Metallophilic interactions between two closed-shell copper(I) molecules

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Organocopper reagents as well as copper catalyzed reactions have become of great importance in organic synthesis. Recently the solid state structure of a cyanocuprate, $[t\text{-BuCu(CN)Li(OEt}_2)_2]_\infty$ [1], was determined. It is interesting to note that this crystal structure shows an experimental evidence for a Cu(I)-Cu(I) interaction in a free dimer. Although intra- and intermolecular Au(I)-Au(I) contacts have been known for a quite some time due to experimental and theoretical investigations[2], only poor attention was given to short Cu(I)-Cu(I) bond distances and possible metallophilic closed-shell interactions in organocopper complexes. Is there a Cu(I)-Cu(I) attraction in **1** and how strong are these interactions? In the present work we report on ab initio calculations of monomers CH_3CuX and the corresponding dimers $(CH_3CuX)_2$. The dependency of Cu(I)-Cu(I) attractions on different X and varying dimer geometries are discussed as well as basis set effects.

1) G. Boche, F. Bosold, M. Marsch, K. Harms, *Angew. Chem. int. ed.* **1998**, *37*, 1684 - 1686.

2) a) H. Schmidbauer, *Chem. Soc. Rev.* **1995**, 391 ; b) P. Pyykkö *Chem. Rev.* **1997**, *97*, 597-636