AB INITIO CALCULATION OF THE ELECTRONIC TRANSITIONS OF SAMARIUM MONOXIDE

TIANXIAO YANG AND RUSSELL M. PITZER, *Department of Chemistry, The Ohio State University, 100 W.18th Avenue, Columbus, OH, 43210.*

Using relativistic effective core potentials, spin-orbit configuration interaction (SOCI) calculations have been performed to compute the electronic transitions of SmO and SmO^+. The ordering and positions of the low-lying states of SmO are shown to be in very good agreement with the experimental measurements[a,b] and those calculated from ligand field theory.[c] The SOCI calculations confirmed that the lowest superconfiguration of SmO is $Sm^{2+}(4f^5 6s)O^{2-}$. The ground electronic state of SmO is $X\ 0^-$. The upper state configuration is $Sm^{2+}(4f^5 5p\pi)O^{2-}$. The electronic transitions of SmO^+ will also be discussed.

[a] C. Linton, B. J. Guo, R. S. Rana and J. A. Gray *J. Mol. Spectrosc.* **126**(370),1987.
[b] B. J. Guo and C. Linton *J. Mol. Spectrosc.* **147**(120),1991.
[c] P. Carette and A. Hocquet *J. Mol. Spectrosc.* **131**(301),1988.