A LABORATORY AND THEORETICAL STUDY OF PROTONATED CARBON DISULFIDE, $HSCS^+$

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The rotational spectrum of protonated carbon disulfide, $HSCS^+$, has been detected in the centimeter-wave band in a molecular beam by Fourier transform microwave spectroscopy. Rotational and centrifugal distortion constants have been determined from transitions in the $K_a = 0$ ladder of the normal isotopic species, $HS^{13}CS^+$, and $DSCS^+$. The present assignment agrees well with high-level coupled cluster calculations of the $HSCS^+$ structure, which, like earlier work, predict this isomer to be the ground state on the HCS_2^+ potential energy surface; $HCSS^+$, an isomer with C_{2v} symmetry, is predicted to lie more than 20 kcal/mol higher in energy. Other properties of $HSCS^+$ including its dipole moment, vibrational frequencies, and infrared intensities have also been calculated at the CCSD(T)/cc-pwCVQZ level of theory. Because carbon disulfide possesses a fairly large proton affinity, and because this nonpolar molecule may plausible exist in astronomical sources, $HSCS^+$ is a good candidate for detection with radio telescopes in the sub-millimeter band where the stronger b-type transitions of this protonated cation are predicted to lie.