

AB INITIO CALCULATION OF THE ELECTRONIC TRANSITIONS OF SAMARIUM MONOXIDE

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Using relativistic effective core potentials, spin-orbit configuration interaction (SOC) 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 SOC calculations confirmed that the lowest superconfiguration of SmO is Sm²⁺(4f⁵6s)O²⁻. The ground electronic state of SmO is X 0⁻. The upper state configuration is Sm²⁺(4f⁵5pπ)O²⁻. The electronic transitions of SmO⁺ will also be discussed.

^aC. Linton, B. J. Guo, R. S. Rana and J. A. Gray *J. Mol. Spectrosc.* **126**(370),1987.

^bB. J. Guo and C. Linton *J. Mol. Spectrosc.* **147**(120),1991.

^cP. Carette and A. Hocquet *J. Mol. Spectrosc.* **131**(301),1988.