Supplementary Material for PCCP

SUPPLEMENTARY INFORMATION FOR

Vibrational Overtone Induced Elimination Reactions Within Hydrogen-Bonded Molecular Clusters: The Dynamics of Water Catalyzed Reactions in $CH_2FOH\cdot(H_2O)_n$

Kaito Takahashi,[a] Zeb C. Kramer,[a] Veronica Vaida,[a,b] and Rex T. Skodje[a]

a) Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309-0215

b) CIRES, University of Colorado, Boulder, CO 80309

Table S1. The calculated equilibrium (EQ) and transition state (TS) geometries of CH_2FOH using B3LYP/6-31+G(d,p) given in Cartesian coordinates in units of angstrom.

		EQ	
C	0.000	0.000	0.000
O	0.000	0.000	1.380
F	1.312	0.000	-0.502
H	-0.482	-0.885	-0.431
H	-0.475	0.926	-0.327
H	0.330	-0.849	1.706
		TS	
C	0.000	0.000	0.000
O	0.000	0.000	1.288
F	1.823	0.000	0.075
H	-0.153	-0.933	-0.556
H	-0.152	0.933	-0.556
H	1.202	0.001	1.119

Table S2. The calculated equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)$ using B3LYP/6-31+G(d,p) given in Cartesian coordinates in units of angstrom.

		EQ	
C	0.000	0.000	0.000
O	0.000	0.000	1.367
F	1.341	0.000	-0.504
H	-0.457	-0.892	-0.443
H	-0.460	0.924	-0.353
H	0.382	-0.847	1.670
O	1.672	-2.241	1.275
H	2.325	-2.664	1.845
H	2.162	-1.719	0.621

		TS	
C	0.000	0.000	0.000
O	0.000	0.000	1.267
F	1.818	0.000	-0.488
H	-0.124	-0.934	-0.558
H	-0.265	0.922	-0.523
H	0.973	-0.744	1.634
O	2.041	-1.177	1.529
H	2.643	-0.828	2.199
H	2.178	-0.670	0.561

Table S3. The calculated equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)_2$ using B3LYP/6-31+G(d,p) given in Cartesian coordinates in units of angstrom.

		EQ	
C	0.000	0.000	0.000
O	1.263	0.000	-0.485
F	0.000	0.000	1.457
H	-0.583	0.890	-0.258
H	-0.503	-0.929	-0.270
H	1.648	0.908	-0.426
O	2.151	2.539	-0.025
H	3.062	2.789	-0.217
H	2.036	2.576	0.952
O	1.486	2.099	2.586
H	0.962	2.650	3.180
H	0.953	1.305	2.395
		TS	
C	0.000	0.000	0.000
O	1.187	0.000	-0.419
F	0.000	0.000	1.886
H	-0.585	0.926	0.015
H	-0.564	-0.934	-0.027
H	1.876	1.084	-0.140

O	2.415	1.954	0.318
H	3.367	1.866	0.177
H	2.103	1.870	1.472
O	1.629	1.600	2.558
H	1.233	2.350	3.020
H	0.865	0.851	2.340

Table S4. The calculated equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)_3$ using B3LYP/6-31+G(d,p) given in Cartesian coordinates in units of angstrom.

		EQ	
C	0.000	0.000	0.000
O	1.004	-0.762	-0.485
F	0.000	0.000	1.459
H	0.076	1.062	-0.256
H	-0.965	-0.435	-0.262
H	1.848	-0.245	-0.511
O	3.209	0.768	-0.438
H	3.817	0.910	-1.172
H	3.749	0.634	0.381
O	4.404	0.345	1.952
H	4.952	-0.436	2.095
H	3.615	0.240	2.535
O	2.082	0.000	3.340
H	1.789	0.620	4.018
H	1.351	-0.068	2.697
		TS	
C	0.000	0.000	0.000
O	0.985	-0.637	-0.452
F	0.000	0.000	1.861
H	0.001	1.097	0.005
H	-0.981	-0.481	-0.004
H	2.198	-0.050	-0.479
O	3.217	0.345	-0.404

H	3.314	1.174	-0.887
H	3.650	0.328	0.795
O	3.965	0.258	1.889
H	4.566	-0.489	2.015
H	3.043	0.147	2.554
O	1.973	0.000	3.230
H	1.839	0.648	3.932
H	1.095	-0.026	2.625

Table S5. The calculated equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)_2H_2O$ using B3LYP/6-31+G(d,p) given in Cartesian coordinates in units of angstrom.

		EQ	
C	0.000	0.000	0.000
O	1.263	0.000	-0.490
F	0.000	0.000	1.449
H	-0.583	0.890	-0.262
H	-0.504	-0.927	-0.276
H	1.650	0.908	-0.423
O	2.157	2.535	-0.041
H	3.102	2.710	-0.130
H	1.940	2.601	0.924
O	1.333	2.315	2.511
H	0.751	2.954	2.964
H	0.830	1.489	2.409
O	-0.305	4.206	3.862
H	-0.038	4.465	4.753
H	-0.593	5.013	3.416
		TS	
C	0.000	0.000	0.000
O	1.189	0.000	-0.436
F	0.000	0.000	1.801
H	-0.593	0.923	-0.030
H	-0.570	-0.931	-0.060

H	1.883	1.095	-0.174
O	2.429	1.967	0.260
H	3.370	1.897	0.055
H	2.156	1.838	1.480
O	1.733	1.549	2.524
H	1.336	2.301	3.016
H	0.985	0.847	2.307
O	0.541	3.573	3.985
H	-0.390	3.748	3.792
H	0.611	3.495	4.945

Table S6. The calculated harmonic frequencies in cm^{-1} of the equilibrium (EQ) and transition state (TS) geometries of CH_2FOH using B3LYP/6-31+G(d,p) .

	EQ	
395.2	533.7	974.2
1061.1	1142.5	1253.8
1382.9	1441.8	1530.2
3053.0	3152.5	3814.3
	TS	
1696.2i	402.5	543.3
656.2	907.3	1216.6
1261.9	1419.2	1599.1
1949.2	3035.8	3128.3

Table S7. The calculated harmonic frequencies in cm^{-1} of the equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)_1$ using B3LYP/6-31+G(d,p).

	EQ	
98.2	113.4	193.7
199.1	316.1	406.0
516.1	726.6	897.5
1097.5	1176.8	1257.8
1418.8	1468.5	1529.6
1610.3	3058.9	3157.1
3642.9	3773.4	3913.9

	TS	
1043.7i	152.3	371.2
466.7	521.0	596.1
626.2	664.2	832.8
1203.6	1232.8	1248.3
1428.3	1456.3	1591.8
1652.8	1781.7	2067.6
3058.8	3157.9	3847.2

Table S8. The calculated harmonic frequencies in cm^{-1} of the equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)_2$ using B3LYP/6-31+G(d,p).

	EQ	
41.3	94.5	119.5
183.2	212.1	234.0
248.4	297.1	353.2
453.0	512.2	623.4
765.5	834.6	950.3
1110.2	1214.3	1268.4
1417.4	1515.2	1529.9
1629.4	1653.4	3062.9
3161.2	3397.2	3514.9
3686.3	3889.6	3898.8
	TS	
998.0i	70.5	136.6
150.7	297.1	408.6
446.3	497.1	525.2
606.1	623.0	716.9
738.1	846.5	1184.9
1219.5	1244.7	1299.2
1469.5	1508.1	1539.6
1616.7	1697.2	1764.3
1839.3	1985.0	3052.1
3157.9	3856.5	3867.6

Table S9. The calculated harmonic frequencies in cm^{-1} of the equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)_3$ using B3LYP/6-31+G(d,p).

	EQ	
27.3	40.0	70.0
83.6	124.2	173.1
209.2	218.9	222.9
258.6	294.1	309.2
361.0	438.3	497.1
559.7	600.0	811.2
836.1	904.4	987.6
1106.1	1220.0	1270.2
1418.8	1492.2	1528.9
1642.3	1660.5	1689.5
3068.0	3157.7	3320.0
3402.9	3463.0	3681.7
3884.9	3893.5	3898.6
	TS	
829.3i	25.3	56.0
93.7	125.7	148.0
262.0	330.1	360.4
408.8	456.2	495.5
557.6	567.6	640.7
690.1	736.1	799.2
862.6	1127.9	1220.1
1224.1	1265.2	1425.8
1471.3	1490.2	1525.9
1611.8	1629.2	1711.9
1734.6	1779.3	1907.5
2238.4	3033.6	3138.8
3854.2	3874.2	3883.3

Table S10. The calculated harmonic frequencies in cm^{-1} of the equilibrium (EQ) and transition state (TS) geometries of $CH_2FOH\cdots(H_2O)_2H_2O$ using B3LYP/6-31+G(d,p).

	EQ	
22.4	40.8	48.4
83.8	92.7	119.8
154.3	188.4	207.8
229.7	240.3	286.1
328.9	459.0	488.7
524.7	608.1	727.7
821.9	857.3	1008.1
1114.1	1209.5	1271.5
1419.9	1525.1	1529.5
1616.8	1643.6	1669.3
3054.9	3151.7	3333.2
3420.7	3661.1	3775.6
3812.8	3887.0	3929.5
	TS	
820.3i	37.3	48.7
71.0	77.6	129.9
143.2	215.6	283.5
307.5	336.6	421.1
458.0	520.0	558.8
677.9	789.3	799.7
859.8	916.7	1131.6
1241.4	1252.4	1294.0
1451.9	1488.6	1557.4
1622.3	1642.0	1730.1
1792.4	1850.4	2469.1
3028.3	3130.3	3536.8
3808.1	3865.0	3921.9