Single-boron complexes of N-confused and N-fused porphyrins.

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Streszczenie

Boron(III) has been inserted into N-confused porphyrin, (*N*CP*H*)H_2 (**1**), and N-fused porphyrin, (*N*FP)H (**2**). The reaction of dichlorophenylborane and **1** yields σ-phenylboron N-confused porphyrin (**4**). The boron atom is bound by two pyrrolic nitrogen atoms and the σ-phenyl ligand. The N-confused pyrrole ring is not involved in the direct coordination because the C(21)−H fragment remains intact. A reaction between $PhBCl_2$ and N-fused porphyrin produces σ-phenylboron N-fused porphyrin ($\mathbf{3^+}$) . **4** converts quantitatively into $\mathbf{3^+}$ under protonation. In σ-phenylboron *N*-fused porphyrin [(*N*FP)BPh]Cl, the coordinating environment of boron(III) resembles a distorted trigonal pyramid, with the nitrogen atoms occupying equatorial positions and with the phenyl ligand lying at the unique apex. Boron(III) is displaced by 0.547(4) Å from the N_3 plane. The B−N distances are as follows: B−N(22), 1.559(4) Å; B−N(23), 1.552(4) Å; B−N(24), 1.568(4) Å; $B-C_{ipsoPh}$, 1.621(4) Å. $\mathbf{3^+}$ can be classified as a boronium cation considering a filled octet and a complete coordination sphere. $\mathbf{3^+}$ is susceptible to alkoxylation at the inner C(9) carbon atom, yielding **5**-OR. The addition of acid results in protonation of the alkoxy group and elimination of alcohol, restoring the original $\mathbf{3^+}$. Density functional theory has been applied to model the molecular and electronic structure of **4**, $\mathbf{3^+}$, and syn and anti isomers of methoxy adducts **5**-OMe.

Adres publiczny

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https://www.acs.org/content/acs/en.html