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An infrared measurement of chemical desorption from interstellar ice analogues

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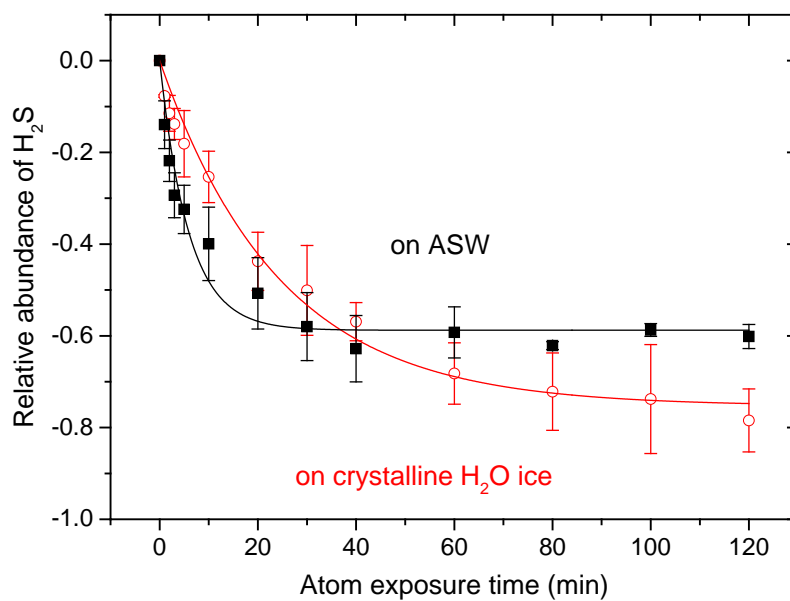
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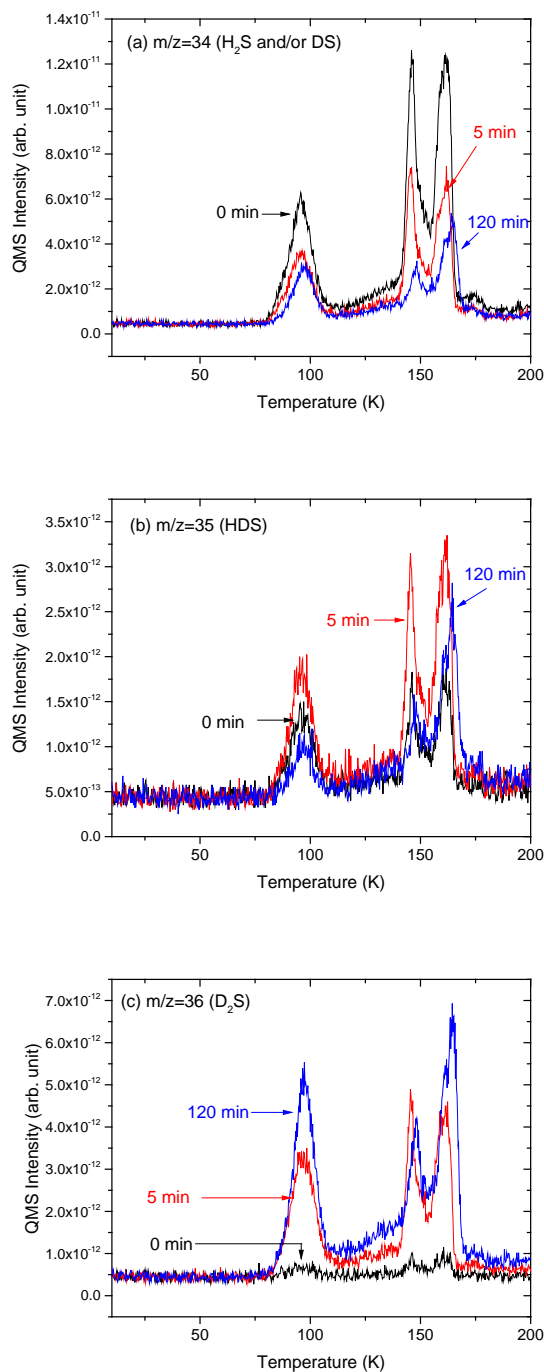
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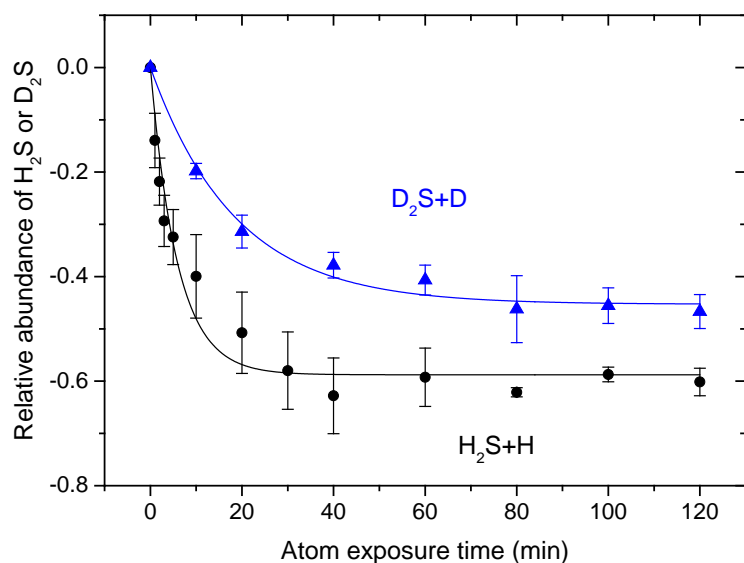


Supplementary Figure 1. **Variations in the relative abundance of H₂S after exposure to H atoms on ASW (black solid squares) and on crystalline H₂O ice (red open circles).** The desorption fraction is larger for the reaction on crystalline ice (~80% of the initial H₂S) than on ASW (~60%). Solid lines are guides for the eyes. Each data point is an average of three measurements with the standard deviation of the mean value.



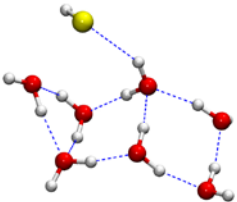
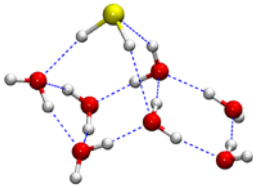

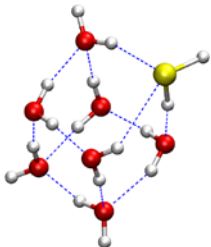
Supplementary Figure 2. **Temperature-programmed desorption (TPD) spectra of H_2S after exposure to D atoms at $m/z =$ (a) 34, (b) 35 and (c) 36 for 0 (black), 5 (red) and 120 min (blue).** The mass peaks at $m/z = 34$ include contributions from either or both H_2S and DS . The DS radical originates from the fragment ions of HDS and D_2S . The TPD results in panel (b) clearly indicate the formation of HDS at the earlier stages of the $\text{H}_2\text{S}+\text{D}$ experiment, followed by the formation of D_2S as shown in

panel (c). This trend is consistent with our proposal that the reaction between $\text{H}_2\text{S} + \text{D}$ proceeds through reactions R3–R6 and hence the reaction between $\text{H}_2\text{S} + \text{H}$ proceeds through reactions R1 and R2. Detection of HDS ($m/z = 35$) and D_2S ($m/z = 36$) in the non-processed sample (0 min) would not be due to the presence of both deuterated sulfides but be mainly due to the low mass resolution of the present QMS setup.



Supplementary Figure 3. **Variations in the relative abundance of solid D_2S after exposure to D atoms on amorphous D_2O ice for 120 min (blue solid triangles). Those of solid H_2S after exposure to H atoms (black solid squares) are also shown for comparison.** The solid lines are guides for the eyes. Each data point is an average of three measurements with the standard deviation of the mean value.

Supplementary Table 1. HS-(H₂O)₇ and H₂S-(H₂O)₇ structures and corresponding binding energies with respect to the separated cluster and adsorbate. The blue dashed lines are a guide to the eye.

Structure	Binding Energy (kJ/mol)	Zero-point energy (kJ/mol)	Total (kJ/mol)
	-16.8	4.7	-12.1
	-23.3	7.2	-16.1
	-12.8	4.0	-8.8
	-13.3	6.7	-6.6