Towards chiral coordination compounds with ephedrine and pseudoephedrine derivatives. On the Cu(II)---HC agostic interaction?

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The stereospecific binding of metal ions towards biological relevant ligands may control the conformation of the molecules and so affect their chemical and biological properties. In this context, we have been interested in the coordination behavior towards metal ions of chiral ephedrine and *pseudo*ephedrine derivatives, specially on the effect of the estereogenic nitrogen in stereoselective reactions[1]. These two diasteromers differ only in the orientation of the methyl and phenyl groups: *erythro* in H_2ceph and *threo* in H_2cpse. Notwithstanding this subtle difference, they have a quite different chemical reactivity in reaction synthesis, giving place to stereoselective compounds. The X-ray crystal structure of $[Cu(Hceph)_2]$, showed a CH---Cu agostic interaction (2.454 Å). To understand the bonding properties of the *threo* and *erythro* ligands, we have performed a DFT study for the complexes and for the bare ligands. All-electron calculations were done, using the Gaussian-98 program, at the B3LYP/6-31G** level of theory. The Bader theory "atoms in molecules" (AIM)[2] was used to characterize the bonding interactions in the complexes**.** For $[Cu(Hceph)_2]$, the behavior of the electronic density along the Cu---H internuclear region indicates the formation of an agostic Cu---H bond, since the associated electronic density shows both, a bond critical point and a bond ring critical point.

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[1] H. López-Sandoval, R. Contreras, A. Escuer, R. Vicente, S. Bernès, H. Nöth, G. Jeffery Leigh, N. Barba-Behrens, *J. Chem.Soc., Dalton Trans*., 2002,2648.

[2] P. L. A Popelier, G. Logothetis, *J. Organomet. Chem*. 1998, **555**, 101.