

AB INITIO STUDY OF GROUND-STATE CS PHOTODISSOCIATION VIA HIGHLY EXCITED ELECTRONIC STATES

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Wavelength-dependent photodissociation cross sections are key data required by modern astrochemical models to simulate the evolution of chemical species in photon-dominated regions. Although photodissociation is considered as the dominant destruction pathway for carbon monosulfide (CS) in these environments, the photodissociation rate of CS is essentially unknown due to a lack of vacuum ultraviolet (VUV) laboratory measurements and accurate theoretical calculations. Here we present a high-level *ab initio* study of CS photodissociation, including for the first time a detailed investigation of its predissociation via the $B^1\Sigma^+$ and $C^1\Sigma^+$ states. Potential energy curves of CS electronic states were calculated at the MRCI+Q/aug-cc-pV(5+C)Z level and photodissociation cross sections from the vibrational and electronic ground state were calculated by solving the coupled-channel Schrödinger equation. We found that the $C - X$ ($0 - 0$) transition followed by spin-orbit coupling into several triplet states is responsible for 73% of the overall photodissociation of CS under the standard interstellar radiation field (ISRF), giving rise to the main atomic products C (3P) and S (1D). Our new calculations of the photodissociation rate are a factor of 2.4 larger than the value currently adopted by the Leiden database, suggesting that this value may be revised for improving the accuracy of astrochemical models.