XXIX Simposio del Grupo Especializado en Cristalografía y Crecimiento Cristalino
19-22 de enero de 2021

COPPER(I) BOROHYDRIDE COMPLEX WITH BIS[(2-DIPHENYLPHOSPHINO)PHENYL] ETHER. STRUCTURE INVESTIGATION BY SINGLE-CRYSTAL X-RAY DIFFRACTION AND DFT CALCULATIONS

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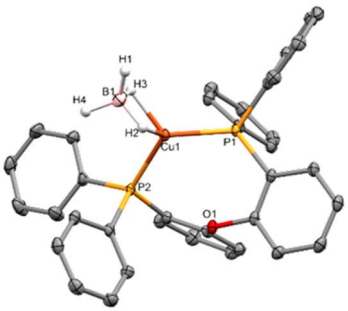
Abstract: the borohydride anion is characterized by a rich coordination chemistry because of the variable denticity and the possibility of behaving as terminal or bridging ligand. The copper(I) complex Cu(κ^2-BH_4)(DPEphos), where DPEphos is bis[(2-diphenylphosphino)phenyl] ether, was recently synthesized from CuCl using $NaBH_4$ as borohydride source. The product crystallized from dichloromethane/ethanol (space group $P\bar{1}$). The asymmetric unit contains two non-equivalent molecules, both exhibiting κ^2 coordination mode of the borohydride ligand, as suggested also by IR and ^{1}H NMR spectra. The same Cu(I)-BH_4 interaction was already observed for the related bis(triphenylphosphine) complex. The Cu-H distances are comprised between 1.67(3) and 1.75(2) Å, while the B-H distances are in the 1.07(2) – 1.20(2) Å range. The H-Cu-H angles for the two non-equivalent molecules are 62.7(12) and 66.3(10)°. DPEphos behaves as chelating ligand, with bite angles of 111.663(16) and 116.190(17)°. The Cu-P distances are between 2.2300(4) and 2.2776(5) Å. Bond lengths and angles of the first coordination sphere were compared with those obtained from DFT geometry optimizations, carried out using hybrid and range-separated functionals with variable percentage of Hartree-Fock exchange.



Key words: borohydride, copper(I), DPEphos, SC-XRD, DFT

Acknowledgments: CACTI (University of Vigo) is gratefully acknowledged for X-ray data collection. We acknowledge Università Ca' Foscari Venezia for financial support (Bando Spin 2018, D. R. 1065/2018 prot. 67416) and CINECA (COLUMN project 2020) for the availability of computing resources.