SPIN-ORBIT CONFIGURATION INTERACTION STUDY ON CUO

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The ground and excited electronic states of linear CUO have been computed using relativistic spin-orbit configuration interaction as implemented in the COLUMBUS suite of programs. Four sets of geometries optimized by ADF[a] and CASPT2[b] method have been investigated. ADF and CASPT2 singlet geometries give that $^1\Sigma_0^+$ is 0.198 eV and 0.181 eV lower than $^3\Phi_2$ respectively. ADF and CASPT2 triplet geometries give that $^3\Phi_2$ is 0.306 eV and 0.455 eV lower than $^1\Sigma_0^+$ respectively. However, the lowest state at the triplet geometry is higher than the lowest state at the singlet geometry by 0.100 eV (ADF geometry) and 0.118 eV (CASPT2 geometry). Calculations[b] by the CASPT2 method give the $^3\Phi_2$ state lower in energy at all geometries. The experiments[a] indicate that in the Ne matrix CUO is in the $^1\Sigma^+$ state and in the Ar matrix CUO is in the $^3\Phi$ state. The electronic states of the system of CUO-noble gas atoms are also being investigated.

[a] J. Li, B. E. Bursten, B. Liang, L. Andrews. *Science* **295**, 2242, 2002.
[b] B. O. Roos, P. Widmark, L. Gagliardi. *Faraday Discuss.* **124**, 57, 2003.