PROBING THE H$_2$C$_4$-(OCS)$_2$ COMPLEXES: A JOINT EXPERIMENTAL STUDY AND COMPUTATIONAL ANALYSIS

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In the present contribution we report on the results of a joint experimental study and computational investigation on the weakly bound trimer H$_2$C$_4$-(OCS)$_2$. From an experimental point of view, the infrared spectra of both H$_2$C$_4$-(OCS)$_2$ and D$_2$C$_4$-(OCS)$_2$ were recorded in the region of the $\nu_1$ fundamental vibration of OCS using a supersonic slit-jet apparatus and a rapid-scan tunable diode laser. From the rovibrational analysis of the assigned transitions the trimer was found to be the ground state isomer having C$_2$ point group symmetry. By performing quantum-chemical calculations, the stationary points on the potential energy surface were identified and characterized in terms of structures and binding energies. The predicted data, obtained by computations carried out employing double hybrid functionals, corrected by anharmonic effects, were in very good agreement with those experimentally determined from the rovibrational analysis of the infrared spectra.