O1—Al—O2	89.23 (7)	O2—Al—O3^{i}	91.32 (8)
O1—Al—O2^{i}	90.77 (7)	Al—O1—C11	126.5 (2)
O1—Al—O3	89.25 (7)	Al—O2—C21	130.2 (2)
O1—Al—O3^{i}	90.75 (7)	Al—O3—C31	129.6 (2)
O2—Al—O3	88.68 (8)		
Al—O1—C11—N1	−163.4 (2)	Al—O3—C31—N3	−160.9 (2)
Al—O2—C21—N2	177.6 (2)		

Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} - y, -z$.

Data were corrected for Lorentz, polarization and absorption effects. Laue class and systematic absences indicated space group *Cc* or *C*2/*c*. The latter was chosen because the comparison of Bijvoet pairs did not suggest a non-centrosymmetric structure; an alternative analysis based on *Cc* gave practically the same structure (two ClO_4^- ions out of three are disordered) as in *C*2/*c*, with a slightly better fit ($R = 0.046$, $wR = 0.142$) probably due to the doubled number of parameters. The structure was solved by direct methods and subsequent difference Fourier syntheses. Full-matrix least-squares refinement was performed. A small empirical extinction parameter (x) was introduced and refined by least squares, where F_c was multiplied by $[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$. All non-H atoms were refined anisotropically. Methyl H atoms were placed at idealized positions with fixed C—H distances and H—C—H angles, and refined using a rotating model, with displacement parameters set as 1.5 times the equivalent isotropic displacement parameter of the methyl C atom. Formyl H atoms were placed at idealized positions and refined using a riding model. Disorder of the two O atoms O13 and O14 was suggested by their highly anisotropic displacement parameters, so that two positions for each atom were calculated by moving along the direction of the largest eigenvalue of the displacement tensor, with a fixed site-occupation factor of 0.5. After the refinement, the displacement parameters for O13 were still somewhat anisotropic and the Cl—O distances showed variation, but further attempts with more disordered positions did not converge. The maximum residual peak in the final difference Fourier map was near O12 (1.20 Å apart).

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *CAD*-4 *Software*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*III (Burnett & Johnson, 1996). Software used to prepare material for publication: *SHELXL*93.

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1-Phenyl-3,3-bis(triethylphosphine)-1,2-dicarba-3-platina-*closo*-dodecaborane 0.5-Dichloromethane Solvate

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Abstract

The title compound, $[Pt(C_8H_{15}B_9)(C_6H_{15}P)_2].0.5CH_2Cl_2$, crystallizes with two carbaplatinaborane molecules and one solvent molecule in the asymmetric unit. The conformation of the $\{Pt(PEt_3)_2\}$ fragment relative to

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the carbaborane ligand is practically the same in both crystallographically independent molecules and similar to that in 1-Ph-3,3-$(PMe_2Ph)_2$-3,1,2-$PtC_2B_9H_{10}$.

Comment

The molecular structures of $L_2PtC_2B_9H_{10}R$ species continue to be of interest. When the cage C atoms are adjacent in the metal-bonded ligand face, identifying the species as the 3,1,2-*closo*-PtC_2B_9 isomer, two extreme conformations of the $\{PtL_2\}$ fragment are defined: $\kappa = 0°$ is when the $\{PtL_2\}$ plane is parallel to the $\{C_2B_9\}$ mirror plane, and $\kappa = 90°$ is when these planes are orthogonal (Fig. 1). Mingos *et al.* (1978) used the results of extended Hückel molecular-orbital calculations to show that the $\kappa = 90°$ conformation is preferred in the case of minimal steric demands of the carbaborane ligand (*i.e.* R = H) and have shown that the solid-state structure of 3,3-$(PEt_3)_2$-3,1,2-*closo*-$PtC_2B_9H_{11}$ is in broad agreement with this prediction, having $\kappa = 75.8°$. Recent work by O'Connell *et al.* (1995, 1996) has revealed that the barrier to rotation of the $\{Pt(PMe_2Ph)_2\}$ fragment in 3,3-$(PMe_2Ph)_2$-3,1,2-*closo*-$PtC_2B_9H_{11}$ is < 30 kJ mol^{-1} and that, in the crystal, this compound exists as a mixture of two conformers with κ values of 78.1 and 44.2°. The presence of two different conformers is entirely consistent with the barrier to $\{Pt(PMe_2Ph)_2\}$ rotation being of the same order as packing forces.

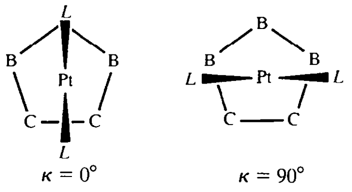
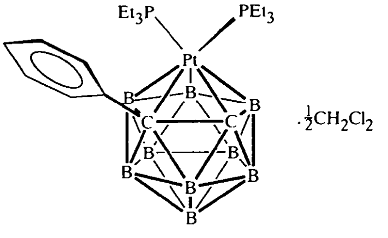


Fig. 1. Extreme conformations of a $\{PtL_2\}$ fragment relative to the C_2B_3 ligand face in the 3,1,2-PtC_2B_9 icosahedra. κ is the dihedral angle between the $\{PtL_2\}$ and B6,B10,X planes, where X is the midpoint of the B9—B12 connectivity.

Given the relatively small energy differences between differing conformations of $L_2PtC_2B_9H_{11}$, the presence of a non-H substituent on one cage C atom would be expected to contribute significantly to the conformation observed. Thus, in 1-Ph-3,3-$(PMe_2Ph)_2$-3,1,2-*closo*-$PtC_2B_9H_{10}$, the measured conformation ($\kappa = 52.8°$) is that which avoids intramolecular crowding between the cage Ph substituent and the phosphine ligands (Baghurst *et al.*, 1993). Surprisingly, the importance of the steric influence of the cage Ph group on the observed conformation in this last compound has recently been questioned (O'Connell *et al.*, 1995, 1996). To establish further experimental evidence in this area, we report herein the structure of the analogous compound 1-Ph-3,3-$(PEt_3)_2$-3,1,2-*closo*-$PtC_2B_9H_{10}$, as its dichloromethane hemisolvate, (I).



(I)

Two crystallographically independent molecules (A and B) of the title compound co-crystallize with one molecule of CH_2Cl_2 of solvation. Figs. 2 and 3 present similar views of molecules A and B and indicate the atomic numbering schemes. The structures of the two molecules are highly congruent. The cages are essentially icosahedral and the Ph substituents on C1 have θ values (Cowie *et al.*, 1994) of 75.6 and 77.4°, resulting in relatively short C1—C2 distances, 1.57 (2) Å in both molecules (Lewis & Welch, 1993). The conformations of the $\{PtP_2\}$ fragments are similarly equivalent in A and B, with κ values of 64.6 and 67.0°, respectively. The Pt—C distances are substantially longer than the Pt—B distances, reflecting localization of the frontier molecular orbitals of the carbaborane ligand on the B atoms of the 'open' face (Mingos *et al.*, 1978), but among the Pt—C connectivities, Pt—C(Ph) [2.701 (12) and 2.672 (13) Å] is significantly longer than Pt—C(H) [2.487 (14) and 2.569 (13) Å]. Thus, the carbaborane ligand is effectively η^4-bonded to platinum. Platinum slip parameters (Mingos *et al.*, 1978) are 0.30 and 0.40 Å in molecules A and B, respectively. The C_2B_3 ligand faces are folded into envelope conformations, with θ and φ values of 2.5 and 5.4°, respectively, in molecule A, and 3.9 and 5.3°, respectively, in molecule B. The Pt—P2 distances (approximately *trans* to CH) are shorter than the Pt—P1 distances (approximately *trans* to B4), reflecting the relative *trans* influences of cage B and cage C atoms.

Thus, the relative conformations of the $\{PtL_2\}$ and cage fragments in the two crystallographically independent molecules of 1-Ph-3,3-$(PEt_3)_2$-3,1,2-*closo*-$PtC_2B_9H_{10}$ are effectively the same. Moreover, this conformation is that found in a second crystalline modification of the same compound ($\kappa = 68.2°$; Thomas *et al.*, 1998) and similar to that in 1-Ph-3,3-$(PMe_2Ph)_2$-3,1,2-*closo*-$PtC_2B_9H_{10}$ ($\kappa = 52.8°$; Baghurst *et al.*, 1993). While we accept that alternative conformations of the non-carbaborane-substituted species 3,3-L_2-3,1,2-*closo*-$PtC_2B_9H_{11}$ are possible in the solid state since the energy differences between them are of the same order as crystal packing forces, it remains invariably true that only one conformation of the substituted compounds 1-Ph-3,3-L_2-3,1,2-*closo*-$PtC_2B_9H_{10}$ has yet been found. We await the report of an alternative conformation with considerable interest.

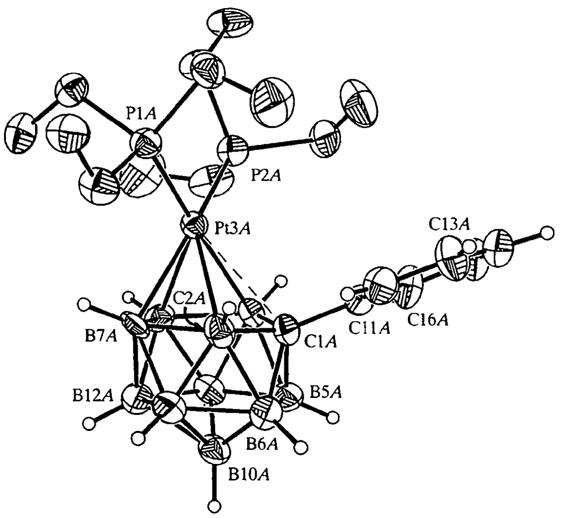


Fig. 2. View of molecule *A* of the title compound with displacement ellipsoids at the 30% probability level for non-H atoms. H atoms are drawn as small circles of arbitary radii for clarity, except for the alkyl H atoms, which have been omitted.

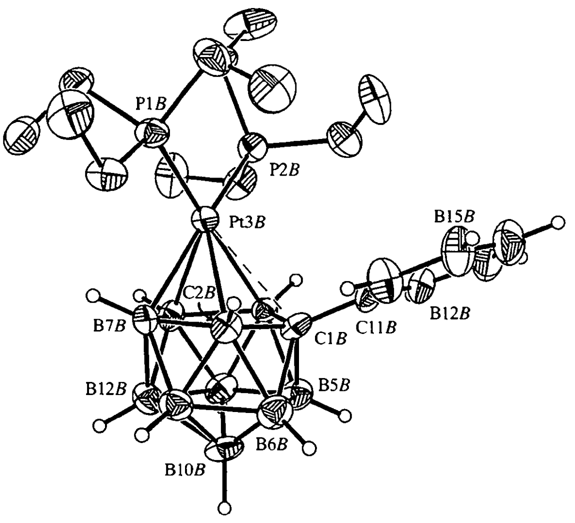


Fig. 3. View of molecule *B* of the title compound with displacement ellipsoids at the 30% probability level for non-H atoms. H atoms are drawn as small circles of arbitary radii for clarity, except for the alkyl H atoms, which have been omitted.

Experimental

The title compound was prepared by a variation of the published method of McGrath & Welch (1995) for the preparation of carbaplatinaboranes, utilizing 1-Ph-1,2-$C_2B_{10}H_{11}$ in place of 1-Ph-2-Me-1,2-$C_2B_{10}H_{10}$. Crystals were grown by slow diffusion of hexane into a dichloromethane solution. Analysis calculated for $C_{20}H_{45}B_9P_2Pt$: C 37.6, H 7.04%; found: C 36.1, H 6.79%. FT-IR (CH_2H_2): ν = 2530 cm^{-1} (B—H). ^{1}H FT-NMR (200 MHz, $CDCl_3$, 298 K, TMS): δ (p.p.m.) 0.83–1.12 (*br m*, 18H, CH_3), 1.80–1.93 (*br m*, 12H, CH_2), 3.89 (C_{cage}—H), 7.13 (*m*, 3H, Ar—H), 7.49 (*d* of *d*, 2H, Ar—H). ^{11}B-{^{1}H} FT-NMR (64.2 MHz, $CDCl_3$, 293 K, $BF_3.Et_2O$): δ (p.p.m.) 13.87 ($^1J^{195}$Pt-B = 254 Hz, 1B), −1.98 (1B), −3.11 (1B), −7.69 (1B), −13.62 (1B), −14.67 (2B), −19.35 (1B), −22.19 (1B). ^{31}P{^{1}H} FT-NMR (81.0 MHz, $CDCl_3$, 293 K, H_3PO_4): δ (p.p.m.) 13.68 (*br d*, $^1J^{195}$Pt-P = 3038 Hz, ^2JP-P not resolved), 8.59 (*br d*, $^1J^{195}$Pt-P = 3388 Hz).

Crystal data

$[Pt(C_8H_{15}B_9)(C_6H_{15}P)_2]$.-
$0.5CH_2Cl_2$
M_r = 682.34
Orthorhombic
$Pna2_1$
a = 33.354 (7) Å
b = 10.260 (2) Å
c = 17.400 (4) Å
V = 5954.5 (2) Å^3
Z = 8
D_x = 1.522 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 11–12°
μ = 4.920 mm^{-1}
T = 293 (2) K
Needle
0.4 × 0.2 × 0.2 mm
Dark orange

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
T_{min} = 0.297, T_{max} = 0.374
5409 measured reflections
5409 independent reflections

4593 reflections with $I > 2\sigma(I)$
θ_{max} = 25°
$h = 0 \rightarrow 39$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 20$
3 standard reflections
frequency: 480 min
intensity decay: 1.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.080
S = 1.063
5409 reflections
592 parameters
H atoms constrained
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 5.2421P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.951 e Å^{-3}
$\Delta\rho_{min}$ = −0.606 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = 0.008 (11)

Table 1. *Selected geometric parameters (Å, °)*

Pt3*A*—P2*A*	2.267 (3)	Pt3*B*—P2*B*	2.269 (3)
Pt3*A*—B8*A*	2.271 (15)	Pt3*B*—B8*B*	2.229 (14)
Pt3*A*—B7*A*	2.279 (12)	Pt3*B*—B7*B*	2.280 (13)
Pt3*A*—P1*A*	2.292 (4)	Pt3*B*—P1*B*	2.291 (4)
Pt3*A*—B4*A*	2.29 (2)	Pt3*B*—B4*B*	2.28 (2)
Pt3*A*—C2*A*	2.487 (14)	Pt3*B*—C2*B*	2.569 (13)
C11*A*—C1*A*	1.515 (14)	C11*B*—C1*B*	1.50 (2)
C1*A*—C2*A*	1.57 (2)	C1*B*—C2*B*	1.57 (2)
P2*A*—Pt3*A*—B8*A*	107.6 (5)	P2*B*—Pt3*B*—B8*B*	110.4 (4)
P2*A*—Pt3*A*—B7*A*	153.7 (4)	P2*B*—Pt3*B*—B7*B*	156.7 (4)
P2*A*—Pt3*A*—P1*A*	98.40 (15)	P2*B*—Pt3*B*—P1*B*	98.83 (15)
P2*A*—Pt3*A*—B4*A*	91.9 (5)	P2*B*—Pt3*B*—B4*B*	90.8 (4)
P2*A*—Pt3*A*—C2*A*	148.5 (3)	P2*B*—Pt3*B*—C2*B*	146.7 (3)

P1*A*—Pt3*A*—B4*A*	164.8 (5)	P1*B*—Pt3*B*—B4*B*	165.3 (4)
P1*A*—Pt3*A*—C2*A*	100.7 (4)	P1*B*—Pt3*B*—C2*B*	100.8 (3)
B8*A*—Pt3*A*—P1*A*	138.0 (4)	B8*B*—Pt3*B*—P1*B*	136.5 (4)
B7*A*—Pt3*A*—P1*A*	99.9 (4)	B7*B*—Pt3*B*—P1*B*	99.3 (4)

The cage C atoms were initially refined as B atoms, being subsequently identified by inspection of the relevant interatomic distances and displacement parameters. The two crystallographically independent molecules appear to be related by the symmetry operation $\frac{3}{4} - x$, $0.068 + y$, $\frac{1}{2} - z$; however, attempts to impose this symmetry on the structure solution or refinement caused the model to become unstable, suggesting that this is merely pseudosymmetry. The need for an absorption correction became apparent when residual peaks of up to 2.46 e Å^{-3} persisted near the Pt atom; the only available method was a refined correction using *DIFABS* (Walker & Stuart, 1983), which resulted in transmission factors consistent with the observed crystal dimensions. After this was applied, a final electron-density map showed a maximum residual electon-density peak of 0.95 e Å^{-3} near Pt3*A*. The H atoms were constrained to ride on the atoms to which they were bonded (C_{aryl}—H = 0.95, C_{alkyl}—H = 0.98 and B—H = 1.08 Å), with displacement parameters set at $1.2U_{eq}$ of that atom (1.5 for CH_3 groups). All alkyl C atoms were constrained to be tetrahedral.

Data collection: *CAD*-4 *Software* (Enraf-Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *CADABS* (Gould & Smith, 1986). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL*/*PC* (Sheldrick, 1994). Software used to prepare material for publication: *SHELXTL*/*PC*.

We thank Heriot–Watt University for the provision of a studentship (RLlT) and the Callery Chemical Company for a generous gift of decaborane.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: MU1341). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1998). C**54**, 591–594

Triaquatris(μ-oxydiacetato)europium(III)-lanthanum(III) Pentahydrate

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Abstract

The new heterobimetallic complex $[\{LaEu(oda)_3(H_2O)_3.5H_2O\}_n]$ (oda = $^-O_2CCH_2OCH_2CO_2^-$) has been synthesized and structurally characterized. Three tridentate oda ligands are coordinated to the smaller Eu^{III} cation, while six adjacent outer carboxylate O atoms and three metal-bound water O atoms are bonded to the larger La^{III} cation. The structure consists of a three-dimensional network with the metal centers bridged by oda carboxylate groups, with Eu···La separations of 6.95 (1) Å.

Comment

Heterometallic carboxylates containing lanthanides are of current interest with regard to chemical processing of lanthanide-containing ceramic materials (Segal, 1989). Among oxodicarboxylic acid derivatives, two heterobimetallic oxydiacetates, $[\{LaLn(oda)_3(H_2O)_3.6H_2O\}_n]$ (Ln = Gd or Y; oda = $^-O_2CCH_2OCH_2CO_2^-$), have been structurally characterized (Baggio *et al.*, 1998). These have been shown to be isomorphous with the reported homometallic complex $[\{La_2(oda)_3(H_2O)_3.5H_2O\}_n]$ (Baggio *et al.*, 1996). In this report, we present the preparation and results of the crystal structure analysis of the related europium–lanthanum heterobimetallic complex $[\{LaEu(oda)_3(H_2O)_3.5H_2O\}_n]$, (1).