THE ELECTRONIC SPECTRUM OF THE NEPTUNYL ION, NpO_2^{2+}

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The electronic spectrum of the neptunyl ion, NpO_2^{2+}, has been calculated using relativistic spin-orbit configuration-interaction calculations. Neptunium in NpO_2^{2+} is in oxidation state VI and has an f^1 configuration. In the lower energies lie the $f \rightarrow f$ transitions while at energies above 20000 cm^{-1} charge transfer transitions occur. The ground state is a $^2\Delta$ state with $\Omega = 3/2$. Equilibrium distances and vibrational frequencies for the symmetric stretch in the ground state are obtained and compared with experimental work.