THE ROTATIONAL SPECTRA AND HYPERFINE CONSTANTS OF ZrS AND ZrO.

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The pure rotational spectra of ZrS and ZrO have been recorded using cavity Fourier transform microwave spectroscopy in the frequency range 9-26 GHz. The molecules were generated by laser ablation of a solid Zr rod with 0.05% of H_2S or O_2, respectively, in either argon or neon.

For ZrS, this is the first measurement of the pure rotational spectrum of the $X^1\Sigma^+$ state. Rotational transitions in the ground vibrational state were observed for all five $Zr^{32}S$ isotopomers and for the $^{90}Zr^{34}S$ isotopomer in natural abundance. Transitions in the first excited vibrational state were measured for the 3 most abundant isotopomers and a value for the equilibrium bond length calculated. For the $^{91}Zr^{32}S$ isotopomer nuclear hyperfine structure due to the zirconium nucleus was observed and values for $eQq(^{91}Zr)$ and $C_1(^{91}Zr)$ were determined.

The microwave spectra of the three most abundant isotopomers of $Zr^{16}O$ had been observed previously (1). The new results from the present work are the observations of the $J = 1 - 0$ transitions for the remaining two $Zr^{16}O$ isotopomers and three $Zr^{18}O$ isotopomers. In addition, the $v = 1 \quad J = 1 - 0$ transition was measured for $^{90}Zr^{16}O$, allowing an accurate determination of r_e. ^{91}Zr nuclear hyperfine structure was observed for $^{91}Zr^{16}O$ and values of the hyperfine constants were determined. The hyperfine parameters for the two molecules are interpreted in terms of the electronic structure and chemical bonding.

(1) R. D. Suenram, F. J. Lovas, G. T. Fraser and K. Matsumura, *J. Chem. Phys.* **92**, 4725-4733 (1990).