plane, as indicated by the O(2)—C(2)—C(1)—O(5) and O(2)—C(2)—C(1)—O(6) conformation angles (Table 10). The maximum displacements of the O(2) atom from this plane are observed in molecule *B* of (IV) [0.51 (1) Å] and in (VIII) [0.49 (1) Å]. Similar trends have been noted in other structures containing the glycolate moiety (Lis, 1980, and references therein). The orientation of the phosphate group relative to the acetate moiety may be described by torsion angles P—O(2)—C(2)—C(1) and O—P—O(2)—C(2) (Table 10). The values of these angles suggest considerable conformational flexibility around the P—O(2) and O(2)—C(2) bonds. It is interesting to note that the carboxylic OH group is *trans* to the O ester atom in (I), (III) and (IV) but *syn* in (II). Both these structural variations were also observed in PEP salts (Lis, 1992).

Bond lengths, bond angles and torsion angles of the ten PG residues described in this work are collected in Table 10. In two crystals, two PG moieties occur in the asymmetric unit. Among the bonds only P—O(2) is partially correlated with the degree of ionization of PG. This bond varies from 1.566 (2) Å in H_3PG (I) to 1.635 (2) Å in the trianion (VIII). However, the values of this bond for the ionized forms with charges 1, 1.5, 2 and 2.5 do not correlate strictly with the degree of ionization of PG. This is in contrast with PEP (Weichsel & Lis, 1991). To facilitate comparison with other phosphate monoester structures, the statistical analysis of the geometry of the singly and doubly ionized phosphate groups in phosphate monoesters was performed (Starynowicz, 1986; Starynowicz, Lis & Weichsel, 1986). Mean values of 1.593 and 1.624 Å were found for P—O(ester) bond lengths in singly and doubly ionized phosphate groups, respectively. In a few examples of non-ionized phosphate groups in non-aromatic phosphate monoesters, the P—O(ester) bond length ranges from 1.567 (4) Å (Srikrishnan, Friday & Parthasarathy, 1979) to 1.594 (3) Å (Weichsel, Lis & Kuczek, 1991); thus, this bond in H_3PG (I) [1.566 (2) Å] is amongst the shortest.

The other bond lengths and angles in the structures are normal within experimental error and do not merit comment. The hydrogen bonds and sodium or potassium coordination are probably the most inportant factors which affect the shape of the system.

Note added in proof. Three new PG structures: $Zn(H_2PG)_2.2H_2O$, $Ca(H_2PG)_2.2H_2O$ and $K_3PG.2H_2O$ were recently determined by the author.

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Structure of 1,2-Diphenylcarbaborane, 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$

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Abstract. 1,2-Diphenyl-1,2-dicarba-*closo*-dodecaborane(12), $C_{14}H_{20}B_{10}$, $M_r = 296.41$, monoclinic, $P2_1/c$, $a = 10.832\ (4)$, $b = 24.890\ (13)$, $c = 13.9243\ (21)$ Å, $\beta = 111.881\ (21)^\circ$, $V = 3483.6$ Å^3, $Z = 8$, $D_x = 1.130$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 0.051$ mm^{-1}, $F(000) = 1232$, $T = 291\ (1)$ K, $R =$

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0.0703 for 3779 independent observed reflections. The C_2B_{10} fragments of the two crystallographically independent molecules are practically superimposable (r.m.s. misfit 0.013 Å), but the phenyl rings of molecule *B* are slightly twisted (in a conrotatory manner) relative to those in molecule *A*. In general terms, however, the phenyl rings in both molecules lie roughly perpendicular to the plane through the atomic sequence C(aryl)—C(cage)—C(cage)—C(aryl). The C(cage)—C(cage) distance is 1.733 (4) Å in molecule *A* and 1.720 (4) Å in molecule *B*.

Introduction. 1,2-Diphenylcarbaborane (1,2-Ph_2-*closo*-$C_2B_{10}H_{10}$) was first reported nearly 30 years ago (Fein, Bobinski, Myers, Schwartz & Cohen, 1963). It is an exceptionally stable compound that has the potential for extensive derivatization, both of the carbaborane polyhedron and of the aromatic rings, the latter being of current interest in the search for new compounds with non-linear optical properties (Murphy, 1992).

Surprisingly, in view of the extensive number of metal compounds with C_2B_9 ligands in which the cage C atoms are substituted with a wide variety of alkyl and/or single aryl functions (Hawthorne, 1975; Grimes, 1981; Housecroft, 1991), there are no reports in the current literature of similar compounds involving $[Ph_2C_2B_9H_9]^{2-}$. We have, however, shown (Lewis & Welch, 1992) that such compounds can have unusual structures that result primarily from steric repulsions between the phenyl groups and the ligands bound to metal vertices. In view of such a finding it was clearly important to characterize fully the stereochemistry of 1,2-diphenylcarbaborane and, accordingly, the study described herein was undertaken.

Table 1. *Coordinates of non-*H *atoms and equivalent isotropic thermal parameters* (Å^2) *for* 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
C(1*A*)	0.8065 (3)	0.06102 (12)	0.20389 (22)	0.0421 (18)
C(2*A*)	0.7619 (3)	0.00084 (13)	0.24464 (24)	0.0491 (20)
B(11*A*)	0.5938 (4)	0.00083 (19)	0.2161 (3)	0.065 (3)
B(3*A*)	0.8413 (4)	0.05004 (15)	0.3334 (3)	0.0500 (24)
B(6*A*)	0.6602 (4)	0.02967 (16)	0.1295 (3)	0.0488 (23)
B(5*A*)	0.6684 (4)	0.10036 (17)	0.1480 (3)	0.0527 (25)
B(4*A*)	0.7829 (4)	0.11293 (16)	0.2752 (3)	0.0526 (25)
B(7*A*)	0.7066 (4)	0.01318 (19)	0.3428 (3)	0.065 (3)
B(12*A*)	0.5637 (5)	0.05374 (19)	0.2885 (4)	0.073 (3)
B(10*A*)	0.5355 (4)	0.06305 (19)	0.1566 (3)	0.060 (3)
B(8*A*)	0.7174 (4)	0.08358 (18)	0.3622 (4)	0.063 (3)
B(9*A*)	0.6092 (4)	0.11480 (19)	0.2471 (4)	0.064 (3)
C(11*A*)	0.9189 (3)	0.06227 (12)	0.16574 (24)	0.0441 (19)
C(12*A*)	1.0480 (3)	0.07209 (15)	0.2339 (3)	0.0615 (24)
C(13*A*)	1.1497 (4)	0.07697 (17)	0.1964 (4)	0.077 (3)
C(14*A*)	1.1240 (4)	0.07352 (17)	0.0928 (4)	0.085 (3)
C(15*A*)	0.9969 (4)	0.06508 (18)	0.0257 (3)	0.081 (3)
C(16*A*)	0.8948 (4)	0.05894 (16)	0.0614 (3)	0.066 (3)
C(21*A*)	0.8366 (3)	−0.04976 (13)	0.2411 (3)	0.0551 (22)
C(22*A*)	0.9466 (4)	−0.06587 (16)	0.3256 (3)	0.069 (3)
C(23*A*)	1.0107 (4)	−0.11389 (18)	0.3235 (4)	0.087 (4)
C(24*A*)	0.9669 (5)	−0.14529 (19)	0.2394 (4)	0.099 (4)
C(25*A*)	0.8582 (6)	−0.13094 (18)	0.1553 (4)	0.103 (4)
C(26*A*)	0.7900 (5)	−0.08261 (15)	0.1556 (3)	0.077 (3)
C(1*B*)	0.4357 (3)	0.22853 (12)	0.52520 (22)	0.0421 (18)
C(2*B*)	0.4043 (3)	0.16842 (12)	0.57262 (23)	0.0416 (18)
B(11*B*)	0.2504 (3)	0.14582 (16)	0.4975 (3)	0.0472 (23)
B(3*B*)	0.4000 (4)	0.22685 (15)	0.6367 (3)	0.0476 (23)
B(6*B*)	0.3508 (4)	0.17871 (15)	0.4409 (3)	0.0476 (23)
B(5*B*)	0.3005 (4)	0.24680 (16)	0.4183 (3)	0.0505 (24)
B(4*B*)	0.3317 (4)	0.27665 (16)	0.5408 (3)	0.0537 (25)
B(7*B*)	0.2812 (4)	0.17586 (17)	0.6200 (3)	0.0517 (24)
B(12*B*)	0.1366 (4)	0.19371 (18)	0.5103 (3)	0.059 (3)
B(10*B*)	0.1824 (4)	0.19514 (17)	0.4007 (3)	0.057 (3)
B(8*B*)	0.2309 (4)	0.24375 (17)	0.5987 (3)	0.059 (3)
B(9*B*)	0.1684 (4)	0.25554 (18)	0.4632 (3)	0.061 (3)
C(11*B*)	0.5753 (3)	0.24146 (12)	0.53702 (23)	0.0458 (19)
C(12*B*)	0.6519 (4)	0.27499 (17)	0.6147 (3)	0.073 (3)
C(13*B*)	0.7808 (4)	0.28702 (18)	0.6252 (3)	0.081 (3)
C(14*B*)	0.8344 (4)	0.26654 (18)	0.5600 (4)	0.080 (3)
C(15*B*)	0.7587 (4)	0.23404 (19)	0.4803 (4)	0.096 (4)
C(16*B*)	0.6299 (4)	0.22111 (15)	0.4693 (3)	0.075 (3)
C(21*B*)	0.5187 (3)	0.13035 (13)	0.62247 (24)	0.0488 (20)
C(22*B*)	0.5996 (4)	0.13668 (17)	0.7253 (3)	0.071 (3)
C(23*B*)	0.7008 (4)	0.10070 (22)	0.7716 (4)	0.091 (4)
C(24*B*)	0.7234 (4)	0.05858 (20)	0.7163 (5)	0.096 (4)
C(25*B*)	0.6430 (5)	0.05245 (17)	0.6152 (4)	0.092 (4)
C(26*B*)	0.5398 (4)	0.08770 (15)	0.5672 (3)	0.071 (3)

Experimental. The title compound was prepared by a modified version of the literature procedure (Fein, Bobinski, Myers, Schwartz & Cohen, 1963) and recrystallized from an acetone–water solution. Colourless diffraction-quality blocks were grown by slow cooling of a methanol solution. Crystal, 0.3 × 0.2 × 0.2 mm, mounted on a glass fibre and set on an Enraf–Nonius CAD-4 diffractometer (graphite monochromator); cell parameters and orientation matrix from least-squares refinement of the setting angles ($6 < \theta < 12°$) of 25 centred reflections; data collection by ω–2θ scans in 96 steps with ω-scan width $(0.8 + 0.34\tan\theta)°$; one quadrant of data (h 0 to 12, k 0 to 29, l −16 to 16) measured for $1 \leq \theta \leq 25°$ over 132 X-ray hours with no appreciable decay or movement; corrections for Lorentz and polarization effects applied (Gould & Smith, 1986); of 6121 data measured, 3779 [$F \geq 2.0\sigma(F)$] used to solve [direct methods (Sheldrick, 1986) for C and B atoms; difference Fourier methods (Sheldrick, 1976) for cage H atoms] and refine (least squares on F) the structure to isotropic convergence; cage H atoms allowed positional refinement, but phenyl H atoms set in idealized positions (C—H 1.08 Å); empirical absorption correction (Walker & Stuart, 1983) applied (correction factors 0.89–1.12); all non-H atoms refined with anisotropic thermal parameters; all H atoms refined with single group thermal parameter, 0.077 (3) Å^2 at convergence; weights assigned according to $w^{-1} = [\sigma^2(F) + 0.006124F^2]$; crystallographically independent molecules refined in alternate cycles (each with 248 variable parameters); $R = 0.0703$, $wR = 0.0992$, $S = 0.928$; max. shift/e.s.d. in final cycle < 0.02 for positional parameters; max. and min. residues in final ΔF synthesis 0.18 and −0.29 e Å^{-3}, respectively; scattering factors inlaid in *SHELX76*; Figs. 1 and 2 drawn using *EASYORTEP* (Mallinson & Muir, 1985); molecular geometry calculations *via CALC* (Gould & Taylor, 1986).

Table 2. *Interatomic distances* (Å) *and interbond angles* (°) *for* 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$

C(1A)—C(2A)	1.733 (4)	C(1B)—C(2B)	1.720 (4)
C(1A)—B(3A)	1.721 (5)	C(1B)—B(3B)	1.735 (5)
C(1A)—B(6A)	1.723 (5)	C(1B)—B(6B)	1.719 (5)
C(1A)—B(5A)	1.713 (5)	C(1B)—B(5B)	1.715 (5)
C(1A)—B(4A)	1.706 (5)	C(1B)—B(4B)	1.712 (5)
C(1A)—C(11A)	1.500 (4)	C(1B)—C(11B)	1.494 (4)
C(2A)- -B(11A)	1.713 (6)	C(2B)—B(11B)	1.700 (5)
C(2A)—B(3A)	1.725 (5)	C(2B)—B(3B)	1.716 (5)
C(2A)—B(6A)	1.727 (5)	C(2B)—B(6B)	1.724 (5)
C(2A)—B(7A)	1.712 (6)	C(2B)—B(7B)	1.705 (5)
C(2A)—C(21A)	1.508 (5)	C(2B)—C(21B)	1.508 (4)
B(11A)—B(6A)	1.771 (6)	B(11B)—B(6B)	1.764 (5)
B(11A)—B(7A)	1.759 (7)	B(11B)—B(7B)	1.777 (6)
B(11A)—B(12A)	1.761 (7)	B(11B)—B(12B)	1.772 (6)
B(11A)—B(10A)	1.759 (6)	B(11B)—B(10B)	1.768 (6)
B(11A)—H(11A)	1.10 (4)	B(11B)—H(11B)	1.07 (4)
B(3A)—B(4A)	1.768 (6)	B(3B)—B(4B)	1.769 (6)
B(3A)—B(7A)	1.770 (6)	B(3B)—B(7B)	1.760 (6)
B(3A)—B(8A)	1.750 (6)	B(3B)—B(8B)	1.757 (6)
B(3A)—H(3A)	1.09 (4)	B(3B)—H(3B)	1.02 (4)
B(6A)—B(5A)	1.776 (6)	B(6B)—B(5B)	1.772 (6)
B(6A)—B(10A)	1.742 (6)	B(6B)—B(10B)	1.746 (6)
B(6A)—H(6A)	1.10 (4)	B(6B)—H(6B)	1.03 (4)
B(5A)—B(4A)	1.771 (6)	B(5B)—B(4B)	1.773 (6)
B(5A)—B(10A)	1.754 (6)	B(5B)—B(10B)	1.766 (6)
B(5A)—B(9A)	1.762 (6)	B(5B)—B(9B)	1.776 (6)
B(5A)—H(5A)	1.03 (4)	B(5B)—H(5B)	1.12 (4)
B(4A)—B(8A)	1.774 (6)	B(4B)—B(8B)	1.781 (6)
B(4A)—B(9A)	1.774 (6)	B(4B)—B(9B)	1.774 (6)
B(4A)—H(4A)	1.11 (4)	B(4B)—H(4B)	1.04 (4)
B(7A)—B(12A)	1.764 (7)	B(7B)—B(12B)	1.789 (6)
B(7A)—B(8A)	1.770 (7)	B(7B)—B(8B)	1.766 (6)
B(7A)—H(7A)	1.15 (4)	B(7B)—H(7B)	1.07 (4)
B(12A)—B(10A)	1.762 (7)	B(12B)—B(10B)	1.773 (6)
B(12A)—B(8A)	1.761 (7)	B(12B)—B(8B)	1.781 (6)
B(12A)—B(9A)	1.760 (7)	B(12B)—B(9B)	1.757 (6)
B(10A)—B(9A)	1.771 (6)	B(10B)—B(9B)	1.772 (6)
B(10A)—H(10A)	1.06 (4)	B(10B)—H(10B)	1.16 (4)
B(8A)—B(9A)	1.774 (7)	B(8B)—B(9B)	1.774 (6)
B(8A)—H(8A)	1.09 (4)	B(8B)—H(8B)	1.10 (4)
B(9A)—H(9A)	1.10 (4)	B(9B)—H(9B)	1.11 (4)
C(11A)—C(12A)	1.388 (5)	C(11B)—C(12B)	1.373 (5)
C(11A)—C(16A)	1.380 (5)	C(11B)—C(16B)	1.382 (5)
C(12A)—C(13A)	1.390 (6)	C(12B)—C(13B)	1.381 (6)
C(13A)—C(14A)	1.365 (6)	C(13B)—C(14B)	1.347 (6)
C(14A)—C(15A)	1.361 (7)	C(14B)—C(15B)	1.371 (7)
C(15A)—C(16A)	1.379 (6)	C(15B)—C(16B)	1.384 (6)
C(21A)—C(22A)	1.386 (5)	C(21B)—C(22B)	1.381 (5)
C(21A)—C(26A)	1.376 (6)	C(21B)—C(26B)	1.379 (5)
C(22A)—C(23A)	1.388 (6)	C(22B)—C(23B)	1.375 (6)
C(23A)—C(24A)	1.338 (8)	C(23B)—C(24B)	1.376 (7)
C(24A)—C(25A)	1.363 (8)	C(24B)—C(25B)	1.360 (8)
C(25A)—C(26A)	1.412 (7)	C(25B)—C(26B)	1.382 (7)

B(3A)—C(1A)—C(2A)	59.91 (20)	B(3B)—C(1B)—C(2B)	59.56 (19)
B(3A)—C(1A)—B(4A)	62.12 (22)	B(3B)—C(1B)—B(4B)	61.75 (22)
B(6A)—C(1A)—C(2A)	59.96 (20)	B(6B)—C(1B)—C(2B)	60.18 (19)
B(6A)—C(1A)—B(5A)	62.23 (22)	B(6B)—C(1B)—B(5B)	62.12 (21)
B(5A)—C(1A)—B(4A)	62.40 (22)	B(5B)—C(1B)—B(4B)	62.31 (22)
C(2A)—C(1A)—C(11A)	119.75 (25)	C(2B)—C(1B)—C(11B)	118.82 (25)
B(3A)—C(1A)—C(11A)	119.0 (3)	B(3B)—C(1B)—C(11B)	117.5 (3)
B(6A)—C(1A)—C(11A)	118.9 (3)	B(6B)—C(1B)—C(11B)	119.5 (3)
B(5A)—C(1A)—C(11A)	120.9 (3)	B(5B)—C(1B)—C(11B)	122.7 (3)
B(4A)—C(1A)—C(11A)	120.5 (3)	B(4B)—C(1B)—C(11B)	121.5 (3)
B(11A)—C(2A)—B(6A)	61.95 (23)	B(11B)—C(2B)—B(6B)	62.01 (21)
B(11A)—C(2A)—B(7A)	61.79 (25)	B(11B)—C(2B)—B(7B)	62.94 (22)
B(3A)—C(2A)—C(1A)	59.69 (20)	B(3B)—C(2B)—C(1B)	60.66 (19)
B(3A)—C(2A)—B(7A)	61.99 (24)	B(3B)—C(2B)—B(7B)	61.93 (22)
B(6A)—C(2A)—C(1A)	59.74 (20)	B(6B)—C(2B)—C(1B)	59.90 (19)
C(1A)—C(2A)—C(21A)	119.5 (3)	C(1B)—C(2B)—C(21B)	118.49 (25)
B(11A)—C(2A)—C(21A)	122.0 (3)	B(11B)—C(2B)—C(21B)	121.6 (3)
B(3A)—C(2A)—C(21A)	119.1 (3)	B(3B)—C(2B)—C(21B)	118.1 (3)
B(6A)—C(2A)—C(21A)	118.7 (3)	B(6B)—C(2B)—C(21B)	118.4 (3)
B(7A)—C(2A)—C(21A)	121.9 (3)	B(7B)—C(2B)—C(21B)	121.2 (3)
C(2A)—B(11A)—B(6A)	59.42 (23)	C(2B)—B(11B)—B(6B)	59.68 (21)
C(2A)—B(11A)—B(7A)	59.07 (24)	C(2B)—B(11B)—B(7B)	58.66 (21)
B(6A)—B(11A)—B(10A)	59.16 (25)	B(6B)—B(11B)—B(10B)	59.25 (23)
B(7A)—B(11A)—B(12A)	60.2 (3)	B(7B)—B(11B)—B(12B)	60.58 (23)
B(12A)—B(11A)—B(10A)	60.1 (3)	B(12B)—B(11B)—B(10B)	60.12 (24)
C(1A)—B(3A)—C(2A)	60.40 (20)	C(1B)—B(3B)—C(2B)	59.78 (19)
C(1A)—B(3A)—B(4A)	58.52 (21)	C(1B)- -B(3B)—B(4B)	58.49 (21)
C(2A)—B(3A)—B(7A)	58.66 (23)	C(2B)—B(3B)—B(7B)	58.71 (21)
B(4A)—B(3A)—B(8A)	60.56 (24)	B(4B)—B(3B)—B(8B)	60.65 (23)
B(7A)—B(3A)—B(8A)	60.4 (3)	B(7B)—B(3B)—B(8B)	60.29 (23)
C(1A)—B(6A)—C(2A)	60.30 (20)	C(1B)—B(6B)—C(2B)	59.92 (19)

Table 2 (*cont.*)

C(1A)—B(6A)—B(5A)	58.60 (21)	C(1B)—B(6B)—B(5B)	58.82 (21)
C(2A)—B(6A)—B(11A)	58.64 (23)	C(2B)—B(6B)—B(11B)	58.31 (20)
B(11A)—B(6A)—B(10A)	60.09 (25)	B(11B)—B(6B)—B(10B)	60.50 (23)
B(5A)—B(6A)—B(10A)	59.80 (24)	B(5B)—B(6B)—B(10B)	60.25 (23)
C(1A)—B(5A)—B(6A)	59.17 (21)	C(1B)—B(5B)—B(6B)	59.06 (21)
C(1A)—B(5A)—B(4A)	58.59 (22)	C(1B)—B(5B)—B(4B)	58.77 (21)
B(6A)—B(5A)—B(10A)	59.15 (24)	B(6B)—B(5B)—B(10B)	59.15 (23)
B(4A)—B(5A)—B(9A)	60.28 (25)	B(4B)—B(5B)—B(9B)	59.99 (24)
B(10A)—B(5A)—B(9A)	60.5 (3)	B(10B)—B(5B)—B(9B)	60.04 (24)
C(1A)—B(4A)—B(3A)	59.36 (21)	C(1B)—B(4B)—B(3B)	59.76 (21)
C(1A)—B(4A)—B(5A)	59.00 (22)	C(1B)—B(4B)—B(5B)	58.92 (21)
B(3A)—B(4A)—B(8A)	59.22 (24)	B(3B)—B(4B)—B(8B)	59.34 (23)
B(5A)—B(4A)—B(9A)	59.61 (24)	B(5B)—B(4B)—B(9B)	60.10 (24)
B(8A)—B(4A)—B(9A)	60.0 (3)	B(8B)—B(4B)—B(9B)	59.89 (24)
C(2A)—B(7A)—B(11A)	59.14 (24)	C(2B)—B(7B)—B(11B)	58.43 (22)
C(2A)—B(7A)—B(3A)	59.36 (23)	C(2B)—B(7B)—B(3B)	59.35 (21)
B(11A)—B(7A)—B(12A)	60.0 (3)	B(11B)—B(7B)—B(12B)	59.58 (23)
B(3A)—B(7A)—B(8A)	59.3 (3)	B(3B)—B(7B)—B(8B)	59.78 (23)
B(12A)—B(7A)—B(8A)	59.8 (3)	B(12B)—B(7B)—B(8B)	60.12 (24)
B(11A)—B(12A)—B(7A)	59.8 (3)	B(11B)—B(12B)—B(7B)	59.89 (23)
B(11A)—B(12A)—B(10A)	59.9 (3)	B(11B)—B(12B)—B(10B)	59.84 (23)
B(7A)—B(12A)—B(8A)	60.3 (3)	B(7B)—B(12B)—B(8B)	59.31 (24)
B(10A)—B(12A)—B(9A)	60.4 (3)	B(10B)—B(12B)—B(9B)	60.27 (25)
B(8A)—B(12A)—B(9A)	60.5 (3)	B(8B)—B(12B)—B(9B)	60.21 (25)
B(11A)—B(10A)—B(6A)	60.8 (3)	B(11B)—B(10B)—B(6B)	60.25 (23)
B(11A)—B(10A)—B(12A)	60.0 (3)	B(11B)—B(10B)—B(12B)	60.03 (24)
B(6A)—B(10A)—B(5A)	61.05 (24)	B(6B)—B(10B)—B(5B)	60.61 (23)
B(5A)—B(10A)—B(9A)	60.0 (3)	B(5B)—B(10B)—B(9B)	60.28 (24)
B(12A)—B(10A)—B(9A)	59.8 (3)	B(12B)—B(10B)—B(9B)	59.39 (25)
B(3A)—B(8A)—B(4A)	60.22 (24)	B(3B)—B(8B)—B(4B)	60.01 (23)
B(3A)—B(8A)—B(7A)	60.4 (3)	B(3B)—B(8B)—B(7B)	59.94 (23)
B(4A)—B(8A)—B(9A)	60.0 (3)	B(4B)—B(8B)—B(9B)	59.88 (24)
B(7A)—B(8A)—B(12A)	59.9 (3)	B(7B)—B(8B)—B(12B)	60.57 (24)
B(12A)—B(8A)—B(9A)	59.7 (3)	B(12B)—B(8B)—B(9B)	59.21 (25)
B(5A)—B(9A)—B(4A)	60.10 (25)	B(5B)—B(9B)—B(4B)	59.92 (24)
B(5A)—B(9A)—B(10A)	59.5 (3)	B(5B)—B(9B)—B(10B)	59.68 (24)
B(4A)—B(9A)—B(8A)	60.0 (3)	B(4B)—B(9B)—B(8B)	60.23 (24)
B(12A)—B(9A)—B(10A)	59.9 (3)	B(12B)—B(9B)—B(10B)	60.33 (25)
B(12A)—B(9A)—B(8A)	59.8 (3)	B(12B)—B(9B)—B(8B)	60.57 (25)
C(1A)—C(11A)—C(12A)	120.4 (3)	C(1B) C(11B)—C(12B)	120.5 (3)
C(1A)—C(11A)—C(16A)	120.8 (3)	C(1B)—C(11B)—C(16B)	121.2 (3)
C(12A)—C(11A)—C(16A)	118.6 (3)	C(12B)—C(11B)—C(16B)	118.3 (3)
C(11A)—C(12A)—C(13A)	119.7 (4)	C(11B)—C(12B)—C(13B)	120.4 (4)
C(12A)—C(13A)—H(13A)	119.6 (5)	C(12B)—C(13B)—C(14B)	121.2 (4)
C(12A)—C(13A)—C(14A)	120.9 (4)	C(13B)—C(14B)—C(15B)	119.4 (4)
C(13A)—C(14A)—C(15A)	119.4 (4)	C(14B)—C(15B)—C(16B)	120.1 (4)
C(14A)—C(15A)—C(16A)	120.8 (4)	C(11B)—C(16B)—C(15B)	120.6 (4)
C(11A)—C(16A)—C(15A)	120.6 (4)	C(2B)—C(21B)—C(22B)	120.0 (3)
C(2A)—C(21A)—C(22A)	121.0 (3)	C(2B)—C(21B)—C(26B)	120.3 (3)
C(2A)—C(21A)—C(26A)	119.8 (3)	C(22B)—C(21B)—C(26B)	119.6 (3)
C(22A)—C(21A)—C(26A)	119.0 (4)	C(21B)—C(22B)—C(23B)	119.9 (4)
C(21A)—C(22A)—C(23A)	120.6 (4)	C(22B)—C(23B)—C(24B)	120.7 (5)
C(22A)—C(23A)—C(24A)	120.3 (5)	C(23B)—C(24B)—C(25B)	119.1 (5)
C(23A)—C(24A)—C(25A)	120.6 (5)	C(24B)—C(25B)—C(26B)	121.3 (5)
C(24A)—C(25A)—C(26A)	120.4 (5)	C(21B)—C(26B)—C(25B)	119.4 (4)
C(21A)—C(26A)—C(25A)	119.0 (4)		

Discussion. Lists of coordinates of refined non-H atoms and equivalent isotropic thermal parameters are given in Table 1.* Table 2 details internuclear distances and selected interbond angles. There are two crystallographically independent molecules (*A* and *B*) in the asymmetric fraction of the unit cell. Figs. 1 and 2 show similar perspective views of single molecules of *A* and *B*, respectively, and give the atomic numbering scheme adopted. There are no close contacts between molecules.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and full geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55794 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: MU1026]

The C_2B_{10} cages of 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ have the expected icosahedral architecture (Wade, 1971). A root-mean-square misfit calculation (Macgregor, Wynd, Gould, Moulden, Taylor, Yellowlees & Welch, 1991) on the C_2B_{10} portions of the two crystallographically independent molecules affords an overall fit of only 0.013 Å, with the greatest individual misfits occurring for C(2) (0.019 Å), B(7) (0.018 Å) and B(12) (0.018 Å). Inclusion of the phenyl ring C atoms in the calculation raises the r.m.s. misfit value to 0.151 Å. This arises from the fact that in molecule *B* (which has approximately C_2 symmetry) the phenyl rings are somewhat twisted, in a conrotatory fashion, about their C(cage)—C(aryl) bonds, relative to those in molecule *A* (which has approximate C_{2v} symmetry). Hence, in the calculation which includes the phenyl ring C atoms, individual misfits for the cage atoms are all <0.07 Å, while the average for the ring C atoms is >0.17 Å.

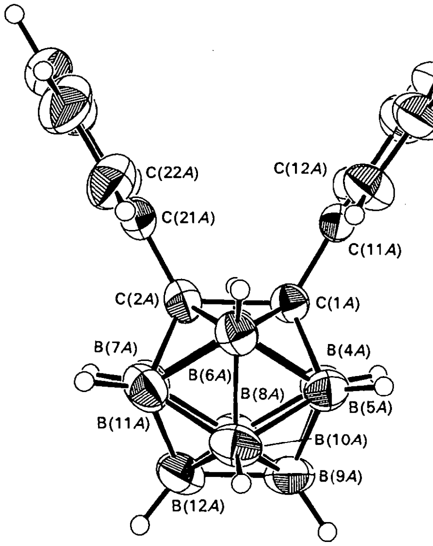

Fig. 1. Perspective view of molecule *A* of 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ (50% thermal ellipsoids, except for H atoms which have artificial radii of 0.1 Å for clarity). H atoms carry the same number as the B or C atom to which they are bound, except that H(12*AX*) is bonded to C(12*A*) and H(12*BX*) is bonded to C(12*B*).

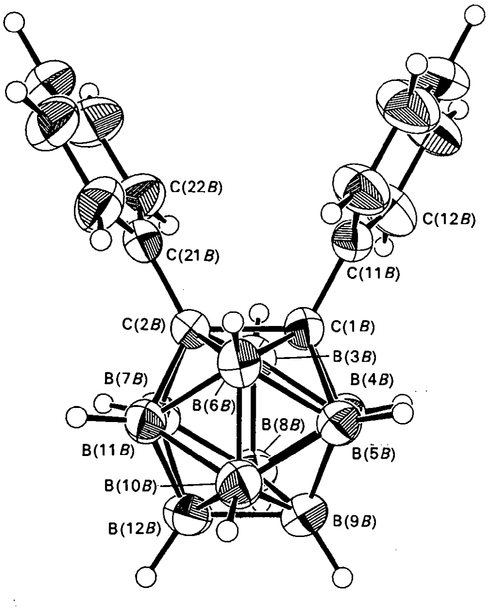

Fig. 2. Perspective view of molecule *B* of 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$.

It is convenient to describe the orientation of the phenyl rings in aryl-substituted 1,2-carbaboranes by θ, the average difference between 90° and the moduli of the C(cage)—C(cage)—C—C torsion angles. In molecule *A*, θ values are 2.4 [ring C(11)–C(16)] and 2.3° [ring C(21)–C(26)] while in molecule *B*, the θ values are 9.2 and 8.0°, respectively. Initially, it would appear reasonable to assume that these generally low θ values are the result of mutual repulsion between the two phenyl groups. Indeed, the idea that some degree of interphenyl intramolecular crowding exists in 1,2-diphenylcarbaborane, given the conformation adopted, seems likely given that the C(1)—C(2) distances, 1.733 (4) Å in molecule *A* and 1.720 (4) Å in molecule *B*, are substantially longer than in 1,2-L_2-1,2-*closo*-$C_2B_{10}H_{10}$ ($L \neq$ aryl) species (*e.g.* Voet & Lipscomb, 1964; Kirillova, Klimova, Struchkov & Stanko, 1979), but fully consistent with the results of a number of structure determinations on such species for which L = aryl (*e.g.* Lindeman, Khotina, Teplyakov, Struchkov & Korshak, 1988; Murphy, 1992).

However, an *electronic* contribution to the long C(1)—C(2) distances in 1,2-L_2-1,2-*closo*-$C_2B_{10}H_{10}$ (L = aryl) at low θ values may be established from the results of a series of extended Hückel molecular-orbital calculations (Howell, Rossi, Wallace, Haraki & Hoffmann, 1977) on idealized models of 1-Ph-1,2-*closo*-$C_2B_{10}H_{11}$ and 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$, constructed with B—B = 1.85, B—C = 1.7575, C(cage)—C(cage) = 1.65, B—H = 1.15, C(cage)—H = 1.65, C(cage)—C(aryl) = 1.50, C(aryl)—C(aryl) = 1.395 and C(aryl)—H = 1.08 Å. These studies were undertaken to probe the optimum conformations of mono- and diphenylcarbaborane as a function of θ. For 1-Ph-1,2-*closo*-$C_2B_{10}H_{11}$, the conformation with $\theta = 0°$ is least stable while that with $\theta = 90°$ is most stable (Fig. 3), by *ca* 0.2 e V.

Reduced overlap populations for C(1)—C(2) and, where appropriate, C(cage)—C(aryl) for 1-Ph-1,2-*closo*-$C_2B_{10}H_{11}$ and 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ are listed in Table 3, along with the C(1)—C(2) population for the parent species 1,2-*closo*-$C_2B_{10}H_{12}$. Clearly, the C(cage)—C(cage) bonding is weakened by the introduction of either one or two phenyl groups at $\theta = 0°$, but strengthened at $\theta = 90°$. Thus, as the Ph groups of 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ synchronously twist, in a conrotatory fashion, from 0 to 90°, the C(1)—C(2) bond is predicted to shorten, and it may be that, although the changes are small, some degree of experimental support for these theoretical conclusions lies in the fact that C(1)—C(2) is just significantly shorter [$\Delta = 0.013$ (6) Å] in molecule *B* ($\langle\theta\rangle = 8.6°$) than in molecule *A* ($\langle\theta\rangle = 2.4°$). Notably, the C(cage)—C(aryl) bonds are also strongest at $\theta = 90°$, implying that this conformation affords the most efficient conjugation between aryl and cage fragments. For 1-Ph-1,2-*closo*-$C_2B_{10}H_{11}$ the $\theta = 90°$ conformation is clearly sterically allowed, but for 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ it is not. Although a conrotatory twisting of both phenyl groups about their C(cage)—C(aryl) bonds, starting at $\theta = 0°$, initially stabilizes this molecule at about the same rate as for the monophenyl analogue (Fig. 4), from $\theta \simeq 40°$ additional twisting produces increasingly unfavourable contacts between approaching H(*ortho*) and C(*ortho*) atoms and results in rapid molecular destabilization.

In spite of this, a carbametallaborane analogue of the $\theta = 90°$ conformation of 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ has recently been reported by us (Lewis & Welch, 1992). In 1,2-Ph_2-3-(η-C_5Me_5)-3,1,2-*pseudocloso*-$RhC_2B_9H_9$, the steric demands of the η-C_5Me_5 ligand force the carbaborane phenyl rings to lie essentially coplanar ($\theta \simeq 90°$) and the H(*ortho*)···H(*ortho*) contact prises open the C(1)—C(2) connectivity to about 2.51 Å. It is clear that the steric requirements of the phenyl substituents in a wide range of derivatives of 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ could have unusual and interesting stereochemical consequences, and future contributions from this laboratory will address such possibilities (*e.g.* Cowie, Donohoe, Douek & Welch, 1993; Lewis & Welch, 1993; Cowie, Lewis & Welch, 1993; Kyd, Yellowlees & Welch, 1993).

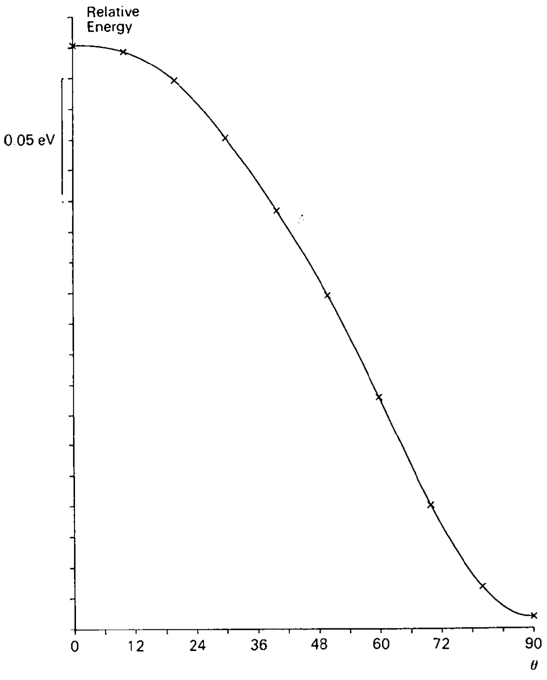

Fig. 3. Relative energy (eV) *versus* θ (°) for 1-Ph-1,2-*closo*-$C_2B_{10}H_{11}$.

Table 3. *Reduced overlap populations for* C—C *interactions in carbaboranes*

	C(cage)—C(cage)	C(cage)—C(aryl)
1,2-*closo*-$C_2B_{10}H_{12}$	0.5346	
1-Ph-1,2-*closo*-$C_2B_{10}H_{11}$ ($\theta = 0°$)	0.5295	0.8416
1-Ph-1,2-*closo*-$C_2B_{10}H_{11}$ ($\theta = 90°$)	0.5414	0.8575
1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ ($\theta = 0°$)	0.5229	0.8438
1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$ ($\theta = 90°$)	0.5447	0.8520

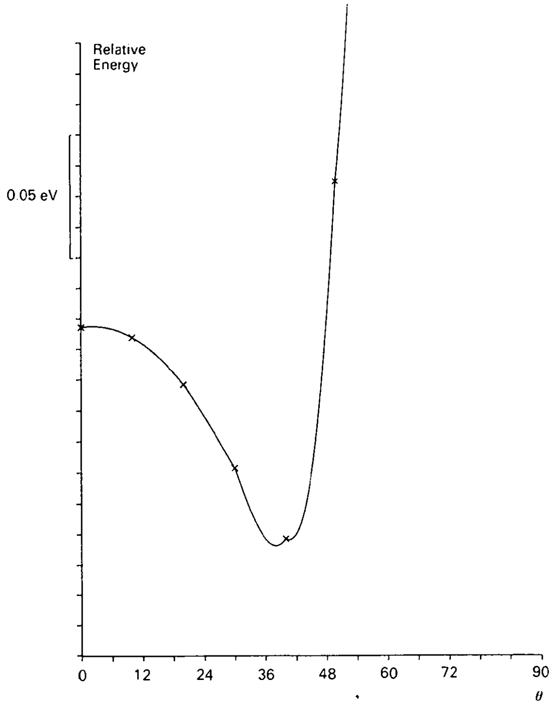

Fig. 4. Relative energy (eV) *versus* θ (°, conrotatory twist) for 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$.

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Structures of $[HNEt_3]^+$ and $[Me_3NCH_2C_6H_5]^+$ Salts of [7,8-Ph_2-7,8-*nido*-$C_2B_9H_{10}]^-$

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Abstract. Triethylammonium 7,8-diphenyl-7,8-dicarba-*nido*-decahydroundecaborate(1−), $C_6H_{16}N^+.C_{14}H_{20}B_9^-$, $M_r = 387.80$, triclinic, $P\bar{1}$, $a = 11.014$ (4), $b = 11.030$ (7), $c = 12.333$ (6) Å, $\alpha = 67.83$ (5), $\beta = 80.78$ (4), $\gamma = 60.20$ (5)°, $V = 1203.3$ Å^3, $Z = 2$, $D_x = 1.070$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 0.052$ mm^{-1}, $F(000) = 416$, $T = 291$ (1) K, $R = 0.1074$ for 3289 independent observed reflections. Benzyltrimethylammonium 7,8-diphenyl-7,8-dicarba-*nido*-decahydroundecaborate(1−), $C_{10}H_{16}N^+.C_{14}H_{20}B_9^-$, $M_r = 435.85$, monoclinic, $P2_1/n$, $a = 10.751$ (4), $b = 21.662$ (4), $c = 11.9745$ (25) Å, $\beta = 106.592$ (23)°, $V = 2672.5$ Å^3, $Z = 4$, $D_x = 1.083$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 0.053$ mm^{-1}, $F(000) = 928$, $T = 185$ (1) K, $R = 0.0637$ for 3857 independent observed reflections. In both determinations, the phenyl substituents lie very roughly orthogonal to the open C_2B_3 face of the anion, pairs of rings being twisted (in a conrotatory manner) by an average of 7.8° for the $[HNEt_3]^+$ salt, and 19.0° for the $[Me_3NCH_2C_6H_5]^+$ salt, from this extreme. In the latter case, this twist is traced to interion contacts. The C(cage)—C(cage) distances, 1.590 (5) and 1.602 (3) Å, respectively, and the mean facial B—B and facial B—C distances are discussed in relation to the equivalent distances in 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$.

Introduction. The preceding paper (Lewis & Welch, 1993*a*) reports the molecular structure of 1,2-Ph_2-1,2-*closo*-$C_2B_{10}H_{10}$, noting the relatively long C(1)—C(2) connectivity [1.727 (6) Å averaged over the two crystallographically independent molecules] and the low θ values [θ is the average difference between 90° and the moduli of the C(cage)—C(cage)—C—C torsion angles] that describe the molecular conformation.

Our interest in diphenylcarbaborane rests primarily in its use as a ligand to *d*- and *f*-block metals, predominantly in the partially degraded form [7,8-Ph_2-7,8-*nido*-$C_2B_9H_9]^{2-}$ [note the change in conventional numbering between related *closo* and *nido* polyhedra (Casey, Evans & Powell, 1983)]. We have already shown (Lewis & Welch, 1992) that unusual structure deformation can arise when the phenyl

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