

Aspects of the structural chemistry of heteroboranes

A. J. Welch, Heriot-Watt University

Plenary talk abstract

The distinction between CH and BH vertices in crystallographic studies of carboranes and heterocarboranes is sometimes tricky, and a number of incorrect examples exist in the literature. To help with this problem we have developed two new methods, the *Vertex-to-Centroid Distance* (VCD) and the *Boron-Hydrogen Distance* (BHD) methods, which will be described in the talk.

Once the CH vertices are correctly positioned a number of consequences follow, driven by the differing trans influences of C and B. I will focus particularly on *Exopolyhedral Ligand Orientation* (ELO). ELO links with the issue of correctly locating the cage C atoms in that an unexpected ELO often signals an incorrect assignment.

Finally I will briefly discuss the question of *Verticity*. Just because an atom looks like it is a vertex is it really one? And just because an atom looks like it's merely a bridge between two 'real' vertices is it, or should we think of it as a vertex itself?