AB INITIO CALCULATION OF UO2

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Ab initio spin-orbit configuration interaction calculations are performed on the UO_2 molecule, which has been observed in matrix isolation and vacuum ultraviolet spectroscopic studies. UO_2 is isoelectronic with PuO_2^{2+}, which has a $5f\delta^1 5f\varphi^1\ {}^3H_{4g}$ ground state. We find, as have other workers, that UO_2 has a $5f\varphi^1 7s\sigma^1\ \ {}^3\Phi_2$ ground state with a moderate mixture of $5f\delta^1 7s\sigma^1\ \ {}^3\Delta_2$. the UO distance is found to be 1.786 $\dot{A}$. The ${}^3H_{4g}$ state is only slightly higher in energy. Oscillator strengths have been calculated for electronic transitions.