THE VISBLE SPECTRUM OF TITANIUM DIOXIDE

XIUJUAN ZHUANG AND <u>TIMOTHY C. STEIMLE</u>, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; RAMYA NAGARAJANN AND JOHN P. MAIER, Department of Chemistry, University of Basel, Basel Switzerland.

Bulk TiO₂ is a widely used photo-activated catalytic material, yet poorly understood. Much of the motivation for studies of molecular TiO₂ is the observation^{*a*} that there is a smooth correlation of the molecular electronic states to the band gap of the bulk. The field-free energy levels of the ground state of the monomer have been fully characterized by microwave spectroscopy.^{*b*} Here we report on the visible spectrum in the region between 18200 cm⁻¹ to 18750 cm⁻¹ of a cold molecular beam sample of TiO₂ using laser induced fluorescence detection and mass-selected REMPI. Bands at 18240 cm⁻¹, 18411 cm⁻¹ and 18470 cm⁻¹ bands were analyzed to produce a set of vibrational parameters for the ground state. The optical Stark spectra of the 18411 cm⁻¹ and 18470 cm⁻¹ bands were recorded and analyzed to determine permanent electric dipole moments and compared with the results for the band at 18655 cm^{-1*c*}

^aH.J. Zhai and L.-S. Wang *JACS* **129** 3022, 2007.

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