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Supporting Information

for

Dissection of the multichannel reaction of acetylene with atomic oxygen: from global potential energy surface to rate coefficients and branching dynamics

Junxiang Zuo,[†] Qixin Chen,[†] Xixi Hu,*[,†] Hua Guo,[‡] and Daiqian Xie[†,§]

[†] *Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China*

[‡] *Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, New Mexico 87131, USA*

[§] *Synergetic Innovation Center of Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China*

*: corresponding author, xxhu@nju.edu.cn (X.H.)

Table S1. Comparison of calculated (UCCSD(T)) and fit geometries of stationary points for the $O(^3P) + C_2H_2$ reaction. Distances and angles are in units of Å and °, respectively. The abbreviated labels of the stationary points can be found in Figure 1.

Species	Method	r_{OC_1}	$r_{C_1C_2}$	$r_{C_1H_1}$	$r_{C_2H_2}$	$\theta_{OC_1C_2}$	$\theta_{H_1C_1C_2}$	$\theta_{C_1C_2H_2}$	$\varphi_{H_1C_1C_2O}$	$\varphi_{OC_1C_2H_2}$
R	PES	-	1.206	1.063	1.063	-	180.0	180.0	-	-
	UCCSD(T)	-	1.206	1.063	1.063	-	180.0	180.0	-	-
Int1	PES	2.957	1.206	1.064	1.064	78.3	179.9	179.9	0	0
	UCCSD(T)	2.965	1.206	1.063	1.063	78.3	179.8	179.8	0	0
Int2	PES	1.232	1.425	1.097	1.082	119.9	118.9	129.3	180.0	0
	UCCSD(T)	1.232	1.425	1.097	1.082	119.8	118.8	129.0	180.0	0
Int3	PES	1.224	1.426	1.108	1.081	125.3	114.3	131.5	180.0	180.0
	UCCSD(T)	1.224	1.426	1.107	1.081	125.3	114.2	131.6	180.0	180.0
Int4	PES	1.195	1.443	2.192	1.085	127.5	25.2	119.5	180.0	0
	UCCSD(T)	1.194	1.445	2.192	1.085	127.7	25.2	119.7	180.0	0
TS1	PES	1.986	1.224	1.065	1.064	99.5	161.3	169.7	180.0	0
	UCCSD(T)	1.982	1.225	1.065	1.065	99.6	161.1	169.7	180.0	0
TS2	PES	1.221	1.441	1.102	1.076	123.2	116.5	144.6	178.7	91.8
	UCCSD(T)	1.221	1.441	1.102	1.076	123.2	116.5	144.6	178.6	92.0
TS3	PES	1.174	1.324	1.731	1.079	171.0	82.9	130.9	180.0	0
	UCCSD(T)	1.176	1.320	1.738	1.078	171.0	84.6	132.7	180.0	0
TS4	PES	1.211	1.381	2.295	1.445	139.3	19.5	55.1	-125.5	-7.1
	UCCSD(T)	1.211	1.381	2.295	1.442	139.2	19.4	55.1	-126.0	-7.1
TS5	PES	1.172	1.328	1.938	1.076	160.5	94.2	128.5	180.0	180.0
	UCCSD(T)	1.172	1.328	1.932	1.076	160.5	94.0	128.6	180.0	180.0
TS6	PES	1.228	1.378	2.247	1.428	127.3	20.9	54.7	-115.2	175.8
	UCCSD(T)	1.227	1.381	2.255	1.427	127.2	20.7	54.6	-116.1	176.7
TS7	PES	1.138	2.244	2.871	1.078	114.4	20.0	113.9	0	180.0
	UCCSD(T)	1.138	2.248	2.875	1.078	114.5	19.9	113.7	0	180.0
P1	PES	1.172	1.302	-	1.073	168.5	-	132.5	180.0	-
	UCCSD(T)	1.172	1.302	-	1.073	168.9	-	132.6	180.0	-

Species	Method	r_{OC_1}	$r_{C_2H_1}$	$r_{C_2H_2}$	$\theta_{H_1C_2H_2}$
P2	PES	1.131	1.077	1.077	133.6
	UCCSD(T)	1.131	1.077	1.077	133.7

Table S2. Comparison of calculated (UCCSD(T)) and fit (PES) energies and frequencies of stationary points for the $O(^3P)$ + C_2H_2 reaction. Energies and frequencies are in units of kcal/mol and cm^{-1}, respectively. The abbreviated labels of the stationary points can be found in Figure 1.

Species	Method	E	E+ZPE	Harmonic Frequencies
R	PES	0	0	3499.1, 3413.7, 2011.3, 746.8, 746.8, 613.4, 613.4
	UCCSD(T)	0	0	3503.0, 3411.0, 2007.5, 748.9, 748.9, 616.2, 616.2
Int1	PES	-1.1	-0.9	3505.8, 3412.3, 2009.0, 758.3, 756.4, 616.7, 613.4, 77.6, 52.2
	UCCSD(T)	-1.1	-0.8	3501.4, 3410.3, 2004.8, 751.9, 748.6, 624.2, 620.0, 75.3, 71.2
Int2	PES	-53.4	-51.1	3215.0, 3023.7, 1549.4, 1407.7, 1139.9, 958.5, 930.2, 599.3, 444.9
	UCCSD(T)	-53.5	-51.1	3216.6, 3030.3, 1552.8, 1404.4, 1144.3, 962.6, 941.5, 607.0, 448.5
Int3	PES	-52.0	-50.1	3232.2, 2902.4, 1584.0, 1384.7, 1120.1, 943.9, 862.8, 477.7, 473.7
	UCCSD(T)	-52.0	-50.1	3222.2, 2909.5, 1583.5, 1388.1, 1121.9, 946.2, 877.9, 464.6, 441.1
Int4	PES	-72.6	-70.3	3289.3, 3131.2, 1774.5, 1448.9, 1071.9, 978.7, 768.5, 466.2, 354.3
	UCCSD(T)	-72.6	-70.3	3275.8, 3125.5, 1784.3, 1443.4, 1067.0, 983.2, 762.2, 464.7, 379.0
TS1	PES	3.6	3.6	3472.1, 3384.9, 1885.4, 806.1, 752.9, 623.3, 548.4, 218.1, 497.7 *i*
	UCCSD(T)	3.6	3.7	3468.8, 3393.2, 1885.0, 808.4, 754.1, 629.6, 559.5, 225.1, 501.5 *i*
TS2	PES	-46.7	-45.7	3296.4, 2973.3, 1612.7, 1399.1, 1080.7, 960.3, 549.2, 473.7, 608.0 *i*
	UCCSD(T)	-46.7	-45.7	3286.1, 2968.0, 1607.6, 1400.7, 1083.4, 963.3, 551.7, 481.8, 602.8 *i*
TS3	PES	-5.2	-8.3	3259.6, 1984.4, 1198.3, 766.1, 650.7, 625.8, 517.0, 463.1, 1137.9 *i*
	UCCSD(T)	-5.2	-8.4	3261.7, 1978.8, 1201.3, 732.8, 666.9, 607.6, 515.2, 463.5, 1156.6 *i*
TS4	PES	-8.0	-9.3	3057.4, 1936.6, 1680.1, 1249.9, 935.6, 788.7, 717.6, 389.3, 1771.1 *i*
	UCCSD(T)	-7.9	-9.3	3054.7, 1952.5, 1673.5, 1224.4, 903.2, 749.7, 696.4, 391.9, 1767.7 *i*
TS5	PES	-12.2	-15.8	3283.0, 1995.5, 1174.9, 732.3, 561.5, 498.9, 471.6, 452.2, 791.5 *i*
	UCCSD(T)	-12.3	-15.7	3291.8, 1995.4, 1176.1, 715.2, 574.4, 516.8, 498.4, 470.1, 773.8 *i*
TS6	PES	-0.3	-1.1	3241.0, 1995.9, 1507.7, 1247.4, 1008.8, 895.1, 729.7, 474.6, 1623.8 *i*
	UCCSD(T)	-0.1	-1.2	3242.9, 1976.5, 1492.5, 1238.5, 989.4, 854.4, 657.4, 445.0, 1663.6 *i*
TS7	PES	-42.7	-44.1	3345.7, 3122.1, 2083.0, 1145.8, 371.5, 284.4, 211.0, 112.9, 325.5 *i*
	UCCSD(T)	-42.7	-44.0	3350.7, 3129.9, 2084.6, 1134.9, 370.6, 307.5, 201.4, 116.6, 324.7 *i*
P1	PES	-14.8	-19.6	3324.1, 2057.9, 1228.9, 601.3, 524.5, 494.5
	UCCSD(T)	-14.7	-19.6	3325.9, 2062.0, 1227.1, 569.4, 515.9, 490.7
P2	PES	-45.6	-48.3	2162.7, 3368.3, 3142.2, 1095.5
	UCCSD(T)	-45.6	-48.3	2164.8, 3371.7, 3142.7, 1095.2