AB INITIO CALCULATION OF THE URANYL ION, UO_2^{2+}

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Relativistic effective core potential calculations are carried out for the ground and low-lying excited states of the uranyl ion, UO_2^{2+}, which has a distinctive and extensively studied visible spectrum. Extensive configuration interaction calculations with spin orbit interaction are used to calculate the potential energy curves of the ground and the first excited state. Average MCSCF calculations are used to generate natural orbitals for the CI calculation. It is found that the ground state is closed-shell $^1\Sigma_g^+$ state and the excited states are $^3\Delta_g$ and $^3\Phi_g$ from $\sigma_u^1\delta_u^1$ and $\sigma_u^1\phi_u^1$ configurations respectively. The assigned Ω values are 1, 2, and 3 from $^3\Delta_g$ and 2, 3 and 4 from $^3\Phi_g$, in agreement with that derived from single crystal experiments, in that order. The excitation energies, symmetrical stretch frequencies for the ground and first excited state and the magnetic moments of the excited states are obtained and compared with experimental values.