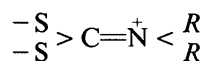


Discussion. There is a crystallographic centre of symmetry in the molecule. The two V atoms are bridged by two (μ - η^2 -S₂) groups. The other coordination sites of each V atom are occupied by two bidentate dithiocarbamate ligands. The arrangement of the ligands is simply described as two distorted hexahedra that share a parallelogram and each has its other five faces strongly twisted. The bond distance of 2.884 (4) Å for V—V, which indicates a direct metal–metal interaction, is consistent with those of diamagnetic complexes (Duraj, Andras & Kibala, 1990; Halbert, Hutchings, Rhodes & Stiefel, 1986), and is much longer than the distance of 2.4 Å postulated for a d^2 — d^2 double bond (Dorfman & Holm, 1983). The average V—S_b (bridge) distance (2.409 Å) is obviously shorter than the average value (2.503 Å) for V—S_t (terminal). The S(1)—S(2) distance of 1.984 (5) Å is not significantly different from those in other similar compounds (Bolinger & Rauchfuss, 1982; Bolinger, Rauchfuss & Rheingold, 1983; Bolinger, Weatherill, Rauchfuss, Rheingold, Day & Wilson, 1986).

Atoms S(n 1), S(n 2), C(n), N(n), C(n 1) and C(n 3) ($n = 1, 2$) are coplanar, which indicates that the dtc ligand coordinates to a V atom in the



form. Although molecular vanadium dimers with S₂ bridges are known, those with a V₂(μ - η^2 -S₂)₂ core that have been hitherto structurally characterized are

found in the mineral patronite (VS₄)_n, V₂(μ - η^2 -S₂)₂(Bu₂NCS₂)₄ (Halbert, Hutchings, Rhodes & Stiefel, 1986) and V₂(μ - η^2 -S₂)₂(S₂CCH₃)₄ (Duraj, Andras & Kibala, 1990).

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References

- BOLINGER, C. M. & RAUCHFUSS, T. B. (1982). *Organometallics*, **1**, 1551–1553.
- BOLINGER, C. M., RAUCHFUSS, T. B. & RHEINGOLD, A. L. (1983). *J. Am. Chem. Soc.* **105**, 6321–6323.
- BOLINGER, C. M., WEATHERILL, J. D., RAUCHFUSS, J. B., RHEINGOLD, A. L., DAY, C. S. & WILSON, S. R. (1986). *Inorg. Chem.* **25**, 634–643.
- CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, Table 2.2B. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- DORFMAN, J. R. & HOLM, R. H. (1983). *Inorg. Chem.* **22**, 3179–3181.
- DURAJ, S. A., ANDRAS, M. T. & KIBALA, P. A. (1990). *Inorg. Chem.* **29**, 1232–1234.
- FRENZ, B. A. (1978). *The Enraf–Nonius CAD-4 SDP – A Real-Time System for Concurrent X-ray Data Collection and Crystal Structure Solution*. In *Computing in Crystallography*, edited by H. SCHENK, R. OLTJOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI. Delft Univ. Press.
- HALBERT, T. R., HUTCHINGS, L. L., RHODES, R. & STIEFEL, E. I. (1986). *J. Am. Chem. Soc.* **108**, 6437–6438.
- KILLEAN, R. C. G. & LAWRENCE, J. L. (1969). *Acta Cryst.* **B25**, 1750–1752.
- WALKER, N. & STUART, D. (1983). *Acta Cryst.* **A39**, 158–166.

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Structure of Benzyltriphenylphosphonium Imidazolebis(*o*-mercaptophenolato)-manganese(III) Acetonitrile Solvate

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Abstract. C₂₅H₂₂P⁺·[Mn(C₆H₄OS)₂(C₃H₄N₂)]⁻·C₂H₃N, $M_r = 765.82$, monoclinic, $P2_1/n$, $a = 16.221$ (4), $b = 9.705$ (2), $c = 24.457$ (5) Å, $\beta = 94.96$ (1)°, $V = 3835$ Å³, $Z = 4$, $D_x = 1.33$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 5.1$ cm⁻¹, $F(000) = 1592$, $T = 296$ K, final $R = 0.054$ and $wR = 0.064$ for 2570 observed reflections with $F > 3\sigma(F)$. The Mn^{III} ion is in a distorted square-pyramidal S₂O₂N coordination environment.

Introduction. On the basis of chemical and spectroscopic evidence, the acid phosphatase from sweet potato appears to contain a mononuclear manganese(III) site with thiolate (cystein), phenolate (tyrosine) (Sugiura, Kawabe, Tanaka, Fujimoto & Ohara, 1981) and imidazole (histidine) (Fujimoto, Murakami & Ohara, 1981) ligands. These discoveries have stimulated research into manganese chemistry, especially in Mn^{III}–thiolate chemistry (Bashkin, Huffman & Christou, 1986; Christou & Huffman, 1983; Costa, Dorfman, Hagen & Holm, 1983; Seela,

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Huffman & Christou, 1985; Gohdes & Armstrong, 1988; Greiwe, Krebs & Henkel, 1989). Complexes with Mn—O or Mn—N ligations have been studied extensively (Wieghardt, 1989; Christou, 1989), while those with Mn—S bonds are less common and those with mixed O,S,N ligations are scarcely reported. To our knowledge, only two complexes of the latter type are reported in the literature (Bashkin, Huffman & Christou, 1986; Gohdes & Armstrong, 1988). In our studies (Kang, Weng, Liu, Wu, Huang, Lu, Cai, Chen & Lu, 1990) on transition metal complexes with *o*-mercaptophenol (H₂mp), a multifunctional bidentate ligand with mixed S,O donors, it was observed that different coordination modes are possible for ligation with transition metals. Imidazole (Him) is a ligand of potential interest in Mn-containing biological systems (Fujimoto, Murakami & Ohara, 1981; Stalling, Patridge, Strong & Ludwig, 1985). We applied the two interesting ligands to the synthesis of the title complex.

Experimental. Crystals of (Ph₃PCH₂Ph)[Mn(mp)₂(Him)].CH₃CN were obtained from the reaction of Mn(CH₃CO₂)₂·4H₂O, H₂mp, Him and NaOCH₃ in 1:2:2:6 molar ratio in CH₃OH by controlled aerial oxidation at room temperature. Single crystals suitable for X-ray diffraction were obtained by recrystallization from CH₃CN solution. Red plate single crystal with dimensions 0.3 × 0.2 × 0.08 mm was mounted on a Rigaku MSC/AFC5R diffractometer with graphite-monochromated Mo K α radiation. 18 reflections whose 2 θ values ranged from 18–27° were used in the least-squares refinement of the orientation matrix and the lattice parameters of the crystal. 5309 reflections were collected in ω -2 θ scan mode, ω scan width (0.8 + 0.35tan θ)°, 2 θ _{max} = 48.2° (0 < *h* < 20, 0 < *k* < 12, -30 < *l* < 30), of which 2570 were observed with *F* > 3 σ (*F*). Three standard reflections with no significant variation in intensity. The systematic absences (*h*0*l*, *h* + *l* = 2*n*; 0*k*0, *k* = 2*n*) indicated the space group to be *P*2₁/*n* exclusively. Anisotropic decay correction was applied with max. and min. correction factors 0.940 and 1.224, respectively. Lp and empirical absorption corrections were made. Max. and min. transmission factors were 1.290 and 0.861, respectively (*DIFABS*; Walker & Stuart, 1983).

The structure was solved by direct methods and refined by full-matrix least-squares refinement on (*F*) of 460 parameters for all non-H atoms, with anisotropic temperature factors. H atoms were added to the structure factor calculations but not refined. Scattering factors and *f*' and *f*'' values were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Final *R* = 0.054, *wR* = 0.064 for 2570 observed reflections, *w* = 1/[$\sigma^2(F_o) + (0.01F_o)^2 + 1.0$], (Δ/σ)_{max} = 0.14, ($\Delta\rho$)_{max} = 0.38, ($\Delta\rho$)_{min} =

-0.34 e Å⁻³. All calculations were carried out on a VAX 11/785 computer with *SDP* (Frenz, 1978).

Discussion. Table 1* contains the atomic positional and thermal parameters. Table 2 gives selected bond distances and bond angles. The unit cell of the title complex consists of well separated cations, anions and acetonitrile solvate with no close contact, in which the structures of cation and solvate are unexceptional. Fig. 1 shows an *ORTEP* (Johnson, 1976) view of the anion which features a distorted square-pyramidal coordination with the imidazole nitrogen N(1) at the apex and the two *cis*-thiolato atoms S(1), S(2) and the two *cis*-phenolato atoms O(1), O(2) from two mp²⁻ in the base plane. Yet, the four basal atoms do not exhibit planarity, with largest deviations of 0.2 Å from the least-squares plane. The Mn atom is nearly in the plane of the imidazole ring which is exactly planar as expected. Only small deviations (± 0.008 , ± 0.074 Å, respectively) are found for the atoms in the two five-membered chelate rings Mn—S(1)—O(1)—C(11)—C(16) (plane 1) and Mn—S(2)—O(2)—C(21)—C(26) (plane 2); the dihedral angle is 153.3°. The imidazole ring tilts markedly to one side of the anion to make dihedral angles of 106.4° with plane 1 and 82.83° with plane 2. The anion has no symmetry. The angle N(1)—Mn—S(*n*) or N(1)—Mn—O(*n*) (*n* = 1,2) can be divided into two sets: that which contains N(1)—Mn—O(1) [91.4 (3)°] and N(1)—Mn—S(2) [97.6 (3)°] and that which contains N(1)—Mn—O(2) [103.6 (2)°] and N(1)—Mn—S(1) [105.4 (2)°]. The two chelate angles (av. 87.0°) and the bite distances (av. 2.90 Å) fall in the range of the other complexes with mp²⁻ ligation (Kang *et al.*, 1990). Compared to other five-coordinate manganese(III) complexes, the bond distances in the title complex can be summarized as follows: (1) The average Mn—S bond length (2.28 Å) is comparable to that in [Mn(tdt)₂MeOH]⁻ (av. 2.282 Å; H₂tdt = toluene-3,4-dithiol; Greiwe, Krebs & Henkel, 1989) and [Mn(thiosal)₂(Him)]⁻ (av. 2.282 Å; H₂thiosal = thio-salicylic acid; Bashkin, Huffman & Christou, 1986), but shorter than those in [Mn(edt)₂(Him)]²⁻ (2.134–2.334 Å; H₂edt = ethanedithiol; Seela, Foltling, Wong, Huffman, Christou, Chang & Hendrickson, 1985) and [Mn₂(edt)₄]²⁻ (terminal Mn—S av. 2.32 Å; Costa, Dorfman, Hagen & Holm, 1983). (2) The Mn—O distances (av. 1.905 Å) are longer than those in [Mn(salen)(S—C₆H₄-*p*-NO₂)] [av. 1.88 Å; salen

* Lists of structure factors, anisotropic thermal parameters, bond distances and angles, least-squares planes and deviations, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54188 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Atomic coordinates and equivalent isotropic thermal parameters for $(\text{Ph}_3\text{PCH}_2\text{Ph})[\text{Mn}(\text{mp})_2(\text{Him})] \cdot \text{CH}_3\text{CN}$

$$B_{\text{eq}} = (4/3)[a^2 B(1,1) + b^2 B(2,2) + c^2 B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$$

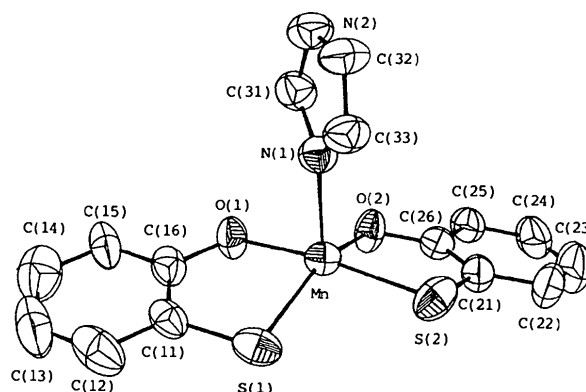
	x	y	z	$B_{\text{eq}} (\text{\AA}^2)$
Mn	0.67546 (9)	0.1856 (2)	0.85523 (5)	3.34 (3)
S(1)	0.7235 (2)	0.1639 (3)	0.9457 (1)	4.57 (6)
S(2)	0.5410 (2)	0.1882 (3)	0.8761 (1)	5.24 (7)
O(1)	0.7875 (3)	0.2137 (7)	0.8404 (2)	3.9 (2)
O(2)	0.6408 (3)	0.2970 (7)	0.7932 (2)	4.1 (1)
N(1)	0.6763 (5)	-0.0202 (8)	0.8220 (3)	3.8 (2)
C(11)	0.8282 (6)	0.1638 (9)	0.9334 (4)	4.0 (2)
C(12)	0.8936 (8)	0.143 (1)	0.9738 (4)	6.7 (3)
C(13)	0.9755 (7)	0.150 (1)	0.9610 (5)	7.7 (4)
C(14)	0.9932 (7)	0.174 (1)	0.9082 (5)	7.2 (3)
C(15)	0.9298 (6)	0.195 (1)	0.8685 (4)	4.9 (3)
C(16)	0.8481 (6)	0.191 (1)	0.8800 (4)	4.0 (2)
C(21)	0.5050 (6)	0.292 (1)	0.8201 (4)	4.0 (2)
C(22)	0.4217 (6)	0.333 (1)	0.8105 (4)	5.8 (3)
C(23)	0.3973 (7)	0.416 (1)	0.7666 (5)	7.6 (4)
C(24)	0.4523 (7)	0.456 (1)	0.7318 (4)	6.2 (3)
C(25)	0.5347 (6)	0.417 (1)	0.7399 (4)	4.5 (3)
C(26)	0.5616 (6)	0.336 (1)	0.7846 (3)	3.7 (2)
C(31)	0.7097 (6)	-0.057 (1)	0.7770 (4)	4.2 (2)
N(2)	0.6885 (5)	-0.1853 (9)	0.7621 (3)	4.4 (2)
C(32)	0.6398 (6)	-0.235 (1)	0.7990 (4)	4.9 (3)
C(33)	0.6338 (6)	-0.135 (1)	0.8358 (4)	4.7 (3)
P	0.7483 (2)	0.5995 (3)	0.0188 (1)	3.55 (6)
C(41)	0.7448 (5)	0.747 (1)	0.0625 (3)	3.5 (2)
C(42)	0.7717 (6)	0.738 (1)	0.1174 (4)	4.5 (3)
C(43)	0.7661 (6)	0.845 (1)	0.1519 (4)	4.8 (3)
C(44)	0.7316 (7)	0.968 (1)	0.1325 (4)	5.5 (3)
C(45)	0.7062 (7)	0.981 (1)	0.0781 (4)	5.6 (3)
C(46)	0.7099 (6)	0.869 (1)	0.0427 (4)	4.5 (3)
C(51)	0.7863 (5)	0.6415 (9)	-0.0461 (3)	3.0 (2)
C(52)	0.7870 (6)	0.5368 (9)	-0.0843 (4)	4.2 (2)
C(53)	0.8151 (7)	0.563 (1)	-0.1351 (4)	5.0 (3)
C(54)	0.8424 (6)	0.692 (1)	-0.1476 (3)	4.5 (2)
C(55)	0.8446 (6)	0.795 (1)	-0.1091 (4)	4.1 (2)
C(56)	0.8163 (5)	0.7720 (9)	-0.0580 (4)	3.5 (2)
C(61)	0.8180 (6)	0.4783 (9)	0.0538 (4)	3.8 (2)
C(62)	0.7912 (7)	0.383 (1)	0.0887 (5)	6.9 (3)
C(63)	0.8470 (8)	0.296 (1)	0.1184 (5)	7.7 (4)
C(64)	0.9284 (8)	0.310 (1)	0.1129 (5)	7.6 (3)
C(65)	0.9574 (7)	0.405 (1)	0.0791 (4)	7.0 (3)
C(66)	0.9019 (6)	0.490 (1)	0.0490 (4)	5.3 (3)
C(71)	0.6480 (6)	0.516 (1)	0.0072 (4)	4.3 (2)
C(72)	0.5829 (5)	0.600 (1)	-0.0270 (4)	3.5 (2)
C(73)	0.5628 (6)	0.564 (1)	-0.0815 (4)	4.1 (2)
C(74)	0.5013 (6)	0.634 (1)	-0.1126 (4)	4.6 (3)
C(75)	0.4612 (6)	0.739 (1)	-0.0909 (4)	5.1 (3)
C(76)	0.4797 (6)	0.777 (1)	-0.0367 (4)	6.2 (3)
C(77)	0.5406 (6)	0.704 (1)	-0.0050 (4)	5.0 (3)
C(81)	0.9017 (9)	0.585 (2)	0.2492 (6)	12.7 (5)
C(82)	0.973 (1)	0.513 (2)	0.2397 (6)	12.8 (5)
N(3)	0.847 (1)	0.638 (2)	0.2568 (6)	21.0 (6)

= N,N' -ethylenebis(salicylideneaminato); Gohdes & Armstrong, 1988], but shorter than those in $[\text{Mn}(\text{thiosal})_2(\text{Him})]^-$; (av. 1.94 Å; Bashkin, Huffman & Christou, 1986). (3) The Mn—N length of 2.157 Å is shorter than any other ones reported for five-coordinate complexes with Mn^{III} —imidazole ligation such as that in $[\text{Mn}(\text{thiosal})_2(\text{Him})]^-$ (2.176 Å), $[\text{Mn}_2(\text{edt})_4(\text{im})]^{2-}$ (2.197 Å) and $[\text{Mn}(\text{edt})_2(\text{Him})]^-$ (2.224 Å). These results compare favourably with each other and the nature of the ligands around Mn^{III} plays an important role in these differences.

The financial support of NNSF, NSFCAS and FNSF is greatly appreciated.

Table 2. Selected bond distances (Å) and bond angles (°)

Mn—S(1)	2.290 (2)	O(1)—C(16)	1.337 (9)
Mn—S(2)	2.284 (3)	O(2)—C(26)	1.338 (9)
Mn—O(1)	1.903 (6)	N(1)—C(31)	1.32 (1)
Mn—O(2)	1.908 (5)	N(1)—C(33)	1.38 (1)
Mn—N(1)	2.157 (7)	C(11)—C(16)	1.40 (2)
S(1)—C(11)	1.751 (9)	C(21)—C(26)	1.38 (2)
S(2)—C(21)	1.761 (8)		
S(1)—Mn—S(2)	92.2 (1)	Mn—S(1)—C(11)	95.1 (3)
S(1)—Mn—O(1)	87.0 (2)	Mn—S(2)—C(21)	95.2 (4)
S(1)—Mn—O(2)	150.8 (2)	Mn—O(1)—C(16)	119.6 (5)
S(1)—Mn—N(1)	105.4 (2)	Mn—O(2)—C(26)	119.7 (5)
S(2)—Mn—O(1)	171.0 (3)	Mn—N(1)—C(31)	125.9 (6)
S(2)—Mn—O(2)	87.1 (2)	Mn—N(1)—C(33)	129.9 (6)
S(2)—Mn—N(1)	97.6 (3)	S(1)—C(11)—C(16)	117.8 (7)
O(1)—Mn—O(2)	89.3 (2)	O(1)—C(16)—C(11)	117.8 (8)
O(1)—Mn—N(1)	91.4 (3)	S(2)—C(21)—C(26)	118.1 (8)
O(2)—Mn—N(1)	103.6 (2)	O(2)—C(26)—C(21)	119.9 (9)

Fig. 1. ORTEP (Johnson, 1976) view of $[\text{Mn}(\text{mp})_2(\text{Him})]^-$.

References

- BASHKIN, J. S., HUFFMAN, J. C. & CHRISTOU, G. (1986). *J. Am. Chem. Soc.* **108**, 5038–5039.
- CHRISTOU, G. (1989). *Acc. Chem. Res.* **22**, 328–335.
- CHRISTOU, G. & HUFFMAN, J. C. (1983). *J. Chem. Soc. Chem. Commun.* pp. 558–560.
- COSTA, T., DORFMAN, J. R., HAGEN, K. S. & HOLM, R. H. (1983). *Inorg. Chem.* **22**, 4091–4099.
- FRENZ, B. A. (1978). *The Enraf-Nonius CAD-4 SDP – A Real-Time System for Concurrent X-ray Data Collection and Crystal Structure Solution*. In *Computing in Crystallography*, edited by H. SCHENK, R. OLTJOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, pp. 64–71. Delft Univ. Press.
- FUJIMOTO, S., MURAKAMI, K. & OHARA, A. (1981). *J. Biochem.* **97**, 1777–1784.
- GOHDES, J. W. & ARMSTRONG, W. H. (1988). *Inorg. Chem.* **27**, 1841–1842.
- GREIWE, K., KREBS, B. & HENKEL, G. (1989). *Inorg. Chem.* **28**, 3713–3720.
- JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- KANG, B. S., WENG, L. H., LIU, H. Q., WU, D. X., HUANG, L. R., LU, C. Z., CAI, J. H., CHEN, X. T. & LU, J. X. (1990). *Inorg. Chem.* **29**, 4873–4877.
- SEELA, J. L., FOLTING, K., WONG, R., HUFFMAN, J. C., CHRISTOU, G., CHANG, H. & HENDRICKSON, D. N. (1985). *Inorg. Chem.* **24**, 4456–4458.
- SEELA, J. L., HUFFMAN, J. C. & CHRISTOU, G. (1985). *J. Chem. Soc. Chem. Commun.* pp. 58–60.

STALLING, W. C., PATTRIDGE, K. A., STRONG, R. K. & LUDWIG, M. L. (1985). *J. Biol. Chem.* **260**, 16424–16432.
 SUGIURA, Y., KAWABE, H., TANAKA, H., FUJIMOTO, S. & OHARA, A. (1981). *J. Biol. Chem.* **256**, 10664–10670.

WALKER, N. & STUART, D. (1983). *Acta Cryst.* **A39**, 158–166.
 WIEGHARDT, K. (1989). *Angew. Chem. Int. Ed. Engl.* **28**, 1153–1172.

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(2-Aminophenyl)diphenylphosphinedichloroplatinum(II) Acetone Solvate, $[PtCl_2(Ph_2PC_6H_4NH_2)] \cdot C_3H_6O$

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Abstract. $C_{18}H_{16}Cl_2NPt \cdot C_3H_6O$, $M_r = 601.4$, triclinic, $P\bar{1}$, $a = 9.381(1)$, $b = 14.352(1)$, $c = 8.944(2)$ Å, $\alpha = 107.37(1)$, $\beta = 103.83(1)$, $\gamma = 78.71(1)^\circ$, $V = 1106(2)$ Å³, $Z = 2$, $D_x = 1.806$ g cm⁻³, $\lambda(Mo K\alpha) = 0.7107$ Å, $\mu = 66.90$ cm⁻¹, $F(000) = 580$, $T = 293(1)$ K, $R = 0.026$ for 3457 observed reflections. The square planar Pt atom is coordinated by two Cl atoms [Pt—Cl 2.369(1), 2.300(1) Å] and the P and N atoms derived from a chelating (2-aminophenyl)diphenylphosphine ligand [Pt—P 2.188(1), Pt—N(1) 2.048(4) Å and P(1)—Pt—N(1) 86.3(1)°]. Centrosymmetric molecules associate *via* N—H...Cl contacts and the acetone molecule of solvation hydrogen bonds to the second amine proton.

Introduction. The hybrid ligand (2-aminophenyl)diphenylphosphine, $Ph_2PC_6H_4NH_2$, displays facile and reversible deprotonation at the aromatic amino group upon coordination to transition metals (Ansell, McPartlin, Tasker, Cooper & Duckworth, 1983; Cooper, Downes, Goodwin, McPartlin & Rosalky, 1983). Bis-chelating complexes of this ligand with Ni^{II}, Pt^{II} and Rh^I have been used to study geometric isomerism (Cooper & Downes, 1981) and metal-templated catalyzed synthesis of the multidentate P,N-ligand, *N,N'*-bis[2-(diphenylphosphino)phenyl]propane-1,3-diamine (Cooper, Duckworth, Hambley, Organ, Henrick, McPartlin & Parekh, 1989). Serendipitous crystallization of the precursor complex $[PtCl_2(Ph_2PC_6H_4NH_2)]$ from acetone gave a novel hydrogen-bonded acetone solvate, the structure of which is reported herein.

Experimental. $[PtCl_2(Ph_2PC_6H_4NH_2)]$ was prepared as in the literature (Downes, 1978) and crystals for the X-ray study were obtained as a mono acetone solvate from an acetone solution of the compound; m.p. 339–343 K (dec.). Enraf–Nonius CAD-4F diffractometer controlled by a PDP8/A computer, graphite-monochromated Mo $K\alpha$ radiation; ω - 2θ scan technique. Cell parameters by least squares on 25 reflections ($2 \leq \theta \leq 11^\circ$) (de Boer & Duisenberg, 1984) on a $0.12 \times 0.12 \times 0.50$ mm crystal. Analytical absorption correction applied; max. and min. transmission factors 0.517 and 0.410 (*SHELX76*; Sheldrick, 1976). 4364 reflections ($1.5 \leq \theta \leq 25.0^\circ$) measured in the range $-11 \leq h \leq 11$, $-17 \leq k \leq 17$, $-10 \leq l \leq 1$. No significant variation in the net intensity of three reference reflections (221, 222, 433) measured every 7200 s. 3894 unique reflections ($R_{merge} 0.011$) and 3457 satisfied $I \geq 2.5\sigma(I)$. Structure solved by Patterson method, full-matrix least-squares refinement on 245 parameters based on F (*SHELX76*; Sheldrick, 1976). Anisotropic thermal parameters for non-H atoms and H atoms included at their calculated positions and assigned a common isotropic thermal parameter. At convergence $R = 0.026$, $wR = 0.027$, $w = [\sigma^2(F) + 0.0018|F|^2]^{-1}$, $S = 0.79$, $(\Delta/\sigma)_{max} \leq 0.001$, $\Delta\rho_{max} = +2.01$, $\Delta\rho_{min} = -1.70$ e Å⁻³; no extinction correction applied. Scattering factors for neutral Pt corrected for f' and f'' from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 99, 149) and for the remaining atoms as incorporated in *SHELX76* (Sheldrick, 1976). All calculations on SUN4/280 computer system. Atomic parameters are given in Table 1,