# AB INITIO CALCULATIONS OF THE NEPTUNYL ION, $NpO_2^{2+}$ AND OF THE DIOXONEPTUNIUM(+) ION, $NpO_2^+$

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Spin-orbit Configuration Interaction calculations based on Relativistic Effective Core Potentials (RECPs) were used for the study of the linear $NpO_2^{2+}$ and $NpO_2^+$ ions. The ground state of $NpO_2^{2+}$ is $\frac{5}{2}u$ ($^2\Delta_u + ^2\Phi_u$) with equilibrium Np-O bond distance, R = 1.66 $\mathring{A}$ and symmetric stretch vibrational frequency, $\omega$ = 1059 $cm^{-1}$. $NpO_2^+$ has a $4_g$ ($^3H_{4g}$, $\delta_u\phi_u$) ground state with R = 1.73 $\mathring{A}$ and $\omega$ = 913 $cm^{-1}$. The spectra for both ions have $f \rightarrow f$ transitions at low energies and charge-transfer type transitions at higher energies.