THE MOLECULAR STRUCTURE AND RENNER-TELLER EFFECT IN THE ELECTRONIC SPECTRUM OF BORON DISULFIDE, BS_2

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The $\tilde{A}\,^2\Pi_u$ - $\tilde{X}\,^2\Pi_g$ electronic band system of jet-cooled boron disulfide has been studied by laser-induced fluorescence and wavelength resolved emission spectroscopy. The free radical was produced in a pulsed electric discharge jet using a precursor mixture of BCl_3 and CS_2 in argon. Detailed analysis of the spectra shows that the ground state exhibits a substantial Renner-Teller effect with $\epsilon = -0.2013$ and a spin-orbit coupling constant $A = -413.80\ \mathrm{cm}^{-1}$. Angular momentum coupling is negligible in the excited state which has a much smaller spin-orbit coupling constant of $A = -239.15\ \mathrm{cm}^{-1}$. Rotational analysis of the 0_0^0 band gave the effective molecular structures as $r_0'' = 1.6648(4)$ Å and $r_0' = 1.7127(5)$ Å. *Ab initio* methods have been used to predict the BS_2 spectroscopic parameters and good agreement with experiment was found. Our present understanding of the LIF spectrum is in accord with the pioneering analysis of the absorption spectrum of matrix isolated BS_2 published by Brom and Weltner [a] three decades ago.

[a] J.M.Brom, Jr. and W. Weltner, Jr., *J. Mol. Spectrosc.* **45**, 82 (1973).