Theoretical study of copper-carbonyls interaction in CU(CO)N (N=1-2) complexes

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We studied the dependence on the attraction between copper(0) and carbonyls in Cu(CO)n (n = 1-2) complexes using ab initio methodology. Oscillation in the equilibrium Cu-C distance, as well as on the interaction energy are sensitive to the electron correlation potential. These effects were evaluated using several levels of theory, ranging from MP2 to CCSD(T). The long-distance behaviour of the CuCO interaction is related to simple induction and dispersion expressions involving the individual properties of both copper and carbonyl. The dispersion interaction is the principal contribution in the stability at long distance and an important term at short distance.