

Supporting Information for:

The catalytic mechanism of KI and the co-catalytic mechanism of hydroxyl substances for cycloaddition of CO₂ with propylene oxide

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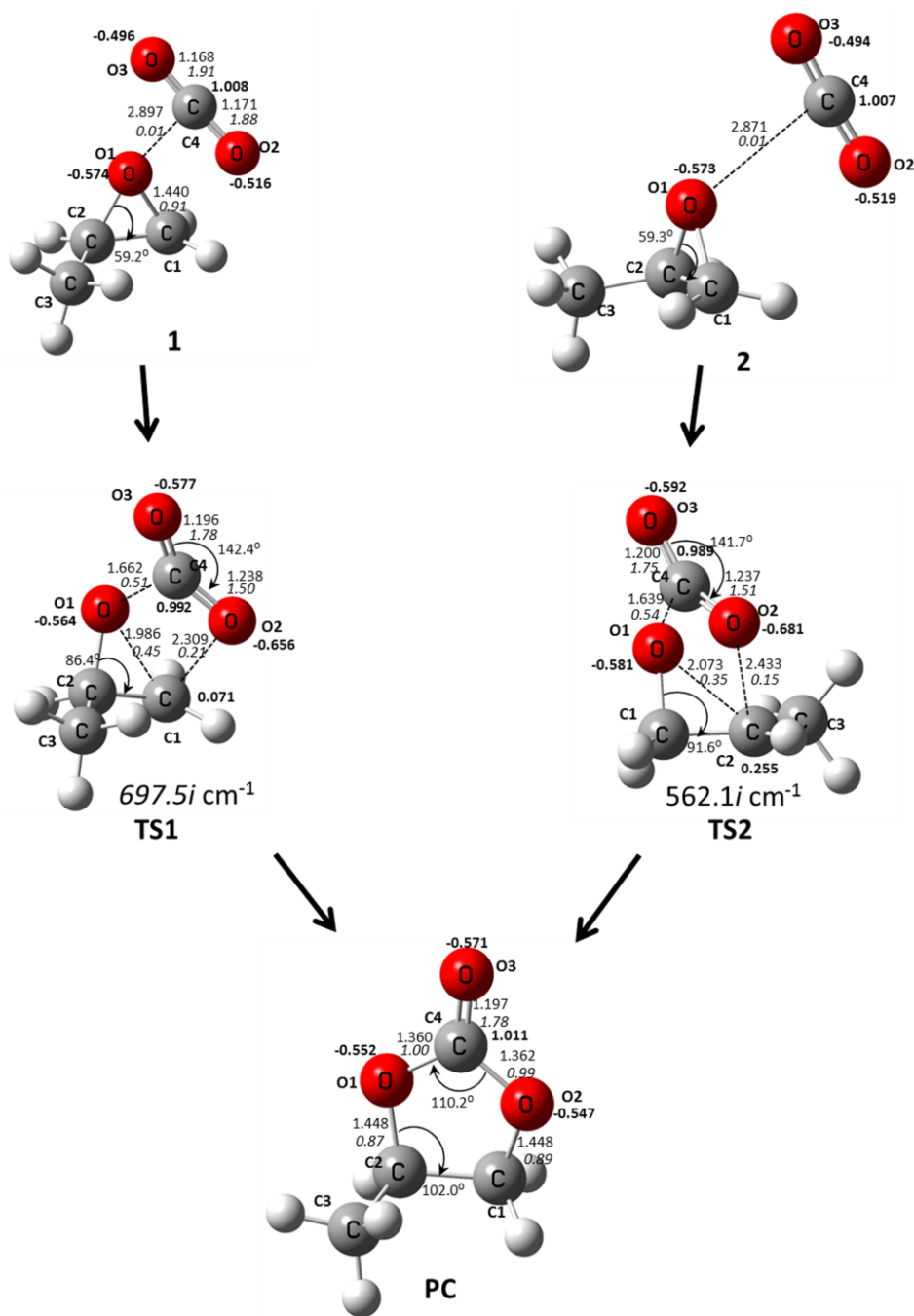


Figure S1. Optimized geometries of the reactants, transition states and PC of the cycloaddition of CO₂ with PO without catalyst (Path 1). The bond distances (in angstroms), bond orders (italic), angles (in degrees) and atomic charges (bold) are labeled in the corresponding positions. For TS1 and TS2, the imaginary vibrational frequencies (cm⁻¹) are shown (in the bracket).

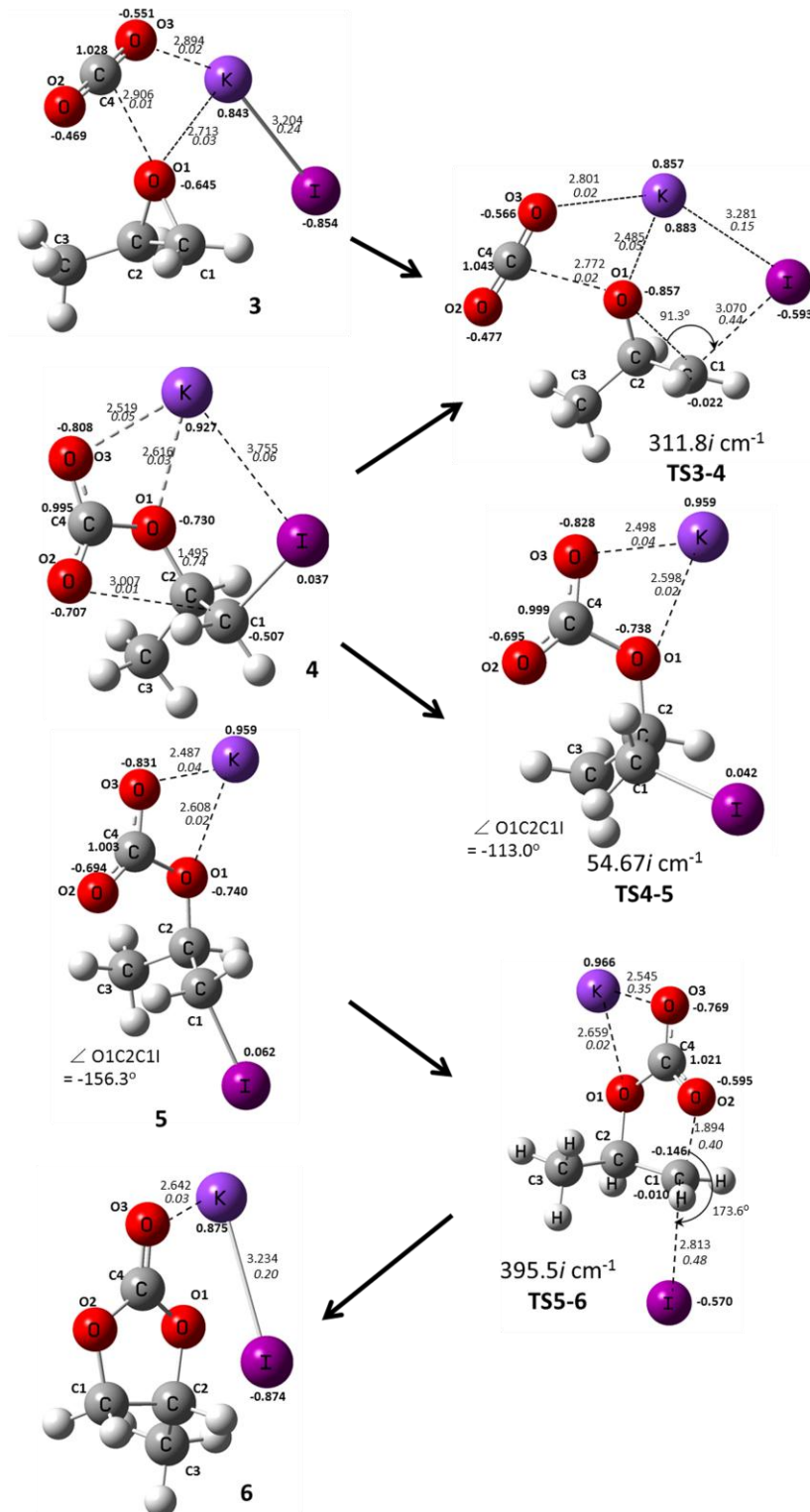


Figure S2. Optimized geometries of the reactants, intermediates, transition states and products of Path 2 of cycloaddition of CO₂ in the presence of KI. The bond distances (in angstroms), bond orders (italic), angles (in degrees) and atomic charges (bold) are labeled in the corresponding positions. For TS1 and TS2, the imaginary vibrational frequencies (cm⁻¹) are shown (in the bracket).

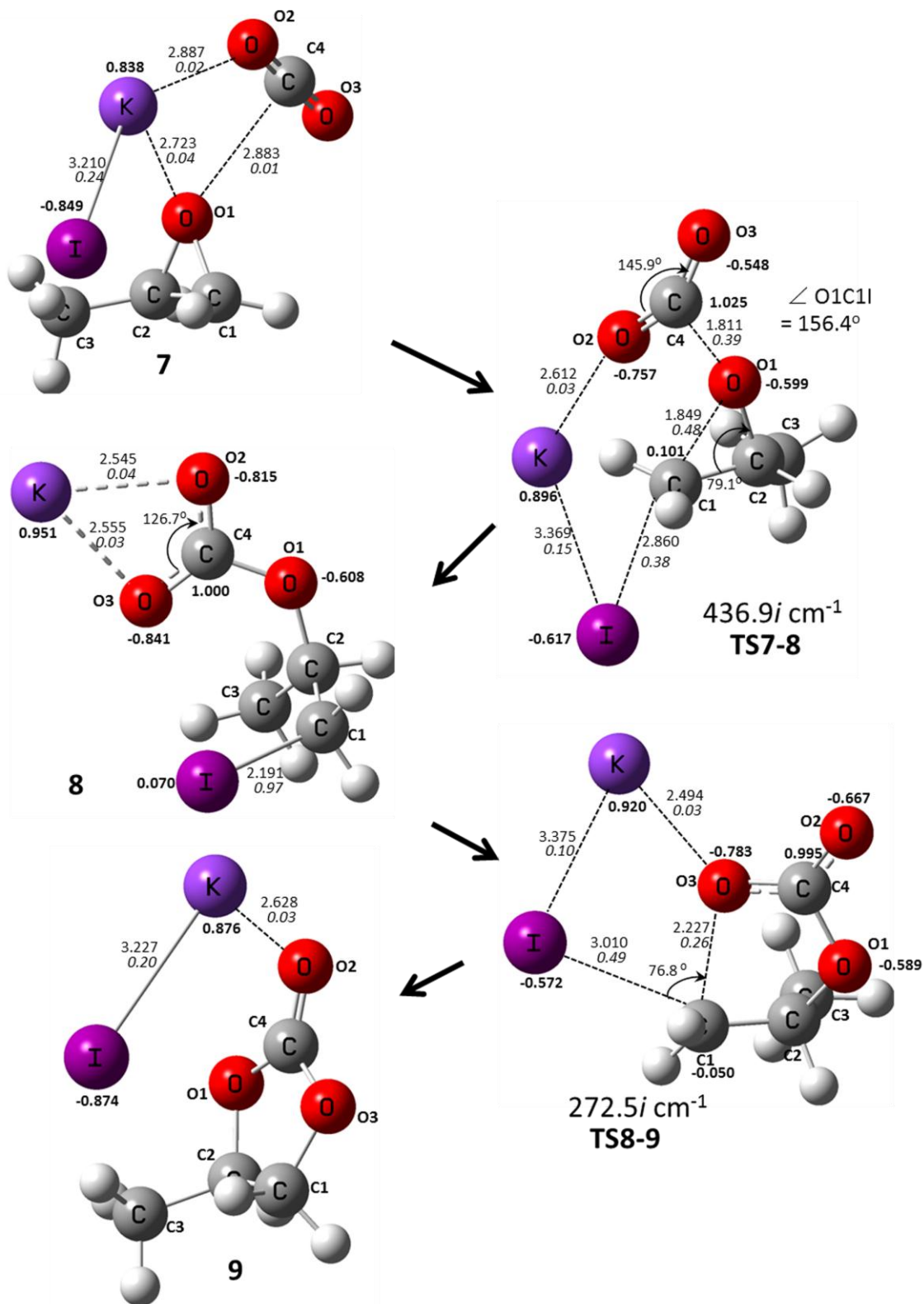


Figure S3. Optimized geometries of the reactants, intermediates, transition states and products of Path 3 of cycloaddition of CO_2 in the presence of KI. For TSN-m, the imaginary vibrational frequencies (cm^{-1}) are shown (in the bracket).

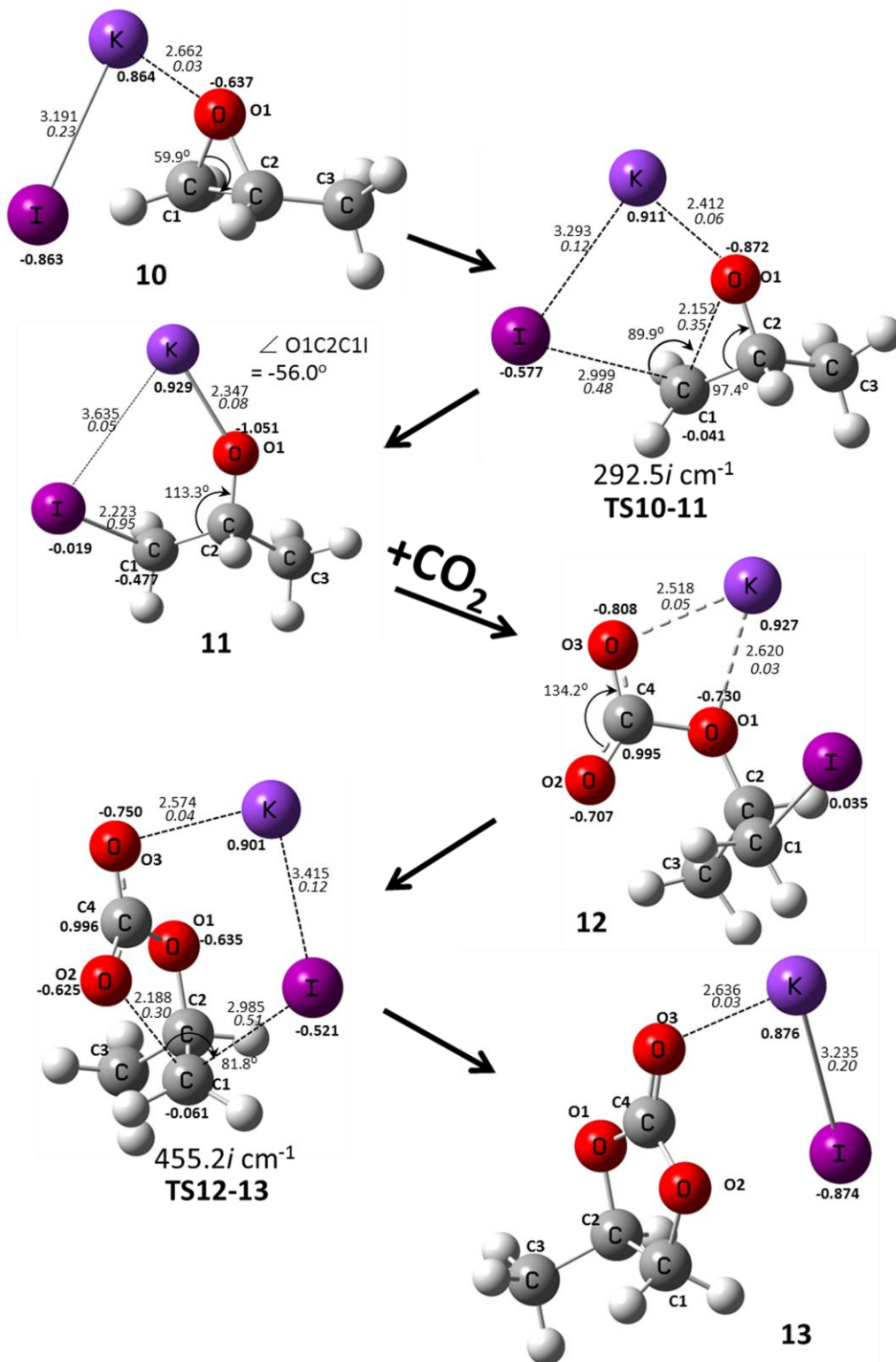


Figure S4. Optimized geometries of the reactants, intermediates, transition states and products in Path 4 of cycloaddition of CO₂ in the presence of KI. The bond distances (in angstroms), bond orders (italic), angles (in degrees) and atomic charges (bold) are labeled in the corresponding positions. For TS_n-m, the imaginary vibrational frequencies (cm⁻¹) are shown (in the bracket).

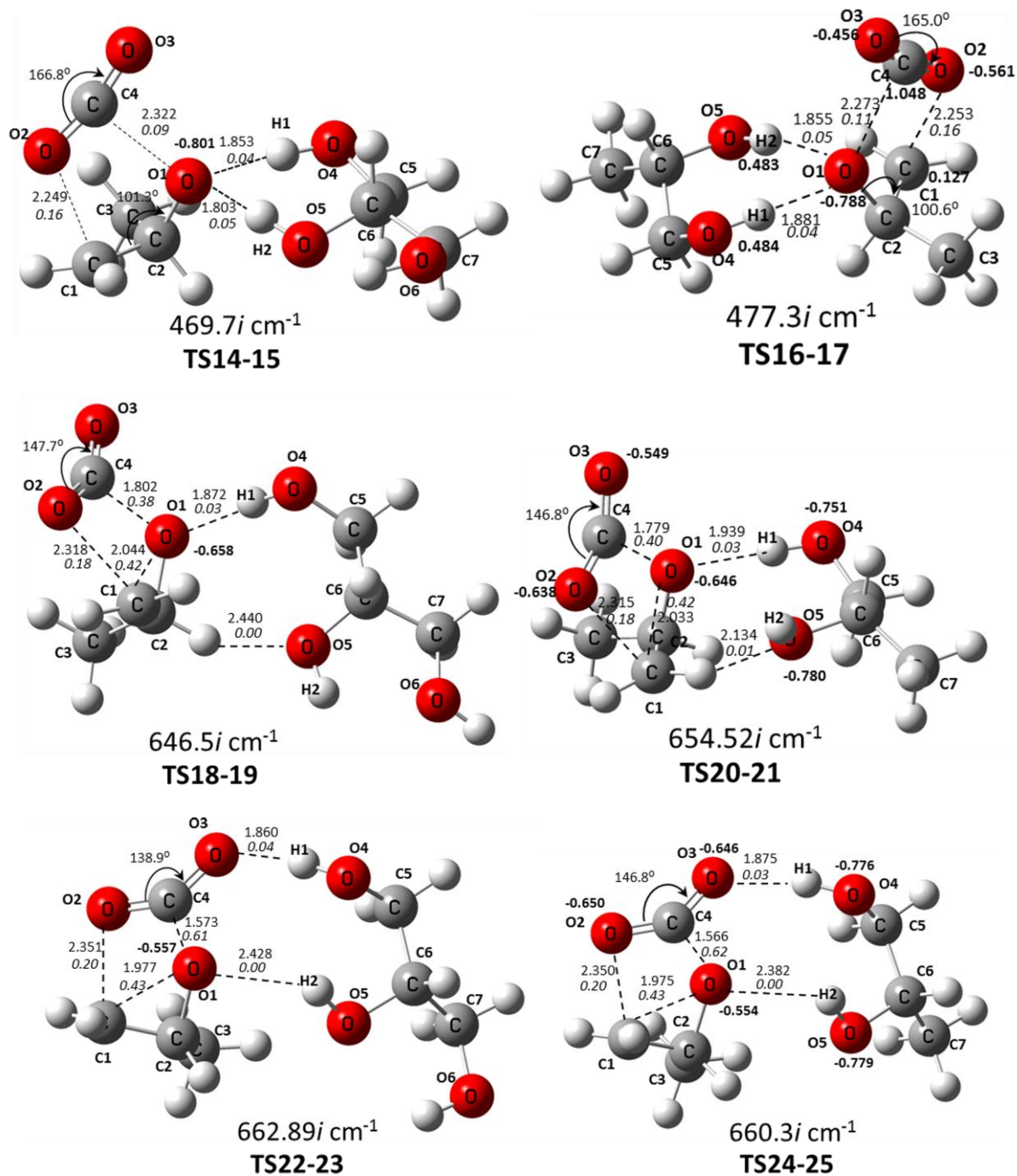
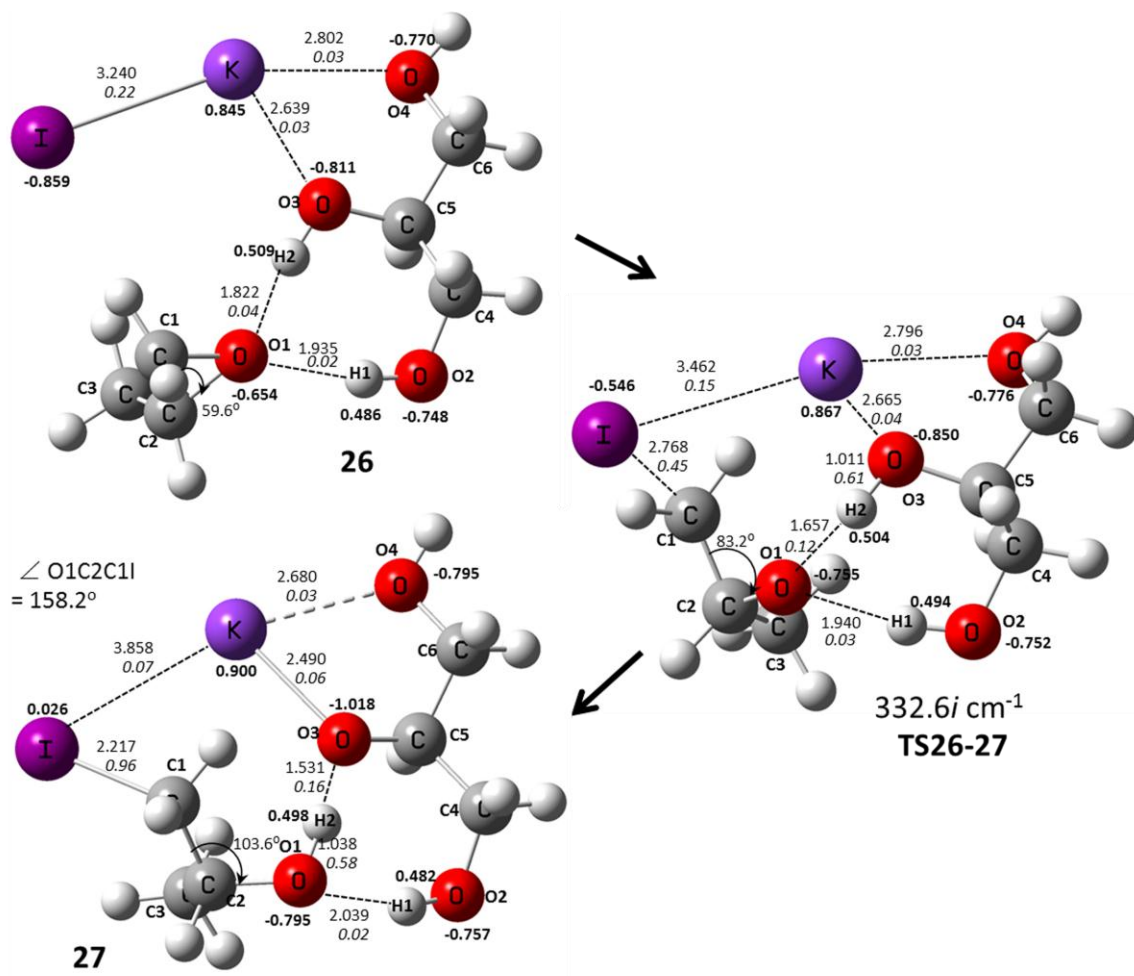


Figure S5. Optimized geometries of the transition states in the pathways of Path 5, Path 6, Path 7, Path 8, Path 9 and Path 10.

Table S1. Potential energy of the pathways of cycloaddition of CO₂ in the presence of glycerol or PG.

<i>Pathway</i>	In the gas phase			In the solution		
	Structure	Potential energy (kcal/mol)	Energy barrier (kcal/mol)	Structure	Potential energy (kcal/mol)	Energy barrier (kcal/mol)
Path 1-a ^a	1	-1.84		41	-0.57	
	TS1	59.56	61.39	TS41-42	51.08	51.64
	PC	-12.28		42	-15.82	
Path 5	14	-10.81		--	--	--
	TS14-15	48.81	59.62	--	--	--
	15	-17.00		--	--	--
Path 6	16	-10.11		--	--	--
	TS16-17	49.23	59.34	--	--	--
	17	-17.45		--	--	--
Path 7	18	-9.14		54	-4.40	
	TS18-19	51.23	60.37	TS54-55	47.21	51.61
	19	-16.75		55	-18.35	
Path 8	20	-6.48		56	-4.48	
	TS20-21	52.25	58.74	TS56-57	46.68	51.52
	21	-19.77		57	-18.97	
Path 9	22	-9.05		58	-5.81	
	TS22-23	50.33	59.38	TS58-59	45.31	51.11
	23	-19.85		59	-20.98	
Path 10	24	-8.89		60	-5.62	
	TS24-25	50.02	59.00	TS60-61	45.08	50.69
	25	-19.93		61	-21.19	

^a The reference reaction pathway cycloaddition of CO₂ and PO without any other reagents.



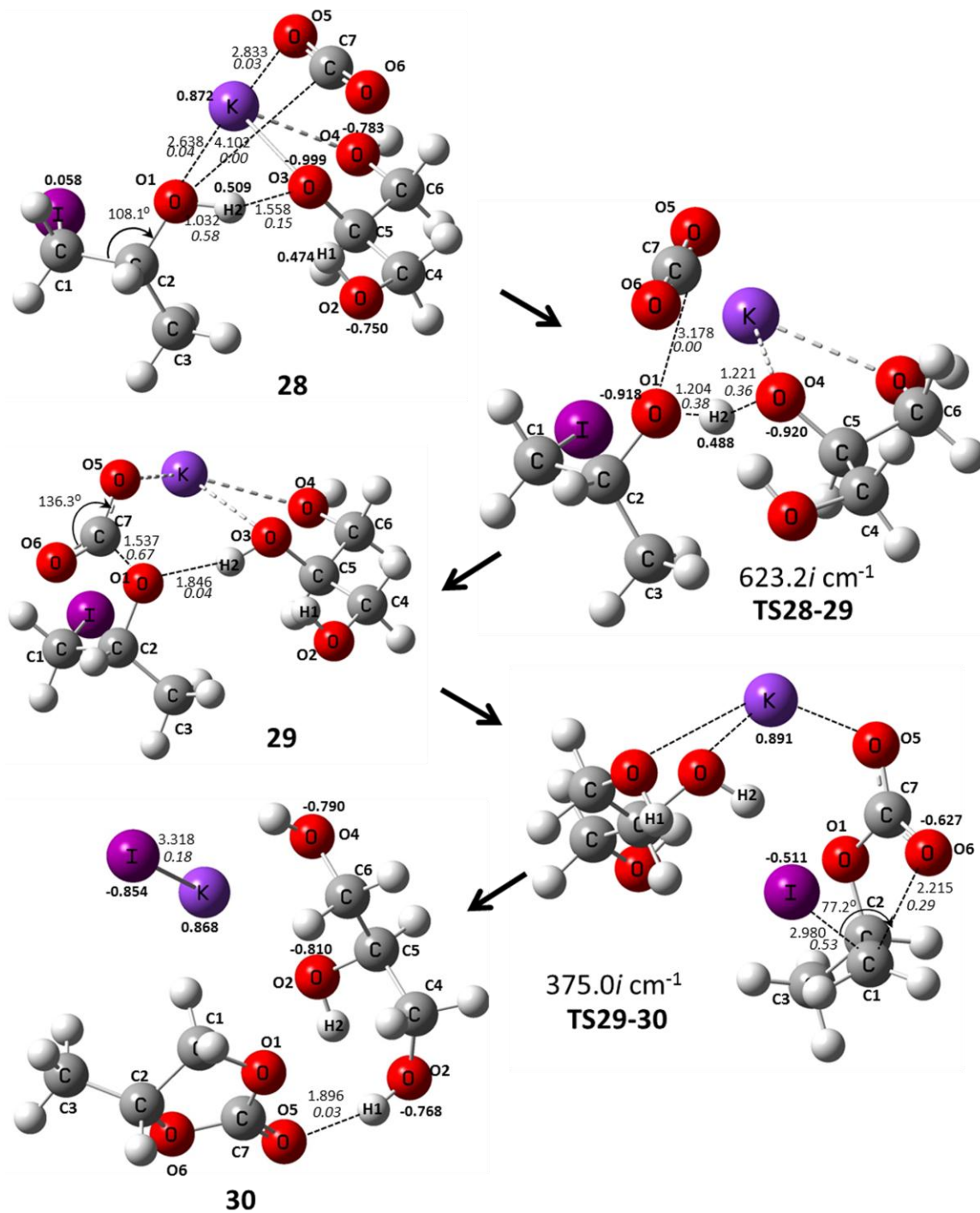
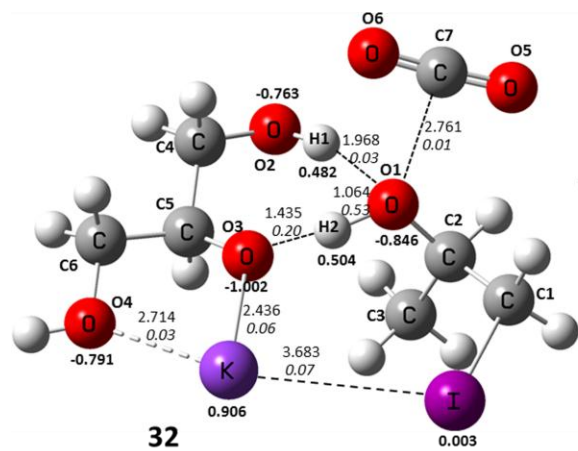
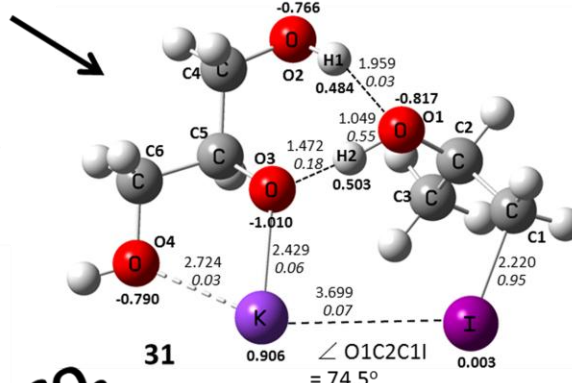
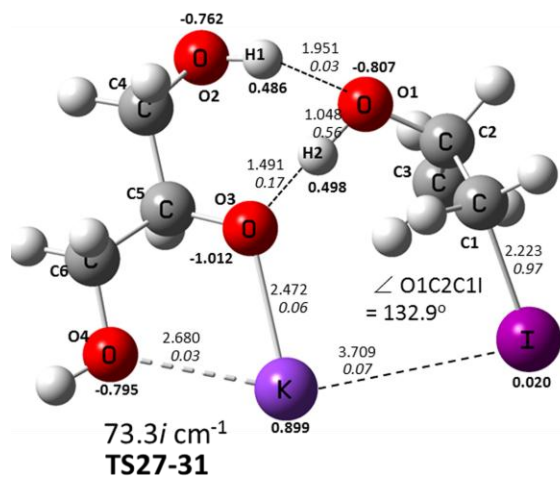
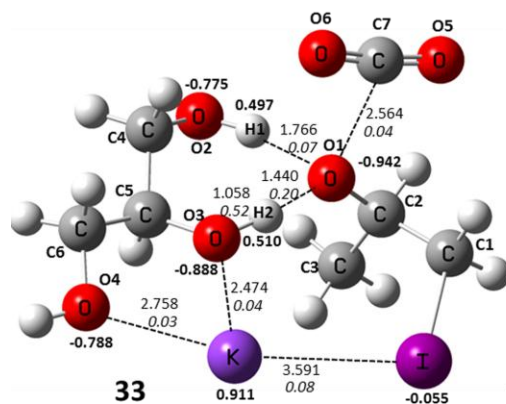
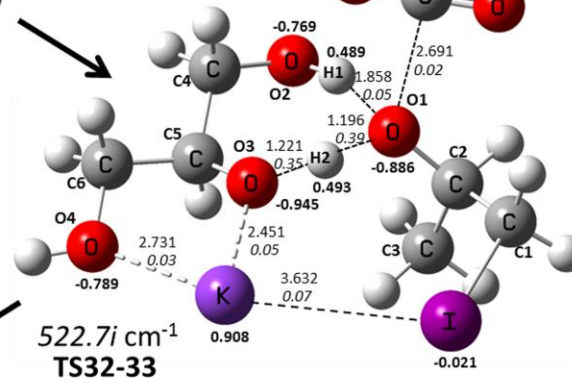


Figure S6. Optimized geometries of the reactants, intermediates, transition states and products of the cycloaddition of CO₂ in the presence of KI/glycerol (Path 11). The bond distances (in angstroms), bond orders (italic), angles (in degrees) and atomic charges (bold) are labeled in the corresponding positions. For TS_n-m, the imaginary vibrational frequencies (cm⁻¹) are shown (in the bracket).



$+\text{CO}_2$



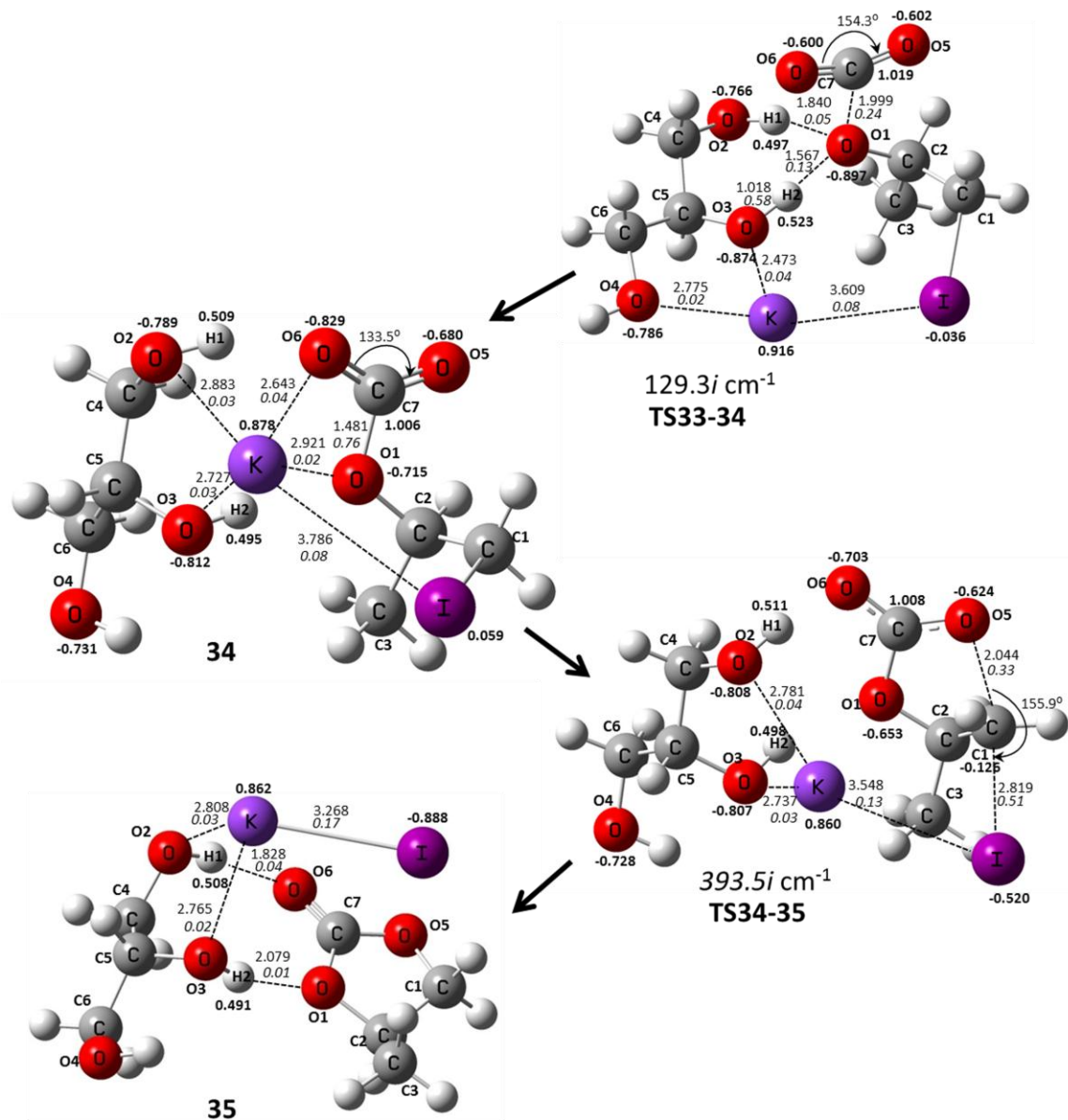
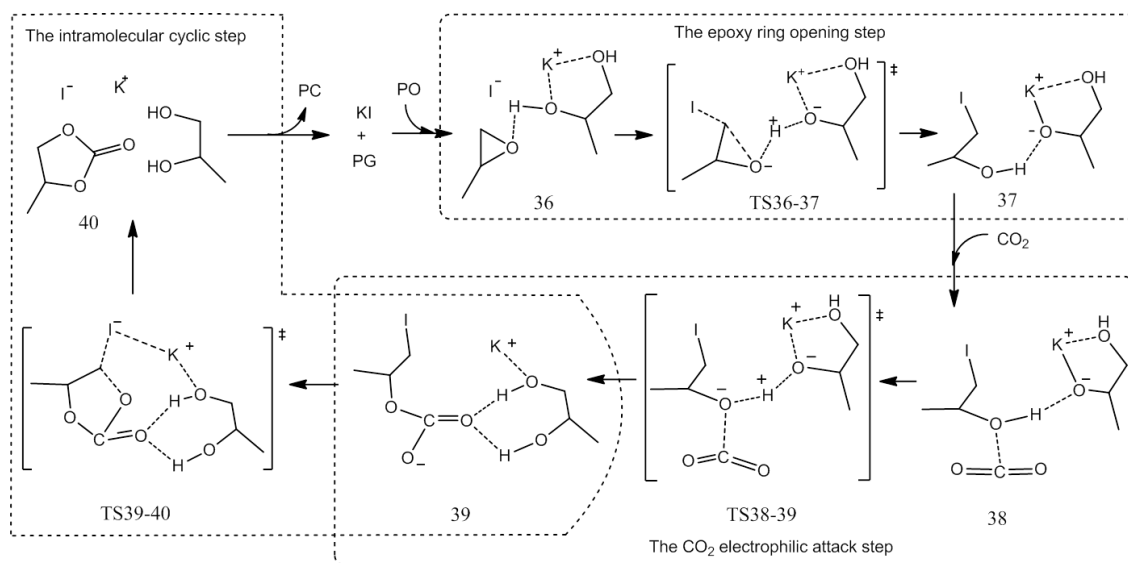


Figure S7. Optimized geometries of the reactants, intermediates, transition states and products of the cycloaddition of CO₂ in the presence of KI/Glycerol (Path 12). The bond distances (in angstroms), bond orders (italic), angles (in degrees) and atomic charges (bold) are labeled in the corresponding positions. For TS_{n-m}, the imaginary vibrational frequencies (cm⁻¹) are shown (in the bracket).



Scheme S1. The co-catalytic mechanism of PG with KI as catalyst for cycloaddition of CO₂ with PO (Path 13).

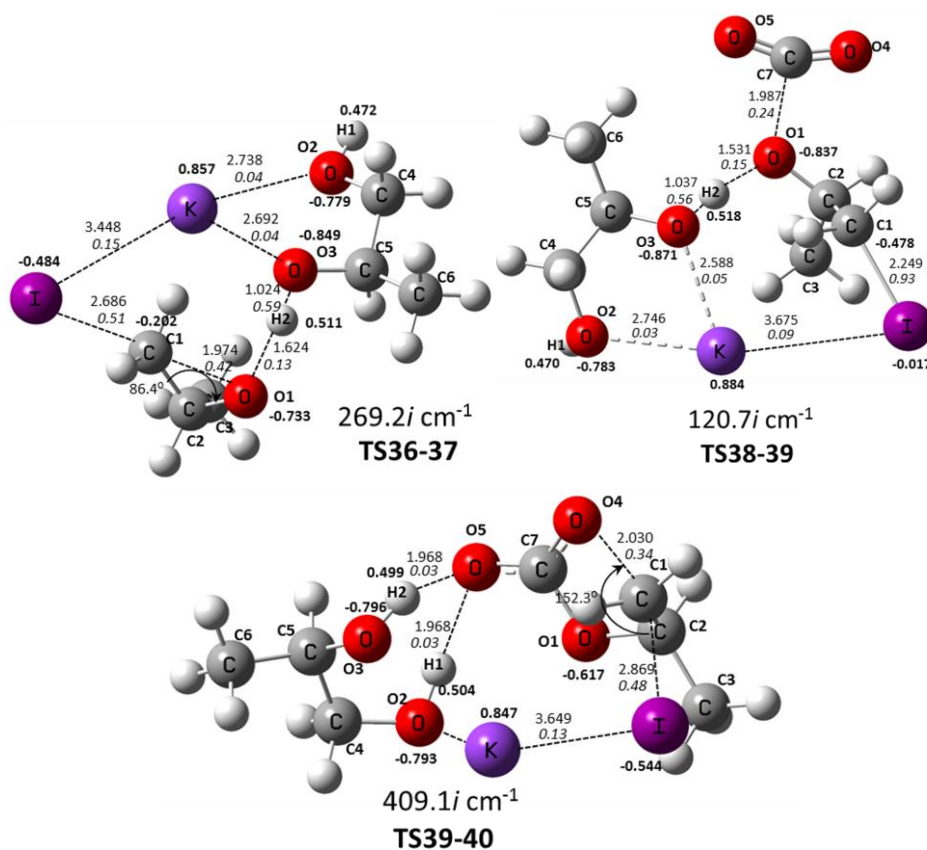


Figure S8. Optimized geometries of the transition state of Path 13. The bond distances (in angstroms), bond orders (*italic*), angles (in degrees) and atomic charges (**bold**) are labelled in the corresponding positions. The imaginary vibrational frequencies (cm⁻¹) are shown.

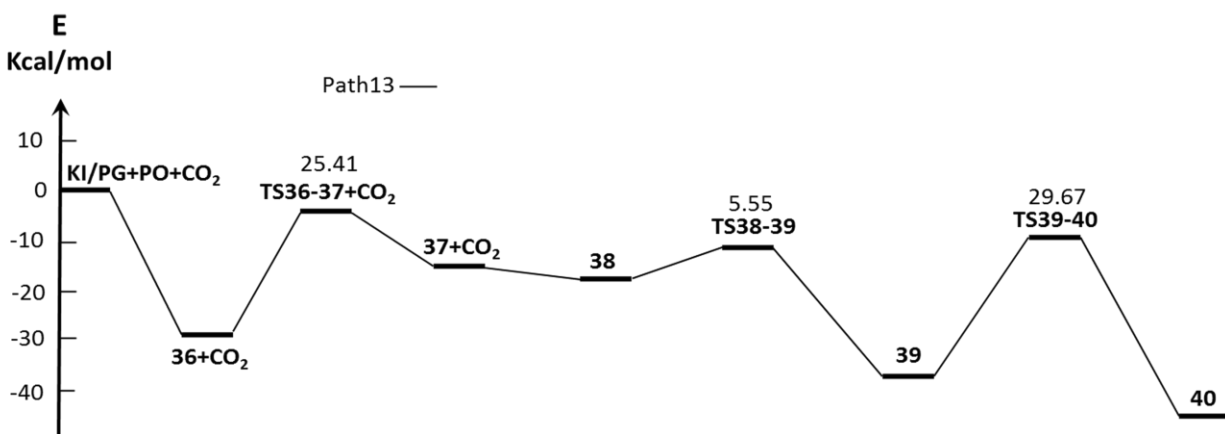


Figure S9. Potential energy curve of the pathway of cycloaddition of CO₂ with PO in the presence of KI/PG.

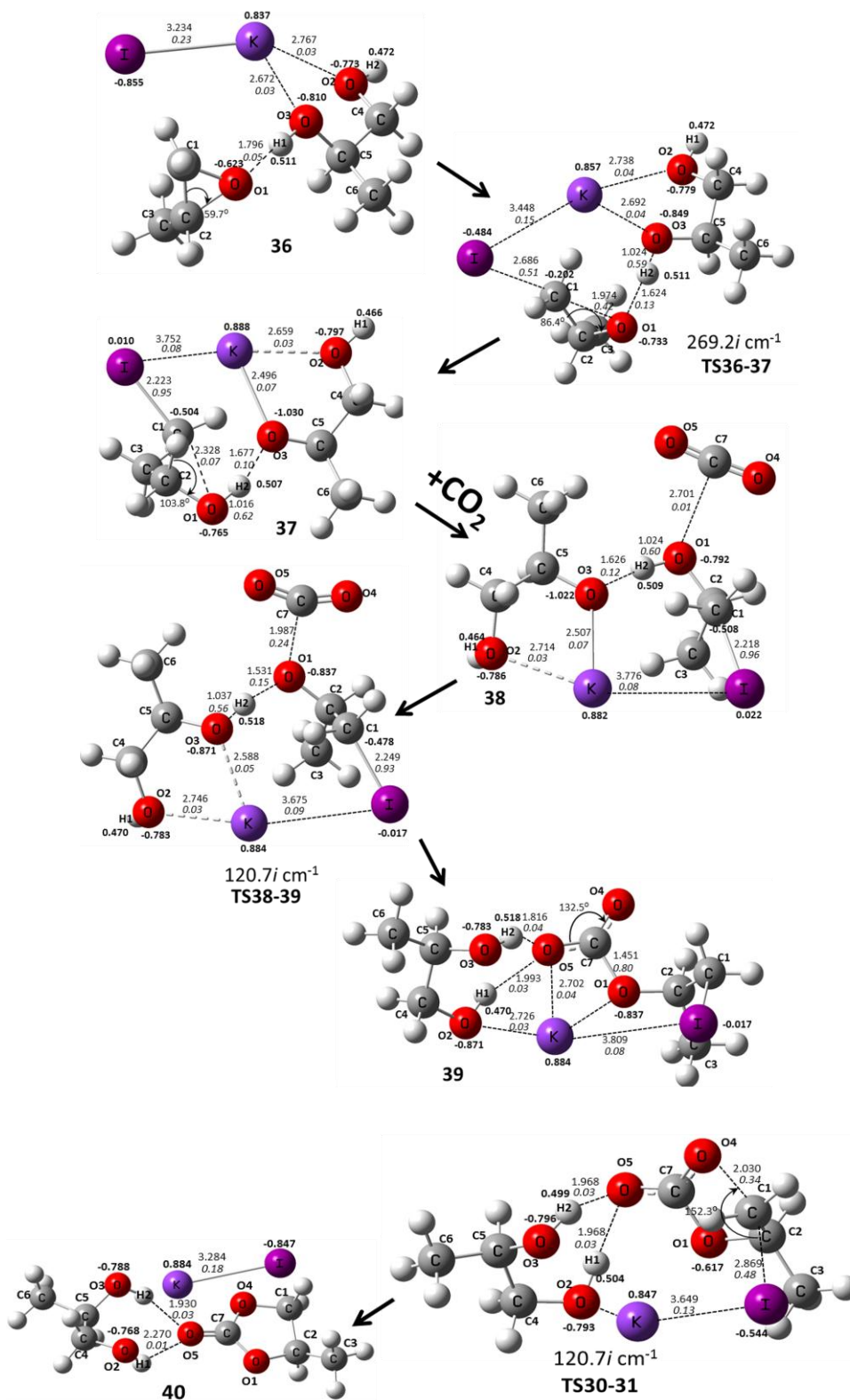


Figure S10. Optimized geometries of the reactants, intermediates, transition states and products of the cycloaddition of CO₂ in the presence of KI/PG (Path 13).

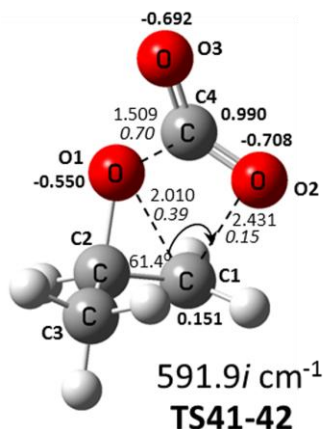


Figure S11. Optimized geometry of transition state of the non-catalyzed cycloaddition of CO₂ by taking into account of solvent effects

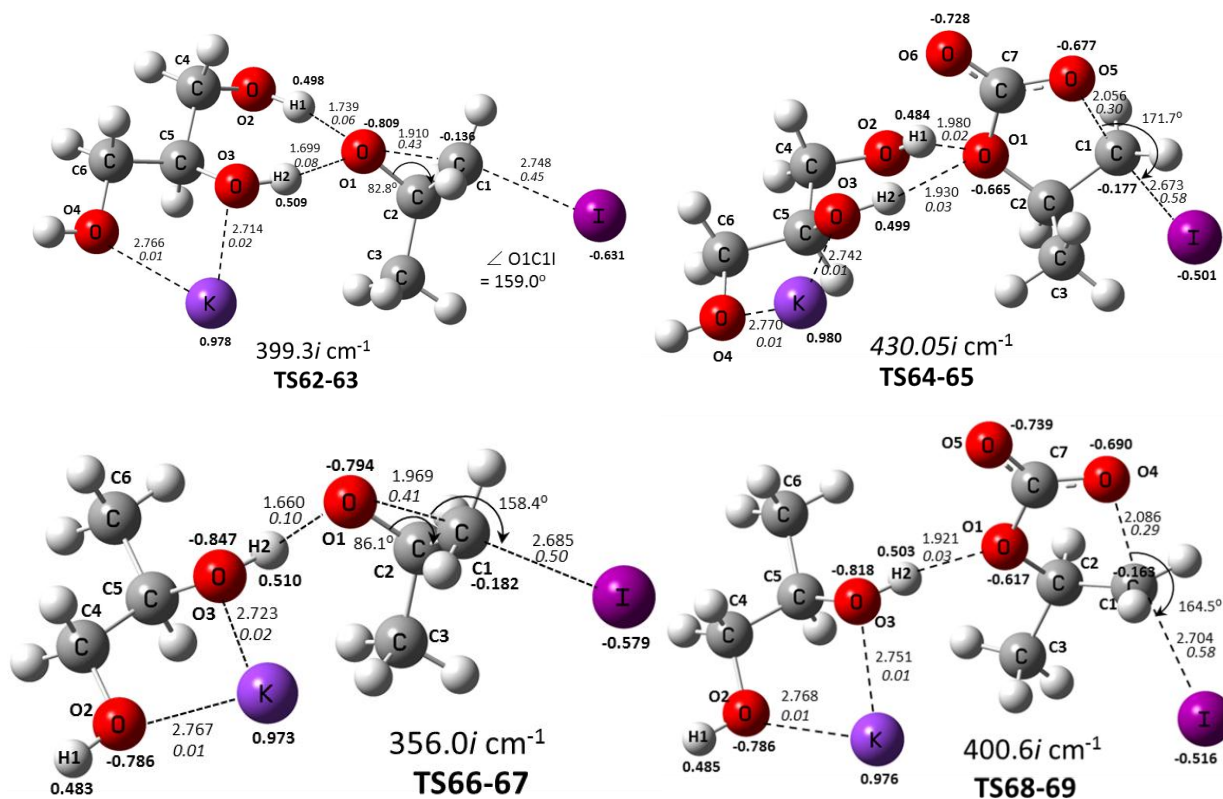


Figure S12. Optimized geometries of the transition state of Path 17 (TS62-63, TS62-63) and Path 18 (TS66-67, TS68-69). The bond distances (in angstroms), bond orders (*italic*), angles (in degrees) and atomic charges (**bold**) are labeled in the corresponding positions. The imaginary vibrational frequencies (cm⁻¹) are shown.

Table S2. Potential energy and relative energies of the reactants, transition states, and products of noncatalyzed cycloaddition of CO₂ with PO.

Species	Potential energy (hartree)	Potential energy (kcal/mol)	Relative energy (kcal/mol)
PO	-193.168445	-121215.1311	
CO ₂	-188.646611	-118377.6349	
CO ₂ +PO	-381.815056	-239592.7660	0.00
1	-381.817983	-239594.6023	-1.84
TS1	-381.720144	-239533.2076	59.56
2	-381.818154	-239594.7099	-1.94
TS2	-381.730040	-239539.4176	53.35
PC	-381.834627	-239605.0469	-12.28

Table S3. Potential energy and relative energies of the reactants, intermediates, transition states, and final products of KI catalyzed cycloaddition of CO₂ with PO.

Species	Potential energy (hartree)	Potential energy (kcal/mol)	Relative energy (kcal/mol)
KI	-611.410637	-383666.2886	
PO+KI	-804.579082	-504881.4197	0.00
PO+CO ₂ +KI	-993.225693	-623259.0546	0.00
3	-993.255330	-623277.6524	-18.60
TS3-4	-993.197443	-623241.3271	17.73
4	-993.250423	-623274.5729	-15.52
TS4-5	-993.2422027	-623269.4146	-10.36
5	-993.2451475	-623271.2625	-12.21
TS5-6	-993.2180253	-623254.2431	4.81
6	-993.275735	-623290.4563	-31.40
7	-993.255683	-623277.8735	-18.82
TS7-8	-993.197436	-623241.3231	17.73
8	-993.243734	-623270.3753	-11.32
TS8-9	-993.196442	-623240.6996	18.36
9	-993.276196	-623290.7457	-31.69
10	-804.602199	-504895.9261	-14.51
TS10-11	-804.542228	-504858.2935	23.13
11	-804.579158	-504881.4674	-0.05
12	-993.250415	-623274.5681	-15.51
TS12-13	-993.185782	-623234.0099	25.04
13	-993.275664	-623290.4119	-31.36

Table S4. Potential energy and relative energies of the reactants, intermediates, transition states, and final products of the cycloaddition of CO₂ with PO in the presence of glycerol (and PG) (Paths 5 to 10).

Species	Potential energy (hartree)	Potential energy (kcal/mol)	Relative energy (kcal/mol)
Glycerol	-344.903431	-216430.3518	
CO ₂ +PO+Glycerol	-726.718487	-456023.1178	0.00
14	-726.735711	-456033.9259	-10.81
TS14-15	-726.640702	-455974.3066	48.81
15	-726.745576	-456040.1167	-17.00
PG	-269.663883	-169216.7832	
CO ₂ +PO+PG	-651.478939	-408809.5492	0.00
16	-651.495043	-408819.6546	-10.11
TS16-17	-651.400483	-408760.3170	49.23
17	-651.506741	-408826.9947	-17.45
18	-726.733047	-456032.2545	-9.14
TS18-19	-726.636839	-455971.883	51.23
19	-726.745184	-456039.8703	-16.75
20	-651.489272	-408816.0333	-6.48
TS20-21	-651.395669	-408757.2963	52.25
21	-651.510438	-408829.3147	-19.77
22	-726.732910	-456032.1683	-9.05
TS22-23	-726.638276	-455972.7843	50.33
23	-726.750118	-456042.9668	-19.85
24	-651.493257	-408818.5336	-8.98
TS24-25	-651.399235	-408759.5338	50.02
25	-651.510692	-408829.4746	-19.93

Table S5. Potential energy and relative energies of the reactants, intermediates, transition states, and final products of KI catalyzed cycloaddition of CO₂ by taking into account of solvent effects (Paths 14 to 16).

Species	Potential energy (hartree)	Potential energy (kcal/mol)	Relative energy (kcal/mol)
Glycerol+KI+PO	-1149.482513	-721311.7715	0.00
26	-1149.530194	-721341.6917	-29.92
TS26-27	-1149.491690	-721317.5301	-5.76
27	-1149.506296	-721326.6955	-14.92
Glycerol+KI+PO+CO ₂	-1338.129124	-839689.4064	0.00
28	-1338.176818	-839719.3352	-29.93
TS28-29	-1338.174785	-839718.0595	-28.65
29	-1338.180396	-839721.5805	-32.17
TS29-30	-1338.119358	-839683.2781	6.13
30	-1338.204658	-839736.8049	-47.40
TS27-31	-1149.505886	-721326.4385	-14.67
31	-1149.512885	-721330.8306	-19.06
32	-1338.164489	-839711.5987	-22.19
TS32-33	-1338.163551	-839711.0099	-21.60
33	-1338.163481	-839710.9657	-21.56
TS33-34	-1338.159968	-839708.7617	-19.36
34	-1338.188407	-839726.607	-37.20
TS34-35	-1338.143555	-839698.462	-9.06
35	-1338.200455	-839734.1672	-44.76
PG+KI+PO	-651.393923	-408756.2007	0.00
36	-1074.289719	-674127.5416	-29.34
TS36-37	-1074.249219	-674102.1272	-3.92
37	-1074.264089	-674111.4588	-13.26
38	-1262.916118	-792492.493	-16.66
TS38-39	-1262.907266	-792486.9383	-11.10
39	-1262.951097	-792514.4427	-38.60
TS39-40	-1262.903816	-792484.7738	-8.94
40	-1262.963141	-792522.0008	-46.16

Table S6. Potential energy and relative energies of the reactants, transition states, and PC of noncatalyzed cycloaddition of CO₂ by taking into account of solvent effects (Paths 5 to 10 with the solven effects).

Species	Potential energy (hartree)	Potential energy (kcal/mol)	Relative energy (kcal/mol)
PO	-193.1734834	-121218.2926	
CO ₂	-188.6494474	-118379.4148	
CO ₂ +PO	-381.822931	-239597.7073	0.00
41	-381.823836	-239598.2753	-0.57
TS41-42	-381.741536	-239546.6311	51.08
42	-381.848141	-239613.5271	-15.82
Glycerol	-344.9155183	-216437.9369	
CO ₂ +PO+Glycerol	-726.7384492	-456035.6442	0.00
54	-726.7454562	-456040.0412	-4.40
TS54-55	-726.6632162	-455988.4348	47.21
55	-726.7676849	-456053.99	-18.35
58	-726.7477004	-456041.4495	-5.81
TS58-59	-726.6662443	-455990.335	45.31
59	-726.7718882	-456056.6276	-20.98
PG	-269.672174	-169221.9859	
CO ₂ +PO+PG	-651.4951049	-408819.6933	
56	-651.5028191	-408824.534	-4.84
TS56-57	-651.4207138	-408773.0121	46.68
57	-651.5253349	-408838.6629	-18.97
60	-651.5040605	-408825.313	-5.62
TS60-61	-651.4232732	-408774.6181	45.08
61	-651.5288712	-408840.882	-21.19

Table S7. Potential energy and relative energies of the reactants, intermediates, transition states, and final products of KI/Glycerol (Path 17) and KI/PG (Path 18) catalyzed cycloaddition of CO₂ by taking into account of solvent effects.

Species	Potential energy (hartree)	Potential energy (kcal/mol)	Relative energy (kcal/mol)
Glycerol+KI+PO	-1149.55492	-721357.208	0.00
62	-1149.573702	-721368.9938	-11.79
TS62-63	-1149.542385	-721349.3421	7.87
63	-1149.556423	-721358.1512	-0.94
Glycerol+KI+PO+CO ₂	-1338.204368	-839736.6228	0.00
64	-1338.215394	-839743.542	-6.92
TS64-65	-1338.19713	-839732.0812	4.54
65	-1338.236623	-839756.8636	-20.24
PG+KI+PO	-1074.311576	-674141.257	0.00
66	-1074.329682	-674152.6185	-11.36
TS66-67	-1074.293774	-674130.0863	11.17
67	-1074.301848	-674135.1526	6.10
PG+KI+PO+CO ₂	-1262.961023	-792520.6718	0.00
68	-1262.975329	-792529.6489	-8.98
TS68-69	-1262.948535	-792512.8352	7.84
69	-1262.996725	-792543.0751	-22.40

Complete Reference 17: Gaussian 09, Revision A.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

The cartesian coordinates of the optimized geometries of the transition states

1. The cartesian coordinates of the optimized geometries of the transition states in Path 1-a and Path 1-b.

Transition state TS1				Transition state TS2			
O	-0.485929	0.483452	0.308451	O	-0.669945	0.561239	0.413978
C	0.174214	-0.710373	1.25815	C	0.039319	-0.553772	1.383882
O	-0.104011	-1.789799	0.720128	O	-0.275576	-1.681144	0.984839
O	0.769931	-0.236876	2.180513	O	0.708954	0.000009	2.211691
C	-1.219098	-0.783625	-1.033164	C	-1.134899	-0.774209	-1.10249
H	-1.43239	-1.840748	-0.955418	H	-1.208332	-1.847437	-0.970933
H	-0.562353	-0.456036	-1.83219	C	-1.8741	0.131805	-0.213771
C	-1.816311	0.250082	-0.191362	H	-2.339745	0.986273	-0.716595
H	-2.099552	1.148551	-0.751349	H	-2.572821	-0.362857	0.465351
C	-2.875334	-0.130572	0.826	C	-0.272795	-0.283864	-2.190561
H	-3.009804	0.687708	1.540138	H	0.737137	-0.705571	-2.104865
H	-3.830753	-0.303868	0.316014	H	-0.683365	-0.696962	-3.128879
H	-2.598145	-1.035634	1.373293	H	-0.217649	0.804295	-2.245535

2. The cartesian coordinates of the optimized geometries of the transition states in Path 2.

Transition state TS3-4				Transition state TS4-5				Transition state TS5-6			
C	-3.475409	-1.00282	-0.56003	C	-0.50583658	0.85603112	0	C	-1.51750974	0.40856031	0.00000000
O	-2.851771	-1.970901	-0.319436	O	-1.55963458	0.22009912	-0.243036	O	-2.73188274	0.53321131	-0.22480500
O	-4.170588	-0.110089	-0.83638	O	-0.01693258	1.89245412	-0.43447	O	-0.60041074	1.28134031	0.05250300
K	-0.251326	-1.799545	0.705989	K	-1.31434958	-1.92402888	1.014234	K	-3.47185374	-1.90006669	-0.32672700
I	2.328401	0.010676	-0.207872	I	4.28358142	-0.47829288	0.562527	I	3.54556226	-0.92348169	-0.14440000
O	-1.355368	0.419264	0.521466	O	0.28150142	0.12628812	1.027756	O	-1.06801374	-0.89819169	0.21108800
C	-0.04475	1.957912	-0.165923	C	2.53762542	0.84585812	0.340121	C	1.01502226	0.29341431	0.02732100
H	-0.165712	1.765106	-1.226246	H	2.11096142	0.57596212	-0.621161	H	1.14000826	0.38660131	-1.04000800
C	-1.223501	1.794928	0.701677	C	1.51956342	0.69529512	1.491139	C	0.34802526	-0.94027169	0.61354900
H	-0.976553	2.052798	1.748465	H	1.88201142	-0.05921988	2.195276	H	0.73847326	-1.84055469	0.14388200
H	0.892447	2.389767	0.158672	H	2.96228442	1.84608012	0.273887	H	1.52801626	1.00299031	0.65521700
C	-2.439802	2.624771	0.271118	C	1.31737142	2.00065612	2.267807	C	0.43986226	-1.02057969	2.13102100
H	-2.682865	2.443	-0.781581	H	0.96538042	2.80007412	1.612513	H	0.02606626	-0.11766469	2.59469900
H	-3.302673	2.320045	0.876464	H	0.58339242	1.84792212	3.067723	H	-0.11029374	-1.89257369	2.50233600
H	-2.272141	3.699865	0.421394	H	2.26549342	2.30381812	2.729834	H	1.48912826	-1.12133469	2.42348200

3. The cartesian coordinates of the optimized geometries of the transition states in Path 3

Transition state TS7-8				Transition state TS8-9			
O	-1.84602600	-1.29549100	.19844700	O	0.27284500	-0.90626300	1.61984000
C	-3.34990700	-2.18792400	-0.27089000	C	-0.43589900	-1.35765600	0.50437700
O	-3.71824500	-1.80732800	-1.37303800	O	-0.22313300	-0.63976600	-0.54089100
O	-3.55677100	-2.92909300	0.63399700	O	-1.14630700	-2.34797300	0.61857900
C	-1.11552300	-0.51746500	-1.31205100	C	1.58821100	0.47474400	0.11956700
H	-1.72221300	-1.05624800	-2.01128300	H	2.09565900	-0.38660000	-0.29550600
H	-0.05620300	-0.73942800	-1.30076900	H	2.06596100	1.42825600	-0.06206500
C	-1.72576300	0.10022200	-0.13047400	C	0.88735400	0.35962000	1.42478400
H	-0.97357900	0.54506600	0.52911500	H	1.71735900	0.38713000	2.15977500
C	-2.96852800	0.96758200	-0.14395000	C	-0.06927300	1.51505500	1.73901400
H	-3.34352900	1.07409500	0.88040200	H	-0.47944800	1.38377500	2.74450000
H	-2.70847400	1.96015400	-0.52623700	H	0.45584600	2.47577300	1.69302000
H	-3.77423600	0.55147900	-0.75276600	H	-0.88795700	1.53358600	1.01447000
K	-3.86565900	-0.39100200	-3.56305400	K	-1.27368800	-0.80607100	-2.79723000
I	-0.96202400	1.31549000	-3.50198900	I	0.93449600	1.73287300	-2.53587200

4. The cartesian coordinates of the optimized geometries of the transition states in Path 4

Transition state TS10-11				Transition state TS12-13			
O	-1.08692800	0.68894300	0.32814900	O	1.01164700	1.37062200	1.69121100
C	-2.74533700	0.95547800	-1.01648100	C	-0.74287100	1.55954200	-0.02432900
H	-2.92990200	0.80179300	-2.07162400	H	-0.66043900	1.41479500	-1.09240900
H	-3.55036700	0.71563200	-0.33099100	H	-1.74365300	1.77976300	0.32180500
C	-1.58546500	1.69693700	-0.48430100	C	0.43676400	2.20158000	0.67165600
H	-0.88416300	1.96402300	-1.29784700	H	1.24057800	2.33425200	-0.06000100
C	-1.96790600	2.97907700	0.26979300	C	0.02504500	3.55602800	1.26541600
H	-1.06579600	3.37071000	0.75720700	H	0.89274800	4.02351700	1.74282400
H	-2.36893300	3.75366600	-0.39856600	H	-0.34401100	4.23195400	0.48445100
H	-2.70723300	2.75822100	1.04895300	H	-0.76028000	3.42183600	2.01651500
K	-0.56608800	-1.61118000	0.83343300	K	2.53942300	-1.10578200	1.66103000
I	-2.69443600	-1.97489500	-1.65249800	I	0.32462800	-1.07343200	-0.93835000
O	-1.08692800	0.68894300	0.32814900	C	0.11973100	0.45564900	2.30613200
C	-2.74533700	0.95547800	-1.01648100	O	-1.04528800	0.44068500	1.83176300
H	-2.92990200	0.80179300	-2.07162400	O	0.64973500	-0.24570900	3.18252100

5. The cartesian coordinates of the optimized geometries of the transition states in Path 5 and 6							
Transition state TS14-15				Transition state TS16-17			
O	-0.660212	0.560803	0.273136	O	-0.842100	0.287875	0.441206
C	0.725566	-0.988887	1.307943	C	-2.337577	-1.424302	0.414823
O	0.169727	-1.906597	0.787877	O	-2.735517	-1.155994	-0.678307
O	1.423920	-0.286245	1.916100	O	-2.146633	-1.914409	1.453361
C	-1.283386	-1.259545	-0.802074	C	-1.483327	0.442614	-1.654931
H	-1.630623	-2.273551	-0.613003	H	-2.394655	0.480498	-2.248241
H	-0.514116	-1.128604	-1.558174	H	-0.684780	-0.215257	-1.991341
C	-1.819404	-0.048928	-0.173259	C	-1.208773	1.266127	-0.470881
H	-2.283222	0.524068	-1.017666	H	-0.336197	1.902353	-0.759166
C	-2.894516	-0.258942	0.899289	C	-2.334779	2.192073	-0.001992
H	-3.208820	0.713110	1.289222	H	-2.009119	2.727875	0.893981
H	-3.769372	-0.769196	0.476661	H	-2.584548	2.925325	-0.779574
H	-2.496609	-0.851099	1.729738	H	-3.230363	1.614565	0.249063
H	-1.906396	3.808022	-0.976465	H	2.453485	1.598401	-0.056128
C	-1.025735	3.980928	-0.335512	C	2.602263	0.806026	0.698647
C	0.234197	3.625352	-1.127753	C	2.637369	-0.549477	-0.016863
O	-1.146566	3.279818	0.896174	O	1.630870	0.891468	1.732441
H	-1.003341	5.044932	-0.070560	H	3.568453	0.984019	1.184666
C	0.465754	4.570671	-2.305191	C	3.804316	-0.650523	-0.991763
O	0.150923	2.312316	-1.703392	O	1.434247	-0.769883	-0.769394
H	1.102435	3.672767	-0.452292	H	2.727111	-1.334461	0.750873
H	-1.002845	2.318768	0.747131	H	0.731135	0.740574	1.367903
O	1.588563	4.169035	-3.079994	H	3.757850	0.151931	-1.738658
H	-0.440642	4.604580	-2.932037	H	4.762571	-0.580892	-0.463810
H	0.676115	5.582840	-1.945654	H	0.665020	-0.594006	-0.185307
H	0.035457	1.649846	-0.983720	H	3.770159	-1.608622	-1.520961
H	1.514479	3.203410	-3.175304				

6. The cartesian coordinates of the optimized geometries of the transition states in Path 7 and 8							
Transition state TS18-19				Transition state TS20-21			
O	-1.381323	0.408560	0.000000	O	-0.914397	-0.038911	0.000000
C	-2.813084	1.420676	0.415881	C	0.048280	1.402486	-0.398940
O	-3.163496	1.008704	1.512202	O	0.247583	1.321859	-1.604643
O	-2.981230	2.199310	-0.462894	O	0.191043	2.041802	0.590905
C	-1.461539	-0.535564	1.811380	C	-1.050789	-0.561461	-1.960342
H	-2.279393	-0.720377	2.497317	H	-0.388369	-0.378001	-2.797583
H	-0.569536	-0.044467	2.187741	H	-2.092057	-0.252026	-2.037477
C	-1.427489	-0.960927	0.413815	C	-0.644073	-1.237482	-0.727551
H	-0.457697	-1.413239	0.170803	H	-1.378837	-1.990681	-0.408897
C	-2.586326	-1.776689	-0.134479	C	0.770869	-1.781418	-0.618316
H	-2.516802	-1.824206	-1.225693	H	0.981711	-2.046524	0.422224
H	-2.542810	-2.800115	0.258619	H	0.874012	-2.683825	-1.233629
H	-3.550376	-1.336175	0.136479	H	1.506512	-1.042465	-0.949146
H	1.934206	0.551569	-0.855601	H	-4.218148	-1.495444	-0.246926
C	2.164648	1.050303	0.097685	C	-4.536832	-0.621208	0.348766
C	2.681046	0.016908	1.095913	C	-5.016975	0.466959	-0.610567
O	1.046218	1.763893	0.587690	O	-3.529136	-0.199711	1.243279
H	2.962352	1.781711	-0.088557	H	-5.380630	-0.939254	0.970886
C	4.012107	-0.588032	0.659783	C	-6.299035	0.076059	-1.344144
O	1.703773	-1.025535	1.234846	O	-3.942078	0.694624	-1.552785
H	2.816847	0.510638	2.070013	H	-5.172933	1.383313	-0.025090
H	0.221997	1.332352	0.281966	H	-2.695404	-0.010479	0.766017
H	3.922237	-1.010568	-0.351481	H	-6.159819	-0.861021	-1.896692
H	4.795735	0.181946	0.661299	H	-7.128776	-0.054406	-0.638772
H	2.155071	-1.755452	1.695300	H	-4.033008	1.582181	-1.931713
O	4.314904	-1.622130	1.607545	H	-6.589013	0.851361	-2.063234
H	5.075963	-2.136512	1.300292				

7. The cartesian coordinates of the optimized geometries of the transition states in Path 9 and 10							
Transition state TS22-23				Transition state TS24-25			
O	-0.680934	0.525292	0.000000	O	0.836576	0.136187	0.000000
C	-2.188813	0.945166	0.158501	C	-0.675466	0.517103	0.143953
O	-2.857366	-0.030545	0.520434	O	-1.326666	-0.476826	0.492495
O	-2.346666	2.125734	-0.073018	O	-0.861904	1.695347	-0.081586
C	-0.921627	-1.363819	0.532039	C	0.637291	-1.766642	0.491752
H	-1.840766	-1.930759	0.590670	H	-0.267609	-2.357740	0.529905
H	-0.310842	-1.287225	1.426044	H	1.236945	-1.692731	1.393434
C	-0.418974	-0.735006	-0.686446	C	1.136776	-1.103778	-0.709688
H	0.668364	-0.782267	-0.791503	H	2.225351	-1.117767	-0.808500
C	-1.122234	-0.957878	-2.007942	C	0.450155	-1.318157	-2.041019
H	-0.774257	-0.211395	-2.726671	H	0.793290	-0.553660	-2.742511
H	-0.861103	-1.952527	-2.389003	H	0.735089	-2.301384	-2.434704
H	-2.208793	-0.894167	-1.906229	H	-0.638506	-1.277755	-1.949321
H	-0.993248	3.216356	-2.646305	H	0.551611	2.748932	-2.677271
C	-0.121135	3.745690	-2.238369	C	1.402321	3.303548	-2.256628
C	1.168179	3.044197	-2.671640	C	2.711350	2.603010	-2.635503
O	-0.162331	3.757881	-0.814864	O	1.310039	3.365416	-0.836467
H	-0.133092	4.777589	-2.615997	H	1.389198	4.322321	-2.669268
C	1.263156	2.801454	-4.170493	C	2.847738	2.363151	-4.131335
O	1.247753	1.757958	-2.037144	O	2.777048	1.339246	-1.961703
H	2.029055	3.650274	-2.349850	H	3.546607	3.231358	-2.285611
H	-0.969772	3.297393	-0.508270	H	0.506456	2.893339	-0.538542
H	0.393365	2.211133	-4.501909	H	2.023015	1.742838	-4.503642
H	1.258974	3.753622	-4.710818	H	2.839679	3.314315	-4.677208
H	0.971647	1.911972	-1.113041	H	2.459234	1.523981	-1.056675
O	2.475435	2.143249	-4.524160	H	3.789332	1.849377	-4.352951
H	2.588018	1.407468	-3.899539				

8. The cartesian coordinates of the optimized geometries of the transition states in Path 11							
Transition state TS26-27				Transition state TS28-29			
O	-1.918917	-0.776739	0.595357	O	-0.003975	0.765957	0.337089
C	-0.889592	-0.370716	-0.972441	C	-2.198855	1.248707	1.147065
H	-1.054307	-1.335554	-1.413680	H	-2.273368	2.128206	0.507496
H	0.121662	-0.173603	-0.637873	H	-2.842072	1.358115	2.022510
C	-2.007827	0.317404	-0.287774	C	-0.741470	0.943995	1.501456
H	-1.670512	1.250167	0.186167	H	-0.426598	1.875262	2.023690
C	-3.341715	0.552944	-0.980505	C	-0.589596	-0.210408	2.501292
H	-4.089801	0.848475	-0.235714	H	0.459589	-0.307666	2.800318
H	-3.249878	1.349545	-1.726535	H	-1.185045	-0.036948	3.407487
H	-3.708591	-0.352909	-1.476572	H	-0.911587	-1.155774	2.048674
K	-2.621432	-2.333989	-3.500073	K	0.284241	-0.532831	-1.839216
I	-0.498320	0.398624	-3.601930	I	-3.166757	-0.328654	-0.059283
H	-3.268113	-4.016842	1.414530	H	4.815912	-0.531885	0.895944
C	-4.135256	-3.414599	1.098847	C	3.929176	-0.760767	1.512418
C	-4.110159	-3.267609	-0.430555	C	2.738766	-1.111434	0.592274
O	-4.169234	-2.164972	1.762730	O	3.599373	0.350143	2.329056
H	-5.047554	-3.940239	1.405066	H	4.178780	-1.591034	2.183047
C	-4.378781	-4.580208	-1.148895	C	3.180891	-2.132409	-0.453935
O	-2.845726	-2.787837	-0.883428	O	2.252466	0.057750	-0.003079
H	-4.902070	-2.551002	-0.706394	H	1.955265	-1.586247	1.212831
H	-3.358610	-1.647173	1.560771	H	3.144277	0.969086	1.724996
O	-4.338343	-4.338714	-2.577824	O	2.040465	-2.535294	-1.256120
H	-3.614765	-5.322931	-0.884546	H	3.939668	-1.685630	-1.110303
H	-5.369486	-4.959111	-0.869026	H	3.606498	-3.017991	0.038607
H	-2.509206	-2.070395	-0.255978	H	1.144745	0.408442	0.370584
H	-4.710228	-5.111454	-3.029278	H	2.256743	-3.369544	-1.697931
				C	1.978549	2.576169	-1.363373
				O	1.536828	2.006914	-2.291434
				O	2.423587	3.199896	-0.486017
Transition state TS29-30							
O	-0.298094	2.015164	0.869074				
C	1.498942	2.160702	-0.760365				
H	2.497537	2.566150	-0.654695				
H	1.289615	1.684614	-1.708278				
C	0.332752	2.869110	-0.098953				
H	0.732844	3.737939	0.439483				
C	-0.716258	3.305421	-1.116320				
H	-1.525524	3.845536	-0.614299				
H	-0.269777	3.976756	-1.859186				
H	-1.151560	2.445491	-1.635422				
K	-0.039315	-1.755594	2.009018				
I	1.976336	-0.777253	-0.900890				
H	-4.581456	-0.652073	-0.380391				
C	-3.817478	-0.110694	-0.959870				
C	-2.424516	-0.624728	-0.576535				
O	-3.938324	1.291864	-0.759181				
H	-4.007964	-0.280990	-2.024478				
C	-2.329922	-2.142644	-0.740577				
O	-2.144897	-0.296861	0.790455				
H	-1.676509	-0.143141	-1.222275				
H	-3.849165	1.459139	0.193604				
O	-1.059526	-2.674815	-0.365508				
H	-3.057857	-2.631760	-0.084080				
H	-2.571572	-2.416885	-1.777481				
H	-1.659773	0.552357	0.833792				
H	-0.358586	-2.279174	-0.924653				
C	0.664223	1.412211	1.711350				
O	0.202323	0.730123	2.637710				
O	1.856573	1.618332	1.357678				

9. The cartesian coordinates of the optimized geometries of the transition states in Path 12

Transition state TS27-31				Transition state TS32-33			
O	0.623376	2.1 2272	-0.684947	O	0.246679	1.471882	0.363819
C	-1.513588	1.188559	-0.991981	C	-2.154981	1.223834	0.708132
H	-0.851774	0.593570	-1.618729	H	-2.300350	1.843673	-0.174894
H	-2.239424	1.702652	-1.622553	H	-2.961188	1.376937	1.428674
C	-0.668613	2.169874	-0.120767	C	-0.766544	1.447391	1.316760
H	-1.096107	3.167864	-0.288423	H	-0.891946	2.480474	1.709498
C	-0.643302	1.923963	1.390572	C	-0.469671	0.545082	2.523204
H	-0.022677	2.696588	1.856314	H	0.466077	0.859346	2.996305
H	-1.646353	1.971634	1.829326	H	-1.274036	0.599059	3.268306
H	-0.198170	0.951492	1.625963	H	-0.356090	-0.499332	2.212124
K	0.466978	-2.158667	0.173828	K	0.511712	-2.477907	-0.933258
I	-2.767844	-0.352975	0.003933	I	-2.601538	-0.820910	-0.063383
H	3.731451	1.357367	-1.305376	H	3.549623	1.304740	-0.468428
C	3.770953	1.249898	-0.208306	C	3.512776	0.937029	0.570323
C	3.011663	-0.035081	0.191593	C	2.876824	-0.468004	0.571847
O	3.270543	2.416959	0.429177	O	2.825367	1.854439	1.404427
H	4.824612	1.180438	0.092834	H	4.540247	0.887106	0.955044
C	3.807672	-1.249807	-0.304624	C	3.796084	-1.436610	-0.176069
O	1.705264	-0.068201	-0.282805	O	1.607749	-0.484696	-0.019507
H	3.040991	-0.070517	1.304003	H	2.821089	-0.802056	1.626818
H	2.364326	2.588307	0.101897	H	1.903342	1.936915	1.065442
O	3.128187	-2.473032	0.111215	O	3.151992	-2.739052	-0.284572
H	3.866345	-1.239134	-1.401653	H	3.994881	-1.061330	-1.189674
H	4.821577	-1.252631	0.118324	H	4.747681	-1.551051	0.359094
H	1.069372	1.254917	-0.542963	H	0.890316	0.474548	0.216909
H	3.751315	-3.208652	0.019816	H	3.840407	-3.404578	-0.429399
				C	0.263725	3.240170	-1.664349
				O	1.253763	2.802507	-2.106965
				O	-0.730595	3.746251	-1.305162
Transition state TS33-34				Transition state TS34-35			
O	0.139831	1.639069	0.068012	O	0.498742	1.425048	0.824260
C	-2.280443	1.284448	0.024437	C	-1.816266	1.545255	0.494675
H	-2.272918	1.486019	-1.044748	H	-1.668137	1.412350	-0.559038
H	-3.222472	1.608503	0.471366	H	-2.750886	2.004258	0.789966
C	-1.059539	1.890597	0.722807	C	-0.752135	1.241580	1.524979
H	-1.300036	2.971514	0.623347	H	-0.837536	2.042191	2.271123
C	-0.984700	1.567034	2.220302	C	-0.714604	-0.081145	2.278099
H	-0.190674	2.156441	2.689757	H	0.081505	-0.031941	3.029589
H	-1.931879	1.795801	2.726439	H	-1.668639	-0.247391	2.784891
H	-0.756781	0.506569	2.377604	H	-0.538204	-0.936169	1.623106
K	0.609181	-2.530309	-0.862730	K	0.237948	-0.918935	-1.434810
I	-2.482998	-0.941395	0.107145	I	-3.075574	-0.888667	-0.166082
H	3.400715	1.427770	-0.361509	H	4.682186	-0.318781	1.439419
C	3.352104	1.123214	0.694399	C	4.615163	-1.136771	0.703341
C	2.853079	-0.329827	0.772094	C	3.458915	-0.864174	-0.260109
O	2.544471	2.010983	1.441550	O	4.462372	-2.389437	1.352173
H	4.361608	1.180956	1.121772	H	5.564312	-1.184432	0.159569
C	3.830050	-1.270078	0.073545	C	3.608924	0.457947	-1.012667
O	1.587048	-0.497548	0.151334	O	2.210817	-0.930410	0.461780
H	2.777419	-0.614247	1.834251	H	3.411450	-1.695267	-0.976723
H	1.671099	2.086134	0.985071	H	3.576202	-2.397813	1.752508
O	3.249000	-2.600847	-0.010210	O	2.449331	0.726105	-1.802132
H	4.037269	-0.911969	-0.943735	H	3.762893	1.280686	-0.301394
H	4.769856	-1.316882	0.637148	H	4.492515	0.402917	-1.662655
H	1.006350	0.338415	0.180219	H	1.968952	-0.043635	0.798066
H	3.968867	-3.241060	-0.110706	H	2.117228	1.612613	-1.516848
C	0.394577	2.572870	-1.680963	C	0.446934	2.640176	0.084467
O	1.399061	2.066492	-2.072641	O	1.464739	2.936063	-0.545767
O	-0.535002	3.315137	-1.757151	O	-0.684878	3.212923	0.154119

10. The cartesian coordinates of the optimized geometries of the transition states in Path 13

Transition state TS36-37				Transition state TS38-39			
O	0.784076	2.535500	-0.95685	O	0.886495	1.674326	0.368048
C	-0.827866	1.454874	-0.657932	C	-1.137585	0.928786	-0.466313
H	-0.235644	0.655890	-1.070901	H	-0.474490	0.298887	-1.058437
H	-1.381881	2.025983	-1.393328	H	-1.492718	1.745587	-1.094445
C	-0.297390	2.197613	0.517649	C	-0.414962	1.456647	0.801074
H	-0.938800	3.065218	0.741019	H	-0.888777	2.417109	1.060877
C	0.018960	1.478486	1.826308	C	-0.457071	0.566166	2.051700
H	0.521784	2.177595	2.505159	H	0.129341	1.056203	2.836102
H	-0.896789	1.118173	2.308097	H	-1.474684	0.406603	2.424590
H	0.703300	0.634946	1.672048	H	0.010109	-0.413267	1.872180
K	0.379540	-1.683891	0.094524	K	0.102107	-2.380755	-0.146601
I	-2.777853	-0.319116	-0.142968	I	-2.965649	-0.357918	-0.224754
H	4.462556	1.030516	-1.715436	H	4.223280	-0.160687	-1.804971
C	4.338380	1.261332	-0.650708	C	4.241030	0.107016	-0.741019
C	3.400261	0.250854	0.016191	C	3.247483	-0.752021	0.046105
H	5.325581	1.267625	-0.171031	H	5.264023	-0.020713	-0.362909
C	3.947216	-1.164098	-0.116187	C	3.551762	-2.239259	-0.117839
O	2.105642	0.271783	-0.568861	O	1.910611	-0.545148	-0.387226
H	3.323173	0.486308	1.091589	H	3.325572	-0.495003	1.118022
O	3.049867	-2.101680	0.531049	O	2.640596	-3.088654	0.624868
H	4.039593	-1.429236	-1.177987	H	3.421668	-2.527105	-1.166595
H	4.935899	-1.218452	0.355269	H	4.585086	-2.464186	0.173147
H	1.700595	1.208886	-0.489073	H	1.586390	0.400838	-0.112731
H	3.547972	-2.902550	0.751975	H	2.925902	-3.109578	1.551544
H	3.913538	2.267014	-0.570010	H	3.967468	1.162834	-0.651883
				C	1.419815	3.516918	-0.149076
				O	0.439048	4.167406	0.037873
				O	2.551793	3.342193	-0.472927
Transition state TS39-40							
O	0.216177	1.859280	0.594246				
C	-1.515698	1.384040	-0.899608				
H	-0.977551	0.532438	-1.265278				
H	-2.303405	1.756620	-1.543020				
C	-1.198384	2.080477	0.402153				
H	-1.346062	3.149986	0.201997				
C	-1.931676	1.751155	1.694270				
H	-1.568908	2.423648	2.479244				
H	-3.005963	1.904020	1.560434				
H	-1.789995	0.713918	2.003745				
K	0.591332	-1.083416	0.807298				
I	-2.913041	-1.024234	-0.209742				
H	4.518019	-2.733454	-0.655029				
C	4.964825	-1.765435	-0.913083				
C	4.070363	-0.623636	-0.444994				
H	5.954295	-1.706829	-0.443209				
C	3.960519	-0.586485	1.089305				
O	2.764568	-0.775149	-1.037189				
H	4.486430	0.332814	-0.788439				
O	2.871697	0.203580	1.565285				
H	3.788930	-1.600213	1.477329				
H	4.911629	-0.231372	1.512989				
H	2.476534	0.131521	-1.268000				
H	2.778605	1.014908	1.016700				
H	5.094378	-1.728920	-1.998977				
C	0.888231	2.101930	-0.610911				
O	0.117563	2.375794	-1.586028				
O	2.118727	1.943737	-0.588266				

11. The cartesian coordinates of the optimized geometries of the transition states in Path 17

Transition state TS62-63				Transition state TS64-65			
O	0.564202	0.89 942	0.000000	O	-1.108949	-0.214008	0.000000
C	2.326359	1.491786	-0.431494	C	-3.504153	-0.039992	-0.275114
H	2.097854	2.422198	-0.933239	H	-4.105767	0.672759	-0.813856
H	2.666807	0.662398	-1.033773	H	-3.766317	-0.261638	0.747690
C	1.649363	1.206629	0.847361	C	-2.219597	-0.597872	-0.867019
H	2.048640	0.322533	1.363517	H	-2.222670	-1.685773	-0.810996
C	1.413314	2.350617	1.818748	C	-1.960336	-0.130991	-2.294626
H	0.653983	2.061753	2.555119	H	-1.016009	-0.543834	-2.662339
H	2.335926	2.601705	2.354193	H	-2.767079	-0.477531	-2.948478
H	1.061623	3.244190	1.289086	H	-1.913886	0.961985	-2.346196
K	-2.306689	4.754863	0.033399	K	3.058336	-0.277987	-2.689263
I	4.932738	2.276486	-0.054341	I	-5.235596	-1.920155	-1.058797
H	-2.329662	-0.255753	-1.352050	H	1.705282	-1.759498	2.062342
C	-2.511205	-0.269251	-0.266130	C	1.244250	-2.544609	1.446032
C	-2.796291	1.164122	0.209361	C	1.747450	-2.418626	0.002563
O	-1.429350	-0.891846	0.420733	O	-0.179219	-2.500363	1.552314
H	-3.389338	-0.895993	-0.075857	H	1.536859	-3.518133	1.851552
C	-4.159164	1.629673	-0.284736	C	3.218807	-2.796742	-0.088376
O	-1.820886	2.100593	-0.261651	O	1.619039	-1.077213	-0.496828
H	-2.803963	1.164506	1.311252	H	1.164251	-3.100902	-0.633716
H	-0.603160	-0.367818	0.261707	H	-0.506197	-1.635100	1.240414
O	-4.401726	2.958053	0.210398	O	3.639151	-2.690645	-1.458353
H	-4.181382	1.630899	-1.383262	H	3.820175	-2.127036	0.541519
H	-4.932986	0.946109	0.085195	H	3.347097	-3.826252	0.266006
H	-0.900383	1.748726	-0.105704	H	0.695335	-0.768324	-0.401070
				H	4.534364	-3.057290	-1.535951
				C	-1.254135	1.064627	0.577130
				O	-0.270661	1.513814	1.167399

12. The cartesian coordinates of the optimized geometries of the transition states in Path 18

Transition state TS66-67				Transition state TS68-69			
O	-1.575876	0.194553	0.000000	O	-2.276265	0.408560	0.000000
C	0.070294	1.273097	-0.045751	C	0.073908	0.070882	0.292457
H	-0.365100	2.262372	-0.106825	H	-0.052396	-0.326187	1.287736
H	0.501801	0.869582	-0.950875	H	0.933430	0.685361	0.090751
C	-0.525707	0.322840	0.920188	C	-1.075579	-0.012314	-0.703349
H	0.064106	-0.602115	1.020478	H	-0.884101	0.724812	-1.491821
C	-0.913733	0.853613	2.293912	C	-1.413899	-1.355953	-1.336658
H	-1.573739	0.134344	2.793907	H	-2.334018	-1.245739	-1.920384
H	-0.028144	1.004581	2.921895	H	-0.613324	-1.675173	-2.005393
H	-1.447564	1.807575	2.206207	H	-1.560866	-2.127186	-0.575026
K	-3.331349	4.367867	0.368687	K	-4.269508	-3.415294	1.520346
I	2.452188	2.226809	0.746468	I	1.777727	-1.986658	-0.128540
H	-5.646532	-0.148856	-0.715754	H	-6.641921	0.857233	-0.477256
C	-5.208655	-0.278324	0.281724	C	-6.033871	0.404810	-1.269591
C	-4.782741	1.071706	0.866469	C	-5.594217	-1.006568	-0.878239
H	-5.946117	-0.772768	0.925967	H	-6.621118	0.386481	-2.195361
C	-5.969475	2.019947	0.955326	C	-6.793371	-1.899500	-0.601252
O	-3.775499	1.697989	0.069100	O	-4.786008	-0.999005	0.310347
H	-4.393027	0.917879	1.885560	H	-5.015397	-1.453701	-1.700637
O	-5.550613	3.245897	1.583203	O	-6.331871	-3.231624	-0.316513
H	-6.352186	2.228861	-0.053783	H	-7.357829	-1.505878	0.255311
H	-6.766557	1.550465	1.544829	H	-7.446141	-1.906903	-1.482274
H	-2.941615	1.133552	0.084308	H	-3.985272	-0.455817	0.156081
H	-6.335941	3.786613	1.762690	H	-7.099590	-3.822969	-0.266564
				H	-5.159822	1.043209	-1.438067
				C	-2.068436	1.518777	0.826222
				O	-3.074760	2.049603	1.306594