

Computational approach for detecting undetected interstellar molecules: CH₂DOD and CHD₂OD

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Observations revealed that complex molecules (COMs) are very abundant in star forming regions (SFRs) either low-mass or massive. Methanol is believed to be the main driver of molecular complexity in the interstellar medium. Some deuterated forms of methanol; namely CH₂DOD and CHD₂OD, could play a role in the formation of deuterated COMs. We found that these undetected forms are detectable in SFRs (with abundances $>10^{-12}n_{\text{H}}$). We ran theoretical models and computed the peak positions of the IR spectral lines of these species and compared them with experimentally predicted IR positions.

Our results are in agreement with experimental data. Given the calculated abundances of these undetected species and their spectral line positions, we recommend searches for these molecules in SFRs.

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