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Mercuric Halide Adducts: Synthesis and Structure of $[Co(NH_3)_5Cl]Hg_3Cl_8$ and $[Co(NH_3)_5HPO_4]_2Hg_3Cl_8$

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Abstract

The crystal structures of $[Co(NH_3)_5Cl]Hg_3Cl_8$ (CHLOR) and $[Co(NH_3)_5HPO_4]_2Hg_3Cl_8$ (PHOS) were determined. CHLOR crystallized in *Pnma* with $Z = 4$, $a = 15.412(2)$ Å, $b = 8.140(2)$ Å, c 15.215(1) Å and $d_{calc} = 3.705$ g/cm^3. PHOS crystallized in $P\bar{1}$ with $Z = 2$, $a = 7.040(2)$ Å, $b = 8.995(2)$ Å, $c = 25.647(7)$ Å, $\alpha = 106.02(2)°$, $\beta = 93.34(2)°$, $\gamma = 72.80(2)°$ and $d_{calc} = 3.038$ g/cm^3. Both structures are polymeric, and mercury is in both tetrahedral and octahedral (2 + 4) environments.

Introduction

The structural chemistry of inorganic mercury complexes has proved difficult to describe [1] in detail. Some success has been achieved [2] in the family of mercuric halide adducts, where at least for some of the coordinated groups (the halides) the variation is limited. Even here mercury is found in effective [1, 2] 3, 4, 5 and 6-coordination, with the complexes being discrete, dimeric or polymeric.

A variety of adducts of $HgCl_2$ have structures containing both $HgCl_2$ complexed to the added Lewis base where mercury achieves 4 or 5-coordination, and also linear $HgCl_2$, held in place by intermolecular interactions with four atoms (usually Cl, O or N) that make relatively long equatorial approaches. These equatorial atoms can be either terminal or bridging. This 2 + 4 coordination geometry is also found in pure crystalline $HgCl_2$, although here the equatorial approaches are quite long (3.37–3.48 Å) and mercury has been considered [1, 2] as having digonal coordination.

In the present work we present the synthesis and structure of $[Co(NH_3)_5Cl]Hg_3Cl_8$ (CHLOR) and $[Co(NH_3)_5HPO_4]_2Hg_3Cl_8$ (PHOS) were mercury exists in both tetrahedral and 2 + 4 coordination, the equatorial atoms being Cl or O and the complexes polymeric.

Experimental

Synthesis

To synthesise CHLOR and PHOS we first prepared the respective complexes $[Co(NH_3)_5Cl]Cl_2$ and $[Co(NH_3)_5PO_4]2H_2O$ by routine methods [3, 4]. Equimolar amounts of $HgCl_2$ and each of these complexes were reacted in 20 ml of H_2O and the solutions heated at 80 °C for 20 minutes. Red precipitates were formed in each case and they were left overnight at room temperature. They were then filtered, washed a few times with ice water and dried over $CaCl_2$. In both cases crystals suitable for X-ray work were obtained by slow evaporation of a water solution.

Collection and Reduction of Intensity Data

Complete crystal and intensity collection data are reported in Table I. Preliminary oscillation and Weissenberg photograms indicated the space groups *Pnma* or *Pna*2$_1$ for CHLOR (systematic absences $0kl$, $k + l = 2n + 1$ and hko, $h = 2n + 1$) and a triclinic space group for PHOS. We noticed in CHLOR that reflections hkl, $h + l = 2n + 1$; $k = 2n + 1$ were generally weaker than the rest. We took this as an indication for the centrosymmetric space group *Pnma* with one or two Hg atoms being on the centers of symmetry. Therefore this space group was assumed, and this was confirmed by the least-squares refinement. For PHOS we assumed $P\bar{1}$, and this was also confirmed by the refinement. Unit cell dimensions were derived from least-squares refinements of the setting angles of 15 automatically centered reflections in the range $20° < 2\theta < 24°$ on a SYNTEX P2$_1$ diffractometer. The intensities of three standards monitored after every 67 reflections were

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TABLE I Summary of Crystal and Intensity Collection Data

Compound	$[Co(NH_3)_5Cl](HgCl_2)_2HgCl_4$	$[Co(NH_3)_5HPO_4]_2(HgCl_2)_2HgCl_4$	
fw	1065	1364	
a, Å	15 412(2)	7 040(2)	7 040[a]
b, Å	8 140(2)	8 995(2)	8 995
c, Å	15 215(1)	25 647(7)	24 725
α, deg	90 0	106 02(2)	85 55
β, deg	90 0	93 34(2)	87 30
γ, deg	90 0	72 80(2)	72 80
V, Å^3	1908 8	1490 6	
Z	4	2	
D_{calcd}, g/cm^3	3 705	3 038	
D_{measd}, g/cm^3	3 65	3 00	
space group	*Pnma*	$P\bar{1}$	
cryst dimens mm	0 1 × 0 2 × 0 15	0 3 × 0 2 × 0 15	
radiation	Zr-filtered Mo$K\alpha$ (λ = 0 71069 Å)		
μ, cm^{-1}	260 73	172 82	
scan type	$\theta/2\theta$		
scan speed	variable with 1° 2θ/min for weak relfs		
scan range	0 7 below Ka_1 to 0 7 above Ka_2	0 9 below Ka_1 to 0 9 above Ka_2	
bkgd counting, s	0 4 of scantime	0 6 of scantime	
2θ limit, deg	44 0	46 0	
data collected/unique	5881/1281	4172/3796	
data used	1214 with $I \geqslant 2\ 0\ \sigma(I)$	3737 with $I \geqslant 3\ 0\ \sigma(I)$	
data form	hkl, $\bar{h}kl$, $hk\bar{l}$ and $\bar{h}k\bar{l}$	$\bar{h}kl$, $\bar{h}\bar{k}l$, $\bar{h}k\bar{l}$ and $\bar{h}\bar{k}\bar{l}$	
R/R (all data)	0 0248/0 0333	0 0448/0 0490	
R_w/R_w (all data)	0 0276/0 0432	0 0606/0 0627	

[a] Reduced cell obtained by the transformation matrix $\begin{pmatrix}1 0 0\\ 0 1 0\\ 0 1 1\end{pmatrix}$

stable, with a scatter of less than 3% from their respective means The integrated intensities, I, and the standard deviations $\sigma(I)$ were calculated as before [5] Lorentz, polarization and numerical absorption corrections were applied and the data were reduced using the SHELX 76 program [6]

Solution and Refinement of the Structures

In both cases the positions of the Hg atoms were deduced from a Patterson synthesis Subsequent structure factor-Fourier calculations revealed the positions of all the non-hydrogen atoms Refinement was carried out by blocked (129 by 129) full matrix least-squares refinement in which $\Sigma\omega\Delta^2$ was minimized The weight for each reflection was initially unity and in the final cycles given by $w = (\sigma(F_o) + cF_o^2)^{-1}$, where c = 0 001 for CHLOR and 0.0004 for PHOS were chosen so that the average values of $\omega\Delta^2$ for ranges of increasing F_o were almost constant Isotropic refinement converged to an R $(= \Sigma||F_o| - |F_c||/\Sigma|F_o|)$ of 0 067 for CHLOR and 0 075 for PHOS, and anisotropic refinement to R = 0 028 for CHLOR and 0 056 for PHOS At this point a difference Fourier synthesis revealed the positions of the 8 hydrogen atoms (CHLOR) from within the 13 highest peaks and the 32 hydrogen atoms (PHOS) from within the 43 highest peaks All NH_3 groups, except that of N3 (CHLOR) which occupies a special position, were idealized to a trigonal pyramid with distance N–H = 0 94 Å and were refined as rigid groups with nitrogen atoms at the pivot The final cycles of refinement also contained an empirical isotropic extinction parameter, and converged to the values of R and R_w $(=|\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2|^{1/2})$ reported in Table I

Anomalous dispersion corrections were applied to all non-hydrogen atoms Nine reflections of CHLOR and three of PHOS, severely affected by secondary extinction, were given zero weight The final difference Fourier maps contained several peaks between 0 5 and 1 e/Å^3 but they were all close to Hg sites

Results and Discussion

The final positional parameters appear in Tables II and III* Bond distances and angles are given in Fig 1 for CHLOR and Table IV for PHOS

TABLE II. Positional ($\times 10^4$) Parameters of the Non-Hydrogen Atoms of CHLOR with e s d s in Parentheses

Atom	*x/a*	*y/b*	*z/c*
Hg1	0	0	0
Hg2	84 0(3)	2500	4864 8(3)
Hg3	574 3(3)	2500	2412 3(3)
Co	2069(1)	2500	−1994(1)
Cl11	1316(1)	−16(3)	708(1)
Cl21	−1379(2)	2500	4518(2)
Cl22	1555(2)	2500	5167(2)
Cl31	−673(1)	2500	1466(2)
Cl32	2130(2)	2500	2524(2)
Cl33	349(1)	−62(2)	3476(1)
Cl	726(1)	2500	−1362(2)
N1	1664(3)	794(7)	−2816(4)
N2	2442(3)	784(7)	−1164(4)
N3	3215(5)	2500	−2557

TABLE III Positional ($\times 10^4$) Parameters of the Non-Hydrogen Atoms of PHOS with e s d s in Parentheses

Atom	*x/a*	*y/b*	*z/c*
Hg1	−827(1)	5144(1)	2564 1(2)
Hg2	−5360(1)	3793(1)	3429 3(2)
Hg3	3721(1)	6049(1)	1526 0(2)
Co1	−1276(2)	9086(2)	970(1)
Co2	2058(2)	845(2)	4022(1)
P1	3080(4)	7458(3)	407(1)
P2	5411(4)	2476(3)	4573(1)
Cl11	412(5)	7334(4)	2475(1)
Cl12	1874(5)	2696(4)	2560(1)
Cl13	−2[illegible]56(6)	4034(4)	1734(2)
Cl14	−3[illegible]24(7)	6008(4)	3302(2)
Cl21	1996(5)	5873(3)	3916(1)
Cl22	6991(4)	1440(4)	2946(1)
Cl31	4487(5)	8398(3)	1999(1)
Cl32	2506(4)	3904(3)	1081(1)
N11	−4110(10)	10300(10)	1139(4)
N12	−1970(10)	8110(10)	226(4)
N13	−560(10)	10050(10)	1707(4)
N14	−1650(10)	7240(10)	1176(4)
N15	−790(20)	10860(10)	742(4)
N21	4010(10)	−930(10)	4237(4)
N22	160(10)	2740(10)	3850(4)
N23	3120(10)	−110(10)	3268(3)
N24	1060(10)	1780(10)	4782(4)
N25	60(10)	−320(10)	3859(4)
O11	1490(10)	7826(9)	844(3)
O12	3200(10)	8987(9)	288(3)
O13	5040(10)	6472(9)	576(3)
O14	2400(10)	6350(10)	−132(3)
O21	3990(10)	2044(8)	4120(3)
O22	6410(10)	3605(8)	4431(3)
O23	4120(10)	3375(9)	5104(3)
O24	6890(10)	984(8)	4672(3)

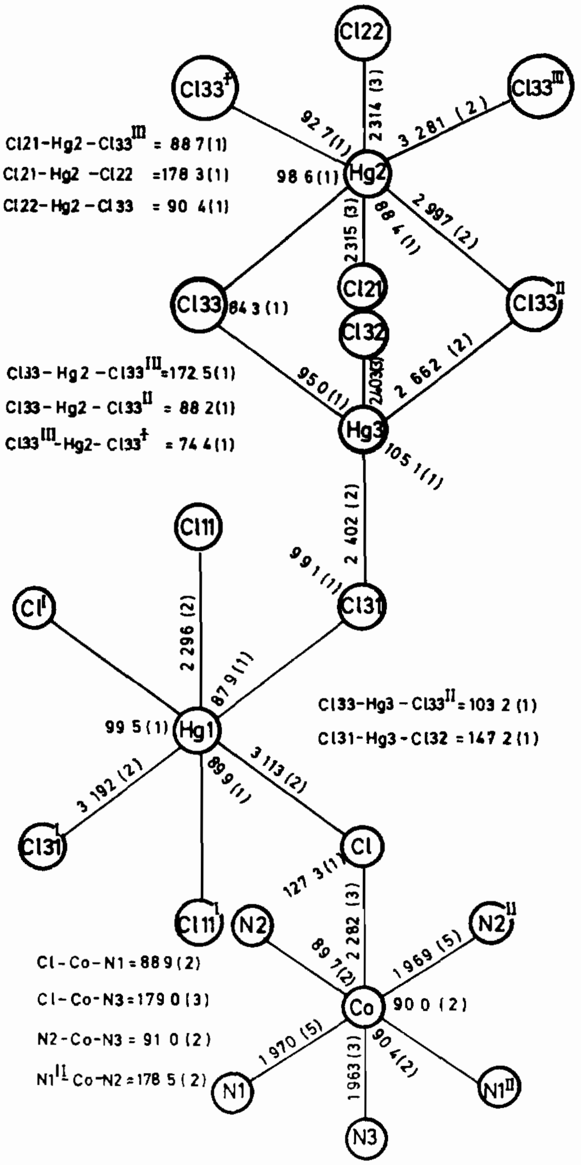

Fig 1 Bond distances and angles for CHLOR (standard deviations in parentheses) Symmetry code (I) $-x, -y, -z$, (II) $x, \frac{1}{2}-y, z$, (III) $-x, \frac{1}{2}+y, 1-z$, (+) $-x, -y, 1-z$

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*Thermal parameters have been deposited with the Editor-in-Chief

TABLE IV Bond Lengths and Angles of PHOS with e s d s in Parentheses [a]

	Distances Å		Angles (°)		Angles (°)
Hg1–Cl11	2 446(4)	Cl11–Hg1–Cl12	112 0(1)	Cl12–Hg1–Cl13	99 4(1)
Hg1–Cl12	2 445(3)	Cl11–Hg1–Cl13	112 9(1)	Cl12–Hg1–Cl14	115 1(1)
Hg1–Cl13	2 541(4)	Cl11–Hg1–Cl14	113 1(1)	Cl13–Hg1–Cl14	103 1(1)
Hg1–Cl14	2 459(5)				
Hg2–Cl12′	3 025(3)	Cl12′–Hg2–Cl14	119 8(1)	Cl4–Hg2–O22′	92 4(2)
Hg2–Cl14	2 869(5)	Cl12′–Hg2–Cl21	91 2(1)	Cl21–Hg2–Cl22	171 0(1)
Hg2–Cl21	2 334(3)	Cl12′–Hg2–Cl22	83 5(1)	Cl21–Hg2–O21′	84 9(2)
Hg2–Cl22	2 339(3)	Cl12′–Hg2–O21′	95 5(1)	Cl21–Hg2–O22′	87 6(2)
Hg2–O21′	2 807(5)	Cl12′–Hg2–O22′	147 8(1)	Cl22–Hg2–O21′	88 4(2)
Hg2–O22′	2 816(5)	Cl14–Hg2–Cl21	92 6(1)	Cl22–Hg2–O22′	93 0(2)
		Cl14–Hg2–Cl22	96 3(1)	O21′–Hg2–O22′	52 4(4)
		Cl14–Hg2–Cl21	144 7(2)		
Hg3–Cl11	3 194(3)	Cl11–Hg3–Cl13″	115 8(1)	Cl13″–Hg3–O13	95 7(1)
Hg3–Cl13″	2 777(3)	Cl11–Hg3–Cl31	81 1(1)	Cl31–Hg3–Cl32	172 2(1)
Hg3–Cl31	2 326(3)	Cl11–Hg3–Cl32	92 7(1)	Cl31–Hg3–O11	87 1(2)
Hg3–Cl32	2 324(4)	Cl11–Hg3–O11	95 9(2)	Cl31–Hg3–O13	87 4(2)
Hg3–O11	2 796(6)	Cl11–Hg3–O13	146 9(2)	Cl32–Hg3–O11	88 9(2)
Hg3–O13	2 814(6)	Cl13″–Hg3–Cl31	93 6(1)	Cl32–Hg3–O13	95 3(2)
		Cl13″–Hg3–Cl32	93 4(1)	O11–Hg3–O13	52 4(2)
		Cl13″–Hg3–O11	148 1(2)		
Co1–O11	1 934(6)	O11–Co1–N11	175 9(4)	N12–Co1–N15	90 8(5)
Co1–N11	1 975(8)	O11–Co1–N12	92 3(3)	N13–Co1–N14	92 0(4)
Co1–N12	1 968(9)	O11–Co1–N13	87 2(3)	N13–Co1–N15	89 1(4)
Co1–N13	1 956(9)	O11–Co1–N14	85 6(4)	N14–Co1–N15	177 1(4)
Co1–N14	1 960(10)	O11–Co1–N15	91 7(4)	Co1–O11–P1	135 7(5)
Co1–N15	1 970(10)	N11–Co1–N12	89 6(4)	O11–P1–O12	111 6(4)
P1–O11	1 531(8)	N11–Co1–N13	80 9(4)	O11–P1–O13	108 9(5)
P1–O12	1 520(10)	N11–Co1–N14	90 8(4)	O11–P1–O14	106 2(5)
P1–O13	1 513(7)	N11–Co1–N15	91 9(4)	O12–P1–O13	113 5(5)
P1–O14	1 607(9)	N12–Co1–N13	179 5(3)	O12–P1–O14	108 4(5)
O14–H1	0 8(1)	N12–Co1–N14	88 2(4)	O13–P1–O14	108 0(4)
				H1–O14–P1	110(10)
Co2–O21	1 936(8)	O21–Co2–N21	90 5(4)	N22–Co2–N25	90 1(4)
Co2–N21	1 956(9)	O21–Co2–N22	86 6(4)	N23–Co2–N24	178 6(4)
Co2–N22	1 968(9)	O21–Co2–N23	85 8(4)	N23–Co2–N25	90 3(4)
Co2–N23	1 978(8)	O21–Co2–N24	93 6(4)	N24–Co2–N25	90 4(4)
Co2–N24	1 977(9)	O21–Co2–N25	174 8(4)	Co2–O21–P2	134 2(5)
Co2–N25	1 960(10)	N21–Co2–N22	175 9(4)	O21–P2–O22	108 7(5)
P2–O21	1 531(7)	N21–Co2–N23	89 4(4)	O21–P2–O23	107 0(4)
P2–O22	1 523(9)	N21–Co2–N24	89 4(4)	O21–P2–O24	111 8(4)
P2–O23	1 562(7)	N21–Co2–N25	93 0(4)	O22–P2–O23	109 6(4)
P2–O24	1 511(7)	N22–Co2–N23	93 4(4)	O22–P2–O24	112 5(4)
O23–H2	0 86(9)	N22–Co2–N24	87 9(4)	O23–P2–O24	107 2(4)
				H2–P2–O23	126(7)

[a] Symmetry code (′) −1 + x, y, z, (″) 1 + x, y, z

Observed and calculated structure amplitudes and positional parameters for hydrogen atoms are available from the author The numbering of the atoms is given in Fig 1 for CHLOR and Fig 2 for PHOS

Hg Coordination

Both structures contain two kinds of mercury atoms In CHLOR we have Hg1 and Hg2 in 2 + 4 coordination and Hg3 is tetrahedral coordination. Hg1 and Hg2 are similar to other adducts of HgCl$_2$

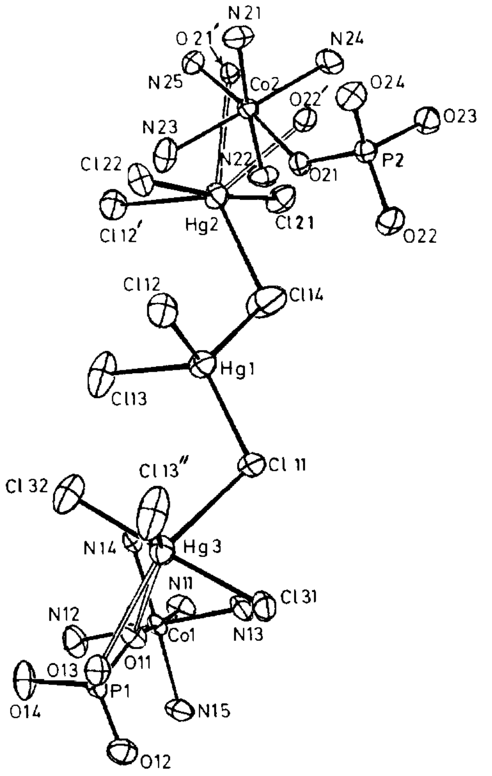

Fig 2 ORTEP plot of PHOS Thermal ellipsoids are at the 50% probability level H atoms not shown Symmetry code (′) –1 + *x*, *y*, *z*, (″) 1 + *x*, *y*, *z*

[2] where Hg is in effective 6-coordination There are two short Hg–Cl axial bonds of 2 296 Å (Hg1) and 2 314 Å (Hg2) and four long equatorial Hg–Cl bonds between 2 997 and 3 281 Å This is very much like the structure of HgCl$_2$ [7] with two short bonds at 2 29 Å, and four long bonds between 3 37 and 3 48 Å In Hg1 and Hg2 the four equatorial chlorine atoms define planes (symmetry dictated) and Hg1 is on the plane and its axial Cl–Hg–Cl angle is 180° (symmetry dictated), while Hg2 is 0 08 Å above the plane with its Cl–Hg–Cl axial angle 178 3° The Cl$_{ax}$–Hg–Cl$_{eq}$ angles range between 87 9° and 92 7° The Hg3 tetrahedron is very distorted (towards a 2 + 4 coordination with two Hg–Cl bonds at 2 403 Å and two at 2 662 Å, and the tetrahedral angles ranging between 95 0° and 147 2° This is because of two longer Hg–Cl approaches at 3 496 Å It is difficult to judge whether these should be considered as bonding interactions, since the value of the Van der Waals radius of mercury is of crucial importance This value has ranged in the literature from as low as 1 50 Å [1, 2] to as high as 1 7–2 0 Å [8] Using the value of 1 73 Å suggested by Canty and Deacon [8] and 1 80 Å for the Van der Waals radius of chlorine [9] we have a sum of 3 53 Å, which indicates that the Hg3····Cl11 approach of 3 496 Å may be a weak interaction

However, the value of 1 8 Å for the Van der Waals radius of chlorine may be too large for the present case A redetermination [7] of the structure of HgCl$_2$ has found a non-bonded Cl···Cl distance of 3 33 Å, so we may have to revise the Van der Waals radius of Cl downwards Values of 1 70–1.77 Å have been suggested before [10] The Hg3–Cl11 approach is a borderline case and the 4 bonds to Hg3, which range between 2 403 and 2 662 Å, strongly indicate a distorted tetrahedral and not a 2 + 4 coordination

In PHOS we again have Hg2 and Hg3 in 2 + 4 coordination and Hg1 in tetrahedral coordination Hg2 and Hg3 each have two short axial Hg–Cl bonds between 2 324 and 2 339 Å and four long equatorial interactions, two Hg–O between 2 796 and 2 814 Å and two Hg–Cl between 2 777 and 3 194 Å The axial Cl–Hg–Cl angle is 171 0° for Hg2 and 172 2° for Hg2 Very similar coordination of Hg has been observed [11] in the uracil and dihydrouracil adducts of HgCl$_2$ The tetrahedron around Hg1 is much less distorted than that of Hg3 in CHLOR, with Hg–Cl bonds between 2 445 and 2 541 Å and angles of 99 4° to 115 1° The next closest approach to Hg1 is by a chlorine atom at 3 888 Å, which clearly constitutes no interaction

Attempts have been made [12–15] to explain the tendency of Hg^{2+} to have linear complexes (2 + 4 coordination) in comparison say to Zn^{2+} and Cd^{2+} If the bonds are ionic [12, 13] crystal-field arguments predict that low promotional energies of nd^{10} → nd^{9} (n + 1)s (9 7 ev, 10 0 ev, 5 3 ev for Zn^{2+}, Cd^{2+}, Hg^{2+}) favor linear complexes If the bonds have appreciable covalent character, hybridization arguments [14, 15] predict that large promotional energies of s^2 → sp (Hg > Cd ≈ Zn) favor again linear complexes It seems likely that both ionic and covalent mechanisms play some part in determining the unusual stereochemistry of Hg^{2+} However, it should be stressed that the balance between the various electronic factors that are involved may be very sensitive to environmental features (crystal packing, hydrogen bonds) which can play a controlling role For example, in both of these structures we find Hg atoms side by side in both 2 + 4 and tetrahedral coordination Also, HgCl$_5^{3-}$ exists as a regular trigonal-bipyramid complex [16] with *two short* axial bonds (2 518 Å) and *three long* equatorial ones when crystallized with Cr(NH$_3$)$_6^{3+}$, but as a distorted trigonal-bipyramid [17] with *two long* axial (2 870 and 3 158 Å) and three short equatorial bonds (2 382 Å to 2 447 Å) when crystallized with Co(NH$_3$)$_6^{3+}$ Differences in the number and strength of the hydrogen bonds are probably sufficient to cause such reversals and both CHLOR and PHOS have extensive Cl···· H–N hydrogen-bond networks

Co and P Coordination

There is nothing unusual about the Co coordination The Co–N, Co–Cl and Co–O bonds fall in the normal ranges [17–19] In the HPO_4 groups we observe a range of P–O bond lengths between 1 511 Å and 1 607 Å We have noted before [20, 21] that H^+ is a better sink for electrons than coordinated metals In the present case we see again that H^+ is more effective than either Co or Hg in effecting structural changes in the PO_4 group The shortest P–O distances (1 511–1.523 Å) are to oxygen atoms which are either not involved in any other interaction (O12, O24), or only to weak 'equatorial' Hg···O interactions (O13, O22) The next longer P–O bond (1 531 Å) is to the oxygen coordinated to the $Co(NH_3)_5^{3+}$ group (O11, O21) and the longest by far P–O distances (1 562 and 1 607 Å) are to oxygens that are bonded to the H^+ (O14, O23) We note a similar behavior in the structures [19] of $[CoHP_2O_7(NH_3)_4]2H_2O$, $[CoH_2P_3O_{10}(NH_3)_4]H_2O$ and $[CoHP_2O_7(NH_3)_5]H_2O$ In the first two structures in which the pyrophosphate and tripolyphosphate hydrogens had been located they reside on the oxygens with the longest P–O terminal bonds (1 548 to 1 565 Å) In the latter structure the pyrophosphate hydrogen was not located but we can safely predict that it resides on O11, since P1–O11 is by far the longest (1 541 Å) P–O terminal bond of that structure

The Molecular Packing

Both structures are polymeric The structure of CHLOR, Fig 3, is made of Hg1 octahedra sharing ***trans*** edges forming long stacks along *b* The Hg2 octahedra form similar stacks along *b* These two kinds of stacks are joined by the Hg3 tetrahedra to form extended sheets in the *bc* plane at $x \approx 0$ and $x \approx ½$ These sheets are held in place by hydrogen bonds The structure of PHOS, Fig 4, is made up of eight-member rings (boat conformation) in which Cl and Hg atoms alternate and which contain four Cl atoms Hg2, Hg3 and two Hg1 atoms at positions diametrically across These eight-member rings are joined at the Hg1 (tetrahedral) corners to form stacks along the *a* axis These stacks are held together by hydrogen bonds There is an extended Cl···H–N hydrogen bond network in both structures All chlorine atoms, with the exception of Cl31 and ClCo in CHLOR, are involved in at least one, and several of them in two, hydrogen bonds in which the Cl···N approach is less than 3 4 Å There exist as well several N–H···O hydrogen bonds in PHOS with N···O approaches between 2 633 and 3 0 Å, and the phosphate hydrogens are involved in two strong O–H···O hydrogen bonds, O14–HO14····O13′ and O23–HO23···O22′ (the primes mean symmetry transformed) where the O···O approaches are 2 633 and 2 570 Å and the angles 170° and 156° respectively

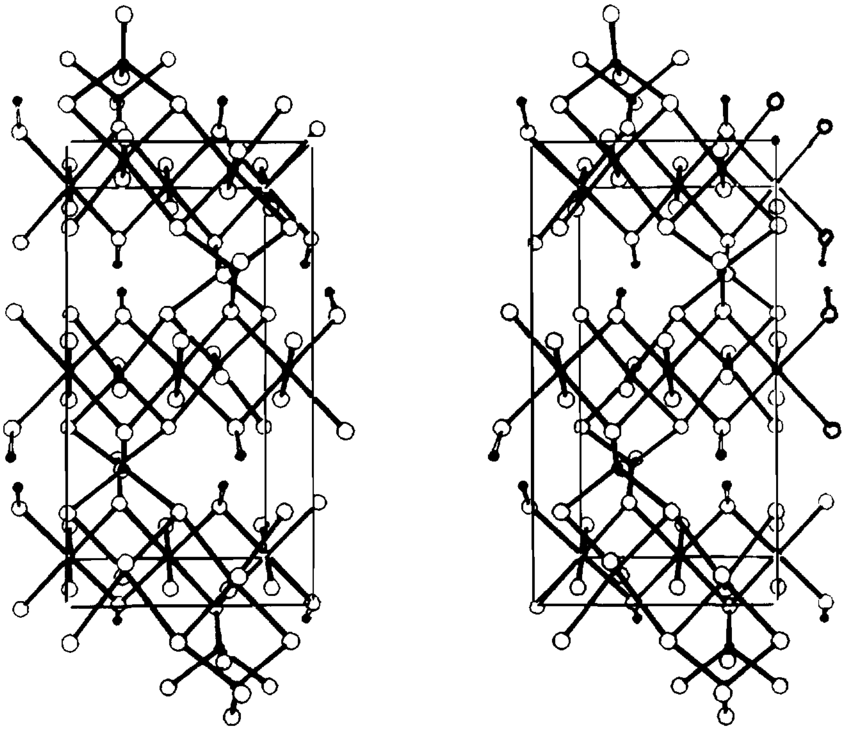

Fig 3 Stereoscopic view of the molecular packing of CHLOR NH_3 groups not shown for clarity ● = Hg, ⊕ = Co, ○ = Cl

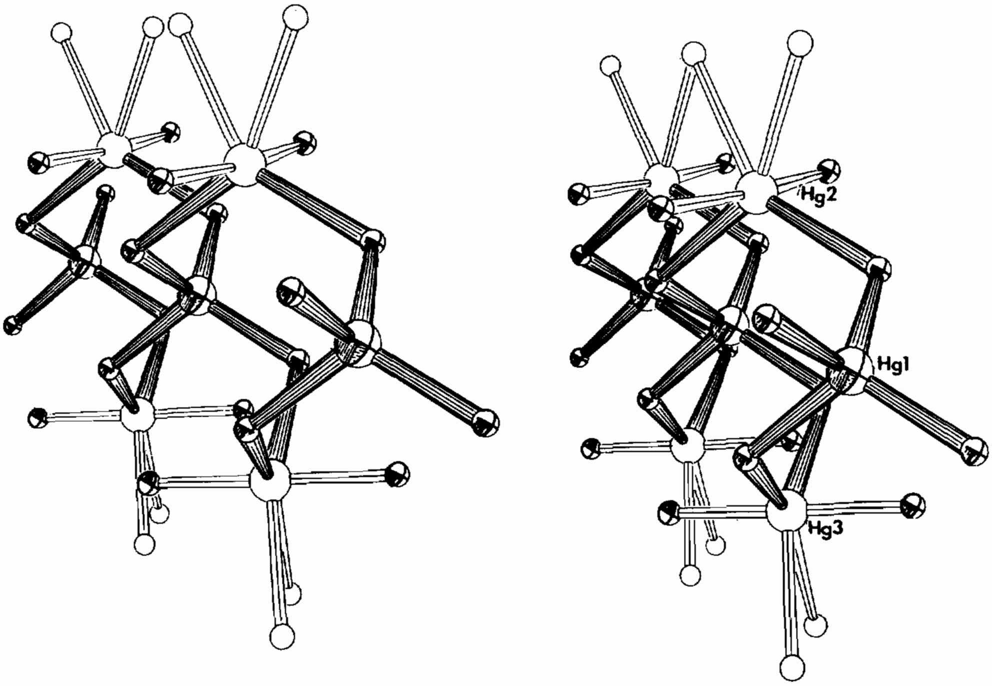

Fig. 4. Stereoscopic view of the eight-member rings in PHOS. ○ = O; ⊕ = Cl; ◯ = Hg (octahedral); ⊕ = Hg (tetrahedral).

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