PURE ROTATIONAL SPECTRUM AND STRUCTURE OF ZIRCONIUM DIOXIDE

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The pure rotational spectrum of the asymmetric top ZrO_2 has been collected using a Fourier transform microwave spectrometer that employed a laser ablation molecular beam source. Four rotational transitions for each of five $Zr^{16}O_2$ isotopomers have been recorded. The rotational constants of the $^{90}Zr^{16}O_2$ isotope were determined to be A = 19881.352 ± 0.068 MHz, B = 7693.895 ± 0.021 MHz, and C = 5533.111 ± 0.036 MHz. The r_0 structure was determined to possess a Zr-O bond length of 1.7710 ± 0.0007 Å, and an O-Zr-O bond angle of 108.11 ± 0.08°. The electric dipole moment has been measured for the $^{90}Zr^{16}O_2$ isotope and found to be μ_b = 7.80 ± 0.02 Debye. The nuclear quadrupole hyperfine structure for the $^{91}Zr^{16}O_2$ isotope has also been recorded and analyzed, yielding χ_{aa} = 115.94 ± 0.16 MHz, χ_{bb} = -37.55 ± 0.33 MHz, and χ_{cc} = -78.39 ± 0.16 MHz. High-level density functional theory calculations have yielded a structure that agrees well with the values determined experimentally.