In Tabelle 1 sind die Atomparameter,* in Tabelle 2 die Bindungsabstände und -winkel zusammengestellt. Fig. 1 zeigt die Struktur in stereoskopischer Darstellung.

Verwandte Literatur. Das $[Re_2Cl_8]^{2-}$-Ion ist mit mehreren Kationen bekannt: Überblick (Cotton & Walton, 1982), $K_2[Re_2Cl_8].2H_2O$ (Cotton & Harris, 1965), $(NH_4)_2[Re_2Cl_8].2H_2O$ (Koz'min, Surazhskaya & Larina, 1979), $(C_5H_5NH)_2[Re_2Cl_8]$ (Bratton & Cotton, 1969), $(Bu_4N)_2[Re_2Cl_8]$ (Cotton, Frenz, Stults & Webb, 1976), $[(DMF)_2H]_2[Re_2Cl_8]$, $[(CH_3)_2NH_2]_2[Re_2Cl_8]$ (Koz'min, Kotel'nikova, Surazhskaya, Larina, Bagirov & Misailova, 1978).

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* Die Liste der anisotropen Temperaturfaktoren und der beobachteten und berechneten Strukturfaktoren sind bei der British Library Document Supply Centre (Supplementary Publication No. SUP 44268: 21 pp.) hinterlegt. Kopien sind erhältlich durch: The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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trans-Bis[dicyclohexylphosphino-*N*-phenyl(thioformamido)]platinum(II): $Pt[(c\text{-}C_6H_{11})_2PC(S){=}N(C_6H_5)]_2$

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Abstract. $[Pt(C_{19}H_{27}NPS)_2]$, M_r = 860·0, monoclinic, $P2_1/c$, a = 12·307 (2), b = 8·456 (2), c = 18·673 (4) Å, β = 104·26 (2)°, U = 1883 (2) Å^3, D_m (by flotation) = 1·50 (1), D_x = 1·517 Mg m^{-3} for $Z = 2$, Mo $K\bar{\alpha}$ radiation, λ = 0·7107 Å, μ = 3·948 mm^{-1}, $F(000)$ = 872, T = 295 (2) K, R = 0·024 for 3164 reflections with $I \geq 2{\cdot}5\sigma(I)$. The anion coordinates *via* the P and S atoms [Pt—P(1) 2·282 (1), Pt—S(1) 2·322 (1) Å and P(1)—Pt—S(1) 74·7 (1)°]; the Pt atom is situated at a centre of inversion (at 0,0,0) so that the *trans*-PtP_2S_2 group is constrained to planarity. The four-membered chelate ring is not planar, however, with the dihedral angle for PtP(1)S(1)/P(1)S(1)C(1) being 7·4°; further, the Pt atom lies 0·3316 (1) Å above the least-squares plane through the P(1), S(1), C(1) and N(1) atoms.

Experimental. The title compound was synthesized by adding excess $N(C_2H_5)_3$ to a stirred dichloromethane solution of $Cl_2Pt[(C_6H_5)CN]_2$ (Hartley, 1973) and $(c\text{-}C_6H_{11})_2PC(S)N(H)(C_6H_5)$ (Kunze & Antoniadis, 1981) in a 1:2 ratio; crystals obtained by the slow evaporation of the filtered solution. Enraf–Nonius CAD-4F diffractometer controlled by a PDP8/A computer, graphite-monochromated Mo $K\bar{\alpha}$ radiation; ω:2θ scan technique. Cell parameters on crystal 0·41 × 0·16 × 0·21 mm from least-squares

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Table 1. *Fractional atomic coordinates and B_{eq} values* (Å^2)

$$B_{\text{eq}} = 8\pi^2(U_{11} + U_{22} + U_{33})/3.$$

	x	y	z	B_{eq}
Pt	0·0	0·0	0·0	2·36
S(1)	0·0615 (1)	0·2133 (1)	0·0777 (1)	3·77
P(1)	0·1574 (1)	0·0890 (1)	−0·0311 (1)	2·36
N(1)	0·2746 (3)	0·3080 (3)	0·0662 (2)	2·73
C(1)	0·1826 (3)	0·2345 (3)	0·0440 (2)	2·56
C(2)	0·2973 (3)	0·4061 (4)	0·1296 (2)	2·77
C(3)	0·2230 (3)	0·5170 (5)	0·1438 (2)	3·69
C(4)	0·2554 (4)	0·6113 (5)	0·2061 (3)	5·11
C(5)	0·3590 (5)	0·5990 (6)	0·2519 (3)	5·42
C(6)	0·4343 (5)	0·4895 (6)	0·2379 (3)	4·89
C(7)	0·4038 (4)	0·3939 (5)	0·1759 (2)	3·82
C(8)	0·2837 (3)	−0·0328 (4)	−0·0136 (2)	2·66
C(9)	0·3088 (4)	−0·1056 (4)	0·0640 (2)	3·47
C(10)	0·4188 (4)	−0·1986 (5)	0·0780 (2)	3·88
C(11)	0·4151 (4)	−0·3247 (5)	0·0203 (2)	4·44
C(12)	0·3853 (4)	−0·2555 (4)	−0·0568 (2)	4·03
C(13)	0·2757 (3)	−0·1613 (4)	−0·0715 (2)	3·35
C(14)	0·1471 (3)	0·1921 (4)	−0·1193 (2)	2·76
C(15)	0·0522 (4)	0·3134 (5)	−0·1325 (2)	4·00
C(16)	0·0391 (4)	0·3944 (6)	−0·2076 (3)	4·71
C(17)	0·1466 (5)	0·4684 (5)	−0·2149 (3)	4·89
C(18)	0·2414 (4)	0·3497 (5)	−0·2009 (3)	4·77
C(19)	0·2569 (3)	0·2689 (5)	−0·1259 (2)	3·75

Table 2. *Interatomic distances* (Å) *and bond angles* (°)

Pt—S(1)	2·322 (1)	Pt—P(1)	2·282 (1)
S(1)—C(1)	1·763 (4)	P(1)—C(1)	1·834 (3)
P(1)—C(8)	1·826 (4)	P(1)—C(14)	1·841 (3)
C(1)—N(1)	1·268 (4)	N(1)—C(2)	1·417 (4)
C(2)—C(3)	1·381 (5)	C(2)—C(7)	1·384 (5)
C(3)—C(4)	1·385 (5)	C(4)—C(5)	1·353 (7)
C(5)—C(6)	1·380 (8)	C(6)—C(7)	1·386 (6)
C(8)—C(9)	1·535 (5)	C(8)—C(13)	1·519 (5)
C(9)—C(10)	1·531 (6)	C(10)—C(11)	1·510 (6)
C(11)—C(12)	1·513 (6)	C(12)—C(13)	1·532 (5)
C(14)—C(15)	1·528 (5)	C(14)—C(19)	1·532 (5)
C(15)—C(16)	1·532 (6)	C(16)—C(17)	1·500 (8)
C(17)—C(18)	1·512 (7)	C(18)—C(19)	1·528 (5)

P(1)—Pt—S(1)	74·7 (1)	Pt—S(1)—C(1)	91·7 (1)
Pt—P(1)—C(1)	91·2 (1)	Pt—P(1)—C(8)	120·5 (1)
C(8)—P(1)—C(1)	105·4 (2)	Pt—P(1)—C(14)	120·5 (1)
C(1)—P(1)—C(14)	109·2 (2)	C(8)—P(1)—C(14)	107·1 (2)
C(1)—N(1)—C(2)	122·4 (3)	P(1)—C(1)—S(1)	101·9 (2)
N(1)—C(1)—S(1)	134·3 (3)	N(1)—C(1)—P(1)	123·2 (3)
N(1)—C(2)—C(3)	123·7 (3)	N(1)—C(2)—C(7)	116·1 (4)
C(3)—C(2)—C(7)	120·1 (3)	C(2)—C(3)—C(4)	119·0 (4)
C(3)—C(4)—C(5)	121·3 (5)	C(4)—C(5)—C(6)	120·2 (4)
C(5)—C(6)—C(7)	119·6 (5)	C(2)—C(7)—C(6)	119·8 (4)
P(1)—C(8)—C(9)	111·1 (3)	P(1)—C(8)—C(13)	112·0 (3)
C(9)—C(8)—C(13)	110·4 (3)	C(8)—C(9)—C(10)	109·4 (3)
C(9)—C(10)—C(11)	111·8 (4)	C(10)—C(11)—C(12)	111·4 (3)
C(11)—C(12)—C(13)	111·6 (4)	C(8)—C(13)—C(12)	110·2 (3)
P(1)—C(14)—C(15)	110·1 (2)	P(1)—C(14)—C(19)	113·9 (3)
C(15)—C(14)—C(19)	110·9 (3)	C(14)—C(13)—C(16)	110·6 (4)
C(15)—C(16)—C(17)	111·9 (4)	C(16)—C(17)—C(18)	111·6 (4)
C(17)—C(18)—C(19)	111·8 (4)	C(14)—C(19)—C(18)	110·5 (4)

procedure on 25 reflections ($11 \leq \theta \leq 19°$). Analytical absorption correction applied (Sheldrick, 1976); max./min. transmission factors 0·5686 and 0·4257. Total of 8342 reflections ($1 \leq \theta \leq 27·5°$) measured in the range $-2 \leq h \leq 16$, $0 \leq k \leq 11$, $-24 \leq l \leq 24$. Average decrease of 6% in the intensities of three reference reflections ($\bar{5}3\bar{3}$, $\bar{7}31$, $\bar{2},0,\overline{10}$) measured every 3600 s; correction applied for variation. 4305 unique reflections ($R_{\text{int}} = 0·023$), 3164 satisfied $I \geq 2·5\sigma(I)$. Structure solved from interpretation of Patterson map, full-matrix least-squares refinement of 208 parameters based on F (Sheldrick, 1976). Anisotropic thermal parameters for non-H atoms, H atoms included in the model at their calculated positions. At convergence $R = 0·024$, $wR = 0·025$, $w = 1·45/[\sigma^2(F) + 0·0003F^2]$, $S = 1·46$, $(\Delta/\sigma)_{\text{max}} \leq 0·001$, $(\Delta\rho)_{\text{max}} = 1·35$, $(\Delta\rho)_{\text{min}} = -1·15$ e Å^{-3}, no extinction correction. Scattering factors for H,C,N,P and S given in *SHELX76* (Sheldrick, 1976) and those for neutral Pt corrected for f' and f'' (Hamilton & Ibers, 1974). All calculations on VAX11/780 computer system. Atomic parameters are given in Table 1, bond distances and angles in Table 2;[*] the numbering scheme used is shown in Fig. 1.

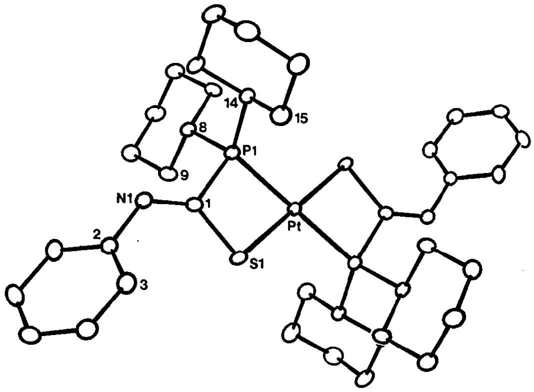

Fig. 1. Molecular structure and numbering scheme for the title compound. Note that the Pt atom is situated on a crystallographic centre of inversion. Atoms otherwise not indicated are carbon atoms (Johnson, 1971).

Related literature. Ligands based on anions of the general formula $[R_2PC(S)NR']^-$ are known to function in a variety of coordination modes involving one, two or, in one case, three donor atoms. Monodentate *S*-coordination has been recently characterized in $(C_6H_5)_3Sn[(c\text{-}C_6H_{11})_2PC(S)N(C_6H_5)]$ (Dakternieks, Hoskins & Rolls, 1986); bidentate *P,S*-coordination has been observed for the ligand in $Mn(CO)_4[(C_6H_5)_2PC(S)N(C_6H_5)]$ (Just, Klein, Kopf, Steinhäuser & Kramolowsky, 1982; Antoniadis, Hiller, Kunze, Schaal & Strähle, 1982); bidentate *S,N*-

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[*] Lists of structure factors, thermal parameters, H-atom parameters and mean plane data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44298 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

chelation is found in $Mo_2[(C_6H_5)_2PC(S)N(CH_3)]_4$ and both *S,N*- and *P,N*-coordination modes exist in an isomer of that compound (Ambrosius, Cotton, Falvello, Hintzen, Melton, Schwotzer, Tomas & Van Der Linden, 1984). A tridentate bridging mode, as well as a bidentate (*P,S*-) mode, has been reported in the dimer: $\{Mo(CO)_2[(C_6H_5)_2PC(S)N(CH_3)]_2\}_2$ (Bosman, Noordik, Ambrosius & Cras, 1980; Ambrosius, Willemse, Cras, Bosman & Noordik, 1984).

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Structure of the Aluminium Alkoxide Complex [Al(O-iPr)(3,5-heptanedione)$_2$]$_2$

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Abstract. 1,1,2,2-Tetrakis(3,5-heptanedionato)-di-μ-isopropoxy-dialuminium(III), $[Al(C_7H_{11}O_2)_2(C_3H_7O)]_2$, $M_r = 734{\cdot}8$, triclinic, $P\bar{1}$, $a = 9{\cdot}150\,(4)$, $b = 10{\cdot}08\,(1)$, $c = 12{\cdot}574\,(7)$ Å, $\alpha = 96{\cdot}64\,(7)$, $\beta = 111{\cdot}15\,(4)$, $\gamma = 112{\cdot}62\,(7)°$, $V = 954{\cdot}0$ Å^3, $Z = 2$, $D_x = 2{\cdot}56$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 3{\cdot}4$ cm^{-1}, $F(000) = 788$, $T = 173$ K, $R = 0{\cdot}0837$, $wR = 0{\cdot}0672$ for 1534 unique observed reflections. Centrosymmetric dimer, with half of the molecule being the asymmetric unit. Aluminium sites contain octahedral coordination with bridging isopropoxide ligands occupying a diastereotopic position. This is the final compound in a series of aluminium alkoxides.

Experimental. Compound obtained by reaction of 3,5-heptanedione with $[Al(O\text{-}iPr)_3]_4$ in dry methylene chloride (Wengrovius, Garbauskas, Williams, Going, Donohue & Smith, 1986), recrystallized from methy lene chloride/pentane at 243 K. Crystal size $0{\cdot}3 \times 0{\cdot}3 \times 0{\cdot}1$ mm plate. Poorly diffracting (hence high R value). Crystal sealed in capillary under dry nitrogen due to moisture sensitivity. Nicolet *P3F* automated diffractometer. ω/θ scan with variable scan speeds. Cell parameters determined from 14 reflections $5 < 2\theta < 22°$. No absorption correction applied. Data collection: $4 < 2\theta < 45°$. $0 \le h \le 10$, $-11 \le k \le 11$, $-14 \le l \le 14$. Standard reflections: 100 and $\bar{1}\bar{1}\bar{1}$ varied less than 1% during data collection. 2689 reflections collected, 2500 unique reflections, 1534 unique reflections observed with $F > 3\sigma(F)$. Structure solved by direct methods, refined on F. H atoms located by

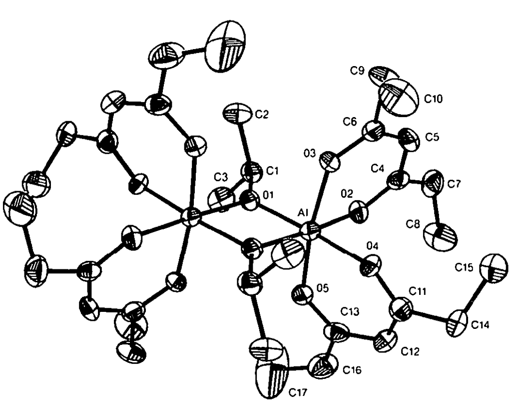

Fig. 1. Thermal-ellipsoid (50% probability) plot.

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