

THE VISIBLE SPECTRUM OF ZIRCONIUM DIOXIDE, ZrO₂

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Zirconia (ZrO₂) is an important material with applications in microelectronics, catalysis, and ceramics. Previously the photoelectron spectrum^{a,b} of the ZrO₂ anion and the pure rotation spectrum of the neutral^c have been recorded and analyzed. Here we present the first observation of the visible spectrum of ZrO₂ via laser induced fluorescence (LIF) and resonance enhanced multi-photon ionization (REMPI). The LIF spectrum was recorded between 17000-18900 cm⁻¹ at a resolution of 0.2 cm⁻¹ using pulsed dye laser excitation and tentatively analyzed to give harmonic vibrational parameters ω_1 , ω_2 , and ω_3 for the \tilde{A}^1B_2 state of 495(1) cm⁻¹, 150(3) cm⁻¹ and 1045(4) cm⁻¹, respectively. Dispersed fluorescence spectra of thirteen bands were recorded and analyzed to give harmonic vibrational parameters ω_1 , ω_2 , and ω_3 for the X¹A₁ state of 898 (1) cm⁻¹, 287(3) cm⁻¹ and 808(4) cm⁻¹, respectively. The radiative lifetimes of numerous bands have been measured and analyzed. Franck-Condon factors were calculated and used to model the REMPI and excitation spectra. A comparison with TiO₂ is made^d.

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