Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Theoretically Derived Mechanisms of HPALD Photolysis in Isoprene Oxidation

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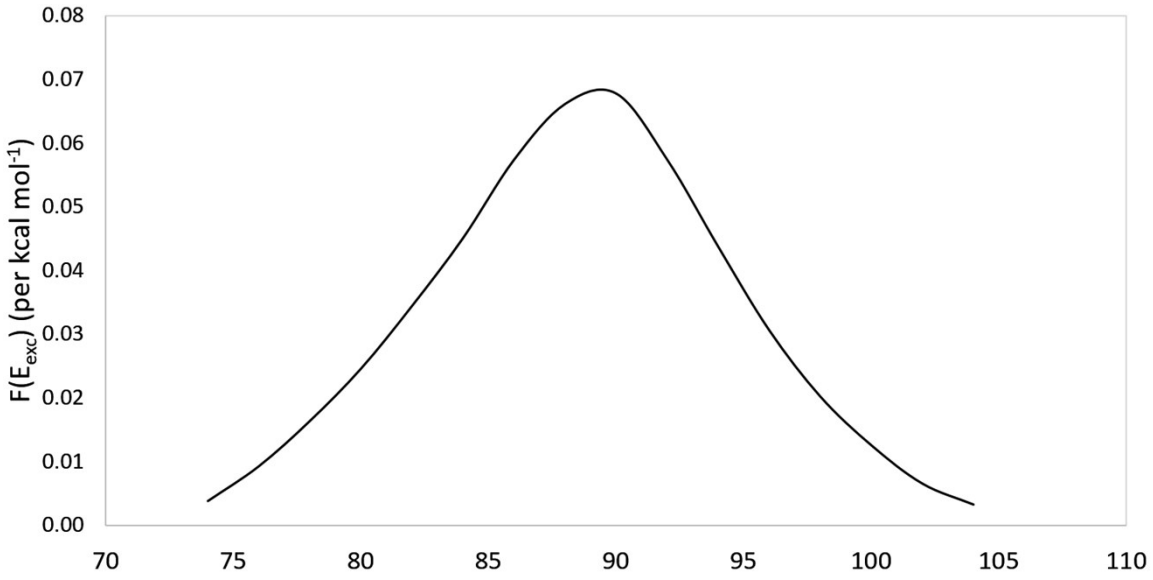

Figure S1. Smoothed, normalized excitation energy distribution F(Eexc) of HPALDs, representing the absorption cross section spectrum of methacrolein O=CH-C(CH3)=CH2 multiplied by the actinic flux at the earth's surface for an overhead sun, and convoluted with the thermal vibration energy distribution of HPALDs at 298 K. The abscissa is the total excitation energy E_{exc} in kcal mol^{-1}.

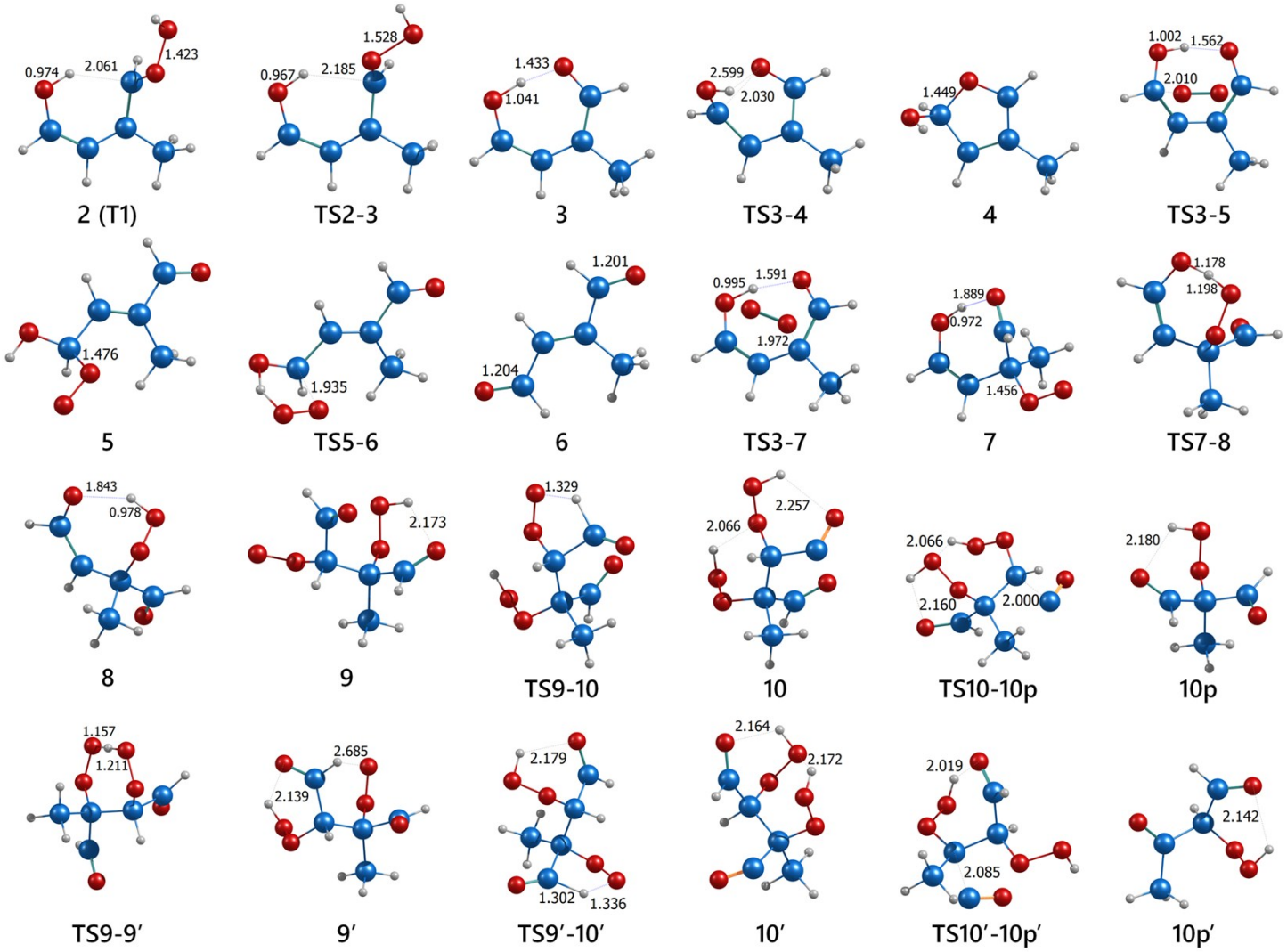

Figure S2. Various structures of the molecules in Figures 1a and 1b in the main text, optimized at M06-2X-D3/6-311++G(2d,p) level of theory. Bond lengths are in angstrom.

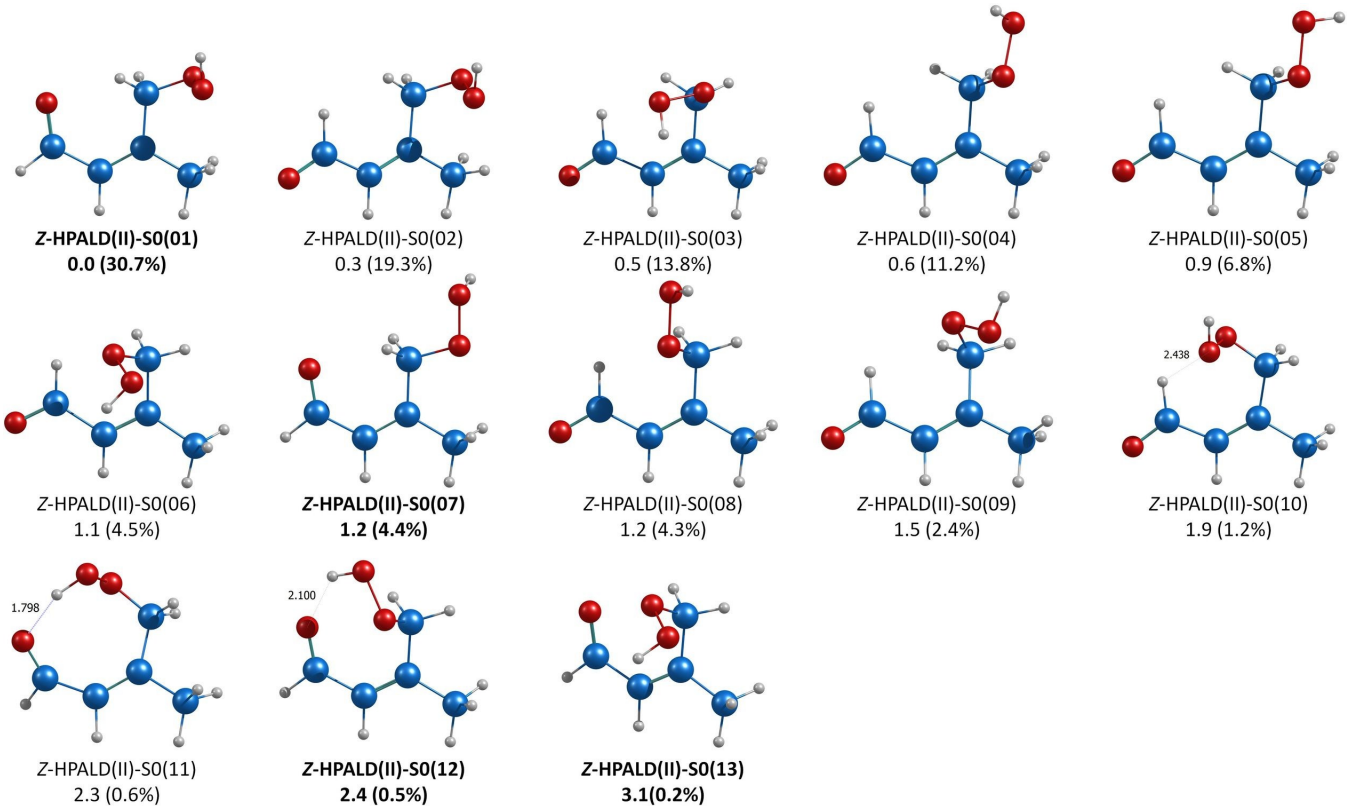

Figure S3. Structures of the 13 singlet Z-HPALD(II) conformers, optimized at M06-2X-D3/6-311++G(2d,p) level of theory, together with the Gibbs free energy and the percentual Boltzmann population. Bond lengths are in angstrom.

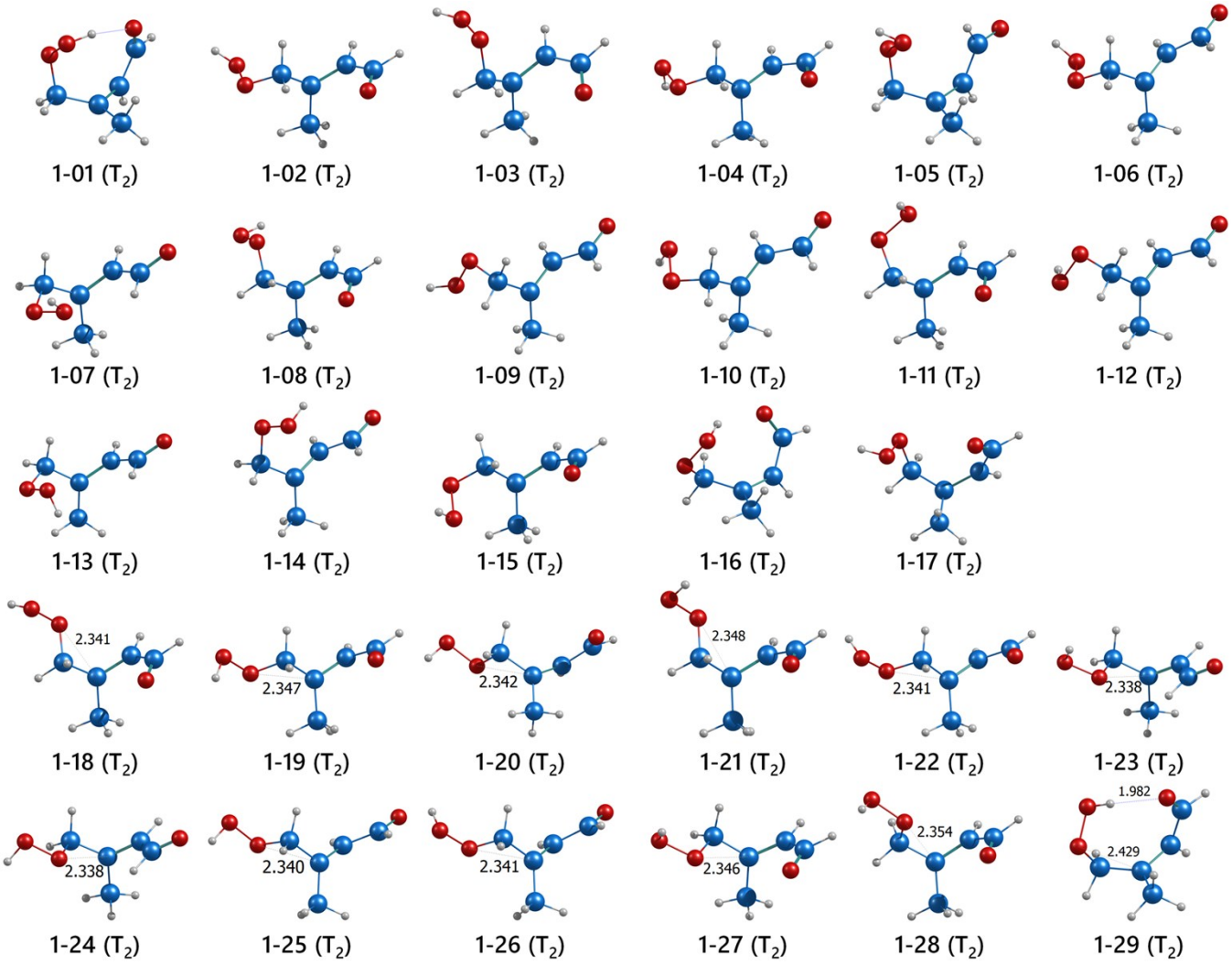

Figure S4. Various structures of the conformers of **1** (T_2), optimized at M06-2X-D3/6-311++G(2d,p) level of theory. The last 12 structures are the 'reactive' conformers, see main text. Bond lengths are in angstrom.

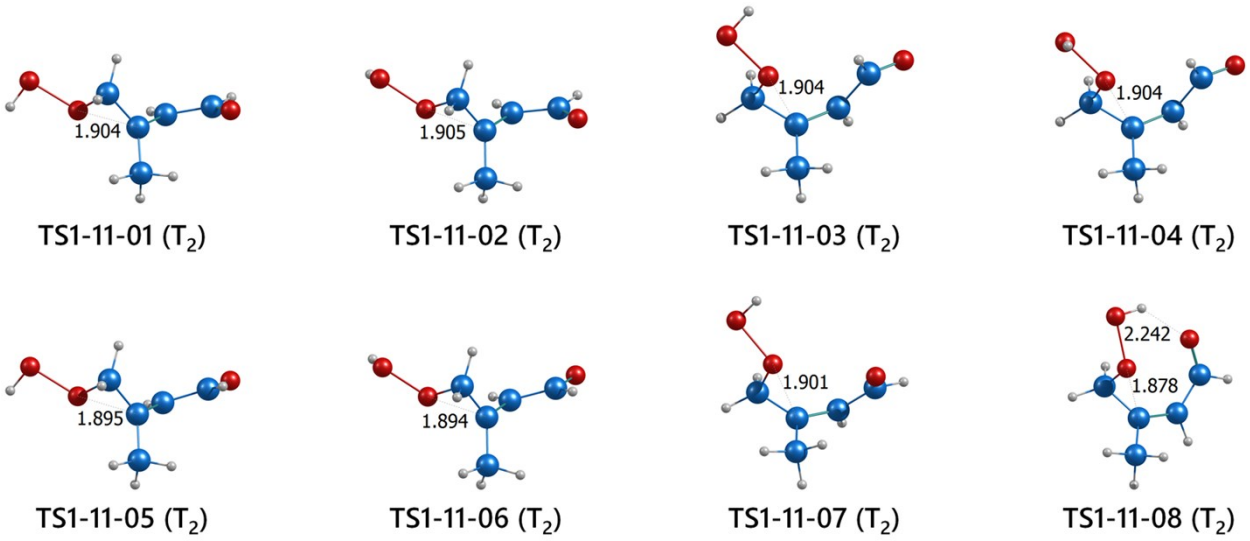

Figure S5. Various structures of the transition states of **TS1-11**, optimized at M06-2X-D3/6-311++G(2d,p) level of theory. Bond lengths are in angstrom.

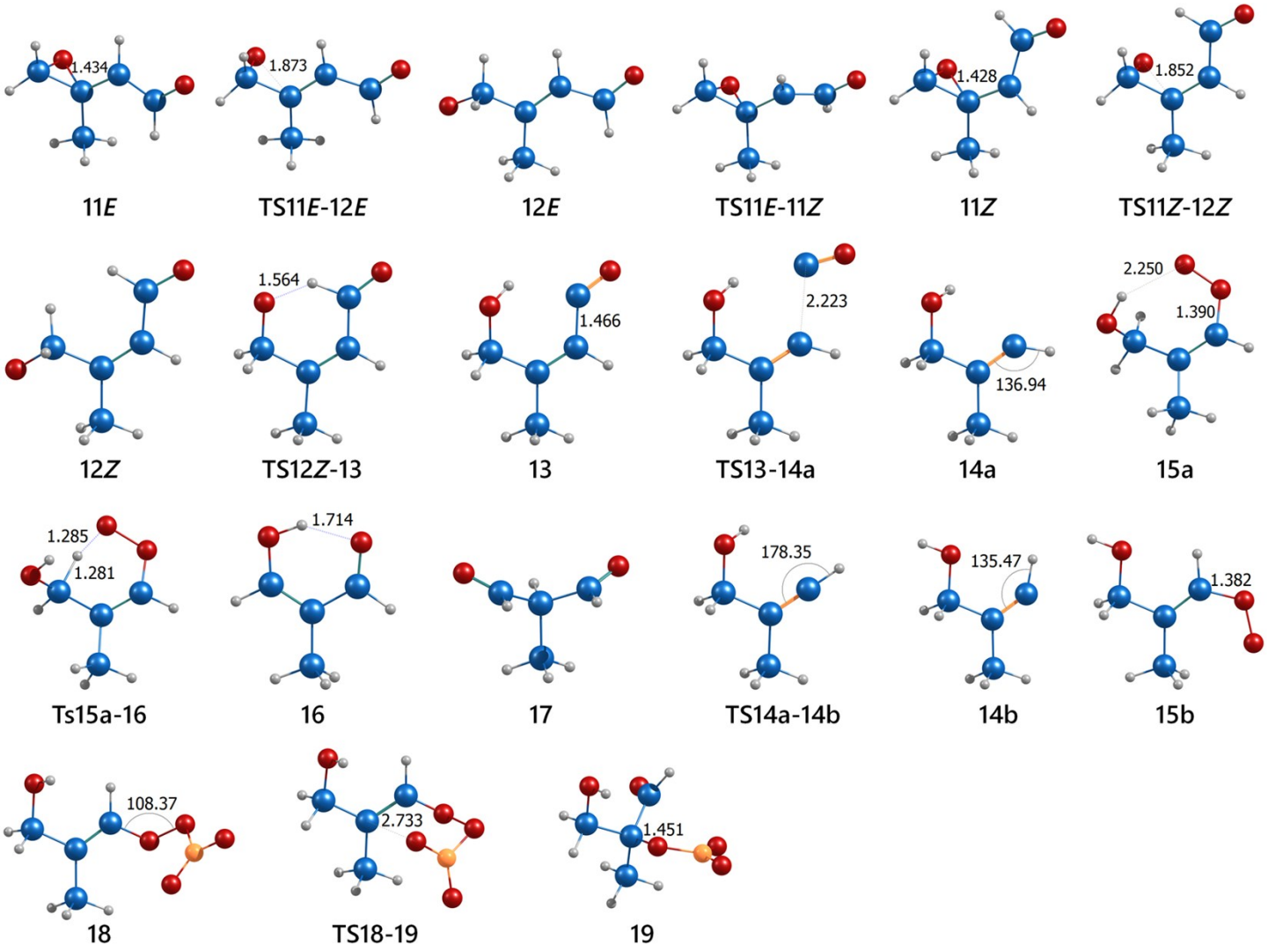

Figure S6. Various structures of the molecules in Figures 3a and 3b in the main text, optimized at M06-2X-D3/6-311++G(2d,p) level of theory. Bond lengths are in angstrom.

Table S1. Relative energies and free energies (kcal mol^{-1}) at 298 K for various conformers of **1** (T_2) and the transition states (TS1-11).

	$\nu_{im}^{\neq}$/i	ΔE_1	ΔG_1 (298 K)	ΔE_2	ΔG_2 (298 K)
1-01 (T_2)		52.5	51.9	55.0	54.3
1-02 (T_2)		56.4	54.2	58.6	56.4
1-03 (T_2)		56.2	54.1	58.6	56.5
1-04 (T_2)		56.5	54.7	58.8	57.0
1-05 (T_2)		56.8	55.3	59.0	57.5
1-06 (T_2)		56.8	55.0	59.0	57.2
1-07 (T_2)		56.9	55.1	59.1	57.3
1-08 (T_2)		57.0	54.9	59.3	57.2
1-09 (T_2)		57.4	55.5	59.4	57.4
1-10 (T_2)		57.4	55.3	59.4	57.4
1-11 (T_2)		57.9	55.6	59.7	57.3
1-12 (T_2)		57.8	55.5	59.7	57.5
1-13 (T_2)		57.5	55.4	59.8	57.7
1-14 (T_2)		57.3	55.5	59.9	58.1
1-15 (T_2)		58.0	56.4	60.1	58.5
1-16 (T_2)		57.6	56.8	60.5	59.6
1-17 (T_2)		58.9	57.4	60.8	59.2
1-18 (T_2) —>TS01		57.7	55.6	59.5	57.5
1-19 (T_2) —>TS01		57.0	54.9	59.6	57.5
1-20 (T_2) —>TS01		57.9	54.9	59.6	56.7
1-21 (T_2) —>TS02		57.5	55.6	59.5	57.6
1-22 (T_2) —>TS02		57.8	55.5	59.6	57.2
1-23 (T_2) —>TS03		58.0	55.8	59.7	57.5
1-24 (T_2) —>TS04		58.3	56.2	59.9	57.8
1-25 (T_2) —>TS05		58.4	56.1	60.0	57.7
1-26 (T_2) —>TS06		58.2	55.9	59.8	57.6
1-27 (T_2) —>TS07		58.8	56.5	60.4	58.2
1-28 (T_2) —>TS07		59.0	56.4	60.7	58.2
1-29 (T_2) —>TS08		54.1	53.1	56.5	55.6
TS1-11-01	-978.1	74.7	72.9	70.7	68.9
TS1-11-02	-975.3	74.8	73.0	70.8	69.0
TS1-11-03	-986.6	75.3	73.7	71.1	69.4
TS1-11-04	-986.1	75.4	73.8	71.1	69.5
TS1-11-05	-999.4	76.4	74.6	72.2	70.4
TS1-11-06	-999.5	76.4	74.7	72.2	70.5
TS1-11-07	-985.8	77.3	75.6	73.1	71.3
TS1-11-08	-1181.0	79.6	78.8	74.7	73.9

ΔE_1, the relative energy with inclusion of ZPVE at M06-2X-D3/6-311++G(2d,p) level of theory; ΔG_1, the relative Gibbs free energy (298 K) at M06-2X-D3/6-311++G(2d,p) level of theory; ΔE_2, the relative energy with inclusion of ZPVE at CCSD(T)-F12/cc-pVDZ-F12//M06-2X-D3/6-311++G(2d, p) level of theory; ΔG_2, the relative Gibbs free energy 298 K at CCSD(T)-F12/cc-pVDZ-F12//M06-2X-D3/6-311++G(2d, p) level of theory; $\nu_{im}^{\neq}$/i , the imaginary frequency of the TSs.

Table S2. Microcanonical rate coefficient k(E) of the isomerization through 1,5-H shift of excited HPALD(II) (S_1) as a function of the initial excitation energy E in kcal mol^{-1}.

Excitation energy E **/**(kcal mol^{-1})	k(E) **/(**s^{-1}**)**
82.0	3.15E+11
84.0	5.23E+11
86.0	6.79E+11
88.0	8.03E+11
90.0	9.09E+11
92.0	9.95E+11
94.0	1.08E+12
96.0	1.14E+12
98.0	1.21E+12
100.0	1.26E+12

Table S3. Microcanonical rate coefficient k(E) for reaction of the HPALD-II triplet state T_2 and fractional reaction yield $f_{react}(E)$ as function of the initial excitation energy E in kcal mol^{-1}.

Excitation energy E /(kcal mol^{-1})	k(E) /(s^{-1})	$f_{react}(E)$
78.0	2.64E+07	0.00
78.5	3.50E+07	0.00
79.0	4.55E+07	0.00
79.5	5.84E+07	0.00
80.0	7.37E+07	0.00
80.5	9.19E+07	0.00
81.0	1.13E+08	0.01
81.5	1.38E+08	0.01
82.0	1.68E+08	0.02
82.5	2.01E+08	0.03
83.0	2.39E+08	0.05
83.5	2.83E+08	0.06
84.0	3.32E+08	0.08
84.5	3.86E+08	0.10
85.0	4.48E+08	0.13
85.5	5.16E+08	0.16
86.0	5.92E+08	0.19
86.5	6.76E+08	0.23
87.0	7.68E+08	0.27
87.5	8.69E+08	0.31
88.0	9.80E+08	0.36
88.5	1.10E+09	0.41
89.0	1.23E+09	0.46
89.5	1.37E+09	0.51
90.0	1.52E+09	0.56
90.5	1.68E+09	0.61
91.0	1.86E+09	0.65
91.5	2.04E+09	0.70
92.0	2.24E+09	0.74
92.5	2.45E+09	0.78
93.0	2.68E+09	0.82
93.5	2.92E+09	0.85
94.0	3.18E+09	0.88
94.5	3.45E+09	0.90
95.0	3.74E+09	0.93
95.5	4.04E+09	0.94
96.0	4.36E+09	0.96
96.5	4.70E+09	0.97
97.0	5.03E+09	0.98
97.5	5.42E+09	0.98
98.0	5.80E+09	0.99
98.5	6.20E+09	0.99
99.0	6.62E+09	1.00
99.5	7.07E+09	1.00
100.0	7.53E+09	1.00

List of Cartesian coordinates.

a. Structures depicted in Figure S2.

1 (S1)

Geometry with 16 atoms:
Total energy: -420.837575980

C	-2.51810	-0.01089	-0.05031
C	-1.45317	0.93188	-0.06202
C	-0.12291	0.68250	0.03425
C	0.42057	-0.70500	0.19824
C	0.87138	1.80541	0.01828
H	-3.55412	0.34148	-0.12872
H	-1.79561	1.95630	-0.14417
H	0.62596	-0.93839	1.24954
H	-0.28420	-1.44771	-0.18762
H	1.60920	1.65382	-0.77271
H	1.42974	1.84310	0.95824
H	0.37705	2.76371	-0.13592
O	-2.40914	-1.27863	0.09873
O	1.60579	-0.93607	-0.55289
O	2.70651	-0.42918	0.19498
H	3.18004	-1.24456	0.40406

TS1-2 (S1)

Geometry with 16 atoms:
Total energy: -420.832176188

C	-2.46467	-0.25191	-0.12061
C	-1.55075	0.83638	-0.11945
C	-0.21260	0.78473	0.09950
C	0.52003	-0.47947	0.40161
C	0.63871	2.01947	0.05758
H	-3.53017	-0.06288	-0.30223
H	-2.02323	1.79297	-0.30739
H	1.00235	-0.43385	1.38203
H	-0.14840	-1.34988	0.38173
H	1.44473	1.89415	-0.66964
H	1.11167	2.19395	1.02958
H	0.05718	2.90109	-0.20860
O	-2.18349	-1.47877	0.10411
O	1.54519	-0.69854	-0.57257
O	2.81165	-0.67398	0.07423
H	3.11476	-1.58042	-0.06345

2 (T_1)

Geometry with 16 atoms:
Total energy: -420.760464251

C	-2.16959	-0.75447	-0.16003
C	-1.65637	0.52731	-0.18329
C	-0.36536	0.93758	0.11531
C	0.69568	-0.00503	0.50127
C	0.03205	2.38691	0.04965
H	-3.19700	-0.95527	-0.42831
H	-2.36905	1.29315	-0.46874
H	1.15449	0.00161	1.48766
H	-0.59093	-1.61315	0.43262
H	-0.80587	3.01280	-0.25739
H	0.38631	2.74047	1.02320
H	0.85210	2.53320	-0.65886
O	-1.49714	-1.86458	0.17846
O	1.58959	-0.22919	-0.51286
O	2.73368	-0.88989	0.01539
H	2.74242	-1.69730	-0.51559

TS2-3

Geometry with 16 atoms:
Total energy: -420.756925491

C	-2.26536	-0.46893	-0.17228
C	-1.55766	0.71593	-0.20625
C	-0.23087	0.95147	0.12013
C	0.69561	-0.09694	0.57160
C	0.37480	2.32375	0.00594
H	-3.30897	-0.50114	-0.45049
H	-2.14158	1.56931	-0.53341
H	1.14706	-0.08754	1.56147
H	-0.85333	-1.62590	0.37624
H	-0.36920	3.05815	-0.30332
H	0.80151	2.64520	0.96103
H	1.19089	2.32882	-0.72300
O	-1.79864	-1.67771	0.17885
O	1.29079	-0.86316	-0.32320
O	2.80588	-0.74434	-0.16008
H	3.05019	-1.65694	-0.36781

3

Geometry with 14 atoms:
Total energy: -345.110271037

C	-1.40374	-1.12283	0.00001
C	-0.02339	-1.17318	0.00002
C	0.92460	-0.13134	0.00000
C	0.61231	1.25440	-0.00002
C	2.37874	-0.51715	0.00003
H	-1.95145	-2.06096	0.00002
H	0.37679	-2.18124	0.00003
H	1.47000	1.93867	-0.00003
H	-1.56539	0.77787	-0.00002
H	2.62194	-1.11751	0.87992
H	3.02645	0.35864	-0.00008
H	2.62192	-1.11770	-0.87974
O	-2.16478	-0.07285	-0.00001
O	-0.52664	1.76570	-0.00003

TS3-4

Geometry with 14 atoms:
Total energy: -345.053030712

C	-1.30444	-0.56087	-0.41457
C	0.04734	-1.00625	-0.44129

C	0.99273	-0.10168	0.02080
C	0.45735	1.21137	0.01611
C	2.44167	-0.39704	0.24510
H	-1.95349	-0.69579	-1.27466
H	0.30927	-1.88228	-1.02304
H	1.09227	2.07799	0.21972
H	-1.44364	-0.39466	1.45753
H	2.60313	-0.91549	1.19257
H	3.02941	0.52158	0.26005
H	2.83396	-1.03865	-0.54709
O	-2.03611	-0.45689	0.69569
O	-0.74874	1.38865	-0.30093

4

Geometry with 14 atoms:
Total energy: -345.092649423

C	-1.22051	-0.17362	-0.41375
C	0.05723	-0.94804	-0.34916
C	1.08254	-0.08582	-0.02642
C	0.52149	1.17868	0.09175
C	2.53142	-0.40490	0.16954
H	-1.70324	-0.15487	-1.39338
H	0.11371	-2.00865	-0.53828
H	0.98016	2.12437	0.33458
H	-1.79372	-0.75430	1.32575
H	2.66310	-1.14969	0.95529
H	3.09260	0.48658	0.44877
H	2.96708	-0.80717	-0.74599
O	-2.21179	-0.57699	0.47486
O	-0.80730	1.18524	-0.12717

TS3-5

Geometry with 16 atoms:
Total energy: -495.410441938

C	-1.25115	-0.23238	-1.01481
C	0.12957	-0.59078	-1.08096
O	-1.73361	0.94502	-0.72276
O	-1.51351	-1.21161	0.72092
C	1.15488	-0.10349	-0.33510
O	-0.66731	-0.89182	1.56392
C	1.08173	1.08579	0.52016
C	2.48482	-0.80715	-0.30110
O	0.24773	1.97565	0.48260
H	-1.95155	-0.85847	-1.55596
H	0.30907	-1.51217	-1.62445
H	-1.02309	1.50724	-0.29475
H	1.91108	1.17853	1.23991
H	3.29815	-0.13701	-0.58898
H	2.49278	-1.66369	-0.97199
H	2.69796	-1.16420	0.70974

5

Geometry with 16 atoms:
Total energy: -495.438015452

C	-1.26022	-0.36789	0.37523
C	0.12209	-0.79637	0.01502
O	-2.11240	-1.43921	0.29985
O	-1.65675	0.66123	-0.60528
C	1.19968	-0.02009	0.11279
O	-2.88642	1.01093	-0.39016
C	2.49361	-0.62157	-0.30435
C	1.24278	1.39659	0.58800
O	3.53780	-0.02883	-0.26119
H	-1.31700	0.14529	1.33973
H	0.20348	-1.81138	-0.36091
H	-3.00020	-1.13411	0.52500
H	2.44015	-1.66740	-0.66165
H	1.54757	2.04691	-0.23419
H	1.99998	1.50181	1.36610
H	0.28057	1.74189	0.96002

TS5-6

Geometry with 16 atoms:
Total energy: -495.414738234

C	-1.17233	-0.27032	0.72835
C	0.10153	-0.71140	0.13808
O	-2.16560	-1.06184	0.73781
O	-1.82558	0.90078	-0.66676
C	1.24754	-0.02387	0.16538
O	-2.95787	0.36857	-0.88407
C	2.42510	-0.67244	-0.47341
C	1.48289	1.33042	0.75098
O	3.51125	-0.16072	-0.51564
H	-1.13451	0.53602	1.46541
H	0.05887	-1.68214	-0.34800
H	-2.88361	-0.51001	-0.09720
H	2.24117	-1.67078	-0.91269
H	1.87166	1.99223	-0.02505
H	2.25590	1.27148	1.51929
H	0.58459	1.77451	1.17131

6

Geometry with 13 atoms:
Total energy: -344.513808245

C	-2.02845	0.20107	-0.00001
C	-0.72925	-0.49835	-0.00001
C	0.47435	0.08662	0.00000
C	1.65311	-0.82739	0.00001
C	0.79336	1.54680	0.00001
H	-0.80426	-1.58245	-0.00001
H	1.41999	-1.90840	0.00000
H	1.40518	1.78234	-0.87264
H	1.40509	1.78235	0.87273
H	-0.08870	2.18000	-0.00004
O	-3.07461	-0.39518	-0.00002
O	2.78684	-0.43104	0.00001
H	-2.01388	1.30340	-0.00000

TS3-7

Geometry with 16 atoms:

Total energy: -495.411227551

C	1.62448	-0.64046	0.88884
C	0.28625	-0.55920	1.14592
C	-0.73126	0.21487	0.52234
C	-0.46818	1.36660	-0.35378
C	-2.10755	0.17742	1.12116
H	2.19395	-1.39423	1.42398
H	-0.06438	-1.28718	1.86724
H	-1.36690	1.92066	-0.66698
H	1.82047	0.76814	-0.35087
H	-2.85694	0.50380	0.39925
H	-2.16356	0.83240	1.99438
H	-2.35363	-0.83544	1.43773
O	2.37986	0.08001	0.10119
O	0.61491	1.71000	-0.78886
O	-1.17105	-0.82286	-1.09595
O	-0.17765	-1.45008	-1.47283

7

Geometry with 16 atoms:

Total energy: -495.433479600

C	-1.93400	-0.94835	-0.35349
C	-0.61940	-1.14019	-0.47192
C	0.44828	-0.22752	0.07150
C	0.31076	1.14618	-0.57088
C	0.47895	-0.14506	1.59008
H	-2.62508	-1.69647	-0.72205
H	-0.27323	-2.03530	-0.97049
H	0.99400	1.36596	-1.40763
H	-1.98107	0.84840	0.32647
H	-0.46243	0.26765	1.95098
H	1.29878	0.49337	1.91799
H	0.60118	-1.14784	1.99733
O	-2.57704	0.09113	0.20256
O	-0.52856	1.92947	-0.21309
O	1.70042	-0.79726	-0.40454
O	2.69772	0.00089	-0.17047

TS7-8

Geometry with 16 atoms:

Total energy: -495.406709198

C	1.59414	0.40403	1.03843
C	0.26187	0.18768	1.30787
C	-0.70760	-0.18669	0.23999
C	-0.83878	0.80492	-0.91734
C	-2.10001	-0.45810	0.78751
H	2.27020	0.66932	1.85070
H	-0.06517	0.16866	2.33919
H	-1.17643	0.35753	-1.86946
H	1.46670	-0.44403	-0.78085
H	-2.77903	-0.74551	-0.01529
H	-2.47383	0.44462	1.27113
H	-2.05432	-1.26681	1.51743
O	2.11635	0.28760	-0.12494
O	-0.67580	1.97956	-0.77699
O	-0.22464	-1.44943	-0.26094
O	0.72837	-1.27957	-1.21859

8

Geometry with 16 atoms:

Total energy: -495.434943749

C	1.78074	-1.13291	-0.28772
C	0.35558	-1.10709	-0.17533
C	-0.50457	-0.01595	0.36739
C	-1.63031	0.30447	-0.63243
C	-1.17658	-0.46859	1.67183
H	2.20708	-2.10994	-0.56076
H	-0.18055	-1.99113	-0.50072
H	-1.88824	1.37842	-0.67255
H	1.58263	1.35746	-0.48027
H	-1.74096	-1.38373	1.49909
H	-1.85215	0.31327	2.02088
H	-0.41265	-0.64136	2.42930
O	2.53285	-0.17780	-0.11146
O	-2.20635	-0.53296	-1.26076
O	0.16022	1.17695	0.69735
O	0.68024	1.73350	-0.49981

9

Geometry with 18 atoms:

Total energy: -645.785390186

C	0.82496	1.49192	-0.13008
C	0.83329	0.00975	-0.48002
C	-0.50058	-0.68997	-0.18309
C	-1.64662	0.06976	-0.85556
C	-0.50236	-2.12589	-0.70013
H	1.51550	1.81352	0.66538
H	1.06575	-0.07283	-1.54521
H	-1.56693	0.20144	-1.94958
H	-1.57828	0.80204	1.64302
H	-0.40701	-2.13716	-1.78651
H	-1.43651	-2.61060	-0.41848
H	0.33069	-2.67358	-0.26197
O	0.11189	2.24066	-0.73376
O	-2.60147	0.45039	-0.24161
O	-0.72015	-0.79947	1.20272
O	-0.66525	0.49542	1.77521
O	1.85354	-0.68066	0.25082
O	3.02453	-0.18837	-0.03505

TS9-10

Geometry with 18 atoms:

Total energy: -645.743607212

C	-1.82632	-0.38703	-0.09712
C	-0.49988	0.26067	-0.62554
C	0.79452	-0.46763	-0.28953
C	0.89928	-0.71873	1.21207
C	0.87846	-1.79586	-1.03121
H	-0.64702	0.34199	-1.70984
H	1.92192	-0.92149	1.57426

H	1.57249	2.01913	-0.06750
H	0.00225	-2.40697	-0.81760
H	1.77853	-2.32771	-0.72369
H	0.93773	-1.60895	-2.10404
O	-2.23800	-1.47576	-0.18440
O	-0.06066	-0.74513	1.92528
O	1.91988	0.27713	-0.72474
O	2.17545	1.31304	0.21367
O	-0.54053	1.51667	-0.01295
O	-1.84381	1.96168	-0.13637
H	-2.34100	0.77420	0.19246

10

Geometry with 18 atoms:
Total energy: -645.781455640

C	-1.43719	-1.16343	-0.40214
C	-0.53424	0.06458	-0.60116
C	0.94932	-0.24716	-0.37058
C	1.19924	-0.84918	1.00745
C	1.45875	-1.22488	-1.42473
H	-0.66996	0.36630	-1.64601
H	2.23399	-0.73990	1.37557
H	0.84804	2.15808	0.57975
H	0.84779	-2.12664	-1.43129
H	2.49417	-1.48664	-1.20760
H	1.42057	-0.75198	-2.40667
O	-2.48989	-1.15425	0.11329
O	0.35467	-1.44751	1.60724
O	1.73374	0.91964	-0.53178
O	1.68807	1.68036	0.66847
O	-0.91255	1.12201	0.25044
O	-2.15001	1.63265	-0.20705
H	-2.78218	1.07795	0.27834

TS10-10p

Geometry with 18 atoms:
Total energy: -645.766524348

C	-2.31844	-0.81820	0.33020
C	-0.75136	-0.03504	-0.80537
C	0.52085	-0.64727	-0.27147
C	0.70042	-0.48946	1.23436
C	0.51686	-2.14655	-0.56752
H	-1.06423	-0.38618	-1.78582
H	-0.18621	-0.73082	1.84404
H	2.53325	1.04697	0.14851
H	-0.33495	-2.62293	-0.08361
H	1.44232	-2.59056	-0.20388
H	0.45008	-2.30037	-1.64488
O	-3.23408	-0.14347	0.31063
O	1.75177	-0.19483	1.73291
O	1.66392	-0.15832	-0.96912
O	1.92972	1.18854	-0.59904
O	-0.92614	1.30631	-0.76613
O	-0.58203	1.78983	0.52264
H	0.32441	2.09846	0.34942

10p

Geometry with 14 atoms:
Total energy: -456.777609061

C	0.40361	-1.12794	-0.59394
C	-0.18854	-0.08190	0.34197
C	-1.22629	0.74965	-0.40792
C	-0.86162	-0.79000	1.51666
H	-0.33276	-1.76131	-1.11840
H	-1.11941	1.84209	-0.28821
H	2.11485	0.83090	-0.44033
H	-1.65284	-1.44027	1.14496
H	-1.29557	-0.05051	2.18974
H	-0.12331	-1.37791	2.06159
O	-2.10232	0.24463	-1.04975
O	0.80591	0.74571	0.89035
O	1.41705	1.45330	-0.18005
O	1.58512	-1.26137	-0.74678

TS9-9′

Geometry with 18 atoms:
Total energy: -645.744276382

C	0.51891	1.73337	-0.29334
C	0.19956	0.35237	-0.86806
O	-0.28133	2.31193	0.37688
C	-0.54497	-0.52167	0.19143
O	1.33110	-0.24250	-1.42864
C	-2.00470	-0.06370	0.23491
C	-0.45601	-1.99745	-0.18445
O	-0.09147	-0.29163	1.51004
O	2.29284	-0.45759	-0.49028
O	-2.67752	-0.03144	-0.75274
O	1.25769	-0.33567	1.63487
H	1.50263	2.15055	-0.57042
H	-0.49199	0.47344	-1.70729
H	-2.38317	0.21122	1.23345
H	-0.85301	-2.12643	-1.19147
H	-1.04552	-2.58903	0.51502
H	0.57812	-2.33664	-0.16298
H	1.76567	-0.42544	0.59974

9′

Geometry with 18 atoms:
Total energy: -645.787387274

C	-0.98974	-1.34686	-0.46560
C	-0.37644	0.00575	-0.80821
O	-2.15582	-1.46579	-0.21022
C	0.78753	0.41128	0.10873
O	-1.35060	0.99834	-0.95277
C	2.01096	-0.46193	-0.16922
C	1.15292	1.87699	-0.04817
O	0.46953	0.23760	1.51184
O	-1.91858	1.25642	0.32405
O	2.25593	-0.91045	-1.25021
O	0.31583	-1.01903	1.80263

H	-0.31300	-2.21517	-0.51797
H	0.06365	-0.09689	-1.80782
H	2.67602	-0.61234	0.70071
H	1.36707	2.08848	-1.09517
H	2.03012	2.11294	0.55528
H	0.31281	2.48953	0.27552
H	-2.57839	0.54536	0.38173

TS9′-10′

Geometry with 18 atoms:
Total energy: -645.743605270

C	-1.60896	-1.21047	-0.02925
C	-0.53883	-0.28761	-0.58490
O	-2.77060	-0.91438	-0.00128
C	0.64838	-0.18878	0.40453
O	-1.04684	0.93765	-1.02364
C	1.70491	0.77887	-0.25393
C	0.32211	0.17366	1.83467
O	1.38015	-1.39222	0.38468
O	-1.64691	1.61402	0.07329
O	1.82201	1.93412	-0.17325
O	1.98016	-1.49037	-0.85908
H	-1.24674	-2.18660	0.34019
H	-0.14503	-0.76171	-1.49159
H	-0.05216	1.19406	1.87262
H	1.22096	0.08406	2.44371
H	-0.44321	-0.49247	2.23680
H	-2.54726	1.25272	0.04301
H	2.30408	-0.19462	-0.87728

10′

Geometry with 18 atoms:
Total energy: -645.782630503

C	0.92936	1.41363	-0.05609
C	0.24839	0.24928	-0.76238
O	2.12019	1.56232	-0.06885
C	-0.92828	-0.39199	0.00600
O	1.17169	-0.70120	-1.22849
C	-1.93408	0.72852	0.39000
C	-1.67878	-1.39938	-0.85441
O	-0.52290	-1.10738	1.13688
O	1.99015	-1.14105	-0.14957
O	-2.28362	1.58579	-0.32898
O	0.25005	-0.24684	1.95536
H	0.26126	2.14465	0.42778
H	-0.18672	0.67358	-1.67654
H	-2.47851	-1.85493	-0.27212
H	-0.97912	-2.17013	-1.17486
H	-2.10463	-0.90342	-1.72588
H	2.72442	-0.50959	-0.22056
H	1.13923	-0.59359	1.77259

TS10′-10p′

Geometry with 18 atoms:
Total energy: -645.768071181

C	0.57800	1.80337	0.07789
C	0.54461	0.29675	-0.11826
O	-0.22803	2.54062	-0.42516
C	-0.66556	-0.30031	0.57833
O	1.67654	-0.30516	0.46612
C	-0.68157	-2.21410	-0.24927
C	-0.62440	-0.55007	2.05079
O	-1.86281	0.24701	0.23683
O	2.78925	0.04401	-0.34156
O	0.04659	-2.37201	-1.11305
O	-1.94419	0.44254	-1.16749
H	1.37803	2.17518	0.74267
H	0.49856	0.07346	-1.18850
H	-0.63157	0.39069	2.60971
H	0.27465	-1.10685	2.30925
H	-1.50159	-1.13070	2.33426
H	2.92084	-0.76619	-0.85505
H	-1.66428	1.37449	-1.23481

10p′

Geometry with 14 atoms:
Total energy: -456.784362270

C	-1.19055	-1.11334	-0.02244
C	-0.14789	-0.21058	-0.66306
O	-2.26430	-0.70159	0.31940
C	1.23314	-0.41870	-0.01897
O	-0.56348	1.12384	-0.73796
C	2.09293	0.79341	0.17404
O	1.57273	-1.54104	0.25238
O	-0.76633	1.59190	0.58939
H	-0.89189	-2.16423	0.11386
H	-0.04124	-0.53157	-1.70798
H	3.07301	0.48201	0.52541
H	1.61800	1.46632	0.88933
H	2.17199	1.34103	-0.76728
H	-1.68463	1.31673	0.74361

b. Structures depicted in Figure S3.

Z-HPALD(II)-S0(01)

Geometry with 16 atoms:
Total energy: -420.850110218

C	-2.42587	-0.09277	-0.26982
C	-1.38711	0.94034	-0.20991
C	-0.10494	0.70754	0.10879
C	0.39968	-0.67354	0.44934
C	0.89419	1.81909	0.18089
H	-3.39330	0.23503	-0.69365
H	-1.70046	1.95008	-0.45187
H	0.05600	-0.96204	1.44679
H	0.02538	-1.42202	-0.25023
H	1.69715	1.65607	-0.53965
H	1.36398	1.83148	1.16718
H	0.42222	2.78117	-0.00808
O	-2.29292	-1.23555	0.10701
O	1.81103	-0.73393	0.53118

O	2.31560	-0.62355	-0.79539
H	2.60367	-1.52947	-0.96863

Z-HPALD(II)-S0(02)

Geometry with 16 atoms:

Total energy: -420.847959008

C	-2.16746	-0.53658	0.04658
C	-1.26363	0.60496	-0.14277
C	0.03685	0.63972	0.16906
C	0.77003	-0.49569	0.84142
C	0.87319	1.85614	-0.08364
H	-1.73879	-1.47440	0.44098
H	-1.73883	1.47977	-0.57481
H	0.85103	-0.29092	1.91386
H	0.28535	-1.46202	0.70288
H	1.64880	1.62550	-0.81672
H	1.38779	2.16232	0.83081
H	0.26513	2.68124	-0.44876
O	-3.34402	-0.48458	-0.21612
O	2.12036	-0.57513	0.42717
O	2.10623	-0.86294	-0.96696
H	2.48503	-1.75144	-0.98484

Z-HPALD(II)-S0(03)

Geometry with 16 atoms:

Total energy: -420.847813584

C	1.88177	-0.27640	0.24599
C	0.97251	0.81514	-0.14784
C	-0.33055	0.89143	0.14157
C	-1.08256	-0.16878	0.90880
C	-1.18484	2.02364	-0.34337
H	1.46040	-1.11535	0.82210
H	1.44851	1.59808	-0.73093
H	-0.45228	-0.78460	1.54793
H	-1.85807	0.29506	1.52293
H	-1.56449	2.59874	0.50579
H	-2.05574	1.63091	-0.87485
H	-0.63710	2.69418	-1.00296
O	3.04866	-0.27480	-0.06012
O	-1.81319	-1.00572	0.02157
O	-0.87646	-1.86696	-0.60556
H	-0.75137	-1.44736	-1.46811

Z-HPALD(II)-S0(04)

Geometry with 16 atoms:

Total energy: -420.845651199

C	2.15320	-0.76498	0.00779
C	1.45846	0.52962	-0.05508
C	0.14755	0.73973	0.10678
C	-0.83657	-0.34012	0.46891
C	-0.44662	2.11133	-0.01060
H	1.54567	-1.67258	0.16273
H	2.11560	1.37018	-0.25467
H	-0.42275	-1.34680	0.42255
H	-1.20825	-0.15886	1.48391
H	-1.03002	2.34871	0.88275
H	-1.13808	2.14965	-0.85422
H	0.32604	2.86557	-0.14603
O	3.34941	-0.86008	-0.11368
O	-1.92184	-0.22415	-0.43832
O	-2.93665	-1.09748	0.03538
H	-2.97172	-1.75565	-0.67089

Z-HPALD(II)-S0(05)

Geometry with 16 atoms:

Total energy: -420.845101310

C	-2.15979	-0.76074	-0.00257
C	-1.45966	0.53219	-0.05384
C	-0.14739	0.73415	0.10369
C	0.83142	-0.35596	0.44903
C	0.45093	2.10552	0.00272
H	-1.55431	-1.67407	0.12204
H	-2.11450	1.37819	-0.23737
H	1.17110	-0.21759	1.48324
H	0.42415	-1.35994	0.34643
H	1.14101	2.15226	-0.84186
H	1.03309	2.33261	0.89992
H	-0.31930	2.86370	-0.12410
O	-3.35873	-0.84569	-0.10192
O	1.93719	-0.21011	-0.42870
O	2.86065	-1.23087	-0.07913
H	3.61272	-0.71272	0.23547

Z-HPALD(II)-S0(06)

Geometry with 16 atoms:

Total energy: -420.847001519

C	-1.86682	-0.27782	0.18849
C	-0.95494	0.81722	-0.18591
C	0.32962	0.88803	0.17674
C	1.01327	-0.21854	0.96028
C	1.20340	2.04207	-0.20089
H	-1.47473	-1.05182	0.87007
H	-1.40550	1.60204	-0.78526
H	2.06293	0.03453	1.12891
H	0.53612	-0.38433	1.92884
H	2.04545	1.68314	-0.79946
H	1.62809	2.50479	0.69457
H	0.65839	2.79983	-0.76074
O	-3.00307	-0.33733	-0.21223
O	0.93626	-1.47759	0.31977
O	1.65057	-1.36044	-0.90282
H	0.93200	-1.29108	-1.54695

Z-HPALD(II)-S0(07)

Geometry with 16 atoms:

Total energy: -420.846998795

C	2.40780	-0.54507	-0.02510
C	1.67170	0.72261	-0.01673
C	0.33363	0.81950	0.00360
C	-0.54655	-0.40104	0.02245

C	-0.34399	2.15545	0.02010
H	3.50821	-0.45234	-0.08164
H	2.26821	1.62800	-0.02819
H	-0.30953	-1.06761	-0.81184
H	-0.39379	-0.97178	0.94271
H	-0.98446	2.24170	0.90014
H	-1.00079	2.26001	-0.84573
H	0.38679	2.96156	0.02037
O	1.89844	-1.64180	0.02531
O	-1.89673	0.03354	-0.05504
O	-2.70300	-1.11897	0.11328
H	-2.99996	-1.29045	-0.79013

Z-HPALD(II)-S0(08)

Geometry with 16 atoms:

Total energy: -420.844919636

C	1.65697	-0.90621	0.13356
C	1.34064	0.51443	-0.09929
C	0.13953	1.05840	0.10915
C	-1.03801	0.23230	0.57813
C	-0.14092	2.50675	-0.14381
H	0.84174	-1.54876	0.50704
H	2.16796	1.11652	-0.46078
H	-0.81124	-0.33417	1.48534
H	-1.90303	0.87091	0.77502
H	-0.49124	2.99358	0.77037
H	-0.94013	2.60678	-0.88365
H	0.74201	3.03150	-0.50397
O	2.75429	-1.36345	-0.06856
O	-1.34393	-0.67089	-0.47425
O	-2.44142	-1.45435	-0.01566
H	-3.10681	-1.26082	-0.68817

Z-HPALD(II)-S0(09)

Geometry with 16 atoms:

Total energy: -420.845420153

C	-1.89971	-0.40427	0.12352
C	-1.05159	0.75687	-0.19034
C	0.22203	0.88424	0.18976
C	0.94501	-0.19726	0.97255
C	1.04431	2.08386	-0.16058
H	-1.44728	-1.21309	0.72253
H	-1.53613	1.53320	-0.77357
H	1.94042	0.15120	1.26235
H	0.39978	-0.47769	1.87577
H	1.90367	1.76946	-0.75946
H	1.43912	2.55654	0.74322
H	0.46917	2.82078	-0.71805
O	-3.04566	-0.48828	-0.24384
O	1.05924	-1.41246	0.25717
O	1.82266	-1.12111	-0.91029
H	2.58112	-1.70621	-0.78661

Z-HPALD(II)-S0(10)

Geometry with 16 atoms:

Total energy: -420.845937231

C	1.74061	0.09986	-0.18971
C	0.62518	1.03282	0.07348
C	-0.68968	0.82717	-0.04220
C	-1.38985	-0.43545	-0.47113
C	-1.66883	1.92868	0.25366
H	1.51134	-0.90912	-0.55164
H	0.96886	2.01166	0.39536
H	-2.25186	-0.60450	0.18437
H	-1.76788	-0.30619	-1.49094
H	-2.27138	1.67533	1.13009
H	-2.36224	2.06529	-0.58126
H	-1.16142	2.87246	0.44060
O	2.88465	0.45221	-0.02385
O	-0.61695	-1.60760	-0.54037
O	-0.24373	-1.93007	0.79767
H	-0.56176	-2.83986	0.86121

Z-HPALD(II)-S0(11)

Geometry with 16 atoms:

Total energy: -420.846531140

C	-1.00914	1.64418	-0.22491
C	0.41662	1.35040	0.02427
C	1.11447	0.20943	-0.01121
C	0.65614	-1.16769	-0.41678
C	2.58785	0.22767	0.28877
H	-1.17193	2.61067	-0.73637
H	0.98120	2.26118	0.21087
H	1.10536	-1.38365	-1.39355
H	1.05723	-1.89778	0.29515
H	3.15463	-0.23144	-0.52546
H	2.78708	-0.36288	1.18680
H	2.95860	1.23811	0.44683
O	-1.97408	1.00551	0.11943
O	-0.71072	-1.38263	-0.59496
O	-1.28346	-1.51893	0.69818
H	-1.72165	-0.64970	0.77369

Z-HPALD(II)-S0(12)

Geometry with 16 atoms:

Total energy: -420.846762371

C	-0.23429	1.93954	-0.06054
C	1.02066	1.18320	-0.19688
C	1.18492	-0.11605	0.08605
C	0.02781	-0.98550	0.51589
C	2.51452	-0.78868	-0.02786
H	-0.13914	3.02093	-0.26691
H	1.87584	1.76665	-0.52175
H	0.37089	-1.98217	0.80874
H	-0.48962	-0.52251	1.35777
H	2.44756	-1.61036	-0.74647
H	2.79304	-1.23395	0.93134
H	3.29908	-0.10197	-0.34024
O	-1.31238	1.49707	0.26748
O	-0.86279	-1.08559	-0.58413

O	-2.17882	-1.21779	-0.07896
H	-2.40748	-0.28118	0.04247

Z-HPALD(II)-S0(13)

Geometry with 16 atoms:
Total energy: -420.843708115

C	2.13468	0.13468	-0.32839
C	0.98699	1.06159	-0.40616
C	-0.20175	0.88927	0.18477
C	-0.56158	-0.36692	0.95231
C	-1.27693	1.92645	0.10259
H	3.04318	0.48997	-0.85137
H	1.16830	1.97247	-0.96865
H	0.24295	-0.66662	1.62264
H	-1.48271	-0.20700	1.51996
H	-0.97346	2.79033	-0.48662
H	-1.54553	2.26344	1.10810
H	-2.17686	1.48245	-0.33034
O	2.15426	-0.92085	0.25396
O	-0.73115	-1.48673	0.10605
O	-1.84139	-1.19302	-0.73960
H	-1.41809	-1.19063	-1.60777

c. Structures depicted in Figure S4.

1-01(T2)

Geometry with 16 atoms:
Total energy: -420.763859499

C	-1.87924	-0.57057	-0.28270
C	-1.22140	0.59572	-0.80007
C	0.05037	1.07359	-0.26564
C	1.30877	0.45947	-0.79926
H	-2.84699	-0.83712	-0.73417
H	1.37821	0.56910	-1.88633
H	2.18326	0.91995	-0.33212
O	1.35360	-0.94711	-0.61535
O	1.40227	-1.18725	0.78402
H	0.45861	-1.33817	0.97671
C	0.04087	1.85743	1.00550
H	1.01583	2.30892	1.19019
H	-0.19004	1.20238	1.85552
H	-0.71599	2.64529	0.98884
H	-1.72283	1.13402	-1.60139
O	-1.42541	-1.25291	0.63080

1-02(T2)

Geometry with 16 atoms:
Total energy: -420.756175213

C	2.45737	-0.34002	0.39605
C	1.24247	0.10262	1.02255
C	0.05056	0.38732	0.23294
C	-0.70346	-0.77149	-0.33779
H	3.32437	-0.51870	1.05339
H	-0.29564	-1.05052	-1.31895
H	-0.64904	-1.64392	0.32133
O	-2.05265	-0.45701	-0.62528
O	-2.68177	-0.14584	0.61601
H	-3.36077	-0.83129	0.65523
C	-0.10090	1.73040	-0.40255
H	-1.13308	1.88400	-0.71786
H	0.54541	1.80798	-1.28701
H	0.18374	2.52902	0.28403
H	1.23628	0.21648	2.10414
O	2.54348	-0.52792	-0.81092

1-03(T2)

Geometry with 16 atoms:
Total energy: -420.756485615

C	-1.81722	-1.07143	-0.33826
C	-0.70853	-0.37566	-0.92965
C	-0.06632	0.73016	-0.22390
C	0.88897	0.37726	0.86843
H	-2.25327	-1.90314	-0.91567
H	1.53040	1.23127	1.11309
H	0.34976	0.06606	1.77390
O	1.67332	-0.76073	0.56185
O	2.43353	-0.44452	-0.60227
H	3.33381	-0.49455	-0.25676
C	-0.72686	2.06822	-0.20542
H	-0.04121	2.83808	0.15354
H	-1.60277	2.05638	0.45614
H	-1.07624	2.35188	-1.19994
H	-0.34114	-0.70741	-1.89635
O	-2.27179	-0.77099	0.75852

1-04(T2)

Geometry with 16 atoms:
Total energy: -420.756226789

C	2.41588	-0.46587	0.37528
C	1.17496	-0.13785	1.02198
C	0.04060	0.35162	0.24713
C	-0.74303	-0.62871	-0.57137
H	3.23920	-0.81882	1.01759
H	-0.64901	-1.64522	-0.18212
H	-0.40038	-0.61712	-1.61412
O	-2.11389	-0.28055	-0.66977
O	-2.69602	-0.48152	0.61016
H	-2.68080	0.40981	0.98452
C	-0.00062	1.79558	-0.13891
H	-0.96901	2.04968	-0.57261
H	0.19144	2.44932	0.71400
H	0.77272	2.00250	-0.89025
H	1.10489	-0.26895	2.09891
O	2.56794	-0.36916	-0.83545

1-05(T2)

Geometry with 16 atoms:
Total energy: -420.755754186

C	1.76739	-0.38593	-0.26047
C	1.12204	0.64263	0.51245
C	-0.29396	0.96980	0.36477

C	-1.28709	0.05387	1.00093
H	1.13056	-0.93317	-0.97523
H	-1.06363	-0.11339	2.05873
H	-2.30427	0.44141	0.89727
O	-1.22220	-1.26853	0.46467
O	-1.52703	-1.15622	-0.92489
H	-2.28749	-1.74702	-0.99633
C	-0.71002	1.93268	-0.69819
H	-1.74312	2.25330	-0.55590
H	-0.64400	1.46238	-1.68804
H	-0.06534	2.81389	-0.71273
H	1.75197	1.17176	1.22428
O	2.95363	-0.65368	-0.13591

1-06(T2)

Geometry with 16 atoms:
Total energy: -420.755699221

C	-2.36063	-0.06842	0.29052
C	-1.06349	-0.11804	-0.31783
C	0.08506	0.62827	0.18450
C	1.09804	-0.06603	1.03621
H	-2.45759	0.58004	1.17971
H	1.44287	0.58456	1.84634
H	0.70377	-0.99413	1.45918
O	2.30335	-0.33319	0.32024
O	1.94869	-1.16411	-0.78078
H	2.38275	-1.99410	-0.54449
C	0.50320	1.88178	-0.51290
H	1.19555	2.45758	0.10382
H	-0.35640	2.50470	-0.76496
H	1.02461	1.64163	-1.44806
H	-0.96095	-0.75099	-1.19826
O	-3.32050	-0.69953	-0.12899

1-07(T2)

Geometry with 16 atoms:
Total energy: -420.755498861

C	1.90428	-0.39857	-0.21005
C	1.18382	0.60641	0.52544
C	-0.22702	0.90307	0.30071
C	-1.29055	0.11353	0.98987
H	1.33000	-0.95634	-0.96748
H	-0.87071	-0.56721	1.73551
H	-2.02176	0.77112	1.47376
O	-2.10351	-0.61357	0.07105
O	-1.24511	-1.52259	-0.61083
H	-1.57370	-2.37346	-0.29252
C	-0.62758	1.79073	-0.83244
H	-1.63769	2.17784	-0.68571
H	-0.63127	1.23162	-1.77652
H	0.06413	2.62678	-0.94911
H	1.76604	1.15983	1.25977
O	3.08827	-0.63399	-0.01507

1-08(T2)

Geometry with 16 atoms:
Total energy: -420.755377501

C	2.00161	-0.91382	0.37897
C	0.82011	-0.32670	0.95230
C	0.03666	0.65005	0.19669
C	-0.85745	0.11949	-0.87995
H	2.54768	-1.64583	0.99635
H	-0.26628	-0.38185	-1.65729
H	-1.43995	0.92413	-1.33581
O	-1.72925	-0.90131	-0.42307
O	-2.70230	-0.28537	0.40972
H	-2.37225	-0.48581	1.29549
C	0.53999	2.05378	0.11076
H	0.87624	2.41758	1.08343
H	1.39792	2.11124	-0.57162
H	-0.23715	2.72214	-0.26303
H	0.53525	-0.63347	1.95507
O	2.39568	-0.62892	-0.74356

1-09(T2)

Geometry with 16 atoms:
Total energy: -420.754721686

C	-2.37338	-0.11253	0.21191
C	-1.05901	-0.08299	-0.36067
C	0.07476	0.56346	0.29567
C	1.05771	-0.31150	1.00322
H	-2.48701	0.37879	1.19522
H	0.55749	-1.01154	1.67838
H	1.78177	0.28579	1.56467
O	1.74935	-1.18553	0.11082
O	2.47745	-0.35408	-0.78977
H	3.38531	-0.62406	-0.60163
C	0.44663	1.95297	-0.10683
H	0.92562	1.95037	-1.09429
H	-0.43210	2.59812	-0.16917
H	1.15611	2.38717	0.59901
H	-0.93791	-0.56890	-1.32703
O	-3.33050	-0.64191	-0.33416

1-10(T2)

Geometry with 16 atoms:
Total energy: -420.754476157

C	-2.36671	-0.08017	0.28632
C	-1.07197	-0.13694	-0.32814
C	0.08253	0.60143	0.17148
C	1.09146	-0.08866	1.03134
H	-2.45287	0.55802	1.18407
H	1.40543	0.55136	1.86210
H	0.70735	-1.03118	1.42885
O	2.31828	-0.33075	0.34867
O	2.01539	-1.25892	-0.69248
H	2.40781	-0.81734	-1.45602
C	0.46717	1.88794	-0.48477
H	1.23688	2.40422	0.09067
H	-0.39514	2.54777	-0.60205

H	0.87095	1.71335	-1.49053
H	-0.98196	-0.76999	-1.20984
O	-3.33534	-0.69256	-0.13928

1-11(T2)

Geometry with 16 atoms:
Total energy: -420.753767001

C	2.47101	-0.60657	0.23391
C	1.45314	0.08679	0.97492
C	0.23511	0.54669	0.31735
C	-0.82530	-0.45454	0.00276
H	3.37374	-0.91211	0.78786
H	-0.72316	-1.35959	0.60664
H	-0.78448	-0.73656	-1.05925
O	-2.08006	0.16139	0.27637
O	-3.08383	-0.77784	-0.08323
H	-3.44322	-0.38550	-0.88952
C	0.26434	1.83672	-0.43662
H	-0.74723	2.17663	-0.65825
H	0.78194	2.61642	0.12441
H	0.80168	1.70174	-1.38474
H	1.61716	0.26315	2.03522
O	2.35561	-0.86089	-0.95768

1-12(T2)

Geometry with 16 atoms:
Total energy: -420.753829336

C	-2.38114	-0.11670	0.21505
C	-1.07451	-0.08581	-0.37715
C	0.07451	0.54127	0.27057
C	1.04779	-0.33672	0.98782
H	-2.47749	0.35774	1.20819
H	1.74353	0.25770	1.58592
H	0.53879	-1.05765	1.63316
O	1.79491	-1.18048	0.11292
O	2.62780	-0.31688	-0.65974
H	2.42515	-0.61385	-1.55560
C	0.42932	1.94747	-0.08756
H	1.18341	2.34424	0.59266
H	-0.44885	2.59721	-0.06562
H	0.84526	2.00055	-1.10176
H	-0.98349	-0.55655	-1.35463
O	-3.34798	-0.63094	-0.32752

1-13(T2)

Geometry with 16 atoms:
Total energy: -420.754345826

C	2.05953	-0.49071	-0.24811
C	1.27759	0.48581	0.45878
C	-0.13205	0.72666	0.17661
C	-1.18879	0.04965	0.99406
H	1.52894	-1.07283	-1.02199
H	-0.77410	-0.77072	1.58428
H	-1.68873	0.75584	1.66962
O	-2.26291	-0.43247	0.20012
O	-1.76274	-1.51643	-0.57057
H	-1.66944	-1.11672	-1.44570
C	-0.52682	1.85487	-0.72208
H	-1.58261	1.78281	-0.98756
H	0.06990	1.86579	-1.63696
H	-0.36907	2.82403	-0.23103
H	1.80705	1.05035	1.22527
O	3.24332	-0.68563	-0.01847

1-14(T2)

Geometry with 16 atoms:
Total energy: -420.754613710

C	1.83463	0.01043	-0.28539
C	0.78691	0.54947	0.53539
C	-0.53345	0.87523	0.00778
C	-1.67464	-0.05644	0.27322
H	1.58858	-0.13101	-1.35253
H	-2.39044	-0.02676	-0.55696
H	-2.21506	0.22167	1.18921
O	-1.28467	-1.38680	0.52756
O	-0.73130	-1.88763	-0.68890
H	0.09709	-2.27061	-0.37032
C	-0.85769	2.28532	-0.36679
H	-0.03651	2.74879	-0.91578
H	-1.75564	2.32517	-0.98684
H	-1.04298	2.90573	0.52050
H	1.03667	0.71088	1.58365
O	2.93893	-0.28405	0.14931

1-15(T2)

Geometry with 16 atoms:
Total energy: -420.753939592

C	2.44623	-0.32894	0.00845
C	1.56251	0.52495	0.75428
C	0.14539	0.63141	0.42171
C	-0.70717	-0.54690	0.78542
H	3.50559	-0.33981	0.31499
H	-0.41690	-1.42674	0.19359
H	-0.58596	-0.79772	1.84447
O	-2.09489	-0.31486	0.63785
O	-2.40169	-0.39462	-0.74941
H	-2.85544	-1.24646	-0.79707
C	-0.27814	1.58103	-0.65140
H	-1.33694	1.82108	-0.55455
H	-0.12929	1.13372	-1.64243
H	0.30502	2.50194	-0.60595
H	1.98536	1.09110	1.58122
O	2.06104	-1.02882	-0.91907

1-16(T2)

Geometry with 16 atoms:
Total energy: -420.754972731

C	2.13826	-0.28702	0.00834
C	1.41275	0.89619	0.36934
C	-0.04181	0.97394	0.27085

C	-0.88158	0.07640	1.12661
H	3.23589	-0.23926	0.07591
H	-1.48025	0.63477	1.85573
H	-0.24472	-0.62966	1.67365
O	-1.86551	-0.62928	0.38898
O	-1.28291	-1.21322	-0.76906
H	-0.46054	-1.62863	-0.45377
C	-0.65138	1.67785	-0.89587
H	-1.73779	1.67586	-0.81107
H	-0.29345	2.70834	-0.96954
H	-0.39704	1.16574	-1.83025
H	1.98920	1.73060	0.76268
O	1.58983	-1.33774	-0.31730

1-17(T2)

Geometry with 16 atoms:
Total energy: -420.752415258

C	-2.00291	-0.64973	-0.24356
C	-1.36444	0.52701	-0.76889
C	-0.08537	1.01039	-0.25386
C	1.16365	0.53578	-0.92214
H	-2.95014	-0.94977	-0.72358
H	1.06055	0.54709	-2.01090
H	2.01495	1.15892	-0.63153
O	1.46495	-0.83074	-0.65232
O	1.74029	-0.91835	0.74211
H	2.66038	-1.21133	0.73024
C	-0.04329	1.62885	1.10274
H	0.90597	2.13834	1.27290
H	-0.14857	0.84341	1.86165
H	-0.86103	2.33903	1.24645
H	-1.88570	1.07666	-1.54961
O	-1.55553	-1.28294	0.70004

1-18(T2)

Geometry with 16 atoms:
Total energy: -420.754251864

C	1.80689	-1.22938	0.24502
C	0.98479	-0.31016	0.98272
C	0.32492	0.80334	0.30217
C	-0.93469	0.49640	-0.43433
H	2.26907	-2.05339	0.81295
H	-1.41620	1.41169	-0.79381
H	-0.73540	-0.16269	-1.29028
O	-1.78877	-0.18798	0.47495
O	-2.88451	-0.68232	-0.28244
H	-3.61205	-0.14401	0.05450
C	1.14197	1.98499	-0.10438
H	0.50634	2.83549	-0.35533
H	1.75124	1.74114	-0.98435
H	1.82795	2.28296	0.69049
H	0.85960	-0.46890	2.04931
O	1.99905	-1.11889	-0.95886

1-19(T2)

Geometry with 16 atoms:
Total energy: -420.755489368

C	1.50303	-1.29959	0.20446
C	0.67124	-0.38900	0.93819
C	0.20211	0.84711	0.31623
C	-0.95477	0.77073	-0.62973
H	1.83187	-2.21057	0.73122
H	-0.69558	0.16966	-1.51314
H	-1.24311	1.77187	-0.95760
O	-2.14247	0.25309	-0.04498
O	-1.92069	-1.12048	0.23980
H	-2.37373	-1.55374	-0.49630
C	1.17530	1.97303	0.17027
H	0.66394	2.90886	-0.06152
H	1.75897	2.11137	1.08198
H	1.88546	1.76103	-0.63969
H	0.38615	-0.64962	1.95248
O	1.83872	-1.09793	-0.95657

1-20(T2)

Geometry with 16 atoms:
Total energy: -420.753779424

C	-2.37770	-0.79686	-0.33203
C	-1.15525	-0.25893	-0.86193
C	-0.24244	0.51701	-0.02841
C	0.94435	-0.16037	0.56013
H	-3.00936	-1.37059	-1.02998
H	1.26880	0.34153	1.47736
H	0.74716	-1.21362	0.77348
O	1.98836	-0.07890	-0.41824
O	3.09639	-0.80878	0.09870
H	3.71896	-0.10007	0.30592
C	-0.39695	2.00015	0.02695
H	0.28827	2.43572	0.75436
H	-1.42027	2.26985	0.30253
H	-0.19232	2.46074	-0.94666
H	-0.92718	-0.43763	-1.91065
O	-2.72301	-0.63630	0.83020

1-21(T2)

Geometry with 16 atoms:
Total energy: -420.754612827

C	1.65208	-1.32035	0.24028
C	1.01940	-0.27642	0.99749
C	0.39790	0.86067	0.32021
C	-0.90716	0.62866	-0.36311
H	2.10094	-2.15039	0.81040
H	-0.74653	0.10794	-1.31978
H	-1.42563	1.57239	-0.55753
O	-1.69539	-0.18935	0.48884
O	-2.91166	-0.44609	-0.19351
H	-2.78507	-1.35694	-0.49089
C	1.27646	1.95361	-0.19592
H	1.81091	1.62064	-1.09514
H	0.69082	2.83656	-0.45682

H	2.02774	2.23886	0.54221
H	0.99919	-0.36273	2.07963
O	1.69399	-1.31247	-0.98355

1-22(T2)

Geometry with 16 atoms:
Total energy: -420.753942108

C	2.48013	-0.61396	0.26870
C	1.41135	0.03675	0.97657
C	0.23043	0.51955	0.27123
C	-0.83978	-0.44297	-0.11709
H	3.35140	-0.93404	0.86367
H	-0.68878	-1.42790	0.33447
H	-0.88273	-0.55712	-1.20732
O	-2.07510	0.11607	0.32658
O	-3.11259	-0.66053	-0.26059
H	-3.47151	-1.12060	0.50888
C	0.26838	1.86160	-0.38343
H	-0.73603	2.17502	-0.66813
H	0.70038	2.61807	0.27438
H	0.89002	1.81919	-1.28718
H	1.51288	0.16713	2.05159
O	2.44035	-0.81873	-0.93678

1-23(T2)

Geometry with 16 atoms:
Total energy: -420.753519664

C	1.85809	-0.69877	-0.30269
C	1.33983	0.29947	0.59366
C	0.07625	0.99545	0.36231
C	-1.19639	0.29449	0.69674
H	1.24784	-0.92017	-1.19477
H	-1.09417	-0.32591	1.59236
H	-2.01851	1.00204	0.83397
O	-1.49652	-0.54599	-0.42280
O	-2.73512	-1.18746	-0.13767
H	-2.45514	-2.10262	-0.00581
C	0.05472	2.19152	-0.53251
H	-0.86881	2.75805	-0.40548
H	0.11313	1.88956	-1.58612
H	0.90514	2.84810	-0.33903
H	1.94774	0.51619	1.46938
O	2.91011	-1.28632	-0.09824

1-24(T2)

Geometry with 16 atoms:
Total energy: -420.753093886

C	1.86285	-0.70682	-0.30348
C	1.34125	0.29216	0.59089
C	0.07742	0.98742	0.35909
C	-1.19541	0.29032	0.69970
H	1.24470	-0.94736	-1.18466
H	-1.09089	-0.33668	1.58878
H	-2.01265	1.00341	0.84830
O	-1.50143	-0.55313	-0.41603
O	-2.65382	-1.30888	-0.05659
H	-3.31729	-0.95086	-0.66024
C	0.05969	2.18790	-0.53017
H	-0.87379	2.74218	-0.42223
H	0.15168	1.89478	-1.58393
H	0.89555	2.85571	-0.31192
H	1.94982	0.51408	1.46482
O	2.92752	-1.27314	-0.10678

1-25(T2)

Geometry with 16 atoms:
Total energy: -420.752916959

C	-2.43237	-0.37323	0.31670
C	-1.23440	-0.07924	-0.41590
C	-0.10156	0.63196	0.17039
C	1.07547	-0.15163	0.64665
H	-2.45519	-0.03756	1.36900
H	0.79171	-1.15125	0.98399
H	1.59419	0.37330	1.45633
O	1.95788	-0.27522	-0.47196
O	3.05371	-1.07615	-0.04269
H	3.77838	-0.43780	-0.05590
C	0.05733	2.09360	-0.09687
H	0.78790	2.53560	0.58244
H	0.41255	2.26576	-1.12070
H	-0.89176	2.62261	0.00832
H	-1.20664	-0.41077	-1.45256
O	-3.38634	-0.95970	-0.17243

1-26(T2)

Geometry with 16 atoms:
Total energy: -420.753290458

C	-2.43840	-0.37137	0.31898
C	-1.24621	-0.07114	-0.42061
C	-0.10330	0.62543	0.16311
C	1.06738	-0.16816	0.63828
H	-2.45363	-0.04383	1.37384
H	0.77691	-1.17452	0.95352
H	1.57681	0.33922	1.46323
O	1.97184	-0.25589	-0.46605
O	3.14241	-0.90919	0.01169
H	3.09134	-1.75979	-0.44328
C	0.07247	2.08622	-0.09721
H	0.80724	2.51540	0.58542
H	0.43571	2.25734	-1.11816
H	-0.87108	2.62529	0.00661
H	-1.23322	-0.38780	-1.46247
O	-3.39447	-0.95707	-0.16738

1-27(T2)

Geometry with 16 atoms:
Total energy: -420.752311740

C	2.21222	-0.82462	0.20554
C	1.53712	0.25312	0.87917
C	0.30993	0.84350	0.35530

C	-1.01686	0.29703	0.75922
H	3.13479	-1.19952	0.68041
H	-0.93050	-0.42963	1.57239
H	-1.69094	1.10430	1.07179
O	-1.58181	-0.32664	-0.39098
O	-2.90961	-0.69991	-0.03426
H	-2.85756	-1.66193	-0.09957
C	0.38738	1.79118	-0.79555
H	-0.55076	2.33520	-0.91253
H	0.57115	1.23700	-1.72341
H	1.20474	2.50520	-0.67166
H	1.99158	0.63938	1.78905
O	1.81001	-1.30986	-0.84084

1-28(T2)

Geometry with 16 atoms:

Total energy: -420.751772084

C	1.70450	-1.23887	0.30245
C	1.13456	-0.13086	1.01984
C	0.38889	0.91935	0.32878
C	-1.09806	0.81492	0.29163
H	2.22807	-2.00020	0.90431
H	-1.53113	0.91601	1.29493
H	-1.53070	1.58120	-0.35783
O	-1.42735	-0.48343	-0.19385
O	-2.83686	-0.62308	-0.03824
H	-3.11454	-0.74436	-0.95493
C	1.13297	1.88600	-0.53024
H	0.51839	2.75027	-0.78394
H	1.44042	1.39253	-1.46123
H	2.04368	2.23599	-0.03896
H	1.30278	-0.07727	2.09302
O	1.64745	-1.33817	-0.91417

1-29(T2)

Geometry with 16 atoms:

Total energy: -420.761203169

C	1.94788	-0.51327	0.28862
C	1.17368	0.52890	0.90539
C	-0.06670	1.02986	0.32206
C	-1.39166	0.44308	0.70033
H	2.90617	-0.76886	0.76619
H	-1.36827	-0.02568	1.68649
H	-2.16054	1.22118	0.68340
O	-1.85886	-0.50514	-0.25227
O	-1.10686	-1.69484	-0.07156
H	-0.32802	-1.54688	-0.63589
C	0.02680	1.87825	-0.90529
H	-0.92312	2.37460	-1.10764
H	0.27474	1.25900	-1.77592
H	0.81074	2.63368	-0.81416
H	1.58778	0.98936	1.79975
O	1.59829	-1.09219	-0.73478

d. Structures depicted in Figure S5.

TS1-11-01(T2)

Geometry with 16 atoms:

Total energy: -420.724163631

C	-2.33793	-0.82660	-0.25390
C	-0.99970	-0.60038	-0.71914
C	-0.14931	0.37746	-0.04705
C	0.92904	-0.10845	0.83758
H	-2.93427	-1.57529	-0.79851
H	1.27431	0.60546	1.58732
H	0.79832	-1.10962	1.25109
O	1.67324	-0.08885	-0.33903
O	3.24944	-0.62407	0.07550
H	3.70522	0.04267	-0.45586
C	-0.39045	1.83008	-0.24841
H	0.43471	2.41743	0.15117
H	-1.31382	2.10176	0.27637
H	-0.52903	2.07177	-1.30388
H	-0.62135	-1.15229	-1.57254
O	-2.81318	-0.21640	0.69483

TS1-11-02(T2)

Geometry with 16 atoms:

Total energy: -420.723908901

C	-2.32608	-0.84690	-0.24421
C	-0.99499	-0.60256	-0.72211
C	-0.15229	0.38772	-0.05932
C	0.92599	-0.07659	0.83691
H	-2.91835	-1.60140	-0.78551
H	1.24806	0.64367	1.59129
H	0.81076	-1.08055	1.24796
O	1.68468	-0.03763	-0.32879
O	3.26313	-0.54593	0.11773
H	3.45708	-0.96937	-0.72935
C	-0.40432	1.83663	-0.27458
H	0.42656	2.43048	0.10268
H	-1.31939	2.11095	0.26345
H	-0.56188	2.06487	-1.33022
H	-0.62268	-1.14705	-1.58300
O	-2.79906	-0.24661	0.71139

TS1-11-03(T2)

Geometry with 16 atoms:

Total energy: -420.723021040

C	1.83961	-0.68715	-0.27278
C	1.27788	0.39383	0.49363
C	-0.04693	0.95307	0.26058
C	-1.22594	0.30723	0.87826
H	1.20496	-1.09940	-1.07224
H	-1.02951	-0.31055	1.75577
H	-2.09775	0.95056	1.01155
O	-1.24452	-0.41119	-0.31243
O	-2.58194	-1.48939	-0.20294
H	-2.10217	-2.25600	-0.54558
C	-0.20838	2.15566	-0.60351
H	-1.25805	2.31440	-0.84554

H	0.36436	2.05888	-1.52768
H	0.16993	3.04099	-0.07909
H	1.90478	0.81039	1.27854
O	2.95471	-1.13007	-0.04873

TS1-11-04(T2)

Geometry with 16 atoms:
Total energy: -420.722916019

C	1.84249	-0.70176	-0.27306
C	1.29082	0.39657	0.47740
C	-0.04114	0.94636	0.26259
C	-1.20660	0.29175	0.89702
H	1.18858	-1.15112	-1.03533
H	-2.08534	0.92512	1.03148
H	-0.99499	-0.31581	1.77836
O	-1.22495	-0.44129	-0.28453
O	-2.55248	-1.52660	-0.15350
H	-2.80373	-1.46331	-1.08515
C	-0.22130	2.14655	-0.60120
H	0.32340	2.04249	-1.54159
H	-1.27632	2.31447	-0.81210
H	0.17941	3.03119	-0.09272
H	1.93186	0.83375	1.23941
O	2.97137	-1.11882	-0.06933

TS1-11-05(T2)

Geometry with 16 atoms:
Total energy: -420.721086436

C	-2.36508	-0.31591	0.28181
C	-1.12108	-0.19954	-0.42507
C	-0.00724	0.58625	0.09664
C	1.05299	-0.08474	0.88231
H	-2.42594	0.18952	1.26227
H	1.62506	0.56387	1.54853
H	0.77551	-1.02672	1.35815
O	1.63009	-0.24601	-0.37001
O	3.13055	-1.04898	-0.10344
H	3.57835	-0.63789	-0.85550
C	0.06489	2.04671	-0.18785
H	1.04167	2.44381	0.08436
H	-0.70242	2.57361	0.39163
H	-0.12886	2.25486	-1.24173
H	-1.03631	-0.71048	-1.37890
O	-3.31988	-0.93590	-0.15854

TS1-11-06(T2)

Geometry with 16 atoms:
Total energy: -420.721261539

C	-2.35212	-0.32903	0.29209
C	-1.11426	-0.19881	-0.42331
C	-0.00710	0.60430	0.08576
C	1.05814	-0.04354	0.88365
H	-2.41525	0.18282	1.26893
H	1.61485	0.61860	1.54979
H	0.79185	-0.98606	1.36428
O	1.64726	-0.20116	-0.36415
O	3.14870	-1.00189	-0.09445
H	3.06203	-1.59708	-0.85173
C	0.05364	2.06057	-0.22164
H	1.03378	2.46365	0.02854
H	-0.70661	2.59274	0.36248
H	-0.15658	2.25202	-1.27538
H	-1.03279	-0.71088	-1.37692
O	-3.29860	-0.96904	-0.13755

TS1-11-07(T2)

Geometry with 16 atoms:
Total energy: -420.719743104

C	1.95811	-0.95622	0.34745
C	1.27351	0.15736	0.95170
C	0.21340	0.89551	0.26947
C	-1.18539	0.72189	0.71809
H	2.70355	-1.46857	0.97746
H	-1.31990	0.35841	1.73917
H	-1.85510	1.55376	0.48758
O	-1.19124	-0.28301	-0.23265
O	-2.76271	-0.99996	-0.15523
H	-2.48975	-1.81669	-0.59520
C	0.55860	1.78082	-0.87441
H	-0.34329	2.17311	-1.34135
H	1.13953	1.22434	-1.61317
H	1.17504	2.61959	-0.53098
H	1.60464	0.49537	1.93007
O	1.76344	-1.30898	-0.80304

TS1-11-08(T2)

Geometry with 16 atoms:
Total energy: -420.717327031

C	0.51777	1.97774	-0.03792
C	-0.77239	1.38239	0.16220
C	-1.10783	-0.04074	0.21229
C	-0.21230	-0.96478	0.93136
H	0.52004	3.07952	-0.03881
H	0.48375	-0.49792	1.62831
H	-0.66204	-1.87601	1.32803
O	1.57317	1.36485	-0.14851
O	0.32950	-1.11162	-0.34942
O	1.90424	-1.64394	-0.22581
H	2.27553	-0.75530	-0.34855
C	-2.34061	-0.51960	-0.47151
H	-2.39757	-1.60609	-0.44109
H	-2.37009	-0.19515	-1.51428
H	-3.22965	-0.10849	0.02229
H	-1.58311	2.07501	0.37546

e. Structures depicted in Figure S6.

11E

Geometry with 14 atoms:
Total energy: -345.054564525

C	-1.83978	0.22180	0.06270

C	-0.61724	-0.50173	-0.07495
C	0.71879	0.08633	0.00812
C	1.77916	-0.74369	0.63719
H	-1.77171	1.31129	0.21689
H	2.61007	-0.22679	1.10730
H	1.52955	-1.72152	1.03516
O	1.69915	-0.62138	-0.76345
C	0.87054	1.58457	0.00905
H	0.41037	2.01951	-0.87942
H	1.92937	1.83840	0.00775
H	0.40500	2.02388	0.89241
H	-0.68870	-1.56896	-0.25106
O	-2.93574	-0.32356	0.01574

TS11E-12E

Geometry with 14 atoms:
Total energy: -345.031556889

C	1.87831	0.19498	0.06391
C	0.60163	-0.46676	-0.18266
C	-0.60408	0.17969	-0.23072
C	-1.82637	-0.64377	-0.52796
H	1.85428	1.28015	0.26199
H	-2.65989	-0.04563	-0.90720
H	-1.65694	-1.54919	-1.11489
O	-1.79419	-0.80342	0.83189
C	-0.81995	1.64040	0.02260
H	-0.14551	2.03986	0.77675
H	-1.84171	1.79821	0.36362
H	-0.67840	2.20092	-0.90497
H	0.64554	-1.53717	-0.34815
O	2.93236	-0.39838	0.04333

12E

Geometry with 14 atoms:
Total energy: -345.045214278

C	-2.05938	0.18566	-0.05915
C	-0.76427	-0.50247	0.04621
C	0.43070	0.09127	0.11714
C	1.65969	-0.77762	0.27744
H	-2.04946	1.28821	-0.09520
H	2.00139	-0.71167	1.33168
H	1.44056	-1.84139	0.11265
O	2.74885	-0.37853	-0.43990
C	0.71134	1.56112	0.07583
H	-0.18416	2.17225	0.02178
H	1.34644	1.78253	-0.78342
H	1.28055	1.85171	0.96313
H	-0.83730	-1.58594	0.06901
O	-3.10716	-0.40941	-0.10566

TS11E-11Z

Geometry with 14 atoms:
Total energy: -345.048342593

C	1.75926	0.10536	0.26565
C	0.63255	-0.29749	-0.52333
C	-0.75197	0.09353	-0.16027
C	-1.83614	-0.87388	-0.36361
H	1.54717	0.70506	1.16766
H	-2.84723	-0.50636	-0.50335
H	-1.61288	-1.84244	-0.79875
O	-1.29252	-0.65763	0.93182
C	-1.04802	1.57152	-0.12471
H	-0.38614	2.07988	0.57834
H	-2.07824	1.73224	0.19200
H	-0.90253	2.01414	-1.11134
H	0.82875	-0.92579	-1.38417
O	2.90715	-0.19875	-0.01967

11Z

Geometry with 14 atoms:
Total energy: -345.054504102

C	1.73313	-0.18991	0.12855
C	0.60299	0.62399	-0.20049
C	-0.78681	0.17827	-0.05966
C	-1.16525	-1.14238	-0.62825
H	1.52256	-1.18862	0.54223
H	-2.19356	-1.28858	-0.94402
H	-0.41163	-1.73802	-1.13373
O	-0.97256	-0.97658	0.75982
C	-1.83712	1.24828	0.08217
H	-1.64607	1.84925	0.97237
H	-2.82275	0.79443	0.17369
H	-1.82791	1.90701	-0.78760
H	0.80168	1.61522	-0.59040
O	2.88456	0.19406	-0.03062

TS11Z-12Z

Geometry with 14 atoms:
Total energy: -345.032136867

C	-1.72408	-0.18722	0.08934
C	-0.57066	0.70552	-0.00930
C	0.73419	0.31977	0.17340
C	1.08538	-1.08490	0.56687
H	-1.52319	-1.25497	0.27126
H	2.10321	-1.16219	0.95984
H	0.36656	-1.63174	1.17978
O	0.97083	-1.24452	-0.78999
C	1.87807	1.26133	-0.02980
H	1.58554	2.12613	-0.62293
H	2.69243	0.74335	-0.53581
H	2.24648	1.60694	0.93938
H	-0.79676	1.73265	-0.27468
O	-2.85729	0.21362	-0.04250

12Z

Geometry with 14 atoms:
Total energy: -345.043859196

C	-1.87936	-0.39982	-0.00000
C	-0.85567	0.65132	0.00000
C	0.46223	0.41872	-0.00000

C	1.04638	-0.98467	-0.00001
H	-1.52704	-1.44887	-0.00001
H	0.69372	-1.56876	0.86731
H	0.69377	-1.56872	-0.86737
O	2.40629	-1.05087	0.00001
C	1.46366	1.52798	-0.00000
H	0.97223	2.49843	0.00000
H	2.11718	1.44822	-0.87175
H	2.11719	1.44822	0.87173
H	-1.23775	1.66661	0.00001
O	-3.06289	-0.16867	0.00000

TS12Z-13

Geometry with 14 atoms:
Total energy: -345.038881297

C	-1.55829	-0.15159	0.02661
C	-0.32998	-0.95057	-0.03135
C	0.86309	-0.35905	0.00196
C	1.04656	1.14677	0.09680
H	-1.30683	0.97161	0.09359
H	1.49971	1.33976	1.08195
H	1.79076	1.40797	-0.67245
O	-0.07611	1.90965	-0.11311
C	2.15203	-1.12088	-0.02113
H	1.98531	-2.19176	0.07377
H	2.80565	-0.79159	0.78993
H	2.68076	-0.93019	-0.95830
H	-0.43795	-2.02849	-0.07072
O	-2.68113	-0.55533	0.01623

13

Geometry with 14 atoms:
Total energy: -345.073010979

C	-1.65145	-0.07692	0.06060
C	-0.44848	-0.90583	-0.05325
C	0.79583	-0.41862	0.00823
C	1.17521	1.03191	0.17002
H	-0.62545	1.76808	0.15118
H	1.49064	1.15351	1.21830
H	2.06663	1.21005	-0.43724
O	0.24317	2.00410	-0.20277
C	1.97959	-1.33651	-0.04206
H	1.68852	-2.38257	0.02560
H	2.67023	-1.10811	0.77384
H	2.52742	-1.18152	-0.97508
H	-0.62143	-1.97477	-0.15646
O	-2.78077	-0.41020	0.02010

TS13-14a

Geometry with 14 atoms:
Total energy: -345.027980640

C	-2.16934	0.13054	0.15154
C	-0.22820	-0.93040	-0.07028
C	0.97290	-0.41015	-0.00790
C	1.27965	1.06512	0.09020
H	-0.57834	1.60419	0.26860
H	1.71815	1.24090	1.08356
H	2.05918	1.29846	-0.64037
O	0.21677	1.94063	-0.15824
C	2.20299	-1.29065	0.00216
H	1.94210	-2.34672	0.02555
H	2.81857	-1.06398	0.87621
H	2.80692	-1.09735	-0.88723
H	-0.58821	-1.94767	-0.13091
O	-3.03257	-0.57496	-0.04048

14a

Geometry with 12 atoms:
Total energy: -231.717177535

C	-0.39569	1.47145	-0.02389
C	-0.48114	0.16631	-0.01215
C	0.74574	-0.71185	0.00039
H	1.89449	0.76183	0.50800
H	0.69566	-1.35680	0.88901
H	0.71978	-1.37083	-0.87189
O	1.96641	-0.01808	-0.05258
C	-1.79834	-0.57288	0.01401
H	-2.64130	0.11545	0.02115
H	-1.85923	-1.20873	0.90044
H	-1.88367	-1.21930	-0.86286
H	-1.08045	2.30480	-0.03339

15a

Geometry with 14 atoms:
Total energy: -382.106517086

C	-0.38437	-1.22221	-0.07922
C	0.67578	-0.45090	0.13090
C	0.59542	0.97260	0.63120
H	-0.34687	1.76015	-0.84517
H	-0.23883	1.09279	1.32687
H	1.51876	1.20562	1.16362
O	0.51510	1.89623	-0.43470
C	2.04675	-0.97500	-0.16977
H	2.02628	-1.98061	-0.58779
H	2.65624	-0.98277	0.73698
H	2.53589	-0.30757	-0.88371
H	-0.34219	-2.25688	-0.39233
O	-1.70914	-0.85302	0.12240
O	-1.98230	0.39708	-0.13734

TS15a-16

Geometry with 14 atoms:
Total energy: -382.068322966

C	-0.39250	-1.24407	-0.18763
C	0.65463	-0.45889	0.06896
C	0.43113	0.93947	0.53183
H	0.13089	1.68932	-1.20337
H	-0.83439	0.85312	0.71061
H	0.96244	1.21842	1.44130
O	0.59080	1.94949	-0.39465

C	2.06825	-0.96125	-0.01256
H	2.10507	-1.99687	-0.35024
H	2.55266	-0.90155	0.96542
H	2.65304	-0.34870	-0.70227
H	-0.31416	-2.28556	-0.47463
O	-1.69192	-0.90299	-0.01950
O	-1.87697	0.46853	0.06533

16

Geometry with 12 atoms:
Total energy: -306.435096955

C	0.08487	1.22390	-0.00000
C	-0.61899	-0.04119	0.00000
C	0.11654	-1.17883	-0.00000
H	1.76542	-0.30578	0.00000
H	-0.35312	-2.15857	-0.00000
O	1.43528	-1.23643	-0.00000
C	-2.12245	-0.05647	0.00000
H	-2.52934	0.44371	0.88129
H	-2.49670	-1.08024	-0.00003
H	-2.52934	0.44377	-0.88126
H	-0.53881	2.13490	-0.00001
O	1.30498	1.34116	0.00000

17

Geometry with 12 atoms:
Total energy: -306.421610458

C	-1.24442	-0.37280	-0.35848
C	-0.00000	0.20077	0.27854
C	1.24442	-0.37281	-0.35848
H	1.26311	-0.35455	-1.46861
O	2.18168	-0.78893	0.25928
C	0.00001	1.72223	0.02842
H	0.00002	1.94440	-1.04128
H	0.88639	2.17378	0.47295
H	-0.88636	2.17380	0.47294
H	-1.26313	-0.35452	-1.46861
O	-2.18169	-0.78892	0.25928
H	-0.00000	-0.02450	1.34408

TS14a-14b

Geometry with 12 atoms:
Total energy: -231.709123776

C	-0.37438	1.48633	-0.02145
C	-0.49777	0.19433	-0.01151
C	0.70045	-0.73992	-0.00529
H	1.91442	0.66212	0.53810
H	0.61855	-1.38886	0.87773
H	0.64482	-1.38605	-0.88534
O	1.94830	-0.09944	-0.05050
C	-1.83183	-0.52299	0.01562
H	-2.65850	0.18356	0.01785
H	-1.90400	-1.15396	0.90480
H	-1.92502	-1.17242	-0.85835
H	-0.25557	2.54468	-0.05495

14b

Geometry with 12 atoms:
Total energy: -231.715421745

C	0.37719	1.50671	0.00004
C	0.52158	0.20779	0.00002
C	-0.66367	-0.72596	-0.00004
H	-2.60563	-0.60738	-0.00012
H	-0.59418	-1.37140	-0.88568
H	-0.59425	-1.37143	0.88558
O	-1.86883	0.00805	-0.00007
C	1.86351	-0.47661	0.00006
H	2.67038	0.25326	0.00011
H	1.96983	-1.11427	-0.88138
H	1.96976	-1.11430	0.88148
H	-0.45696	2.18953	0.00003

15b

Geometry with 14 atoms:
Total energy: -382.104019056

C	-0.31762	-0.80454	-0.09921
C	0.28353	0.37775	-0.05142
C	1.78259	0.41539	0.02419
H	3.28295	-0.82304	0.10624
H	2.15346	0.94866	-0.86098
H	2.06226	1.01018	0.90435
O	2.32503	-0.88379	0.09642
C	-0.36941	1.72896	-0.07950
H	-1.23073	1.74643	-0.74472
H	0.35181	2.47928	-0.41024
H	-0.72645	2.00966	0.91246
H	0.21487	-1.74293	-0.12864
O	-1.68049	-1.03487	-0.17990
O	-2.44237	-0.07303	0.26563

18

Geometry with 17 atoms:
Total energy: -587.207262688

C	-0.56590	-0.36755	0.69346
C	-1.45598	0.43067	0.12409
C	-2.75366	-0.13704	-0.38671
H	-2.23123	-1.87877	-1.07264
H	-3.57046	0.20740	0.25302
H	-2.94186	0.27477	-1.38610
O	-2.82350	-1.54383	-0.39272
C	-1.28609	1.91164	-0.01922
H	-1.38933	2.19899	-1.06818
H	-0.31430	2.23987	0.33900
H	-2.06507	2.43669	0.53987
H	-0.68518	-1.43410	0.82738
O	0.57973	0.16677	1.27308
O	1.68346	0.87713	-0.82957
N	2.21278	-0.07460	-0.36037
O	1.67647	-0.59870	0.86902
O	3.14357	-0.71999	-0.71726

TS18-19

Geometry with 17 atoms:
Total energy: -587.183979206

C	-0.47534	-0.61540	0.94681
C	-1.06733	0.48176	0.37283
C	-2.39403	0.34826	-0.30194
H	-2.21892	-1.35781	-1.20658
H	-3.15559	0.80960	0.33642
H	-2.36032	0.94693	-1.22184
O	-2.80482	-0.96878	-0.54781
C	-0.48518	1.84866	0.43044
H	-0.28062	2.19938	-0.58380
H	0.43423	1.87574	1.00868
H	-1.21757	2.53453	0.86696
H	-0.93138	-1.59902	0.89313
O	0.67744	-0.48977	1.52403
O	2.42256	0.82683	-0.62154
N	1.73133	-0.16105	-0.58639
O	1.89423	-1.01447	0.42399
O	0.82836	-0.43652	-1.36330

19

Geometry with 17 atoms:
Total energy: -587.315080264

C	1.65441	-0.98483	0.48541
C	0.53577	0.06030	0.38703
C	0.80479	0.89541	-0.86394
H	0.36744	0.51810	-1.80435
O	1.51029	1.85910	-0.82599
C	0.45559	0.88548	1.65452
H	1.38095	1.45089	1.75884
H	-0.36793	1.59512	1.61479
H	0.33320	0.23035	2.51745
H	1.46916	-1.61468	1.36154
O	1.78649	-1.74231	-0.69062
O	-0.63255	-0.77831	0.19661
N	-1.81443	-0.12584	-0.12115
O	-1.75891	1.05608	-0.32998
O	-2.75488	-0.85355	-0.15409
H	1.01943	-2.31767	-0.77619
H	2.59182	-0.44755	0.63041