A computational investigation on the substituent effect on the chemo- and stereoselectivity of crossed intermolecular radical anion [2+2] cycloadditions of enones

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Table S1 Main geometrical and electronic parameters[a] of critical structures for the cycloadditions.

Reactions	Structures	C1-C3		C2-C4		μ [D]	t [e]
		r [Å]	l	r [Å]	l		
1 (R1a+R2a)	**PC**	3.01		4.62		2.22	0.39
	TS1	2.16	0.67	4.03	0.96	4.73	0.43
	IM	1.63		3.86		4.93	0.52
	TS2-trans	1.54	1.00	2.00	0.75	2.29	0.78
	P-trans	1.55		1.60		2.29	0.45
	TS2-cis	1.54	1.00	2.02	0.74	6.06	0.84
	P-cis	1.55		1.60		4.75	0.40
2 (R1b+R2a)	**PC**	3.72		5.19		0.81	0.23
	TS1	2.14	0.69	4.01	0.96	5.80	0.41
	IM	1.63		3.86		5.76	0.52
	TS2-trans	1.54	1.00	2.04	0.72	5.75	0.53
	P-trans	1.55		1.59		1.93	0.41
	TS2-cis	1.54	1.00	2.05	0.72	6.54	0.58
	P-cis	1.55		1.60		4.56	0.41
3 (R1c+R2a)	**PC**	3.00		4.61		7.41	0.43
	TS1	2.17	0.67	4.04	0.95	9.56	0.51
	IM	1.63		3.86		9.60	0.58
	TS2-trans	1.54	1.00	1.96	0.78	5.65	0.63
	P-trans	1.55		1.61		3.13	0.50
	TS2-cis	1.54	1.00	1.97	0.78	8.45	0.62
	P-cis	1.55		1.60		4.94	0.43
4 (R1d+R2a)	**PC**	5.20		6.24		8.55	0.02
	TS1	1.99	0.77	3.91	0.98	2.68	0.40
	IM	1.62		3.85		1.92	0.45
	TS2-trans	1.54	1.00	2.39	0.48	1.47	0.60
	P-trans	1.55		1.57		10.50	0.26
	TS2-cis	1.54	1.00	2.38	0.50	4.29	0.56

	P-cis	1.55		1.59		10.35	0.37
5 (R1e+R2a)	**PC**	3.00		4.63		7.23	0.46
	TS1	2.17	0.67	4.05	0.95	8.84	0.51
	IM	1.63		3.86		8.96	0.59
	TS2-trans	1.54	1.00	1.94	0.80	4.86	0.65
	P-trans	1.55		1.61		3.15	0.51
	TS2-cis	1.54	1.00	1.96	0.78	7.73	0.63
	P-cis	1.55		1.61		5.29	0.44
6 (R1f+R2a)	**PC**	3.00		4.58		2.49	0.40
	TS1	2.14	0.69	4.02	0.96	4.46	0.52
	IM	1.63		3.86		4.73	0.61
	TS2-trans	1.54	1.00	2.01	0.74	1.72	0.71
	P-trans	1.55		1.60		3.32	0.48
	TS2-cis	1.54	1.00	2.02	0.74	5.78	0.69
	P-cis	1.55		1.60		5.28	0.48
7 (R1g+R2a)	**PC**	4.74		6.11		2.59	0.13
	TS1	2.11	0.63	4.02	0.42	4.31	0.50
	IM	1.54		2.54		3.18	0.75
	TS2-trans	1.54	1.00	2.01	0.74	2.44	0.72
	P-trans	1.55		1.60		4.35	0.47
	TS2-cis	1.55	1.00	2.02	0.74	6.10	0.66
	P-cis	1.55		1.60		6.04	0.35
8 (R1a+R2b)	**PC**	3.49		5.01		5.11	0.21
	TS1	2.14	0.70	4.01	0.96	2.28	0.43
	IM	1.64		3.86		2.97	0.43
	TS2-trans	1.54	1.00	2.00	0.73	1.13	0.49
	P-trans	1.55		1.58		3.07	0.15
	TS2-cis	1.54	1.00	2.01	0.75	5.17	0.47
	P-cis	1.55		1.61		5.32	0.12
9 (R1a+R2c)	**PC**	3.58		5.07		4.62	0.14
	TS1	2.11	0.71	4.01	0.96	2.97	0.49
	IM	1.63		3.86		2.86	0.60
	TS2-trans	1.54	1.00	2.05	0.72	2.77	0.69
	P-trans	1.55		1.60		4.90	0.56
	TS2-cis	1.54	1.00	2.03	0.73	4.31	0.65
	P-cis	1.55		1.60		3.99	0.53
10 (R1a+R2d)	**PC**	8.61		6.70		4.88	0.10
	TS1	2.13	0.69	3.99	0.96	10.32	0.34
	IM	1.63		3.85		11.96	0.21
	TS2-trans	1.54	1.00	2.16	0.63	6.11	0.24
	P-trans	1.55		1.58		10.64	0.23
	TS2-cis	1.54	1.00	2.10	0.66	7.85	0.07
	P-cis	1.55		1.57		10.45	0.19
	PC	4.34		6.22		2.11	0.37

11 (R1a+R2e)	**TS1**	2.04	0.77	3.92	0.98	3.75	0.49
	IM	1.66		3.83		5.64	0.57
	TS2-trans	1.54	1.00	2.72	0.29	4.01	0.54
	P-trans	1.55		1.59		4.11	0.52
	TS2-cis	1.54	1.00	2.00	0.73	6.06	0.83
	P-cis	1.56		1.58		4.91	0.51
12 (R1a+R2f)	**PC**	6.01		6.60		7.18	0.09
	TS1	1.98	0.79	4.00	0.97	4.64	0.30
	IM	1.63		3.89		6.23	0.41
	TS2-trans	1.54	1.00	1.96	0.77	4.31	0.32
	P-trans	1.55		1.59		5.42	0.29
	TS2-cis	1.56	1.00	2.00	0.76	5.00	0.24
	P-cis	1.53		1.61		5.23	0.52
13 (R1a+R1a)	**PC**	3.31		4.61		2.03	0.52
	TS1	2.07	0.75	3.95	0.97	1.10	0.51
	IM	1.66		3.85		0.74	0.52
	TS2-trans	1.54	1.00	2.10	0.70	2.70	0.50
	P-trans	1.55		1.61		1.00	0.48
	TS2-cis	1.54	1.00	2.02	0.75	5.72	0.51
	P-cis	1.55		1.62		4.12	0.59
14 (R1b+R1b)	**PC**	3.31		4.59		1.81	0.51
	TS1	2.07	0.75	3.94	0.98	1.70	0.50
	IM	1.66		3.85		0.79	0.48
	TS2-trans	1.54	1.00	2.47	0.46	3.04	0.50
	P-trans	1.55		1.60		0.86	0.52
	TS2-cis	1.54	1.00	2.05	0.73	6.12	0.52
	P-cis	1.55		1.61		4.83	0.66
15 (R1c+R1c)	**PC**	3.30		4.60		2.74	0.52
	TS1	2.08	0.75	3.96	0.97	1.73	0.49
	IM	1.66		3.85		1.71	0.52
	TS2-trans	1.54	1.00	2.06	0.72	7.03	0.50
	P-trans	1.55		1.61		5.09	0.45
	TS2-cis	1.54	1.00	2.03	0.75	9.69	0.53
	P-cis	1.55		1.62		7.88	0.59
16 (R1f+R1f)	**PC**	3.34		4.67		2.16	0.50
	TS1	2.06	0.77	3.95	0.97	1.38	0.51
	IM	1.67		3.85		1.04	0.51
	TS2-trans	1.54	1.00	2.11	0.69	1.30	0.50
	P-trans	1.55		1.61		1.24	0.38
	TS2-cis	1.54	1.00	2.03	0.75	5.19	0.62
	P-cis	1.55		1.62		4.28	0.73

[a] The indexes l were calculated according to the equation[1]: $l_{X-Y} = 1-(r^{TS}{}_{X-Y} - r^{P}{}_{X-Y}) / r^{P}{}_{X-Y}$, where $r^{TS}{}_{X-Y}$ is the distance between the atoms X

and Y in the transition state and r^{P}_{X-Y} is the corresponding distance in product. The charge transfer (t) was calculated according to the expression[2]: $t = -\sum q_A$, where q_A is the charge on atom A, and the summation is over all of the neutral molecule.

[1] R. Jasiński, M. Kwiatkowska, A. Barański, J. Mol. Struct: Theo. Chem. 2009, **910**, 80.

[2] G. Leroy, M. Sana, L. A. Burke, M. T. Nguyen, Quantum Theory Chem. React., 1980, **1**, 91.

Table S2 The enthalpies at 298 K in solvent (CH_3CN) for the pr-reaction complexes, transition states, intermediates, and products along the cycloaddition pathways. All values are given in kcal/mol.

Reactions	R1+R2	PC	TS1	IM	TS2-trans	P-trans	TS2-cis	P-cis
1 (R1a+R2a)	0	1.6	3.9	-2.3	1.1	-5.5	4.0	-2.5
2 (R1b+R2a)	0	-0.1	5.0	-1.3	1.6	-5.9	4.4	-3.0
3 (R1c+R2a)	0	0.0	1.9	-4.3	-0.1	-4.2	3.0	-1.2
4 (R1d+R2a)	0	0.0	21.5	16.3	16.6	-9.6	18.4	-6.1
5 (R1e+R2a)	0	-1.5	1.0	-5.2	-0.7	-3.9	2.6	-0.9
6 (R1f+R2a)	0	2.3	5.5	-0.5	1.5	-5.2	4.4	-2.3
7 (R1g+R2a)	0	-1.6	9.7	0.4	3.5	-3.6	6.8	-0.5
8 (R1a+R2b)	0	1.7	12.1	5.4	6.3	0.7	12.0	7.8
9 (R1a+R2c)	0	1.0	7.3	2.0	5.0	-4.0	7.4	-0.5
10 (R1a+R2d)	0	1.0	19.3	11.5	16.6	-3.3	18.5	-4.5
11 (R1a+R2e)	0	-6.2	20.0	17.0	16.4	9.6	18.3	13.1
12 (R1a+R2f)	0	1.1	25.9	22.9	23.6	16.5	29.1	23.4
13 (R1a+R1a)	0	3.8	10.7	1.9	2.9	-2.0	9.4	5.2
14 (R1b+R1b)	0	4.9	12.5	4.7	6.1	2.8	12.2	10.7
15 (R1c+R1c)	0	5.0	12.8	5.2	5.2	1.0	11.5	6.9
16 (R1f+R1f)	0	4.8	13.1	5.7	6.2	1.7	12.7	8.8

Cartesian Coordinates (Å), SCF Energies, Enthalpies, and Free Energies at 298 K and 1 atm and NBO charges for the main Optimized Structures

TS1-1

B3LYP SCF energy: -693.503216 a.u.

B3LYP enthalpy: -693.485787 a.u.

B3LYP free energy: -693.550745 a.u.

Cartesian coordinate

C	-0.000000182	-0.000000811	-0.000004365
H	0.000001148	-0.000003414	-0.000001749
C	-0.000000562	-0.000004659	-0.000002845
H	-0.000001661	-0.000002796	0.000008620
C	-0.000003001	-0.000002857	-0.000002135
O	0.000002522	-0.000002426	-0.000003266
C	0.000000001	-0.000004579	0.000002042
H	-0.000000587	-0.000003664	0.000004152
H	0.000000024	-0.000006218	-0.000000319
H	0.000000445	-0.000001443	0.000000147
H	-0.000003328	-0.000002873	0.000002808
C	0.000000290	0.000002784	0.000002987
H	0.000000934	0.000000562	0.000000431
C	0.000002756	0.000003699	0.000001374
H	-0.000001210	0.000002673	-0.000002257
C	-0.000001067	-0.000001762	-0.000000799
O	-0.000001027	0.000001701	0.000003900
C	0.000000534	0.000000405	-0.000000877
C	-0.000000727	0.000002407	-0.000001306
C	0.000000940	0.000001382	0.000001445
C	0.000002152	0.000001121	-0.000003461
H	0.000002203	0.000001005	-0.000003662
C	-0.000000839	0.000001403	0.000001752
H	-0.000001473	0.000001095	0.000003925
C	0.000000022	0.000001168	-0.000002235
H	0.000001228	0.000001441	-0.000005794
H	-0.000000880	0.000001495	0.000002164
H	0.000000349	0.000001346	-0.000002613
C	-0.000003055	-0.000000971	-0.000002401
H	0.000003388	0.000005517	0.000008399
H	0.000000943	0.000003073	-0.000002968
H	-0.000000279	0.000004198	-0.000001096

NBO Charges

C	1	-0.13022
H	2	0.10401
C	3	-0.11235
H	4	0.08741
C	5	0.24613
O	6	-0.27891
C	7	-0.32572
H	8	0.09256
H	9	0.10307
H	10	0.10375
H	11	0.10621
C	12	-0.01961
H	13	0.10606
C	14	-0.11685
H	15	0.08726
C	16	0.24037
O	17	-0.26432
C	18	-0.04675
C	19	-0.08689
C	20	-0.07580
C	21	-0.11520
H	22	0.10083
C	23	-0.11604
H	24	0.11381
C	25	-0.09734
H	26	0.09585
H	27	0.09555
H	28	0.09445
C	29	-0.29681
H	30	0.10614
H	31	0.10007
H	32	0.09928

IM-1

B3LYP SCF energy: -693.511163 a.u.

B3LYP enthalpy: -693.493835 a.u.

B3LYP free energy: -693.558230 a.u.

Cartesian coordinates

C	-0.000012398	-0.000003881	-0.000012960
H	-0.000000707	0.000006143	0.000008069

C	0.000010867	0.000009252	-0.000003635
H	-0.000003965	-0.000000914	-0.000009460
C	-0.000000913	0.000021740	-0.000013080
O	0.000003083	-0.000006114	0.000018035
C	-0.000006023	0.000012368	-0.000003373
H	0.000008263	0.000002757	-0.000007016
H	0.000000160	0.000010189	0.000000856
H	-0.000002161	-0.000001586	-0.000000812
H	0.000004349	0.000010575	-0.000004083
C	0.000018760	-0.000003921	0.000004048
H	-0.000000480	-0.000001966	-0.000003059
C	-0.000005188	-0.000005933	-0.000006917
H	0.000000781	0.000005275	0.000010775
C	-0.000010270	-0.000007445	0.000010882
O	-0.000003241	0.000006600	-0.000017256
C	0.000019506	-0.000022039	-0.000004411
C	-0.000004088	0.000005280	0.000006299
C	-0.000009508	-0.000002167	-0.000010834
C	-0.000000449	0.000005334	0.000006935
H	0.000001708	-0.000004754	0.000010056
C	0.000004962	-0.000006078	-0.000004403
H	0.000002456	-0.000002566	-0.000011553
C	-0.000003352	0.000001524	0.000000483
H	-0.000001572	-0.000003361	0.000011491
H	0.000002885	0.000000794	-0.000009632
H	0.000001319	-0.000001086	0.000002079
C	-0.000008244	0.000000379	0.000007346
H	-0.000007002	-0.000005574	0.000005110
H	-0.000000410	-0.000005276	0.000014610
H	0.000000874	-0.000013547	0.000005410

NBO Charges

C	1	-0.41571
H	2	0.21260
C	3	-0.26449
H	4	0.17132
C	5	0.39675
O	6	-0.67329
C	7	-0.64135
H	8	0.18488
H	9	0.20001
H	10	0.20003
H	11	0.21702
C	12	-0.24252
H	13	0.20564
C	14	-0.28974
H	15	0.17439
C	16	0.37316
O	17	-0.70234
C	18	-0.06981
C	19	-0.19584
C	20	-0.19043
C	21	-0.22170
H	22	0.20430
C	23	-0.21703
H	24	0.22948
C	25	-0.23140
H	26	0.19116
H	27	0.19096
H	28	0.19011
C	29	-0.56792
H	30	0.20059
H	31	0.19426
H	32	0.18690

TS2-trans-1

B3LYP SCF energy: -693.504927 a.u.

B3LYP enthalpy: -693.488372 a.u.

B3LYP free energy: -693.550208 a.u.

Cartesian coordinate

C	0.000013515	0.000001690	-0.000000030
H	-0.000001035	0.000000706	0.000001298
C	-0.000021325	-0.000033159	-0.000004222
H	0.000005570	0.000005086	-0.000002673
C	0.000020824	0.000035527	0.000043151
O	-0.000014397	-0.000017134	-0.000017305
C	-0.000010873	0.000019671	0.000005258
H	0.000007437	0.000007923	0.000004395
H	0.000014136	-0.000007573	-0.000008552
H	-0.000005587	-0.000011330	0.000008507
H	-0.000000560	-0.000001895	0.000000169
C	0.000000235	-0.000016623	0.000007229
H	-0.000001071	0.000000768	-0.000000550
C	0.000026793	0.000036511	0.000004111
H	-0.000002478	-0.000010204	0.000006166
C	-0.000029922	-0.000021848	-0.000027616
O	0.000004268	0.000012059	0.000007440
C	0.000012647	0.000000907	0.000001271

C	-0.000002378	0.000002791	0.000002241
C	-0.000007170	0.000002205	-0.000007326
C	0.000001515	-0.000000508	0.000000812
H	-0.000001372	-0.000001321	0.000003282
C	0.000001400	-0.000001536	-0.000008026
H	-0.000000368	0.000001002	-0.000002395
C	-0.000004751	0.000003851	-0.000000497
H	-0.000001398	-0.000000685	0.000001553
H	-0.000000656	0.000002310	-0.000003745
H	-0.000001367	0.000001215	-0.000001784
C	-0.000002914	-0.000003058	-0.000006860
H	0.000000362	-0.000002092	-0.000002507
H	0.000000282	-0.000003183	-0.000001355
H	0.000000640	-0.000002073	-0.000001439

NBO charges

C	1	-0.19787
H	2	0.08981
C	3	-0.06312
H	4	0.09866
C	5	0.26061
O	6	-0.27854
C	7	-0.32523
H	8	0.09889
H	9	0.10507
H	10	0.10193
H	11	0.10526
C	12	-0.12197
H	13	0.10706
C	14	-0.06316
H	15	0.09705
C	16	0.24999
O	17	-0.23746
C	18	-0.04824
C	19	-0.07913
C	20	-0.06678
C	21	-0.11973
H	22	0.10267
C	23	-0.12322
H	24	0.11145
C	25	-0.08639
H	26	0.09527
H	27	0.09380
H	28	0.09235
C	29	-0.28388
H	30	0.09194
H	31	0.09322
H	32	0.09970

TS2-cis-1

B3LYP SCF energy: -693.497148 a.u.

B3LYP enthalpy: -693.480704 a.u.

B3LYP free energy: -693.541692 a.u.

Cartesian coordinate

C	0.000014579	-0.000004427	-0.000000212
H	0.000004332	-0.000002663	0.000002046
C	0.000025273	0.000013402	-0.000005162
H	-0.000000027	0.000004959	0.000000254
C	-0.000035942	0.000015267	0.000032032
O	0.000020007	-0.000006059	-0.000013045
C	0.000008564	-0.000000064	0.000005046
H	-0.000002074	0.000000718	0.000003514
H	-0.000001340	-0.000002011	0.000003212
H	-0.000000273	0.000000595	0.000001453
H	0.000000178	-0.000000442	0.000003017
C	0.000000790	-0.000026790	0.000003906
H	-0.000000111	0.000001864	-0.000001099
C	-0.000043095	0.000002596	-0.000035650
H	-0.000001055	-0.000002904	-0.000002446
C	-0.000000315	0.000015728	0.000033048
O	0.000003880	-0.000012035	-0.000014220
C	-0.000007567	-0.000005997	-0.000005933
C	0.000002113	0.000005261	-0.000003133
C	0.000002904	-0.000003287	0.000002567
C	-0.000002990	0.000006307	-0.000001208
H	0.000000117	0.000002597	0.000000468
C	0.000000863	-0.000001917	0.000002757
H	0.000000692	-0.000004280	0.000000835
C	0.000005716	0.000004475	0.000001098
H	0.000000207	0.000005501	0.000000284
H	0.000001753	-0.000001425	0.000001130
H	0.000000990	0.000003034	0.000000815
C	0.000002689	-0.000004216	-0.000006262
H	-0.000001837	-0.000000495	-0.000002566
H	0.000000024	0.000000551	-0.000003729
H	0.000000952	-0.000003845	-0.000002817

NBO charges

C	1	-0.19957

H	2	0.10452
C	3	-0.05698
H	4	0.09306
C	5	0.25657
O	6	-0.27085
C	7	-0.32672
H	8	0.09388
H	9	0.10044
H	10	0.11471
H	11	0.08838
C	12	-0.12316
H	13	0.11477
C	14	-0.06696
H	15	0.08982
C	16	0.24294
O	17	-0.22232
C	18	-0.04620
C	19	-0.08065
C	20	-0.06465
C	21	-0.12219
H	22	0.09782
C	23	-0.12325
H	24	0.11211
C	25	-0.08440
H	26	0.09362
H	27	0.09389
H	28	0.09198
C	29	-0.28443
H	30	0.09263
H	31	0.08891
H	32	0.10228

TS1-2

B3LYP SCF energy: -1153.140687 a.u.

B3LYP enthalpy: -1153.121985 a.u.

B3LYP free energy: -1153.190456 a.u.

Cartesian coordinate

C	-0.000001173	-0.000001551	0.000000450
H	0.000000159	-0.000002565	0.000001315
C	-0.000001063	-0.000003641	-0.000001973
H	0.000000075	-0.000001273	-0.000002225
C	-0.000001422	0.000001791	-0.000002777
O	0.000000354	-0.000005482	0.000008538
C	0.000001270	-0.000002684	-0.000000630
H	0.000000299	-0.000001834	-0.000001100
H	0.000001463	-0.000001959	0.000002275
H	-0.000001138	0.000000420	0.000001779
H	-0.000001091	-0.000001976	-0.000002961
C	-0.000000493	0.000004692	-0.000001265
H	0.000000696	0.000001716	-0.000000247
C	0.000001090	0.000004235	0.000001376
H	-0.000000097	0.000000022	0.000001847
C	0.000003724	-0.000004115	-0.000003460
O	-0.000001434	0.000006150	-0.000008214
C	-0.000001659	0.000003631	-0.000000404
C	0.000002025	0.000001139	0.000002023
C	-0.000001514	-0.000001122	-0.000004866
C	0.000000172	0.000002248	0.000004200
H	0.000001437	0.000001128	0.000002375
C	-0.000001460	-0.000001610	-0.000003211
H	-0.000000453	-0.000000911	-0.000003078
C	0.000000360	-0.000003775	-0.000000300
H	0.000000967	-0.000000899	0.000002774
H	-0.000001581	-0.000002299	-0.000002465
C	-0.000000600	0.000006692	0.000002900
H	0.000002263	0.000002635	0.000001131
H	-0.000000140	0.000001907	0.000002796
H	0.000000091	0.000004037	0.000000317
Cl	-0.000001129	-0.000004747	0.000003081

NBO charges

C	1	-0.13728
H	2	0.10478
C	3	-0.10447
H	4	0.08760
C	5	0.24504
O	6	-0.27636
C	7	-0.32584
H	8	0.09287
H	9	0.10355
H	10	0.10409
H	11	0.10766
C	12	-0.01468
H	13	0.10622
C	14	-0.12319
H	15	0.08698
C	16	0.23969
O	17	-0.26411

C	18	-0.04753
C	19	-0.07768
C	20	-0.06506
C	21	-0.12774
H	22	0.10280
C	23	-0.12868
H	24	0.11737
C	25	-0.00271
H	26	0.10537
H	27	0.10525
C	28	-0.29721
H	29	0.10598
H	30	0.10075
H	31	0.09993
Cl	32	-0.02340

IM-2

B3LYP SCF energy: -1153.148684 a.u.

B3LYP enthalpy: -1153.130095 a.u.

B3LYP free energy: -1153.197978 a.u.

Cartesian coordinate

C	0.000026971	-0.000009551	0.000030131
H	-0.000001617	0.000005605	-0.000006870
C	-0.000014136	0.000005929	0.000003294
H	0.000002656	-0.000000794	0.000006490
C	0.000003823	-0.000000232	-0.000004249
O	-0.000000210	0.000009938	-0.000003280
C	-0.000004914	0.000008023	0.000001520
H	0.000002009	0.000001600	0.000003732
H	0.000000422	0.000007350	0.000000702
H	-0.000000059	0.000001395	-0.000001499
H	-0.000004954	0.000004593	-0.000004807
C	-0.000019931	0.000014303	-0.000023616
H	0.000005593	-0.000005744	0.000006560
C	0.000008046	-0.000008381	-0.000003186
H	-0.000005489	0.000003043	-0.000006940
C	-0.000008826	0.000007289	0.000007312
O	0.000005069	-0.000007916	0.000006979
C	0.000006700	-0.000005269	-0.000002628
C	0.000001459	-0.000000899	0.000005507
C	-0.000004719	-0.000002335	0.000007739
C	-0.000001846	-0.000003644	-0.000009114
H	0.000002610	-0.000002031	-0.000005914
C	0.000003931	-0.000000573	0.000002620
H	0.000000953	0.000000733	0.000007342
C	-0.000001840	0.000002031	0.000001318
H	-0.000000450	-0.000001837	-0.000008474
H	0.000000488	0.000000406	0.000006749
C	0.000000486	-0.000006388	0.000000857
H	-0.000001331	-0.000003494	-0.000004653
H	-0.000000245	-0.000004278	-0.000007424
H	-0.000000487	-0.000008418	-0.000005058
Cl	-0.000000162	-0.000000456	-0.000001139

NBO Charges

C	1	-0.20432
H	2	0.10719
C	3	0.07343
H	4	0.08034
C	5	0.19610
O	6	-0.23607
C	7	-0.32199
H	8	0.09280
H	9	0.10167
H	10	0.10267
H	11	0.11624
C	12	-0.10333
H	13	0.10469
C	14	-0.04480
H	15	0.08413
C	16	0.18758
O	17	-0.28454
C	18	-0.03590
C	19	-0.08696
C	20	-0.08347
C	21	-0.12408
H	22	0.10454
C	23	-0.12144
H	24	0.11790
C	25	-0.01913
H	26	0.10521
H	27	0.10510
C	28	-0.28015
H	29	0.09915
H	30	0.09780
H	31	0.09414
Cl	32	-0.02450

TS2-trans-2

B3LYP SCF energy: -1153.143205 a.u.

B3LYP enthalpy: -1153.125512 a.u.

B3LYP free energy: -1153.189953 a.u.

Cartesian coordinate

C	-0.000012190	0.000004476	-0.000001479
H	0.000000035	0.000000417	-0.000002442
C	0.000022085	-0.000042756	0.000009998
H	-0.000006866	0.000004553	0.000003487
C	-0.000018401	0.000040863	-0.000041904
O	0.000010022	-0.000016506	0.000030776
C	0.000005279	-0.000000492	0.000010820
H	-0.000001150	0.000000628	0.000000781
H	0.000000589	0.000001573	0.000001465
H	-0.000003269	0.000001452	-0.000000558
H	-0.000000690	-0.000000553	-0.000001644
C	-0.000002266	-0.000015763	-0.000012009
H	0.000000123	-0.000000270	0.000000303
C	-0.000025865	0.000041792	-0.000009188
H	0.000001392	-0.000011034	-0.000006933
C	0.000027604	-0.000027030	0.000028076
O	-0.000002088	0.000006980	-0.000015585
C	-0.000015278	0.000001239	-0.000005132
C	0.000005549	0.000004625	-0.000001672
C	0.000007251	-0.000003724	0.000003888
C	-0.000002154	0.000005588	-0.000001453
H	0.000000323	0.000000359	-0.000002704
C	0.000002395	-0.000000170	0.000003109
H	0.000001434	-0.000001193	0.000000385
C	-0.000002108	-0.000000695	0.000003843
H	0.000001056	0.000001999	0.000000064
H	0.000002653	0.000000184	0.000003052
C	0.000001210	-0.000001218	0.000000446
H	-0.000002199	-0.000000903	-0.000000213
H	-0.000001127	-0.000000752	-0.000001398
H	-0.000001213	-0.000001862	-0.000001917
Cl	0.000007865	0.000008190	0.000005737

NBO Charges

C	1	-0.19929
H	2	0.09054
C	3	-0.05246
H	4	0.09801
C	5	0.25553
O	6	-0.27648
C	7	-0.32495
H	8	0.09863
H	9	0.10498
H	10	0.10258
H	11	0.10569
C	12	-0.12215
H	13	0.10710
C	14	-0.06384
H	15	0.09705
C	16	0.24569
O	17	-0.23573
C	18	-0.04773
C	19	-0.07078
C	20	-0.05753
C	21	-0.13190
H	22	0.10567
C	23	-0.13534
H	24	0.11447
C	25	0.00872
H	26	0.10525
H	27	0.10382
C	28	-0.28397
H	29	0.09246
H	30	0.09345
H	31	0.09985
Cl	32	-0.02736

TS2-cis-2

B3LYP SCF energy: -1153.135704a.u.

B3LYP enthalpy: -1153.117974 a.u.

B3LYP free energy: -1153.182448 a.u.

Cartesian coordinate

C	-0.000015572	0.000009086	-0.000005774
H	-0.000002917	0.000001656	-0.000002082
C	0.000030712	-0.000034924	0.000000059
H	0.000000135	0.000004298	0.000000126
C	-0.000065732	0.000025971	0.000051157
O	0.000035102	-0.000007250	-0.000015786
C	0.000010865	0.000002538	0.000007757
H	-0.000001241	0.000000873	0.000005525
H	-0.000003169	0.000001590	0.000006047
H	0.000001973	0.000000858	0.000006393

H	0.000000961	0.000000486	-0.000000768
C	-0.000000004	-0.000014711	-0.000005348
H	-0.000003012	-0.000000901	0.000000627
C	-0.000015799	0.000026554	-0.000044397
H	0.000001908	-0.000011075	0.000001951
C	0.000023207	-0.000005788	0.000045857
O	-0.000001185	-0.000010153	-0.000022440
C	-0.000015170	-0.000005809	-0.000007304
C	0.000005502	0.000004837	-0.000006538
C	0.000004338	-0.000006024	0.000003479
C	0.000000247	0.000007419	-0.000002473
H	0.000000224	0.000001837	-0.000000650
C	0.000003871	-0.000003818	0.000003408
H	0.000001531	-0.000005269	0.000000871
C	-0.000004693	0.000000747	0.000001265
H	0.000001106	0.000005122	-0.000001016
H	0.000001543	-0.000001529	0.000000629
C	-0.000000555	0.000004370	-0.000008184
H	-0.000001964	0.000000720	-0.000003097
H	-0.000001868	0.000001436	-0.000005565
H	-0.000000624	-0.000003068	-0.000004930
Cl	0.000010276	0.000009921	0.000001200

NBO Charges

C	1	-0.20074
H	2	0.10489
C	3	-0.04640
H	4	0.09251
C	5	0.25196
O	6	-0.26865
C	7	-0.32621
H	8	0.09380
H	9	0.10113
H	10	0.11388
H	11	0.08889
C	12	-0.12338
H	13	0.11518
C	14	-0.06846
H	15	0.08977
C	16	0.23902
O	17	-0.22079
C	18	-0.04562
C	19	-0.07236
C	20	-0.05539
C	21	-0.13421
H	22	0.10088
C	23	-0.13548
H	24	0.11512
C	25	0.01119
H	26	0.10366
H	27	0.10394
C	28	-0.28455
H	29	0.09319
H	30	0.08912
H	31	0.10242
Cl	32	-0.02828

TS1-3

B3LYP SCF energy: -808.026278 a.u.

B3LYP enthalpy: -808.006164 a.u.

B3LYP free energy: -808.077717 a.u.

Cartesian coordinate

C	0.000006378	0.000004150	-0.000000922
H	-0.000006347	-0.000002016	-0.000001849
C	-0.000000911	0.000002208	-0.000000567
H	0.000000347	-0.000001455	-0.000000225
C	0.000000442	0.000000723	0.000004572
O	-0.000000719	0.000003204	-0.000001565
C	0.000000304	0.000000845	-0.000000631
H	-0.000000495	-0.000000265	-0.000000046
H	-0.000000410	0.000002387	-0.000000706
H	0.000000410	0.000001683	0.000001855
H	-0.000000214	-0.000000556	-0.000000965
C	0.000005368	0.000006908	0.000000973
H	-0.000000999	-0.000003956	0.000002437
C	-0.000000361	-0.000001619	0.000002889
H	-0.000000005	-0.000000677	0.000001218
C	0.000000940	0.000000609	-0.000001252
O	-0.000001463	-0.000002121	0.000001041
C	-0.000000427	-0.000001423	-0.000000151
C	0.000001047	0.000001387	0.000000202
C	0.000000211	-0.000001787	-0.000001161
C	-0.000000143	0.000000611	0.000000014
H	0.000000855	0.000001017	0.000001046
C	0.000000182	-0.000001182	-0.000002002
H	-0.000000371	-0.000002362	-0.000002079
C	-0.000000727	-0.000001432	-0.000001302
H	0.000000080	0.000001473	0.000000597

H	-0.000000142	-0.000002475	-0.000002561
C	-0.000000930	-0.000001517	0.000002871
H	-0.000000674	-0.000001241	0.000000990
H	0.000001995	0.000001361	0.000002947
H	0.000000499	0.000000171	0.000004534
O	0.000000044	0.000001771	-0.000000455
C	-0.000001383	-0.000001717	-0.000002269
H	-0.000000842	-0.000000324	-0.000002359
H	-0.000001187	-0.000000582	-0.000003182
H	-0.000000354	-0.000001801	-0.000001935

NBO Charges

C	1	-0.12697
H	2	0.10361
C	3	-0.11447
H	4	0.08723
C	5	0.24718
O	6	-0.27870
C	7	-0.32576
H	8	0.09240
H	9	0.10297
H	10	0.10360
H	11	0.10660
C	12	-0.01706
H	13	0.10561
C	14	-0.11868
H	15	0.08681
C	16	0.24381
O	17	-0.27217
C	18	-0.06214
C	19	-0.07751
C	20	-0.06306
C	21	-0.13464
H	22	0.10161
C	23	-0.15705
H	24	0.11465
C	25	0.16502
H	26	0.10312
H	27	0.09972
C	28	-0.29744
H	29	0.10670
H	30	0.09986
H	31	0.09914
O	32	-0.27634
C	33	-0.10183
H	34	0.08953
H	35	0.08251
H	36	0.08213

IM-3

B3LYP SCF energy: -808.034258 a.u.

B3LYP enthalpy: -808.014314a.u.

B3LYP free energy: -808.084654 a.u.

Cartesian coordinate

C	-0.000018754	0.000012067	-0.000028821
H	0.000000643	0.000000055	0.000011795
C	0.000013176	-0.000020441	0.000024502
H	0.000003124	-0.000003731	-0.000003322
C	-0.000002416	0.000035787	-0.000099364
O	-0.000004886	-0.000011255	0.000046264
C	0.000000067	-0.000023024	0.000023507
H	-0.000003741	-0.000006810	-0.000002554
H	0.000007638	-0.000006761	0.000004425
H	-0.000004876	0.000003813	-0.000001927
H	0.000001326	-0.000006533	0.000007029
C	0.000014690	-0.000011737	0.000026855
H	-0.000003397	-0.000001042	-0.000009665
C	-0.000005277	0.000006996	0.000003045
H	0.000004001	-0.000003428	0.000008289
C	0.000000600	0.000013624	-0.000033587
O	0.000000713	-0.000011057	0.000007686
C	-0.000008054	0.000007100	0.000009293
C	0.000000901	-0.000003592	0.000003757
C	0.000012985	0.000007884	-0.000004883
C	-0.000003175	0.000000136	0.000001072
H	-0.000002010	0.000000521	0.000004030
C	-0.000000033	-0.000004157	0.000000660
H	-0.000001892	-0.000000461	-0.000003630
C	-0.000002318	-0.000000108	-0.000009555
H	0.000000871	0.000002251	0.000003615
H	0.000002538	0.000002103	-0.000003710
C	-0.000003940	0.000004859	-0.000002250
H	0.000004451	-0.000000219	0.000002362
H	0.000001221	0.000003535	0.000008398
H	-0.000002281	0.000004803	-0.000001223
O	0.000007726	0.000005400	0.000017166
C	-0.000005221	0.000005072	-0.000009682
H	-0.000005104	0.000003368	0.000000553

H	-0.000000630	-0.000003244	0.000004559
H	0.000001335	-0.000001770	-0.000004689

NBO Charges

C	1	-0.19989
H	2	0.10651
C	3	0.04560
H	4	0.08051
C	5	0.19663
O	6	-0.24944
C	7	-0.32151
H	8	0.09214
H	9	0.10058
H	10	0.10167
H	11	0.11350
C	12	-0.10706
H	13	0.10490
C	14	-0.02033
H	15	0.08313
C	16	0.19070
O	17	-0.27882
C	18	-0.05088
C	19	-0.08452
C	20	-0.08034
C	21	-0.13064
H	22	0.10274
C	23	-0.15172
H	24	0.11519
C	25	0.15349
H	26	0.10299
H	27	0.09955
C	28	-0.27956
H	29	0.09969
H	30	0.09749
H	31	0.09348
O	32	-0.27789
C	33	-0.10180
H	34	0.08954
H	35	0.08227
H	36	0.08210

TS2-trans-3

B3LYP SCF energy: -808.027084 a.u.

B3LYP enthalpy: -808.007961a.u.

B3LYP free energy: -808.075552 a.u.

Cartesian coordinate

C	-0.000003175	0.000000497	-0.000002226
H	-0.000002093	0.000000356	-0.000001489
C	0.000005189	0.000010249	-0.000003145
H	-0.000001745	0.000001338	0.000000212
C	-0.000006047	-0.000010756	-0.000012286
O	0.000002369	0.000003916	0.000008126
C	-0.000004710	0.000005858	-0.000000053
H	0.000004125	0.000009663	0.000010991
H	0.000007433	-0.000003376	-0.000004805
H	-0.000008471	-0.000006995	0.000006097
H	0.000000357	-0.000000761	-0.000002982
C	0.000000510	0.000001851	-0.000009423
H	-0.000000282	0.000000183	-0.000001490
C	-0.000004876	-0.000009411	-0.000000575
H	-0.000000532	0.000000881	-0.000000704
C	0.000000682	0.000012438	0.000006321
O	-0.000000148	-0.000004018	-0.000010546
C	-0.000001639	0.000000167	-0.000002224
C	0.000001181	-0.000003162	0.000000736
C	0.000000134	0.000002293	-0.000000183
C	-0.000000422	-0.000002081	0.000002520
H	0.000000945	-0.000000982	0.000001145
C	-0.000001239	0.000001253	0.000002064
H	-0.000000426	0.000001423	-0.000000699
C	0.000002171	-0.000000293	0.000004774
H	0.000000335	-0.000001042	0.000002073
H	0.000000430	0.000001009	0.000000583
C	0.000001718	-0.000001642	-0.000005960
H	0.000000355	-0.000000375	-0.000003402
H	0.000001207	-0.000001313	-0.000002792
H	0.000001362	-0.000000081	-0.000002975
O	0.000000829	-0.000001187	0.000003975
C	0.000001839	-0.000000318	0.000009621
H	0.000001212	-0.000001449	0.000003198
H	0.000001576	-0.000002228	0.000001535
H	-0.000000155	-0.000001906	0.000003986

NBO Charges

C	1	-0.19688
H	2	0.08996
C	3	-0.05220
H	4	0.10451
C	5	0.38765

O	6	-0.30683
H	7	0.10314
C	8	-0.12321
H	9	0.10723
C	10	-0.05696
H	11	0.09616
C	12	0.24429
O	13	-0.23489
C	14	-0.04663
C	15	-0.07985
C	16	-0.06806
C	17	-0.11964
H	18	0.10274
C	19	-0.12286
H	20	0.11210
C	21	-0.08938
H	22	0.09506
H	23	0.09400
H	24	0.09255
C	25	-0.28443
H	26	0.09183
H	27	0.09265
H	28	0.10059
O	29	-0.28179
C	30	-0.10517
H	31	0.08314
H	32	0.08629
H	33	0.08486

TS2-cis-3

B3LYP SCF energy: -808.019085 a.u.

B3LYP enthalpy: -807.999964 a.u.

B3LYP free energy: -808.067312 a.u.

Cartesian coordinate

C	-0.000000762	0.000003378	-0.000006521
H	0.000000509	-0.000000534	-0.000002102
C	0.000007325	-0.000007961	0.000001791
H	-0.000001074	0.000004884	0.000001794
C	-0.000003581	-0.000000852	0.000012228
O	-0.000000561	-0.000010806	0.000007480
C	-0.000005798	-0.000005340	0.000012578
H	0.000000578	0.000001597	0.000003731
H	-0.000003799	0.000003174	0.000010818
H	0.000002477	-0.000004377	0.000009882
H	0.000001212	0.000003101	-0.000003534
C	0.000001260	-0.000004884	-0.000008329
H	0.000000257	-0.000003523	-0.000003409
C	-0.000006654	0.000010616	-0.000009469
H	0.000001523	0.000001287	-0.000002726
C	0.000006501	-0.000004703	-0.000004050
O	-0.000002570	-0.000014233	-0.000004978
C	-0.000004496	-0.000001846	-0.000001392
C	0.000001555	0.000007593	-0.000000130
C	0.000001223	-0.000005883	0.000000107
C	0.000000262	0.000009256	0.000002724
H	0.000000123	0.000004406	0.000000028
C	-0.000001345	-0.000002534	0.000001754
H	-0.000000469	-0.000005188	-0.000001110
C	0.000000761	0.000001950	0.000002863
H	0.000000485	0.000006498	0.000001833
H	-0.000000266	-0.000003073	0.000000819
C	0.000002322	-0.000000066	-0.000018476
H	0.000001531	-0.000000782	-0.000008744
H	0.000001622	0.000002065	-0.000008268
H	0.000000988	-0.000001599	-0.000008409
O	0.000000822	0.000013814	0.000007554
C	-0.000000765	0.000001527	0.000004084
H	-0.000000680	0.000002594	0.000003590
H	-0.000000072	0.000000347	0.000004871
H	-0.000000442	0.000000099	0.000001117

NBO Charges

C	1	-0.19821
H	2	0.10457
C	3	-0.06598
H	4	0.09349
C	5	0.26276
O	6	-0.27130
C	7	-0.32753
H	8	0.09405
H	9	0.10045
H	10	0.11531
H	11	0.08821
C	12	-0.12177
H	13	0.11450
C	14	-0.07101
H	15	0.08867
C	16	0.25232

O	17	-0.22997
C	18	-0.06416
C	19	-0.06974
C	20	-0.04591
C	21	-0.14385
H	22	0.09856
C	23	-0.16666
H	24	0.11218
C	25	0.17945
H	26	0.10123
H	27	0.09825
C	28	-0.28430
H	29	0.09249
H	30	0.08892
H	31	0.10217
O	32	-0.27638
C	33	-0.10109
H	34	0.08770
H	35	0.08159
H	36	0.08100

TS1-4

B3LYP SCF energy: -898.082278 a.u.

B3LYP enthalpy: -898.062357 a.u.

B3LYP free energy: -898.133710 a.u.

Cartesian coordinate

C	0.000009496	0.000008518	0.000000068
H	0.000002541	0.000001496	0.000001400
C	-0.000005901	0.000002808	0.000001840
H	-0.000000943	-0.000000840	0.000000204
C	0.000001095	-0.000003363	0.000003537
O	-0.000000144	-0.000001719	-0.000002904
C	0.000000045	0.000000297	-0.000000488
H	-0.000000313	0.000002126	0.000000100
H	-0.000000111	0.000000976	-0.000000502
H	-0.000000089	0.000001166	-0.000000843
H	-0.000000486	0.000002638	0.000003528
C	-0.000010327	-0.000009866	0.000001499
H	0.000000093	0.000003441	-0.000003381
C	0.000006006	-0.000005144	-0.000003294
H	0.000001582	0.000002251	-0.000002303
C	0.000000625	0.000005289	-0.000006876
O	-0.000002735	0.000000132	0.000006097
C	-0.000000506	0.000000147	0.000001502
C	0.000000043	-0.000002091	0.000000670
C	0.000000287	-0.000000139	0.000002146
C	-0.000000631	-0.000002361	-0.000000100
H	-0.000001414	-0.000001088	-0.000000214
C	-0.000000567	0.000000241	0.000001297
H	0.000000017	0.000002980	0.000002034
C	-0.000000185	-0.000003230	0.000000524
H	0.000000435	-0.000003102	-0.000000150
H	-0.000000174	0.000000856	0.000002855
C	-0.000000499	0.000000566	-0.000003429
H	0.000000557	0.000001016	-0.000003211
H	-0.000000834	-0.000001450	-0.000002789
H	-0.000000615	0.000001149	-0.000004823
N	0.000003194	0.000007747	0.000008095
O	-0.000000493	-0.000002992	-0.000001501
O	0.000000949	-0.000008454	-0.000000588

NBO Charges

C	1	-0.16935
H	2	0.10841
C	3	-0.06252
H	4	0.08818
C	5	0.23456
O	6	-0.26843
C	7	-0.32563
H	8	0.09411
H	9	0.10498
H	10	0.10523
H	11	0.11369
C	12	-0.03593
H	13	0.10931
C	14	-0.12732
H	15	0.09036
C	16	0.22245
O	17	-0.25676
C	18	-0.02333
C	19	-0.09077
C	20	-0.08027
C	21	-0.09130
H	22	0.10255
C	23	-0.09791
H	24	0.11749
C	25	0.04508
H	26	0.11517

H	27	0.11523
C	28	-0.29408
H	29	0.10401
H	30	0.10359
H	31	0.10073
N	32	0.24613
O	33	-0.19718
O	34	-0.20046

TS2-trans-4

B3LYP SCF energy: -898.086536 a.u.

B3LYP enthalpy: -898.067370 a.u.

B3LYP free energy: -898.136014 a.u.

Cartesian coordinate

C	-0.000003639	-0.000000050	-0.000001421
H	0.000001970	-0.000001202	0.000001258
C	-0.000003093	-0.000005815	0.000000405
H	0.000000581	-0.000001860	-0.000004236
C	0.000005138	0.000006362	-0.000006403
O	0.000000183	-0.000003079	0.000002129
C	-0.000003248	0.000000748	-0.000003307
H	0.000000790	0.000001690	-0.000001551
H	0.000000239	0.000002318	0.000000452
H	-0.000000275	0.000000523	0.000000759
H	-0.000000472	-0.000001251	0.000001569
C	-0.000002421	-0.000000350	0.000004034
H	0.000000669	-0.000001838	0.000000365
C	0.000000615	0.000009516	0.000009395
H	0.000000598	0.000000296	-0.000001175
C	0.000015870	-0.000010366	-0.000009802
O	0.000001174	0.000003662	0.000003580
C	-0.000008323	0.000000561	0.000005008
C	0.000000921	0.000001070	-0.000001166
C	0.000001184	-0.000002295	-0.000003709
C	-0.000004812	0.000001308	0.000001974
H	-0.000002042	0.000000745	0.000000550
C	-0.000003130	-0.000002368	0.000005945
H	0.000002131	0.000000413	0.000000120
C	0.000002987	-0.000001138	-0.000012460
H	-0.000001610	-0.000000060	-0.000000069
H	-0.000001003	0.000001622	-0.000001010
C	0.000001746	-0.000000313	0.000002543
H	0.000001466	-0.000001697	0.000001679
H	0.000000339	-0.000001657	0.000002010
H	0.000000994	-0.000001332	0.000001909
N	0.000002500	0.000007063	0.000014460
O	-0.000005381	0.000000460	-0.000007163
O	-0.000002644	-0.000001688	-0.000006673

NBO Charges

C	1	-0.21278
H	2	0.09556
C	3	0.06516
H	4	0.09176
C	5	0.21226
O	6	-0.24343
C	7	-0.32202
H	8	0.09697
H	9	0.10548
H	10	0.10246
H	11	0.10705
C	12	-0.12597
H	13	0.10618
C	14	-0.06871
H	15	0.09539
C	16	0.20100
O	17	-0.25659
C	18	-0.01632
C	19	-0.09161
C	20	-0.08559
C	21	-0.09378
H	22	0.10830
C	23	-0.09834
H	24	0.11792
C	25	0.03666
H	26	0.11581
H	27	0.11478
C	28	-0.28374
H	29	0.09332
H	30	0.09347
H	31	0.10110
N	32	0.24324
O	33	-0.20245
O	34	-0.20251

TS2-cis-4

B3LYP SCF energy: -898.080567 a.u.

B3LYP enthalpy: -898.061424 a.u.

B3LYP free energy: -898.129784 a.u.

Cartesian coordinate

C	0.000168431	-0.000235887	-0.000006185
H	-0.000146787	0.000026097	0.000000122
C	0.000011872	0.000189789	0.000008212
H	-0.000002251	0.000000216	-0.000000818
C	-0.000027741	0.000010637	-0.000036299
O	0.000007814	-0.000004766	0.000025259
C	0.000003670	0.000004363	0.000005604
H	0.000001031	0.000000886	0.000000532
H	0.000004971	0.000000692	-0.000000332
H	-0.000003832	0.000000216	0.000003696
H	-0.000004011	-0.000001551	0.000005735
C	-0.000008020	0.000013784	0.000005049
H	0.000008470	0.000001967	-0.000008795
C	0.000007562	-0.000023002	-0.000007080
H	-0.000003729	-0.000001036	-0.000001467
C	-0.000027859	0.000030186	0.000014729
O	0.000007786	-0.000010442	0.000002425
C	0.000012242	-0.000000358	-0.000007982
C	-0.000009829	-0.000001793	0.000004002
C	-0.000002674	0.000002557	0.000005276
C	0.000006816	-0.000007445	-0.000006037
H	-0.000000312	-0.000000735	0.000003386
C	0.000006296	0.000000972	-0.000002289
H	0.000000574	0.000000920	0.000000209
C	-0.000005120	0.000005714	0.000028713
H	0.000002031	-0.000000017	0.000001524
H	0.000000143	0.000002365	0.000002785
C	-0.000001467	0.000000053	-0.000008410
H	-0.000000882	-0.000002243	0.000000091
H	-0.000000474	0.000000884	0.000001361
H	-0.000000964	0.000000303	-0.000001319
N	-0.000046071	0.000001447	-0.000023912
O	0.000021862	-0.000006797	-0.000009154
O	0.000020451	0.000002024	0.000001371

NBO Charges

C	1	-0.21286
H	2	0.10739
C	3	0.06180
H	26	0.11466
H	27	0.11490
C	28	-0.28513
H	29	0.09432
H	30	0.08970
H	31	0.10371
N	32	0.24453
O	33	-0.20033
O	34	-0.20341

TS1-5

B3LYP SCF energy: -748.860390 a.u.

B3LYP enthalpy: -748.841377 a.u.

B3LYP free energy: -748.910117 a.u.

Cartesian coordinate

C	0.000001631	-0.000002305	0.000001852
H	0.000002252	-0.000002399	0.000002708
C	0.000003820	-0.000000157	0.000000640
H	0.000002191	0.000002774	0.000003555
C	0.000002862	-0.000001631	0.000005277
O	-0.000000705	-0.000005911	0.000002656
C	0.000002906	-0.000003069	0.000002921
H	0.000001620	-0.000001086	0.000004515
H	0.000002195	-0.000004356	0.000006496
H	0.000000303	-0.000003930	0.000002657
H	0.000000838	-0.000002944	0.000001863
C	-0.000001029	0.000002775	0.000001407
H	-0.000000380	0.000002393	-0.000001119
C	-0.000001741	-0.000000933	-0.000000582
H	-0.000001691	-0.000003420	-0.000002396
C	0.000000885	0.000002545	-0.000001156
O	0.000001564	0.000004789	-0.000000736
C	0.000000066	0.000002301	-0.000001209
C	-0.000001223	0.000000127	-0.000002246
C	0.000000483	0.000004888	-0.000000563
C	-0.000001605	-0.000000496	-0.000002586
H	-0.000002726	-0.000001628	-0.000002309
C	0.000001130	0.000004803	-0.000001057
H	0.000001864	0.000005775	-0.000000072
C	-0.000001185	0.000002070	-0.000000289
H	-0.000002260	-0.000002028	-0.000002834
H	0.000001441	0.000006180	-0.000000295
C	-0.000001377	-0.000000175	-0.000000911
H	-0.000004995	-0.000005818	-0.000001719
H	-0.000002627	-0.000004374	-0.000002122
H	-0.000002642	-0.000001790	-0.000004319
N	-0.000000665	0.000002022	-0.000003666

H	-0.000001047	0.000001710	-0.000002485
H	-0.000000153	0.000003297	-0.000001877

NBO Charges

C	1	-0.12417
H	2	0.10329
C	3	-0.11702
H	4	0.08712
C	5	0.24759
O	6	-0.27965
C	7	-0.32571
H	8	0.09229
H	9	0.10279
H	10	0.10341
H	11	0.10606
C	12	-0.01994
H	13	0.10571
C	14	-0.11519
H	15	0.08604
C	16	0.24396
O	17	-0.27405
C	18	-0.06608
C	19	-0.07495
C	20	-0.06335
C	21	-0.14015
H	22	0.10061
C	23	-0.13772
H	24	0.11457
C	25	0.08858
H	26	0.09458
H	27	0.09429
C	28	-0.29718
H	29	0.10659
H	30	0.09970
H	31	0.09872
N	32	-0.40086
H	33	0.18004
H	34	0.18009

TS2-trans-5

B3LYP SCF energy: -748.860914 a.u.

B3LYP enthalpy: -748.842904 a.u.

B3LYP free energy: -748.907272 a.u.

Cartesian coordinate

C	-0.000013028	-0.000055252	-0.000054128
H	-0.000007807	0.000075292	-0.000001051
C	0.000044312	0.000025479	0.000036658
H	-0.000011970	-0.000017987	-0.000001835
C	-0.000030820	-0.000033904	-0.000041329
O	-0.000015023	0.000009740	-0.000024945
C	0.000006159	0.000007813	0.000019258
H	-0.000000176	-0.000003533	-0.000011165
H	0.000001828	0.000013273	0.000005137
H	0.000002055	-0.000010492	0.000011099
H	0.000014922	0.000022455	0.000015236
C	0.000007898	-0.000034624	0.000056766
H	-0.000002194	-0.000001235	0.000003562
C	0.000024402	-0.000039211	0.000003978
H	0.000006176	0.000014857	0.000008676
C	-0.000059775	0.000002275	0.000008756
O	0.000010624	0.000000020	-0.000005063
C	-0.000013580	-0.000028601	-0.000038568
C	0.000000292	-0.000020079	0.000005641
C	0.000126046	0.000050498	0.000083761
C	-0.000008334	0.000013910	0.000002473
H	-0.000000660	0.000003104	-0.000009751
C	-0.000056365	-0.000022474	-0.000041387
H	-0.000011218	0.000002328	0.000006486
C	-0.000032824	0.000015727	0.000003301
H	0.000010370	0.000002360	0.000005651
H	-0.000027095	0.000000674	-0.000022972
C	-0.000000394	0.000013909	-0.000024138
H	-0.000000218	-0.000009579	0.000000577
H	-0.000005727	0.000009263	0.000010712
H	0.000005746	0.000006352	-0.000011318
N	0.000041405	-0.000007020	-0.000012184
H	-0.000001664	-0.000003474	0.000006980
H	-0.000003362	-0.000001867	0.000005125

NBO Charges

C	1	-0.19519
H	2	0.08936
C	3	-0.07865
H	4	0.09940
C	5	0.27105
O	6	-0.28004
C	7	-0.32604
H	8	0.09854
H	9	0.10504

H	10	0.10209
H	11	0.10505
C	12	-0.12048
H	13	0.10739
C	14	-0.06963
H	15	0.09692
C	16	0.26183
O	17	-0.24754
C	18	-0.07022
C	19	-0.06457
C	20	-0.05041
C	21	-0.14669
H	22	0.10261
C	23	-0.14722
H	24	0.11132
C	25	0.10213
H	26	0.09428
H	27	0.09274
C	28	-0.28367
H	29	0.09162
H	30	0.09322
H	31	0.09962
N	32	-0.40088
H	33	0.17873
H	34	0.17829

TS2-cis-5

B3LYP SCF energy: -748.852739 a.u.

B3LYP enthalpy: -748.834715 a.u.

B3LYP free energy: -748.898979a.u.

Cartesian coordinate

C	0.000365753	0.000334678	0.000025959
H	-0.000348110	-0.000148910	0.000000110
C	-0.000013484	-0.000198270	-0.000005285
H	0.000001027	-0.000008583	-0.000007922
C	0.000010856	0.000019000	0.000001735
O	0.000002368	0.000010060	0.000003489
C	-0.000004087	-0.000016058	-0.000003507
H	0.000002045	0.000004963	0.000005043
H	0.000000057	-0.000008518	0.000000217
H	-0.000002801	0.000002634	-0.000006306
H	-0.000001728	-0.000000784	-0.000001270
C	0.000018965	0.000008199	-0.000005020
H	-0.000015798	-0.000000099	0.000005560
C	-0.000030024	0.000005197	-0.000000477
H	-0.000006034	-0.000014884	-0.000008858
C	-0.000071438	-0.000005304	-0.000039626
O	-0.000011772	-0.000003544	-0.000000820
C	0.000209441	0.000034237	0.000124172
C	-0.000034176	-0.000002867	-0.000018266
C	-0.000165907	-0.000015987	-0.000097515
C	-0.000016152	0.000007874	-0.000004765
H	0.000035033	0.000003003	0.000017649
C	0.000058011	-0.000000401	0.000026689
H	0.000037926	0.000003224	0.000013280
C	0.000000164	-0.000011222	0.000012325
H	-0.000015963	-0.000002237	-0.000009715
H	0.000023777	0.000000083	0.000014538
C	0.000000704	0.000006283	-0.000011752
H	-0.000000779	0.000001168	0.000000103
H	0.000000299	-0.000000200	-0.000000588
H	-0.000000890	-0.000000762	0.000000118
N	-0.000039738	-0.000002709	-0.000051683
H	0.000008293	-0.000002808	0.000011991
H	0.000004161	0.000003546	0.000010394

NBO Charges

C	1	-0.19762
H	2	0.10460
C	3	-0.07149
H	4	0.09352
C	5	0.26526
O	6	-0.27213
C	7	-0.32779
H	8	0.09377
H	9	0.10025
H	10	0.11561
H	11	0.08800
C	12	-0.12172
H	13	0.11442
C	14	-0.07011
H	15	0.08865
C	16	0.25410
O	17	-0.23212
C	18	-0.06873
C	19	-0.06542
C	20	-0.04770
C	21	-0.14954

H	22	0.09763
C	23	-0.14809
H	24	0.11185
C	25	0.10490
H	26	0.09269
H	27	0.09282
C	28	-0.28422
H	29	0.09233
H	30	0.08883
H	31	0.10227
N	32	-0.40108
H	33	0.17804
H	34	0.17820

TS1-6

B3LYP SCF energy: -732.797621 a.u.

B3LYP enthalpy: -732.778992 a.u.

B3LYP free energy: -732.846450 a.u.

Cartesian coordinate

C	-0.000003461	0.000000154	-0.000005905
H	-0.000000631	0.000001168	0.000000876
C	0.000001628	0.000001951	0.000001531
H	0.000000053	0.000001087	0.000002331
C	0.000000617	-0.000001897	-0.000005116
O	-0.000001317	0.000000874	-0.000001608
C	-0.000000359	0.000001152	-0.000001424
H	0.000000214	0.000001241	-0.000001243
H	-0.000000736	0.000000171	-0.000003396
H	0.000000335	0.000001875	-0.000003595
H	-0.000000574	0.000001761	0.000002276
C	0.000002866	-0.000005694	-0.000009156
H	-0.000000570	0.000001787	0.000009559
C	-0.000002579	0.000000245	-0.000001146
H	0.000000324	0.000000055	0.000000293
C	0.000002194	-0.000000060	0.000000833
O	0.000000308	-0.000000408	0.000002893
C	-0.000000288	-0.000000795	0.000002570
C	0.000000464	-0.000001505	0.000001303
C	-0.000000098	-0.000001305	0.000002319
C	-0.000000809	-0.000001331	0.000000626
H	-0.000000153	-0.000000242	0.000000172
C	-0.000000015	-0.000001686	0.000002582
H	0.000000182	-0.000001635	0.000003835
C	-0.000000792	-0.000002494	0.000003474
H	-0.000000666	-0.000001456	0.000001002
H	-0.000000219	-0.000002784	0.000004362
H	-0.000000691	-0.000002479	0.000002994
C	0.000002109	0.000005844	0.000001139
H	0.000000201	0.000001280	-0.000003735
H	0.000001603	0.000001569	-0.000000939
C	-0.000000065	-0.000001397	-0.000002836
H	-0.000000721	0.000001153	-0.000002249
H	0.000000859	0.000001074	-0.000001856
H	0.000000788	0.000002724	-0.000002767

NBO Charges

C	1	-0.13238
H	2	0.10366
C	3	-0.11074
H	4	0.08748
C	5	0.24745
O	6	-0.28159
C	7	-0.32529
H	8	0.09265
H	9	0.10315
H	10	0.10382
H	11	0.10805
C	12	-0.01770
H	13	0.10809
C	14	-0.11651
H	15	0.08872
C	16	0.24064
O	17	-0.26525
C	18	-0.04693
C	19	-0.08687
C	20	-0.07601
C	21	-0.11514
H	22	0.10032
C	23	-0.11566
H	24	0.11449
C	25	-0.09764
H	26	0.09575
H	27	0.09565
H	28	0.09450
C	29	-0.20273
H	30	0.10292
H	31	0.09786
C	32	-0.29012

H	33	0.11379
H	34	0.08923
H	35	0.09233

TS2-trans-6

B3LYP SCF energy: -732.800716 a.u.

B3LYP enthalpy: -732.782823 a.u.

B3LYP free energy: -732.847781 a.u.

Cartesian coordinate

C	0.000002633	0.000001987	0.000001603
H	0.000000885	0.000001154	0.000001424
C	-0.000000658	0.000006988	-0.000001397
H	0.000001855	-0.000000865	0.000000428
C	0.000005930	-0.000004608	0.000012631
O	0.000000782	0.000004341	-0.000003691
C	0.000005438	0.000003967	0.000001960
H	-0.000000928	0.000002361	-0.000003983
H	-0.000002613	-0.000003133	0.000005250
H	0.000005556	-0.000007317	-0.000002105
H	0.000000231	0.000001633	0.000001293
C	-0.000000056	0.000004382	0.000001296
H	-0.000000012	0.000000665	-0.000000354
C	0.000002389	-0.000005051	0.000002698
H	-0.000000157	0.000001639	0.000000749
C	-0.000003403	0.000006367	-0.000007811
O	-0.000001539	-0.000004223	0.000002975
C	0.000000342	-0.000003093	0.000000219
C	-0.000000899	-0.000001749	-0.000000154
C	-0.000002222	-0.000003539	-0.000002546
C	-0.000000071	-0.000003145	-0.000000946
H	-0.000000094	0.000000103	0.000000606
C	-0.000001402	-0.000004712	-0.000003128
H	-0.000001097	-0.000001568	-0.000001242
C	-0.000001899	-0.000004795	-0.000001930
H	-0.000000440	-0.000000989	0.000000090
H	-0.000001385	-0.000002929	-0.000001953
H	-0.000001216	-0.000002659	-0.000001270
C	-0.000002091	0.000003513	-0.000000568
H	-0.000000360	0.000002109	0.000000273
H	-0.000000682	0.000001836	-0.000000324
C	-0.000001799	0.000004861	0.000000179
H	-0.000000048	0.000002081	0.000000420
H	-0.000000619	0.000002655	-0.000000199
H	-0.000000352	0.000001732	-0.000000493

NBO Charges

C	1	-0.20032
H	2	0.09055
C	3	-0.06067
H	4	0.09852
C	5	0.26006
O	6	-0.27770
C	7	-0.32510
H	8	0.09921
H	9	0.10479
H	10	0.10193
H	11	0.10577
C	12	-0.12072
H	13	0.10800
C	14	-0.06276
H	15	0.09739
C	16	0.24976
O	17	-0.23803
C	18	-0.04823
C	19	-0.07932
C	20	-0.06720
C	21	-0.11950
H	22	0.10278
C	23	-0.12299
H	24	0.11155
C	25	-0.08680
H	26	0.09536
H	27	0.09387
H	28	0.09243
C	29	-0.18785
H	30	0.09131
H	31	0.09790
C	32	-0.28578
H	33	0.09542
H	34	0.09186
H	35	0.09452

TS2-cis-6

B3LYP SCF energy: -732.792932 a.u.

B3LYP enthalpy: -732.775054 a.u.

B3LYP free energy: -732.839747 a.u.

Cartesian coordinate

C	-0.000006949	0.000000254	0.000000601
H	-0.000000713	-0.000001257	0.000000974
C	0.000005129	-0.000016518	0.000002986
H	-0.000001650	0.000002463	0.000000789
C	-0.000001371	0.000002609	0.000004486
O	-0.000002500	-0.000003809	0.000004872
C	-0.000005592	-0.000002069	-0.000000220
H	-0.000001892	0.000000170	0.000001687
H	-0.000003131	0.000002212	0.000002667
H	-0.000001361	0.000000491	0.000004520
H	0.000000229	0.000000465	0.000001264
C	0.000000131	-0.000004796	0.000002598
H	0.000001264	-0.000002142	0.000000076
C	-0.000005749	0.000014659	-0.000006830
H	0.000001991	-0.000002315	-0.000001492
C	0.000021243	-0.000004073	-0.000004216
O	-0.000001479	-0.000001988	0.000004669
C	-0.000009847	0.000001185	0.000001326
C	0.000000903	0.000002645	-0.000003162
C	0.000004330	0.000001911	-0.000001441
C	-0.000002469	0.000004044	-0.000001874
H	-0.000001453	0.000000349	-0.000001161
C	-0.000001319	0.000003406	-0.000002429
H	0.000001176	0.000000762	-0.000001255
C	0.000001610	0.000004870	-0.000004008
H	-0.000000723	0.000001468	-0.000001136
H	0.000000662	0.000002036	-0.000001528
H	-0.000000008	0.000002332	-0.000001557
C	0.000002672	-0.000001503	-0.000000817
H	0.000000562	-0.000000264	-0.000000759
H	0.000001283	-0.000000817	-0.000000900
C	0.000002390	-0.000003104	0.000000492
H	0.000000301	-0.000000540	0.000000317
H	0.000001029	-0.000001547	-0.000000311
H	0.000001302	-0.000001587	0.000000771

NBO Charges

C	1	-0.20152
H	2	0.10527
C	3	-0.05671
H	4	0.09300
C	5	0.25674
O	6	-0.27065
C	7	-0.32654
H	8	0.09381
H	9	0.10054
H	10	0.11443
H	11	0.08884
C	12	-0.12193
H	13	0.11547
C	14	-0.06657
H	15	0.09059
C	16	0.24358
O	17	-0.22245
C	18	-0.04600
C	19	-0.08070
C	20	-0.06494
C	21	-0.12207
H	22	0.09811
C	23	-0.12309
H	24	0.11190
C	25	-0.08463
H	26	0.09370
H	27	0.09392
H	28	0.09205
C	29	-0.18816
H	30	0.08673
H	31	0.10063
C	32	-0.28568
H	33	0.09436
H	34	0.09087
H	35	0.09709

TS1-7

B3LYP SCF energy: -811.384583 a.u.

B3LYP enthalpy: -811.363325 a.u.

B3LYP free energy: -811.435734 a.u.

Cartesian coordinate

C	-0.000004577	-0.000001577	-0.000003383
H	0.000002368	0.000000165	-0.000001689
C	0.000000947	-0.000000593	0.000001468
H	-0.000000463	-0.000000881	0.000000950
C	0.000001992	-0.000000040	-0.000002316
O	0.000000743	0.000002873	-0.000003623
C	0.000000124	0.000001834	-0.000002385
H	0.000000089	0.000000857	-0.000000078
H	0.000001211	0.000001412	-0.000002624
H	-0.000000071	0.000003305	-0.000001478

H	0.000001235	-0.000001534	-0.000000220
O	0.000003722	0.000001781	0.000001190
H	-0.000001551	-0.000000173	0.000002281
C	-0.000001857	-0.000001575	-0.000000666
H	0.000000956	0.000001030	-0.000000814
C	0.000000007	-0.000003185	0.000001821
O	-0.000000474	-0.000003156	0.000002544
C	0.000000743	-0.000003501	0.000000670
C	0.000001320	-0.000002720	-0.000000893
C	0.000000460	-0.000005506	0.000001935
C	0.000002012	-0.000003910	-0.000001092
H	0.000001548	-0.000001498	-0.000001835
C	0.000000965	-0.000006631	0.000001695
H	0.000000000	-0.000006023	0.000003385
C	0.000001995	-0.000005764	0.000000032
H	0.000002542	-0.000003358	-0.000002491
H	0.000001017	-0.000007934	0.000002571
H	0.000002313	-0.000006614	-0.000000278
C	-0.000001280	0.000003580	0.000000987
C	-0.000001673	0.000002928	0.000001221
H	-0.000002515	0.000005409	0.000000829
H	-0.000002676	0.000003924	0.000002393
H	-0.000002324	0.000003642	0.000000905
C	0.000000709	0.000004092	-0.000001375
H	0.000000327	0.000003609	-0.000002142
H	0.000000838	0.000003576	-0.000002479
H	-0.000001089	0.000005571	-0.000002208
C	-0.000002791	0.000003759	0.000001871
H	-0.000002897	0.000003351	0.000003444
H	-0.000002856	0.000006061	0.000001139
H	-0.000001091	0.000003414	0.000000736

TS2-trans-7

B3LYP SCF energy: -811.392034 a.u.

B3LYP enthalpy: -811.371535 a.u.

B3LYP free energy: -811.441382 a.u.

Cartesian coordinate

C	0.000000274	0.000004872	-0.000002634
H	0.000001081	0.000007315	-0.000002500
C	0.000000029	0.000004464	-0.000003319
H	0.000000872	0.000005961	-0.000002055
C	-0.000001227	0.000003414	-0.000006418
O	-0.000002374	0.000002449	-0.000008531
C	-0.000001518	0.000003832	-0.000007259
H	-0.000000620	0.000004332	-0.000005107
H	-0.000002426	0.000001533	-0.000008133
H	-0.000001614	0.000005802	-0.000009112
H	-0.000000609	0.000003607	-0.000004390
C	0.000000805	0.000002540	0.000000924
H	0.000002030	0.000004336	0.000002470
C	0.000000229	0.000000719	0.000000067
H	-0.000000895	-0.000001294	-0.000001551
C	0.000000722	-0.000000114	0.000002510
O	0.000002144	0.000001868	0.000004781
C	0.000000005	-0.000002541	0.000001884
C	-0.000001460	-0.000004375	-0.000000793
C	0.000000647	-0.000003341	0.000004410
C	-0.000002183	-0.000006788	-0.000001108
H	-0.000002002	-0.000003829	-0.000002849
C	-0.000000082	-0.000005780	0.000004164
H	0.000001750	-0.000001937	0.000006526
C	-0.000001516	-0.000007532	0.000001404
H	-0.000003290	-0.000008102	-0.000003284
H	0.000000455	-0.000006303	0.000006121
H	-0.000002080	-0.000009422	0.000001188
C	0.000001048	0.000000921	0.000002129
C	0.000001959	0.000003319	0.000001596
H	0.000001240	0.000004972	-0.000000159
H	0.000001745	0.000002384	0.000003026
H	0.000003048	0.000005308	0.000003637
C	-0.000000683	-0.000001617	-0.000000149
H	-0.000000431	-0.000002747	0.000000629
H	-0.000001029	-0.000000532	-0.000002741
H	-0.000001061	-0.000003620	-0.000000407
C	0.000001460	-0.000000379	0.000005705
H	0.000001242	-0.000002633	0.000005461
H	0.000002741	0.000000865	0.000007275
H	0.000001575	-0.000001928	0.000006594

TS2-cis-7

B3LYP SCF energy: -811.382862 a.u.

B3LYP enthalpy: -811.362663 a.u.

B3LYP free energy: -811.431362 a.u.

Cartesian coordinate

C	0.000002116	-0.000010232	0.000007597
H	-0.000005828	-0.000000913	0.000000162

C	-0.000018007	0.000005909	-0.000012689
H	-0.000003348	-0.000004470	-0.000005763
C	0.000014310	-0.000035823	0.000006602
O	0.000002899	0.000014927	-0.000006693
C	-0.000003704	0.000013635	0.000005735
H	-0.000001344	-0.000000129	0.000007001
C	-0.000005701	0.000007299	-0.000005087
H	0.000005423	-0.000004931	0.000002847
C	-0.000014638	0.000019241	0.000010546
H	-0.000000990	-0.000001769	0.000004306
C	0.000039640	-0.000014749	-0.000032420
O	-0.000006152	-0.000004068	0.000005942
C	-0.000012897	-0.000003969	0.000030005
C	0.000000409	0.000008345	-0.000010222
C	0.000004262	-0.000004181	-0.000007113
C	-0.000004226	0.000001293	0.000006399
H	-0.000002577	-0.000002751	-0.000001015
C	-0.000000737	-0.000002098	0.000006171
H	0.000004392	-0.000001159	-0.000000313
C	-0.000000347	0.000000529	-0.000006087
H	-0.000005136	-0.000000515	-0.000000486
H	0.000002133	0.000001048	-0.000000985
H	-0.000002407	0.000000354	-0.000000499
C	0.000004521	-0.000011717	0.000009791
H	0.000002855	-0.000006152	0.000002786
H	-0.000002243	-0.000007590	0.000001667
H	0.000004162	-0.000007028	0.000004618
C	-0.000000107	0.000003748	-0.000000357
H	-0.000001825	0.000007231	-0.000001437
H	-0.000001248	0.000003559	-0.000001820
H	0.000000117	0.000005687	-0.000004454
C	-0.000002590	0.000007216	-0.000002440
H	-0.000002597	0.000003977	-0.000000664
H	-0.000003103	0.000003493	-0.000002993
H	-0.000001090	0.000002647	0.000000107
O	0.000005359	0.000000327	-0.000004823
H	0.000006898	0.000005034	-0.000001180
H	0.000001236	0.000001847	0.000002596
H	0.000002109	0.000006896	-0.000005339

TS1-8

B3LYP SCF energy: -772.093982 a.u.

B3LYP enthalpy: -772.073904 a.u.

B3LYP free energy: -772.145299 a.u.

Cartesian coordinate

C	0.000015585	0.000005182	-0.000016810
H	0.000000346	-0.000001703	0.000005692
C	-0.000016563	0.000001351	0.000001236
H	-0.000001281	0.000003607	-0.000003429
C	0.000003732	0.000002356	0.000008275
O	0.000000199	-0.000005592	0.000008037
C	-0.000003075	-0.000004565	0.000003757
H	0.000001060	0.000005118	-0.000000560
H	0.000000142	-0.000003050	-0.000006763
C	-0.000015406	-0.000005961	0.000011221
H	-0.000000395	0.000000240	-0.000004332
C	0.000015871	-0.000006464	-0.000001565
H	0.000000988	-0.000003526	0.000002499
C	-0.000003802	0.000005629	-0.000008113
O	-0.000003359	-0.000000615	-0.000010934
C	0.000008328	-0.000006624	0.000000829
C	-0.000000348	0.000006572	0.000003416
C	-0.000005606	-0.000003072	-0.000005774
C	0.000006978	0.000008696	0.000006732
H	0.000002781	0.000004375	0.000002384
C	-0.000000225	-0.000001629	-0.000002118
H	-0.000001298	-0.000003288	-0.000003542
C	-0.000004385	0.000000506	0.000003271
H	0.000001565	0.000004771	0.000004433
H	-0.000004171	-0.000002790	-0.000002290
H	-0.000001261	0.000001842	0.000001934
C	0.000002246	-0.000010002	-0.000007252
H	0.000000582	-0.000003989	-0.000000350
H	0.000000169	-0.000002784	0.000002382
H	-0.000000428	-0.000006088	-0.000000481
C	0.000000796	0.000001241	0.000001166
H	-0.000001155	0.000001918	0.000005947
H	0.000003927	-0.000001750	0.000002117
H	-0.000000132	0.000002374	0.000006830
C	-0.000002601	0.000008613	0.000003577
H	-0.000001983	0.000002635	-0.000004917
H	0.000001863	0.000001124	-0.000002564
H	0.000000318	0.000005343	-0.000003944

NBO Charges

C	1	-0.04240
H	2	0.10662
C	3	-0.10763

H	4	0.08691
C	5	0.24698
O	6	-0.28368
C	7	-0.22450
H	8	0.09094
H	9	0.10054
C	10	-0.02489
H	11	0.10509
C	12	-0.10494
H	13	0.08813
C	14	0.23489
O	15	-0.26115
C	16	-0.04597
C	17	-0.08790
C	18	-0.07761
C	19	-0.11439
H	20	0.10242
C	21	-0.11526
H	22	0.11327
C	23	-0.09903
H	24	0.09630
H	25	0.09569
H	26	0.09474
C	27	-0.29400
H	28	0.10280
H	29	0.10420
H	30	0.09826
C	31	-0.28488
H	32	0.10567
H	33	0.08868
H	34	0.09351
C	35	-0.29395
H	36	0.09669
H	37	0.11137
H	38	0.09849

TS2-trans-8

B3LYP SCF energy: -772.099921 a.u.

B3LYP enthalpy: -772.080626 a.u.

B3LYP free energy: -772.148542 a.u.

Cartesian coordinate

C	0.000026310	-0.000015189	-0.000015716
C	0.000018080	0.000061285	-0.000008887
H	0.000000569	-0.000003040	-0.000000904
C	-0.000032756	-0.000044768	0.000021258
O	0.000020250	0.000002160	0.000003328
C	-0.000006271	0.000010693	0.000000894
H	0.000008452	-0.000013461	-0.000009942
H	0.000017078	0.000005432	0.000007700
H	-0.000007158	-0.000000072	0.000011211
C	-0.000023188	0.000013401	-0.000030262
H	-0.000003660	0.000005629	0.000009723
C	-0.000031909	-0.000062244	-0.000012435
H	0.000000626	0.000003863	-0.000003505
C	-0.000004386	0.000052098	0.000067560
O	0.000011492	-0.000003233	-0.000015409
C	0.000015846	-0.000010483	-0.000045172
C	-0.000014522	-0.000004566	0.000013939
C	0.000003210	0.000008078	0.000015124
C	0.000004448	-0.000006003	-0.000002028
H	0.000001223	0.000002662	0.000007287
C	0.000009658	-0.000007805	-0.000005494
H	-0.000001366	0.000001529	-0.000000888
C	-0.000004238	0.000002687	0.000006045
H	0.000003137	-0.000001908	0.000004241
H	0.000000493	-0.000000631	-0.000000579
H	0.000003676	-0.000002863	0.000001936
C	0.000012127	-0.000002625	-0.000002428
H	-0.000005571	0.000004307	0.000000566
H	-0.000004822	-0.000000302	0.000000693
H	-0.000007149	0.000000147	0.000001024
C	-0.000002406	-0.000005347	-0.000002002
H	-0.000000872	0.000001410	-0.000000818
H	0.000010091	-0.000002274	-0.000005175
H	0.000008598	0.000002067	0.000005373
C	-0.000017566	0.000004205	-0.000010865
H	-0.000000446	0.000002528	-0.000001001
H	-0.000005741	0.000000718	0.000001471
H	-0.000001332	0.000001916	-0.000005862

NBO Charges

C	1	-0.12142
C	2	-0.06634
H	3	0.09990
C	4	0.26591
O	5	-0.27741
C	6	-0.22459
H	7	0.09609

H	8	0.10337
H	9	0.10532
C	10	-0.11876
H	11	0.10801
C	12	-0.06002
H	13	0.09721
C	14	0.25097
O	15	-0.23762
C	16	-0.04840
C	17	-0.07941
C	18	-0.06724
C	19	-0.11932
H	20	0.10264
C	21	-0.12268
H	22	0.11152
C	23	-0.08691
H	24	0.09548
H	25	0.09399
H	26	0.09259
C	27	-0.28423
H	28	0.09209
H	29	0.09345
H	30	0.10013
C	31	-0.28127
H	32	0.09022
H	33	0.10262
H	34	0.09255
C	35	-0.28303
H	36	0.09812
H	37	0.09243
H	38	0.09405

TS2-cis-8

B3LYP SCF energy: -772.088934 a.u.

B3LYP enthalpy: -772.069642 a.u.

B3LYP free energy: -772.137344 a.u.

Cartesian coordinate

C	-0.000000384	0.000002678	-0.000001222
C	0.000010140	0.000000633	-0.000004676
H	-0.000000798	-0.000004881	0.000003906
C	-0.000023337	0.000002898	-0.000002166
O	0.000008375	-0.000004533	-0.000000286
C	-0.000000583	0.000003724	-0.000001435
H	-0.000005317	0.000000800	0.000001053
H	-0.000006283	0.000000756	-0.000003135
H	0.000003638	0.000002320	0.000000677
C	0.000005762	-0.000002023	0.000000501
H	0.000002914	-0.000004866	-0.000004704
C	0.000011104	0.000006224	-0.000000111
H	0.000001722	-0.000002664	0.000000474
C	-0.000010111	-0.000006337	0.000013109
O	0.000005771	-0.000003042	-0.000006543
C	-0.000000002	0.000004535	-0.000006879
C	0.000001765	0.000000795	0.000005057
C	-0.000003251	-0.000000905	0.000004357
C	-0.000001427	0.000004861	0.000003767
H	0.000000349	0.000002628	0.000004346
C	-0.000003784	0.000001924	0.000000248
H	-0.000000362	-0.000001074	-0.000001869
C	-0.000001548	0.000000807	0.000006663
H	-0.000002187	0.000004040	0.000007046
H	-0.000002735	0.000000736	0.000001267
H	-0.000003493	0.000003288	0.000005777
C	0.000005839	-0.000000717	0.000000191
H	0.000008514	-0.000003046	-0.000001143
H	0.000008096	-0.000001938	0.000002492
H	0.000007352	-0.000003138	-0.000000170
C	-0.000006689	0.000000611	-0.000003982
H	-0.000007705	0.000002093	-0.000003556
H	-0.000007964	0.000001551	-0.000004975
H	-0.000007641	-0.000000920	-0.000005451
C	0.000004496	-0.000003063	-0.000002714
H	0.000001381	0.000000029	0.000000325
H	0.000006641	-0.000002044	-0.000002041
H	0.000001740	-0.000002742	-0.000004198

NBO Charges

C	1	-0.11285
C	2	-0.05897
H	3	0.09409
C	4	0.26390
O	5	-0.27661
C	6	-0.23011
H	7	0.09231
H	8	0.11385
H	9	0.08664
C	10	-0.12118
H	11	0.11624

C	12	-0.06494
H	13	0.08999
C	14	0.24425
O	15	-0.21793
C	16	-0.04734
C	17	-0.07933
C	18	-0.06317
C	19	-0.12261
H	20	0.09783
C	21	-0.12376
H	22	0.11180
C	23	-0.08262
H	24	0.09364
H	25	0.09389
H	26	0.09192
C	27	-0.28529
H	28	0.09281
H	29	0.08940
H	30	0.10375
C	31	-0.28563
H	32	0.09011
H	33	0.09160
H	34	0.10694
C	35	-0.28896
H	36	0.09228
H	37	0.08923
H	38	0.11483

TS1-9

B3LYP SCF energy: -768.750127 a.u.

B3LYP enthalpy: -768.731776 a.u.

B3LYP free energy: -768.799026 a.u.

Cartesian coordinate

C	-0.000221792	0.000022255	0.000093290
H	0.000180243	0.000063323	-0.000000681
C	0.000065828	-0.000168767	-0.000094190
H	-0.000024394	0.000022743	-0.000000706
C	-0.000029058	0.000019723	-0.000069010
O	0.000008078	-0.000003978	0.000082335
H	-0.000002738	-0.000011773	-0.000012739
C	0.000096060	0.000008552	-0.000035175
H	0.000007277	0.000011109	-0.000006317
C	-0.000096296	0.000040099	0.000026387
H	-0.000017492	-0.000003774	-0.000000210
C	0.000000067	-0.000052547	0.000125189
O	-0.000009639	0.000028136	-0.000068285
C	0.000189327	-0.000052483	-0.000035282
C	-0.000024698	0.000016822	0.000093255
C	-0.000080550	0.000057198	-0.000129687
C	0.000034917	0.000004300	0.000017937
H	0.000002877	0.000009106	-0.000009389
C	-0.000082704	-0.000001288	0.000089105
H	-0.000026009	0.000004738	0.000011982
C	0.000001069	0.000009753	-0.000034362
H	0.000012198	-0.000027642	-0.000007519
H	0.000001753	-0.000006131	-0.000008808
H	-0.000012052	0.000006440	-0.000025299
C	0.000018924	-0.000017329	0.000000919
H	0.000018328	0.000014561	0.000014453
H	-0.000003851	-0.000012273	0.000001027
H	0.000000864	0.000021815	-0.000018399
O	-0.000020638	0.000004155	-0.000005422
C	0.000018835	-0.000009119	0.000009215
H	-0.000002271	0.000009817	0.000000876
H	-0.000004218	-0.000005635	0.000003986
H	0.000001753	-0.000001906	-0.000008475

NBO Charges

C	1	-0.18793
H	2	0.12427
C	3	-0.11825
H	4	0.11365
C	5	0.37884
O	6	-0.30782
H	7	0.12975
C	8	-0.04160
H	9	0.12996
C	10	-0.13411
H	11	0.10208
C	12	0.24188
O	13	-0.26165
C	14	-0.05102
C	15	-0.10295
C	16	-0.09241
C	17	-0.13635
H	18	0.11815
C	19	-0.13710
H	20	0.13261

C	21	-0.11594
H	22	0.11524
H	23	0.11519
H	24	0.11350
C	25	-0.35225
H	26	0.12297
H	27	0.11809
H	28	0.11915
O	29	-0.28691
C	30	-0.16848
H	31	0.10770
H	32	0.10473
H	33	0.10701

TS2-trans-9

B3LYP SCF energy: -858.786696 a.u.

B3LYP enthalpy: -858.769282 a.u.

B3LYP free energy: -858.833629 a.u.

Cartesian coordinate

C	0.000035180	-0.000010094	-0.000043169
C	-0.000058393	0.000051833	0.000032653
H	0.000000210	-0.000015246	-0.000002131
C	-0.000051970	0.000029768	-0.000123981
O	0.000119720	-0.000052150	0.000093693
H	-0.000029005	-0.000003094	0.000014443
C	-0.000005049	-0.000001902	0.000016848
H	0.000008882	-0.000003280	-0.000005682
C	-0.000001906	-0.000052227	-0.000011953
H	0.000011768	0.000006005	-0.000003154
C	-0.000010643	0.000004029	-0.000006217
O	-0.000004127	0.000003497	0.000010611
C	0.000002900	0.000025040	-0.000018544
C	-0.000002680	-0.000005143	0.000020787
C	0.000014118	-0.000016109	0.000023823
C	-0.000001127	0.000025497	-0.000016705
H	-0.000016686	0.000018970	0.000000437
C	0.000007968	0.000021360	-0.000017898
H	0.000012579	0.000003944	-0.000006415
C	0.000005278	-0.000014769	0.000024976
H	-0.000015968	0.000005965	0.000014576
H	0.000014549	-0.000011010	0.000001966
H	-0.000002119	0.000003267	-0.000000240
C	0.000001454	-0.000020060	0.000001134
H	-0.000004401	-0.000009346	-0.000002936
H	-0.000019605	0.000006258	0.000001948
H	0.000016338	0.000010336	0.000000961
N	0.000149303	0.000022458	0.000139153
O	0.000046731	-0.000027089	-0.000046559
O	-0.000195017	0.000001002	-0.000102572
H	-0.000028282	0.000002293	0.000010146

NBO Charges

C	1	-0.19566
H	2	0.09022
C	3	-0.07120
H	4	0.10068
C	5	0.38719
O	6	-0.28791
H	7	0.10556
C	8	-0.12179
H	9	0.10747
C	10	-0.06280
H	11	0.09670
C	12	0.24717
O	13	-0.23497
C	14	-0.05135
C	15	-0.07928
C	16	-0.06640
C	17	-0.11904
H	18	0.10325
C	19	-0.12337
H	20	0.11159
C	21	-0.08583
H	22	0.09602
H	23	0.09399
H	24	0.09259
C	25	-0.28384
H	26	0.09217
H	27	0.09330
H	28	0.10026
O	29	-0.28694
C	30	-0.10676
H	31	0.08614
H	32	0.07831
H	33	0.09452

TS2-cis-9

B3LYP SCF energy: -858.785043 a.u.

B3LYP enthalpy: -858.767600 a.u.

B3LYP free energy: -858.832198 a.u.

Cartesian coordinate

C	0.000043837	-0.000227220	-0.000002576
C	-0.000158035	0.000435382	0.000024294
H	0.000016815	-0.000233742	-0.000018846
C	0.000017150	0.000090996	-0.000095196
O	-0.000006744	-0.000015386	0.000032100
H	-0.000006724	-0.000026662	-0.000003944
C	0.000069287	-0.000088494	0.000027760
H	-0.000003601	0.000031262	0.000002939
C	0.000035370	0.000036519	-0.000034136
H	-0.000001636	-0.000001833	0.000009042
C	0.000023160	0.000006041	-0.000016548
O	0.000001106	0.000000783	0.000046349
C	0.000004831	-0.000045307	-0.000006130
C	-0.000002504	0.000026830	0.000005249
C	-0.000003170	0.000004659	-0.000013161
C	-0.000012526	0.000000512	-0.000017249
H	-0.000001569	0.000003912	-0.000013441
C	-0.000027511	-0.000009990	-0.000018051
H	-0.000002244	-0.000000911	-0.000003359
C	0.000031185	-0.000001076	0.000032571
H	-0.000002685	-0.000005148	-0.000000631
H	-0.000000662	0.000000242	-0.000002661
H	0.000001399	-0.000000182	0.000003338
C	-0.000020185	0.000001666	-0.000000553
H	0.000014670	0.000010666	0.000006008
H	-0.000000493	-0.000019946	0.000006051
H	-0.000013246	0.000006148	-0.000012963
N	-0.000010720	0.000001173	-0.000018240
O	0.000017670	-0.000018671	0.000032143
O	-0.000005037	0.000027547	0.000045462
H	0.000002810	0.000010233	0.000004380

NBO Charges

C	1	-0.19133
C	2	-0.11390
H	3	0.11341
C	4	0.30318
O	5	-0.19231
H	6	0.09128
C	7	-0.13135
H	8	0.11426
C	9	-0.00698
H	10	0.09370
C	11	0.23452
O	12	-0.23556
C	13	-0.04898
C	14	-0.08813
C	15	-0.08257
C	16	-0.10792
H	17	0.11404
C	18	-0.11305
H	19	0.11038
C	20	-0.10230
H	21	0.09915
H	22	0.09619
H	23	0.09557
C	24	-0.28320
H	25	0.09466
H	26	0.09033
H	27	0.10202
N	28	0.22255
O	29	-0.18468
O	30	-0.19714
H	31	0.10417

TS1-10

B3LYP SCF energy: -748.855528 a.u.

B3LYP enthalpy: -748.837087 a.u.

B3LYP free energy: -748.903579 a.u.

Cartesian coordinate

C	-0.000000278	0.000002791	-0.000002439
H	-0.000001129	0.000001458	-0.000006114
C	-0.000003955	0.000002633	-0.000003820
H	-0.000002949	-0.000007809	-0.000003713
C	-0.000000605	0.000006617	-0.000002358
O	-0.000000120	0.000005926	-0.000004394
C	-0.000001030	0.000003635	-0.000004025
H	-0.000001305	0.000001014	-0.000004157
H	-0.000001344	0.000006641	-0.000006606
H	0.000000287	0.000005868	-0.000000416
C	0.000001332	-0.000008867	0.000003175
H	-0.000000001	-0.000000557	0.000003300
C	0.000003110	-0.000001005	0.000001035
H	0.000000890	0.000001434	0.000002980

C	0.000000384	-0.000002677	0.000002172
O	-0.000002506	-0.000005224	-0.000000598
C	-0.000000336	-0.000002196	0.000000241
C	0.000002379	0.000004410	0.000003430
C	0.000000223	-0.000004855	0.000000757
C	0.000001463	0.000004216	0.000003047
H	0.000002445	0.000005752	0.000003004
C	0.000000340	-0.000001312	0.000000939
H	-0.000001279	-0.000005639	-0.000000004
C	0.000001461	0.000002051	0.000002706
H	0.000002687	0.000007846	0.000004049
H	-0.000000299	-0.000004086	0.000000825
H	0.000001607	0.000003271	0.000002884
C	-0.000003369	0.000003687	0.000002144
H	0.000004147	-0.000008314	0.000004579
H	0.000003121	0.000001864	0.000004021
H	0.000002681	-0.000000732	0.000006848
N	0.000000439	-0.000006882	-0.000002440
H	-0.000005925	-0.000004795	-0.000006022
H	-0.000002567	-0.000006166	-0.000005031

NBO Charges

C	1	0.03302
H	2	0.10119
C	3	-0.09660
H	4	0.09054
C	5	0.23841
O	6	-0.27946
C	7	-0.32467
H	8	0.09245
H	9	0.10207
H	10	0.10311
C	11	-0.03009
H	12	0.11284
C	13	-0.10033
H	14	0.08819
C	15	0.24122
O	16	-0.28217
C	17	-0.04663
C	18	-0.08554
C	19	-0.07700
C	20	-0.11492
H	21	0.10189
C	22	-0.11554
H	23	0.11415
C	24	-0.09809
H	25	0.09629
H	26	0.09569
H	27	0.09466
C	28	-0.29640
H	29	0.10115
H	30	0.10602
H	31	0.09737
N	32	-0.43735
H	33	0.17640
H	34	0.19815

TS2-trans-10

B3LYP SCF energy: -748.858412a.u.

B3LYP enthalpy: -748.840863 a.u.

B3LYP free energy: -748.905360a.u.

Cartesian coordinate

C	-0.000000605	0.000001349	0.000017865
H	-0.000002877	-0.000000870	-0.000001259
C	0.000004476	-0.000013319	-0.000008972
H	-0.000001787	0.000000627	0.000005372
C	-0.000005776	0.000003448	0.000002408
O	0.000010127	-0.000011188	0.000002003
C	-0.000000716	-0.000007276	0.000004326
H	-0.000000024	-0.000000484	0.000001959
H	0.000006716	-0.000003302	0.000003521
H	-0.000000853	-0.000003350	0.000005156
C	-0.000004408	0.000005567	-0.000004955
H	0.000000745	-0.000000794	-0.000003033
C	-0.000003026	-0.000003202	-0.000002175
H	0.000008722	0.000005338	0.000001439
C	-0.000006943	-0.000001146	-0.000004423
O	-0.000002417	0.000000227	-0.000001212
C	-0.000000486	0.000000659	-0.000000723
C	0.000001345	0.000000622	0.000000719
C	-0.000003462	0.000000353	-0.000002660
C	0.000001149	0.000001494	0.000000138
H	0.000001268	0.000001177	0.000000320
C	-0.000002654	0.000001122	-0.000001620
H	-0.000004044	0.000000467	-0.000002744
C	-0.000000268	0.000001510	-0.000000733
H	0.000002711	0.000001613	0.000001082
H	-0.000003424	0.000001041	-0.000002490

H	0.000000230	0.000001586	-0.000000433
C	-0.000001046	0.000000338	-0.000000373
H	-0.000002322	0.000003406	-0.000002549
H	-0.000000695	0.000003237	-0.000002816
H	-0.000002944	0.000002770	-0.000001878
N	0.000005915	0.000001033	-0.000005614
H	0.000002071	0.000002897	-0.000000227
H	0.000005297	0.000003050	0.000004579

NBO Charges

C	1	-0.02570
H	2	0.07901
C	3	0.01081
H	4	0.09465
C	5	0.20292
O	6	-0.26836
C	7	-0.31993
H	8	0.10269
H	9	0.10077
H	10	0.09803
C	11	-0.13824
H	12	0.10621
C	13	0.04226
H	14	0.09847
C	15	0.18428
O	16	-0.24950
C	17	-0.03772
C	18	-0.09301
C	19	-0.09123
C	20	-0.11109
H	21	0.10747
C	22	-0.11086
H	23	0.11306
C	24	-0.11081
H	25	0.09677
H	26	0.09528
H	27	0.09493
C	28	-0.28001
H	29	0.09134
H	30	0.09564
H	31	0.10202
N	32	-0.43835
H	33	0.16511
H	34	0.19308

TS2-cis-10

B3LYP SCF energy: -748.852860 a.u.

B3LYP enthalpy: -748.835261 a.u.

B3LYP free energy: -748.898464 a.u.

Cartesian coordinate

C	-0.000005951	0.000011775	-0.000001088
C	0.000006484	0.000008690	0.000006588
H	-0.000006974	0.000006769	0.000005475
C	0.000000160	-0.000003666	-0.000013899
O	-0.000005255	-0.000004991	0.000013516
C	-0.000000900	-0.000002693	0.000010783
H	-0.000003712	0.000001478	0.000008825
H	-0.000001919	-0.000003821	0.000011677
H	0.000000078	-0.000002100	0.000007476
H	0.000000567	0.000001542	0.000000201
C	-0.000001000	-0.000000901	0.000004632
H	0.000002160	-0.000007339	-0.000000836
C	0.000002568	-0.000009053	0.000003112
H	0.000001417	0.000003481	-0.000003792
C	-0.000012340	-0.000003742	-0.000005814
O	0.000003794	-0.000003892	-0.000001603
C	0.000007525	0.000002593	-0.000002869
C	-0.000002302	0.000003486	0.000000492
C	-0.000001489	-0.000001914	-0.000003910
C	0.000000802	0.000006244	-0.000001106
H	-0.000002203	0.000005607	-0.000000316
C	0.000002235	0.000001129	-0.000003408
H	0.000001845	-0.000004081	-0.000003345
C	-0.000002139	0.000004105	-0.000001940
H	-0.000002004	0.000009196	-0.000000661
H	0.000001050	-0.000000918	-0.000003431
H	-0.000000784	0.000005943	-0.000002156
C	0.000002059	-0.000001983	-0.000008745
H	0.000002789	-0.000002944	-0.000007253
H	0.000001853	0.000001337	-0.000007926
H	0.000003122	-0.000002393	-0.000007842
N	-0.000008801	-0.000012378	0.000004018
H	0.000007891	-0.000004294	-0.000001597
H	0.000009374	-0.000000273	0.000006741

NBO Charges

C	1	-0.01536
C	2	-0.08022
H	3	0.09481

C	4	0.26602
O	5	-0.28181
C	6	-0.32659
H	7	0.09430
H	8	0.10137
H	9	0.11575
H	10	0.08350
C	11	-0.12527
H	12	0.11700
C	13	-0.06114
H	14	0.08997
C	15	0.24559
O	16	-0.21907
C	17	-0.04723
C	18	-0.07971
C	19	-0.06358
C	20	-0.12220
H	21	0.09778
C	22	-0.12321
H	23	0.11202
C	24	-0.08318
H	25	0.09378
H	26	0.09410
H	27	0.09213
C	28	-0.28505
H	29	0.09927
H	30	0.08846
H	31	0.10127
N	32	-0.43005
H	33	0.19071
H	34	0.16585

TS1-11

B3LYP SCF energy: -898.079402a.u.

B3LYP enthalpy: -898.059666 a.u.

B3LYP free energy: -898.130041 a.u.

Cartesian coordinate

C	-0.000002591	-0.000000017	-0.000001437
H	0.000000552	0.000003534	-0.000001910
C	-0.000000688	0.000000795	-0.000002917
H	0.000000307	-0.000003559	-0.000003506
C	-0.000000088	0.000002932	-0.000002733
O	0.000000448	0.000004803	-0.000000327
C	-0.000000304	0.000001127	-0.000002148
H	0.000000019	-0.000000911	-0.000003025
H	-0.000000014	0.000002758	-0.000003886
H	0.000000180	0.000001437	0.000000030
C	0.000001173	-0.000004667	-0.000000144
H	0.000001252	-0.000002230	0.000001830
C	-0.000001539	0.000001431	0.000003374
H	0.000001229	0.000001482	0.000001761
C	-0.000000682	-0.000003244	0.000001920
O	-0.000000079	-0.000004615	0.000000145
C	0.000000398	-0.000000082	0.000001330
C	-0.000000473	0.000001745	-0.000000231
C	0.000000032	-0.000003747	0.000001733
C	0.000001044	0.000002741	0.000000085
H	-0.000000130	0.000003210	-0.000000049
C	-0.000000346	-0.000002244	0.000002230
H	-0.000000317	-0.000005979	0.000002388
C	-0.000000288	0.000000416	0.000000507
H	0.000000340	0.000005318	-0.000000542
H	-0.000000209	-0.000004156	0.000002129
H	0.000000191	0.000001428	0.000000993
C	0.000000314	0.000001688	0.000003634
H	-0.000000180	0.000000090	0.000003432
H	0.000000018	0.000002888	0.000004007
H	0.000000131	-0.000000136	0.000006283
N	-0.000000738	0.000002371	-0.000007275
O	0.000000308	-0.000005780	-0.000003407
O	0.000000727	-0.000000829	-0.000004274

NBO Charges

C	1	-0.01080
H	2	0.11708
C	3	-0.04168
H	4	0.10210
C	5	0.22957
O	6	-0.25980
C	7	-0.32310
H	8	0.09485
H	9	0.10426
H	10	0.10429
C	11	-0.09848
H	12	0.11395
C	13	-0.03798
H	14	0.08903
C	15	0.22484

O	16	-0.24578
C	17	-0.04438
C	18	-0.08863
C	19	-0.08326
C	20	-0.10983
H	21	0.10670
C	22	-0.11080
H	23	0.11223
C	24	-0.10435
H	25	0.09757
H	26	0.09674
H	27	0.09601
C	28	-0.28649
H	29	0.10461
H	30	0.10255
H	31	0.09866
N	32	0.24802
O	33	-0.19837
O	34	-0.19932

TS2-trans-11

B3LYP SCF energy: -898.085426 a.u.

B3LYP enthalpy: -898.066271 a.u.

B3LYP free energy: -898.134996 a.u.

Cartesian coordinate

C	0.000016646	0.000035420	-0.000015169
C	0.000003101	0.000021308	-0.000001452
H	0.000000875	0.000005546	-0.000001609
C	-0.000016742	-0.000014866	0.000005176
O	0.000009598	-0.000001872	0.000004505
C	0.000001752	0.000013131	-0.000002985
H	0.000002708	-0.000005196	0.000000323
H	0.000003321	-0.000002238	0.000001528
H	-0.000001116	-0.000007397	-0.000003955
H	-0.000002702	-0.000008299	0.000001984
C	-0.000028763	-0.000018375	-0.000011323
H	0.000001249	-0.000002398	0.000000774
C	0.000001258	-0.000014169	0.000004147
H	-0.000008119	-0.000010125	0.000006396
C	-0.000018497	0.000038761	0.000023994
O	0.000014812	-0.000001868	-0.000004570
C	0.000018059	-0.000017069	-0.000020997
C	-0.000004749	-0.000002137	0.000004676
C	0.000000785	0.000007099	0.000008244
C	0.000004034	-0.000001343	0.000000055
H	0.000001310	-0.000002136	-0.000000504
C	0.000008231	-0.000003289	-0.000003364
H	0.000002335	-0.000000691	0.000000307
C	-0.000001575	-0.000001056	0.000006818
H	0.000002116	-0.000001882	0.000003576
H	0.000003770	-0.000001231	0.000001317
H	0.000003935	-0.000001786	0.000003142
C	0.000011093	0.000006443	0.000000689
H	-0.000002743	0.000002004	0.000000806
H	-0.000005060	0.000003230	0.000000615
H	-0.000003096	0.000001273	0.000000792
N	-0.000034052	-0.000013370	0.000001448
O	-0.000006609	-0.000002145	-0.000027707
O	0.000022837	0.000000723	0.000012322

NBO Charges

C	1	-0.03976
C	2	-0.08802
H	3	0.11412
C	4	0.27001
O	5	-0.27373
C	6	-0.32551
H	7	0.10274
H	8	0.10524
H	9	0.10623
H	10	0.12247
C	11	-0.11797
H	12	0.11721
C	13	-0.06020
H	14	0.09929
C	15	0.25443
O	16	-0.23039
C	17	-0.05241
C	18	-0.07849
C	19	-0.06488
C	20	-0.11902
H	21	0.10211
C	22	-0.12167
H	23	0.11182
C	24	-0.08389
H	25	0.09644
H	26	0.09519
H	27	0.09359

C	28	-0.28610
H	29	0.10182
H	30	0.09520
H	31	0.10269
N	32	0.24947
O	33	-0.18981
O	34	-0.20820

TS2-cis-11

B3LYP SCF energy: -898.075534a.u.

B3LYP enthalpy: -898.056456 a.u.

B3LYP free energy: -898.124596 a.u.

Cartesian coordinate

C	-0.000016137	-0.000020025	0.000017094
H	-0.000000591	0.000008039	-0.000005030
C	0.000006068	-0.000004336	0.000000935
H	0.000001982	0.000012622	0.000004328
C	-0.000000619	0.000000762	-0.000009294
O	0.000002251	0.000008793	0.000001996
C	0.000006132	-0.000003418	0.000003022
H	-0.000002865	0.000003999	-0.000006264
H	-0.000002155	0.000001102	-0.000000358
H	-0.000001617	0.000006123	-0.000002573
C	-0.000005255	0.000023539	-0.000000944
H	0.000004333	-0.000002159	-0.000002811
C	-0.000003855	-0.000008939	-0.000017804
H	0.000007611	0.000000320	0.000001410
C	-0.000009838	-0.000009461	0.000011400
O	0.000004185	0.000002478	-0.000003261
C	0.000004092	-0.000013232	-0.000007740
C	0.000000444	-0.000000868	0.000000698
C	-0.000000971	0.000003004	0.000004758
C	0.000000439	0.000000512	0.000000840
H	-0.000000354	-0.000000442	0.000002517
C	0.000002980	-0.000002101	-0.000000265
H	0.000002250	0.000000141	0.000001855
C	0.000000451	-0.000001929	0.000003170
H	0.000000043	-0.000002424	0.000000214
H	0.000001227	-0.000000360	0.000002384
H	0.000000961	-0.000001826	0.000001488
C	-0.000002718	-0.000006617	0.000002552
H	0.000000392	-0.000000242	0.000001148
H	0.000000672	-0.000002424	0.000000038
H	0.000000776	-0.000001011	0.000002752
N	0.000000290	0.000010446	0.000003246
O	-0.000002268	0.000003470	-0.000004617
O	0.000001663	-0.000003538	-0.000006888

NBO Charges

C	1	-0.03462
H	2	0.12117
C	3	-0.08214
H	4	0.11142
C	5	0.26285
O	6	-0.26729
C	7	-0.32608
H	8	0.09653
H	9	0.10301
H	10	0.11561
C	11	-0.11520
H	12	0.12233
C	13	-0.06397
H	14	0.09968
C	15	0.24630
O	16	-0.22487
C	17	-0.05149
C	18	-0.07990
C	19	-0.06557
C	20	-0.11930
H	21	0.10010
C	22	-0.12083
H	23	0.11271
C	24	-0.08552
H	25	0.09563
H	26	0.09528
H	27	0.09359
C	28	-0.29110
H	29	0.09891
H	30	0.09838
H	31	0.10588
N	32	0.25174
O	33	-0.19901
O	34	-0.20425