Vibrational Spectrum and Gas-Phase Structure of Disulfur Dinitride, S_2N_2

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The vibrational spectrum of S_2N_2 (D_{2h}) in solid Ar has been recorded and completed by the frequencies of all IR active fundamentals and four additional combination bands. Their agreement with calculated anharmonic frequencies utilizing either VPT2 or VCI theory based on (explicitly correlated) coupled-cluster surfaces is superior. Gas-phase FTIR spectra of the ν_6 (B-type) and the v4 (C-type) fundamental bands have been recorded with a resolution of $\leq$ 0.004 cm^{-1}. Their analysis provided accurate rotational constants for the vibrational ground and the two vibrational excited states of $^{32}S_2{}^{14}N_2$. A precise ground-state r_z structure (R_z(SN) = 1.647808(93) Å, α_z(NSN) = 91.1173(20)°) and a semi-experimental equilibrium structure (R_e(SN) = 1.64188(33) Å, α_e(NSN) = 91.0777(12)°) of S2N2 have been established, which will be compared to results of ab initio CCSD(T)-F12a structure calculations, the solid-state structure of S_2N_2, and structural properties of related sulfur nitrogen compounds.

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