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# Exploring Chemical Pathways in Molecular Clouds: Unraveling CS Chemistry through CH + S, CS + H, and C2 + S Reactions

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Carbon monosulphide (CS) is among a few sulfur-bearing species that have been widely observed in all environments, including the most extreme ones such as diffuse clouds. Moreover, it has been widely used as a tracer of gas density in the interstellar medium in our Galaxy and external galaxies. Therefore, a full understanding of its chemistry in all environments is of paramount importance for the study of interstellar matter. We performed ab initio calculations to characterize the main features of all the electronic states correlating to the open shell reactants. For CH + S, we calculated the full potential energy surfaces (PES) for the lowest doublet states and the reaction rate constant using a quasi-classical method. For C2 + S, the reaction can only occur through the three lower triplet states, all of which exhibit deep insertion wells. A detailed study of the long-range interactions for these triplet states allowed us to apply a statistical adiabatic method to determine the rate constants [1].
Our comprehensive theoretical study of the CH + S ⟶ CS + H reaction provides valuable insights into its temperature dependence. We have observed that the reaction rate remains nearly constant within a wide temperature range of 10−500 K, with a consistent value of 5.5 × 10−11 cm3 s−1 at temperatures above 100 K. Notably, this rate is consistently lower by a factor of approximately 2-3 compared to the rate predicted by the capture model. In contrast, the rate of the C2 + S ⟶ CS + C reaction exhibits pronounced temperature dependence. At lower temperatures, the rate is approximately 2.0 × 10−10 cm3 s−1, gradually increasing to around 5.0 × 10−10 cm3 s−1 for temperatures exceeding 200 K. Importantly, our detailed modeling, which takes into account electronic and spin states, yields a rate that is approximately twice as high as the currently employed rate.
[1] Carlos M. R. Rocha, Octavio Roncero at al. https://arxiv.org/pdf/2307.00311.pdf

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