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# Tetraethylammonium 12-phenylethynyl-carba-*closo*-dodecaborate, [Et<sub>4</sub>N][12-PhCC-*closo*-CB<sub>11</sub>H<sub>11</sub>]

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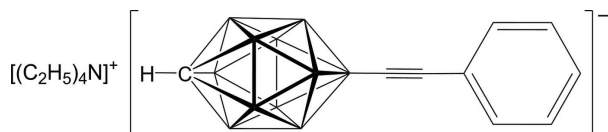
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.101; data-to-parameter ratio = 11.6.

The asymmetric unit of the title compound,  $\text{C}_8\text{H}_{20}\text{N}^+\cdot\text{C}_9\text{H}_{16}\text{B}_{11}^-$  or  $[\text{Et}_4\text{N}][12\text{-PhCC-}i\text{closo-CB}_{11}\text{H}_{11}]^-$  anion is close to possessing a non-crystallographic plane of mirror symmetry with a nearly linear  $\text{B}-\text{C}\equiv\text{C}-\text{C}$  group, with  $\text{B}-\text{C}\equiv\text{C}$  and  $\text{C}\equiv\text{C}-\text{C}$  angles of  $177.15$  (16) and  $176.64$  (17)°, respectively.

## Related literature

Carba-*closo*-dodecaborate anions with functional groups are potential building blocks for a variety of applications, for example ionic liquids and liquid crystals, see: Körbe *et al.* (2006). Recently, we have shown that  $\{i\text{closo-CB}_{11}\}$  clusters with one or two alkynyl groups bonded to boron are accessible by Pd-catalysed Kumada-type cross-coupling reactions starting from the corresponding mono- and diiodinated clusters, see: Finze (2008, 2009).



## Experimental

### Crystal data

$\text{C}_8\text{H}_{20}\text{N}^+\cdot\text{C}_9\text{H}_{16}\text{B}_{11}^-$   
 $M_r = 373.38$   
Triclinic,  $P\bar{1}$   
 $a = 8.8201$  (6) Å  
 $b = 12.0929$  (11) Å  
 $c = 12.1858$  (11) Å  
 $\alpha = 81.032$  (7)°  
 $\beta = 79.899$  (7)°

$\gamma = 71.553$  (7)°  
 $V = 1206.82$  (18) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.05$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.30 \times 0.25 \times 0.20$  mm

### Data collection

Stoe Stadi CCD diffractometer  
Absorption correction: none  
17081 measured reflections

4219 independent reflections  
3228 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.051$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.101$   
 $S = 1.00$   
4219 reflections  
363 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.16$  e Å<sup>-3</sup>

Data collection: *CrysAlis CCD* (Kuma, 2000); cell refinement: *CrysAlis RED* (Kuma, 2000); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2103).

## References

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**supplementary materials**

*Acta Cryst.* (2009). E65, o1048 [ doi:10.1107/S1600536809013300 ]

**Tetraethylammonium 12-phenylethynylcarba-*closo*-dodecaborate, [Et<sub>4</sub>N][12-PhCC-*closo*-CB<sub>11</sub>H<sub>11</sub>]**

**M. Finze and G. J. Reiss**

**Comment**

Carba-*closo*-dodecaborate anions with functional groups are potential building blocks for a variety of applications, for example ionic liquids and liquid crystals (Körbe, 2006). Recently, we have shown that {*closo*-CB<sub>11</sub>} clusters with one or two alkynyl groups bonded to boron are accessible by Pd-catalyzed Kumada-type cross-coupling reactions starting from the corresponding mono- and diiodinated clusters, respectively (Finze, 2008, 2009). The title compound [Et<sub>4</sub>N][12-PhCC-*closo*-CB<sub>11</sub>H<sub>11</sub>] crystallizes in the triclinic centrosymmetric space group P $\bar{1}$  with one formula unit in the asymmetric unit. The bond lengths and angles in the [12-PhCC-*closo*-CB<sub>11</sub>H<sub>11</sub>]<sup>-</sup> anion in its [Et<sub>4</sub>N]<sup>+</sup> salt are close to the values reported for the respective Cs<sup>+</sup> salt (Finze, 2008). However, the quality of the data for the [Et<sub>4</sub>N]<sup>+</sup> salt described herein is significantly better than the quality of the data obtained for the Cs<sup>+</sup> salt. The thermal properties of [Et<sub>4</sub>N][12-PhCC-*closo*-CB<sub>11</sub>H<sub>11</sub>] were studied by differential scanning calorimetry (DSC). The salt melts at 433 K and is thermally stable up to 518 K.

**Experimental**

[Et<sub>4</sub>N][12-PhCC-*closo*-CB<sub>11</sub>H<sub>11</sub>] was synthesized according to a published procedure (Finze, 2008). The spectroscopic data have been reported earlier (Finze, 2008). The salt was dissolved in acetonitrile and slow evaporation of the solvent resulted in colorless crystals.

**Refinement**

All hydrogen atom positions were obtained from difference fourier maps. The hydrogen atoms of the methyl groups were included in the latest stages of the refinement with a riding model and for each methyl group a common  $U_{iso}$  value was refined. The positional parameters and the isotropic displacement parameters of all other hydrogen atoms were refined freely.

**Figures**

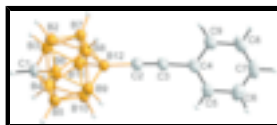


Fig. 1. : The 12-phenylethynylcarba-*closo*-dodecaborate cation in [Et<sub>4</sub>N][12-PhCC-*closo*-CB<sub>11</sub>H<sub>11</sub>]. Hydrogen atoms are drawn with an arbitrary radius and the displacement ellipsoids are shown at the 40% probability level.

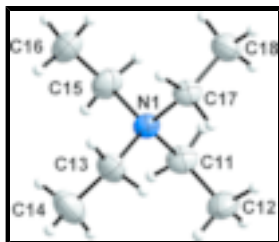


Fig. 2. : The tetraethylammonium cation in  $[\text{Et}_4\text{N}][12\text{-PhCC-}closo\text{-CB}_{11}\text{H}_{11}]$ . Hydrogen atoms are drawn with an arbitrary radius and the displacement ellipsoids are shown at the 40% probability level.

## Tetraethylammonium 12-phenylethynylcarba-*closo*-dodecaborate

### Crystal data



$$M_r = 373.38$$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$$a = 8.8201 (6) \text{ \AA}$$

$$b = 12.0929 (11) \text{ \AA}$$

$$c = 12.1858 (11) \text{ \AA}$$

$$\alpha = 81.032 (7)^\circ$$

$$\beta = 79.899 (7)^\circ$$

$$\gamma = 71.553 (7)^\circ$$

$$V = 1206.82 (18) \text{ \AA}^3$$

$$Z = 2$$

$$F_{000} = 400$$

$$D_x = 1.031 \text{ Mg m}^{-3}$$

Melting point: 433 K

Mo  $K\alpha$  radiation

$$\lambda = 0.71073 \text{ \AA}$$

Cell parameters from 4623 reflections

$$\theta = 6.8\text{--}20.7^\circ$$

$$\mu = 0.05 \text{ mm}^{-1}$$

$$T = 293 \text{ K}$$

Block, colourless

$$0.3 \times 0.25 \times 0.2 \text{ mm}$$

### Data collection

Stoe Stadi CCD  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$$T = 293 \text{ K}$$

$\omega$  scans

Absorption correction: none

17081 measured reflections

4219 independent reflections

3228 reflections with  $I > 2\sigma(I)$

$$R_{\text{int}} = 0.051$$

$$\theta_{\text{max}} = 25.0^\circ$$

$$\theta_{\text{min}} = 5.1^\circ$$

$$h = -10 \rightarrow 10$$

$$k = -14 \rightarrow 14$$

$$l = -14 \rightarrow 14$$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.048$$

$$wR(F^2) = 0.101$$

$$S = 1.00$$

4219 reflections

Hydrogen site location: difference Fourier map

H atoms treated by a mixture of  
independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 0.45P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} < 0.001$$

$$\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$$

363 parameters

Extinction correction: SHELXL97 (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.037 (3)

Secondary atom site location: difference Fourier map

### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{iso}^*/U_{eq}$
N1	0.02767 (14)	0.15270 (10)	0.23820 (10)	0.0443 (3)
C11	0.1693 (2)	0.11482 (16)	0.30484 (17)	0.0572 (4)
H11A	0.145 (2)	0.1795 (17)	0.3523 (15)	0.075 (6)*
H11B	0.264 (2)	0.1153 (15)	0.2471 (15)	0.067 (5)*
C12	0.1927 (2)	-0.00116 (17)	0.37487 (17)	0.0756 (6)
H12A	0.0981	0.0009	0.4282	0.115 (5)*
H12B	0.2842	-0.0170	0.4139	0.115 (5)*
H12C	0.2110	-0.0617	0.3274	0.115 (5)*
C13	0.0403 (3)	0.06144 (18)	0.16256 (17)	0.0621 (5)
H13A	0.034 (2)	-0.0082 (16)	0.2173 (15)	0.071 (5)*
H13B	-0.055 (2)	0.0949 (16)	0.1246 (15)	0.074 (6)*
C14	0.1930 (3)	0.0312 (2)	0.08048 (18)	0.0937 (7)
H14A	0.1895	-0.0262	0.0355	0.149 (6)*
H14B	0.2844	0.0001	0.1208	0.149 (6)*
H14C	0.2024	0.1005	0.0329	0.149 (6)*
C15	0.0310 (3)	0.26924 (16)	0.17111 (18)	0.0655 (5)
H15A	0.021 (2)	0.3226 (17)	0.2329 (15)	0.074 (6)*
H15B	0.140 (2)	0.2534 (16)	0.1284 (16)	0.075 (6)*
C16	-0.0984 (3)	0.32222 (19)	0.09677 (17)	0.0891 (7)
H16A	-0.0897	0.2691	0.0434	0.126 (5)*
H16B	-0.0861	0.3948	0.0577	0.126 (5)*
H16C	-0.2023	0.3366	0.1416	0.126 (5)*
C17	-0.12997 (19)	0.16523 (15)	0.31589 (15)	0.0494 (4)
H17A	-0.119 (2)	0.0852 (16)	0.3536 (14)	0.062 (5)*
H17B	-0.207 (2)	0.1839 (14)	0.2658 (14)	0.060 (5)*
C18	-0.1717 (2)	0.25361 (16)	0.39823 (15)	0.0660 (5)
H18A	-0.1861	0.3305	0.3586	0.101 (4)*
H18B	-0.0860	0.2361	0.4430	0.101 (4)*

## supplementary materials

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H18C	-0.2697	0.2509	0.4459	0.101 (4)*
C1	0.8578 (2)	-0.42097 (13)	0.37589 (14)	0.0537 (4)
H1	0.905 (2)	-0.5044 (15)	0.4091 (13)	0.064 (5)*
B2	0.7262 (3)	-0.39328 (16)	0.28148 (17)	0.0561 (5)
H2	0.6959 (19)	-0.4675 (14)	0.2554 (13)	0.064 (5)*
B3	0.9243 (2)	-0.38352 (16)	0.23998 (17)	0.0555 (5)
H3	1.012 (2)	-0.4499 (15)	0.1888 (13)	0.065 (5)*
B4	0.9825 (2)	-0.33524 (16)	0.35199 (17)	0.0535 (5)
H4	1.108 (2)	-0.3739 (14)	0.3728 (13)	0.064 (5)*
B5	0.8195 (2)	-0.31531 (15)	0.46186 (16)	0.0516 (5)
H5	0.8448 (19)	-0.3415 (14)	0.5490 (14)	0.062 (5)*
B6	0.6607 (2)	-0.35139 (16)	0.41916 (17)	0.0560 (5)
H6	0.588 (2)	-0.3994 (14)	0.4814 (13)	0.065 (5)*
B7	0.7589 (2)	-0.27118 (15)	0.19136 (16)	0.0503 (4)
H7	0.7377 (18)	-0.2580 (13)	0.1044 (13)	0.057 (4)*
B8	0.5950 (2)	-0.25187 (16)	0.30200 (17)	0.0523 (5)
H8	0.465 (2)	-0.2256 (14)	0.2866 (13)	0.067 (5)*
B9	0.6529 (2)	-0.20266 (15)	0.41506 (16)	0.0496 (4)
H9	0.5641 (19)	-0.1430 (14)	0.4736 (13)	0.057 (4)*
B10	0.8521 (2)	-0.19299 (14)	0.37266 (15)	0.0463 (4)
H10	0.8952 (18)	-0.1288 (13)	0.4032 (12)	0.054 (4)*
B11	0.9180 (2)	-0.23517 (15)	0.23469 (16)	0.0486 (4)
H11	1.002 (2)	-0.1994 (14)	0.1743 (13)	0.063 (5)*
B12	0.7131 (2)	-0.15303 (14)	0.27349 (14)	0.0436 (4)
C2	0.64183 (18)	-0.02308 (13)	0.22826 (12)	0.0467 (4)
C3	0.58462 (17)	0.07904 (13)	0.19784 (12)	0.0446 (4)
C4	0.51356 (16)	0.20251 (12)	0.16824 (12)	0.0420 (3)
C5	0.46196 (19)	0.27790 (14)	0.25139 (15)	0.0503 (4)
H5A	0.4757 (19)	0.2488 (14)	0.3277 (14)	0.059 (5)*
C6	0.3917 (2)	0.39677 (15)	0.22449 (18)	0.0633 (5)
H6A	0.357 (2)	0.4489 (17)	0.2854 (16)	0.078 (6)*
C7	0.3720 (2)	0.44060 (16)	0.11525 (18)	0.0662 (5)
H7A	0.318 (2)	0.5237 (19)	0.0958 (16)	0.089 (6)*
C8	0.4210 (2)	0.36716 (16)	0.03291 (18)	0.0647 (5)
H8A	0.408 (2)	0.3951 (16)	-0.0451 (16)	0.074 (5)*
C9	0.4921 (2)	0.24830 (15)	0.05830 (15)	0.0536 (4)
H9A	0.530 (2)	0.1947 (15)	-0.0011 (14)	0.062 (5)*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0430 (7)	0.0412 (7)	0.0525 (7)	-0.0178 (6)	-0.0068 (6)	-0.0043 (5)
C11	0.0394 (9)	0.0633 (11)	0.0709 (12)	-0.0172 (8)	-0.0107 (9)	-0.0057 (9)
C12	0.0600 (12)	0.0723 (13)	0.0766 (13)	0.0020 (10)	-0.0135 (10)	0.0039 (10)
C13	0.0695 (13)	0.0592 (11)	0.0616 (11)	-0.0210 (10)	-0.0051 (10)	-0.0189 (9)
C14	0.1051 (18)	0.0901 (16)	0.0746 (14)	-0.0207 (13)	0.0179 (13)	-0.0270 (12)
C15	0.0741 (13)	0.0518 (10)	0.0705 (12)	-0.0272 (10)	-0.0061 (11)	0.0080 (9)
C16	0.1112 (18)	0.0705 (13)	0.0693 (13)	-0.0084 (12)	-0.0202 (13)	0.0107 (10)

C17	0.0387 (9)	0.0518 (10)	0.0590 (10)	-0.0155 (7)	-0.0070 (8)	-0.0048 (8)
C18	0.0640 (12)	0.0628 (11)	0.0675 (11)	-0.0110 (9)	-0.0052 (9)	-0.0162 (9)
C1	0.0603 (10)	0.0321 (8)	0.0662 (10)	-0.0067 (7)	-0.0200 (8)	-0.0001 (7)
B2	0.0654 (13)	0.0385 (9)	0.0701 (12)	-0.0170 (9)	-0.0233 (10)	-0.0037 (9)
B3	0.0587 (12)	0.0423 (10)	0.0620 (12)	-0.0061 (9)	-0.0080 (10)	-0.0137 (9)
B4	0.0475 (11)	0.0417 (9)	0.0684 (12)	-0.0036 (8)	-0.0184 (9)	-0.0056 (8)
B5	0.0625 (12)	0.0394 (9)	0.0506 (10)	-0.0089 (8)	-0.0179 (9)	0.0007 (8)
B6	0.0575 (12)	0.0431 (10)	0.0645 (12)	-0.0158 (9)	-0.0070 (10)	0.0033 (9)
B7	0.0608 (12)	0.0420 (9)	0.0505 (10)	-0.0138 (8)	-0.0177 (9)	-0.0041 (8)
B8	0.0461 (11)	0.0437 (10)	0.0675 (12)	-0.0125 (8)	-0.0165 (9)	0.0008 (8)
B9	0.0509 (11)	0.0395 (9)	0.0523 (10)	-0.0063 (8)	-0.0056 (9)	-0.0030 (8)
B10	0.0515 (10)	0.0353 (8)	0.0540 (10)	-0.0106 (8)	-0.0171 (8)	-0.0035 (7)
B11	0.0454 (10)	0.0439 (9)	0.0554 (11)	-0.0124 (8)	-0.0055 (8)	-0.0056 (8)
B12	0.0453 (10)	0.0358 (8)	0.0496 (10)	-0.0092 (7)	-0.0126 (8)	-0.0035 (7)
C2	0.0472 (9)	0.0422 (9)	0.0512 (9)	-0.0130 (7)	-0.0127 (7)	-0.0004 (7)
C3	0.0393 (8)	0.0413 (8)	0.0530 (9)	-0.0125 (7)	-0.0115 (7)	0.0025 (7)
C4	0.0329 (7)	0.0374 (7)	0.0552 (9)	-0.0127 (6)	-0.0097 (6)	0.0057 (7)
C5	0.0447 (9)	0.0457 (9)	0.0557 (10)	-0.0120 (7)	-0.0045 (7)	0.0034 (7)
C6	0.0558 (11)	0.0453 (9)	0.0826 (13)	-0.0113 (8)	-0.0001 (10)	-0.0065 (9)
C7	0.0557 (11)	0.0400 (9)	0.0959 (15)	-0.0129 (8)	-0.0150 (10)	0.0160 (10)
C8	0.0676 (12)	0.0563 (11)	0.0693 (12)	-0.0228 (9)	-0.0242 (10)	0.0227 (10)
C9	0.0554 (10)	0.0491 (9)	0.0581 (10)	-0.0189 (8)	-0.0156 (8)	0.0055 (8)

*Geometric parameters (Å, °)*

N1—C13	1.511 (2)	B3—H3	1.106 (17)
N1—C17	1.5173 (19)	B4—B5	1.767 (3)
N1—C11	1.519 (2)	B4—B10	1.768 (2)
N1—C15	1.521 (2)	B4—B11	1.772 (3)
C11—C12	1.498 (2)	B4—H4	1.112 (17)
C11—H11A	0.991 (19)	B5—B10	1.764 (2)
C11—H11B	0.996 (19)	B5—B9	1.768 (3)
C12—H12A	0.9600	B5—B6	1.771 (3)
C12—H12B	0.9600	B5—H5	1.101 (16)
C12—H12C	0.9600	B6—B8	1.771 (3)
C13—C14	1.509 (3)	B6—B9	1.771 (3)
C13—H13A	1.000 (19)	B6—H6	1.117 (17)
C13—H13B	0.973 (19)	B7—B12	1.773 (2)
C14—H14A	0.9600	B7—B11	1.777 (3)
C14—H14B	0.9600	B7—B8	1.778 (3)
C14—H14C	0.9600	B7—H7	1.087 (15)
C15—C16	1.501 (3)	B8—B12	1.779 (2)
C15—H15A	1.041 (19)	B8—B9	1.791 (3)
C15—H15B	0.98 (2)	B8—H8	1.127 (17)
C16—H16A	0.9600	B9—B10	1.778 (3)
C16—H16B	0.9600	B9—B12	1.782 (3)
C16—H16C	0.9600	B9—H9	1.118 (16)
C17—C18	1.497 (2)	B10—B12	1.777 (2)
C17—H17A	0.987 (17)	B10—B11	1.778 (3)

## supplementary materials

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C17—H17B	0.942 (17)	B10—H10	1.101 (15)
C18—H18A	0.9600	B11—B12	1.785 (3)
C18—H18B	0.9600	B11—H11	1.092 (16)
C18—H18C	0.9600	B12—C2	1.548 (2)
C1—B5	1.692 (2)	C2—C3	1.202 (2)
C1—B4	1.698 (3)	C3—C4	1.4393 (19)
C1—B2	1.698 (2)	C4—C5	1.389 (2)
C1—B3	1.699 (3)	C4—C9	1.389 (2)
C1—B6	1.703 (3)	C5—C6	1.385 (2)
C1—H1	1.010 (17)	C5—H5A	0.956 (16)
B2—B8	1.762 (3)	C6—C7	1.373 (3)
B2—B7	1.767 (3)	C6—H6A	0.993 (19)
B2—B3	1.767 (3)	C7—C8	1.366 (3)
B2—B6	1.773 (3)	C7—H7A	0.98 (2)
B2—H2	1.118 (16)	C8—C9	1.383 (2)
B3—B7	1.767 (3)	C8—H8A	0.973 (18)
B3—B11	1.769 (3)	C9—H9A	0.990 (17)
B3—B4	1.775 (3)		
C13—N1—C17	106.34 (12)	C3—C2—B12	177.15 (16)
C13—N1—C11	110.83 (14)	C2—C3—C4	176.64 (17)
C17—N1—C11	110.72 (13)	C5—C4—C9	118.84 (14)
C13—N1—C15	111.48 (14)	C5—C4—C3	119.59 (14)
C17—N1—C15	111.00 (13)	C9—C4—C3	121.55 (14)
C11—N1—C15	106.54 (13)	C6—C5—C4	120.32 (16)
C12—C11—N1	115.71 (14)	C7—C6—C5	120.04 (19)
C14—C13—N1	115.43 (16)	C8—C7—C6	120.15 (17)
C16—C15—N1	115.55 (16)	C7—C8—C9	120.53 (18)
C18—C17—N1	116.43 (13)	C8—C9—C4	120.11 (18)
C2—C3—C4—C5	8(3)	C5—C6—C7—C8	0.2 (3)
C2—C3—C4—C9	-171 (3)	C6—C7—C8—C9	-0.5 (3)
C9—C4—C5—C6	-0.6 (2)	C7—C8—C9—C4	0.2 (3)
C3—C4—C5—C6	-179.29 (14)	C5—C4—C9—C8	0.3 (2)
C4—C5—C6—C7	0.4 (3)	C3—C4—C9—C8	178.98 (15)

Fig. 1

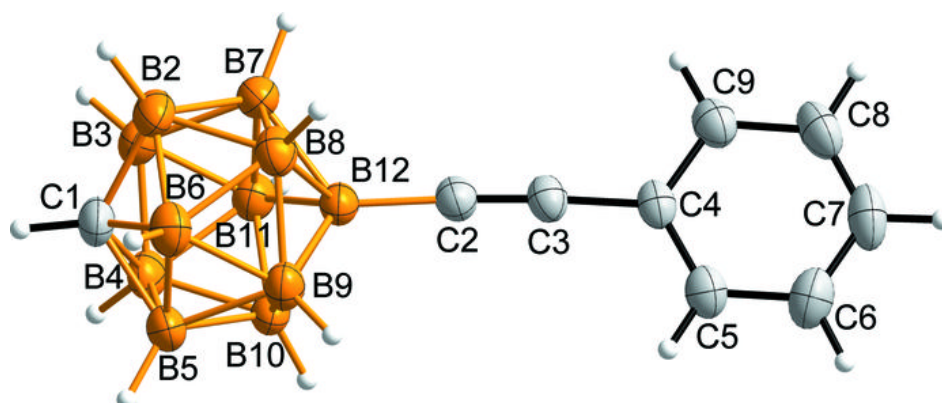


Fig. 2

