

THE PREFERRED CONFORMATION AND NON-COVALENT INTERACTIONS OF THE METHYL ALLYL DISULFIDE-FORMALDEHYDE COMPLEX REVEALED BY ROTATIONAL SPECTROSCOPY

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The methyl allyl disulfide-formaldehyde adduct were probed using Fourier transform microwave spectroscopy and quantum chemical computations. The low energy isomers of the adduct were sampled using the conformer-rotamer ensemble sampling tool (CREST) and geometrically optimized at the B3LYP-D3BJ/def2-TZVP level of theory. Although many isomers of the adduct were theoretically predicted to have close stability, only one isomer of the methyl allyl disulfide-formaldehyde adduct have been detected in the helium supersonic jet. Each observed transition exhibited multiple splitting arising from internal rotation of formaldehyde and methyl internal rotations. In the observed isomer, the non-covalent bonding distance between the carbon atom of formaldehyde and the nearest sulfur atom of methyl allyl disulfide has been found to be well within the corresponding sum of van der Waals radii, indicating the existence of a  $n \rightarrow \pi^*$  interaction. Also, formaldehyde acts as a lone pair donor forming a weak CH...O hydrogen bond with methyl allyl disulfide. Detailed spectral analysis, spectroscopic and computational results will be presented.