

THE MILLIMETER/SUBMILLIMETER SPECTRUM OF BaSH(\tilde{X}^2A'): EVEN FURTHER INVESTIGATIONS OF THE METAL-SULFUR BOND

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The pure rotational spectrum of BaSH (\tilde{X}^2A') and one of its isotopomers, BaSD, were recorded using millimeter/submillimeter wave direct absorption techniques in the range 320-364 GHz. This radical was produced by reacting barium vapor with H₂S in the presence of a d.c. discharge. Ten transitions, ranging from J=66 → 67 to 75 → 76, were measured for BaSH, as well as 5 transitions for the deuterium isotopomer. The spectra exhibit complex K_a ladder structure for both molecules, consistent with a bent geometry. Spin-rotation splittings of approximately 54 MHz were also observed in every transition. Rotational and fine structure constants have been determined for both isotopomers, as well as an r₀ structure for BaSH. This study shows that barium hydrosulfide is bent with an angle of $\Theta = 88^\circ$, and therefore is significantly different from linear BaOH. This structural change indicates more covalent bonding character in the BaSH, relative to its hydroxide analog.