Electronic supplementary information

Table S1. Cartesian coordinates of optimized geometry (in Å) of CH_3---HOH radical complex calculated at the MP2/aug-cc-pVTZ level of theory.

CH_3---HOH			
	x	y	z
1	0.664212	-0.058152	0.000002
8	1.615726	0.100374	-0.000013
1	2.001058	-0.780302	0.000007
6	-1.718446	0.000679	0.000011
1	-1.876016	-0.514300	-0.931165
1	-1.876058	-0.514170	0.931253
1	-1.528332	1.059856	-0.000059

Table S2. Vibrational frequencies for the CH_3---HOH complex calculated at the MP2/aug-cc-pVDZ level of theory. Vibrational frequencies of isolated CH_3 and H_2O monomers are given as well.

	MP2/aug-cc-pVDZ		description	MP2/aug-cc-pVDZ	
	frequency (cm^{-1})	intensity (km mol^{-1})		frequency (cm^{-1})	intensity (km mol^{-1})
			intermolecular	isolated monomers	
ν_1	36.60	100.00	CH_3 & H_2O torsional motion about the hydrogen bond		
ν_2	77.13	34.72	in plane wagging of CH_3 & concerted motion of H_2O		
ν_3	100.67	8.64	out of plane wagging of CH_3		
ν_4	102.73	3.80	van der Waals stretch		
ν_5	216.68	60.44	in plane wagging of H_2O & concerted motion of CH_3		
ν_6	316.49	59.09	out of plane wagging of H_2O		
			intramolecular		
ν_7	564.40	81.94	CH_3 out of plane bend (umbrella)	494.71	76.94
ν_8	1422.52	2.34	CH_3 in plane bend	1424.51	1.76
ν_9	1423.42	1.93	CH_3 in plane bend	1424.51	1.76
ν_{10}	1624.80	43.03	H_2O bend	1622.30	67.46
ν_{11}	3156.41	0.25	CH_3 symmetric stretch	3165.08	0.00
ν_{12}	3354.99	0.97	CH_3 antisymmetric stretch	3364.48	3.01
ν_{13}	3358.22	1.38	CH_3 antisymmetric stretch	3364.48	3.01
ν_{14}	3768.75	57.98	H_2O symmetric stretch	3803.30	4.14
ν_{15}	3914.40	124.27	H_2O antisymmetric stretch	3937.52	67.02

Table S3. Cartesian coordinates of optimized geometry (in Å) of higher energy CH_3---OHH radical complex calculated at the MP2/aug-cc-pVTZ level of theory.

CH_3---OHH			
	x	y	z
6	-0.000080	1.926523	0.000000
1	-0.000129	0.850406	0.000000
1	0.928479	2.469342	0.000000
1	-0.928592	2.469425	0.000000
8	-0.000080	-1.616763	0.000000
1	0.000684	-2.207101	0.759016
1	0.000684	-2.207101	-0.759016

Table S4. Vibrational frequencies for the higher energy CH_3---OHH radical complex calculated at both the MP2/aug-cc-pVDZ and MP2/aug-cc-pVTZ level of theory.

	MP2/aug-cc-pVDZ		MP2/aug-cc-pVTZ	
	frequency (cm^{-1})	intensity (km mol^{-1})	frequency (cm^{-1})	intensity (km mol^{-1})
		intermolecular		
ν_1	18.41	228.91	17.03	61.11
ν_2	33.03	64.06	33.01	225.37
ν_3	58.64	0.00	60.86	0.00
ν_4	100.49	0.51	90.40	0.45
ν_5	107.02	0.38	98.35	0.49
ν_6	234.37	0.68	208.06	2.10
		intramolecular		
ν_7	548.35	78.16	529.70	77.71
ν_8	1426.64	0.86	1438.20	1.10
ν_9	1437.60	0.91	1451.13	1.09
ν_{10}	1623.35	64.67	1628.48	68.66
ν_{11}	3156.41	10.79	3164.85	9.87
ν_{12}	3354.17	5.84	3354.37	3.90
ν_{13}	3361.52	2.39	3358.14	3.10
ν_{14}	3800.76	5.22	3819.45	6.93
ν_{15}	3934.96	71.55	3945.30	79.68