Radical species on interstellar ices: some clues from a quantum mechanics/molecular mechanics study

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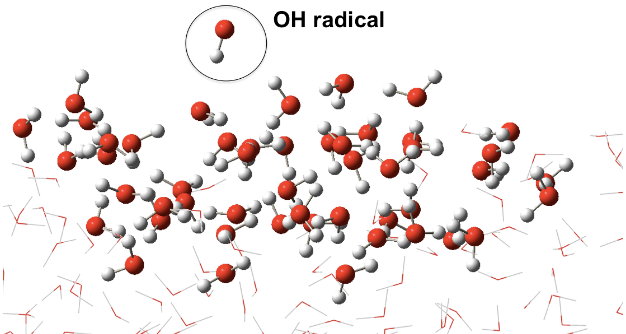
The origin of radical species in the interstellar medium (ISM) and mechanistic details of their reactions remain a mystery. The radical species in the ISM play an important role in the formation of more complex molecules or radicals. These chemical processes occur on the icy mantles of interstellar grains at very low temperatures (typically 10 K). Radicals may adsorb on ice, diffuse, and subsequently react with other species adsorbed at the ice.[1,2] The rates of these processes are difficult to characterize from experimental studies alone, whereby quantum chemistry becomes a critical tool.[3,4,5]



A QM/MM model for an OH radical on amorphous solid water ice
(QM region is in "ball and sticks" and MM region in "wireframe")

We have used quantum mechanics/molecular mechanics (QM/MM) methods to study OH, HCO, CH_3, CH_3O, SH, and O radicals binding on crystalline hexagonal water ice (I_h) and amorphous solid water (ASW). Calculated binding energies of the radicals are sensitive to the number of dangling hydrogen (*d*-H) or dangling oxygen (*d*-O) at the binding sites. A range of strong binding energies was observed for each radical when the binding sites consist of *d*-Hs or *d*-Os, indicating that radical diffusion would be slow. In the absence of dangling atoms at the binding sites, the calculated binding energies are significantly weaker, allowing radicals to diffuse on the ice. Our study provides important insights into radical desorption and diffusion on interstellar ices.

References

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