

Relativistic Electronic Structure of Tantalum Metallocavitands

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Cavitands are a category of supramolecular assemblies which are able to host several molecules depending of the size of its cavity. This ability is useful to incorporate smaller guest molecules and with this, to serve as nanovessels for catalysis, for drug delivery and for molecular recognition [1]. The functionalization and tailoring of these systems can achieve an increase in their selectivity for some substrates or to incorporate several molecular fragments. Several Metallo-Cavitands have been obtained by Fontaine *et al.* [2]. These compounds exhibit a relativistic Ta₃B₃O₁₀ core (see Figure 1). With the aim to understand the electronic structure and the Ta-Ta interactions, and how these changes when a Lewis base enter into the acidic cavity, with the Tantalum core at the bottom; Relativistic density functional theory (DFT) calculations were done, including Spin-Orbit coupling via ZORA Hamiltonian. These systems are studied within C_{3v}* double valued point group according to the inclusion of the spin-orbit coupling into the calculations. The μ³-OH – Ta₃ (4f⁴) interaction play an important role into the Lewis acid activity.

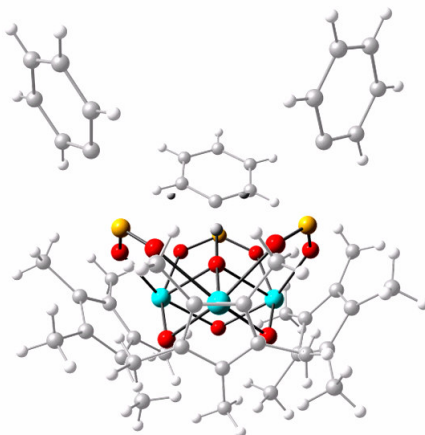


Figure 1: Scheme of the [(Cp*Ta)₃(μ²-PhB(O)₂)₃(μ²-O)₂(μ²-OH)(μ³-OH)], denoting the Ta₃B₃O₁₀ core.

References

- [1] S. M. Biro, J. Chem. Soc. Rev. 36 (2007) 93.
[2] F.-G. Fontaine, et al. Inorg. Chem. 48 (2009) 1699.

Acknowledgment

The authors thanks the financial support of FONDECYT Grants 1070345, Apoyo de Tesis Doctoral Grants N° 23070215, UNAB-DI-02-09/R, UNAB-DI-09-09/I. PROJECT MILLENNIUM No. P07-006-F; Beca Doctoral CONICYT; Beca Doctoral UNAB.