

Erratum

Erratum to “Bond rotamers and calculated  $^{11}\text{B}$ -NMR chemical shifts in boron-containing cluster chemistry. Some effects in the  $\{nido\text{-}7,8,10\text{-PC}_2\text{B}_8\}$  system” [JOM, 614/615C (2000) 61–65]☆

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Fig. 2 and caption should be as follows.

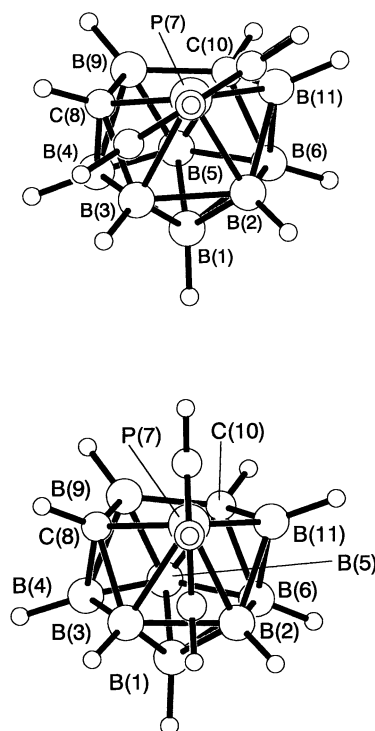


Fig. 2. Views, approximately along the P(7)–C(71) rotamer axis, of the DFT B3LYP/6-31G\* energy/geometry-optimised structures for the two minima associated with contrarotation about the P(cluster)–C(phenyl) linkage of [7-Ph-7,8,10-*nido*-PC<sub>2</sub>[B<sub>8</sub>H<sub>10</sub>]: (top) rotamer **1a** (energy arbitrarily at zero kJ mol<sup>-1</sup>), and (bottom) the more stable of the two **1b** (energy at –3.4 kJ mol<sup>-1</sup> relative to **1a**). The dihedral angles C(71)–C(72)/P(7)–C(8) for **1a** and **1b** differ by 47.6°. The plane of the aromatic group approximately bisects the B(2)–B(3) vector in **1a** and the B(3)–C(8) vector in **1b**. There appear to be no other rotamer minima, in particular there is no apparent minimum for the plane of the aromatic group intersecting the B(2)–B(11) vector (Figure 3).

☆ PII of original article: S0022-328X(00)00613-6

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