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A multivalent chelator and its application for stabilizing a boron complex with potential for achieving hypercoordination

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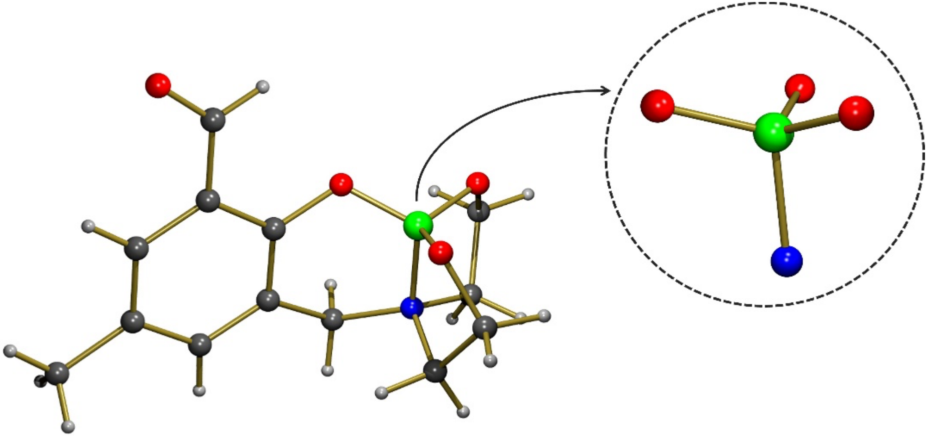
Theoretical studies have pointed out that boron can form thermodynamically stable pentacoordinate compounds through the formation of at least one multicenter bond[1]. The single crystal X-ray analysis of a boron complex containing an anthracene-type ligand has shown that the boron center achieved pentacoordination with an N-B-N tree-center four-electron bond, whose formation was supported by DFT calculations[2]. Here, aiming to produce a boron complex with potential for achieving hypercoordination, a likely tetradentate trivalent chelator, named 3-((bis-(2-hydroxyethyl)amino)methyl)-2-hydroxy-5-methylbenzaldehyde (abbreviated as H_3L), was synthesized, characterized, and used to prepare a neutral tetracoordinated boron complex, [B(L-k^4-N,O,O,O)]. Both the free ligand and its boron complex were characterized by diverse techniques, including FT-IR, UV-Vis and NMR spectroscopies, mass spectrometry, and single crystal X-ray diffraction structure determination. The boron complex possesses a distorted tetrahedral coordination geometry. The ligand coordinates trianionically as L^{3-}, upon deprotonation of all tree hydroxyl groups, whose oxygen atoms form the coordination sphere together with the nitrogen atom. The crystal and molecular structure of the complex [B(L-k^4-N,O,O,O)] is depicted below. The boron atom lies just 0.384(2) Å apart from the plane formed by the three coordinated oxygen atoms, being clearly dislocated from the distorted tetrahedron center, and might favor the formation of a trigonal bipyramid coordination geometry by adding a strong nucleophile species in the position trans to the nitrogen atom. This hypothesis is currently being investigated in our research group.



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