SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE DETERMINATION OF THIOPHENE (C_4H_4S)

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Thiophene (C_4H_4S, C_{2v} symmetry, μ_a = 0.55 D) is the sulfur analog of furan. With the intent of improving its gas-phase structure determination, its rotational spectrum was collected from 8 – 360 GHz, and 21 deuterium containing isotopologues were synthesized and their rotational spectra were collected from 130 – 360 GHz. The heavy atom ^{13}C, ^{34}S, and ^{33}S isotopologues were observable in the rotational spectra of the normal isotopologue and several deuterium containing forms at natural abundance. The resultant determinable rotational constants (A'', B'', C'') were computationally corrected for vibration-rotation interactions and electron mass with CCSD(T) calculations and 24 total isotopologues were least-squares fit to afford the semi-experimental equilibrium structure (${r_e}^{SE}$). For comparison, theoretical structures were determined at several levels of theory up to CCSD(T)/cc-pCV5Z. The quintuple zeta structure was further refined to account for extrapolation to the complete basis set limit, residual electron correlation beyond CCSD(T), relativistic effects, and the diagonal Born-Oppenheimer correction. The resultant ${r_e}^{SE}$ structure and ”best” theoretical structure are compared.