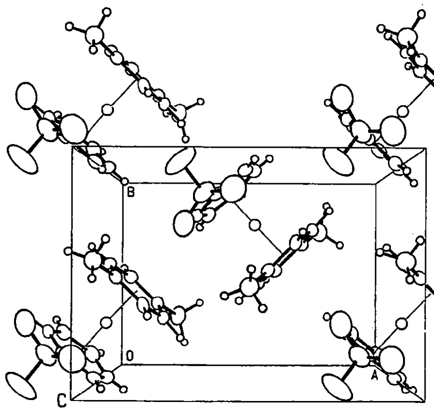

Fig. 2. Packing diagram of (1) as viewed down the *c* axis. The closest intermolecular contact is 2·51 (5) Å for H(10)···H(14*B*)(1−*x*, 1−*y*, *z*−0·5).

packing in Fig. 2. Principal computer programs are given by Gadol & Davis (1982); program for least-squares-planes calculations from Cordes (1983).

Related literature. A (benzene)(napthalene)Cr^0 complex has recently been reported (Kündig, Perret, Spicahiger & Bernardinelli, 1985). Jellinek (1963), Cotton, Dollase & Wood (1963), Ibers (1964) and Keulen & Jellinek (1966) have reported the structures of bisbenzeneCr^0. Elschenbroich, Mockel, Massa, Birkhahn & Zenneck (1982) reported a bisnaphthalene complex. Eyring, Zuerner & Radonovich (1981) and Larson, Seymour & Lagowski (1987) have reported trifluoromethylbenzene complexes of Cr^0.

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Structure of Chloro(isothiocyanato)bis(triphenylphosphine oxide)manganese(II)

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Abstract. $[\mathrm{MnCl(NCS)\{OP(C_6H_5)_3\}_2}]$, $M_r = 705{\cdot}06$, orthorhombic, *Pbca*, $a = 10{\cdot}992\,(3)$, $b = 22{\cdot}331\,(2)$, $c = 27{\cdot}722\,(4)$ Å, $V = 6805\,(3)$ Å^3, $Z = 8$, $D_m = 1{\cdot}37\,(1)$, $D_x = 1{\cdot}376\,(5)$ g cm^{-3}, $\lambda(\mathrm{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $\mu = 5{\cdot}98$ cm^{-1}, $F(000) = 2904$, $T = ca$ 293 K, $R = 0{\cdot}102$ for 2486 observed reflections. Pairs of molecules of the complex link through Mn—Cl′(1 − *x*, 1 − *y*, 1 − *z*) bonds to form dimeric units. Because of this dimerization, the Mn atom assumes a distorted trigonal-bipyramidal geometry. The Mn atom is 0·08 Å out of the equatorial plane formed by Cl, O and N atoms. Pairs of these bipyramids share Cl—Cl′ edges.

Experimental. Synthesized and characterized by Davolos (1978), colourless plates, 0·2 × 0·2 × 0·4 mm, D_m by flotation ($\mathrm{CH_3OH + CHBr_3}$), CAD-4 diffractometer, ω–2θ scan mode, unit-cell dimensions from 25 reflections ($10 < \theta < 17°$), absorption ignored, $\theta < 24°$, $0 \leq h \leq 12$, $0 \leq k \leq 25$, $0 \leq l \leq 31$, three standard reflections showed no appreciable intensity variation, 4141 independent reflections, 2486 observed reflections [$I > 3\sigma(I)$], Lorentz and polarization corrections. Structure solved partially by *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), subsequent difference Fourier maps showed all other atoms. Refinement by least squares using *SHELX*76 (Sheldrick, 1976), $\sum w(|F_o| - |F_c|)^2$ minimized, atomic coordinates, anisotropic thermal parameters and scale factor refined, isotropic thermal parameters for H atoms located geometrically and not refined, final $R = 0{\cdot}102$, $wR = 0{\cdot}079$ (poor quality of crystal and hence of agreement indices), $w = 2{\cdot}5795/\sigma^2(F_o)$, maximum Δ/σ in final refinement cycle 0·05, maximum and minimum height in final difference Fourier map 1·1 and $-1{\cdot}1$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Calculations performed on the VAX 11/780 computer.

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters (Hamilton, 1959) with e.s.d.'s in parentheses*

	x	y	z	B_{eq}(Å^2)
Mn	0·4302 (2)	0·4777 (1)	0·4394 (1)	3·20 (7)
Cl	0·4980 (4)	0·5702 (1)	0·4800 (1)	4·1 (1)
S	0·7063 (5)	0·3423 (2)	0·3597 (1)	6·0 (2)
P(*A*)	0·1625 (4)	0·3951 (1)	0·4293 (1)	3·6 (1)
P(*B*)	0·3514 (4)	0·5770 (1)	0·3450 (1)	3·6 (1)
O(*A*)	0·2772 (8)	0·4279 (3)	0·4438 (3)	3·8 (3)
O(*B*)	0·3530 (9)	0·5293 (3)	0·3835 (3)	4·7 (4)
N	0·553 (1)	0·4309 (5)	0·3963 (4)	4·6 (5)
C	0·614 (1)	0·3926 (6)	0·3807 (5)	4·0 (6)
C(1*A*)	0·146 (1)	0·3252 (5)	0·4631 (4)	3·1 (5)
C(2*A*)	0·066 (2)	0·2815 (5)	0·4471 (5)	4·7 (6)
C(3*A*)	0·056 (2)	0·2289 (6)	0·4719 (5)	5·7 (7)
C(4*A*)	0·127 (2)	0·2202 (6)	0·5131 (6)	4·7 (7)
C(5*A*)	0·212 (2)	0·2639 (6)	0·5292 (5)	5·9 (8)
C(6*A*)	0·222 (2)	0·3181 (6)	0·5035 (5)	4·8 (7)
C(7*A*)	0·032 (1)	0·4388 (5)	0·4379 (4)	3·4 (6)
C(8*A*)	0·031 (2)	0·5008 (5)	0·4271 (4)	4·2 (6)
C(9*A*)	−0·066 (2)	0·5365 (6)	0·4319 (6)	6·0 (8)
C(10*A*)	−0·172 (2)	0·5131 (7)	0·4487 (5)	5·7 (8)
C(11*A*)	−0·182 (2)	0·4532 (7)	0·4595 (5)	5·0 (7)
C(12*A*)	−0·081 (2)	0·4175 (6)	0·4541 (5)	4·1 (6)
C(13*A*)	0·165 (2)	0·3734 (6)	0·3659 (5)	5·0 (7)
C(14*A*)	0·059 (2)	0·3782 (6)	0·3376 (5)	5·0 (7)
C(15*A*)	0·063 (3)	0·3577 (8)	0·2909 (7)	9 (1)
C(16*A*)	0·171 (3)	0·3331 (9)	0·2739 (8)	11 (1)
C(17*A*)	0·276 (3)	0·3276 (9)	0·3024 (7)	11 (1)
C(18*A*)	0·270 (2)	0·3473 (7)	0·3486 (6)	7·4 (9)
C(1*B*)	0·486 (2)	0·6226 (6)	0·3442 (4)	3·9 (6)
C(2*B*)	0·487 (2)	0·6822 (6)	0·3292 (5)	5·6 (7)
C(3*B*)	0·589 (2)	0·7150 (6)	0·3264 (6)	6·1 (8)
C(4*B*)	0·695 (2)	0·6903 (7)	0·3385 (5)	5·5 (8)
C(5*B*)	0·698 (2)	0·6312 (6)	0·3540 (6)	6·0 (8)
C(6*B*)	0·597 (2)	0·5988 (6)	0·3558 (5)	4·5 (7)
C(7*B*)	0·227 (1)	0·6279 (6)	0·3547 (5)	3·2 (5)
C(8*B*)	0·203 (2)	0·6471 (6)	0·4014 (5)	5·3 (7)
C(9*B*)	0·114 (2)	0·6866 (7)	0·4103 (6)	5·2 (7)
C(10*B*)	0·037 (2)	0·7081 (6)	0·3747 (7)	6·7 (9)
C(11*B*)	0·061 (2)	0·6898 (7)	0·3279 (6)	6·4 (8)
C(12*B*)	0·153 (1)	0·6492 (6)	0·3176 (5)	4·5 (7)
C(13*B*)	0·334 (2)	0·5453 (5)	0·2849 (4)	4·2 (6)
C(14*B*)	0·244 (2)	0·5060 (6)	0·2761 (5)	5·5 (7)
C(15*B*)	0·232 (2)	0·4792 (6)	0·2315 (6)	6·2 (8)
C(16*B*)	0·313 (2)	0·4926 (7)	0·1963 (6)	6·1 (9)
C(17*B*)	0·404 (2)	0·5309 (8)	0·2042 (6)	8 (1)
C(18*B*)	0·420 (2)	0·5580 (6)	0·2497 (6)	5·4 (7)

Table 2. *Selected bond angles* (°)

Cl—Mn—O(*A*)	133·2 (3)	O(*B*)—Mn—N	96·5 (4)
Cl—Mn—N	119·1 (3)	Cl—Mn—Cl′	82·0 (1)
O(*A*)—Mn—N	107·3 (4)	Cl′—Mn—O(*A*)	88·5 (2)
Cl—Mn—O(*B*)	90·0 (2)	Cl′—Mn—N	95·2 (3)
O(*A*)—Mn—O(*B*)	90·6 (3)	Cl′—Mn—O(*B*)	168·0 (2)

Positional and equivalent isotropic thermal parameters are listed in Table 1* and selected bond angles are presented in Table 2. The atom-numbering scheme and bond lengths are shown in Fig. 1 and a stereoview of the molecule is shown in Fig. 2 (Johnson, 1965).

Related literature. The author is studying the structure of a series of manganese(II) complexes (Tomita, 1985).

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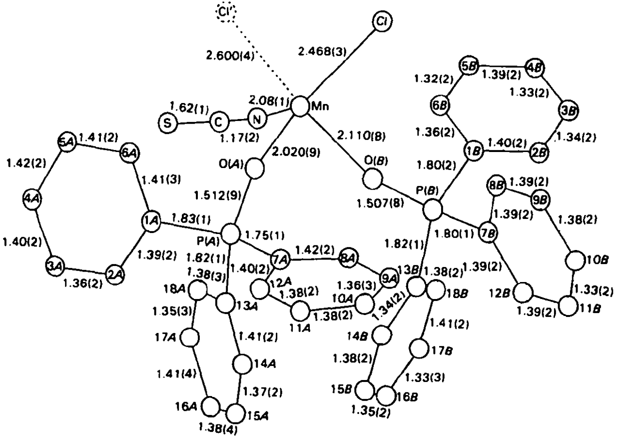

Fig. 1. Numbering scheme and bond lengths (Å) with e.s.d.'s in parentheses. Numbers refer to C atoms unless otherwise indicated.

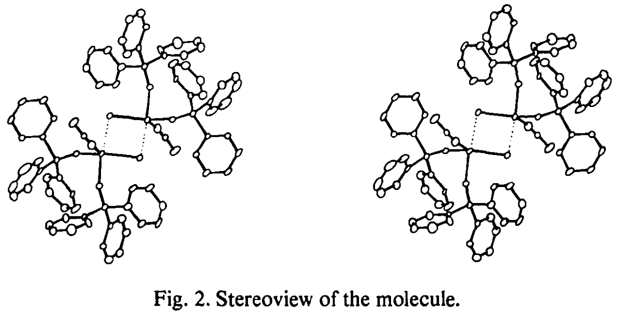

Fig. 2. Stereoview of the molecule.

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* Lists of structure factors, anisotropic thermal parameters and bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43868 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of (Tetrahydroborato)bis(tetrahydrofuran)uranium(IV): a Model for Hydrogen–Uranium Bonding

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Abstract. [$U(BH_4)_4(C_4H_8O)_2$], $M_r = 441{\cdot}6$, orthorhombic, *Pnma*, $a = 10{\cdot}439$ (3), $b = 7{\cdot}120$ (2), $c = 11{\cdot}315$ (3) Å, $V = 841{\cdot}0$ (7) Å^3, $Z = 2$, $D_x = 1{\cdot}74$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 9{\cdot}13$ mm^{-1}, $F(000) = 416$, $T = 295$ K, $R = 0{\cdot}037$ for 216 unique observed data. The molecular geometry is in essential agreement with that reported by Rietz, Edelstein, Ruben, Templeton & Zalkin [*Inorg. Chem.* (1978), **17**, 658–660], the major difference being the relatively high accepted thermal parameters at room temperature for the C and B atoms instead of disorder in both the C atoms of tetrahydrofuran (THF) and the B atoms. The complex is confirmed as a monomer with an octahedral arrangement around the U atom of four BH_4^- and two *trans* THF molecules. The ligation of BH_4^- to the U atom is through bridging H atoms, the four equivalent BH_4^- acting as tridentate ligands [U—B 2·53 (6) Å]. However, the bending of the line U—B—HB(4) [164 (4)°] makes the three bridging H atoms unequivalent, one being as close as 2·16 Å to the U atom.

Experimental. Tetrahydrofuran added to a solution of $U(BH_4)_4$ in deuterated toluene; after recording the NMR spectrum of the adduct at 213 K the solution is stored at 243 K and emerald-green crystals obtained; crystal 0·40 × 0·30 × 0·25 mm; Enraf–Nonius CAD-4 diffractometer controlled by a PDP 11/23 Plus computer, graphite-monochromatized Mo $K\alpha$ radiation; $\omega/2\theta$ scan technique; cell parameters obtained from least-squares procedure on 25 reflections ($8 < \theta < 12°$); decay of 11·8% (in 10 h) in intensities of three standard reflections monitored every 100 measurements, linearly corrected; Lorentz and polarization corrections; max. and min. transmission factors for an empirical absorption correction 1·21 and 0·75 (Walker & Stuart, 1983); total of 921 reflections measured in range $1 < \theta < 20°$; $0 < h < 10$, $0 < k < 6$, $-10 < l < 10$; 355 unique reflections, 216 with $I > 2\sigma(I)$. Structure solved by Patterson method for U; remaining atoms located by difference Fourier techniques; full-matrix least-squares refinement based on F; anisotropic thermal parameters for U; scattering factors including anomalous-dispersion terms from *International Tables for X-ray Crystallography* (1974). H atoms of the THF

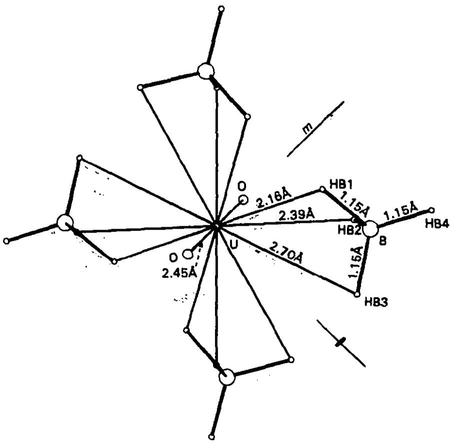

Fig. 1. *ORTEP* (Johnson, 1976) representation of the coordination sphere of the U atom, giving bond lengths (Å) and atomic numbering (symmetry of the U site 2/*m*).

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