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 laser ablation vacuum ultraviolet spectroscopic studies. We found the ground state to be $5f^1 7s^1\ {}^3\Phi_{2u}$. There are four excited states below 32,000 cm^{-1}that have large transition moments with the gound state. The highest of these excited state is $5f^1 \sigma_u^1\ {}^3\Phi_{2g}$. It has two minima in its potential curve. The σ_u orbital at the minimum with shorter bond distance has mostly 7p character, while it has mostly 5f character at the longer bond distance minimum. There are only a few dipole-allowed emission lines from this state to lower-energy states. Most electronic states in this region of the spectrum have g symmetry because most of the orbitals involved (5f,7s,7p) have the same (u) inversion symmetry.