

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

Mariana A. Figueira, Victor M. Miranda, Julyanna C. D. Andrade and Victor M. Deflon

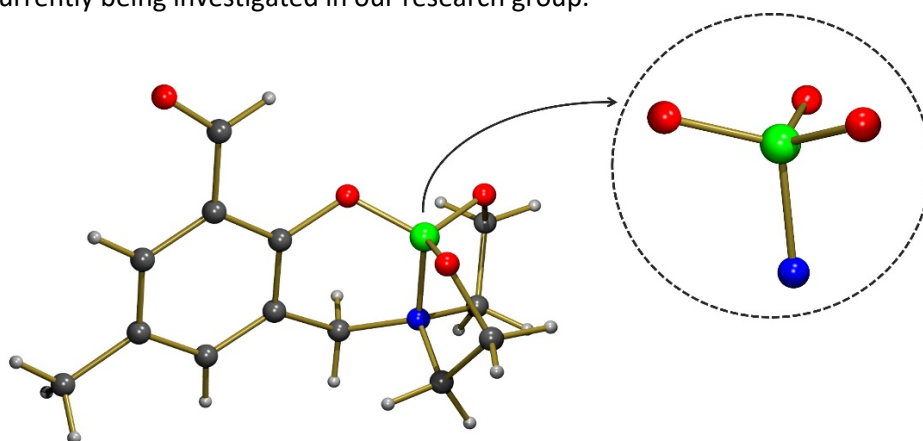
Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, Brasil

E-mail: marianafigueira@usp.br

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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 bond¹. 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 calculations². 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 H₃L), was synthesized, characterized, and used to prepare a neutral tetracoordinated boron complex, [B(L-k⁴-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 L³⁻, upon deprotonation of all three hydroxyl groups, whose oxygen atoms form the coordination sphere together with the nitrogen atom. The crystal and molecular structure of the complex [B(L-k⁴-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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References

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