

INTENSITIES OF THE ELECTRONIC SPECTRUM OF NpO_2^+

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

The ground and excited states of the linear NpO_2^+ ion have been studied theoretically using relativistic spin-orbit configuration interaction methods based on effective core potentials. Transitions of both the $f \rightarrow f$ and charge-transfer types have been calculated. The effect of the equatorial ligands on the intensities of the electronic spectrum of NpO_2^+ is of particular interest. We have surrounded the ion with ligands (water molecules or chloride ions) and calculated the intensities. It has been found that five ligands of either type give an intense peak near $10,000 \text{ cm}^{-1}$, as observed experimentally. Both our calculations and perturbation theory analysis explain this transition. This study has enabled us to assign several transitions in the experimental spectrum.