THE VISIBLE SPECTRUM OF ZIRCONIUM DIOXIDE, ZrO_2

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Zirconia (ZrO_2) is an important material with applications in microelectronics, catalysis, and ceramics. Previously the photoelectron spectrum[a,b] of the ZrO_2 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 ZrO_2 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 X^1A_1 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 TiO_2 is made[d].

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