D/H equilibrium fractionation between water and methanol ices

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The deuterium fractionation of gas-phase molecules in hot cores and cometary comae is believed to reflect the composition of the primitive ices. The deuteration of protostellar methanol is, however, a major puzzle because the isotopologue ratio $[CH_2DOH]/[CH_3OD]$ is about a factor of 20 larger in low mass hot-corinos than in high-mass hot cores. In this talk, we will report a new rate equation model of deuterium surface chemistry applied to the hot-core phase of protostellar sources, during which amorphous water ice is heated, crystallizes and eventually sublimates. According to recent experimental data, crystallization is accompanied in its very initial phase by H/D exchanges between water and molecules (more specifically functional groups within them) able to form hydrogen bonds, such as methanol and ammonia. The D/H ratios of such species are thus expected to equilibrate with the D/H ratio of water. As a result, the $[CH_2DOH]/[CH_3OD]$ ratio is predicted to scale inversely with $[HDO]/[H_2O]$. We will show that our model is able to reproduce the $[CH_2DOH]/[CH_3OD]$ ratios observed in the hot-corino of IRAS 16293-2422 and in the hot-core of Orion KL, provided that the primitive fractionation of water ice $[HDO]/[H_2O]$ is about 1% in both sources. We conclude that gas-phase molecular D/H ratios measured in hot cores, protoplanetary disks or comets may not be representative of the original ices in the case of molecules with exchangeable deuterium atoms.