

Structural Studies of Boracalixarenes

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Boracalixarenes have significant potential as fluorescent sensors [1]. Davidson [2] and Mair [3] have recently reported the ease and difficulties associated with organoboron derivatisation at the lower rim of calix[4]arenes. We have developed new synthetic routes to such species avoiding the use of thermally unstable [(Ar^R)₂BF·Et₂O] reagents. Structures have been determined, in part, at Daresbury Laboratory stations 9.8 and the recently commissioned 16.2 SMX; both now equipped with Bruker AXS APEX II CCD detectors. The structures presented include those with bulky, electron-withdrawing perfluoroaryl ligands, halides (including those where halide exchange has occurred), and an example where calix[4]arenes have been coupled via B–O–B bridges. Rare examples of organometallic intramolecular π - π interactions are presented. Calixarene conformations are discussed as a consequence of the degree of substitution with arylboron groups versus halide.

[1] Gutsche C.D., *Calixarenes Revisited*, Royal Society of Chemistry, London, 1998. [2] Arimori S., Davidson M.G., Fyles T.M., Hibbert T.G., James T.D., Kociok-Köhn G.I., *Chem. Commun.*, 2004, 1640. [3] Cross W.I., Lightfoot M.P., Mair F.S., Pritchard R.G., *Inorg. Chem.*, 2000, **39**, 2690.

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