Supporting Information

Chemiluminogenic Features of 10-Methyl-9-(phenoxycarbonyl)acridinium Trifluoromethanesulfonates Alkyl Substituted at the Benzene Ring in Aqueous Media

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TABLE 1S. Elemental Analyses, MS Data, Retention Factors (R_f; TLC) and Retention Times (R_t; HPLC) for the Compounds Investigated or Their Precursors

cpd no.	elemental analyses[a]			$(M+1)^{+b}$	R_t[c]	R_f[d]
	C	H	N			
1	79.8/80.2	4.44/4.38	4.25/4.68	314	2.10	0.38
2	80.7/80.5	4.81/4.82	4.45/4.47	328	2.37	0.39
3	80.6/80.5	4.84/4.82	4.41/4.47	329	2.39	0.39
4	80.4/80.5	4.86/4.82	4.32/4.47	328	2.45	0.40
5	80.9/80.7	5.12/5.23	4.33/4.28	342	2.67	0.42
6	80.8/80.9	5.52/5.61	4.08/4.10	356	2.92	0.42
7	80.8/81.1	6.02/5.96	3.86/3.94	370	3.53	0.45
8	80.5/80.7	5.09/5.23	4.22/4.28	343	2.66	0.41
9	80.5/80.7	5.24/5.23	4.18/4.28	343	2.55	0.42
10	80.5/80.7	5.29/5.23	4.21/4.28	343	2.99	0.41
11	80.7/80.7	5.18/5.23	4.30/4.28	342	2.96	0.41
12	80.5/80.9	5.60/5.61	4.08/4.10	356	3.19	0.43

[a] Elemental analysis of phenyl acridine-9-carboxylates (PAC) (% found/calculated).

[b] m/z of 10-methyl-9-(phenoxycarbonyl)acridinium cation ($MPCA^+$) (matrix-glycerin).

[c] Retention time (minutes) of $MPCA^+$ determined by HPLC (multisolvent delivery system, dual absorbance detector, λ_{obs} = 254 nm and 367 nm, Waters C-8 symmetry column, mobile phase: acetonitrile/0.1 M trifluoroacetic acid (1/1 v/v)).

[d] Retention factor of PAC determined by TLC (Silica Gel 60 plates, mobile phase: cyclohexane/ethyl acetate (1/1 v/v)).

TABLE 2S. Content of products in post CL mixtures determined by HPLC[a]

cpd no. (Scheme 1)	products[b] 10MeA-9CO_2H		phenol		10Me-9-Aone	
	R_t	Cont.	R_t	Cont.	R_t	Cont.
1	3.19 (3.16)	4.3	4.88 (4.83)	100	6.30 (6.29)	95.7
2[c]	3.20	9.4	5.44 (5.42)	99.9	6.32	90.6
9	3.14	14.7	6.30 (6.37)		6.30	

[a] Waters HPLC system equipped with absorbance Dual W2487 detector set at 268 nm and 366 nm; stationary phase: 150 × 4.60 Gemini 5 μm C6 phenyl 110 column (*Phenomenex*); mobile phase: 3/2 v/v acetonitrile/water mixture containing 2 mM phosphates (Na_2HPO_4+$NaHPO_4$) with pH adjusted to 3.5 (H_3PO_4) (0,5 mL/min).

[b] 10MeA-9CO_2H – 9-carboxy-10-methylacridinium acid; 10Me-9Aone – 10-methyl-9-acridinone.

R_t denotes retention time in minutes (mean of 3–5 measurements); the values in parentheses represent R_t of a pure substance. Cont. denotes the content of a substance in the post-reaction mixture in mole % (the mean values obtained on the basis of calibration plots from 3–5 measurements).

[c] The chromatogram is shown in Figure 8S.

FIGURE 1S. Retention time (R_t) against base 10 logarithm of partition coefficient (P) n-octanol/water and molar refractivity ($MR = (n^2-1) / (n^2+2) \times M/d$, where n – refractive index, M – molar mass, d – density) of $MPCA^+$. Numbers indicate entities listed in Chart 1. Empty circles denote log P values, filled circles denote MR values. The red line corresponds to the equation: $MR = 1.18R_t + 7.24$, the green line corresponds to the equation: $\log P = 1.13R_t - 2.14$.

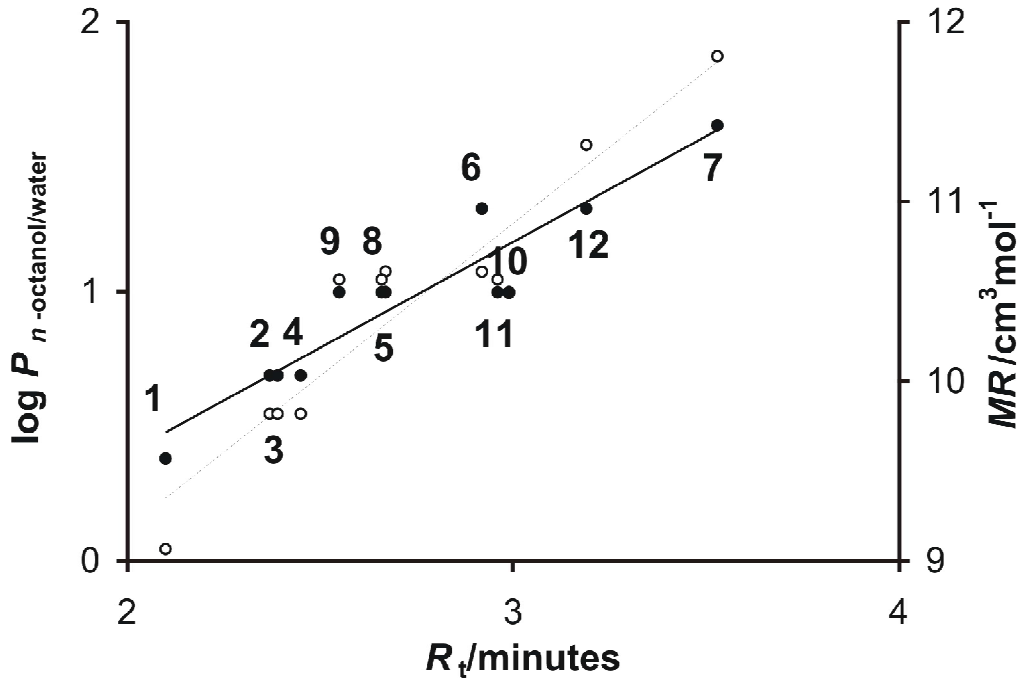


FIGURE 2S. FAB mass spectrum of **1**.

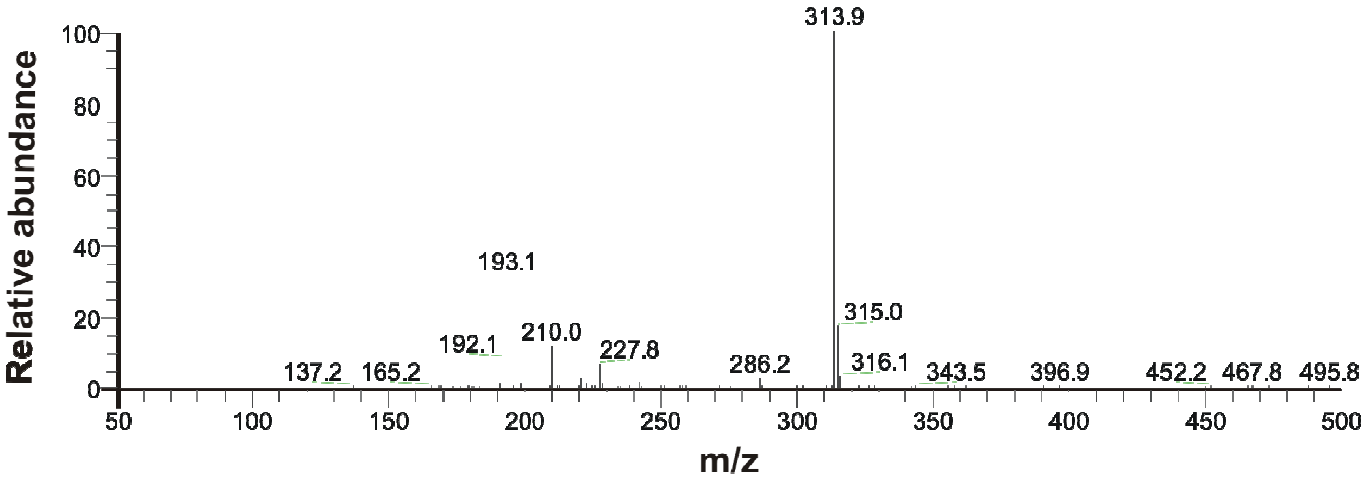
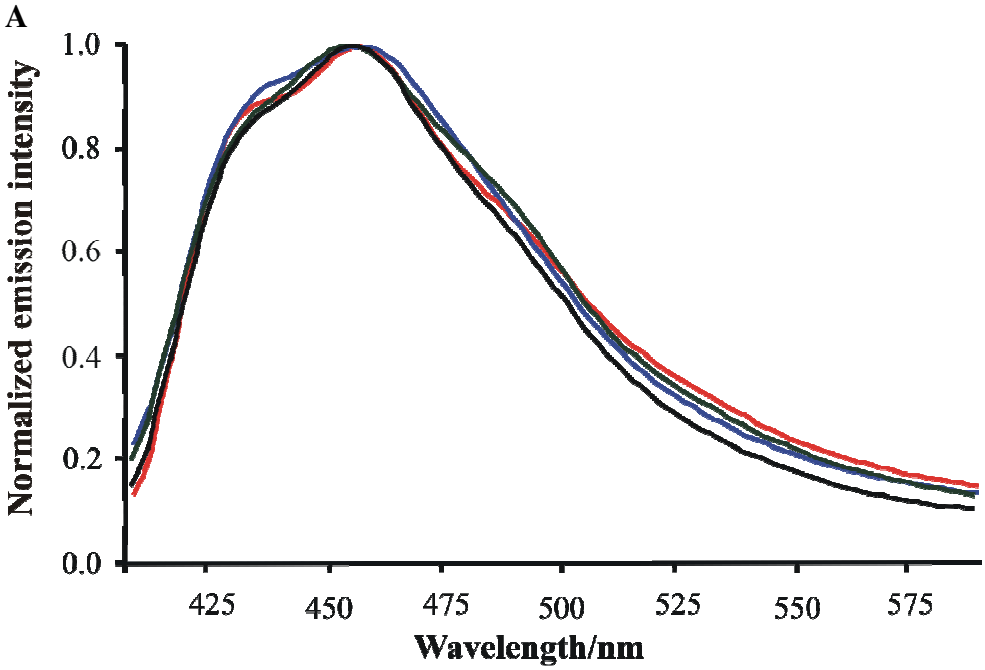


FIGURE 3S. A. Stationary fluorescence spectrum of 10-methyl-9-acridone ($c = 2 \times 10^{-5}$ M in water, pH = 11.6) (red) and stationary chemiluminescence spectra derived from the reaction of **1** (black), **2** (blue) and **9** (green) ($c = 2 \times 10^{-5}$ M) with H_2O_2 ($c = 4.9$ mM) at pH = 11.6, recorded 1–30 s after mixing the reagents. **B.** Stationary fluorescence spectrum of 10-methyl-9-acridone ($c = 2 \times 10^{-5}$ M in water, pH = 11.6) (red) and solutions on completion of reactions of **1** (black), **2** (blue) and **9** (green) described above.



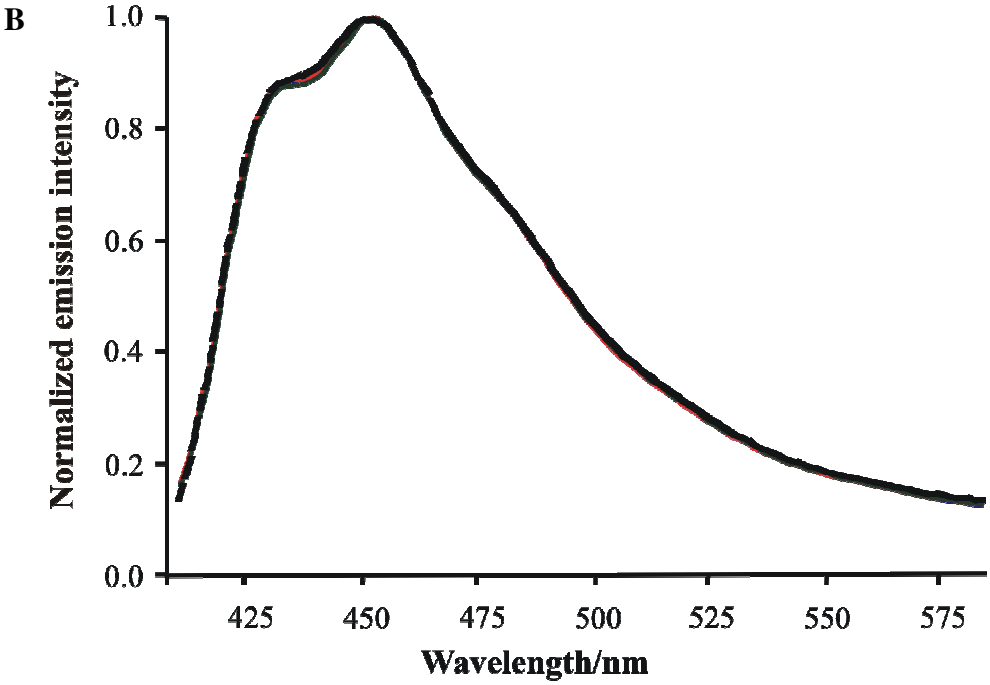


FIGURE 4S. Fluorescence decay of 10-methyl-9-acridinone (c = 1–5 × 10^{-5} M) dissolved in H_2O/acetonitrile (9/1 v/v); excitation and observation at 270 and 425 nm, respectively.

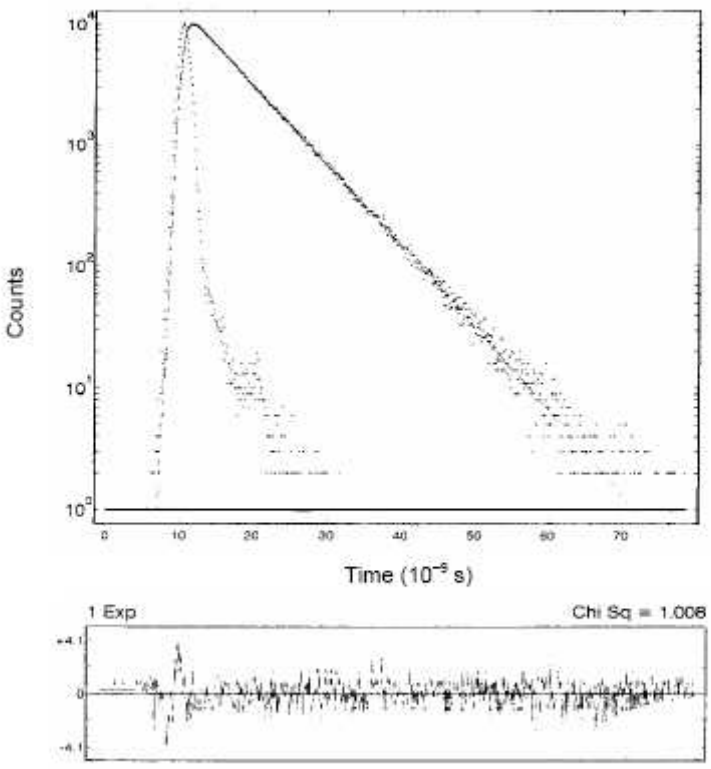


FIGURE 5S. Chemiluminescence intensity versus time profiles for **1** ($c = 2 \times 10^{-8}$ M) at various H_2O_2 concentrations and pH = 11.6.

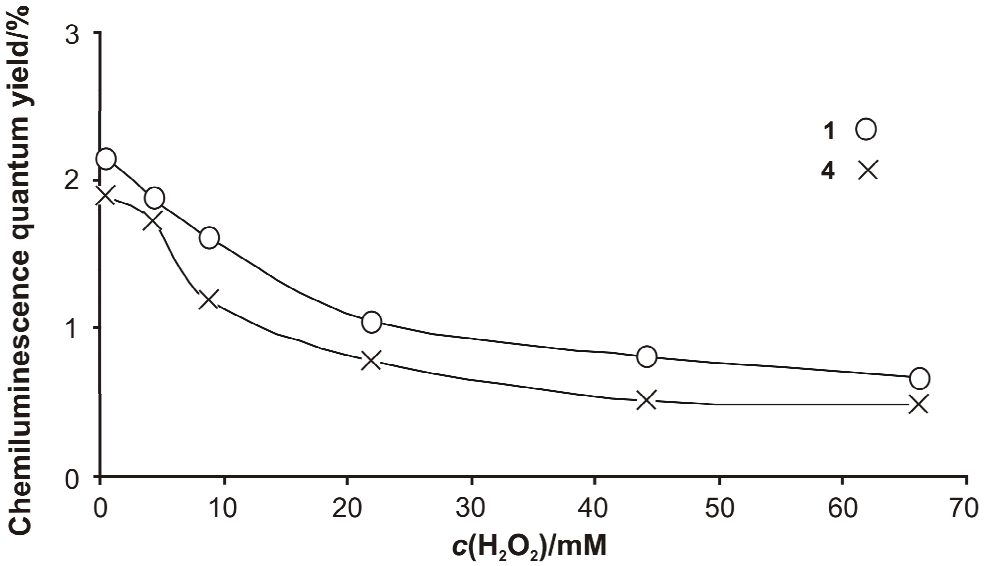


FIGURE 6S. Chemiluminescence quantum yield versus H_2O_2 concentration for compounds **1**, **2** and **4** (c(MPCA$^+$) = 2×10^{-8} M, pH = 11.6).

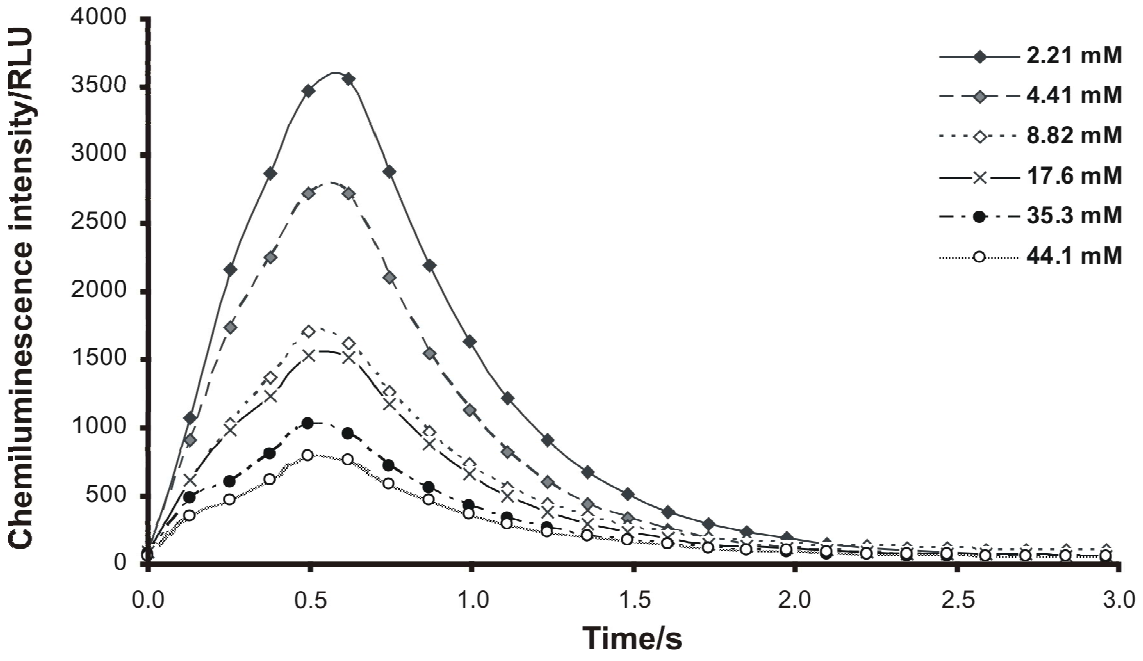
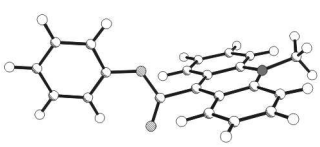
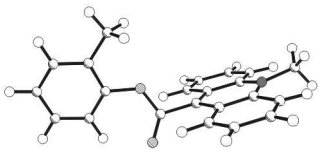
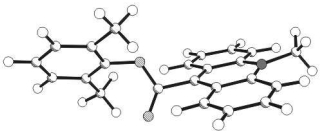
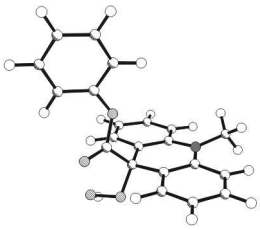
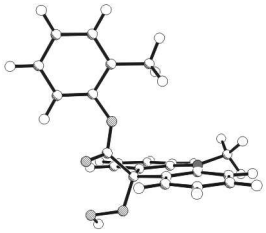
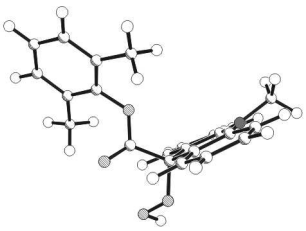
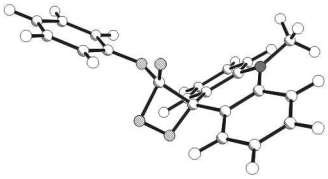
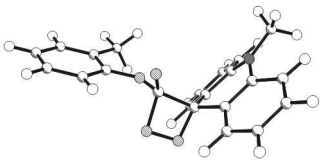
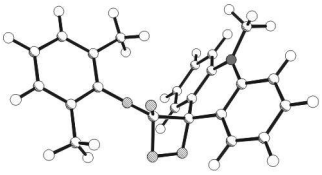
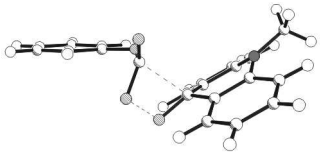
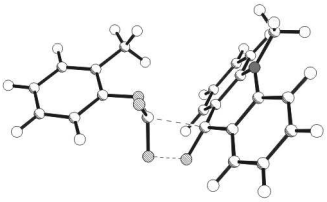
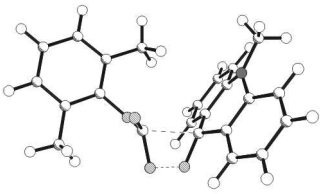
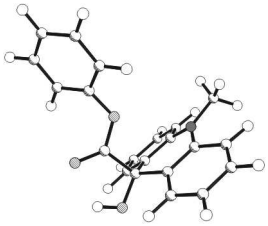
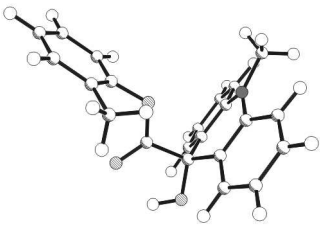
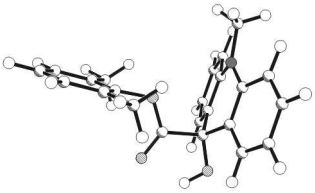
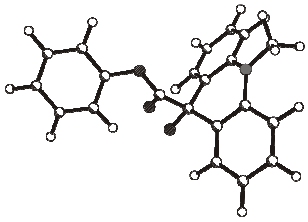
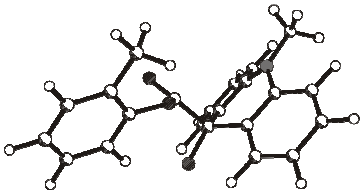
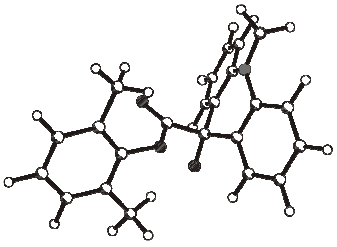
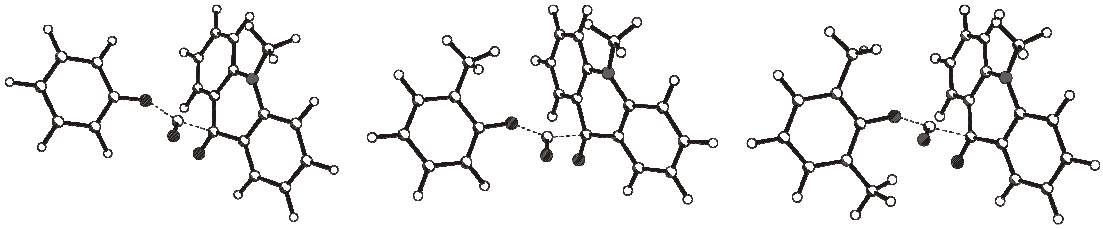


FIGURE 7S. DFT (6-31G**) optimized geometries of selected entities occurring on the reaction pathways of $MPCA^+$ with OOH^- and OH^- (**17** → **19** + **20**, **24** → **19** + **21** + **25** and **27** → **19** + **18** + **22** represent transition state geometries; the dotted lines denote the bonds formed and broken during the course of the reaction).

Entity no.	**Cpd no. (Chart 1)**		
(Scheme 1)	**1**	**2**	**9**
13			
16			
17			
17 → **19** + **20**			
23			
24			

24 → 19 + 21 + 25



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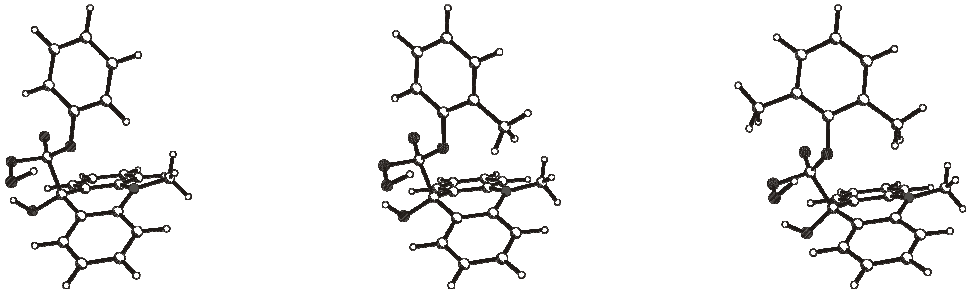

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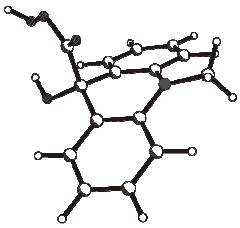
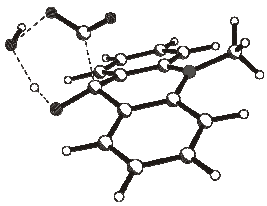


27 → 19 + 18 + 22



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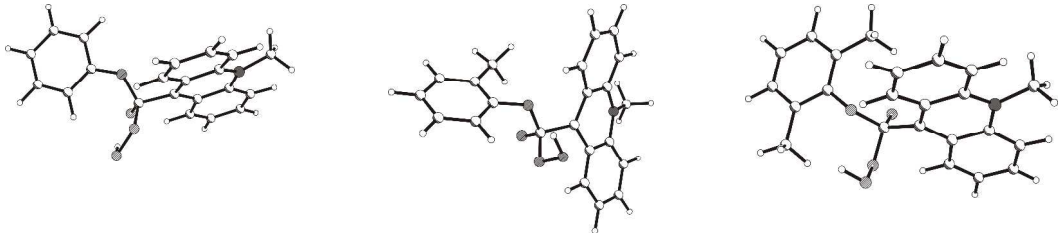

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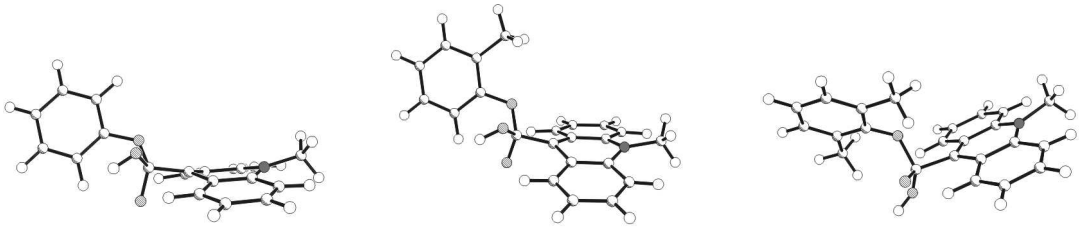

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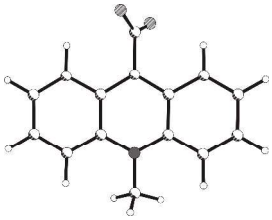

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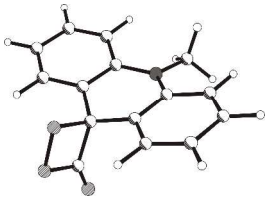


31 → 19 + 22

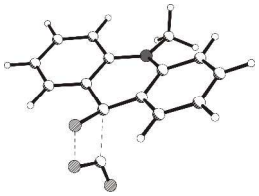


FIGURE 8S. Products of chemiluminogenic oxidation of **2** (c = 8.3 × 10^{-4} M) by H_2O_2 (c = 2.0 mM) at pH = 3.5 identified by HPLC: A – mixture of substrate and expected products, B – post-reaction mixture.

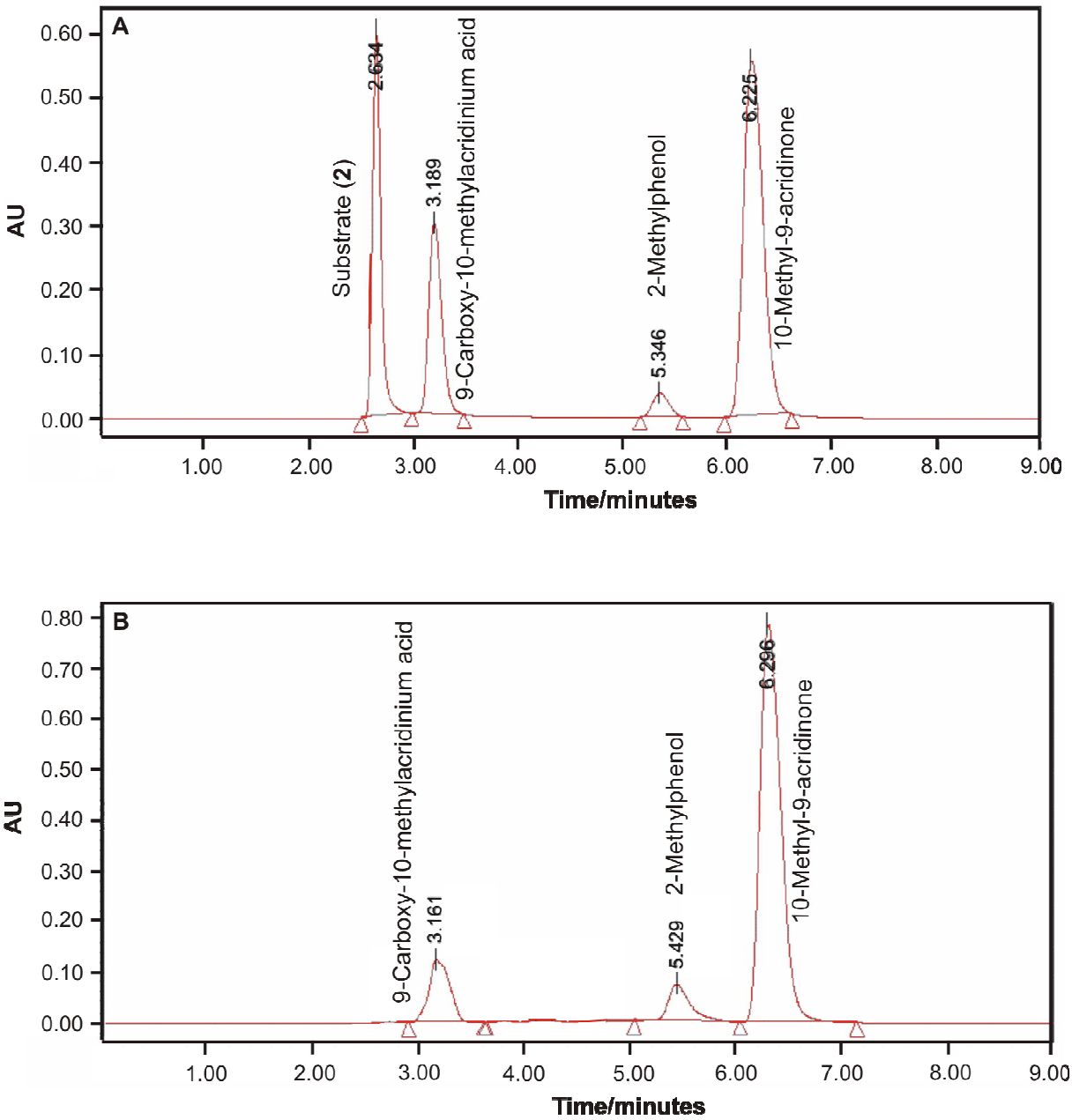
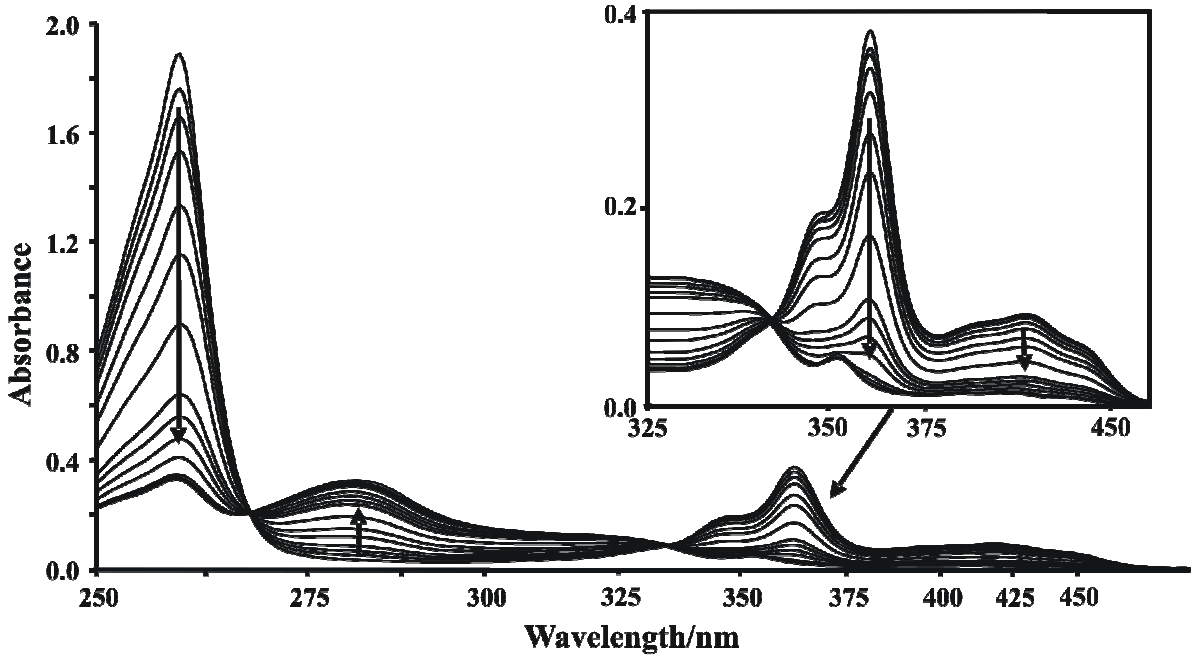


FIGURE 9S. The absorption spectra of **1** ($c = 4 \times 10^{-4}$ M – 2×10^{-5} M) in aqueous environments of various acidity (pH range: 2.0–12.0).



Cartesian coordinates and values (in Hartree) of the:

- total energy, E_{total}
- total energy plus zero point energy, E_0
- total energy plus zero point energy and thermal energy at 298.15 K and standard pressure, E_{298}
- total energy plus zero point energy and thermal enthalpy at 298.15 K and standard pressure, H_{298}
- total energy plus zero point energy, thermal enthalpy and entropy at 298.15 K and standard pressure, G_{298}

Compound **13**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.186072	2.343925	-0.457313
2	6	0	-0.997240	1.190007	-0.226578
3	6	0	-2.386485	1.376297	0.096512
4	6	0	-2.911778	2.691251	0.134862
5	6	0	-2.092450	3.771702	-0.109723
6	6	0	-0.717456	3.604990	-0.397357
7	6	0	-0.490003	-0.118912	-0.331039
8	6	0	-1.344336	-1.230791	-0.196518
9	6	0	-2.723032	-1.010092	0.150299
10	7	0	-3.175490	0.276414	0.357280
11	6	0	-3.588877	-2.124818	0.266359
12	6	0	-3.104009	-3.400590	0.076178
13	6	0	-1.743769	-3.633845	-0.233837
14	6	0	-0.887171	-2.573934	-0.372859
15	6	0	0.967357	-0.354909	-0.672001
16	8	0	1.307884	-0.937368	-1.673100
17	6	0	-4.541646	0.479659	0.885099
18	8	0	1.754789	0.154267	0.287711
19	6	0	3.165677	-0.000169	0.270254
20	6	0	3.926271	0.101134	-0.891867
21	6	0	5.314500	-0.000747	-0.776862
22	6	0	5.915867	-0.194201	0.467251
23	6	0	5.128076	-0.284537	1.616760
24	6	0	3.740786	-0.185005	1.523878
25	1	0	-1.387206	-4.647595	-0.377430
26	1	0	0.145577	-2.739670	-0.649635
27	1	0	-3.787241	-4.239941	0.156237
28	1	0	-4.642183	-1.993362	0.467826
29	1	0	-3.962796	2.866250	0.314654
30	1	0	0.862780	2.207986	-0.686116
31	1	0	-0.093490	4.472210	-0.581656
32	1	0	-2.518586	4.769559	-0.090643
33	1	0	-4.566436	1.390663	1.476173
34	1	0	-5.270481	0.541509	0.072664
35	1	0	-4.795039	-0.342645	1.548743

36	1	0	3.106850	-0.245525	2.401789
37	1	0	5.590272	-0.430267	2.587612
38	1	0	6.995513	-0.272409	0.541455
39	1	0	5.924579	0.072315	-1.671331
40	1	0	3.459686	0.242337	-1.857180

E_{total} = -1014.895082

E_0 = -1014.575880

E_{298} = -1014.557039

H_{298} = -1014.556094

G_{298} = -1014.624852

Compound **13**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.450370	-1.095632	-1.259237
2	6	0	3.013640	-0.090279	-0.405945
3	6	0	3.872610	0.668525	0.393790
4	6	0	5.235118	0.350522	0.307351
5	6	0	5.704377	-0.660136	-0.531289
6	6	0	4.812656	-1.385382	-1.320883
7	8	0	1.613095	0.192541	-0.448053
8	6	0	0.843103	-0.230859	0.568318
9	8	0	1.218613	-0.710933	1.609335
10	6	0	3.385687	1.778310	1.290334
11	1	0	2.729812	-1.631467	-1.868080
12	6	0	-0.631145	-0.074616	0.248811
13	6	0	-1.428591	-1.236164	0.220448
14	6	0	-2.841799	-1.106309	-0.011789
15	7	0	-3.400041	0.150098	-0.122599
16	6	0	-2.625475	1.288707	-0.178763
17	6	0	-1.203853	1.190734	0.022616
18	6	0	-3.629668	-2.277763	-0.126368
19	6	0	-3.050088	-3.519092	0.020921
20	6	0	-1.669800	-3.659929	0.295982
21	6	0	-0.878964	-2.545308	0.389185
22	6	0	-0.425384	2.388736	0.003745
23	6	0	-1.006989	3.607183	-0.226024
24	6	0	-2.399486	3.683931	-0.462737
25	6	0	-3.195000	2.559279	-0.439865
26	6	0	-4.872799	0.279550	-0.163560
27	1	0	-0.404631	4.508497	-0.241407
28	1	0	0.642441	2.314534	0.156693
29	1	0	-2.854871	4.645710	-0.675586
30	1	0	-4.248157	2.663763	-0.657108
31	1	0	-4.681960	-2.220363	-0.364826
32	1	0	0.177288	-2.643649	0.603037
33	1	0	-1.240746	-4.647443	0.423181
34	1	0	-3.669261	-4.404243	-0.083189
35	1	0	5.937679	0.914766	0.913560

36	1	0	6.767076	-0.875963	-0.570871
37	1	0	5.169524	-2.168067	-1.981928
38	1	0	-5.164303	1.214601	0.306501
39	1	0	-5.240091	0.248398	-1.192692
40	1	0	-5.319636	-0.524256	0.414646
41	1	0	4.225269	2.247993	1.806702
42	1	0	2.877529	2.563372	0.717645
43	1	0	2.692544	1.406231	2.051400

E_{total} = -1054.214923

E_0 = -1053.868084

E_{298} = -1053.847613

H_{298} = -1053.846669

G_{298} = -1053.918451

Compound **13**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.412098	-0.926217	1.085195
2	6	0	-2.923023	0.068277	0.233158
3	6	0	-3.721938	0.862950	-0.593098
4	6	0	-5.098942	0.608003	-0.559918
5	6	0	-5.631391	-0.382159	0.262369
6	6	0	-4.795074	-1.138674	1.080644
7	8	0	-1.513295	0.307158	0.311697
8	6	0	-0.727377	-0.121048	-0.689437
9	8	0	-1.087667	-0.574039	-1.748356
10	6	0	-3.157225	1.955087	-1.466215
11	6	0	-2.492315	-1.727464	1.973065
12	6	0	0.742698	-0.009392	-0.330158
13	6	0	1.519039	-1.186483	-0.347541
14	6	0	2.927806	-1.097761	-0.071586
15	7	0	3.506094	0.139021	0.122661
16	6	0	2.751662	1.287926	0.221957
17	6	0	1.334084	1.230356	-0.020490
18	6	0	3.691207	-2.288902	0.000068
19	6	0	3.094784	-3.508941	-0.231603
20	6	0	1.720950	-3.607308	-0.553036
21	6	0	0.952794	-2.474270	-0.605614
22	6	0	0.580865	2.443234	0.043037
23	6	0	1.180813	3.634329	0.354869
24	6	0	2.567208	3.668204	0.632822
25	6	0	3.339777	2.529430	0.568093
26	6	0	4.979344	0.238964	0.206962
27	1	0	0.596441	4.546289	0.402960
28	1	0	-0.483177	2.401545	-0.142677
29	1	0	3.035821	4.606752	0.910741
30	1	0	4.388591	2.598247	0.818030
31	1	0	4.736804	-2.264623	0.271232
32	1	0	-0.097044	-2.539880	-0.858397
33	1	0	1.278435	-4.577573	-0.748562

34	1	0	3.694929	-4.410218	-0.159226
35	1	0	-5.755221	1.201712	-1.188976
36	1	0	-6.702004	-0.559414	0.270836
37	1	0	-5.212572	-1.903249	1.728767
38	1	0	5.298953	1.187122	-0.216671
39	1	0	5.318582	0.159583	1.243117
40	1	0	5.427527	-0.548480	-0.391976
41	1	0	-3.959396	2.466162	-2.002350
42	1	0	-2.631121	2.712793	-0.873231
43	1	0	-2.459872	1.557916	-2.210240
44	1	0	-1.794772	-2.341488	1.390729
45	1	0	-1.890515	-1.078911	2.617756
46	1	0	-3.067234	-2.401219	2.611515

E_{total} = -1093.535666

E_0 = -1093.161086

E_{298} = -1093.138931

H_{298} = -1093.137987

G_{298} = -1093.213153

Compound **14** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.056402	-0.711435	0.000000
2	8	0	0.056402	0.816441	0.000000
3	1	0	-0.902429	-0.840045	0.000000

E_{total} = -150.892218

E_0 = -150.879631

E_{298} = -150.876677

H_{298} = -150.875732

G_{298} = -150.901449

Compound **15** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.109225
2	1	0	0.000000	0.000000	-0.873803

E_{total} = -75.726292

E_0 = -75.718308

E_{298} = -75.715948

H_{298} = -75.715004

G_{298} = -75.734597

Compound **16**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.235251	-1.307020	-0.727072
2	6	0	2.620680	-0.155765	-0.244172
3	6	0	3.320909	1.037659	-0.084592
4	6	0	4.676576	1.064432	-0.413017
5	6	0	5.313716	-0.080134	-0.896600
6	6	0	4.590702	-1.263581	-1.054569
7	8	0	1.239990	-0.239403	-0.011163
8	6	0	0.715785	0.155625	1.169805
9	8	0	1.360498	0.578947	2.105603
10	1	0	2.818540	1.920174	0.291894
11	1	0	2.649379	-2.212628	-0.841810
12	6	0	-0.829735	0.064915	1.132402
13	6	0	-1.302338	1.312626	0.392648
14	6	0	-1.685284	1.236201	-0.963559
15	7	0	-1.682687	0.008346	-1.627297
16	6	0	-1.740351	-1.182930	-0.888398
17	6	0	-1.344994	-1.204266	0.466609
18	6	0	-2.072972	2.422251	-1.617859
19	6	0	-2.054188	3.642602	-0.950902
20	6	0	-1.659691	3.717735	0.385047
21	6	0	-1.287104	2.550502	1.044714
22	6	0	-1.423552	-2.403075	1.183145
23	6	0	-1.877393	-3.576669	0.586057
24	6	0	-2.269262	-3.553587	-0.751021
25	6	0	-2.210954	-2.370238	-1.479652
26	6	0	-1.794407	-0.030896	-3.076556
27	1	0	-1.926270	-4.495199	1.161951
28	1	0	-1.120864	-2.402930	2.222274
29	1	0	-2.638823	-4.454612	-1.232131
30	1	0	-2.564062	-2.365797	-2.503438
31	1	0	-2.417866	2.389331	-2.643770
32	1	0	-0.979321	2.580513	2.082944
33	1	0	-1.643920	4.669028	0.906488
34	1	0	-2.362282	4.538663	-1.481957
35	1	0	5.234844	1.987539	-0.290311
36	1	0	6.368786	-0.048839	-1.150240
37	1	0	5.079022	-2.156558	-1.432631
38	1	0	-1.310547	-0.934419	-3.450403
39	1	0	-2.834254	-0.016068	-3.432871
40	1	0	-1.267826	0.824763	-3.502236
41	8	0	-1.330599	0.247473	2.470686
42	8	0	-0.647568	-0.615033	3.421268
43	1	0	0.187344	-0.115577	3.521416

E_{total} = -1166.055920

E_0 = -1165.719231

E_{298} = -1165.698134

H_{298} = -1165.697189

G_{298} = -1165.770951

Compound **16**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.449495	0.663742	-0.266628
2	6	0	-2.486491	-0.338986	-0.421876
3	6	0	-2.790913	-1.612978	-0.885339
4	6	0	-4.112317	-1.921064	-1.207517
5	6	0	-5.101028	-0.947836	-1.063847
6	6	0	-4.766789	0.325351	-0.601136
7	8	0	-1.129524	-0.040410	-0.185055
8	6	0	-0.668437	-0.078116	1.083536
9	8	0	-1.354253	-0.325827	2.053235
10	1	0	-1.994436	-2.342283	-0.989098
11	6	0	-3.083549	2.032687	0.246330
12	6	0	0.859431	0.167197	1.115143
13	6	0	1.513541	-1.135127	0.666875
14	6	0	2.063372	-1.260309	-0.626400
15	7	0	2.041916	-0.181395	-1.511223
16	6	0	1.858604	1.121295	-1.025956
17	6	0	1.287500	1.342434	0.246076
18	6	0	2.636381	-2.494687	-0.993399
19	6	0	2.631219	-3.572858	-0.114934
20	6	0	2.065843	-3.453360	1.154669
21	6	0	1.514344	-2.233577	1.533846
22	6	0	1.109419	2.656077	0.695463
23	6	0	1.485556	3.748415	-0.082156
24	6	0	2.062609	3.527738	-1.331362
25	6	0	2.255889	2.231436	-1.795694
26	6	0	2.332500	-0.396302	-2.920247
27	1	0	1.335569	4.757056	0.289148
28	1	0	0.675406	2.809420	1.675074
29	1	0	2.379569	4.364302	-1.947388
30	1	0	2.746069	2.083760	-2.749854
31	1	0	3.114296	-2.606175	-1.958579
32	1	0	1.076293	-2.112136	2.517317
33	1	0	2.058244	-4.293681	1.840828
34	1	0	3.083916	-4.509629	-0.427021
35	1	0	-4.363388	-2.913439	-1.568699
36	1	0	-6.132189	-1.176686	-1.315290
37	1	0	-5.541019	1.080570	-0.495579
38	1	0	1.812888	0.356465	-3.514684
39	1	0	3.405408	-0.349657	-3.154385
40	1	0	1.952393	-1.373400	-3.222617
41	1	0	-2.881465	2.002198	1.323109
42	1	0	-2.182494	2.416904	-0.241023
43	1	0	-3.897864	2.741394	0.077326
44	8	0	1.279859	0.292784	2.489664

45	8	0	0.465278	1.249050	3.222926
46	1	0	-0.334608	0.702990	3.361123

E_{total} = -1205.377441

E_0 = -1205.013060

E_{298} = -1204.990273

H_{298} = -1204.989329

G_{298} = -1205.066754

Compound **16**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.296210	1.008890	-0.235471
2	6	0	-2.448077	-0.098778	-0.319683
3	6	0	-2.875490	-1.383558	-0.665513
4	6	0	-4.238007	-1.547142	-0.941645
5	6	0	-5.118713	-0.469325	-0.870055
6	6	0	-4.650012	0.795771	-0.520464
7	8	0	-1.063574	0.106997	-0.124713
8	6	0	-0.569807	0.037606	1.128699
9	8	0	-1.236185	-0.202787	2.114127
10	6	0	-1.906786	-2.537171	-0.728674
11	6	0	-2.769034	2.365648	0.157616
12	6	0	0.966327	0.235082	1.128585
13	6	0	1.568871	-1.098307	0.699066
14	6	0	2.057526	-1.277478	-0.612588
15	7	0	2.032473	-0.221612	-1.525068
16	6	0	1.932146	1.099249	-1.063211
17	6	0	1.423475	1.372575	0.224836
18	6	0	2.572216	-2.540488	-0.968677
19	6	0	2.571973	-3.592722	-0.059025
20	6	0	2.071000	-3.417989	1.231118
21	6	0	1.575633	-2.170374	1.598263
22	6	0	1.337847	2.700754	0.657388
23	6	0	1.739323	3.757452	-0.156192
24	6	0	2.248436	3.485011	-1.424540
25	6	0	2.353350	2.172313	-1.871257
26	6	0	2.265812	-0.479557	-2.937310
27	1	0	1.660431	4.778918	0.201747
28	1	0	0.952814	2.894842	1.650163
29	1	0	2.581942	4.292853	-2.069462
30	1	0	2.793718	1.982207	-2.842096
31	1	0	3.002118	-2.695099	-1.950362
32	1	0	1.186386	-2.005993	2.595830
33	1	0	2.069590	-4.237548	1.942012
34	1	0	2.978876	-4.552831	-0.363074
35	1	0	-4.604358	-2.532843	-1.214720
36	1	0	-6.172015	-0.614971	-1.090330
37	1	0	-5.337163	1.635554	-0.466148
38	1	0	1.752690	0.277909	-3.531450
39	1	0	3.330915	-0.477257	-3.209056
40	1	0	1.841181	-1.448954	-3.203006

41	1	0	-2.401687	-3.435376	-1.105941
42	1	0	-1.055118	-2.313866	-1.378555
43	1	0	-1.497676	-2.769024	0.260901
44	1	0	-2.475879	2.380688	1.213833
45	1	0	-1.883908	2.639474	-0.424286
46	1	0	-3.531856	3.134186	0.011688
47	8	0	1.411004	0.382654	2.492608
48	8	0	0.625043	1.372061	3.212552
49	1	0	-0.179423	0.842250	3.383595

E_{total} = -1244.698725

E_0 = -1244.306627

E_{298} = -1244.28216

H_{298} = -1244.281217

G_{298} = -1244.361966

Compound **17**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.541999	-1.419233	-0.454162
2	6	0	2.984304	-0.132530	-0.307811
3	6	0	3.839627	0.985107	-0.394319
4	6	0	5.204807	0.825967	-0.612712
5	6	0	5.758962	-0.449929	-0.751026
6	6	0	4.912447	-1.558639	-0.669694
7	8	0	1.686867	0.133759	-0.077709
8	6	0	0.692572	-1.002786	0.049387
9	8	0	0.967232	-1.574135	1.461705
10	8	0	-0.081937	-0.689105	2.043278
11	6	0	-0.590034	-0.301483	0.756415
12	6	0	-1.857227	-1.038622	0.402519
13	6	0	-2.779005	-0.466038	-0.496203
14	7	0	-2.538213	0.827090	-0.994251
15	6	0	-1.741950	1.708922	-0.243685
16	6	0	-0.790067	1.183747	0.658997
17	6	0	-2.096685	-2.316874	0.905747
18	6	0	-3.232690	-3.038239	0.539915
19	6	0	-4.147379	-2.468159	-0.344613
20	6	0	-3.930724	-1.189373	-0.855840
21	6	0	-1.891031	3.103320	-0.354543
22	6	0	-1.108388	3.962182	0.415277
23	6	0	-0.179678	3.446417	1.319151
24	6	0	-0.032759	2.065291	1.433857
25	6	0	-3.305103	1.321661	-2.115925
26	8	0	0.640694	-1.806976	-0.884034
27	1	0	-2.728516	2.088956	-2.637786
28	1	0	-4.279555	1.754618	-1.833358
29	1	0	-3.484657	0.503966	-2.817581
30	1	0	-4.674155	-0.747734	-1.510303
31	1	0	-5.043282	-3.011339	-0.636600
32	1	0	-3.395666	-4.038212	0.932611
33	1	0	-1.352819	-2.736329	1.573329

34	1	0	0.687264	1.631533	2.117058
35	1	0	0.430100	4.112365	1.923685
36	1	0	-1.241477	5.036774	0.314035
37	1	0	-2.640652	3.521648	-1.017058
38	1	0	2.887126	-2.279316	-0.423883
39	1	0	5.324632	-2.560079	-0.779996
40	1	0	6.825190	-0.576680	-0.921200
41	1	0	5.841407	1.706950	-0.672808
42	1	0	3.397725	1.970652	-0.280686

E_{total} = -1165.480666

E_0 = -1165.158979

E_{298} = -1165.138353

H_{298} = -1165.137409

G_{298} = -1165.209333

Compound **17**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.314280	-1.735308	-0.279572
2	6	0	2.832073	-0.413936	-0.248931
3	6	0	3.729458	0.659422	-0.479943
4	6	0	5.075782	0.378048	-0.717110
5	6	0	5.560272	-0.932568	-0.737986
6	6	0	4.665904	-1.980708	-0.519635
7	8	0	1.555585	-0.063633	0.004560
8	6	0	0.490134	-1.139785	0.106504
9	8	0	0.702566	-1.743690	1.516791
10	8	0	-0.327259	-0.829723	2.086663
11	6	0	-0.767322	-0.377919	0.797132
12	6	0	-2.064659	-1.021594	0.377109
13	6	0	-2.894160	-0.375842	-0.561176
14	7	0	-2.534850	0.903099	-1.025149
15	6	0	-1.737036	1.720945	-0.206688
16	6	0	-0.875594	1.118459	0.737437
17	6	0	-2.420130	-2.283513	0.850585
18	6	0	-3.583622	-2.918028	0.415903
19	6	0	-4.406095	-2.276425	-0.509272
20	6	0	-4.072127	-1.011585	-0.991942
21	6	0	-1.799150	3.123559	-0.287051
22	6	0	-1.024500	3.915559	0.559529
23	6	0	-0.192582	3.323691	1.509639
24	6	0	-0.128141	1.933218	1.590187
25	6	0	-3.203304	1.466638	-2.176913
26	8	0	0.409270	-1.928070	-0.837142
27	1	0	-2.548223	2.201614	-2.650477
28	1	0	-4.160918	1.959998	-1.939301
29	1	0	-3.397264	0.674356	-2.903462
30	1	0	-4.744574	-0.511831	-1.680494
31	1	0	-5.320829	-2.751968	-0.855638
32	1	0	-3.838240	-3.907193	0.786622
33	1	0	-1.744857	-2.760971	1.551364

34	1	0	0.516390	1.440665	2.308451
35	1	0	0.406778	3.937657	2.176394
36	1	0	-1.089886	4.998254	0.481868
37	1	0	-2.477122	3.601270	-0.985723
38	1	0	2.616637	-2.549637	-0.140926
39	1	0	5.018919	-3.009970	-0.537834
40	1	0	6.613129	-1.128058	-0.926114
41	1	0	5.757424	1.209855	-0.891068
42	6	0	3.207088	2.072862	-0.463446
43	1	0	3.998179	2.787446	-0.716027
44	1	0	2.380624	2.196980	-1.171773
45	1	0	2.797084	2.339632	0.517043

E_{total} = -1204.801584

E_0 = -1204.452322

E_{298} = -1204.429991

H_{298} = -1204.429047

G_{298} = -1204.504663

Compound **17**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.655600	-1.097990	0.023176
2	6	0	2.707288	-0.058858	-0.105452
3	6	0	2.979040	1.056609	-0.927730
4	6	0	4.200903	1.128616	-1.602460
5	6	0	5.146264	0.110106	-1.485502
6	6	0	4.863503	-0.989024	-0.676545
7	8	0	1.550012	-0.032539	0.609536
8	6	0	0.523692	-1.129903	0.398202
9	8	0	0.486722	-1.869399	1.770628
10	8	0	-0.692779	-1.071755	2.199514
11	6	0	-0.891803	-0.492097	0.901852
12	6	0	-2.046648	-1.130424	0.172681
13	6	0	-2.784061	-0.396871	-0.777544
14	7	0	-2.470125	0.957034	-0.996114
15	6	0	-1.831018	1.684414	0.021827
16	6	0	-1.065810	0.996750	0.990866
17	6	0	-2.355754	-2.473688	0.388266
18	6	0	-3.385285	-3.101916	-0.310700
19	6	0	-4.122131	-2.371378	-1.242413
20	6	0	-3.832338	-1.027601	-1.472707
21	6	0	-1.957460	3.083462	0.108698
22	6	0	-1.331852	3.788733	1.134797
23	6	0	-0.586556	3.111395	2.100605
24	6	0	-0.465551	1.725438	2.020876
25	6	0	-3.013506	1.645332	-2.146442
26	8	0	0.658148	-1.825426	-0.610311
27	1	0	-2.356254	2.475147	-2.416280
28	1	0	-4.028345	2.046580	-1.986670
29	1	0	-3.047142	0.957428	-2.994222
30	1	0	-4.442937	-0.466961	-2.171794

31	1	0	-4.935182	-2.840331	-1.791915
32	1	0	-3.602746	-4.152311	-0.137398
33	1	0	-1.747887	-3.014494	1.104520
34	1	0	0.114923	1.169627	2.747175
35	1	0	-0.099678	3.656992	2.904320
36	1	0	-1.444379	4.869311	1.182463
37	1	0	-2.571452	3.621680	-0.604754
38	6	0	3.384888	-2.292146	0.900106
39	1	0	5.596977	-1.787137	-0.573884
40	1	0	6.093869	0.173917	-2.015504
41	1	0	4.405523	1.993467	-2.231521
42	6	0	1.947370	2.147713	-1.061549
43	1	0	2.288914	2.925013	-1.754006
44	1	0	0.998118	1.744971	-1.429203
45	1	0	1.722518	2.614178	-0.097043
46	1	0	4.306904	-2.851791	1.094097
47	1	0	2.935152	-1.989553	1.850412
48	1	0	2.654490	-2.952050	0.421647

E_{total} = -1244.119672

E_0 = -1243.742619

E_{298} = -1243.718782

H_{298} = -1243.717837

G_{298} = -1243.795672

Compound **18** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.119188	0.000000
2	1	0	0.759276	-0.476723	0.000000
3	1	0	-0.759276	-0.476781	0.000000

E_{total} = -76.419737

E_0 = -76.398367

E_{298} = -76.395532

H_{298} = -76.394587

G_{298} = -76.416678

Compound **19** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.471751	-1.439958	-0.016324
2	6	0	1.243483	-0.761720	0.036337
3	6	0	1.214770	0.654063	0.006502
4	6	0	2.441461	1.345016	-0.115286
5	6	0	3.640235	0.648079	-0.169110
6	6	0	3.669000	-0.752039	-0.111146
7	7	0	0.000006	1.337837	0.091152
8	6	0	-1.214764	0.654069	0.006514
9	6	0	-1.243485	-0.761714	0.036348
10	6	0	-0.000019	-1.548941	0.109286
11	6	0	-2.441452	1.345028	-0.115284
12	6	0	-3.640229	0.648098	-0.169118
13	6	0	-3.669001	-0.752020	-0.111154
14	6	0	-2.471735	-1.439941	-0.016310
15	8	0	-0.000041	-2.779144	0.192515
16	6	0	0.000015	2.784851	0.287254
17	1	0	-4.613356	-1.284963	-0.152250
18	1	0	-2.431992	-2.523613	0.017927
19	1	0	-4.566685	1.206629	-0.268084
20	1	0	-2.463341	2.423897	-0.198084
21	1	0	2.463355	2.423884	-0.198101
22	1	0	2.432006	-2.523630	0.017896
23	1	0	4.613362	-1.284972	-0.152222
24	1	0	4.566695	1.206605	-0.268069
25	1	0	0.876566	3.074470	0.865866
26	1	0	-0.000021	3.338278	-0.660058
27	1	0	-0.876481	3.074469	0.865949

E_{total} = -670.130875

E_0 = -669.914750

E_{298} = -669.902855

H_{298} = -669.901911

G_{298} = -669.952687

Compound **20**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.542630	-0.976388	0.161276
2	6	0	-1.195818	-1.325082	0.133186
3	6	0	-0.183931	-0.354561	-0.064256
4	6	0	-0.592564	0.991086	-0.225232
5	6	0	-1.945728	1.323105	-0.188379
6	6	0	-2.937150	0.355670	0.001890
7	8	0	1.069307	-0.805222	-0.136780

8	6	0	2.369653	0.095325	0.060728
9	1	0	-0.881056	-2.357794	0.256229
10	1	0	-3.292153	-1.752427	0.311541
11	1	0	-3.988589	0.632300	0.026245
12	1	0	-2.231651	2.366689	-0.315079
13	1	0	0.170289	1.746563	-0.351212
14	8	0	3.334748	-0.568746	-0.279345
15	8	0	2.144965	1.212685	0.515750

E_{total} = -495.500002

E_0 = -495.394574

E_{298} = -495.386321

H_{298} = -495.385377

G_{298} = -495.429123

Compound **20**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.800042	-0.888135	-0.006993
2	6	0	2.513205	0.477504	0.085505
3	6	0	1.203470	0.955435	0.045693
4	6	0	0.123333	0.038882	-0.101038
5	6	0	0.418043	-1.338823	-0.194099
6	6	0	1.738482	-1.784115	-0.145045
7	8	0	-1.093511	0.581314	-0.191482
8	6	0	-2.468838	-0.201719	0.056153
9	8	0	-2.330933	-1.299794	0.583486
10	8	0	-3.374324	0.516155	-0.332347
11	6	0	0.891834	2.426808	0.142486
12	1	0	3.327030	1.194635	0.193828
13	1	0	3.828240	-1.240697	0.029586
14	1	0	1.937419	-2.852476	-0.218442
15	1	0	-0.408359	-2.030893	-0.278161
16	1	0	0.204289	2.629832	0.971631
17	1	0	1.803702	3.017712	0.286944
18	1	0	0.380407	2.785471	-0.758615

E_{total} = -534.821456

E_0 = -534.688415

E_{298} = -534.678473

H_{298} = -534.677529

G_{298} = -534.725015

Compound **20**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.871307	-0.400703	0.313374
2	6	0	2.407075	0.912856	0.224964
3	6	0	1.071210	1.184896	-0.079806
4	6	0	0.172695	0.115646	-0.313276
5	6	0	0.638517	-1.219275	-0.226235
6	6	0	1.981362	-1.451848	0.085634
7	8	0	-1.081813	0.406592	-0.689554
8	6	0	-2.320234	0.091893	0.296980
9	8	0	-1.962971	-0.404580	1.358942
10	8	0	-3.348263	0.437340	-0.258341
11	6	0	0.548694	2.596042	-0.170889
12	1	0	3.089887	1.743860	0.399655
13	1	0	3.913347	-0.602850	0.551305
14	1	0	2.334726	-2.480857	0.145190
15	6	0	-0.316038	-2.354635	-0.487239
16	1	0	0.083788	2.783173	-1.144891
17	1	0	-0.235577	2.772695	0.574241
18	1	0	1.349436	3.327824	-0.013468
19	1	0	0.214143	-3.310371	-0.570402
20	1	0	-1.053113	-2.417302	0.319597
21	1	0	-0.879800	-2.180224	-1.410655

E_{total} = -574.140952

E_0 = -573.980423

E_{298} = -573.9688062

H_{298} = -573.967862

G_{298} = -574.018519

Compound **21**: $R_2 = H$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.212672	0.287706	0.000000
2	6	0	0.000000	1.084412	0.000000
3	6	0	-1.213011	0.284776	0.000000
4	6	0	-1.200447	-1.102716	0.000000
5	6	0	0.001675	-1.830811	0.000000
6	6	0	1.201238	-1.100989	0.000000
7	8	0	-0.002260	2.350617	0.000000
8	1	0	-2.156384	0.830798	0.000000
9	1	0	-2.150399	-1.643463	0.000000
10	1	0	0.002188	-2.918978	0.000000
11	1	0	2.152689	-1.639159	0.000000
12	1	0	2.157219	0.831597	0.000000

E_{total} = -306.892396

E_0 = -306.801763

E_{298} = -306.796519

H_{298} = -306.795575

G_{298} = -306.830594

Compound **21**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.954691	-0.243271	0.000000
2	6	0	0.352742	-1.557309	0.000000
3	6	0	-1.023041	-1.752963	0.000000
4	6	0	-1.914321	-0.670371	0.000000
5	6	0	-1.370327	0.625354	0.000000
6	6	0	0.000000	0.857445	0.000000
7	1	0	1.035381	-2.406658	0.000000
8	1	0	-1.417517	-2.771987	0.000000
9	1	0	-2.991360	-0.825420	0.000000
10	1	0	-2.045708	1.485590	0.000000
11	6	0	0.581884	2.245688	0.000000
12	8	0	2.207905	-0.041939	0.000000
13	1	0	-0.198548	3.018248	0.000000
14	1	0	1.232371	2.404148	0.871682
15	1	0	1.232371	2.404148	-0.871682

E_{total} = -346.215469

E_0 = -346.097259

E_{298} = -346.090336

H_{298} = -346.089391

G_{298} = -346.128257

Compound **21**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.772499	0.000000
2	6	0	-1.227759	-0.000278	0.000000
3	6	0	-1.202499	-1.391236	0.000000
4	6	0	0.000384	-2.113303	0.000000
5	6	0	1.202746	-1.390869	0.000000
6	6	0	1.227556	0.000353	0.000000
7	6	0	-2.513628	0.782796	0.000000
8	1	0	-2.151596	-1.933922	0.000000

9	1	0	0.000320	-3.201436	0.000000
10	1	0	2.152237	-1.932822	0.000000
11	6	0	2.513646	0.783211	0.000000
12	8	0	-0.000543	2.045021	0.000000
13	1	0	-3.393473	0.125720	0.000000
14	1	0	-2.574198	1.449181	0.871896
15	1	0	-2.574198	1.449181	-0.871896
16	1	0	3.393193	0.125798	0.000000
17	1	0	2.574687	1.449550	-0.871933
18	1	0	2.574687	1.449550	0.871933

E_{total} = -385.538246

E_0 = -385.392570

E_{298} = -385.383867

H_{298} = -385.382923

G_{298} = -385.425972

Compound **22** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000486
2	8	0	0.000000	1.169042	-0.000182
3	8	0	0.000000	-1.169042	-0.000182

E_{total} = -188.580940

E_0 = -188.570803

E_{298} = -188.567822

H_{298} = -188.566878

G_{298} = -188.587322

Compound **23**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.834176	-1.214385	-0.433703
2	6	0	3.290609	-0.152252	0.288446
3	6	0	4.090700	0.885521	0.764143
4	6	0	5.460776	0.866369	0.506585
5	6	0	6.022673	-0.183821	-0.221070
6	6	0	5.207077	-1.216781	-0.685417
7	8	0	1.941774	-0.086599	0.655658
8	6	0	0.937249	-0.419797	-0.215128
9	8	0	1.110926	-0.812157	-1.339795
10	6	0	-0.440056	-0.150398	0.441308

11	6	0	-1.432891	-1.241559	0.088136
12	6	0	-2.806522	-0.925289	0.055882
13	7	0	-3.224150	0.403871	0.209706
14	6	0	-2.335539	1.448288	-0.056713
15	6	0	-0.942795	1.209511	-0.035901
16	6	0	-3.740835	-1.958463	-0.151133
17	6	0	-3.319477	-3.275435	-0.295287
18	6	0	-1.962305	-3.593587	-0.248925
19	6	0	-1.036282	-2.572887	-0.058776
20	6	0	-2.800581	2.738670	-0.375863
21	6	0	-1.907280	3.766683	-0.658663
22	6	0	-0.532780	3.534119	-0.646557
23	6	0	-0.067766	2.258473	-0.336335
24	8	0	-0.341033	-0.177950	1.871945
25	6	0	-4.626633	0.695633	0.462374
26	1	0	-1.629254	-4.620389	-0.358573
27	1	0	0.019732	-2.815816	-0.020173
28	1	0	-4.059649	-4.053709	-0.457237
29	1	0	-4.797267	-1.732865	-0.226081
30	1	0	-3.863766	2.935519	-0.436339
31	1	0	1.002741	2.079584	-0.320978
32	1	0	0.167406	4.330780	-0.875352
33	1	0	-2.294290	4.750453	-0.907878
34	1	0	-4.706418	1.633633	1.014055
35	1	0	-5.225221	0.776118	-0.456112
36	1	0	-5.051095	-0.090906	1.087847
37	1	0	3.633855	1.688188	1.333634
38	1	0	6.086306	1.672933	0.876774
39	1	0	7.089052	-0.198222	-0.423573
40	1	0	5.638394	-2.037828	-1.250114
41	1	0	3.200987	-2.010115	-0.800799
42	1	0	0.315099	0.487531	2.126093

E_{total} = -1090.921470

E_0 = -1090.588682

E_{298} = -1090.568431

H_{298} = -1090.567487

G_{298} = -1090.639230

Compound **23**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.805965	-2.279912	1.491972
2	6	0	1.595489	-1.151451	0.700496
3	6	0	1.944773	-1.174699	-0.665950
4	6	0	2.493738	-2.355015	-1.200144
5	6	0	2.675283	-3.479475	-0.398379
6	6	0	2.338013	-3.450217	0.954184
7	7	0	1.765998	-0.028182	-1.453349
8	6	0	1.722371	1.229264	-0.835050
9	6	0	1.365955	1.332535	0.526106
10	6	0	0.947744	0.090225	1.305320

11	6	0	2.051137	2.404754	-1.535203
12	6	0	2.012584	3.643872	-0.900284
13	6	0	1.670892	3.741487	0.448091
14	6	0	1.357192	2.579436	1.150542
15	6	0	-0.596324	-0.060893	1.248690
16	1	0	1.653047	4.705159	0.946849
17	1	0	1.108061	2.618760	2.205329
18	1	0	2.272596	4.534601	-1.465052
19	1	0	2.368513	2.353777	-2.569584
20	1	0	2.810514	-2.390410	-2.235381
21	1	0	1.551891	-2.218643	2.544474
22	1	0	2.489758	-4.322263	1.582050
23	1	0	3.102903	-4.376715	-0.836676
24	8	0	-1.283162	-0.070330	2.248992
25	8	0	-1.060903	-0.177581	-0.007847
26	6	0	-2.442581	-0.366667	-0.214732
27	6	0	-3.316214	0.723611	-0.137966
28	6	0	-4.659614	0.471509	-0.444380
29	6	0	-5.103227	-0.800161	-0.808739
30	6	0	-4.200633	-1.861035	-0.879792
31	6	0	-2.856039	-1.641361	-0.582231
32	6	0	-2.835267	2.095100	0.260045
33	1	0	-5.366777	1.295235	-0.396291
34	1	0	-6.151809	-0.959407	-1.041134
35	1	0	-4.535978	-2.853018	-1.165782
36	1	0	-2.123077	-2.439609	-0.633162
37	6	0	1.870755	-0.120453	-2.899312
38	1	0	1.286560	0.680922	-3.354833
39	1	0	2.905142	-0.052850	-3.266829
40	1	0	1.445045	-1.068853	-3.231577
41	1	0	-3.600853	2.847947	0.057560
42	1	0	-2.600516	2.127893	1.329543
43	1	0	-1.924980	2.374121	-0.279459
44	8	0	1.277087	0.218044	2.674906
45	1	0	0.431848	0.156843	3.155290

E_{total} = -1130.253626

E_0 = -1129.892588

E_{298} = -1129.870986

H_{298} = -1129.870042

G_{298} = -1129.944066

Compound **23**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.706367	-2.515318	1.192716
2	6	0	1.584332	-1.283446	0.550751
3	6	0	1.913340	-1.166262	-0.816033
4	6	0	2.348608	-2.314159	-1.503993
5	6	0	2.440508	-3.541172	-0.850999
6	6	0	2.126110	-3.651194	0.503026
7	7	0	1.826595	0.080297	-1.451846

8	6	0	1.895639	1.250641	-0.682471
9	6	0	1.566298	1.212647	0.688768
10	6	0	1.052024	-0.077142	1.317723
11	6	0	2.313157	2.473312	-1.240568
12	6	0	2.388194	3.622629	-0.456838
13	6	0	2.074113	3.578917	0.900882
14	6	0	1.671601	2.368269	1.461983
15	6	0	-0.500128	-0.093325	1.276203
16	1	0	2.144959	4.470915	1.514927
17	1	0	1.440344	2.296078	2.519079
18	1	0	2.715618	4.552307	-0.913389
19	1	0	2.612977	2.525374	-2.280148
20	1	0	2.647840	-2.247845	-2.542917
21	1	0	1.473789	-2.563277	2.250897
22	1	0	2.209669	-4.604081	1.015575
23	1	0	2.780955	-4.410335	-1.406500
24	8	0	-1.172090	-0.186943	2.282526
25	8	0	-0.989045	0.000853	0.027708
26	6	0	-2.389832	0.011726	-0.160320
27	6	0	-3.072741	-1.207044	-0.200641
28	6	0	-4.444949	-1.155669	-0.473908
29	6	0	-5.088602	0.060300	-0.695444
30	6	0	-4.367593	1.252359	-0.651081
31	6	0	-2.994109	1.252610	-0.381723
32	6	0	-2.361514	-2.513098	0.046436
33	1	0	-5.007206	-2.084505	-0.513048
34	1	0	-6.153356	0.078644	-0.907958
35	1	0	-4.869326	2.199799	-0.827000
36	6	0	-2.192172	2.528613	-0.330023
37	6	0	1.904977	0.160475	-2.900191
38	1	0	1.383763	1.056848	-3.240687
39	1	0	2.936608	0.189543	-3.280158
40	1	0	1.397568	-0.701449	-3.336719
41	1	0	-3.009048	-3.357789	-0.200755
42	1	0	-1.446755	-2.593764	-0.548477
43	1	0	-2.071384	-2.607243	1.098775
44	8	0	1.406130	-0.148186	2.685186
45	1	0	0.563869	-0.204136	3.171670
46	1	0	-1.779002	2.703562	0.669410
47	1	0	-1.342568	2.498860	-1.019290
48	1	0	-2.817199	3.386613	-0.589254

E_{total} = -1169.574893

E_0 = -1169.186401

E_{298} = -1169.162931

H_{298} = -1169.161987

G_{298} = -1169.240655

Compound **24**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.392905	-0.865017	-0.571794

2	6	0	-2.973508	0.010389	0.437644
3	6	0	-3.895555	0.577598	1.319489
4	6	0	-5.250929	0.265632	1.193174
5	6	0	-5.682687	-0.615215	0.200196
6	6	0	-4.746252	-1.174771	-0.677209
7	8	0	-1.657569	0.389415	0.522291
8	6	0	-0.678206	-0.628407	0.435736
9	8	0	-0.812133	-1.654993	1.059758
10	6	0	0.332002	-0.337578	-0.707913
11	6	0	1.596352	-1.175186	-0.449308
12	6	0	2.603529	-0.708448	0.416855
13	7	0	2.471703	0.588771	0.964316
14	6	0	1.804274	1.560642	0.184824
15	6	0	0.784741	1.132263	-0.688379
16	6	0	3.716567	-1.524091	0.682111
17	6	0	3.816185	-2.785192	0.088540
18	6	0	2.830009	-3.235708	-0.788858
19	6	0	1.728734	-2.418260	-1.053536
20	6	0	2.149523	2.922246	0.226095
21	6	0	1.489072	3.836165	-0.599470
22	6	0	0.504802	3.405238	-1.489141
23	6	0	0.167395	2.050401	-1.528536
24	8	0	-0.407290	-0.707250	-1.767559
25	6	0	3.376109	1.015152	2.007580
26	1	0	2.915368	-4.215440	-1.253204
27	1	0	0.921635	-2.703563	-1.721997
28	1	0	4.684081	-3.404786	0.305151
29	1	0	4.519671	-1.175649	1.323539
30	1	0	2.948983	3.272906	0.870828
31	1	0	-0.589085	1.644297	-2.193725
32	1	0	0.001710	4.118918	-2.137505
33	1	0	1.767786	4.887046	-0.554547
34	1	0	4.367743	1.330751	1.638875
35	1	0	2.932347	1.854388	2.549068
36	1	0	3.521730	0.196301	2.716534
37	1	0	-3.537996	1.255106	2.088719
38	1	0	-5.969351	0.709289	1.878990
39	1	0	-6.737539	-0.861462	0.107433
40	1	0	-5.077889	-1.853137	-1.460175
41	1	0	-2.630690	-1.240845	-1.252708

E_{total} = -1090.342577

E_0 = -1090.024762

E_{298} = -1090.004989

H_{298} = -1090.004046

G_{298} = -1090.073653

Compound **24**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.044694	-2.474134	-0.877397
2	6	0	-1.824477	-1.197362	-0.378032

3	6	0	-2.763478	-0.617322	0.496088
4	6	0	-3.897574	-1.354818	0.876651
5	6	0	-4.084839	-2.650612	0.388491
6	6	0	-3.166881	-3.214015	-0.497633
7	7	0	-2.545631	0.709952	0.933462
8	6	0	-1.875366	1.585701	0.049586
9	6	0	-0.922703	1.042546	-0.835392
10	6	0	-0.538500	-0.445328	-0.762231
11	6	0	-2.155201	2.962058	0.000500
12	6	0	-1.496690	3.776586	-0.924791
13	6	0	-0.580273	3.231218	-1.824146
14	6	0	-0.307754	1.862218	-1.773387
15	6	0	0.514632	-0.695564	0.352205
16	1	0	-0.079474	3.867890	-2.549870
17	1	0	0.394470	1.369086	-2.439341
18	1	0	-1.724519	4.840341	-0.949314
19	1	0	-2.904080	3.399805	0.652710
20	1	0	-4.650599	-0.919957	1.525943
21	1	0	-1.287617	-2.848520	-1.560256
22	1	0	-3.320762	-4.220435	-0.879967
23	1	0	-4.967767	-3.208394	0.694084
24	8	0	0.628833	-1.670645	1.057422
25	8	0	1.547180	0.270718	0.302867
26	6	0	2.840809	-0.181939	0.189364
27	6	0	3.822982	0.418087	0.992759
28	6	0	5.149330	0.007313	0.814825
29	6	0	5.489055	-0.971956	-0.120421
30	6	0	4.489032	-1.550209	-0.907218
31	6	0	3.161269	-1.154906	-0.760903
32	6	0	3.434621	1.468510	2.001839
33	1	0	5.925063	0.462121	1.428535
34	1	0	6.526094	-1.278135	-0.234622
35	1	0	4.745301	-2.306704	-1.645275
36	1	0	2.344388	-1.539217	-1.370025
37	6	0	-3.377178	1.257248	1.980802
38	1	0	-2.871321	2.114109	2.433069
39	1	0	-4.371831	1.589186	1.635220
40	1	0	-3.521454	0.502788	2.758085
41	1	0	4.302910	1.795494	2.583145
42	1	0	2.994140	2.346390	1.515600
43	1	0	2.675549	1.086714	2.693034
44	8	0	0.125761	-0.930340	-1.824582

E_{total} = -1129.663856

E_0 = -1129.318377

E_{298} = -1129.296863

H_{298} = -1129.295919

G_{298} = -1129.369366

Compound **24**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.179647	-2.296437	-1.307876
2	6	0	-1.907008	-1.131448	-0.603875
3	6	0	-2.721706	-0.764820	0.484041
4	6	0	-3.782837	-1.603462	0.864122
5	6	0	-4.021625	-2.788560	0.162912
6	6	0	-3.229913	-3.136987	-0.931277
7	7	0	-2.458290	0.463788	1.135446
8	6	0	-1.947024	1.518400	0.344087
9	6	0	-1.122877	1.190568	-0.750775
10	6	0	-0.693706	-0.268864	-1.005814
11	6	0	-2.264862	2.864963	0.589644
12	6	0	-1.773719	3.863874	-0.255627
13	6	0	-0.991439	3.534413	-1.362715
14	6	0	-0.679884	2.194067	-1.602721
15	6	0	0.478617	-0.658733	-0.051088
16	1	0	-0.623230	4.314788	-2.024864
17	1	0	-0.077380	1.862846	-2.443734
18	1	0	-2.028562	4.901945	-0.051853
19	1	0	-2.917990	3.140604	1.411484
20	1	0	-4.443072	-1.330044	1.681050
21	1	0	-1.519451	-2.503206	-2.145357
22	1	0	-3.424355	-4.057272	-1.477328
23	1	0	-4.846862	-3.427841	0.470210
24	8	0	0.679596	-1.734044	0.468599
25	8	0	1.453038	0.348548	-0.034049
26	6	0	2.765881	-0.021929	0.213769
27	6	0	3.224155	-0.122708	1.535650
28	6	0	4.574844	-0.424699	1.740543
29	6	0	5.434787	-0.629924	0.661593
30	6	0	4.949654	-0.525529	-0.641178
31	6	0	3.607150	-0.214446	-0.893137
32	6	0	2.272351	0.083659	2.685881
33	1	0	4.948935	-0.505803	2.759075
34	1	0	6.480661	-0.870675	0.837031
35	1	0	5.617546	-0.687125	-1.484839
36	6	0	3.071342	-0.059925	-2.295553
37	6	0	-3.143321	0.772206	2.369799
38	1	0	-2.594908	1.554052	2.901328
39	1	0	-4.183048	1.116807	2.231053
40	1	0	-3.161725	-0.117322	3.004435
41	1	0	2.805194	0.082280	3.642086
42	1	0	1.732697	1.031444	2.586786
43	1	0	1.519828	-0.710891	2.698208
44	8	0	-0.182987	-0.524956	-2.217907
45	1	0	2.021053	-0.373666	-2.375076
46	1	0	3.101641	0.995827	-2.598128
47	1	0	3.688607	-0.621731	-3.005263

E_{total} = -1168.987033

E_0 = -1168.613670

E_{298} = -1168.590681

H_{298} = -1168.589737

G_{298} = -1168.665731

Compound **25** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.650245
2	8	0	0.000000	0.000000	0.487684

E_{total} = -113.309454

E_0 = -113.304422

E_{298} = -113.302061

H_{298} = -113.301118

G_{298} = -113.323561

Compound **26**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.721074	2.254154	1.904201
2	6	0	-1.463613	1.128589	1.102497
3	6	0	-1.369909	1.274863	-0.299741
4	6	0	-1.604585	2.531683	-0.857142
5	6	0	-1.861639	3.649762	-0.062167
6	6	0	-1.904151	3.508585	1.323697
7	6	0	-1.035357	0.067097	-1.168790
8	6	0	-1.650036	-1.162713	-0.523732
9	6	0	-1.731327	-1.256194	0.879534
10	7	0	-1.345306	-0.153373	1.661851
11	6	0	-2.228435	-2.433666	1.466559
12	6	0	-2.630500	-3.503306	0.668066
13	6	0	-2.560219	-3.409062	-0.720918
14	6	0	-2.069676	-2.239521	-1.301635
15	6	0	0.542080	-0.262315	-1.406073
16	8	0	1.023350	0.591033	-2.562395
17	8	0	0.988043	2.033130	-2.265844
18	8	0	-1.573240	0.234409	-2.478631
19	6	0	-1.155828	-0.310790	3.086036
20	8	0	1.249478	0.436246	-0.185489
21	6	0	2.477925	0.013142	0.194682
22	6	0	2.847254	0.273460	1.526962
23	6	0	4.113142	-0.070223	1.996333
24	6	0	5.035024	-0.693717	1.152214
25	6	0	4.666016	-0.959172	-0.169519
26	6	0	3.407980	-0.610767	-0.659243
27	8	0	0.842344	-1.439418	-1.646502

28	1	0	3.117535	-0.825694	-1.678028
29	1	0	-2.019951	4.621221	-0.523120
30	1	0	-1.553377	2.618329	-1.934482
31	1	0	-2.102977	4.367188	1.961092
32	1	0	-1.815921	2.148670	2.979482
33	1	0	-2.329430	-2.507491	2.543777
34	1	0	-1.987073	-2.137054	-2.376471
35	1	0	-2.869262	-4.242339	-1.346427
36	1	0	-3.012251	-4.405421	1.140904
37	1	0	5.373495	-1.444144	-0.839212
38	1	0	6.021747	-0.967870	1.517026
39	1	0	4.378361	0.147985	3.029052
40	1	0	2.119361	0.756638	2.172086
41	1	0	-0.489066	0.474299	3.449929
42	1	0	-2.091906	-0.266282	3.668879
43	1	0	-0.676082	-1.272684	3.280430
44	1	0	-0.787637	0.430518	-3.023864
45	1	0	1.283336	1.995193	-1.334049

E_{total} = -1241.922068

E_0 = -1241.573470

E_{298} = -1241.550984

H_{298} = -1241.550040

G_{298} = -1241.625065

Compound **26**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.244805	-1.306467	0.423212
2	6	0	-2.477943	-0.279766	-0.154360
3	6	0	-3.011218	0.476141	-1.225645
4	6	0	-4.296391	0.181535	-1.687206
5	6	0	-5.060403	-0.841142	-1.121394
6	6	0	-4.521594	-1.579149	-0.067267
7	8	0	-1.241430	0.093178	0.273275
8	6	0	-0.426018	-0.869521	1.198447
9	8	0	-0.545146	-2.087918	1.008990
10	6	0	1.092208	-0.266122	1.175385
11	6	0	1.264790	1.186362	0.743090
12	6	0	1.484255	1.506921	-0.615903
13	7	0	1.614382	0.467504	-1.553208
14	6	0	2.104279	-0.773618	-1.103420
15	6	0	1.907635	-1.144066	0.240646
16	6	0	1.242661	2.223169	1.677311
17	6	0	1.364784	3.559534	1.295589
18	6	0	1.539473	3.872229	-0.051141
19	6	0	1.614815	2.853778	-0.999846
20	6	0	2.816029	-1.633549	-1.960454
21	6	0	3.310498	-2.848403	-1.489587
22	6	0	3.121279	-3.215140	-0.158247
23	6	0	2.423318	-2.358123	0.691512
24	8	0	1.572207	-0.438482	2.507525

25	6	0	1.630771	0.768707	-2.967784
26	8	0	-1.022491	-0.549324	2.564090
27	8	0	-1.202191	0.894603	2.794958
28	1	0	-2.815220	-1.881780	1.230580
29	1	0	1.322301	4.346104	2.044404
30	1	0	1.098020	1.955531	2.715507
31	1	0	1.642064	4.906768	-0.370634
32	1	0	1.811156	3.110710	-2.034637
33	1	0	3.011522	-1.346262	-2.987286
34	1	0	2.251877	-2.614232	1.729273
35	1	0	3.501824	-4.163128	0.212571
36	1	0	3.857201	-3.498491	-2.169006
37	1	0	-5.100842	-2.379613	0.388220
38	1	0	-6.057320	-1.055696	-1.498523
39	1	0	-4.701802	0.770255	-2.508923
40	6	0	-2.187315	1.579313	-1.837711
41	1	0	0.900810	1.552346	-3.180545
42	1	0	2.614759	1.101870	-3.339653
43	1	0	1.335544	-0.120743	-3.528795
44	1	0	0.756390	-0.558945	3.031194
45	1	0	-1.478721	1.153589	1.893819
46	1	0	-2.718734	2.051444	-2.670993
47	1	0	-1.935095	2.353197	-1.103827
48	1	0	-1.230652	1.192367	-2.202353

E_{total} = -1281.242071

E_0 = -1280.865523

E_{298} = -1280.841467

H_{298} = -1280.840523

G_{298} = -1280.918529

Compound **26**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.601052	-0.390033	-0.161734
2	6	0	2.412038	0.100099	0.432409
3	6	0	2.359013	0.305876	1.831394
4	6	0	3.467496	0.000861	2.624137
5	6	0	4.631782	-0.511779	2.057528
6	6	0	4.682055	-0.694588	0.679294
7	8	0	1.297356	0.501025	-0.260992
8	6	0	0.599506	-0.470093	-1.289406
9	8	0	0.921802	-1.662096	-1.236463
10	6	0	-1.009738	-0.127021	-1.244230
11	6	0	-1.442638	1.196718	-0.617157
12	6	0	-1.964031	1.258371	0.694925
13	7	0	-2.102850	0.079157	1.447504
14	6	0	-2.221149	-1.149304	0.770837
15	6	0	-1.713956	-1.275521	-0.535948
16	6	0	-1.396635	2.376115	-1.366044
17	6	0	-1.785818	3.605327	-0.837030
18	6	0	-2.270950	3.663468	0.467897

19	6	0	-2.373977	2.498156	1.222935
20	6	0	-2.866909	-2.248026	1.372624
21	6	0	-2.983495	-3.458374	0.694967
22	6	0	-2.479111	-3.589043	-0.598213
23	6	0	-1.858596	-2.496366	-1.198609
24	8	0	-1.422890	-0.147513	-2.613033
25	6	0	-2.448397	0.157321	2.851025
26	8	0	1.106914	0.109619	-2.625577
27	8	0	1.238764	1.574780	-2.617293
28	6	0	3.777508	-0.568231	-1.649257
29	1	0	-1.714815	4.505467	-1.441833
30	1	0	-1.016917	2.312382	-2.376879
31	1	0	-2.592738	4.608526	0.899355
32	1	0	-2.809158	2.552714	2.213969
33	1	0	-3.308158	-2.152817	2.357832
34	1	0	-1.461225	-2.564148	-2.202481
35	1	0	-2.563824	-4.531535	-1.132316
36	1	0	-3.485103	-4.292801	1.179950
37	1	0	5.592356	-1.077062	0.221715
38	1	0	5.490648	-0.755236	2.678402
39	1	0	3.407243	0.167349	3.698082
40	6	0	1.108037	0.866008	2.454287
41	1	0	-1.925771	0.999646	3.308002
42	1	0	-3.529145	0.277227	3.034241
43	1	0	-2.112616	-0.750321	3.356479
44	1	0	-0.581691	-0.042198	-3.102595
45	1	0	1.476885	1.682075	-1.670833
46	1	0	1.229541	0.975649	3.537515
47	1	0	0.848577	1.841686	2.030503
48	1	0	0.252708	0.215313	2.257779
49	1	0	4.806917	-0.872837	-1.868236
50	1	0	3.078553	-1.315209	-2.029437
51	1	0	3.563603	0.355868	-2.194665

E_{total} = -1320.554895

E_0 = -1320.149956

E_{298} = -1320.124673

H_{298} = -1320.123728

G_{298} = -1320.20337

Compound **27** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.212792	-1.365928	-1.019535
2	6	0	1.247113	-0.539119	-0.448979
3	6	0	1.613641	0.714331	0.078453
4	6	0	2.963360	1.100239	0.037310
5	6	0	3.919304	0.254782	-0.521272
6	6	0	3.550736	-0.976772	-1.061434
7	6	0	-0.196901	-0.988533	-0.318665
8	6	0	-1.105895	0.232229	-0.478097

9	6	0	-0.674142	1.462161	0.068328
10	7	0	0.617600	1.555907	0.602945
11	6	0	-1.538850	2.569825	0.018074
12	6	0	-2.788964	2.461226	-0.584993
13	6	0	-3.193791	1.261506	-1.169831
14	6	0	-2.346299	0.157101	-1.111242
15	6	0	0.994433	2.715781	1.391953
16	6	0	-0.380592	-1.531023	1.139019
17	8	0	0.365157	-1.330066	2.058964
18	8	0	-0.437708	-2.013679	-1.263472
19	8	0	-1.497618	-2.276456	1.497050
20	1	0	4.295917	-1.630851	-1.502794
21	1	0	1.898192	-2.321364	-1.422339
22	1	0	4.957213	0.574228	-0.546741
23	1	0	3.267227	2.069484	0.414177
24	1	0	-1.222723	3.527408	0.413785
25	1	0	-2.650068	-0.779685	-1.562796
26	1	0	-4.158376	1.183881	-1.660891
27	1	0	-3.438093	3.331481	-0.617931
28	1	0	1.832909	2.450044	2.037846
29	1	0	1.281223	3.584668	0.781101
30	1	0	0.158469	3.001360	2.033065
31	1	0	-1.277065	-2.430405	-1.014357
32	8	0	-2.454978	-2.528905	0.412131
33	1	0	-2.722524	-3.425591	0.675336

E_{total} = -934.991179

E_0 = -934.735665

E_{298} = -934.719016

H_{298} = -934.728877

G_{298} = -934.792617

Compound **28**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.256866	-2.608108	0.135084
2	6	0	1.556315	-1.214898	0.018861
3	6	0	2.883958	-0.850046	-0.394497
4	6	0	3.845576	-1.859919	-0.630044
5	6	0	3.508565	-3.191018	-0.488292
6	6	0	2.206209	-3.570323	-0.115326
7	7	0	3.209673	0.479924	-0.563858
8	6	0	2.364052	1.483128	-0.126521
9	6	0	1.033445	1.158016	0.296670
10	6	0	0.593977	-0.201525	0.292558
11	6	0	2.807087	2.826152	-0.093888
12	6	0	1.959519	3.828540	0.331161
13	6	0	0.644185	3.535631	0.733979
14	6	0	0.194735	2.236469	0.717306
15	6	0	-0.891293	-0.556898	0.621913
16	1	0	-0.013093	4.330405	1.069620

17	1	0	-0.805113	2.002938	1.046176
18	1	0	2.324615	4.850718	0.364731
19	1	0	3.825427	3.078321	-0.355359
20	1	0	4.866141	-1.603070	-0.878278
21	1	0	0.245128	-2.852677	0.433037
22	1	0	1.954139	-4.620335	-0.010935
23	1	0	4.269308	-3.947754	-0.656645
24	8	0	-1.298878	-1.759320	0.602963
25	8	0	-1.610922	0.372326	-0.271061
26	6	0	-2.940047	0.152370	-0.542602
27	6	0	-3.872931	-0.249577	0.421863
28	6	0	-5.214138	-0.373255	0.060033
29	6	0	-5.639420	-0.092856	-1.240492
30	6	0	-4.703484	0.315041	-2.192546
31	6	0	-3.357914	0.432047	-1.848370
32	1	0	-3.550087	-0.457417	1.434769
33	1	0	-5.935629	-0.687640	0.809438
34	1	0	-6.687533	-0.190171	-1.507853
35	1	0	-5.018392	0.537926	-3.208512
36	1	0	-2.614192	0.740978	-2.576184
37	6	0	4.466661	0.836948	-1.234998
38	1	0	4.330640	1.770129	-1.777106
39	1	0	5.291828	0.945243	-0.523621
40	1	0	4.714698	0.068387	-1.963597
41	8	0	-0.947088	0.035715	2.022041
42	8	0	-1.662248	-0.887017	2.861675
43	1	0	-1.724039	-1.634584	2.191261

E_{total} = -1166.010899

E_0 = -1165.675358

E_{298} = -1165.654427

H_{298} = -1165.653483

G_{298} = -1165.725957

Compound **28**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.934849	-0.948370	0.658001
2	6	0	-3.026320	-0.040869	0.111400
3	6	0	-3.394538	0.807904	-0.946853
4	6	0	-4.707919	0.716070	-1.422176
5	6	0	-5.626110	-0.184333	-0.879946
6	6	0	-5.237193	-1.021497	0.164143
7	8	0	-1.760272	0.071477	0.681015
8	6	0	-0.728943	-0.846231	0.104493
9	8	0	-0.993887	-2.093597	0.795767
10	8	0	-0.863359	-1.854102	2.230196
11	6	0	-2.412762	1.781271	-1.547907
12	1	0	-3.609329	-1.598546	1.463076
13	6	0	0.695268	-0.292114	0.322330
14	6	0	1.804992	-1.166370	0.033815
15	6	0	3.060262	-0.611389	-0.362754

16	7	0	3.199687	0.762460	-0.487318
17	6	0	2.272856	1.612042	0.080986
18	6	0	1.006137	1.098567	0.512805
19	6	0	4.156052	-1.461404	-0.634716
20	6	0	4.017938	-2.831759	-0.534403
21	6	0	2.785093	-3.398599	-0.171983
22	6	0	1.708163	-2.584771	0.101870
23	6	0	0.126721	2.004977	1.172860
24	6	0	0.450403	3.330722	1.358566
25	6	0	1.678118	3.822329	0.884265
26	6	0	2.576723	2.981973	0.258414
27	6	0	4.358768	1.313827	-1.195247
28	8	0	-0.732778	-0.975280	-1.163682
29	1	0	-0.238516	3.989194	1.876911
30	1	0	-0.813120	1.618541	1.532312
31	1	0	1.942331	4.865354	1.031730
32	1	0	3.538514	3.373920	-0.043522
33	1	0	5.123683	-1.046741	-0.883923
34	1	0	0.755513	-3.008974	0.380978
35	1	0	2.679237	-4.475937	-0.101001
36	1	0	4.876736	-3.467441	-0.728676
37	1	0	-5.012036	1.365865	-2.239185
38	1	0	-6.637548	-0.230423	-1.273258
39	1	0	-5.938967	-1.730273	0.594057
40	1	0	4.076787	2.253282	-1.667742
41	1	0	5.209266	1.486077	-0.526224
42	1	0	4.655219	0.624973	-1.984283
43	1	0	-1.506263	-1.124260	2.327293
44	1	0	-2.869589	2.328713	-2.377221
45	1	0	-2.067367	2.513041	-0.809035
46	1	0	-1.533155	1.246586	-1.915199

E_{total} = -1205.322278

E_0 = -1204.958960

E_{298} = -1204.936187

H_{298} = -1204.935243

G_{298} = -1205.011681

Compound **28**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.721465	-2.584496	-0.060352
2	6	0	1.874281	-1.164487	-0.038096
3	6	0	3.153479	-0.631174	-0.388125
4	6	0	4.223845	-1.502860	-0.699521
5	6	0	4.031353	-2.868477	-0.684945
6	6	0	2.771861	-3.414183	-0.372118
7	7	0	3.335225	0.740691	-0.432116
8	6	0	2.409385	1.591153	0.132420
9	6	0	1.121603	1.087327	0.521811
10	6	0	0.796119	-0.285995	0.304606
11	6	0	2.727964	2.953715	0.346990

12	6	0	1.821773	3.793041	0.960387
13	6	0	0.569301	3.312800	1.385880
14	6	0	0.232138	1.997472	1.170155
15	6	0	-0.637287	-0.911821	0.192570
16	1	0	-0.125076	3.975214	1.891618
17	1	0	-0.723398	1.613400	1.489006
18	1	0	2.095923	4.829078	1.136310
19	1	0	3.703543	3.339356	0.084573
20	1	0	5.210609	-1.112446	-0.908473
21	1	0	0.754737	-2.990347	0.193542
22	1	0	2.631217	-4.489741	-0.367857
23	1	0	4.868730	-3.523561	-0.906455
24	8	0	-0.751565	-1.418050	-0.958252
25	8	0	-1.667712	0.121626	0.561938
26	6	0	-2.856801	0.112601	-0.155446
27	6	0	-2.928329	0.756147	-1.404136
28	6	0	-4.167708	0.807120	-2.051857
29	6	0	-5.306702	0.244135	-1.480869
30	6	0	-5.215522	-0.378186	-0.238627
31	6	0	-3.995263	-0.456721	0.442183
32	6	0	-1.711134	1.386908	-2.031563
33	1	0	-4.233099	1.299656	-3.018940
34	1	0	-6.260288	0.294368	-1.998817
35	1	0	-6.100706	-0.815257	0.216801
36	6	0	-3.915209	-1.126198	1.792413
37	6	0	4.532112	1.292180	-1.079194
38	1	0	4.289475	2.256613	-1.521163
39	1	0	5.360267	1.413707	-0.373042
40	1	0	4.838805	0.629588	-1.885830
41	8	0	-0.782184	-1.922186	1.250719
42	8	0	-0.540725	-1.277653	2.537188
43	1	0	-1.353713	-0.744653	2.601140
44	1	0	-1.975235	1.890272	-2.966077
45	1	0	-1.256354	2.127626	-1.364529
46	1	0	-0.958412	0.622130	-2.239546
47	1	0	-3.176017	-1.931734	1.791487
48	1	0	-3.631713	-0.411872	2.577066
49	1	0	-4.884719	-1.546142	2.073847

E_{total} = -1244.641252

E_0 = -1244.250505

E_{298} = -1244.226030

H_{298} = -1244.225085

G_{298} = -1244.304036

Compound **29**: R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.428510	2.975739	-0.008700
2	6	0	-2.139868	1.594607	0.056725
3	6	0	-0.849942	1.125410	-0.332045

4	6	0	0.082374	2.070742	-0.833916
5	6	0	-0.221622	3.413452	-0.903923
6	6	0	-1.480234	3.866579	-0.476364
7	6	0	-0.543656	-0.277095	-0.209662
8	6	0	-1.663961	-1.176979	-0.121624
9	6	0	-2.943146	-0.660477	0.250608
10	7	0	-3.097327	0.693815	0.500347
11	6	0	-4.040718	-1.541451	0.375178
12	6	0	-3.890322	-2.890805	0.115973
13	6	0	-2.645766	-3.408459	-0.277016
14	6	0	-1.560220	-2.566481	-0.389615
15	6	0	0.877630	-0.768035	-0.342554
16	8	0	1.119279	-2.008800	0.303659
17	6	0	-4.289620	1.178478	1.196614
18	8	0	1.740764	0.205511	0.349006
19	6	0	3.095612	0.008242	0.323801
20	6	0	3.788608	-0.522561	-0.775281
21	6	0	5.176660	-0.658255	-0.711085
22	6	0	5.887550	-0.252676	0.419061
23	6	0	5.192426	0.291458	1.502073
24	6	0	3.805810	0.415684	1.460757
25	1	0	3.249335	0.821013	2.299637
26	8	0	0.909527	-0.789484	-1.651721
27	1	0	3.235239	-0.803469	-1.663737
28	1	0	0.503363	4.112873	-1.306450
29	1	0	1.024894	1.695227	-1.201239
30	1	0	-1.730631	4.921406	-0.539738
31	1	0	-3.412145	3.342528	0.253343
32	1	0	-5.022352	-1.158740	0.621590
33	1	0	-0.602142	-2.943455	-0.708247
34	1	0	-2.539782	-4.463728	-0.505157
35	1	0	-4.753293	-3.545164	0.195693
36	1	0	5.731282	0.612351	2.389613
37	1	0	6.968079	-0.354370	0.454728
38	1	0	5.706315	-1.073481	-1.564611
39	1	0	-4.033500	2.069346	1.768730
40	1	0	-5.106980	1.417797	0.506245
41	1	0	-4.627806	0.419412	1.900779
42	1	0	1.680353	-2.486771	-0.325194

E_{total} = -1090.875673

E_0 = -1090.543970

E_{298} = -1090.523643

H_{298} = -1090.522699

G_{298} = -1090.593771

Compound **29**: $R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.559546	2.960728	-0.115572
2	6	0	-2.267753	1.582120	-0.020159
3	6	0	-0.995021	1.101212	-0.448633

4	6	0	-0.084985	2.029932	-1.016219
5	6	0	-0.392205	3.370644	-1.114007
6	6	0	-1.632150	3.836914	-0.648959
7	6	0	-0.684137	-0.298579	-0.296986
8	6	0	-1.801740	-1.194449	-0.138607
9	6	0	-3.062770	-0.665698	0.272892
10	7	0	-3.205156	0.695900	0.491547
11	6	0	-4.154516	-1.541122	0.466864
12	6	0	-4.015951	-2.897334	0.236861
13	6	0	-2.790002	-3.426955	-0.195770
14	6	0	-1.709655	-2.589549	-0.376541
15	6	0	0.725953	-0.800282	-0.461385
16	8	0	0.987824	-2.011960	0.228796
17	6	0	-4.365812	1.201673	1.224420
18	8	0	1.632469	0.194429	0.132507
19	6	0	2.983852	-0.045495	0.068389
20	6	0	3.615730	-0.539418	-1.080027
21	6	0	4.999044	-0.729590	-1.081013
22	6	0	5.754253	-0.409571	0.045625
23	6	0	5.113920	0.095579	1.179742
24	6	0	3.729304	0.279316	1.218847
25	6	0	3.027487	0.799940	2.446830
26	8	0	0.683833	-0.879038	-1.770024
27	1	0	3.014365	-0.758112	-1.954927
28	1	0	0.315390	4.057131	-1.566681
29	1	0	0.843291	1.643781	-1.408090
30	1	0	-1.885907	4.889456	-0.733577
31	1	0	-3.531629	3.335817	0.176277
32	1	0	-5.124722	-1.150553	0.744505
33	1	0	-0.766698	-2.974893	-0.729236
34	1	0	-2.694704	-4.487769	-0.401917
35	1	0	-4.875135	-3.547924	0.370338
36	1	0	5.698344	0.343823	2.062772
37	1	0	6.831508	-0.547655	0.044556
38	1	0	5.483545	-1.116333	-1.973506
39	1	0	-4.085939	2.109702	1.757185
40	1	0	-5.213687	1.419947	0.564414
41	1	0	-4.671284	0.464441	1.965874
42	1	0	3.732517	0.939819	3.271059
43	1	0	2.534151	1.758768	2.250998
44	1	0	2.243084	0.107706	2.769922
45	1	0	1.556791	-2.506007	-0.380575

E_{total} = -1130.196789

E_0 = -1129.837512

E_{298} = -1129.815428

H_{298} = -1129.814484

G_{298} = -1129.889803

Compound **29**: $R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.637949	-2.477617	-0.870162
2	6	0	-1.815179	-1.163493	-0.370588
3	6	0	-3.090945	-0.815023	0.164099
4	6	0	-4.109523	-1.791702	0.225696
5	6	0	-3.887220	-3.069398	-0.254276
6	6	0	-2.648611	-3.414886	-0.816149
7	6	0	-0.765129	-0.171046	-0.389266
8	6	0	-1.181596	1.208116	-0.282198
9	6	0	-2.472233	1.504671	0.246940
10	7	0	-3.321342	0.473099	0.624562
11	6	0	-2.872769	2.851114	0.391483
12	6	0	-2.033301	3.878284	0.000240
13	6	0	-0.773475	3.599392	-0.551258
14	6	0	-0.360632	2.290225	-0.687780
15	6	0	0.667095	-0.543816	-0.647163
16	8	0	1.015765	-1.826715	-0.159718
17	6	0	-4.483247	0.752991	1.466778
18	8	0	1.561635	0.423744	0.002704
19	6	0	2.879851	0.065923	0.242412
20	6	0	3.218362	-0.407257	1.523297
21	6	0	4.560647	-0.695817	1.790613
22	6	0	5.540853	-0.519223	0.815468
23	6	0	5.185279	-0.031828	-0.440115
24	6	0	3.854357	0.277236	-0.750139
25	6	0	2.154508	-0.588468	2.575611
26	6	0	3.493464	0.864061	-2.094226
27	8	0	0.542701	-0.435918	-1.952649
28	1	0	-0.130653	4.407574	-0.883774
29	1	0	0.592635	2.054329	-1.135205
30	1	0	-2.370987	4.905631	0.099877
31	1	0	-3.862125	3.089920	0.759121
32	1	0	-5.091840	-1.532689	0.598679
33	1	0	-0.690277	-2.715188	-1.326050
34	1	0	-2.489522	-4.408459	-1.221700
35	1	0	-4.692425	-3.797127	-0.217367
36	1	0	4.834597	-1.062704	2.776728
37	1	0	6.578805	-0.751727	1.036442
38	1	0	5.949267	0.121998	-1.198211
39	1	0	-4.248739	1.578256	2.138235
40	1	0	-5.373669	1.010064	0.880532
41	1	0	-4.700928	-0.120793	2.080129
42	1	0	1.624506	-2.177615	-0.827841
43	1	0	4.326522	0.761365	-2.795682
44	1	0	2.603984	0.392012	-2.517390
45	1	0	3.271314	1.935268	-2.001338
46	1	0	2.601540	-0.816352	3.547411
47	1	0	1.543422	0.314257	2.675733
48	1	0	1.477524	-1.403232	2.301139

E_{total} = -1169.514664

E_0 = -1169.127780

E_{298} = -1169.104027

H_{298} = -1169.103083

G_{298} = -1169.181468

Compound **30** (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.470286	1.027600	-0.035828
2	6	0	1.220331	0.350531	-0.008393
3	6	0	1.206503	-1.077142	-0.029856
4	6	0	2.431825	-1.771578	-0.165596
5	6	0	3.622970	-1.072833	-0.224991
6	6	0	3.652720	0.333061	-0.141621
7	7	0	-0.000044	-1.752279	0.086957
8	6	0	-1.209917	-1.076859	0.028996
9	6	0	-1.220688	0.351051	-0.012000
10	6	0	0.000041	1.079026	0.026784
11	6	0	-2.441739	-1.771857	-0.006711
12	6	0	-3.632323	-1.072136	-0.067973
13	6	0	-3.654685	0.335630	-0.108637
14	6	0	-2.467557	1.030099	-0.092047
15	6	0	0.003700	2.605297	0.099153
16	1	0	-4.599753	0.863990	-0.172979
17	1	0	-2.439860	2.110227	-0.177200
18	1	0	-4.564819	-1.627604	-0.104483
19	1	0	-2.472011	-2.852779	-0.021782
20	1	0	2.453862	-2.848997	-0.258600
21	1	0	2.456278	2.107612	0.049750
22	1	0	4.599976	0.860775	-0.166541
23	1	0	4.550321	-1.626254	-0.339289
24	8	0	-0.408909	3.173271	-0.928417
25	8	0	0.421536	3.027977	1.194801
26	6	0	0.002546	-3.204254	0.296739
27	1	0	-0.836061	-3.479124	0.933668
28	1	0	-0.064723	-3.752505	-0.648878
29	1	0	0.912007	-3.493197	0.818451

E_{total} = -783.422015

E_0 = -783.196978

E_{298} = -783.182818

H_{298} = -783.181874

G_{298} = -783.238525

Compound **31**

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000006	-1.748523	0.345099
2	6	0	-1.210677	-1.124937	0.024794
3	6	0	-2.410889	-1.857676	-0.065641
4	6	0	-3.607307	-1.223911	-0.381072

5	6	0	-3.645291	0.150065	-0.628159
6	6	0	-2.465210	0.880052	-0.552931
7	6	0	-1.251703	0.263037	-0.229998
8	6	0	0.000011	1.083089	-0.116175
9	6	0	1.251704	0.263026	-0.229979
10	6	0	2.465216	0.880026	-0.552915
11	6	0	3.645285	0.150025	-0.628151
12	6	0	3.607279	-1.223954	-0.381066
13	6	0	2.410855	-1.857704	-0.065635
14	6	0	1.210658	-1.124948	0.024804
15	8	0	0.000021	2.234610	-1.051142
16	6	0	-0.000006	-3.102553	0.880382
17	1	0	0.879565	-3.240955	1.510376
18	1	0	-0.000159	-3.874905	0.099107
19	1	0	-0.879409	-3.240861	1.510635
20	1	0	-2.406577	-2.930825	0.077956
21	1	0	-4.515461	-1.815714	-0.447889
22	1	0	-4.578907	0.641992	-0.879444
23	1	0	-2.463125	1.945709	-0.755947
24	1	0	2.463131	1.945684	-0.755934
25	1	0	4.578907	0.641937	-0.879439
26	1	0	4.515422	-1.815774	-0.447887
27	1	0	2.406523	-2.930857	0.077952
28	6	0	-0.000018	2.146213	0.998455
29	8	0	0.000107	3.188514	0.100579
30	8	0	-0.000042	2.216266	2.187380

E_{total} = -858.564180

E_0 = -858.334887

E_{298} = -858.320472

H_{298} = -858.319527

G_{298} = -858.376298

Transition state of stage VI (**17 → 19 + 20**):

R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.756827	-1.453687	0.471062
2	6	0	-3.043079	-0.246876	0.437962
3	6	0	-3.732877	0.966183	0.294139
4	6	0	-5.120736	0.971142	0.189478
5	6	0	-5.840869	-0.227086	0.216813
6	6	0	-5.147354	-1.430343	0.355826
7	8	0	-1.687555	-0.148119	0.560557
8	6	0	-0.911198	-1.335926	0.458019
9	8	0	-0.944071	-1.885848	-0.842995
10	8	0	-0.118328	-0.894767	-1.636320
11	6	0	0.722187	-0.326019	-0.663339
12	6	0	2.006042	-0.988554	-0.463307
13	6	0	3.002838	-0.313202	0.292628

14	7	0	2.684851	0.962671	0.812462
15	6	0	1.744791	1.773590	0.136046
16	6	0	0.720905	1.126856	-0.614450
17	6	0	2.294887	-2.272679	-0.945216
18	6	0	3.527006	-2.884616	-0.695555
19	6	0	4.504541	-2.210099	0.027984
20	6	0	4.244208	-0.917468	0.509024
21	6	0	1.786968	3.168905	0.203141
22	6	0	0.807770	3.949953	-0.429350
23	6	0	-0.200334	3.326494	-1.157903
24	6	0	-0.232265	1.932812	-1.257210
25	6	0	3.544231	1.553242	1.809097
26	8	0	-0.773393	-2.068393	1.413305
27	1	0	2.976372	2.289276	2.384834
28	1	0	4.434955	2.058906	1.394578
29	1	0	3.887714	0.773634	2.494470
30	1	0	5.024944	-0.383559	1.041038
31	1	0	5.470534	-2.669576	0.222712
32	1	0	3.715333	-3.888875	-1.068603
33	1	0	1.522731	-2.786980	-1.506082
34	1	0	-1.006702	1.436852	-1.830887
35	1	0	-0.963290	3.918871	-1.658380
36	1	0	0.852977	5.033447	-0.352715
37	1	0	2.591226	3.662177	0.739156
38	1	0	-3.226606	-2.389609	0.595059
39	1	0	-5.692844	-2.370879	0.380395
40	1	0	-6.924032	-0.222012	0.130779
41	1	0	-5.643304	1.918599	0.079660
42	1	0	-3.152186	1.882309	0.261052

E_{total} = -1165.459300

E_0 = -1165.140104

E_{298} = -1165.119465

H_{298} = -1165.118521

G_{298} = -1165.190641

Transition state of stage VI (**17** → **19 + 20**):

$R_2 = CH_3$, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005279	1.771137	1.681770
2	6	0	-0.857369	1.043085	0.848940
3	6	0	-1.707693	1.769514	-0.030928
4	6	0	-1.672763	3.167431	-0.040688
5	6	0	-0.781911	3.870725	0.783301
6	6	0	0.055412	3.167558	1.644466
7	6	0	-0.944953	-0.412935	0.847812
8	6	0	-2.211575	-0.992302	0.401366
9	6	0	-3.027087	-0.235483	-0.481982
10	7	0	-2.560035	1.036151	-0.887969

11	6	0	-4.243492	-0.759550	-0.928990
12	6	0	-4.647168	-2.049898	-0.553387
13	6	0	-3.842085	-2.805056	0.292578
14	6	0	-2.640235	-2.273474	0.770162
15	8	0	-0.299757	-1.057811	1.879046
16	8	0	0.657558	-2.061513	1.116130
17	6	0	0.702917	-1.438446	-0.138743
18	8	0	0.558594	-2.097201	-1.143833
19	6	0	-3.207196	1.708981	-1.987795
20	8	0	1.545563	-0.287526	-0.158697
21	6	0	2.896416	-0.476315	-0.266351
22	6	0	3.538485	-1.697867	-0.027570
23	6	0	4.926502	-1.785664	-0.142743
24	6	0	5.681229	-0.667253	-0.491412
25	6	0	5.028354	0.545400	-0.728857
26	6	0	3.641121	0.667532	-0.626898
27	1	0	-2.512094	2.428040	-2.429825
28	1	0	-4.126555	2.252907	-1.705644
29	1	0	-3.471356	0.974720	-2.753650
30	1	0	-4.894105	-0.165873	-1.562888
31	1	0	-5.588842	-2.445736	-0.925977
32	1	0	-4.141552	-3.809325	0.583786
33	1	0	-1.998376	-2.849582	1.427259
34	1	0	0.647171	1.211607	2.352962
35	1	0	0.746287	3.699159	2.295185
36	1	0	-0.763145	4.957135	0.749984
37	1	0	-2.348240	3.722623	-0.683190
38	1	0	2.952271	-2.563142	0.254832
39	1	0	5.414217	-2.738903	0.046272
40	1	0	6.762269	-0.734246	-0.580722
41	1	0	5.606448	1.424388	-1.008049
42	6	0	2.930605	1.967550	-0.901133
43	1	0	3.642310	2.745060	-1.197038
44	1	0	2.190105	1.848091	-1.699425
45	1	0	2.370986	2.314409	-0.026769

E_{total} = -1204.780454

E_0 = -1204.433831

E_{298} = -1204.411325

H_{298} = -1204.410381

G_{298} = -1204.486559

Transition state of stage VI (**17** → **19** + **20**):

$R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.490386	1.642399	2.129929
2	6	0	-1.129587	0.941172	1.094277
3	6	0	-1.854682	1.696543	0.126779
4	6	0	-1.936489	3.086496	0.242222

5	6	0	-1.270498	3.764098	1.276124
6	6	0	-0.545949	3.036159	2.215223
7	6	0	-1.087788	-0.504606	0.953333
8	6	0	-2.173850	-1.123568	0.201359
9	6	0	-2.867111	-0.341492	-0.762101
10	7	0	-2.444296	0.996861	-0.952949
11	6	0	-3.919134	-0.900797	-1.491818
12	6	0	-4.270293	-2.249336	-1.322604
13	6	0	-3.580682	-3.027576	-0.398965
14	6	0	-2.550439	-2.464783	0.359770
15	8	0	-0.670266	-1.191128	2.096226
16	8	0	0.467758	-2.061725	1.594072
17	6	0	0.857557	-1.411307	0.400925
18	8	0	0.984882	-2.045763	-0.624534
19	6	0	-2.940427	1.735815	-2.088444
20	8	0	1.688704	-0.311591	0.706006
21	6	0	2.781562	-0.092051	-0.118262
22	6	0	3.910661	-0.918249	0.016819
23	6	0	5.044343	-0.616384	-0.745915
24	6	0	5.053919	0.469675	-1.619282
25	6	0	3.918218	1.269300	-1.738322
26	6	0	2.762360	1.003760	-0.994531
27	1	0	-2.252059	2.554358	-2.315642
28	1	0	-3.946602	2.167975	-1.940359
29	1	0	-2.982822	1.073315	-2.957198
30	1	0	-4.485177	-0.290435	-2.187763
31	1	0	-5.079575	-2.670873	-1.913797
32	1	0	-3.838171	-4.075799	-0.263879
33	1	0	-2.002356	-3.060058	1.081169
34	1	0	0.067490	1.064139	2.857377
35	1	0	-0.023435	3.546754	3.021268
36	1	0	-1.334344	4.847611	1.336784
37	1	0	-2.526385	3.656582	-0.467951
38	6	0	3.885388	-2.098521	0.953796
39	1	0	5.927218	-1.244508	-0.647251
40	1	0	5.943144	0.693085	-2.203633
41	1	0	3.918712	2.116232	-2.420902
42	6	0	1.528564	1.857339	-1.123243
43	1	0	0.665473	1.254210	-1.420080
44	1	0	1.260406	2.324394	-0.171453
45	1	0	1.678825	2.643943	-1.869549
46	1	0	4.897399	-2.467805	1.147338
47	1	0	3.408769	-1.838688	1.903457
48	1	0	3.293393	-2.915316	0.526128

E_{total} = -1244.103111

E_0 = -1243.728536

E_{298} = -1243.704550

H_{298} = -1243.703605

G_{298} = -1243.782223

Transition state of stage IX (**24** → **19** + **21** + **25**):

R_2 = H, R_6 = H (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.566273	2.295513	-1.735468
2	6	0	1.036983	1.287471	-0.898218
3	6	0	1.464440	1.609147	0.408082
4	6	0	1.399221	2.944319	0.840290
5	6	0	0.903769	3.936426	-0.009059
6	6	0	0.486224	3.618588	-1.301279
7	6	0	1.108476	-0.124750	-1.401560
8	6	0	2.097718	-0.953771	-0.633167
9	6	0	2.493270	-0.578954	0.669260
10	7	0	1.952599	0.585319	1.238729
11	6	0	3.424842	-1.376248	1.356091
12	6	0	3.938266	-2.531063	0.762215
13	6	0	3.548463	-2.899783	-0.525201
14	6	0	2.635441	-2.100039	-1.212665
15	6	0	-0.604715	-0.858113	-0.149638
16	8	0	-0.847168	-1.941802	0.300110
17	8	0	0.832561	-0.396324	-2.588488
18	6	0	2.109868	0.828141	2.657554
19	8	0	-1.796490	0.089777	-0.367339
20	6	0	-3.058208	-0.271601	-0.038703
21	6	0	-3.857123	0.671138	0.635650
22	6	0	-5.184104	0.388132	0.951128
23	6	0	-5.742898	-0.849639	0.619498
24	6	0	-4.950898	-1.792971	-0.040524
25	6	0	-3.625068	-1.517147	-0.373277
26	1	0	3.949785	-3.799318	-0.985098
27	1	0	2.293172	-2.339258	-2.214797
28	1	0	4.656738	-3.134064	1.312952
29	1	0	3.770985	-1.092203	2.343967
30	1	0	1.753376	3.221874	1.827236
31	1	0	0.249974	1.990073	-2.727790
32	1	0	0.101328	4.392558	-1.960502
33	1	0	0.860039	4.963596	0.346076
34	1	0	3.066736	1.308529	2.921160
35	1	0	1.296607	1.468620	3.005274
36	1	0	2.041791	-0.120115	3.194950
37	1	0	-3.017540	-2.250623	-0.886787
38	1	0	-5.372839	-2.760118	-0.307194
39	1	0	-6.777069	-1.073881	0.868843
40	1	0	-5.785870	1.138140	1.461201
41	1	0	-3.408072	1.626973	0.889088

E_{total} = -1090.323898

E_0 = -1090.009054

E_{298} = -1089.988506

H_{298} = -1089.987562

G_{298} = -1090.061277

Transition state of stage IX (**24** → **19** + **21** + **25**):

$R_2 = CH_3$, $R_6 = H$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.329767	-1.921984	0.406159
2	6	0	2.845706	-0.627922	0.150832
3	6	0	3.688740	0.324503	-0.471645
4	6	0	4.994005	-0.044650	-0.803722
5	6	0	5.476603	-1.332671	-0.552432
6	6	0	4.634791	-2.266433	0.052120
7	8	0	1.605220	-0.211946	0.506193
8	6	0	0.350233	-1.054885	0.231812
9	8	0	0.513954	-2.138976	-0.250256
10	6	0	-1.325977	-0.184271	1.425306
11	6	0	-1.068952	1.225148	0.975479
12	6	0	-1.377966	1.627731	-0.341926
13	7	0	-1.937707	0.691209	-1.228501
14	6	0	-2.644701	-0.413287	-0.724490
15	6	0	-2.366413	-0.866815	0.583156
16	6	0	-1.123483	2.954270	-0.728888
17	6	0	-0.561944	3.857245	0.177274
18	6	0	-0.266083	3.460984	1.481623
19	6	0	-0.532186	2.147518	1.869234
20	6	0	-3.626831	-1.073975	-1.482145
21	6	0	-4.305592	-2.172996	-0.951583
22	6	0	-4.032463	-2.618507	0.341572
23	6	0	-3.068313	-1.953083	1.098902
24	8	0	-1.148356	-0.518371	2.615665
25	6	0	-1.986113	0.986035	-2.645414
26	1	0	-4.563160	-3.473777	0.752183
27	1	0	-2.811445	-2.257190	2.108971
28	1	0	-5.060267	-2.670560	-1.556550
29	1	0	-3.882791	-0.725530	-2.476907
30	1	0	-1.380610	3.297876	-1.725102
31	1	0	-0.313774	1.780682	2.867167
32	1	0	0.167713	4.166783	2.185482
33	1	0	-0.371581	4.878871	-0.143734
34	1	0	-2.860721	1.587992	-2.942651
35	1	0	-1.082728	1.528758	-2.931836
36	1	0	-2.005597	0.049845	-3.207232
37	1	0	2.672802	-2.641181	0.877246
38	1	0	4.994828	-3.272674	0.256757
39	1	0	6.495313	-1.598890	-0.823831
40	1	0	5.644392	0.693575	-1.271252
41	6	0	3.157067	1.708668	-0.743211
42	1	0	3.907663	2.328146	-1.246125
43	1	0	2.256945	1.671439	-1.366334
44	1	0	2.851068	2.207969	0.182344

E_{total} = -1129.645630

E_0 = -1129.303157

E_{298} = -1129.280922

H_{298} = -1129.279978

G_{298} = -1129.356829

Transition state of stage IX (**24** → **19** + **21** + **25**):

$R_2 = CH_3$, $R_6 = CH_3$ (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.493217	-1.210411	0.509963
2	6	0	2.884306	-0.077925	-0.073764
3	6	0	3.617476	0.768466	-0.933519
4	6	0	4.961690	0.483633	-1.186245
5	6	0	5.578672	-0.629348	-0.612014
6	6	0	4.840402	-1.463075	0.228348
7	8	0	1.598465	0.251933	0.213751
8	6	0	0.433733	-0.615491	-0.327460
9	8	0	0.735403	-1.485708	-1.093098
10	6	0	-1.188304	-0.388695	1.277981
11	6	0	-1.324006	1.089183	1.080895
12	6	0	-1.981789	1.606622	-0.056529
13	7	0	-2.495150	0.716682	-1.015010
14	6	0	-2.806004	-0.603081	-0.653850
15	6	0	-2.177620	-1.175179	0.474359
16	6	0	-2.110324	2.998580	-0.197168
17	6	0	-1.576311	3.857036	0.766616
18	6	0	-0.926790	3.344895	1.889762
19	6	0	-0.815705	1.962948	2.039263
20	6	0	-3.736256	-1.369186	-1.377736
21	6	0	-4.021501	-2.680683	-0.993892
22	6	0	-3.402356	-3.244237	0.122032
23	6	0	-2.490728	-2.480230	0.849366
24	8	0	-0.689589	-0.857475	2.320761
25	6	0	-2.889437	1.213925	-2.317134
26	1	0	-3.627255	-4.265334	0.419077
27	1	0	-1.976771	-2.868218	1.723294
28	1	0	-4.743653	-3.254785	-1.569938
29	1	0	-4.258583	-0.943232	-2.227359
30	1	0	-2.642096	3.420198	-1.043226
31	1	0	-0.314249	1.510563	2.888576
32	1	0	-0.510940	4.015121	2.637643
33	1	0	-1.684515	4.931359	0.636014
34	1	0	-3.921666	1.599472	-2.348698
35	1	0	-2.213091	2.017359	-2.615813
36	1	0	-2.798516	0.411340	-3.051995
37	6	0	2.695437	-2.111070	1.419141
38	1	0	5.317135	-2.329660	0.684131
39	1	0	6.626294	-0.841245	-0.813117
40	1	0	5.528680	1.142267	-1.842661
41	6	0	2.925257	1.958846	-1.547907
42	1	0	3.353055	-2.681764	2.084519
43	1	0	1.980556	-1.538333	2.016425
44	1	0	2.100312	-2.820268	0.832677
45	1	0	3.624871	2.565953	-2.132873
46	1	0	2.108886	1.641133	-2.206803

47	1	0	2.465013	2.588174	-0.779146

E_{total} = -1168.967193

E_0 = -1168.597258

E_{298} = -1168.573206

H_{298} = -1168.572262

G_{298} = -1168.653313

Transition state of stage XII (**27** → **18** + **19** + **22**) (Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.202045	-1.468988	-0.876621
2	6	0	1.228921	-0.556777	-0.449624
3	6	0	1.616590	0.742272	-0.036623
4	6	0	2.985721	1.084685	-0.053061
5	6	0	3.929038	0.162434	-0.476082
6	6	0	3.542803	-1.119709	-0.896762
7	6	0	-0.197732	-0.964009	-0.355098
8	6	0	-1.125168	0.212702	-0.470146
9	6	0	-0.684764	1.489184	-0.037843
10	7	0	0.647539	1.672249	0.328565
11	6	0	-1.594197	2.568537	-0.050957
12	6	0	-2.894471	2.384096	-0.496066
13	6	0	-3.321392	1.129964	-0.952586
14	6	0	-2.437057	0.060124	-0.934114
15	6	0	1.041562	2.875806	1.055862
16	6	0	-0.368212	-1.393252	1.313493
17	8	0	0.453236	-0.886533	2.072816
18	8	0	-0.483496	-2.048807	-1.146441
19	8	0	-1.348570	-2.118438	1.628902
20	1	0	4.289328	-1.832201	-1.232236
21	1	0	1.868459	-2.451363	-1.188558
22	1	0	4.976762	0.447079	-0.493330
23	1	0	3.307768	2.078827	0.229809
24	1	0	-1.275248	3.558737	0.249085
25	1	0	-2.745555	-0.915292	-1.291101
26	1	0	-4.332721	0.997212	-1.323045
27	1	0	-3.576141	3.229027	-0.506841
28	1	0	1.884611	2.639431	1.704421
29	1	0	1.320350	3.698631	0.385781
30	1	0	0.217147	3.197817	1.691440
31	1	0	-1.300322	-2.494184	-0.762033
32	8	0	-2.325803	-3.025209	0.202062
33	1	0	-3.072268	-2.469985	0.475305

E_{total} = -934.952419

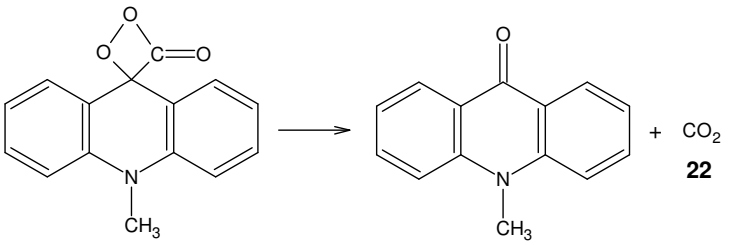
E_0 = -934.701052

E_{298} = -934.684501

H_{298} = -934.683556

G_{298} = -934.744435

Transition state of the reaction:



31 **19** **22**

(for numbers of some of the compounds see Scheme 1)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211491	-1.170696	0.055375
2	7	0	-0.000088	-1.776908	0.404411
3	6	0	-1.211502	-1.170578	0.055191
4	6	0	-1.244948	0.205340	-0.274341
5	6	0	0.000089	0.994734	-0.207002
6	6	0	1.245061	0.205233	-0.274181
7	6	0	-2.460925	0.805933	-0.629389
8	6	0	-3.640755	0.075399	-0.662667
9	6	0	-3.607784	-1.284121	-0.339319
10	6	0	-2.413630	-1.903712	0.009795
11	6	0	2.413596	-1.903909	0.009795
12	6	0	3.607792	-1.284371	-0.339281
13	6	0	3.640870	0.075174	-0.662477
14	6	0	2.461084	0.805764	-0.629177
15	6	0	-0.000408	-3.105371	1.001639
16	8	0	0.000211	2.165236	-1.078142
17	8	0	0.000181	3.221933	-0.044865
18	6	0	0.000001	2.409039	1.059971
19	8	0	-0.000172	2.752068	2.193955
20	1	0	0.878714	-3.214982	1.637614
21	1	0	-0.000125	-3.911246	0.255312
22	1	0	-0.880186	-3.214853	1.636756
23	1	0	-2.413613	-2.967148	0.213119
24	1	0	-4.518418	-1.874906	-0.372169
25	1	0	-4.573903	0.554367	-0.939851
26	1	0	-2.455144	1.859377	-0.886995
27	1	0	2.455366	1.859213	-0.886770
28	1	0	4.574045	0.554091	-0.939660
29	1	0	4.518374	-1.875227	-0.372265
30	1	0	2.413550	-2.967381	0.212850

E_{total} = -858.539179

E_0 = -858.311795

E_{298} = -858.297693

H_{298} = -858.296749

G_{298} = -858.352544