QUANTUM CHEMICAL STUDY OF HYDROXIDE ANION IN AMORPHOUS ASTROPHYSICAL ICE AND ITS INTERACTION WITH HCO^+

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Recent experimental work[a] confirmed our 2011 prediction[b] that some cation-ice reactions are efficient at low temperature. Some workers have suggested, however, that cations may be neutralized by electrons expected to be present in ice before chemistry can occur[c]. The present work assesses the hypothesis that electrons can be trapped as anions in deep potential wells, allowing cation-ice reactions to occur. Clusters with 16-31H_2O molecules containing the hydroxide anion (OH^-) were formed by various routes, including adding an electron to a cluster containing the hydroxyl radical (OH) or to a H atom loosely bound to the surface. When HCO^+ is deposited on an (OH^-)-nH_2O cluster, formic acid (HCOOH) forms, as found previously when OH^- is not present. The reaction introduces a proton into the cluster in the form the hydronium ion, H_3O^+. The H_3O^+ and OH^- entities are attracted to each other and often result in neutralization of the positive and negative charge via formation of H_2O. Vibrational spectra of clusters with OH^- will be shown.

[a]Nakai et al., Astrophys. J. 953, 162 (2023)
[b]Woon, Astrophys. J. 728, 44 (2011)
[c]Rimola et al., Front. Astron. Space Sci. 8, 655405 (2021)