

Atmospheric Vinyl Alcohol to Acetaldehyde Tautomerization Revisited

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Supporting Information

Figure S1. Optimized geometries of all structures

Table S1. Absolute potential energies of all structures

Table S2. Unscaled vibrational frequencies and rotational constants of all structures

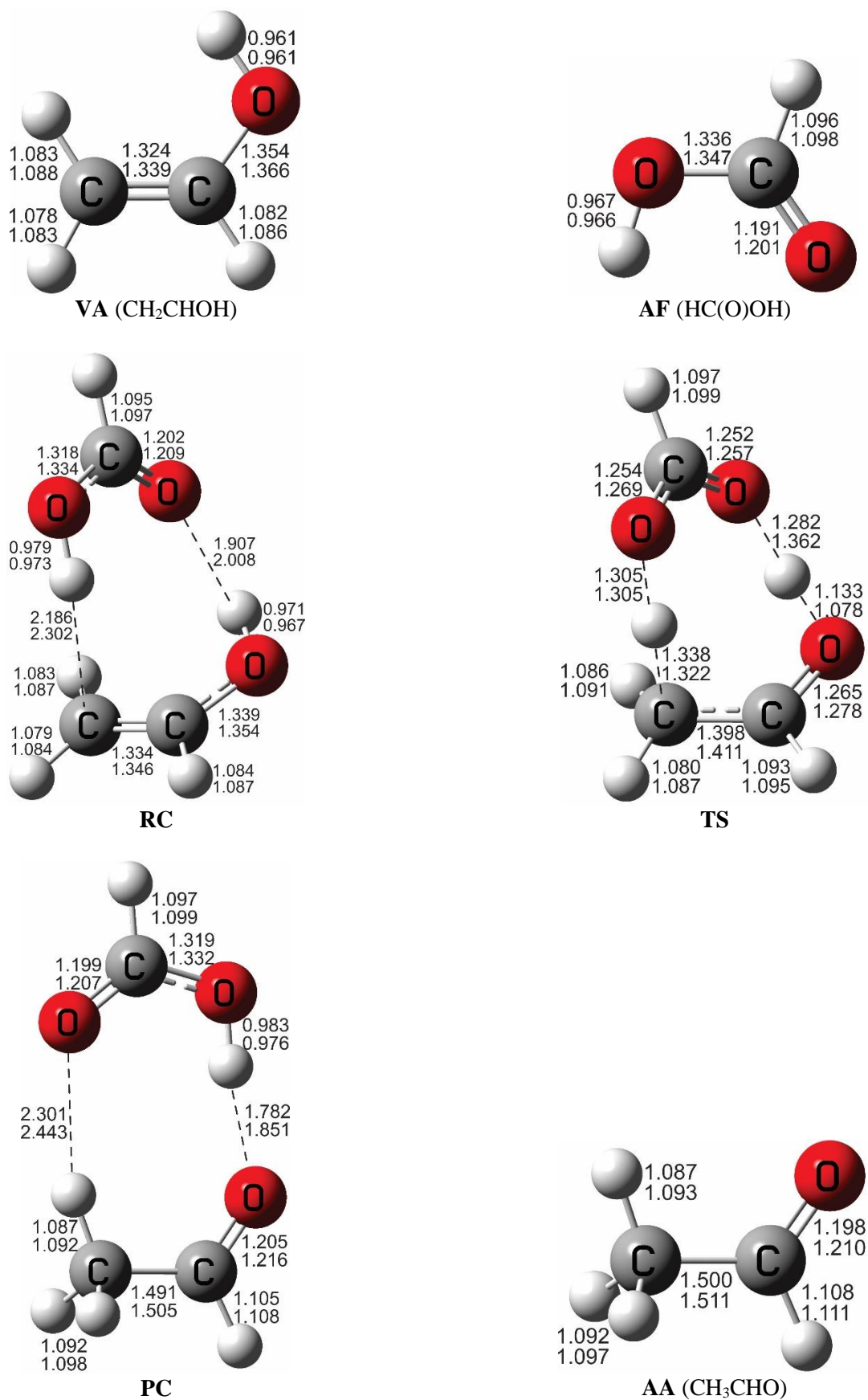


Figure S1. The optimized geometries and absolute energies of all structures in the tautomerization of Vinyl Alcohol (VA) to Acetaldehyde (AA) catalyzed by Formic Acid (FA) at the 2 levels of theory: upper: UM06-2x/6-311++G(3df,2p) and lower: UQCISD/6-311++G(d,p).

Table S1: Absolute potential energies and zero-point vibration energies (ZPVE) of all structures in the tautomerization of Vinyl Alcohol (VA) to Acetaldehyde (AA) catalyzed by Formic Acid (FA), in hartree.

Methods Structures	ZPVE ^{a)} UM06-2x/ 6-311++G(3df,2p)	UM06-2x/ 6-311++G(3df,2p)	UQCISD/ 6-311G(d,p)	CCSD(T)/ aVDZ	CCSD(T)/ aVTZ	CCSD(T)/ aVQZ	CBS/ CCSD(T)
VA (CH ₂ CHOH)	0.057052	-153.8014086	-153.4561889	-153.4451699	-153.5828631	-153.6228215	-153.6450626
AF (HC(O)OH)	0.034397	-189.7625879	-189.3719885	-189.355588	-189.5177349	-189.5676756	-189.5958196
VA + AF	0.091449	-343.5639965	-342.8281774	-342.8007579	-343.100598	-343.1904971	-343.2408822
RC	0.093923	-343.5810788	-342.8410145	-342.8169143	-343.1162045		
TS	0.08697	-343.5533987	-342.8061703	-342.7875148	-343.0867517	-343.1753904	-343.2249436
PC	0.09248	-343.5928551	-342.8611451	-342.8338583	-343.1317778		
AA + AF	0.090219	-343.5774061	-342.8475137	-342.8178733	-343.1161399	-343.2053476	-343.2553197
AA (CH ₃ CHO)	0.055822	-153.8148182	-153.4755252	-153.4622852	-153.598405	-153.637672	-153.6595000

^{a)} Zero-Point Vibration Energy obtained at UM06-2x/6-311++G(3df,2p) level of theory, in hartree, unscaled

Table S2. Unscaled vibrational frequencies, in cm^{-1} , and rotational constants A,B,C, in GHz, obtained at UM06-2x/6-311++G(3df,2p) level, of all structures in the tautomerization of Vinyl Alcohol (VA) to Acetaldehyde (AA) catalyzed by Formic Acid (FA).

465.6818	1015.3633	1725.2045	647.2096	1162.7081	1877.1815
498.4688	1135.9079	3157.3277	678.5136	1317.2315	3109.7125
726.7706	1328.2422	3200.7268	1074.494	1413.7117	3817.9846
865.8597	1353.8401	3264.0837			
969.8375	1449.9746	3885.6768		78.17141	
				12.23964	
	60.71739			10.58266	
	10.68616				
	9.08688				
VA (CH₂CHOH)			FA (HC(O)OH)		
70.7418	777.8456	1459.177	-1499.9702	835.5445	1489.1815
112.1378	882.8812	1699.9672	116.6847	1022.6075	1524.8889
143.5333	980.9371	1832.6648	177.3742	1074.3133	1654.6532
167.6812	1048.0061	3121.0001	254.2828	1095.9083	1711.2699
198.058	1089.6123	3149.2886	317.8556	1242.5431	1824.2261
222.8588	1195.2293	3193.9813	446.4299	1311.5882	3097.2938
514.4834	1226.4188	3253.7406	540.8685	1384.6016	3114.264
668.9235	1347.056	3539.507	606.9407	1402.3298	3119.1558
693.6637	1367.7385	3685.8928	703.2337	1425.2978	3231.6616
753.5303	1427.7585		798.1537	1459.968	
	5.44662			5.56866	
	2.12941			2.70387	
	1.80194			2.0365	
RC			TS		
29.1881	910.1975	1485.4906	157.2569		1466.4845
105.6749	917.6057	1833.6286	510.3252		1473.9691
108.5057	1089.8058	1860.6447	775.0313		1876.0744
132.6999	1152.7475	2996.2882	897.9048		2954.3536
170.0768	1239.2406	3037.9513	1135.566		3038.9333
200.5463	1384.4929	3093.0466	1143.29		3106.1395
201.783	1391.1252	3098.971	1378.9111		3157.4308
531.537	1429.5487	3177.148		78.17141	
691.2344	1441.6264	3475.6464		12.23964	
779.5424	1468.3411			10.58266	
	5.70734				
	1.82541				
	1.39485				
PC			AA (CH₃CHO)		