Poster Presentation

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The enhanced structural carborane effect

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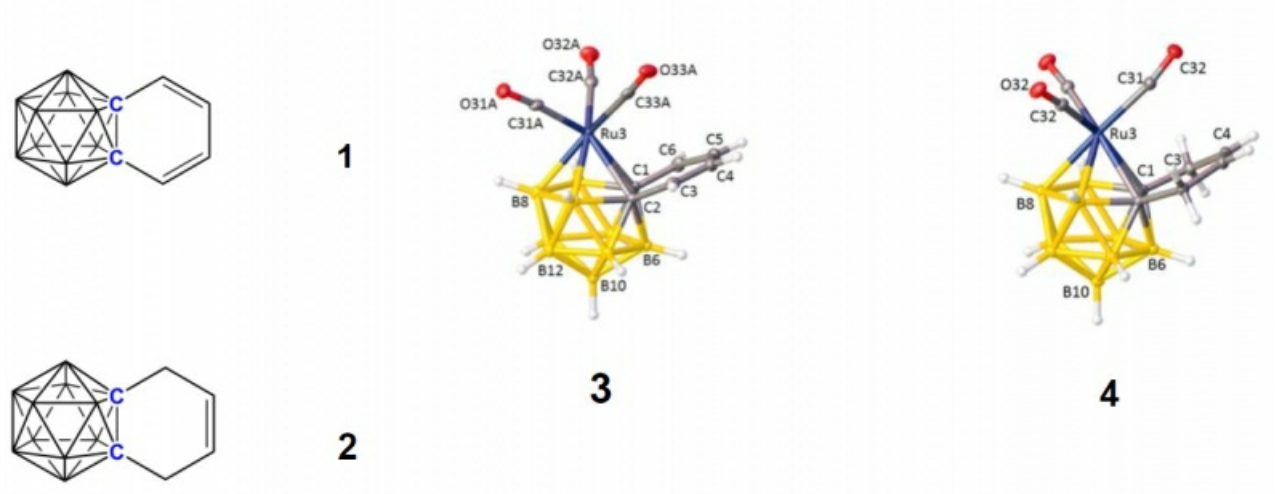
The question of the degree of aromaticity in the exopolyhedral C6 ring of the well-known species benzocarborane (1) is an old one, and most authors conclude that there is little, if any, aromatic character present.[1]

In this work we describe detailed comparisons of the structures of benzocarborane, dihydrobenzocarborane (2) and their transition-metal derivatives (3) and (4) which provide evidence for an enhanced structural carborane effect (ESCE).[2]

The ESCE is related to the difference in the ways in which cyclopentadienyl and indenyl ligands bind to transition metals. Moreover, the presence of an ESCE provides clear evidence for a degree of aromaticity in the C6 ring of benzocarborane, albeit small.[3]

1. Copley, R. C. B. et al., (1996) Chem. Commun., 2033-2034.
2. Powley, S. L. et al., (2015) J. Organomet. Chem., 792, 51-54.
3. Powley, S. L. et al., (2016) Dalton Trans., 45, 11742-11752.



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