Experimental and computational studies on the physicochemical behavior of phosphine induced by reactions with H and D atoms on interstellar ice grains

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Phosphine (PH_3) is an important molecule for the chemistry of phosphorus (P-) bearing species in the interstellar medium (ISM). Interstellar PH_3 is thought to primarily form on icy grains, where several surface processes may occur during and after its formation. To better understand the physicochemical behavior of PH_3 on ice grains in dense molecular clouds, we performed experimental and computational studies on the reactions of phosphine with H and D atoms at low temperatures. We found that phosphine and its deuterated isotopologue PD_3 are released into the gas phase from ice surfaces via chemical desorption. We confirmed that H-D substitution reactions of PH_3 and D-H substitution reactions of PD_3 occurred following reactions with D and H atoms, respectively, at 10 K on icy surface. Because the activation barrier for the abstraction of H and D atoms from phosphine is ~1500 K, quantum tunneling should play a role at low temperatures. On the other hand, the D-H substitution reactions of PD_3 was slightly faster than the H-D substitution reactions of PH_3, meaning that the rates of the H-D and D-H substitution reactions are not constrained by tunneling reactions but rather by other elementary processes such as atoms diffusion on ice.