.00	4.108 (5)	This study
$Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$	C_2	2.53 (5)	3.194 (8)	+0.66	4.059 (4)	This study

[a] Number corresponds to the average value (plus its associated rms deviation) of the four short covalent bonds. [b] See ref 24. [c] See ref 25. [d] See ref 26.

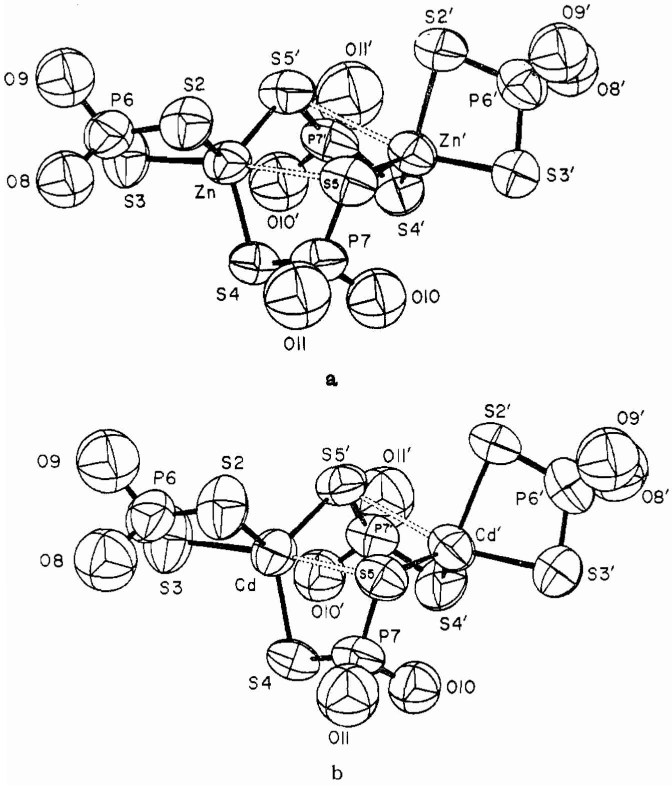


Figure 4.—A parallel projection of the dimers of (a) $Zn_2[(i\text{-}C_3H_7O)_2PS_2]_4$ and (b) $Cd_2[(i\text{-}C_3H_7O)_2PS_2]_4$, illustrating the root-mean-square thermal displacements of atoms in the inner coordination sphere. The ellipsoidal boundaries are at the 60% probability level.

thiocarbamate in benzene[24] and zinc dimethyldithiocarbamate in chloroform.[21] The $Cd_2(dtp)_4$ compound, however, is dimeric in benzene.[2]

In the dimers four "normal" covalent metal–sulfur bonds exist. Their averages, 2.35 (5) Å (range 2.302–2.409 Å) in $Zn_2(dtp)_4$ and 2.53 (5) Å (range 2.486–2.590 Å) in $Cd_2(dtp)_4$, are in excellent agreement with the values 2.35 Å (Zn–S) and 2.52 Å (Cd–S) calculated from the sum of the zinc, cadmium, and sulfur tetrahedral covalent radii.[27a] They also appear to be in accord with those found in the zinc and cadmium dialkyldithiocarbamate dimers,[24–26] summarized in Table VII.

When a dimer forms from two monomers, an intrachelating dtp group of each *monomer* is converted to a bridging group. The bonds M(1)–S(5) and M(1′)–S(5′) are lengthened in the process at the expense of the formation of the new bonds M(1)–S(5′) and M(1′)–S(5) (see Figure 3 for location of primed atoms). The existence of M(1)···S(5) as a *partial* bond in the dimer is open to question. A comparison of this "long-range" distance in $Zn_2(dtp)_4$, $Cd_2(dtp)_4$, and the related dialkyldithiocarbamates is summarized in Table VII. For the zinc complexes the amount by which the M–S bond increases with formation of a dimer does not appear to be constant. The type of alkyl group and the choice of symmetry, C_2 or C_i, assumed by the dimer may be partially responsible for this large variation. Although the number of compounds of this type is rather limited for a truly qualitative comparison, the data in Table VII suggest that a dimer with C_i symmetry tends to contain a shorter M···S distance than is possible with C_2 symmetry. From the single-bond metallic covalent radius of 1.249 Å for zinc and 1.413 Å for cadmium[27b] and the van der Waals radius of 1.85 Å for sulfur with two unshared electron pairs,[27c] the lower limit for zero-bond formation between the metal and sulfur atoms is estimated to be 3.10 Å for Zn–S and 3.26 Å for Cd–S. From a comparison of the observed distances in the phosphorodithioates no appreciable M(1)···S(5) interaction is evident.

The metal–metal distances in the dimers appear to be in direct relation with long-range M···S distances, as might have been expected: the shorter the M···S distance the shorter the M···M distance (Table VII). By comparison with the Zn–Zn and Cd–Cd bonds in metallic zinc and cadmium, 2.665 and 2.979 Å, respectively,[28] it is evident that no metal–metal interaction exists.

The intrachelating and interchelating (bridging) dtp groups deviate only slightly from planarity with the metal atom. As shown in Table VIII the atoms within each group do not deviate by more than 0.09 Å from the respective planes.

Finally, the symmetry of sulfur about the metal atom is of some significance and deserves comment.

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[27] L. Pauling, "The Nature of the Chemical Bond," Cornell University Press, Ithaca, N. Y., 1960: (a) pp 246, 248; (b) p 256; (c) p 260; (d) p 224.

[28] L. E. Sutton, "Tables of Interatomic Distances and Configuration in Molecules and Ions," Special Publication No. 11, The Chemical Society, London, 1958.

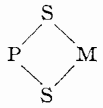
Table VIII

Weighted Least-Squares Planes and Distances of the Atoms from Their Respective Planes in $M_2[(i\text{-}C_3H_7O)_2PS_2]_4$[a,b]

$Zn_2(dtp)_4$		$Cd_2(dtp)_4$	
Atom	Dist, Å	Atom	Dist, Å
(A) Best Plane through M(1), S(2), S(3), P(6)			
$7.580x + 10.138y +$		$7.441x + 9.851y +$	
$7.499z - 11.772 = 0$		$8.571z - 11.590 = 0$	
Zn(1)	−0.007 (2)	Cd(1)	−0.003 (2)
S(2)	0.063 (5)	S(2)	0.071 (9)
S(3)	0.075 (6)	S(3)	0.079 (9)
P(6)	−0.081 (5)	P(6)	−0.100 (9)
(B) Best Plane through M(1), S(4), S(5), P(7)			
$5.330x - 7.061y +$		$5.133x - 6.866y +$	
$17.429z - 1.389 = 0$		$18.345z - 1.632 = 0$	
Zn(1)	−0.005 (2)	Cd(1)	−0.000 (2)
S(4)	0.079 (5)	S(4)	0.009 (8)
S(5)	0.056 (5)	S(5)	0.004 (7)
P(7)	−0.088 (5)	P(7)	−0.009 (8)

[a] Weights were based on the variance–covariance matrix as obtained from the final cycle of least-squares refinement. The least-squares-plane refinement and standard deviations were obtained with Function 16 of ORFFE, written by W. C. Hamilton, Brookhaven National Laboratory, Upton, N. Y. [b] x, y, and z are fractional coordinates of the atoms in the monoclinic cell.

This symmetry deviates considerably from strict tetrahedral coordination in which all angles would be ideally 109° 28′. This deviation is due primarily to the presence of the four-membered ring formed by the dtp group chelating with the metal atom. In the zinc complex the angle S(2)–M(1)–S(3) is 85.5° and in cadmium it is 79.1°. Klug[24] has pointed out that in zinc dimethyldithiocarbamate this sharp decrease of nearly 30° may be responsible for the existence of the complex as a dimer in the crystalline state, a suggestion which could be applied equally well to the present compounds. As a monomer two dtp groups would be present as four-membered rings by ring closure, thereby resulting in two angles of ~80° and four angles of ~126°. As a dimer, one of these four-membered rings is opened and the new angle S(4)–M(1)–S(5′) of ~121° is formed which compensates for the remaining S(2)–M(1)–S(3) angle; the other 126° angles, as shown in Table VI, are then relaxed to near-normal tetrahedral angles.



Several different interpretations of this coordination have been proposed for the related dialkyldithiocarbamate compounds. Among these is the five-coordinate trigonal-bipyramid configuration favored by Bonamico, *et al.*,[25] in describing the zinc diethyldithiocarbamate complex and the four-coordinate distorted tetrahedral configuration favored by Klug[24] in describing the zinc dimethyldithiocarbamate complex. In the application of the trigonal-bipyramid description to $Zn_2(dtp)_4$ and $Cd_2(dtp)_4$ atoms S(2), S(4), and S(5′) would comprise the equatorial positions, and S(3) and S(5) the axial positions. The three S–M–S angles in the equatorial plane are 112.1, 114.6, and 121.3° for $Zn_2(dtp)_4$ and 115.1, 115.5, and 121.6° for $Cd_2(dtp)_4$. These angles are greater than 109° 28′ but they do not satisfy the ideal angle 120°. Moreover, the metal atom is substantially out of this plane by 0.468 (2) Å in $Zn_2(dtp)_4$ and 0.408 (2) Å in $Cd_2(dtp)_4$. In considering the axial bonds it is noted that the M(1)–S(3) bond is only slightly longer than the three equatorial M–S bonds, whereas the M(1)···S(5) distance is essentially a "zero" bond. For a molecule to possess trigonal-bipyramid symmetry, both sulfur atoms in the axial position must be within the coordination sphere of the metal atom. In the zinc and cadmium diethyldithiocarbamates the axial M···S distance is 2.815 and 2.770 Å, respectively.[25,26] Being less than the upper limit of 3.10 and 3.26 Å, respectively, these values are believed to represent the presence of partial bond character in these cases,[25] as compared to a "zero" bond order for the same atom pair in $Zn_2(dtp)_4$ and $Cd_2(dtp)_4$. Thus, in view of the observed bonding and geometrical considerations in $Zn_2(dtp)_4$ and $Cd_2(dtp)_4$, the present authors favor the distorted tetrahedral description.

These compounds are reported to contain 1 mol of water per metal atom, as determined by the Karl Fischer method.[2,4] The final results of the present crystallographic investigation, based on the final difference $(F_o - F_c)$ Fourier syntheses, indicate that no water of crystallization exists in the crystals. This absence is supported by the complete absence of OH bands in the infrared spectrum of the two complexes (recrystallized from an equal mixture of 95% ethanol and acetone) when run using the Nujol mull technique.

The Phosphorus Coordination.—Owing to the lack of structural data, information on the bond orders of phosphorus–sulfur bonds in metal O,O-dialkylphosphorodithioates was previously obtained primarily from their infrared spectra. These spectra have indicated the presence of both single and double bonds. The P–S double bond stretching frequency for the ionic potassium salt (run as a KBr pellet) has been reported[3b] to occur in the region 675–702 cm^{-1} and for the zinc, cadmium, copper, and nickel derivatives and the free acid (run as liquid samples) in the region 635–668 cm^{-1}. The P–S single bond stretching frequency has been reported[3a,3c] to occur in the region 510–556 cm^{-1}. Samples of $Zn_2(dtp)_4$ and $Cd_2(dtp)_4$, run as KBr pellets, were also found to produce absorption bands in these same regions of the spectrum, thus indicating the presence of both single and double P–S bonds in these complexes as well.

The results of the present investigation indicate, however, that in the solid state all phosphorus–sulfur bonds are equivalent and that although each sulfur atom is shared by two atoms, they do, in fact, exhibit *considerable* double-bond character; further, our results indicate that the phosphorus–oxygen bonds also exhibit partial double-bond character. These conclusions are consistent with the following evidence: (A) The four independent P–S bonds average 1.97 (1) Å in length, compared with the hypothetical lengths of a single (2.14 Å) and a double (1.94 Å) P–S bond.[27d] (B) The four independent P–O bonds average 1.58 (2) Å in length, compared with the hypothetical lengths of a single (1.76 Å) and double (1.44 Å) P–O bond.[29] The following two results are also noteworthy: (C) Within the coordination sphere of each phosphorus atom, the S–P–S angle is larger than the O–P–O angle. (D) The oxygen valency angle, P–O–C, is considerably larger (average 123 (7)°) than a tetrahedral angle. These four results are fully consistent with the bond lengths and angles found in the other known molecular O,O-dialkylphosphorodithioates, $Ni[(C_2H_5O)_2PS_2]_2$,[30] $Ni[(C_2H_5O)_2PS_2]_2 \cdot 2C_2H_5N$,[31] and $Te[(CH_3O)_2PS_2]_2$,[32] and may be interpreted variously in terms of sp^3d hybridization,[33,34] repulsion of valence shell electron pairs,[35] π bonding due to delocalization of lone-pair electrons from one atom (*e.g.*, oxygen or sulfur) into the vacant orbitals of another (*e.g.*, phosphorus),[29,33,35c,36–38] and electronegativity effects on atom hybridization.[39]

Molecular Packing.—The crystals are tabular with the plate surface having Miller indices (001) (parallel with the *ab* plane). The molecules (Figure 2) are aligned in such a way as to form layers or sheets of dimeric molecules with the longest dimension of the dimer approximately normal to these planes. These sheets intersect the unit cell *c* axis at the points $^1/_4$ and $^3/_4$. The sheets and all molecules within the sheets are held together by van der Waals forces. All van der Waals contacts between dimers involve only the center carbon (and associated hydrogen) atoms, terminal methyl groups, and sulfur atoms. There are approximately twice as many C···S contacts involving carbon atoms in the isopropyl groups at P(7) as compared with those at P(6) [in crystals of $Zn_2(dtp)_4$, six *vs.* two such contacts and in $Cd_2(dtp)_4$, seven *vs.* four, at distances ≤ 4.5 Å]. The C···C contacts (≤ 4.5 Å) are about equal in number for each of the four isopropyl groups, averaging about five such contacts per group. Thus, forces between the sheets are probably considerably less than those within the sheets, thereby enabling the sheets to slide over one another and form cleavage planes. This would explain the greasy-like feel of the crystals. The spiral-staircase growth effect parallel to *c* occasionally exhibited by these crystals is also similarly explained.

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The Crystal and Molecular Structure of Hexaaquoaluminum Hexachlororuthenate Tetrahydrate[1]

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An X-ray diffraction study of a single crystal of $Al(H_2O)_6RuCl_6 \cdot 4H_2O$ showed that it is monoclinic with $a = 10.492$ (5) Å, $b = 11.415$ (5) Å, $c = 7.069$ (5) Å, $\beta = 92.69$ (2)°, $Z = 2$, and $D_x = 2.045$ g/cm^3. The space group is $P2_1/n$. The ruthenium and aluminum ions are found to lie at the centers of slightly distorted octahedra of chlorines and water molecules, respectively. The hydrogen bond network connecting the octahedra is discussed. The average Ru–Cl and Al–O distances are found to be 2.375 (5) and 1.880 (4) Å.

Introduction

The aqueous ruthenium species are being studied in this laboratory by Professor R. E. Connick and others, and this research has provided a number of interesting ruthenium salts. We have investigated the structures of several of these compounds to help in the correlation of the optical spectra of the solutions with the environment of the ruthenium ion. Structures involving the aquotetrachloro and aquopentachloro ruthenium species are reported elsewhere.[2] In this paper we

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