

cyclohexane (Bucourt & Hainaut, 1965). The Sn—C lengths range from 2.11 (1) to 2.14 (1) Å and S—Sn—C angles from 102.2 (5) to 115.6 (5)°. The dihedral angles between the two phenyl rings attached to each Sn atom range from 85 (1) to 123 (1)°.

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## Structure of [PhCH<sub>2</sub>NMe<sub>3</sub>]<sub>2</sub>[(B<sub>10</sub>H<sub>12</sub>)<sub>2</sub>Pt]

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**Abstract.** [PhCH<sub>2</sub>NMe<sub>3</sub>]<sub>2</sub><sup>+</sup>·[Pt(B<sub>10</sub>H<sub>12</sub>)<sub>2</sub>]<sup>2-</sup>,  $M_r = 735.97$ , triclinic,  $P\bar{1}$ ,  $a = 9.023$  (3),  $b = 10.440$  (4),  $c = 11.172$  (3) Å,  $\alpha = 111.55$  (3),  $\beta = 108.794$  (24),  $\gamma = 101.29$  (3)°,  $V = 865.7$  Å<sup>3</sup>,  $Z = 1$ ,  $D_x = 1.411$  Mg m<sup>-3</sup>, Mo  $K\alpha$ ,  $\lambda = 0.71069$  Å,  $\mu = 4.111$  mm<sup>-1</sup>,  $F(000) = 368$ ,  $T = 185$  (1) K,  $R = 0.0166$  for 3039 independent observed reflections. The anion resides on a crystallographic inversion centre, and is slightly, but significantly, distorted from  $C_{2h}$  point symmetry as a result of crystal packing. Molecular-geometry calculations suggest that the {B<sub>10</sub>H<sub>12</sub>} ligand does not fit particularly well with either a *nido*-{B<sub>10</sub>H<sub>12</sub>}<sup>2-</sup> or an *arachno*-{B<sub>10</sub>H<sub>12</sub>}<sup>4-</sup> formalism.

**Introduction.** The precise structures of metallaboranes of the general family  $MB_{10}H_{12}$  are of current interest because the {B<sub>10</sub>H<sub>12</sub>} ligand could formally be present in such species as either the *nido* fragment {B<sub>10</sub>H<sub>12</sub>}<sup>2-</sup> or the *arachno* fragment {B<sub>10</sub>H<sub>12</sub>}<sup>4-</sup>. The structural differences between these are subtle (the pattern of connectivities is exactly the same), and only recently have they really been successfully delineated *via* application of the 'root-mean-square misfit' technique (Wynd, 1988; Wynd, Welch & Parish, 1990; Macgregor, Yellowlees & Welch, 1990).

It is important to attempt to distinguish between the formalisms of {B<sub>10</sub>H<sub>12</sub>}<sup>2-</sup> and {B<sub>10</sub>H<sub>12</sub>}<sup>4-</sup> ligands in  $MB_{10}H_{12}$  metallaboranes for two reasons. Firstly, it allows access to the formal oxidation state of the metal in the complex, something that is very rarely probed. Cases where independent measure-

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ment of the metal oxidation state is possible are welcome, since these afford a check on the validity of the approach to distinction of the two formalisms. Secondly, it allows assessment of the 'verticity' of the metal atom, *i.e.* (the rough measure of) the extent to which it is truly involved in cluster skeletal bonding, as opposed to acting as a simple bridge between several B atoms.

The dianion [(B<sub>10</sub>H<sub>12</sub>)<sub>2</sub>Pt]<sup>2-</sup> has been known for many years (Klanberg, Wegner, Parshall & Muetteries, 1968). Although it is well accepted that its gross structure is the same as that of the crystallographically characterized anions [(B<sub>10</sub>H<sub>12</sub>)<sub>2</sub>Ni]<sup>2-</sup> (Guggenberger, 1972) and [(B<sub>10</sub>H<sub>12</sub>)<sub>2</sub>Au]<sup>-</sup> (Wynd & Welch, 1987), molecular parameters are not known, and so the precise form of the {B<sub>10</sub>H<sub>12</sub>} ligand in this species cannot be assessed. To remedy this we have resynthesized [(B<sub>10</sub>H<sub>12</sub>)<sub>2</sub>Pt]<sup>2-</sup> for the purposes of the accurate structural study described herein. Suitable crystals were afforded as the [PhCH<sub>2</sub>NMe<sub>3</sub>]<sup>+</sup> salt.

**Experimental.** The salt [PhCH<sub>2</sub>NMe<sub>3</sub>]<sub>2</sub>[(B<sub>10</sub>H<sub>12</sub>)<sub>2</sub>Pt] was prepared in an analogous manner to that which previously afforded the [NMe<sub>4</sub>]<sup>+</sup> salt (Klanberg, Wegner, Parshall & Muetteries, 1968), and its purity confirmed by microanalysis (found: C, 32.3; H, 7.49; N, 3.83%. C<sub>20</sub>H<sub>56</sub>B<sub>20</sub>N<sub>2</sub>Pt requires: C, 32.7; H, 7.62; N, 3.81%); golden-yellow blocks grown by slow diffusion of diethyl ether into an acetonitrile solution at 243 K; slightly irregular crystal, *ca* 0.3 × 0.25 × 0.15 mm, mounted in glass capillary and slowly cooled to 185 (1) K on an Enraf–Nonius CAD-4

diffractometer (Mo K $\alpha$  radiation, graphite monochromator, ULT-1 attachment); orientation matrix and cell parameters from least-squares refinement of the setting angles ( $13 < \theta < 15^\circ$ ) of 25 centred reflections; data collection by  $\omega$ - $2\theta$  scans in 96 steps with  $\omega$ -scan width ( $0.8 + 0.34 \tan \theta$ ) $^\circ$ ; nearly one full sphere of data ( $h$ : 0 to 10,  $k$ : -12 to 12,  $l$ : -13 to 13;  $h$ : -10 to 0,  $k$ : -12 to 12,  $l$ : -13 to 4) measured for  $1 \leq \theta \leq 25^\circ$  over *ca* 82 X-ray hours with no perceptible crystal movement or decay (average net intensity of the 5 $\bar{2}1$  and  $\bar{6}11$  reflections varied between 98.3 and 101.5% of their mean values); 5403 intensities corrected for Lorentz and polarization effects (Gould & Smith, 1986), all having  $F \geq 6.0\sigma(F)$ ; solution *via* iterative application of full-matrix least-squares refinement (on  $F/\Delta F$  syntheses (Pt at inversion centre) (Sheldrick, 1976); empirical absorption correction (Walker & Stuart, 1983) following isotropic convergence (correction factors 0.828–1.262); merging afforded 3039 data ( $R_{\text{merge}}$  0.0134); all non-H atoms allowed anisotropic thermal vibration, and all H atoms freely refined with group isotropic thermal parameters [ $U_{\text{cage H}} = 0.0375$  (24),  $U_{\text{benzyl H}} = 0.047$  (4),  $U_{\text{methyl H}} = 0.041$  (3)  $\text{\AA}^2$  at convergence]; the weighting scheme  $w^{-1} = \sigma^2(F) + 0.000422(F^2)$  afforded satisfactory analysis of variance against parity group,  $\text{abs}(h)$ ,  $\text{abs}(k)$ ,  $\text{abs}(l)$ ,  $(F/F_{\text{max}})^{1/2}$ , and  $\sin \theta$ ; 283 variables, data:variable ratio  $> 10.7:1$ ; max. shift/e.s.d. in final cycle  $< 0.02$ ;  $R = 0.0166$ ,  $wR = 0.0212$ ,  $S = 1.032$ ; max. and min. residues in final  $\Delta F$  synthesis 1.48 and  $-1.42 \text{ e \AA}^{-3}$  respectively (near Pt); scattering factors for C, H, B and N inlaid in *SHELX76*. Those for Pt from *International Tables for X-ray Crystallography* (1974); figures drawn using *EASYORTEP* (Mallinson & Muir, 1985) and *PLUTO* (Motherwell, 1976);

Table 1. Fractional atomic coordinates and equivalent isotropic temperature factors

$$U_{\text{eq}} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$$

	x	y	z	$U_{\text{eq}}(\text{\AA}^2)$
Pt	0.00000	0.00000	0.00000	0.0218 (1)
C(1)	0.7779 (3)	0.4894 (3)	0.3868 (3)	0.0351 (17)
C(2)	0.7429 (4)	0.3618 (3)	0.2671 (3)	0.0444 (20)
C(3)	0.7363 (4)	0.2313 (4)	0.2751 (4)	0.0576 (25)
C(4)	0.7666 (4)	0.2291 (4)	0.4028 (5)	0.066 (3)
C(5)	0.8051 (4)	0.3564 (4)	0.5237 (4)	0.062 (3)
C(6)	0.8090 (4)	0.4861 (4)	0.5154 (3)	0.0449 (20)
C(7)	0.7967 (3)	0.6335 (3)	0.3830 (3)	0.0340 (17)
N(1)	0.6346 (3)	0.66296 (25)	0.33214 (23)	0.0331 (14)
C(8)	0.6803 (4)	0.8187 (3)	0.3547 (4)	0.0445 (21)
C(9)	0.5272 (4)	0.5620 (4)	0.1775 (3)	0.0436 (21)
C(10)	0.5377 (4)	0.6451 (4)	0.4148 (3)	0.0417 (20)
B(a)	0.1163 (4)	0.2424 (3)	0.0634 (3)	0.0307 (17)
B(c)	0.0954 (3)	0.1181 (3)	-0.1060 (3)	0.0290 (17)
B(d)	-0.1101 (4)	-0.0279 (3)	-0.2201 (3)	0.0293 (17)
B(b)	-0.2605 (3)	-0.0253 (3)	-0.1484 (3)	0.0317 (18)
B(i)	-0.2739 (4)	0.1574 (4)	-0.0997 (3)	0.0368 (19)
B(j)	-0.1517 (4)	0.2480 (3)	-0.1597 (3)	0.0368 (19)
B(e)	-0.0583 (4)	0.1316 (3)	-0.2430 (3)	0.0337 (18)
B(g)	-0.2627 (4)	0.0548 (3)	-0.2619 (3)	0.0334 (18)
B(f)	0.0675 (4)	0.2894 (3)	-0.0763 (3)	0.0346 (19)
B(h)	-0.0505 (4)	0.3169 (3)	0.0253 (3)	0.0377 (20)

molecular-geometry calculations (including r.m.s. misfit calculations) *via* *CALC* (Gould & Taylor, 1986).

**Discussion.** Fig. 1 shows a perspective view of the dianion and one adjacent cation. The  $[(\text{B}_{10}\text{H}_{12})_2\text{Pt}]^{2-}$  anion resides on a crystallographic inversion centre; the  $[\text{C}_6\text{H}_5\text{CH}_2\text{NMe}_3]^+$  cation crystallizes in general space. Table 1\* lists fractional coordinates of refined atoms (excluding H atoms), and Table 2 details selected interatomic distances and interbond angles. Fig. 1 also shows the numbering scheme adopted; we have chosen to number the B atoms in the anion as B(a)–B(j) (Fig. 2b) to avoid any prejudice about the best description of the  $\{\text{B}_{10}\text{H}_{12}\}$  fragment. If formally present as *nido*- $\{\text{B}_{10}\text{H}_{12}\}^{2-}$  this would be numbered as in Fig. (2a), whereas if the best description was that of *arachno*- $\{\text{B}_{10}\text{H}_{10}\}^{4-}$  the appropriate numbering scheme would be that of Fig. (2c).

In fact, use of the r.m.s. misfit approach places the  $\{\text{B}_{10}\text{H}_{12}\}$  fragment of the present complex essentially equidistant from idealized *nido*-B<sub>10</sub> and *arachno*-B<sub>10</sub> cages, since the r.m.s. misfit values are 0.085  $\text{\AA}$  versus B<sub>10</sub>H<sub>14</sub> (Brill, Dietrich & Dierks, 1971) and 0.125  $\text{\AA}$  versus the appropriate B<sub>10</sub> fragment of  $[\text{B}_{11}\text{H}_{13}]^{2-}$

\* Lists of structure factors, H-atom positions, additional interatomic distances and interbond angles and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52783 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

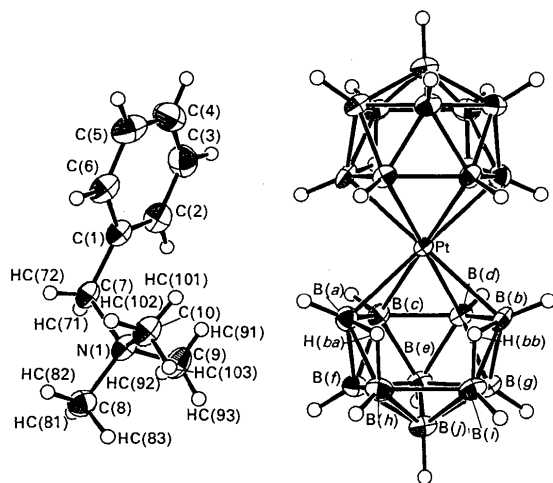


Fig. 1. Perspective view of the  $[(\text{B}_{10}\text{H}_{12})_2\text{Pt}]^{2-}$  anion and one  $[\text{PhCH}_2\text{NMe}_3]^+$  cation (50% thermal ellipsoids, except for H atoms which have an artificial radius of 0.1  $\text{\AA}$  for clarity).

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

Pt—B(a)	2.274 (3)	B(c)—B(d)	1.825 (5)
Pt—B(c)	2.231 (3)	B(c)—B(e)	1.776 (5)
Pt—B(d)	2.215 (3)	B(c)—B(f)	1.779 (5)
Pt—B(b)	2.295 (3)	B(d)—B(b)	1.784 (5)
C(1)—C(2)	1.385 (5)	B(d)—B(e)	1.772 (5)
C(1)—C(6)	1.386 (5)	B(d)—B(g)	1.791 (5)
C(1)—C(7)	1.498 (4)	B(d)—B(i)	1.821 (5)
C(2)—C(3)	1.388 (6)	B(b)—B(g)	1.754 (5)
C(3)—C(4)	1.373 (6)	B(i)—B(j)	1.758 (5)
C(4)—C(5)	1.382 (6)	B(i)—B(g)	1.783 (5)
C(5)—C(6)	1.386 (6)	B(i)—B(h)	1.987 (5)
C(7)—N(1)	1.525 (4)	B(j)—B(e)	1.769 (5)
N(1)—C(8)	1.499 (4)	B(j)—B(g)	1.776 (5)
N(1)—C(9)	1.489 (5)	B(j)—B(f)	1.775 (5)
N(1)—C(10)	1.495 (4)	B(j)—B(h)	1.748 (5)
B(a)—B(c)	1.781 (5)	B(e)—B(g)	1.770 (5)
B(a)—B(f)	1.754 (5)	B(e)—B(f)	1.767 (5)
B(a)—B(h)	1.828 (5)	B(f)—B(h)	1.779 (5)
B(a)—Pt—B(c)	46.55 (12)	B(e)—B(d)—B(g)	59.56 (19)
B(c)—Pt—B(d)	48.46 (2)	Pt—B(b)—B(d)	64.36 (14)
B(d)—Pt—B(b)	46.56 (12)	B(d)—B(b)—B(g)	60.81 (19)
C(2)—C(1)—C(6)	119.3 (3)	B(i)—B(b)—B(g)	59.77 (19)
C(2)—C(1)—C(7)	121.3 (3)	B(b)—B(i)—B(g)	58.23 (19)
C(6)—C(1)—C(7)	119.3 (3)	B(j)—B(i)—B(g)	60.19 (20)
C(1)—C(2)—C(3)	120.4 (3)	B(j)—B(i)—B(h)	55.23 (19)
C(2)—C(3)—C(4)	119.8 (4)	B(i)—B(j)—B(g)	60.58 (20)
C(3)—C(4)—C(5)	120.3 (4)	B(i)—B(j)—B(h)	69.05 (21)
C(4)—C(5)—C(6)	119.8 (4)	B(e)—B(j)—B(g)	59.91 (19)
C(1)—C(6)—C(5)	120.3 (3)	B(e)—B(j)—B(f)	59.83 (19)
C(1)—C(7)—N(1)	115.67 (25)	B(f)—B(j)—B(h)	60.66 (20)
C(7)—N(1)—C(8)	107.85 (24)	B(c)—B(e)—B(d)	61.90 (18)
C(7)—N(1)—C(9)	111.01 (24)	B(c)—B(e)—B(f)	60.30 (19)
C(7)—N(1)—C(10)	111.24 (24)	B(d)—B(e)—B(g)	60.74 (19)
C(8)—N(1)—C(9)	108.8 (3)	B(j)—B(e)—B(g)	60.24 (19)
C(8)—N(1)—C(10)	108.83 (25)	B(j)—B(e)—B(f)	60.25 (19)
C(9)—N(1)—C(10)	109.1 (3)	B(d)—B(g)—B(b)	60.43 (19)
Pt—B(a)—B(c)	65.46 (15)	B(d)—B(g)—B(e)	59.70 (19)
B(c)—B(a)—B(f)	60.45 (19)	B(b)—B(g)—B(i)	62.00 (19)
B(f)—B(a)—B(h)	59.51 (19)	B(i)—B(g)—B(j)	59.23 (19)
Pt—B(c)—B(a)	67.99 (15)	B(j)—B(g)—B(e)	59.85 (19)
Pt—B(c)—B(d)	65.30 (14)	B(a)—B(f)—B(c)	60.53 (19)
B(a)—B(c)—B(f)	59.02 (18)	B(a)—B(f)—B(h)	62.33 (20)
B(d)—B(c)—B(e)	58.96 (18)	B(c)—B(f)—B(e)	60.09 (19)
B(e)—B(c)—B(f)	59.61 (19)	B(j)—B(f)—B(e)	59.93 (19)
Pt—B(d)—B(c)	66.24 (14)	B(j)—B(f)—B(h)	58.93 (20)
Pt—B(d)—B(b)	69.07 (15)	B(a)—B(h)—B(f)	58.15 (19)
B(c)—B(d)—B(e)	59.14 (18)	B(i)—B(h)—B(j)	55.72 (19)
B(b)—B(d)—B(g)	58.77 (18)	B(j)—B(h)—B(f)	60.41 (20)

(Fritchie, 1967). Misfits for the  $B_{10}$  cages of  $[(B_{10}H_{12})_2Ni]^{2-}$  and  $[(B_{10}H_{12})_2Au]^-$  versus these standards are similar, viz 0.080, 0.136 Å (Ni) and 0.107, 0.110 Å (Au) respectively. Naturally, mutual r.m.s. misfit values between the three  $[(B_{10}H_{12})_2M]$  anions are considerably lower (Ni—Au 0.065, Ni—Pt 0.029, Pt—Au 0.054 Å). The verticity of the Pt atom is calculated to be 40.1%.

We have previously (Macgregor, Yellowlees & Welch, 1990) identified a number of key parameters that may ultimately be of use in classifying the  $\{B_{10}H_{12}\}$  ligand, and in the present determination the values of these are as follows: B(c)—B(d) 1.825 (5), B(h)—B(i) 1.987 (5), B(a)⋯B(b) 3.347 (7) Å; height of Pt above the B(a)B(h)B(i)B(b) plane 0.537 (3) Å.

Although it appears that the  $[(B_{10}H_{12})_2Pt]^{2-}$  anion might have non-crystallographic  $C_{2h}$  point-group symmetry, there are small but significant distortions

within the polyhedron that do not accord with this. Specifically, B(b)—B(d)—B(c) is wider than B(a)—B(c)—B(d) by  $1.93 (32)^\circ$ , allowing Pt—B(a) to be shorter than Pt—B(b) [ $\Delta = 0.021 (4) \text{ \AA}$ ] whilst at the same time Pt—B(c) is longer than Pt—B(d) [ $\Delta = 0.016 (4) \text{ \AA}$ ]. Since there is no obvious intramolecular reason for this slight but apparently real asymmetry,

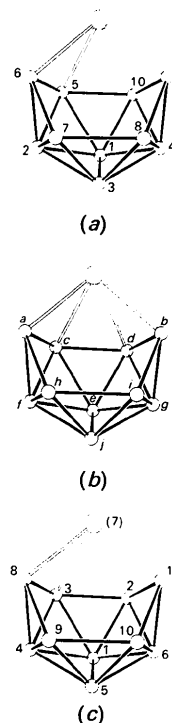


Fig. 2. Numbering schemes for  $B_{10}$  ligands and their inter-relationship; (a) *nido*- $B_{10}$ ; (b) present complex; (c) *arachno*- $B_{10}$ .

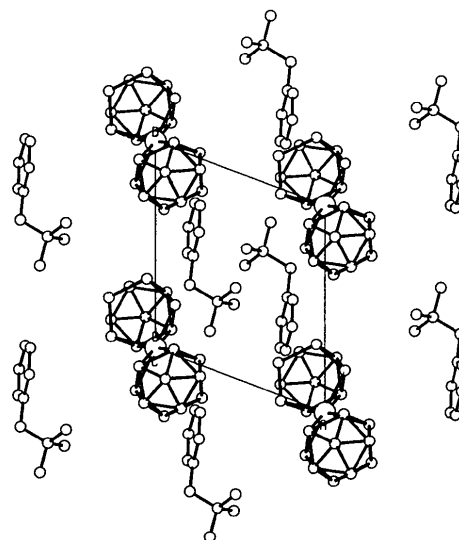


Fig. 3. Packing diagram down the crystallographic  $c$  axis.

it is likely that its origin lies in crystal-packing effects. Although there are no H<sub>cage</sub>···H<sub>cation</sub> contacts < 2.6 Å, it is clear from the packing diagram (Fig. 3) that the two sides of the {B<sub>10</sub>H<sub>12</sub>} ligand [that containing B(*a*) and that containing B(*b*)] experience quite different crystal environments. Distances and angles within the [PhCH<sub>2</sub>NMe<sub>3</sub>]<sup>+</sup> cation are quite normal (e.g. Mitchell & Welch, 1987; Wynd & Welch, 1989; Macgregor, Yellowlees & Welch, 1990).

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## A (Dithioformato)rhodadicarborane Complex: 3-(Dithioformato-*S,S'*)-3-(triphenylphosphine)-1,2-dicarb-3-rhoda-*closo*-dodecaborane(12) Cyclohexane Solvate, [3-(S<sub>2</sub>CH-*S,S'*)-3-(PPh<sub>3</sub>)-3,1,2-RhC<sub>2</sub>B<sub>9</sub>H<sub>11</sub>].C<sub>6</sub>H<sub>12</sub>

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**Abstract.** C<sub>21</sub>H<sub>27</sub>B<sub>9</sub>PRhS<sub>2</sub>.C<sub>6</sub>H<sub>12</sub>, *M<sub>r</sub>* = 658.9, monoclinic, *P*2<sub>1</sub>/*n*, *a* = 20.085 (5), *b* = 16.055 (3), *c* = 10.074 (2) Å, β = 98.69 (2)°, *V* = 3211 (2) Å<sup>3</sup>, *Z* = 4, *D<sub>x</sub>* = 1.36 g cm<sup>-3</sup>, λ = 0.70926 Å, μ(Mo *K*α) = 7.1 cm<sup>-1</sup>, *F*(000) = 1352, *T* = 294 K, *R* = 0.029 for 5595 observed reflections. The Rh atom is bonded symmetrically to the bidentate S<sub>2</sub>CH ligand [Rh—S 2.352 (1) and 2.356 (1) Å]. Each S atom is *trans* to a C atom in the C<sub>2</sub>B<sub>3</sub> face of the C<sub>2</sub>B<sub>9</sub>-carborane

ligand which is bonded to the Rh atom [Rh—C 2.195 (3) and 2.201 (3), Rh—B 2.204 (3), 2.205 (3) and 2.239 (3), and C—C 1.631 (3) Å]. The C—Rh—S angles are 164.29 (6) and 165.88 (6)°. The Rh—P distance is 2.374 (1) Å and the PPh<sub>3</sub> ligand is opposite the unique B atom in the C<sub>2</sub>B<sub>3</sub> face. The P—Rh—B angle is 175.35 (8)°.

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**Introduction.** A study of the reactions of CS<sub>2</sub> with the rhodaheteroborane complexes [2,2-(PPh<sub>3</sub>)<sub>2</sub>-2-(H)-1,2-*XRh*B<sub>10</sub>H<sub>10</sub>] [(I) *X* = Se, Te] has produced several interesting products (Faridoon, Spalding, Ferguson, Kennedy & Fontaine, 1989) including the dithio-