Methoxy radical on interstellar ices: a quantum mechanics/molecular mechanics study

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The origin of the radical species in the interstellar medium (ISM), the mechanistic details of their formation, and their reactions are still not fully understood. These complex chemical processes are challenging to characterise from experimental studies. In this direction, theoretical and computational chemistry provides important contributions. The methoxy radical (CH_3O) is a primary radical species in the ISM. The CH_3O radical was observed in the cold and dense core Barnard-1b.[1] We have used a quantum mechanics/molecular mechanics (QM/MM) method to rationalise CH_3O radical binding on crystalline hexagonal water ice (I_h) and amorphous solid water (ASW).[2] In our QM/MM method,[3]-[6] the electronically important region (i.e. the binding site) is described by a quantum mechanical method, while a classical force field method is used for the remaining part. Therefore, our QM/MM approach provides accurate binding energies, and large ice clusters can be calculated at a low computational cost.

Depending on the dangling-hydrogen (*d*-H) or dangling-oxygen (*d*-O) at the binding site, a range of binding energies is observed. Computed averaged binding energies on I_h and ASW are comparable, while I_h with defects show relatively strong binding. Therefore, the distribution of *d*-Os and *d*-Hs on ice surfaces and the nature of the ice surface play a key role on the radical binding energies. Our study gives important insights about CH_3O radical binding on interstellar ices.

References

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