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Supporting Information

Kinetic study of the reactions of AlO with H_2O and H_2; precursors to stellar dust formation

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Table S1. List of measured second-order rate coefficients for reaction R1 and R2, as a function of temperature and pressure (and bath gas for R2).

$AlO + H_2O (+ N_2) \rightarrow Al(OH)_2$ (R1)			$AlO + H_2 \rightarrow AlOH + H$ (R2)			
T / K	Pressure / Torr	Rate coefficient / cm^3 $molecule^{-1}$ s^{-1}	T / K	Pressure / Torr	Bath gas	Rate coefficient / cm^3 $molecule^{-1}$ s^{-1}
295	3.2	$(7.49 \pm 0.89) \times 10^{-11}$	463	14.9	He	$(2.04 \pm 0.15) \times 10^{-14}$
	5.4	$(9.17 \pm 0.94) \times 10^{-11}$	471	5.0	He	$(2.46 \pm 0.2) \times 10^{-14}$
	9.0	$(1.14 \pm 0.13) \times 10^{-10}$	532	10.6	N_2	$(4.92 \pm 0.33) \times 10^{-14}$
	12.1	$(1.31 \pm 0.19) \times 10^{-10}$	533	24.1	N_2	$(3.66 \pm 0.25) \times 10^{-14}$
433	5.4	$(5.49 \pm 0.65) \times 10^{-11}$	546	14.9	He	$(5.34 \pm 0.57) \times 10^{-14}$
	7.1	$(6.02 \pm 0.76) \times 10^{-11}$	548	5.0	He	$(5.38 \pm 0.75) \times 10^{-14}$
	9.0	$(6.45 \pm 0.81) \times 10^{-11}$	580	8.0	N_2	$(7.3 \pm 0.6) \times 10^{-14}$
	12.1	$(7.01 \pm 0.92) \times 10^{-11}$	613	3.9	He	$(8.38 \pm 1.83) \times 10^{-14}$
590	5.9	$(4.97 \pm 0.51) \times 10^{-11}$	625	5.0	He	$(7.47 \pm 0.92) \times 10^{-14}$
	8.9	$(5.36 \pm 0.55) \times 10^{-11}$	627	14.9	He	$(9.31 \pm 0.61) \times 10^{-14}$
	11.9	$(5.79 \pm 0.61) \times 10^{-11}$	686	9.1	N_2	$(2.95 \pm 0.32) \times 10^{-13}$
640	5.9	$(5.43 \pm 0.6) \times 10^{-11}$	694	4.1	He	$(2.58 \pm 0.24) \times 10^{-13}$
	9.0	$(5.91 \pm 0.84) \times 10^{-11}$	694	10.2	He	$(2.64 \pm 0.55) \times 10^{-13}$
	12.1	$(6.23 \pm 0.67) \times 10^{-11}$	702	5.0	He	$(2.42 \pm 0.28) \times 10^{-13}$
700	5.8	$(5.78 \pm 0.78) \times 10^{-11}$	707	14.6	He	$(2.13 \pm 0.08) \times 10^{-13}$
	9.0	$(6.59 \pm 0.89) \times 10^{-11}$	773	4.0	He	$(5.77 \pm 0.77) \times 10^{-13}$
	12.0	$(6.74 \pm 0.75) \times 10^{-11}$	781	4.5	He	$(4.75 \pm 0.22) \times 10^{-13}$
760	5.8	$(6.83 \pm 0.78) \times 10^{-11}$	782	10.0	N_2	$(4.87 \pm 0.25) \times 10^{-13}$
	9.0	$(7.19 \pm 0.82) \times 10^{-11}$	785	10.4	He	$(6.22 \pm 1.02) \times 10^{-13}$
	12.0	$(7.45 \pm 1.11) \times 10^{-11}$				

Table S2. Molecular properties and heats of formation (at 0 K) of the stationary points on the $AlO + H_2O$ potential energy surface.

Molecule (electronic state)	Geometry (Cartesian co-ordinates in Å) [a]	Rotational constants (GHz) [a]	Vibrational frequencies (cm^{-1}) [a]	$\Delta_f H^o$(0 K) (kJ mol^{-1}) [b]
$AlO + H_2O \rightarrow Al(OH)_2$, AlOH + OH				
AlO	Al, 0., 0., 0.002 O, 0., 0., 1.628	19.0158	967	70.3
H_2O	O, 0.001, 0., 0.001 H 0, 0.0123, 0., 0.963 H, 0.933, 0., -0.237	798.21 438.23 282.91	1672, 3802, 3906	-238.9 (JANAF value [1])
TS from $AlO + H_2O$ to AlOH + H (TS1)	Al, 1.657, 0.017, 0.012 O, -2.294, -0.144, 0.040 H, -1.067, -0.139, -0.124 O, 0.006, 0.096, 0.027 H, -2.555, 0.779, -0.089	479.41 3.0467 3.0286	1232*i*, 72, 78, 419, 613, 841, 1041, 1373, 3774	-108.4
$AlO\text{-}OH_2$	Al, -0.404, -0.685, -0.001 O, 1.446, 0.159, -0.127 H, 0.795, 0.937, -0.037 O, -0.977, 0.854, 0.041 H, 2.046, 0.163, 0.629	19.292 8.6097 6.0356	153, 315, 437, 583, 898, 951, 1541, 2923, 3799	-227.1
TS from $AlO\text{-}OH_2$ to $Al(OH)_2$ (TS2)	Al, -0.432, -0.702, 0.014 O, 1.366, 0.163, -0.121 H, 0.636, 0.914, -0.041 O, -0.992, 0.848, 0.026 H, 1.965, 0.206, 0.634	18.950 9.1058 6.2382	228*i*, 352, 478, 615, 932, 958, 1483, 2488, 3802	-229.6
$Al(OH)_2$	Al, -0.010, -0.497, 0.000 O, 1.518, 0.245, -0.000 H, 1.609, 1.201, -0.000 O, -1.427, 0.453, 0.000 H, -2.296, 0.048, 0.000	41.154 6.5228 5.6304	214, 284, 318, 630, 647, 774, 917, 3874, 3906	-476.1
TS from $AlO\text{-}OH_2$ to OAlOH (TS3)	Al, -0.180, 0.145, 0.000 O, 1.536, -0.149, -0.002 H, 2.178, 0.575, -0.012 O, -1.778, 0.057, 0.006 H, 2.293, -1.398, 0.008	194.01 5.0721 4.9429	1295*i*, 57, 166, 211, 298, 688, 873, 1143, 3749	-81.8
AlOH	Al, 0.026, 0., 0.018 O, -0.063, 0., 1.702 H, 0.364, 0., 2.555	2590.6 15.754 15.658	215, 849, 3960	-191.3
OAlOH	Al, 0.081, -0.016, -0.000 O, -1.587, -0.124, 0.000 H, -2.227, 0.586, 0.000 O, 1.678, 0.039, 0.000	992.82 5.5791 5.5479	210, 221, 544, 786, 1196, 3938	-358.3
OH	O, 0., 0., 0.002 H, 0., 0., 0.978	559.17	3691	38.4 (JANAF value [1])

[a] Calculated at the G4 level of theory. [2, 3] [b] Calculated using the reaction enthalpies at 0 K for R1a-1d, and the bond energy D_0(Al-O) = 503 kJ mol^{-1}, all determined at the G4 level of theory,[2, 3] combined with reference values for $\Delta_f H^o$(Al) = 327.3 kJ mol^{-1}, $\Delta_f H^o$(O) = 246.8 kJ mol^{-1}, $\Delta_f H^o(H_2O)$ = -238.9 kJ

mol^{-1}, and $\Delta_f H^o$(H) = 216.0 kJ mol^{-1} from the JANAF Tables,[1] and $\Delta_f H^o$(OH) = 37.3 kJ mol^{-1} from the Active Thermochemical Tables.[4]

Table S3. Molecular properties and heats of formation (at 0 K) of the stationary points on the AlO + H_2 potential energy surface.

Molecule (electronic state)	Geometry (Cartesian co-ordinates in Å) [a]	Rotational constants (GHz) [a]	Vibrational frequencies (cm^{-1}) [a]	$\Delta_f H^o$(0 K) (kJ mol^{-1}) [b]
AlO + H_2 → AlOH + H, Al + H_2O				
AlO	Al, 0., 0., 0.002 O, 0., 0., 1.628	19.016	967	70.3
TS from AlO + H_2 to AlOH + H (TS1)	Al, 0., 0., -0.868 O, 0., 0., 0.7856 H, ,0., 0., 2.066 H, 0., 0., 2.939	11.895	1197*i*, 90, 90, 867, 874, 874 2141	115.8
TS from AlO + H_2 to *cis*-HAlOH (TS2)	Al, -0.658, -0.133, -0.000 O, 1.016, -0.171, 0.000 H, 0.542, 1.229, 0.000 H, -0.149, 1.772, 0.000	93.758 17.734 14.913	1010*i*, 515, 845, 1037, 1526, 2325	133.4
cis-HAlOH	Al, -0.597, -0.209, 0.000 O, 1.055, 0.205, -0.000 H, 1.756, -0.450, -0.000 H, -0.997, -1.771, -0.000	198.10 15.0139 13.9561	386, 511, 662, 857, 761, 3886	-101.2
TS from *cis*-HAlOH to *trans*-HAlOH (TS3)	Al, 0.637, -0.134, -0.035 O, -1.038, 0.033, 0.119 H, -1.779, 0.225, -0.449 H, 1.534, 1.206, 0.0275	223.01 14.755 14.121	423*i*, 368, 579, 861, 1745, 3971	-96.2
trans-HAlOH	Al, 0.356, -0.071, 0.0276 O, -1.346, -0.143, 0.0915 H, -1.902, 0.620, -0.071 H, 1.076, -1.471, 0.333	203.28 14.995 13.965	430, 535, 683, 842, 1803, 3913	-104.5
TS from *trans*-HAlOH to Al-OH_2 (TS4)	Al, -0.862, -0.154, -0.077 O, 0.995, 0.083, 0.381 H, 1.717, -0.173, -0.214 H, 0.465, 1.129, -0.093	259.86 12.210 11.986	1336*i*, 437, 516, 795, 1268, 3717	105.7
Al-OH_2	Al, -0.668, -0.963, -0.015 O, 0.007, 1.137, -0.003 H, -0.139, 1.678, 0.782 H, -0.137, 1.687, -0.782	363.15 9.0640 8.8926	177.6715 237.2009 327.5853 1605.6061 3760.8304 3875.3572	60.2
AlOH	Al, 0.026, 0., 0.018 O, -0.063, 0., 1.702 H, 0.364, 0., 2.555	2590.6 15.754 15.658	215, 849, 3960	-186.7
TS from AlOH + H to Al-OH_2 (TS5)	Al, 0.858, -0.009, 0.066 O, -0.962, 0.009, 0.088 H, -1.919, 0.904, 0.096 H, -1.448, -0.825, 0.098	338.36 12.593 12.141	1814*i*, 228, 512, 632, 1020, 3777	115.2

[a] Calculated at the G4 level of theory. [2, 3]

[b] Calculated using the reaction enthalpies at 0 K for reactions 2a and b, and the bond energy D_0(Al-O) = 503 kJ mol^{-1}, all at the G4 level of theory [2, 3] with JANAF reference values[1] for $\Delta_f H^o$(Al) = 327.3 kJ mol^{-1}, $\Delta_f H^o$(O) = 246.8 kJ mol^{-1}, $\Delta_f H^o$(H_2O) = -238.9 kJ mol^{-1} and $\Delta_f H^o$(H) = 216.0 kJ mol^{-1}. Note that

$\Delta_f H^o$(AlOH) is different in Table S2 and S3, because the entry in Table S2 uses $\Delta_r H^o$(AlO + $H_2O \rightarrow$ AlOH + OH), and the entry in Table S3 uses $\Delta_r H^o$(AlO + $H_2 \rightarrow$ AlOH + H), both determined at the G4 level.

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