AB INITIO STUDY OF THE AMERICYL AND CURYL IONS

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Restricted Hartree-Fock (RHF) and spin-orbit configuration-interaction (SOCI) calculations were performed on the ground and low-lying excited states of the americyl ion, AmO_2^{2+}. The RHF $\delta_u^2\,\phi_u^1\,,{}^4\Phi_u$ ground state symmetric stretch potential energy curve yields a frequency of 900 cm^{-1} compared to an experimental value of 730 cm^{-1} from Raman spectroscopy on aqueous solutions[a] of AmO_2^{1+}. The SOCI ground state is $\delta_u^2\,\phi_u^1\,,{}^4\Phi_{3/2u}$; the excited states are regular components from the above term followed by irregular components from the $\delta_u^1\,\phi_u^2\,,{}^4\Delta_u$ term. The low energy transitions are $f \rightarrow f$. Analogous calculations are planned for the curyl ion, CmO_2^{2+}. The actinides are modeled with relativistic effective core potentials and Gaussian correlation consistent double-zeta plus polarization (cc-pVDZ) basis sets.

[a]G. M. Begun *et al.*, *Inorg. Chem.* **23**, 1914 (1984).