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Supporting Information

Interstellar Enolization-Acetaldehyde (CH_3CHO) and Vinyl Alcohol ($H_2CCH(OH)$) as a Case Study

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Supporting Information

Table S1. IR features associated with acetaldehyde in pure acetaldehyde ices.[1]

Absorption (cm^{-1})	Assignment	Approximate type of mode
3416	$2\nu_4$	overtone
3123	$\nu_4 + \nu_6$	combination
3001	ν_1	$\nu_{as}(CH_3)$
2964	ν_{11}	$\nu(CH_3)$
2916	ν_2	$\nu_s(CH_3)$
2858	$2\nu_6$	overtone
2843	$2\nu_6$	overtone
2759	ν_3	$\nu(CH)$
2736	ν_3	$\nu(CH)$
2598	$\nu_4 + \nu_9$	combination
2466	$\nu_7 + \nu_8$	combination
2234	$\nu_7 + \nu_9$	combination
2003	$\nu_8 + \nu_9$	combination
1769	$2\nu_9$	overtone
1726	ν_4	$\nu(CO)$
1718	ν_4	$\nu(CO)$
1680	ν_4 ($CH_3{}^{13}CHO$)	$\nu({}^{13}CO)$
1641	$\nu_8 + \nu_{10}$	combination
1546	$2\nu_{14}$	overtone
1430	ν_{12} / ν_5	$\delta(CH_3)$ / $\delta_{as}(CH_3)$
1406	$\nu_9 + \nu_{10}$	combination
1392	ν_6	$\delta(CH)$
1347	ν_7	$\delta_s(CH_3)$
1123	ν_8	$\gamma_r(CH_3)$
1107	ν_8 (${}^{13}CH_3CHO$)	$\gamma_r({}^{13}CH_3)$
886	$\nu_{14} + \nu_{15}$	combination
772	ν_{14}	$\gamma(CH)$

Table S2. IR features associated with solid acetaldehyde-d4 in the acetaldehyde-d4 ice.[1]

Absorption (cm^{-1})	Assignment	Approximate type of mode
3384	$2\nu_4$	overtone
2472	$\nu_4 + \nu_9$	combination
2312	$2\nu_5$	overtone
2254	ν_1	$\nu_{as}(CD_3)$
2219	ν_{11}	$\nu(CD_3)$
2180	$\nu_5+\nu_7$	combination
2134	ν_2	$\nu_s(CD_3)$
2104	ν_2	$\nu_s(CD_3)$
2088		
2076	$\nu_2/2\nu_{12}$ (Fermi resonance)	ν(CD)/overtone
2068		
1908	$\nu_5 + \nu_9$	combination
1884	$\nu_8 + \nu_{12}$	combination
1870	$2\nu_8$	overtone
1709	ν_4	ν(CO)
1693	$\nu_9+\nu_8$	ν(CO)
1662	ν_4 ($CD_3{}^{13}CDO$)	$\nu(^{13}CO)$
1597	$\nu_5 + \nu_{10}$	combination
1157	ν_5	ν(CC)
1042	ν_{12}	$\delta(CD_3)$
1021	ν_6	$\delta_{as}(CD_3)$
952	ν_{13}	γ (CD)
941	ν_8	$\delta_s(CD_3)$

Table S3. Detected mass-to-charge ratios in the irradiated ice and tentative assignment of molecules.

Mass-to-charge ratio			
CH_3CHO	CD_3CDO	Formula	Assignment
42	44	C_2H_2O	Ketene
44	48	C_2H_4O	Vinyl alcohol
45	50	$C_2H_5O^+$	Protonated acetaldehyde
58	64	C_3H_6O	Acetone
70	76	C_4H_6O	?
72	80	C_4H_8O	?
86	92	$C_4H_6O_2$	2,3-Butanedione
88	96	$C_4H_8O_2$	$(CH_3CHO)_2$
89	98	$C_4H_9O_2$	$(CH_3CHO)H(CH_3CHO)$
101	110	$C_5H_9O_2$	$(CH_3CHCO)H(CH_3CHO)$
117*	126*	$C_5H_9O_3$	$(CH_3COCHO)H(CH_3CHO)$
131	142	$C_6H_{11}O_3$	$(CH_3COCOCH_3)H(CH_3CHO)$
132	144	$C_6H_{12}O_3$	$(CH_3CHO)_3$
133	146	$C_6H_{13}O_3$	$(CH_3CHO)_3H$
145	158	$C_7H_{13}O_3$	$(CH_3CHCO)H(CH_3CHO)_2$
149	162	$C_6H_{13}O_4$	$(CH_3COOH)H(CH_3CHO)_2$
159	174	$C_8H_{15}O_3$	$(CH_3COCOCH_3)H(C_4H_8O)$
176	192	$C_8H_{16}O_4$	$(CH_3CHO)_4$
177	194	$C_8H_{17}O_4$	$(CH_3CHO)_4H$

Notes: * also detected in unirradiated acetaldehyde ices

Table S4. Relative signals of vinyl alcohol isotopologues expected assuming only ketene hydrogenation as formation pathway compared to relative signals detected.

m/z	Molecular formula	Relative signal detected	Relative signal expected
44	C_2H_4O	1	1
45	C_2H_3DO	0.83 ± 0.05	2.05
46	$C_2H_2D_2O$	0.34 ± 0.03	1.47
47	C_2HD_3O	0.57 ± 0.04	0.77
48	C_2D_4O	0.45 ± 0.03	0.36

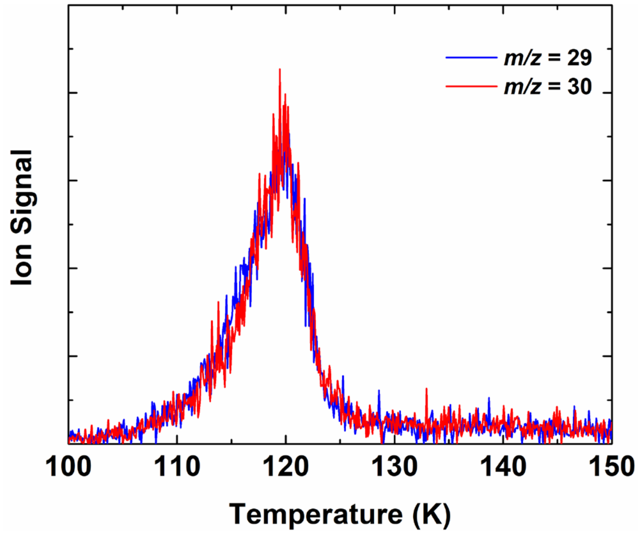

Figure S1. QMS signal of the HCO^+ (*m/z* =29, blue line) and DCO^+ (*m/z* = 30, red line) fragments of CH_3CHO and CD_3CDO, respectively.

References

[1] H. Hollenstein, H. H. Günthard, *Spectrochim Acta A* **1971**, *27*, 2027-2060.