Supporting Information

Chromane Helicity Rule – Scope and Challenges Based on ECD Study of Various Trolox Derivatives

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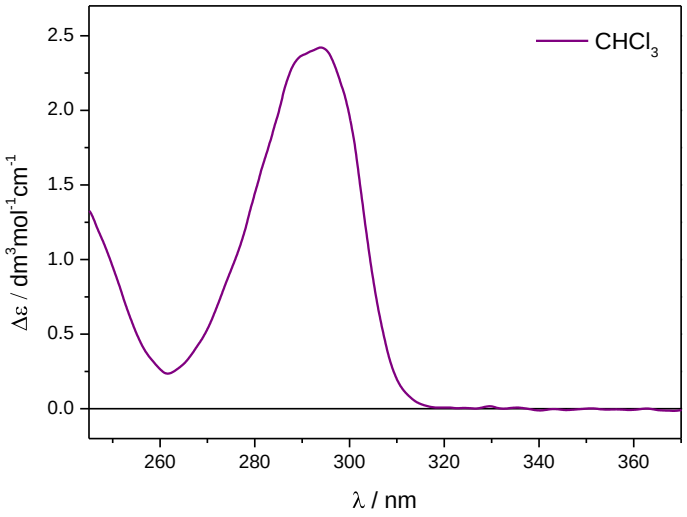


Figure S1. ECD spectrum of chromane **2** recorded in chloroform at room temperature. The symbol Δε denotes the difference of the molar decadic absorption coefficients of left and right circularly polarized light, and λ – the wavelength.

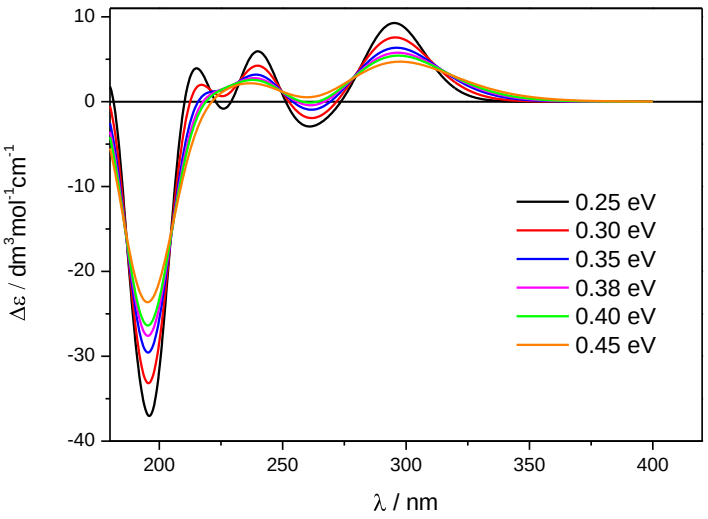


Figure S2. Boltzmann averaged ECD spectra of chromane **2** calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) level of theory simulated with different values of the Gaussian band-width.

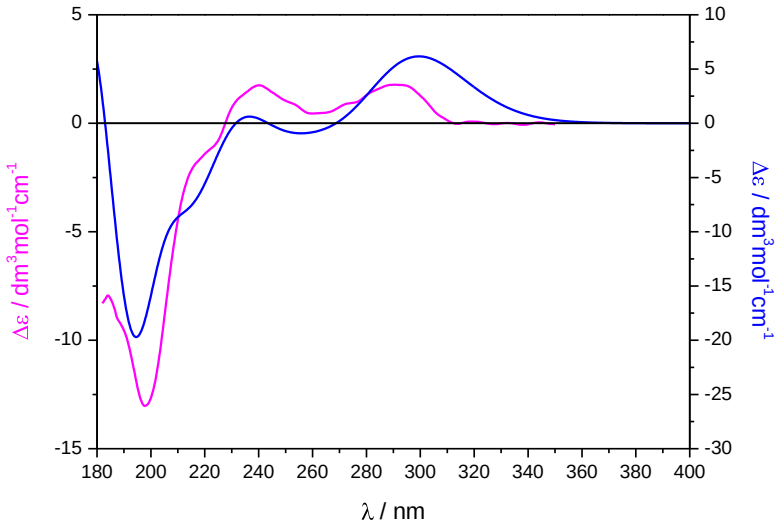
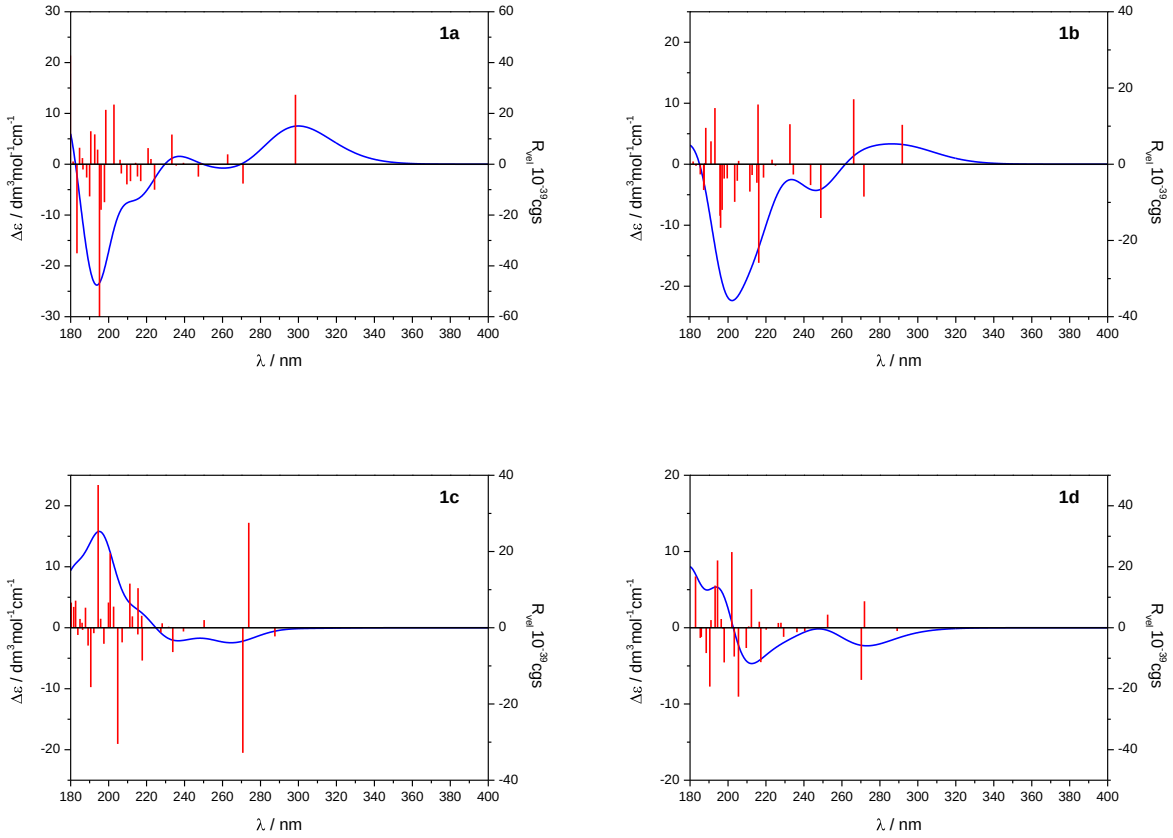


Figure S3. The experimental (pink line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) ECD spectra (blue line) for compound **1**.



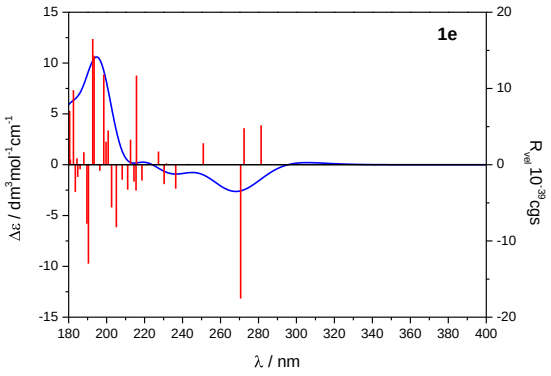


Figure S4. ECD spectra of individual conformers of compound **1** calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) level.

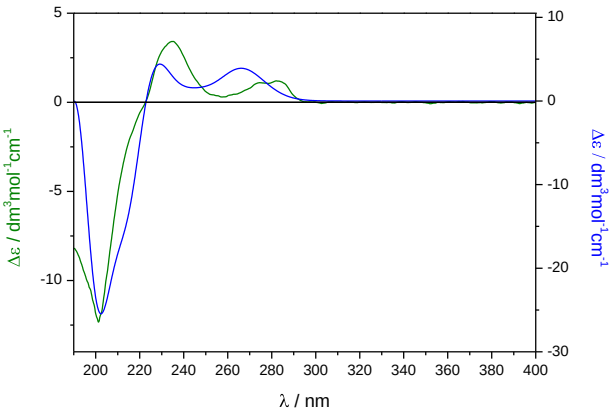


Figure S5. The experimental (green line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) ECD spectra (blue line) for compound **3**.

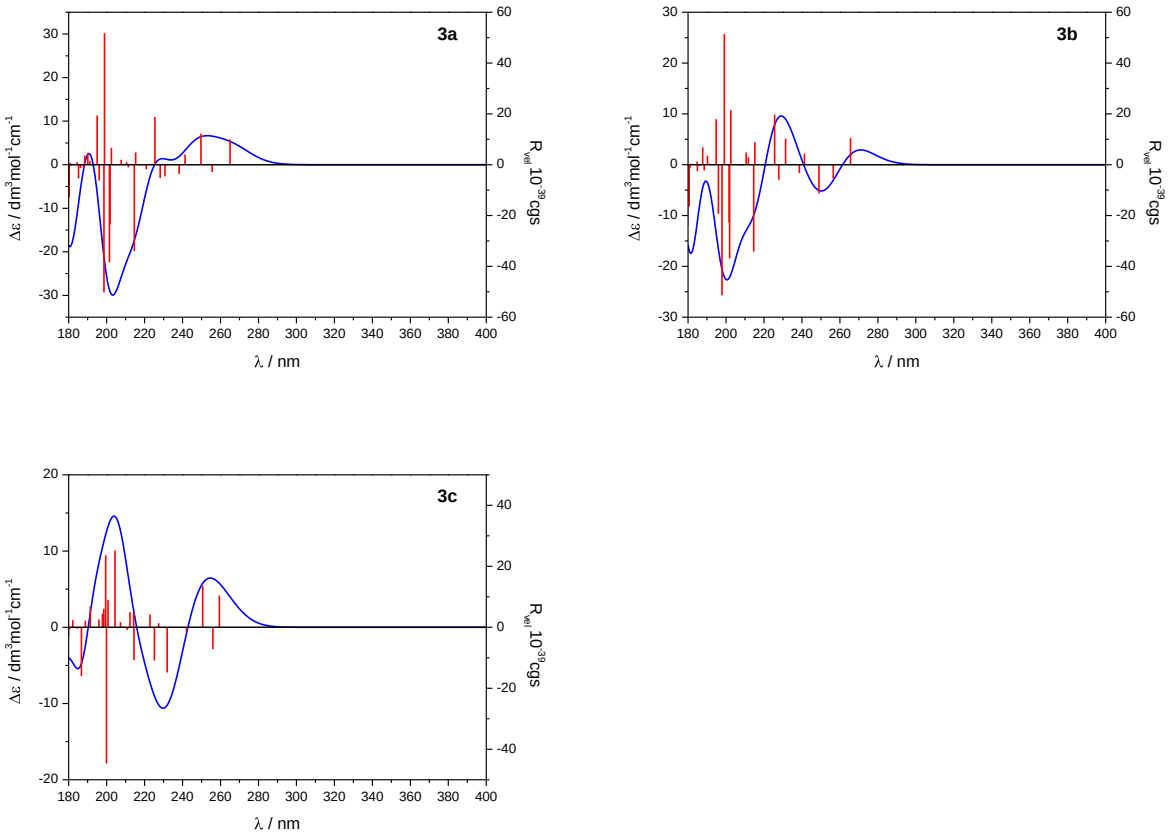


Figure S6. ECD spectra of individual conformers of compound **3** calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) level.

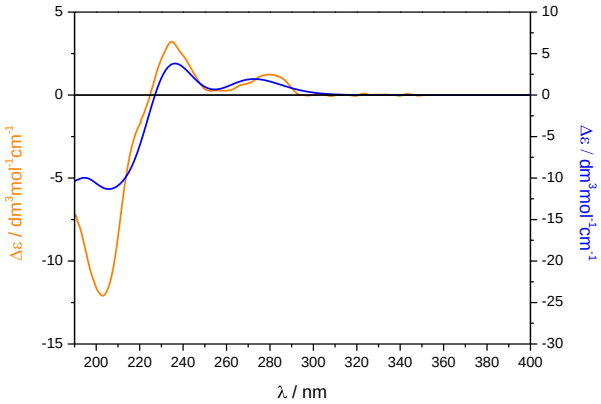


Figure S7. The experimental (orange line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) ECD spectra (blue line) for compound **4**.

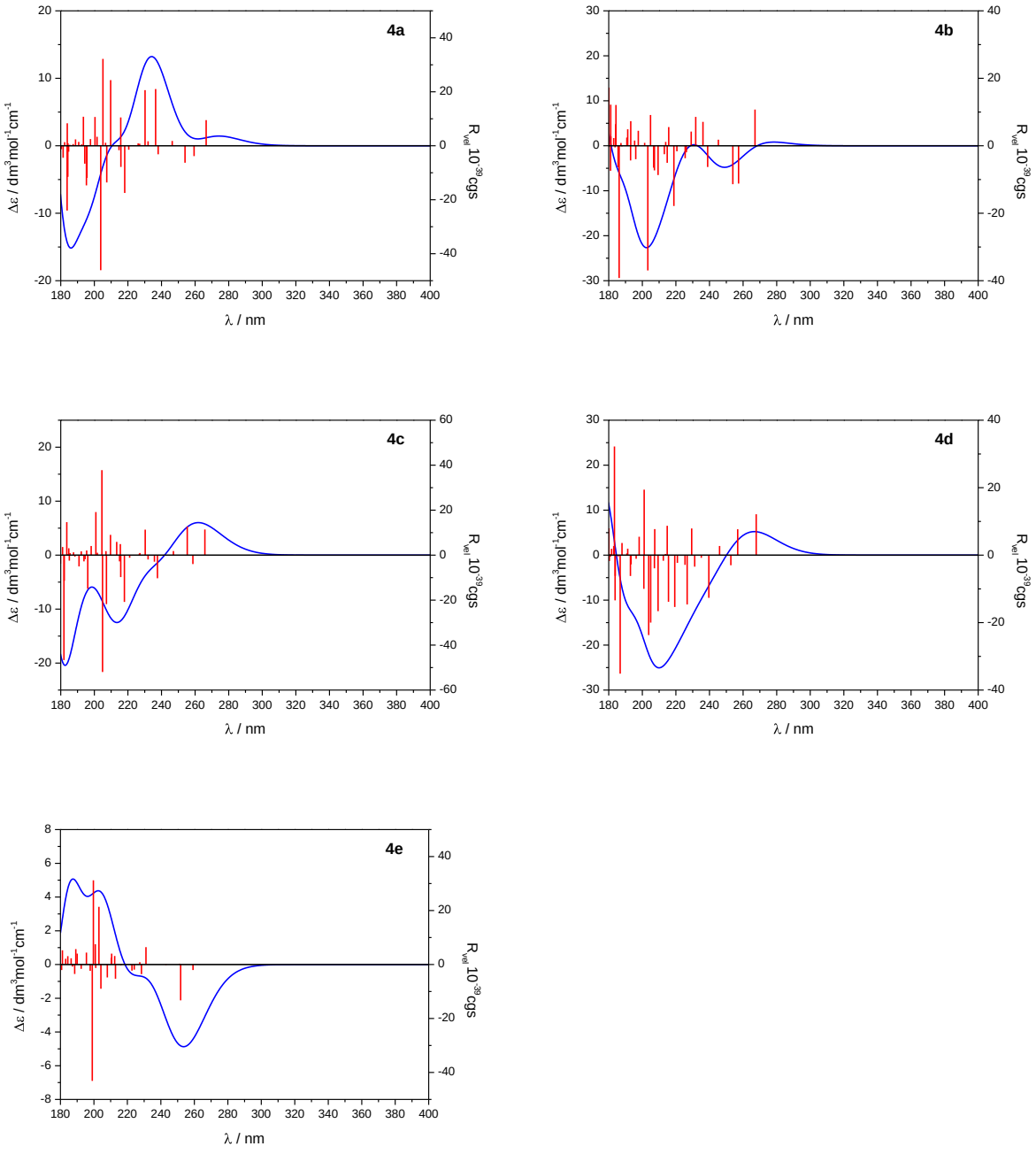


Figure S8. ECD spectra of individual conformers of compound **4** calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) level.

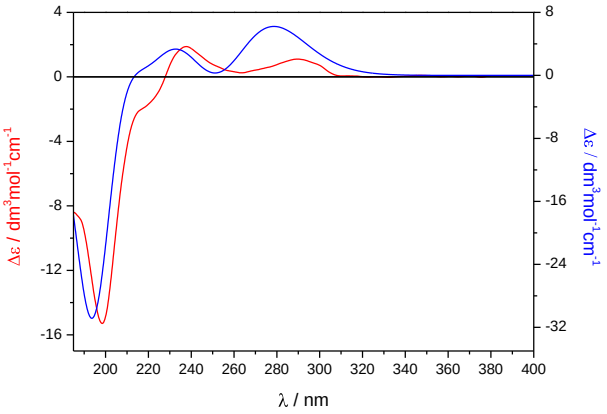


Figure S9. The experimental (red line) and Boltzmann averaged calculated at B3LYP/TZVP/PCM(CH_3CN) ECD spectra (blue line) for compound **5**.

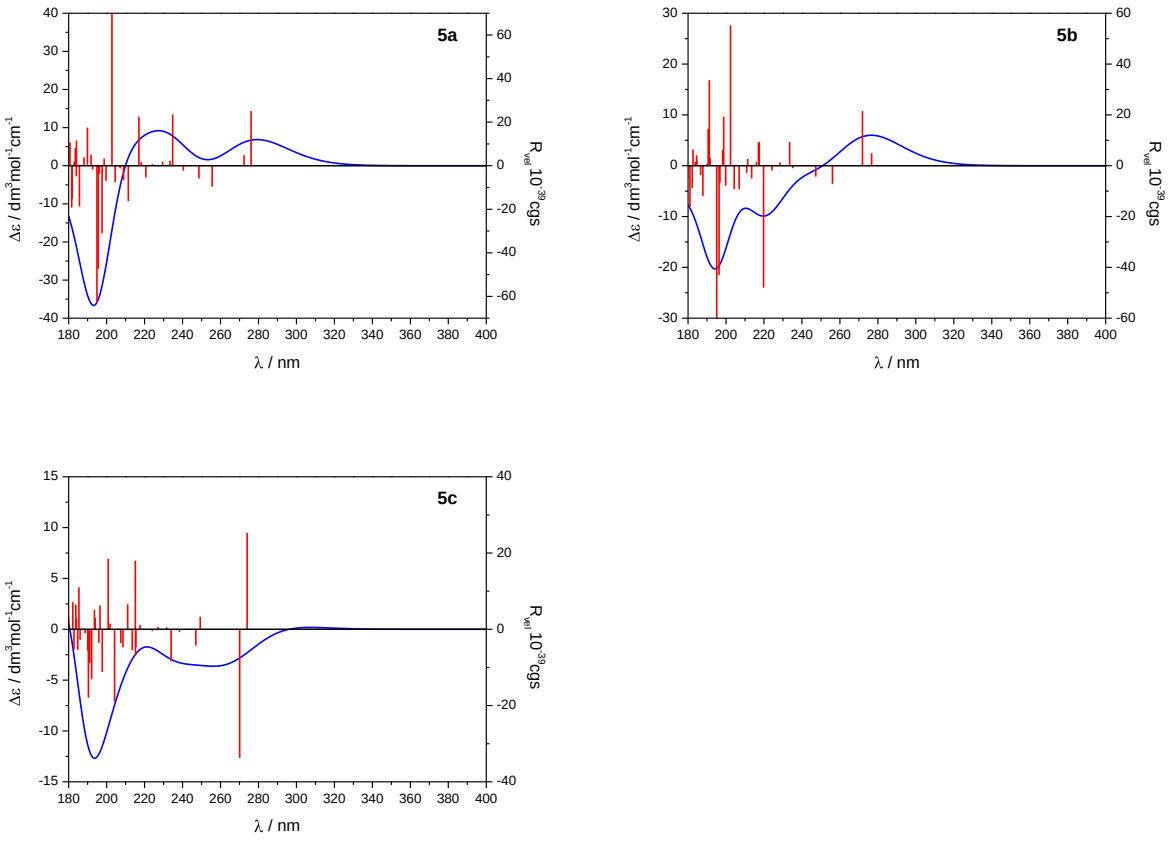


Figure S10. ECD spectra of individual conformers of compound **5** calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) level.

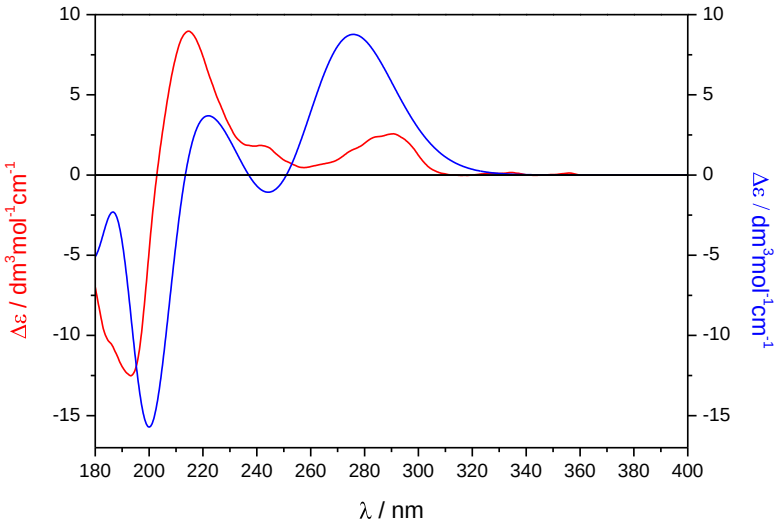


Figure S11. The experimental (red line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) ECD spectra (blue line) for compound **6**.

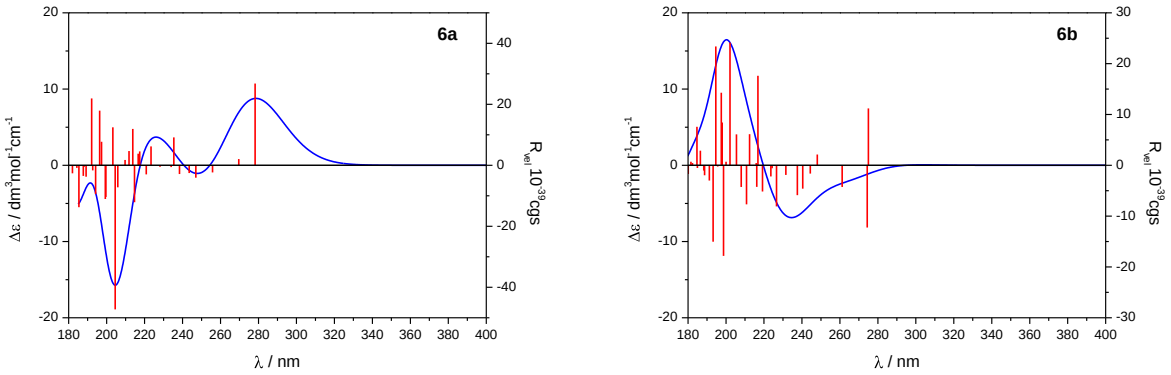


Figure S12. ECD spectra of individual conformers of compound **6** calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) level.

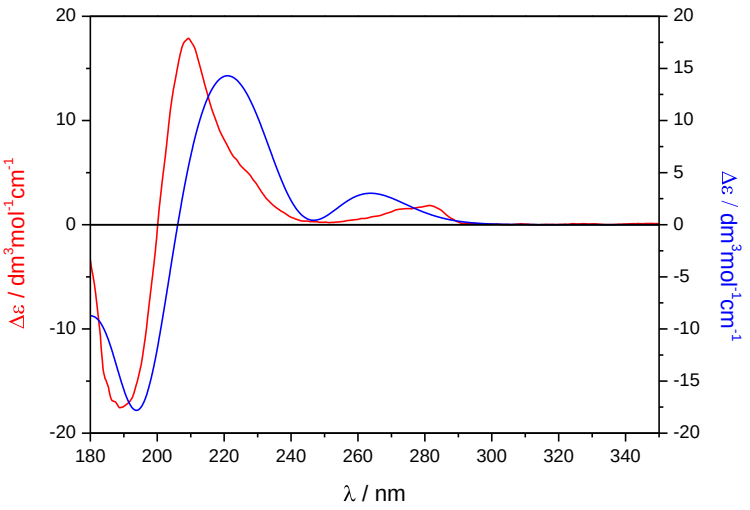


Figure S13. The experimental (red line) and Boltzmann averaged calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) ECD spectra (blue line) for compound **7**.

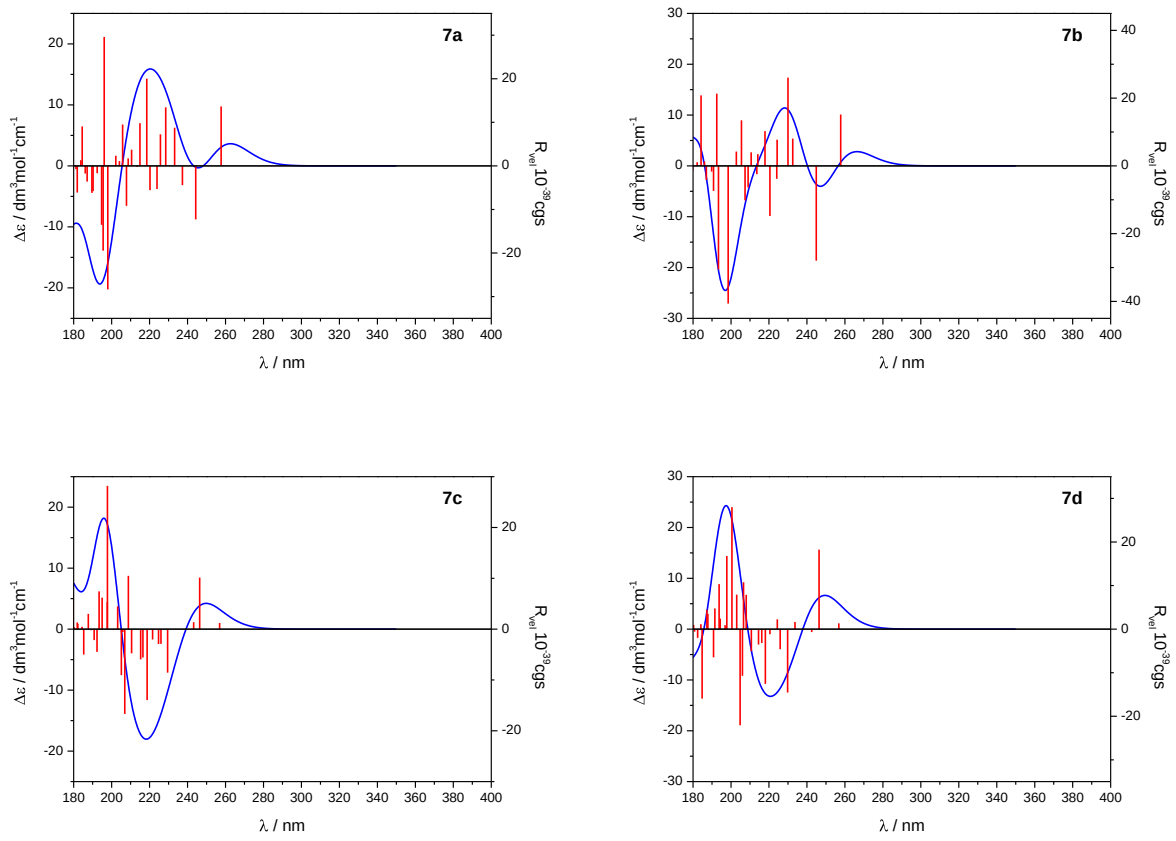


Figure S14. ECD spectra of individual conformers of compound **7** calculated at B3LYP/6-311++G(d,p)/PCM(CH_3CN) level.

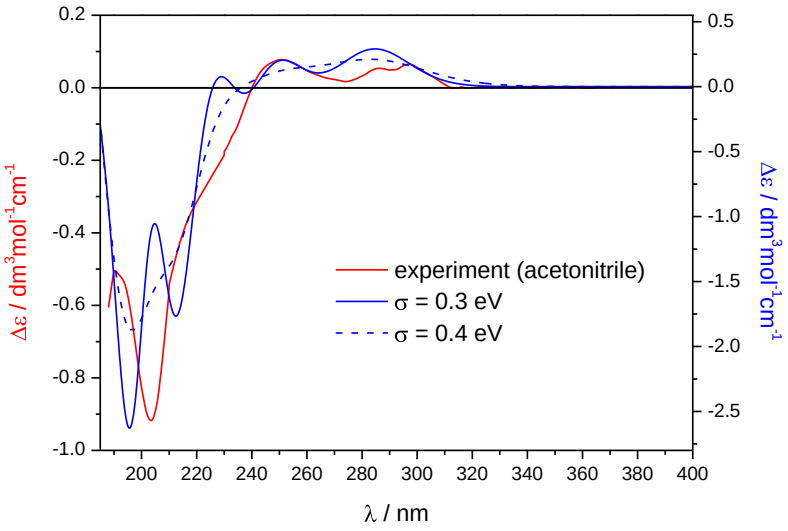


Figure S15. The experimental (red line) and Boltzmann averaged calculated at B3LYP/TZVP/PCM(CH_3CN) ECD spectra (blue line) using 0.3 and 0.4 eV Gaussian band-shape as a half-height width for compound **8**.

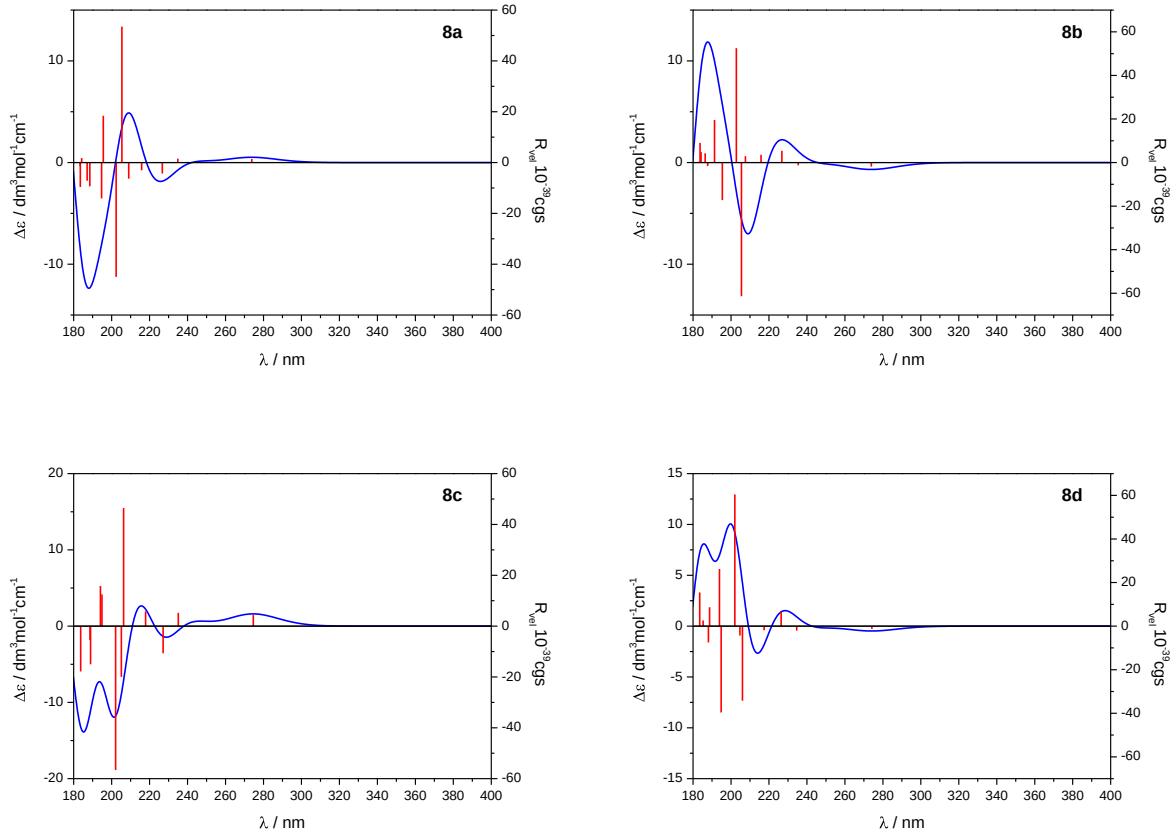
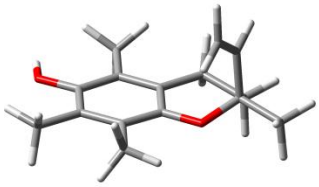
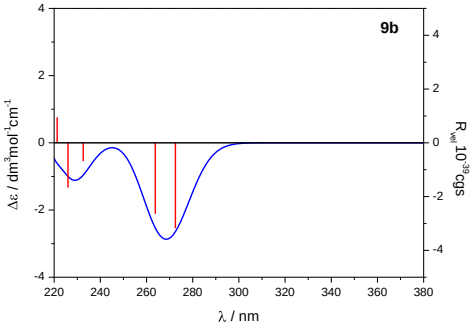


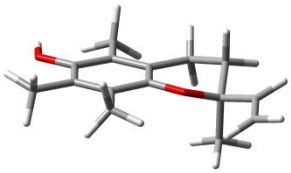
Figure S16. ECD spectra of individual conformers of compound **8** calculated at B3LYP/TZVP/PCM(CH_3CN) level.

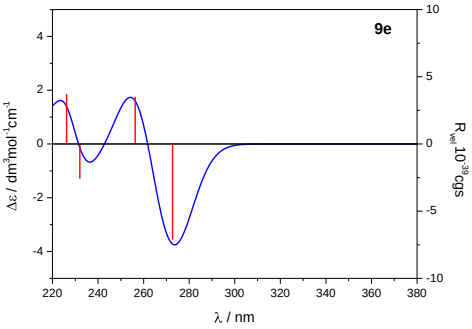
9b



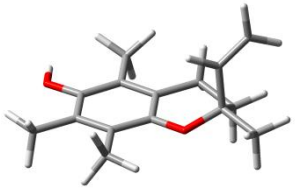

9b
Δε / dm³mol⁻¹cm⁻¹
R_vel 10⁻³⁹ cgs
λ / nm

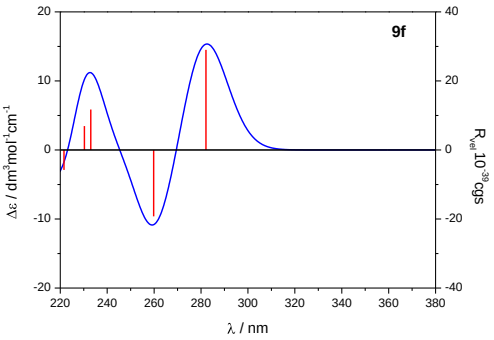
9e



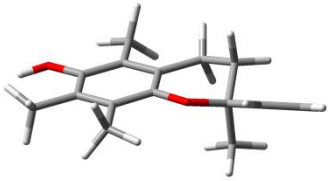

9e
Δε / dm³mol⁻¹cm⁻¹
R_vel 10⁻³⁹ cgs
λ / nm

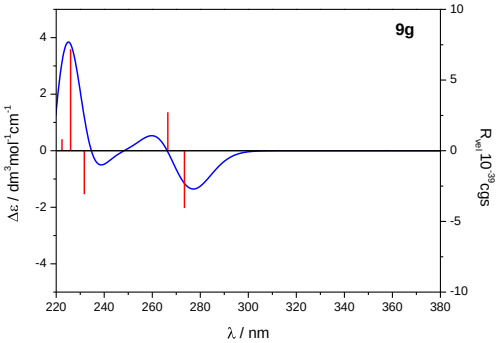
9f



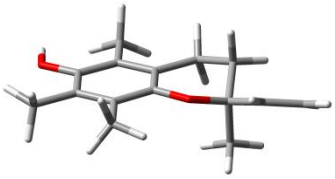

9f
Δε / dm³mol⁻¹cm⁻¹
R_vel 10⁻³⁹ cgs
λ / nm

9g




9g
Δε / dm³mol⁻¹cm⁻¹
R_vel 10⁻³⁹ cgs
λ / nm

9h



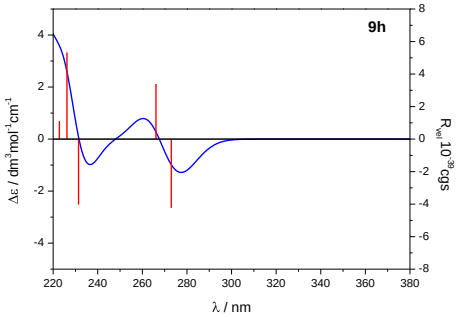
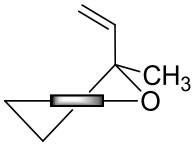
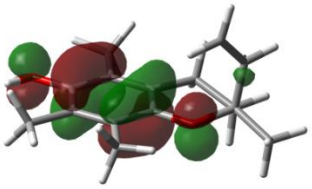


Figure S17. Simulated ECD spectra and structures of conformers of compound **9** calculated at the B3LYP/TZVP/PCM(CH_3CN) level of theory (remaining conformers and their spectra are given in main text).

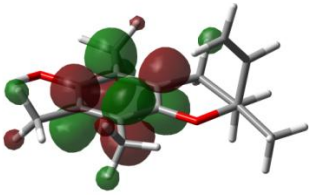
9a



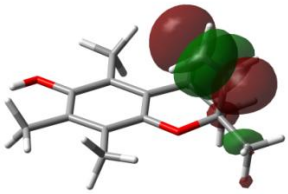
HOMO



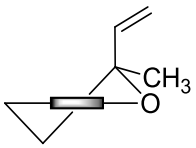
LUMO



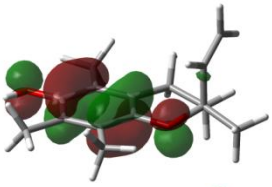
LUMO+1



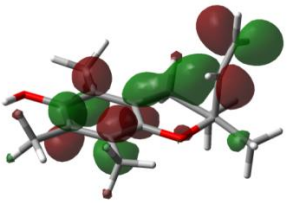
9c



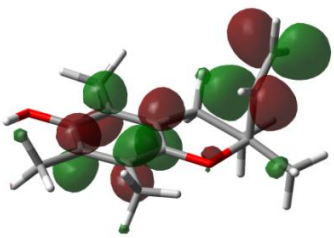
HOMO



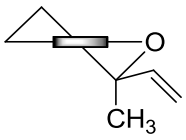
LUMO



LUMO+1



9d



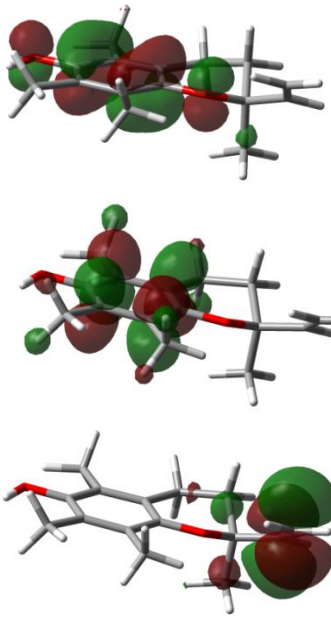


Figure S18. MOs of compound **9** (for conformers **9a**, **9c** and **9d**).

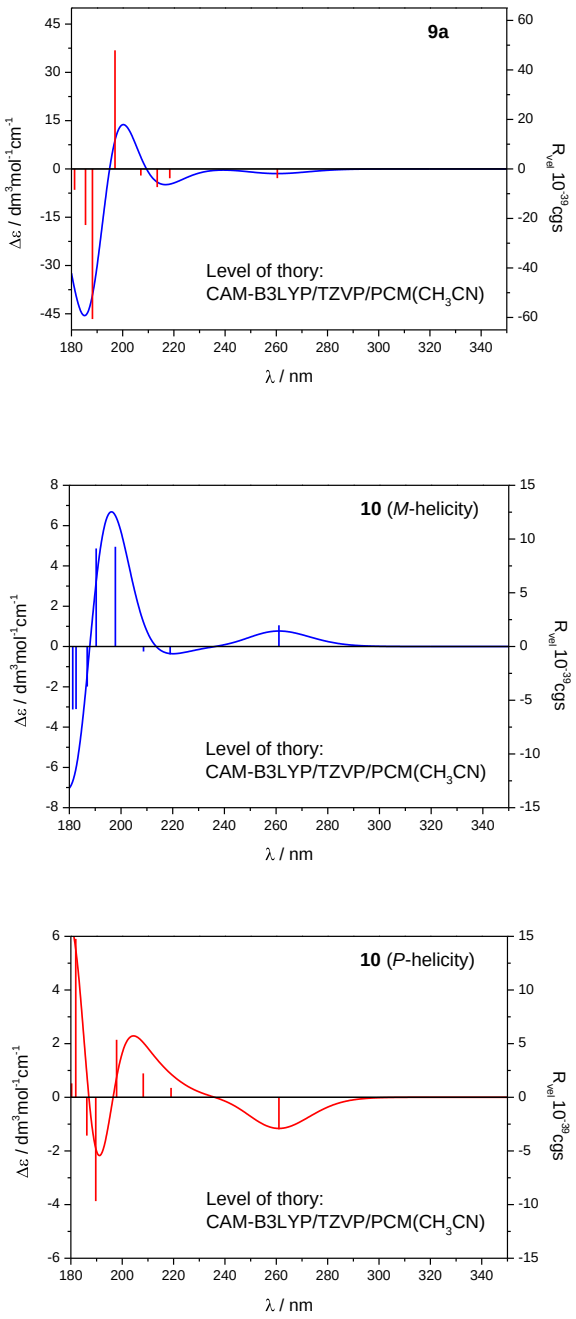


Figure S19. ECD spectra of individual conformers **9a**, **10 (*M*-helicity)** and **10 (*P*-helicity)** calculated at CAM-B3LYP/TZVP/PCM(CH_3CN) level.

Table S1. Electric (μ_e) and magnetic (μ_m) transition dipole moments, and their angles (θ) for two lowest transitions of most stable conformers of compounds **1-11** calculated at: B3LYP/6-311++G(d,p)/PCM(CH_3CN)[a] and B3LYP/TZVP/PCM(CH_3CN)[b] levels of theory.

Comp.	$\lvert\mu_e\rvert$	$\lvert\mu_m\rvert$	θ / deg	MO→MO*
1a[a]	0.50	0.36	51	HOMO-LUMO
	0.34	0.28	110	HOMO-LUMO+1
2a[a]	0.57	0.40	58	HOMO-LUMO
	0.29	0.28	115	HOMO-LUMO+1
3a[a]	0.37	0.23	61	HOMO-LUMO
	0.41	0.39	95	HOMO-LUMO+1
4a[a]	0.53	0.42	80	HOMO-LUMO
	0.28	0.32	109	HOMO-LUMO+1
5a[a]	0.83	0.45	74	HOMO-LUMO
	0.12	0.25	47	HOMO-LUMO+1
6a[a]	0.80	0.43	71	HOMO-LUMO
	0.07	0.28	69	HOMO-LUMO+1
7a[a]	0.51	0.38	72	HOMO-LUMO
	0.36	0.29	121	HOMO-LUMO+1
8a[b]	0.96	0.49	89.6	HOMO-LUMO
	0.06	0.39	80	HOMO-LUMO+1
9a[b]	0.95	0.47	93	HOMO-LUMO
	0.16	0.08	130	HOMO-LUMO+1
10 *P*-helicity[a]	0.39	0.49	60	HOMO-LUMO
	0.87	0.93	98	HOMO-LUMO+1
10 *M*-helicity[a]	0.26	0.32	136	HOMO-LUMO
	0.91	0.81	85	HOMO-LUMO+1
10 *P*-helicity[b]	0.96	1.00	90.2	HOMO-LUMO
	0.06	0.43	102	HOMO-LUMO+1
10 *M*-helicity[b]	0.95	0.83	90.4	HOMO-LUMO
	0.08	0.37	75	HOMO-LUMO+1
11 *P*-helicity[a]	0.45	0.46	58	HOMO-LUMO
	0.84	0.76	102	HOMO-LUMO+1
11 *M*-helicity[a]	0.24	0.35	45	HOMO-LUMO
	0.84	0.74	91	HOMO-LUMO+1
11 *P*-helicity[b]	0.96	0.83	90.3	HOMO-LUMO
	0.34	0.35	93	HOMO-LUMO+1
11 *M*-helicity[b]	0.87	0.76	84	HOMO-LUMO
	0.32	0.41	124	HOMO-LUMO+1

Cartesian coordinates for individual conformers of compounds 1-11 calculated by means of DFT at B3LYP/6-31G(d) level of theory.

Compound 1

Conf. 1a

Imaginary frequencies = 0
Sum of electronic and thermal Enthalpies (Hartree) = -844.99381400

1	6	0	-2.632155	0.453360	0.102271
2	6	0	-2.401701	-0.929046	0.016821
3	6	0	-1.603766	1.392490	-0.054116
4	6	0	-0.299976	0.939969	-0.337602
5	6	0	-0.069711	-0.440048	-0.402638
6	6	0	-1.095986	-1.382313	-0.218393
7	6	0	0.843968	1.913640	-0.563889
8	6	0	2.087372	1.225865	-1.139046
9	6	0	2.316805	-0.134905	-0.476028
10	8	0	1.181696	-0.970177	-0.683970
11	6	0	-1.931585	2.864131	0.088894
12	6	0	-3.548259	-1.898755	0.188300
13	6	0	-0.781920	-2.858624	-0.286343
14	6	0	3.501973	-0.889179	-1.092370
15	8	0	-3.926783	0.851259	0.364302
16	1	0	1.113108	2.407068	0.379672
17	1	0	0.533521	2.712115	-1.248098
18	1	0	2.968975	1.858942	-1.008855
19	1	0	1.958506	1.038689	-2.211569
20	1	0	-2.481820	3.062949	1.019554
21	1	0	-1.035578	3.485474	0.122623
22	1	0	-2.546707	3.239540	-0.743497
23	1	0	-3.538135	-2.669018	-0.591008
24	1	0	-3.495399	-2.419594	1.154300
25	1	0	-4.506854	-1.379846	0.146052
26	1	0	0.275585	-3.036386	-0.085437
27	1	0	-1.374275	-3.425920	0.438397
28	1	0	-1.002875	-3.273524	-1.279961
29	1	0	4.430519	-0.329021	-0.946359
30	1	0	3.603372	-1.876890	-0.633470
31	1	0	3.327582	-1.019244	-2.164739
32	6	0	2.609068	0.040896	1.027842
33	1	0	-3.985726	1.812693	0.271129
34	8	0	3.176836	1.000781	1.504257
35	8	0	2.230402	-1.025584	1.762716
36	1	0	2.494239	-0.823136	2.680610

Conf. 1b

Imaginary frequencies = 0
Sum of electronic and thermal Enthalpies (Hartree) = -844.99231000

1	6	0	4.673018	5.030154	-5.491672
2	6	0	5.710499	4.186365	-5.058302
3	6	0	3.660639	5.475915	-4.631573
4	6	0	3.697565	5.093779	-3.275896
5	6	0	4.723317	4.243699	-2.851280
6	6	0	5.722177	3.772839	-3.719239
7	6	0	2.654322	5.570504	-2.280932
8	6	0	3.087802	5.317490	-0.832792

9	6	0	3.720818	3.927113	-0.684505
10	8	0	4.852686	3.823069	-1.535776
11	6	0	2.557410	6.347789	-5.194166
12	6	0	6.771041	3.737829	-6.039695
13	6	0	6.765466	2.830315	-3.168344
14	6	0	4.244599	3.679253	0.736026
15	8	0	4.684449	5.394209	-6.822858
16	1	0	1.692896	5.068877	-2.466845
17	1	0	2.462551	6.642274	-2.408597
18	1	0	2.241168	5.425170	-0.149286
19	1	0	3.852814	6.045148	-0.536166
20	1	0	2.097338	5.889311	-6.081280
21	1	0	1.750276	6.507600	-4.477735
22	1	0	2.919655	7.344578	-5.489931
23	1	0	7.779549	3.919409	-5.650867
24	1	0	6.695499	2.663247	-6.251878
25	1	0	6.672063	4.269337	-6.986783
26	1	0	6.287953	2.054647	-2.561770
27	1	0	7.338932	2.347376	-3.961770
28	1	0	7.473070	3.352572	-2.510641
29	1	0	3.425506	3.702987	1.459877
30	1	0	4.742693	2.706416	0.790023
31	1	0	4.972951	4.454924	0.991249
32	6	0	2.731955	2.797487	-1.037783
33	1	0	3.991753	6.052383	-6.975077
34	8	0	2.958467	1.855903	-1.757467
35	8	0	1.546655	2.957550	-0.388817
36	1	0	1.002952	2.184182	-0.632254

Conf. 1c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -844.99101300

1	6	0	-2.856136	-0.233405	-0.031594
2	6	0	-2.443422	1.107994	-0.041490
3	6	0	-1.940088	-1.294104	-0.048989
4	6	0	-0.561715	-1.008365	-0.101747
5	6	0	-0.151065	0.331689	-0.087184
6	6	0	-1.070800	1.394890	-0.055550
7	6	0	0.477073	-2.114311	-0.170205
8	6	0	1.864276	-1.582313	-0.545236
9	6	0	2.163004	-0.282347	0.208682
10	8	0	1.183533	0.701079	-0.134346
11	6	0	-2.468458	-2.712774	-0.005187
12	6	0	-3.466978	2.218709	-0.024820
13	6	0	-0.584115	2.825382	-0.050193
14	6	0	2.223342	-0.459815	1.739248
15	8	0	-4.215399	-0.465543	0.009777
16	1	0	0.529138	-2.646882	0.790743
17	1	0	0.182301	-2.866816	-0.910800
18	1	0	2.642995	-2.321664	-0.341753
19	1	0	1.903258	-1.361593	-1.617988
20	1	0	-2.998790	-2.990421	-0.929222
21	1	0	-1.673522	-3.447078	0.132080
22	1	0	-3.169488	-2.853151	0.829950
23	1	0	-3.461807	2.754746	0.934162
24	1	0	-3.259795	2.962198	-0.803571
25	1	0	-4.472871	1.827506	-0.181642
26	1	0	-0.838037	3.336122	-0.989040
27	1	0	-1.051800	3.400736	0.757942

28	1	0	0.498205	2.871400	0.072483
29	1	0	2.989593	-1.192986	2.012088
30	1	0	2.459964	0.496337	2.214433
31	1	0	1.256993	-0.801199	2.120229
32	6	0	3.516386	0.279061	-0.243090
33	1	0	-4.377948	-1.410543	-0.120480
34	8	0	4.438479	-0.406995	-0.627363
35	8	0	3.608168	1.617969	-0.103758
36	1	0	4.515530	1.849462	-0.379958

Conf. 1d

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -844.99073900

1	6	0	5.707854	4.266895	2.010105
2	6	0	4.853372	3.403411	2.719264
3	6	0	5.541240	4.530166	0.644490
4	6	0	4.493747	3.895296	-0.052984
5	6	0	3.629828	3.056938	0.659208
6	6	0	3.794224	2.796276	2.031533
7	6	0	4.287977	4.091354	-1.543210
8	6	0	3.356264	3.025304	-2.129066
9	6	0	2.128853	2.812928	-1.219371
10	8	0	2.560925	2.398944	0.077437
11	6	0	6.491123	5.495243	-0.033942
12	6	0	5.091320	3.160897	4.194034
13	6	0	2.811918	1.865017	2.701902
14	6	0	1.234854	4.054879	-1.106231
15	8	0	6.726861	4.859214	2.727844
16	1	0	5.246997	4.037755	-2.071311
17	1	0	3.885723	5.093360	-1.750580
18	1	0	3.888043	2.069229	-2.201737
19	1	0	3.025825	3.300702	-3.135687
20	1	0	6.185952	5.727550	-1.055287
21	1	0	6.538409	6.454927	0.500712
22	1	0	7.517355	5.101044	-0.092576
23	1	0	4.240482	3.496460	4.800029
24	1	0	5.238501	2.095223	4.407721
25	1	0	5.976934	3.696705	4.536456
26	1	0	3.053290	1.700795	3.753161
27	1	0	1.792276	2.265109	2.643869
28	1	0	2.786806	0.892822	2.196461
29	1	0	0.857619	4.347701	-2.088907
30	1	0	0.380298	3.839169	-0.458237
31	1	0	1.793017	4.886448	-0.668197
32	6	0	1.314736	1.660088	-1.817808
33	1	0	7.299021	5.346959	2.118812
34	8	0	0.483278	1.813544	-2.686841
35	8	0	1.660841	0.446999	-1.341508
36	1	0	1.110236	-0.191549	-1.834059

Conf. 1e

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -844.98973000

1	6	0	3.299369	6.771414	1.794180
2	6	0	2.040839	7.070224	1.248960
3	6	0	3.932727	5.541301	1.571755
4	6	0	3.280265	4.565923	0.792194

5	6	0	2.035790	4.875570	0.226703
6	6	0	1.403144	6.112051	0.448028
7	6	0	3.892965	3.197319	0.555591
8	6	0	2.877819	2.204219	-0.021418
9	6	0	2.031441	2.875455	-1.117755
10	8	0	1.331405	3.982081	-0.560469
11	6	0	5.302224	5.307592	2.175102
12	6	0	1.392415	8.407782	1.516496
13	6	0	0.050973	6.398299	-0.162216
14	6	0	2.858899	3.331377	-2.334909
15	8	0	3.896053	7.752904	2.558436
16	1	0	4.758778	3.275966	-0.117882
17	1	0	4.281814	2.786693	1.494683
18	1	0	2.194619	1.871994	0.769736
19	1	0	3.378977	1.317567	-0.419344
20	1	0	5.754235	4.376434	1.830445
21	1	0	6.002803	6.110894	1.904743
22	1	0	5.271133	5.255595	3.274339
23	1	0	1.244028	8.972772	0.586838
24	1	0	0.401387	8.286089	1.971905
25	1	0	2.002667	9.014109	2.186469
26	1	0	-0.697981	6.603779	0.613494
27	1	0	0.085995	7.285561	-0.807773
28	1	0	-0.300328	5.554047	-0.755358
29	1	0	3.397887	2.490137	-2.779188
30	1	0	2.198418	3.767221	-3.090992
31	1	0	3.578102	4.098316	-2.034832
32	6	0	0.931765	1.915938	-1.589141
33	1	0	4.702419	7.395815	2.956480
34	8	0	-0.258933	2.092581	-1.518426
35	8	0	1.478041	0.792462	-2.128305
36	1	0	0.724246	0.239817	-2.408371

Compound 2

Conf. 2a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -884.27501600

1	6	0	-2.786258	0.356519	0.243020
2	6	0	-2.505879	-0.986226	-0.058381
3	6	0	-1.821563	1.365923	0.124073
4	6	0	-0.534317	1.032173	-0.341264
5	6	0	-0.251998	-0.310394	-0.622821
6	6	0	-1.211830	-1.326748	-0.476875
7	6	0	0.538315	2.090454	-0.531767
8	6	0	1.751150	1.557997	-1.304232
9	6	0	2.100337	0.133292	-0.864354
10	8	0	0.984739	-0.724819	-1.093520
11	6	0	3.251437	-0.461499	-1.684219
12	6	0	2.522753	0.116468	0.621743
13	8	0	3.079242	1.042336	1.175353
14	8	0	2.268927	-1.064894	1.209449
15	6	0	2.678562	-1.168180	2.583922
16	6	0	-2.198062	2.783274	0.502843

17	8	0	-4.063610	0.640703	0.680612
18	6	0	-3.588023	-2.032490	0.082925
19	6	0	-0.832947	-2.757084	-0.781049
20	1	0	0.874142	2.467195	0.443512
21	1	0	0.128865	2.954083	-1.069044
22	1	0	2.612343	2.215946	-1.161736
23	1	0	1.530790	1.513720	-2.377336
24	1	0	3.433610	-1.497348	-1.383593
25	1	0	2.986152	-0.447978	-2.745823
26	1	0	4.166567	0.120277	-1.537294
27	1	0	2.401563	-2.175535	2.894970
28	1	0	3.757516	-1.017525	2.675375
29	1	0	2.161993	-0.421628	3.192675
30	1	0	-2.640880	2.825803	1.508207
31	1	0	-1.334757	3.450010	0.517819
32	1	0	-2.926038	3.224277	-0.195677
33	1	0	-4.171389	1.600946	0.733451
34	1	0	-3.633530	-2.681010	-0.799193
35	1	0	-3.410572	-2.682659	0.950603
36	1	0	-4.564783	-1.565474	0.216063
37	1	0	-1.384573	-3.460198	-0.150291
38	1	0	-1.047673	-3.019796	-1.826593
39	1	0	0.236198	-2.910585	-0.622620

Conf. 2b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -884.27344500

1	6	0	-2.839171	0.602212	0.189516
2	6	0	-2.716050	-0.796321	0.260212
3	6	0	-1.771424	1.430766	-0.180088
4	6	0	-0.536858	0.843998	-0.521954
5	6	0	-0.413702	-0.546463	-0.437746
6	6	0	-1.476081	-1.375629	-0.041456
7	6	0	0.652816	1.678677	-0.961291
8	6	0	1.750383	0.820218	-1.599825
9	6	0	1.965947	-0.475128	-0.806116
10	8	0	0.754241	-1.216972	-0.766219
11	6	0	2.993168	-1.397254	-1.474577
12	6	0	2.426857	-0.206019	0.644344
13	8	0	1.967848	-0.725081	1.633384
14	8	0	3.465518	0.664093	0.665145
15	6	0	4.016290	0.929604	1.967194
16	6	0	-1.982811	2.930574	-0.189988
17	8	0	-4.069728	1.134431	0.517904
18	6	0	-3.907816	-1.633666	0.669847
19	6	0	-1.228853	-2.862346	0.051284
20	1	0	1.071226	2.225583	-0.103217
21	1	0	0.341352	2.443922	-1.681860
22	1	0	2.686312	1.380430	-1.674191
23	1	0	1.455026	0.525094	-2.614029
24	1	0	2.664630	-1.627648	-2.492682
25	1	0	3.974490	-0.916613	-1.513712
26	1	0	3.075880	-2.335728	-0.917772
27	1	0	3.255076	1.357100	2.624779
28	1	0	4.396443	0.008539	2.416870
29	1	0	4.826858	1.640199	1.803043
30	1	0	-2.367610	3.288833	0.775885
31	1	0	-1.057412	3.478205	-0.374129
32	1	0	-2.696882	3.247804	-0.965728

33	1	0	-4.055060	2.087106	0.349606
34	1	0	-4.097046	-2.439707	-0.048397
35	1	0	-3.752012	-2.104270	1.649456
36	1	0	-4.807317	-1.020691	0.736534
37	1	0	-2.033609	-3.377970	0.578680
38	1	0	-1.131448	-3.317103	-0.943552
39	1	0	-0.288097	-3.054189	0.576569

Conf. 2c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -884.27071200

1	6	0	-2.625472	-0.845490	-0.831320
2	6	0	-2.642073	0.555914	-0.753549
3	6	0	-1.433307	-1.579228	-0.767059
4	6	0	-0.210924	-0.890562	-0.639466
5	6	0	-0.230891	0.507185	-0.535395
6	6	0	-1.429064	1.241566	-0.596090
7	6	0	1.116844	-1.625956	-0.614028
8	6	0	2.303976	-0.675951	-0.808404
9	6	0	2.112754	0.605135	0.021976
10	8	0	0.919777	1.261263	-0.396242
11	6	0	2.067506	0.347878	1.539990
12	6	0	3.237252	1.606776	-0.287597
13	8	0	3.101120	2.713158	-0.749696
14	8	0	4.437438	1.071951	0.044310
15	6	0	5.571743	1.923333	-0.189382
16	6	0	-1.503936	-3.090830	-0.831956
17	8	0	-3.845235	-1.476740	-0.965647
18	6	0	-3.949615	1.308105	-0.829582
19	6	0	-1.405768	2.749335	-0.501933
20	1	0	1.147414	-2.384156	-1.405278
21	1	0	1.232672	-2.175464	0.331574
22	1	0	3.244862	-1.163517	-0.539285
23	1	0	2.372747	-0.381518	-1.862854
24	1	0	1.206530	-0.277165	1.792495
25	1	0	2.981046	-0.148187	1.878886
26	1	0	1.961626	1.297312	2.074255
27	1	0	6.440636	1.346845	0.129421
28	1	0	5.647308	2.179497	-1.249420
29	1	0	5.486019	2.844701	0.392639
30	1	0	-1.833322	-3.452155	-1.818401
31	1	0	-0.539373	-3.560016	-0.632817
32	1	0	-2.204273	-3.492433	-0.085408
33	1	0	-3.696270	-2.420826	-1.116340
34	1	0	-4.143656	1.866436	0.095741
35	1	0	-3.939218	2.043624	-1.643963
36	1	0	-4.785850	0.628281	-0.995388
37	1	0	-1.833785	3.208904	-1.402209
38	1	0	-2.005135	3.104041	0.346769
39	1	0	-0.387802	3.120754	-0.384448

Compound 3

Conf. 3a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -997.62424500

1	8	0	-1.985423	0.972939	-0.591779
2	6	0	-3.042454	0.021901	-0.534712
3	6	0	-2.597304	-1.297691	-1.181187
4	1	0	-3.419517	-2.018449	-1.170765
5	1	0	-2.357491	-1.076117	-2.228120
6	6	0	-1.365390	-1.858365	-0.465585
7	1	0	-1.672016	-2.339126	0.476050
8	1	0	-0.924995	-2.655593	-1.075457
9	6	0	-0.338374	-0.777813	-0.193049
10	6	0	0.989498	-1.111483	0.130250
11	6	0	1.898349	-0.074211	0.337062
12	6	0	1.546832	1.278712	0.260665
13	6	0	0.220278	1.611672	-0.053316
14	6	0	-0.702584	0.572769	-0.267964
15	6	0	-4.217038	0.666670	-1.280388
16	1	0	-3.932020	0.836566	-2.322996
17	1	0	-4.467577	1.631769	-0.829199
18	1	0	-5.096761	0.018899	-1.248644
19	6	0	-3.440285	-0.182193	0.940804
20	8	0	-4.399744	-1.139195	1.060604
21	8	0	-3.000211	0.422586	1.887292
22	6	0	1.418007	-2.556070	0.239058
23	1	0	1.524132	-3.020298	-0.750986
24	1	0	0.685982	-3.150013	0.797224
25	1	0	2.378466	-2.642265	0.750227
26	8	0	3.216307	-0.411385	0.707106
27	6	0	4.172631	-0.430132	-0.272406
28	8	0	3.959808	-0.170926	-1.430952
29	6	0	5.507904	-0.815160	0.319962
30	1	0	5.441489	-1.799142	0.795733
31	1	0	5.796538	-0.098491	1.095949
32	1	0	6.262298	-0.833385	-0.467137
33	6	0	2.580228	2.352182	0.504469
34	1	0	3.397804	1.977196	1.124791
35	1	0	2.146281	3.220091	1.008964
36	1	0	3.015763	2.703664	-0.440371
37	6	0	-0.215633	3.055113	-0.157655
38	1	0	-0.160614	3.559802	0.815939
39	1	0	-1.244314	3.127751	-0.509407
40	1	0	0.425354	3.616145	-0.848085
41	1	0	-4.612691	-1.186559	2.012061

Conf. 3b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -997.62390700

1	8	0	1.357378	6.072991	7.501715
2	6	0	1.899662	7.387013	7.440909
3	6	0	1.416085	8.207670	8.644344
4	1	0	1.798637	9.230159	8.582704
5	1	0	0.322255	8.253578	8.580867
6	6	0	1.841007	7.541216	9.956294
7	1	0	2.902692	7.756458	10.151258
8	1	0	1.287690	7.995318	10.786131
9	6	0	1.605658	6.043271	9.926528
10	6	0	1.606424	5.287683	11.112408

11	6	0	1.335928	3.920956	11.025294
12	6	0	1.098420	3.264310	9.812850
13	6	0	1.123529	4.014463	8.626158
14	6	0	1.378569	5.393457	8.705165
15	6	0	1.416523	7.970588	6.107678
16	1	0	0.323614	8.022227	6.112161
17	1	0	1.728524	7.328624	5.278030
18	1	0	1.823711	8.973388	5.955521
19	6	0	3.437616	7.284219	7.410854
20	8	0	4.010631	8.517870	7.432619
21	8	0	4.082265	6.266302	7.350645
22	6	0	1.879233	5.934915	12.449379
23	1	0	2.278219	5.206494	13.159830
24	1	0	0.961867	6.350905	12.886144
25	1	0	2.606766	6.747387	12.363878
26	8	0	1.372371	3.141383	12.199189
27	6	0	0.291185	3.180847	13.037561
28	8	0	-0.687407	3.861073	12.851011
29	6	0	0.518775	2.258291	14.212018
30	1	0	1.434223	2.539785	14.742574
31	1	0	0.650072	1.228796	13.862460
32	1	0	-0.335273	2.313443	14.887692
33	6	0	0.822680	1.780260	9.770216
34	1	0	1.003378	1.313567	10.739602
35	1	0	1.458195	1.280103	9.030454
36	1	0	-0.217953	1.577303	9.484376
37	6	0	0.881951	3.351204	7.290844
38	1	0	1.646863	2.592467	7.080228
39	1	0	0.902987	4.080242	6.481501
40	1	0	-0.088598	2.839514	7.269121
41	1	0	4.973648	8.366258	7.382789

Conf. 3c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -997.62122100

1	8	0	1.695090	6.049563	7.542660
2	6	0	1.815236	7.471285	7.544536
3	6	0	2.888504	7.895116	8.563747
4	1	0	3.021465	8.980102	8.539644
5	1	0	3.838175	7.438502	8.259089
6	6	0	2.511187	7.415290	9.969061
7	1	0	3.392413	7.489758	10.617423
8	1	0	1.765139	8.092380	10.410478
9	6	0	1.986316	5.994440	9.959959
10	6	0	1.858106	5.264059	11.156966
11	6	0	1.383047	3.954656	11.082482
12	6	0	1.047434	3.328783	9.874565
13	6	0	1.150174	4.064404	8.684620
14	6	0	1.611086	5.392960	8.751091
15	6	0	0.439235	8.112050	7.804163
16	1	0	0.050655	7.790859	8.774263
17	1	0	-0.270916	7.793246	7.034888
18	1	0	0.508702	9.203107	7.790505
19	6	0	2.274929	7.821094	6.123726
20	8	0	2.447591	9.163963	5.996270
21	8	0	2.463027	7.049090	5.216771

22	6	0	2.227943	5.891715	12.479876
23	1	0	2.095184	5.188644	13.302819
24	1	0	1.615450	6.778337	12.687728
25	1	0	3.275487	6.218894	12.489611
26	8	0	1.311944	3.208724	12.276426
27	6	0	0.083073	3.026680	12.852726
28	8	0	-0.947115	3.464711	12.403869
29	6	0	0.223017	2.202005	14.110614
30	1	0	0.905271	2.692839	14.812385
31	1	0	0.652045	1.222964	13.872615
32	1	0	-0.756853	2.074779	14.571708
33	6	0	0.563765	1.898563	9.864119
34	1	0	0.960934	1.343158	10.717780
35	1	0	0.870188	1.378215	8.952850
36	1	0	-0.531588	1.852302	9.921469
37	6	0	0.774574	3.457457	7.351739
38	1	0	0.808829	4.206068	6.560263
39	1	0	-0.233072	3.026090	7.380283
40	1	0	1.462450	2.648304	7.072414
41	1	0	2.730878	9.308843	5.073802

Compound 4

Conf. 4a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -1037.216861

1	6	0	1.207120	-1.044537	0.198125
2	6	0	2.041602	0.059759	0.323698
3	6	0	1.635370	1.362096	0.033491
4	6	0	0.327037	1.569465	-0.417988
5	6	0	-0.522191	0.462214	-0.551309
6	6	0	-0.100266	-0.839554	-0.268523
7	6	0	1.698610	-2.429590	0.532531
8	8	0	3.346312	-0.134674	0.826191
9	6	0	2.584851	2.521717	0.192077
10	6	0	-0.160217	2.955138	-0.758834
11	6	0	-1.038575	-2.008007	-0.480960
12	6	0	-2.253510	-1.619456	-1.320137
13	6	0	-2.804549	-0.262577	-0.881825
14	8	0	-1.793853	0.736982	-1.012698
15	6	0	-3.961669	0.203176	-1.767617
16	6	0	-3.335833	-0.350291	0.566821
17	8	0	-3.952777	-1.301305	0.983583
18	8	0	-3.093120	0.754499	1.282349
19	6	0	-3.604271	0.757749	2.629348
20	6	0	4.343074	-0.442542	-0.055297
21	6	0	5.652525	-0.594924	0.672396
22	8	0	4.178194	-0.568995	-1.237964
23	1	0	2.005865	-2.968847	-0.369039
24	1	0	0.922927	-3.021431	1.019571
25	1	0	2.555957	-2.390298	1.201745
26	1	0	3.428980	2.258325	0.825743
27	1	0	2.085966	3.383780	0.636819
28	1	0	2.980218	2.841779	-0.777067
29	1	0	-1.147546	2.921986	-1.209742
30	1	0	-0.222415	3.584988	0.134040

31	1	0	0.520136	3.451543	-1.454862
32	1	0	-1.372995	-2.404854	0.483670
33	1	0	-0.507489	-2.825324	-0.973645
34	1	0	-1.973585	-1.525956	-2.372339
35	1	0	-3.033277	-2.376037	-1.242489
36	1	0	-3.624510	0.248593	-2.803616
37	1	0	-4.293680	1.197543	-1.467280
38	1	0	-4.798939	-0.490830	-1.693698
39	1	0	-3.310077	1.716407	3.046807
40	1	0	-3.169759	-0.060365	3.202934
41	1	0	-4.689175	0.655293	2.625565
42	1	0	5.909107	0.337421	1.178242
43	1	0	5.569190	-1.367519	1.438354
44	1	0	6.432406	-0.857248	-0.037381

Conf. 4b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -1037.216407

1	6	0	1.179413	-1.126598	-0.634909
2	6	0	2.075349	-0.069958	-0.522650
3	6	0	1.687097	1.270274	-0.558578
4	6	0	0.324834	1.568542	-0.666875
5	6	0	-0.588412	0.509860	-0.771918
6	6	0	-0.185525	-0.826991	-0.776761
7	6	0	1.645373	-2.559316	-0.607561
8	8	0	3.452073	-0.368362	-0.432560
9	6	0	2.713891	2.369460	-0.459626
10	6	0	-0.164997	2.994739	-0.667429
11	6	0	-1.207166	-1.933412	-0.921366
12	6	0	-2.572454	-1.406949	-1.360401
13	6	0	-2.915712	-0.107176	-0.633495
14	8	0	-1.913500	0.873804	-0.904481
15	6	0	-4.230781	0.498881	-1.125934
16	6	0	-3.061137	-0.367930	0.883067
17	8	0	-3.568117	-1.367288	1.333457
18	8	0	-2.624003	0.652043	1.630526
19	6	0	-2.758777	0.494346	3.056636
20	6	0	4.032788	-0.387715	0.803429
21	6	0	5.500249	-0.703216	0.683932
22	8	0	3.440743	-0.177838	1.826943
23	1	0	2.728416	-2.625601	-0.547851
24	1	0	1.331902	-3.095439	-1.507104
25	1	0	1.224461	-3.095439	0.247492
26	1	0	2.811167	2.726835	0.570274
27	1	0	2.440962	3.223540	-1.079009
28	1	0	3.693853	2.022766	-0.783237
29	1	0	0.008590	3.477077	-1.635222
30	1	0	-1.232295	3.034743	-0.467623
31	1	0	0.349704	3.590213	0.088211
32	1	0	-1.309497	-2.472321	0.026522
33	1	0	-0.857361	-2.672192	-1.646248
34	1	0	-2.566232	-1.180179	-2.429386
35	1	0	-3.348068	-2.149260	-1.176002
36	1	0	-4.166420	0.673089	-2.200523
37	1	0	-4.418947	1.452166	-0.631109
38	1	0	-5.059833	-0.179254	-0.922990
39	1	0	-2.353331	1.405598	3.486610
40	1	0	-2.194590	-0.373254	3.396810
41	1	0	-3.806782	0.371183	3.328658

42	1	0	6.001013	0.075606	0.105935
43	1	0	5.939125	-0.765203	1.676101
44	1	0	5.642380	-1.644575	0.151252

Conf. 4c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -1037.216356

1	6	0	1.213758	-0.867208	-0.860073
2	6	0	2.179120	0.040992	-0.441505
3	6	0	1.881420	1.347446	-0.051221
4	6	0	0.543673	1.756646	-0.047213
5	6	0	-0.437468	0.849461	-0.469880
6	6	0	-0.125196	-0.446201	-0.884745
7	6	0	1.582254	-2.267916	-1.277184
8	8	0	3.532447	-0.358744	-0.480948
9	6	0	2.978426	2.288468	0.376692
10	6	0	0.151087	3.139683	0.407254
11	6	0	-1.223222	-1.381825	-1.336703
12	6	0	-2.515318	-0.633326	-1.653873
13	6	0	-2.814679	0.416183	-0.580402
14	8	0	-1.729984	1.335537	-0.490065
15	6	0	-4.041752	1.261031	-0.927112
16	6	0	-3.036330	-0.223303	0.809502
17	8	0	-2.505995	0.125851	1.828980
18	8	0	-3.949966	-1.216495	0.740892
19	6	0	-4.282070	-1.852353	1.990658
20	6	0	4.116252	-0.807224	0.669535
21	6	0	5.557375	-1.163123	0.415048
22	8	0	3.546390	-0.895939	1.722422
23	1	0	2.658964	-2.414567	-1.270030
24	1	0	1.227052	-2.488944	-2.287024
25	1	0	1.135376	-3.009872	-0.609468
26	1	0	3.086208	2.296760	1.465692
27	1	0	2.770910	3.310056	0.059201
28	1	0	3.936689	1.995083	-0.048719
29	1	0	0.359069	3.889138	-0.363889
30	1	0	-0.911219	3.183077	0.631239
31	1	0	0.702159	3.431876	1.302214
32	1	0	-1.410380	-2.136757	-0.563510
33	1	0	-0.905065	-1.938971	-2.220452
34	1	0	-2.415279	-0.098018	-2.601803
35	1	0	-3.353587	-1.322941	-1.745470
36	1	0	-3.877782	1.752728	-1.886540
37	1	0	-4.199760	2.028919	-0.168908
38	1	0	-4.931311	0.635408	-0.992526
39	1	0	-5.021482	-2.609350	1.744114
40	1	0	-4.694932	-1.125591	2.689770
41	1	0	-3.396852	-2.308762	2.432519
42	1	0	6.106894	-0.277084	0.092147
43	1	0	5.998701	-1.559266	1.325617
44	1	0	5.628515	-1.899210	-0.387079

Conf. 4d

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -1037.214187

1	6	0	-1.211617	-1.034106	-0.001811
2	6	0	-2.126852	-0.052244	-0.362526
3	6	0	-1.816096	1.306912	-0.393780

4	6	0	-0.525798	1.707710	-0.028960
5	6	0	0.402879	0.726607	0.342353
6	6	0	0.077261	-0.631130	0.376805
7	6	0	-1.595158	-2.491816	-0.001837
8	8	0	-3.415610	-0.449633	-0.780426
9	6	0	-2.847114	2.326287	-0.805009
10	6	0	-0.138031	3.164537	-0.041741
11	6	0	1.107214	-1.645218	0.823064
12	6	0	2.267364	-0.984028	1.562329
13	6	0	2.732089	0.275014	0.824750
14	8	0	1.650133	1.193431	0.707530
15	6	0	3.824701	1.022820	1.590299
16	6	0	3.253806	-0.056313	-0.592220
17	8	0	2.883191	0.459028	-1.612107
18	8	0	4.222418	-0.997019	-0.536900
19	6	0	4.821994	-1.358257	-1.795996
20	6	0	-4.379343	-0.635049	0.168394
21	6	0	-5.675458	-1.043727	-0.480395
22	8	0	-4.199198	-0.491572	1.347080
23	1	0	-1.829583	-2.841013	1.008644
24	1	0	-0.787545	-3.116418	-0.385951
25	1	0	-2.471394	-2.666580	-0.622920
26	1	0	-3.671420	1.861279	-1.341272
27	1	0	-2.411784	3.088865	-1.452054
28	1	0	-3.262114	2.840842	0.067406
29	1	0	0.837507	3.312869	0.411693
30	1	0	-0.090151	3.550552	-1.064758
31	1	0	-0.866737	3.772238	0.499557
32	1	0	1.487877	-2.200487	-0.042945
33	1	0	0.643439	-2.389522	1.473630
34	1	0	1.946993	-0.669937	2.559138
35	1	0	3.101024	-1.675344	1.680141
36	1	0	3.448723	1.291828	2.577852
37	1	0	4.096576	1.938607	1.063894
38	1	0	4.710593	0.398809	1.701191
39	1	0	5.566652	-2.112710	-1.557589
40	1	0	5.290046	-0.489550	-2.258273
41	1	0	4.070410	-1.761155	-2.474329
42	1	0	-5.988326	-0.288158	-1.202651
43	1	0	-5.540286	-1.978723	-1.026840
44	1	0	-6.439014	-1.168175	0.282707

Conf. 4e

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -1037.214091

1	6	0	1.583458	-1.094305	-0.220870
2	6	0	2.347915	0.059034	-0.350385
3	6	0	1.793933	1.336280	-0.443945
4	6	0	0.402326	1.467728	-0.392877
5	6	0	-0.380270	0.310006	-0.267805
6	6	0	0.187978	-0.962390	-0.158799
7	6	0	2.234307	-2.450756	-0.131623
8	8	0	3.749820	-0.064170	-0.456342
9	6	0	2.675722	2.550330	-0.587644
10	6	0	-0.252943	2.824110	-0.468672
11	6	0	-0.699161	-2.170410	0.040579
12	6	0	-2.105296	-1.770084	0.477927

13	6	0	-2.622620	-0.595963	-0.368338
14	8	0	-1.740802	0.520801	-0.233113
15	6	0	-2.786456	-0.949799	-1.852568
16	6	0	-3.997498	-0.194078	0.185090
17	8	0	-4.961307	-0.914889	0.076802
18	8	0	-4.017152	0.989464	0.805828
19	6	0	-5.287275	1.382982	1.361323
20	6	0	4.486484	-0.142172	0.691268
21	6	0	5.952035	-0.246667	0.362030
22	8	0	4.013838	-0.128127	1.795021
23	1	0	2.316837	-2.782394	0.908093
24	1	0	3.237984	-2.431996	-0.552092
25	1	0	1.662176	-3.204876	-0.673165
26	1	0	2.781840	3.075816	0.366723
27	1	0	2.258095	3.260554	-1.302288
28	1	0	3.671583	2.275964	-0.928805
29	1	0	-0.194753	3.239659	-1.480205
30	1	0	-1.302765	2.763483	-0.195546
31	1	0	0.236716	3.535402	0.199440
32	1	0	-0.267666	-2.827886	0.798388
33	1	0	-0.745681	-2.765608	-0.878308
34	1	0	-2.799688	-2.606477	0.400656
35	1	0	-2.086564	-1.449710	1.523273
36	1	0	-1.826837	-1.232490	-2.283973
37	1	0	-3.162059	-0.085261	-2.401397
38	1	0	-3.490575	-1.772410	-1.970457
39	1	0	-5.113385	2.354682	1.814727
40	1	0	-5.616221	0.662335	2.109491
41	1	0	-6.041022	1.452834	0.577607
42	1	0	6.274547	0.640468	-0.185790
43	1	0	6.523690	-0.340783	1.281347
44	1	0	6.132753	-1.109026	-0.281428

Compound 5

Conf. 5a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -825.119498

1	6	0	-2.455227	-0.894415	0.035746
2	6	0	-2.661979	0.491565	0.103445
3	6	0	-1.611173	1.407994	-0.043452
4	6	0	-0.309126	0.928407	-0.285315
5	6	0	-0.100028	-0.456826	-0.324442
6	6	0	-1.155409	-1.375164	-0.180958
7	6	0	0.858336	1.869665	-0.516267
8	6	0	2.037883	1.151991	-1.176073
9	6	0	2.322531	-0.179438	-0.482666
10	8	0	1.155737	-1.021778	-0.516032
11	6	0	-1.915506	2.887123	0.073439
12	8	0	-3.954454	0.916629	0.326289
13	6	0	-3.617086	-1.846532	0.196593
14	6	0	-0.897958	-2.862783	-0.264248
15	1	0	-3.979833	1.883216	0.288310
16	6	0	2.781870	0.065017	0.979252

17	6	0	3.420834	-0.975404	-1.195070
18	8	0	3.556177	0.972510	1.256773
19	7	0	2.322814	-0.839045	1.883455
20	1	0	1.193532	2.314011	0.431151
21	1	0	0.550642	2.705547	-1.154580
22	1	0	1.814221	0.941552	-2.229060
23	1	0	2.935053	1.773941	-1.133211
24	1	0	-2.467952	3.110550	0.997668
25	1	0	-2.519288	3.257841	-0.768789
26	1	0	-1.010195	3.494362	0.105774
27	1	0	-4.530231	-1.310994	0.457963
28	1	0	-3.807927	-2.405383	-0.729530
29	1	0	-3.419709	-2.590089	0.978728
30	1	0	-1.060290	-3.355815	0.704605
31	1	0	0.123826	-3.071060	-0.582662
32	1	0	-1.580740	-3.343179	-0.975077
33	1	0	3.146284	-1.133897	-2.242741
34	1	0	3.557007	-1.951486	-0.718746
35	1	0	4.366407	-0.427851	-1.148612
36	1	0	1.614847	-1.508617	1.623016
37	1	0	2.567189	-0.715429	2.855463

Conf. 5b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -825.119177

1	6	0	-2.460997	-0.872358	0.034983
2	6	0	-2.657057	0.517251	0.111101
3	6	0	-1.602187	1.424715	-0.037000
4	6	0	-0.308790	0.925169	-0.270203
5	6	0	-0.106288	-0.460247	-0.318051
6	6	0	-1.167144	-1.374303	-0.182472
7	6	0	0.858357	1.866473	-0.481760
8	6	0	2.034115	1.158316	-1.157161
9	6	0	2.319217	-0.184651	-0.484230
10	8	0	1.149067	-1.025138	-0.512636
11	6	0	-1.859998	2.911236	0.047246
12	8	0	-3.911360	1.047771	0.326064
13	6	0	-3.660677	-1.782220	0.194000
14	6	0	-0.902164	-2.862466	-0.281397
15	1	0	-4.543518	0.325211	0.447332
16	6	0	2.798225	0.041212	0.974215
17	6	0	3.405858	-0.976280	-1.218906
18	8	0	3.596983	0.928527	1.247016
19	7	0	2.326319	-0.853964	1.880828
20	1	0	1.191347	2.289275	0.476769
21	1	0	0.545231	2.720224	-1.093509
22	1	0	1.806228	0.965264	-2.212649
23	1	0	2.934369	1.775321	-1.107842
24	1	0	-1.135902	3.407018	0.704073
25	1	0	-2.861846	3.110754	0.429699
26	1	0	-1.779844	3.391771	-0.937716
27	1	0	-4.143635	-1.656732	1.175028
28	1	0	-4.424031	-1.589717	-0.574384
29	1	0	-3.392357	-2.836039	0.112781
30	1	0	-1.137791	-3.383819	0.655951
31	1	0	0.144405	-3.054694	-0.518272
32	1	0	-1.509137	-3.328017	-1.067376
33	1	0	3.118517	-1.121227	-2.265090
34	1	0	3.544051	-1.958518	-0.755787

35	1	0	4.353822	-0.432676	-1.176774
36	1	0	1.602122	-1.507736	1.625712
37	1	0	2.583400	-0.738267	2.850514

Conf. 5c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -825.118429

1	6	0	-2.458641	1.086585	0.014680
2	6	0	-2.850785	-0.259693	-0.050277
3	6	0	-1.919554	-1.306001	-0.100728
4	6	0	-0.544592	-1.001060	-0.117817
5	6	0	-0.154745	0.342221	-0.032237
6	6	0	-1.089758	1.389508	0.046401
7	6	0	0.509459	-2.089044	-0.221175
8	6	0	1.889199	-1.521245	-0.567061
9	6	0	2.185878	-0.254414	0.248192
10	8	0	1.176035	0.732129	-0.043107
11	6	0	-2.428585	-2.732099	-0.132085
12	8	0	-4.206677	-0.511717	-0.048121
13	6	0	-3.505610	2.175878	0.059383
14	6	0	-0.611533	2.819427	0.149659
15	1	0	-4.353517	-1.451109	-0.228382
16	6	0	3.540521	0.313623	-0.223128
17	6	0	2.257101	-0.498519	1.761152
18	8	0	4.574025	-0.310906	-0.018035
19	7	0	3.487360	1.501282	-0.875847
20	1	0	0.229002	-2.817118	-0.991144
21	1	0	0.564120	-2.654430	0.720301
22	1	0	2.680366	-2.255698	-0.393960
23	1	0	1.921213	-1.249801	-1.629664
24	1	0	-1.626711	-3.460844	-0.006504
25	1	0	-2.932169	-2.976216	-1.080232
26	1	0	-3.147352	-2.917557	0.678646
27	1	0	-3.570305	2.633511	1.056134
28	1	0	-3.276020	2.980590	-0.648211
29	1	0	-4.491339	1.777174	-0.183687
30	1	0	-1.277928	3.420180	0.775721
31	1	0	-0.570626	3.306415	-0.835432
32	1	0	0.391720	2.863331	0.578395
33	1	0	1.318132	-0.913679	2.137977
34	1	0	2.444325	0.446368	2.281180
35	1	0	3.075691	-1.186571	1.985811
36	1	0	2.604752	1.970144	-1.011144
37	1	0	4.347927	1.909300	-1.210534

Compound 6

Conf. 6a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -748.679605

1	6	0	1.379448	-1.388250	-0.073451
2	6	0	2.421080	-0.462367	0.054378

3	6	0	2.195694	0.925022	0.024502
4	6	0	0.884270	1.407364	-0.116170
5	6	0	-0.156664	0.474383	-0.253139
6	6	0	0.070391	-0.906744	-0.247405
7	6	0	1.665949	-2.870789	-0.028114
8	8	0	3.692615	-0.971951	0.200942
9	6	0	3.384045	1.854167	0.152002
10	6	0	0.579906	2.889828	-0.126737
11	6	0	-1.085635	-1.873967	-0.407114
12	6	0	-2.351137	-1.177317	-0.913949
13	6	0	-2.557689	0.167262	-0.198607
14	8	0	-1.430455	1.012971	-0.426750
15	6	0	-3.769634	0.937324	-0.732754
16	6	0	-2.722548	-0.051547	1.266164
17	1	0	4.306046	-0.245358	0.380994
18	7	0	-2.868356	-0.224370	2.404720
19	1	0	0.993459	-3.387690	0.666785
20	1	0	2.692577	-3.057440	0.289083
21	1	0	1.532077	-3.340058	-1.012698
22	1	0	3.103646	2.900073	0.023291
23	1	0	4.149494	1.636862	-0.606932
24	1	0	3.866062	1.775731	1.138458
25	1	0	-0.496033	3.062792	-0.136170
26	1	0	0.993112	3.391064	0.756267
27	1	0	1.004001	3.384417	-1.010347
28	1	0	-1.295026	-2.364183	0.554306
29	1	0	-0.814260	-2.677696	-1.101374
30	1	0	-2.263485	-0.948649	-1.982768
31	1	0	-3.232071	-1.813872	-0.779498
32	1	0	-3.640375	1.102713	-1.806343
33	1	0	-3.852902	1.906516	-0.233966
34	1	0	-4.689963	0.370988	-0.563296

Conf. 6b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -748.675473

1	6	0	-1.572633	-1.316017	-0.058628
2	6	0	-2.538850	-0.301592	-0.020818
3	6	0	-2.192448	1.058821	-0.022410
4	6	0	-0.835959	1.413585	-0.047318
5	6	0	0.132886	0.396340	-0.099518
6	6	0	-0.210773	-0.961676	-0.122494
7	6	0	-2.030800	-2.759158	-0.023847
8	8	0	-3.883233	-0.599464	0.033218
9	6	0	-3.270062	2.116510	0.014417
10	6	0	-0.423643	2.867034	-0.033949
11	6	0	0.876959	-2.017526	-0.209653
12	6	0	2.233030	-1.419172	-0.597625
13	6	0	2.479170	-0.107210	0.170823
14	8	0	1.450925	0.834495	-0.156683
15	6	0	2.571934	-0.293307	1.696489
16	6	0	3.733597	0.511915	-0.315905

17	1	0	-4.002735	-1.551431	-0.093060
18	7	0	4.740950	0.955485	-0.682067
19	1	0	-2.703170	-2.945370	0.825726
20	1	0	-1.199536	-3.457633	0.082321
21	1	0	-2.570067	-3.047723	-0.939132
22	1	0	-3.284419	2.640738	0.979699
23	1	0	-4.256004	1.676636	-0.139638
24	1	0	-3.106781	2.877937	-0.757205
25	1	0	-0.937477	3.417168	0.762939
26	1	0	0.651551	2.972045	0.111378
27	1	0	-0.682395	3.362639	-0.979360
28	1	0	0.612670	-2.775566	-0.955700
29	1	0	0.965638	-2.555199	0.745248
30	1	0	3.045774	-2.126580	-0.403539
31	1	0	2.248951	-1.183052	-1.666965
32	1	0	1.625229	-0.678437	2.084078
33	1	0	2.776821	0.667538	2.175479
34	1	0	3.373306	-0.993628	1.952534

Compound 7

Conf. 7a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -901.310594

1	6	0	0.828871	-1.001116	0.225439
2	6	0	1.666936	0.109838	0.340027
3	6	0	1.214150	1.427596	0.212676
4	6	0	-0.147916	1.647286	-0.050802
5	6	0	-0.993133	0.534301	-0.184015
6	6	0	-0.529451	-0.782706	-0.066004
7	6	0	1.374258	-2.398524	0.397906
8	8	0	3.021257	-0.089297	0.669114
9	6	0	2.160998	2.594909	0.355361
10	6	0	-0.687208	3.051299	-0.193477
11	6	0	-1.481960	-1.948025	-0.254417
12	6	0	-2.788417	-1.510218	-0.921061
13	6	0	-3.300939	-0.200406	-0.303981
14	8	0	-2.320535	0.827329	-0.467013
15	6	0	-4.566359	0.321619	-0.991386
16	6	0	-3.572609	-0.390277	1.148242
17	7	0	-3.798316	-0.546735	2.276015
18	6	0	3.877665	-0.485631	-0.324559
19	8	0	3.539944	-0.697392	-1.462789
20	6	0	5.277792	-0.615677	0.225922
21	1	0	1.665319	-2.834220	-0.566813
22	1	0	0.639400	-3.064766	0.858688
23	1	0	2.261803	-2.393082	1.035418
24	1	0	2.316769	3.099833	-0.607234
25	1	0	3.134224	2.273956	0.729108
26	1	0	1.763873	3.345981	1.047636
27	1	0	-0.560443	3.622456	0.735366
28	1	0	-0.156835	3.602508	-0.979978

29	1	0	-1.748621	3.044059	-0.439818
30	1	0	-1.703707	-2.414557	0.715865
31	1	0	-1.011831	-2.725590	-0.866673
32	1	0	-2.628039	-1.310539	-1.987150
33	1	0	-3.553467	-2.289118	-0.837324
34	1	0	-4.359905	0.463830	-2.056121
35	1	0	-4.864687	1.279895	-0.558194
36	1	0	-5.387953	-0.391077	-0.875287
37	1	0	5.949494	-0.947448	-0.566310
38	1	0	5.617887	0.346415	0.623264
39	1	0	5.293532	-1.332117	1.053744

Conf. 7b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -901.309166

1	6	0	0.751983	-1.127224	-0.491541
2	6	0	1.672524	-0.079483	-0.439069
3	6	0	1.296984	1.267950	-0.360936
4	6	0	-0.069086	1.580598	-0.284124
5	6	0	-1.001023	0.530121	-0.335831
6	6	0	-0.619313	-0.810878	-0.455464
7	6	0	1.202350	-2.565555	-0.585716
8	8	0	3.038302	-0.401623	-0.549841
9	6	0	2.344274	2.355471	-0.342106
10	6	0	-0.537178	3.011215	-0.144829
11	6	0	-1.667933	-1.902405	-0.527325
12	6	0	-3.056978	-1.336873	-0.833767
13	6	0	-3.325788	-0.072671	-0.002742
14	8	0	-2.333828	0.916621	-0.290895
15	6	0	-4.670188	0.579886	-0.339353
16	6	0	-3.288178	-0.398422	1.449820
17	7	0	-3.279146	-0.662119	2.580121
18	6	0	3.816530	-0.336632	0.577598
19	8	0	3.406765	-0.011633	1.663573
20	6	0	5.237148	-0.724292	0.242402
21	1	0	0.833512	-3.154240	0.263361
22	1	0	2.290027	-2.639680	-0.602974
23	1	0	0.823613	-3.046285	-1.496916
24	1	0	1.989752	3.261767	-0.840346
25	1	0	3.255902	2.029752	-0.849774
26	1	0	2.617618	2.623222	0.686503
27	1	0	-1.586958	3.050574	0.146733
28	1	0	0.048353	3.546971	0.609635
29	1	0	-0.434358	3.564599	-1.088372
30	1	0	-1.695895	-2.457618	0.421071
31	1	0	-1.402037	-2.635659	-1.297398
32	1	0	-3.126768	-1.038436	-1.886593
33	1	0	-3.836732	-2.081968	-0.644540
34	1	0	-4.691028	0.821972	-1.405884
35	1	0	-4.797927	1.501309	0.234711
36	1	0	-5.495278	-0.099624	-0.107179
37	1	0	5.638367	-0.057171	-0.527642

38	1	0	5.850462	-0.664928	1.141941
39	1	0	5.266717	-1.741468	-0.161997

Conf. 7c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -901.307432

1	6	0	-0.935028	-1.009797	0.312374
2	6	0	-1.749834	0.122886	0.347725
3	6	0	-1.253664	1.426322	0.226570
4	6	0	0.128158	1.607688	0.055988
5	6	0	0.954702	0.471754	0.008886
6	6	0	0.446769	-0.830615	0.116983
7	6	0	-1.526327	-2.391018	0.462916
8	8	0	-3.129104	-0.034182	0.582175
9	6	0	-2.179374	2.618213	0.275524
10	6	0	0.712741	2.994047	-0.083470
11	6	0	1.376848	-2.022927	0.007419
12	6	0	2.738265	-1.629749	-0.572251
13	6	0	3.238956	-0.326637	0.078548
14	8	0	2.302381	0.731111	-0.174281
15	6	0	3.497819	-0.450614	1.590876
16	6	0	4.487686	0.104111	-0.590831
17	7	0	5.487126	0.399607	-1.100068
18	6	0	-3.922678	-0.427956	-0.464404
19	8	0	-3.507958	-0.678662	-1.568456
20	6	0	-5.363723	-0.497451	-0.018751
21	1	0	-1.737246	-2.841970	-0.515439
22	1	0	-2.468326	-2.353163	1.015348
23	1	0	-0.852450	-3.063415	1.002074
24	1	0	-1.798970	3.389627	0.954287
25	1	0	-3.176619	2.332804	0.613438
26	1	0	-2.277944	3.084678	-0.713723
27	1	0	0.228255	3.547711	-0.896833
28	1	0	0.567318	3.582783	0.832031
29	1	0	1.781841	2.953801	-0.290423
30	1	0	0.931084	-2.789566	-0.636392
31	1	0	1.509564	-2.499806	0.989408
32	1	0	3.475710	-2.425681	-0.427135
33	1	0	2.651944	-1.451790	-1.649496
34	1	0	2.568696	-0.699473	2.110133
35	1	0	3.869760	0.499521	1.982617
36	1	0	4.238633	-1.230578	1.793270
37	1	0	-5.706803	0.492776	0.299447
38	1	0	-5.981289	-0.853878	-0.843649
39	1	0	-5.463490	-1.167297	0.841399

Conf. 7d

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -901.306494

1	6	0	-0.860625	-1.152904	-0.405687
2	6	0	-1.738846	-0.069249	-0.426570

3	6	0	-1.312216	1.264295	-0.371590
4	6	0	0.060000	1.526712	-0.242092
5	6	0	0.951793	0.439187	-0.212035
6	6	0	0.519472	-0.889398	-0.309616
7	6	0	-1.364636	-2.574236	-0.484726
8	8	0	-3.112317	-0.337014	-0.583196
9	6	0	-2.315743	2.390925	-0.431027
10	6	0	0.579129	2.942437	-0.134620
11	6	0	1.523367	-2.024001	-0.295550
12	6	0	2.953822	-1.527154	-0.523498
13	6	0	3.212384	-0.248665	0.296434
14	8	0	2.290756	0.776090	-0.107047
15	6	0	3.132544	-0.464392	1.818281
16	6	0	4.549158	0.287612	-0.046862
17	7	0	5.616465	0.664925	-0.299823
18	6	0	-3.918366	-0.242253	0.521854
19	8	0	-3.523441	0.055941	1.621405
20	6	0	-5.345905	-0.558981	0.145072
21	1	0	-0.944866	-3.101087	-1.351105
22	1	0	-2.450728	-2.604331	-0.576138
23	1	0	-1.082156	-3.149457	0.406101
24	1	0	-2.615920	2.706509	0.576608
25	1	0	-3.219981	2.082248	-0.961676
26	1	0	-1.907232	3.264759	-0.945520
27	1	0	0.523894	3.465450	-1.098939
28	1	0	-0.006909	3.526308	0.583312
29	1	0	1.621717	2.952908	0.183704
30	1	0	1.278519	-2.756328	-1.073763
31	1	0	1.460324	-2.574023	0.654598
32	1	0	3.687315	-2.294938	-0.257158
33	1	0	3.104119	-1.280023	-1.579913
34	1	0	2.128044	-0.792637	2.097340
35	1	0	3.347552	0.472719	2.338006
36	1	0	3.856358	-1.220264	2.138990
37	1	0	-5.410453	-1.562430	-0.288236
38	1	0	-5.977390	-0.495240	1.031646
39	1	0	-5.699427	0.145646	-0.615007

Compound 8

Conf. 8a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -735.015217

1	6	0	2.571860	-0.293857	0.118592
2	6	0	2.210820	1.050368	-0.058256
3	6	0	1.626834	-1.327297	0.076379
4	6	0	0.276375	-1.013088	-0.172568
5	6	0	-0.090655	0.332561	-0.326320
6	6	0	0.861398	1.368435	-0.269519
7	6	0	-0.780553	-2.097368	-0.276482
8	6	0	-2.087502	-1.566361	-0.874231
9	6	0	-2.469918	-0.194973	-0.296597

10	8	0	-1.390934	0.727429	-0.574230
11	6	0	2.093972	-2.750042	0.305482
12	6	0	3.265259	2.131227	-0.008459
13	6	0	0.435894	2.807118	-0.447931
14	6	0	-3.670000	0.384249	-1.047348
15	8	0	3.907461	-0.555893	0.349950
16	1	0	-0.418581	-2.921242	-0.903216
17	1	0	-0.971732	-2.538441	0.712624
18	1	0	-2.902009	-2.282718	-0.713471
19	1	0	-1.970977	-1.447672	-1.958643
20	1	0	2.680873	-2.835473	1.231313
21	1	0	1.261729	-3.448589	0.402606
22	1	0	2.723858	-3.121468	-0.517675
23	1	0	3.189326	2.803136	-0.871730
24	1	0	3.159227	2.755659	0.889303
25	1	0	4.266997	1.700019	0.003519
26	1	0	0.787502	3.213566	-1.406385
27	1	0	-0.650207	2.899657	-0.428331
28	1	0	0.854842	3.446255	0.338377
29	1	0	-4.570125	-0.208211	-0.848540
30	1	0	-3.860544	1.417646	-0.745221
31	1	0	-3.480376	0.378499	-2.125427
32	6	0	-2.715571	-0.264613	1.228900
33	6	0	-3.095414	1.063455	1.892804
34	1	0	4.046419	-1.513359	0.335337
35	1	0	-1.806590	-0.645525	1.708257
36	1	0	-3.499848	-1.012196	1.412342
37	1	0	-4.073194	1.428550	1.560506
38	1	0	-2.352763	1.836372	1.671052
39	1	0	-3.142837	0.944365	2.980962

Conf. 8b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -735.015127

1	6	0	-2.670760	-0.135764	0.020143
2	6	0	-2.192373	1.183192	-0.011537
3	6	0	-1.808851	-1.239548	-0.018012
4	6	0	-0.420737	-1.022747	-0.120930
5	6	0	0.061272	0.294637	-0.131321
6	6	0	-0.808192	1.400413	-0.068061
7	6	0	0.555208	-2.180673	-0.220236
8	6	0	1.946684	-1.718649	-0.663600
9	6	0	2.378749	-0.431665	0.055052
10	8	0	1.404546	0.596200	-0.237557
11	6	0	-2.403650	-2.630680	0.054728
12	6	0	-3.164221	2.340266	0.024245
13	6	0	-0.247673	2.803500	-0.078527
14	6	0	2.471355	-0.621541	1.576705
15	8	0	-4.039010	-0.300337	0.105996
16	1	0	0.625338	-2.703121	0.745254
17	1	0	0.188334	-2.927115	-0.934972
18	1	0	2.685150	-2.510919	-0.492345

19	1	0	1.937618	-1.511779	-1.741069
20	1	0	-3.105454	-2.721943	0.895816
21	1	0	-2.951862	-2.901271	-0.861100
22	1	0	-1.643000	-3.398483	0.203098
23	1	0	-3.144034	2.854885	0.994885
24	1	0	-2.921227	3.088797	-0.738477
25	1	0	-4.185573	1.996386	-0.144901
26	1	0	-0.314512	3.258123	-1.077131
27	1	0	-0.795622	3.457228	0.608127
28	1	0	0.804610	2.803411	0.208759
29	1	0	2.749582	0.315680	2.066084
30	1	0	1.512380	-0.939248	1.996009
31	1	0	3.223173	-1.379594	1.826288
32	6	0	3.699796	0.083419	-0.547050
33	6	0	4.206595	1.425328	-0.007927
34	1	0	-4.251877	-1.234477	-0.029678
35	1	0	3.553741	0.167075	-1.631350
36	1	0	4.462737	-0.691486	-0.392015
37	1	0	4.473611	1.371588	1.052969
38	1	0	3.449717	2.205806	-0.128990
39	1	0	5.103661	1.736631	-0.554810

Conf. 8c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -735.015051

1	6	0	-2.561791	0.554936	0.102153
2	6	0	-2.407217	-0.841992	0.119372
3	6	0	-1.477818	1.417126	-0.092271
4	6	0	-0.199895	0.861978	-0.282927
5	6	0	-0.035324	-0.530252	-0.240517
6	6	0	-1.126964	-1.396746	-0.038713
7	6	0	0.997204	1.757168	-0.529010
8	6	0	2.199591	0.968111	-1.055428
9	6	0	2.396214	-0.343521	-0.282399
10	8	0	1.191610	-1.136351	-0.425398
11	6	0	-1.688383	2.913472	-0.105197
12	6	0	-3.637359	-1.703899	0.311178
13	6	0	-0.900355	-2.892886	-0.004226
14	6	0	3.483656	-1.202537	-0.929361
15	8	0	-3.803542	1.135877	0.264904
16	1	0	0.736703	2.544738	-1.246571
17	1	0	1.268445	2.284745	0.398032
18	1	0	2.036178	0.708297	-2.108753
19	1	0	3.109739	1.576757	-1.014739
20	1	0	-0.962771	3.427162	0.536918
21	1	0	-1.571182	3.330398	-1.115211
22	1	0	-2.690885	3.167286	0.241813
23	1	0	-3.410552	-2.767062	0.224856
24	1	0	-4.096331	-1.558782	1.301451
25	1	0	-4.407348	-1.483367	-0.442477
26	1	0	-1.310607	-3.343868	0.907504
27	1	0	-1.375689	-3.396572	-0.856434

28	1	0	0.165441	-3.117971	-0.041003
29	1	0	3.583244	-2.157347	-0.402030
30	1	0	3.225673	-1.413416	-1.971977
31	1	0	4.451857	-0.692301	-0.910227
32	6	0	2.650456	-0.144990	1.230087
33	6	0	3.887421	0.682145	1.601207
34	1	0	-4.445957	0.445959	0.483100
35	1	0	2.728748	-1.144865	1.675144
36	1	0	1.760637	0.314492	1.675736
37	1	0	3.987800	0.744347	2.690530
38	1	0	3.824724	1.708373	1.221293
39	1	0	4.810969	0.238128	1.213298

Conf. 8d

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -735.014903

1	6	0	-2.685473	-0.416660	0.007177
2	6	0	-2.414900	0.962523	-0.023827
3	6	0	-1.665057	-1.372219	-0.032205
4	6	0	-0.331754	-0.932227	-0.112963
5	6	0	-0.054302	0.442382	-0.117700
6	6	0	-1.082740	1.403452	-0.071976
7	6	0	0.803793	-1.931846	-0.186276
8	6	0	2.123163	-1.274452	-0.606552
9	6	0	2.343385	0.061596	0.116211
10	8	0	1.231961	0.935983	-0.198952
11	6	0	-1.998103	-2.845588	0.004596
12	6	0	-3.580567	1.928883	-0.000797
13	6	0	-0.733702	2.876227	-0.082811
14	6	0	2.424835	-0.096426	1.642117
15	8	0	-3.982200	-0.886713	0.066320
16	1	0	0.556281	-2.731921	-0.894659
17	1	0	0.926974	-2.431571	0.786248
18	1	0	2.107860	-1.072485	-1.685168
19	1	0	2.960326	-1.955013	-0.416109
20	1	0	-1.796443	-3.330942	-0.960454
21	1	0	-1.399196	-3.373557	0.756661
22	1	0	-3.052298	-2.999985	0.238221
23	1	0	-4.140733	1.880932	0.945813
24	1	0	-3.258278	2.963757	-0.121328
25	1	0	-4.292124	1.723467	-0.813793
26	1	0	0.345744	3.011957	-0.018061
27	1	0	-1.076039	3.368671	-1.002627
28	1	0	-1.193306	3.407845	0.759216
29	1	0	2.638263	0.870952	2.109176
30	1	0	1.478913	-0.463850	2.050434
31	1	0	3.213604	-0.800707	1.927888
32	6	0	3.556244	0.827618	-0.443853
33	6	0	4.923966	0.173241	-0.219799
34	1	0	-4.582710	-0.136989	0.182672
35	1	0	3.548626	1.827636	0.008067
36	1	0	3.387295	0.974389	-1.517970

37	1	0	5.713362	0.792425	-0.659832
38	1	0	4.988328	-0.816129	-0.686342
39	1	0	5.154742	0.057933	0.844951

Compound 9

Conf. 9a

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.80250000

1	6	0	-2.463288	0.432466	0.046800
2	6	0	-2.194701	-0.943822	-0.047979
3	6	0	-1.446473	1.391132	-0.011633
4	6	0	-0.119484	0.957317	-0.177049
5	6	0	0.156176	-0.414748	-0.246944
6	6	0	-0.866850	-1.379793	-0.186064
7	6	0	1.013883	1.955219	-0.276481
8	6	0	2.255944	1.321288	-0.905277
9	6	0	2.568349	-0.033967	-0.249043
10	8	0	1.438771	-0.910388	-0.405503
11	6	0	-1.779678	2.861029	0.098462
12	6	0	-3.357337	-1.912584	0.004313
13	6	0	-0.520851	-2.851054	-0.276272
14	6	0	3.716646	-0.748405	-0.974147
15	8	0	-3.755070	0.897646	0.190149
16	1	0	1.262290	2.340901	0.723442
17	1	0	0.704641	2.823944	-0.868965
18	1	0	2.089573	1.149787	-1.976209
19	1	0	3.122208	1.987060	-0.812468
20	1	0	-2.810752	3.001104	0.426047
21	1	0	-1.120683	3.369331	0.812138
22	1	0	-1.666049	3.376608	-0.865457
23	1	0	-3.041079	-2.943807	-0.156538
24	1	0	-3.872211	-1.889023	0.977187
25	1	0	-4.106644	-1.687807	-0.768701
26	1	0	-0.909966	-3.412770	0.581889
27	1	0	-0.939740	-3.311791	-1.180512
28	1	0	0.559765	-2.989459	-0.306372
29	1	0	3.867304	-1.743717	-0.545664
30	1	0	3.484212	-0.854588	-2.038993
31	1	0	4.649190	-0.182825	-0.872904
32	6	0	2.925744	0.143695	1.216062
33	6	0	2.377258	-0.506851	2.240291
34	1	0	-4.348538	0.143152	0.311853
35	1	0	1.582394	-1.231400	2.094701
36	1	0	2.707102	-0.332293	3.260752
37	1	0	3.725357	0.864000	1.397371

Conf. 9b

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.80217800

1	6	0	5.127178	0.746318	2.845751
2	6	0	5.121331	-0.344880	1.964209

3	6	0	4.299746	1.861044	2.653086
4	6	0	3.415998	1.877648	1.556943
5	6	0	3.426682	0.798628	0.662082
6	6	0	4.270041	-0.311888	0.849868
7	6	0	2.457754	3.028580	1.321101
8	6	0	1.321812	2.621818	0.379969
9	6	0	1.871462	1.901545	-0.861736
10	8	0	2.598845	0.734506	-0.445119
11	6	0	4.395718	3.015265	3.629417
12	6	0	6.027303	-1.527679	2.214659
13	6	0	4.247535	-1.462281	-0.130147
14	6	0	0.733183	1.358725	-1.736119
15	8	0	6.000671	0.681192	3.913045
16	1	0	2.995691	3.888124	0.895034
17	1	0	2.028479	3.371738	2.269196
18	1	0	0.635490	1.936734	0.893259
19	1	0	0.739588	3.499467	0.075046
20	1	0	3.995803	2.759779	4.622970
21	1	0	5.438219	3.335363	3.767722
22	1	0	3.847892	3.894096	3.286247
23	1	0	6.833340	-1.582071	1.470012
24	1	0	6.489805	-1.463882	3.200412
25	1	0	5.475355	-2.473143	2.153235
26	1	0	3.685701	-1.201558	-1.027331
27	1	0	5.262076	-1.753169	-0.426911
28	1	0	3.778696	-2.353795	0.309049
29	1	0	0.076856	0.711854	-1.144552
30	1	0	0.137695	2.179702	-2.149852
31	1	0	1.145039	0.777186	-2.566189
32	6	0	2.745545	2.830849	-1.685342
33	6	0	3.986694	2.578269	-2.096339
34	1	0	5.818755	1.418449	4.512717
35	1	0	4.493997	1.653084	-1.842071
36	1	0	4.536456	3.293561	-2.701950
37	1	0	2.263768	3.770321	-1.961870

Conf. 9c

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.80111300

1	6	0	2.469927	-0.545372	0.068921
2	6	0	2.314078	0.851237	0.096211
3	6	0	1.385916	-1.408396	-0.123005
4	6	0	0.105621	-0.854378	-0.299846
5	6	0	-0.058192	0.536220	-0.245932
6	6	0	1.031614	1.404671	-0.049715
7	6	0	-1.088780	-1.753999	-0.539620
8	6	0	-2.321931	-0.969876	-1.000514
9	6	0	-2.478648	0.340494	-0.217625
10	8	0	-1.291320	1.138929	-0.422682
11	6	0	1.598189	-2.904111	-0.148537
12	6	0	3.544219	1.713601	0.285506
13	6	0	0.803356	2.900408	-0.007704
14	6	0	-3.611912	1.202841	-0.788255
15	8	0	3.713336	-1.125215	0.218757
16	1	0	-1.321063	-2.306630	0.380820
17	1	0	-0.841469	-2.514235	-1.290989
18	1	0	-3.226634	-1.581398	-0.909953
19	1	0	-2.222208	-0.703039	-2.059536
20	1	0	1.460416	-3.315271	-1.158299

21	1	0	2.607479	-3.159037	0.177104
22	1	0	0.885510	-3.421450	0.505069
23	1	0	3.314321	2.777220	0.214065
24	1	0	4.013301	1.557978	1.269395
25	1	0	4.307288	1.503826	-0.478279
26	1	0	-0.262283	3.125832	-0.048486
27	1	0	1.209045	3.346554	0.908555
28	1	0	1.282567	3.409160	-0.854560
29	1	0	-4.568606	0.679319	-0.698482
30	1	0	-3.683706	2.150766	-0.245166
31	1	0	-3.419575	1.423934	-1.843535
32	6	0	-2.685395	0.158803	1.278341
33	6	0	-3.307831	-0.851695	1.884828
34	1	0	4.357559	-0.435070	0.430850
35	1	0	-3.703241	-1.707632	1.343012
36	1	0	-3.450978	-0.859396	2.961925
37	1	0	-2.315247	0.996157	1.869570

Conf. 9d

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.80100000

1	6	0	-2.576597	-0.254702	-0.040601
2	6	0	-2.171047	1.090463	0.010722
3	6	0	-1.654506	-1.304544	-0.102210
4	6	0	-0.282075	-0.997125	-0.121951
5	6	0	0.127497	0.341755	-0.049299
6	6	0	-0.800970	1.397545	0.024651
7	6	0	0.749987	-2.102288	-0.212573
8	6	0	2.138159	-1.558241	-0.563332
9	6	0	2.456800	-0.277052	0.231322
10	8	0	1.458943	0.711998	-0.073815
11	6	0	-2.132466	-2.736931	-0.156817
12	6	0	-3.236097	2.166069	0.050813
13	6	0	-0.306626	2.825473	0.111674
14	6	0	2.483802	-0.513175	1.753577
15	8	0	-3.914156	-0.594244	-0.043809
16	1	0	0.448620	-2.838207	-0.967905
17	1	0	0.790454	-2.657137	0.736653
18	1	0	2.909485	-2.315441	-0.380414
19	1	0	2.182122	-1.300773	-1.627831
20	1	0	-3.206627	-2.795798	0.023046
21	1	0	-1.933540	-3.192144	-1.136910
22	1	0	-1.625129	-3.358844	0.590874
23	1	0	-2.809812	3.168228	-0.005164
24	1	0	-3.934916	2.074403	-0.793413
25	1	0	-3.831788	2.127102	0.975952
26	1	0	-0.507298	3.384155	-0.812504
27	1	0	-0.788692	3.371206	0.931054
28	1	0	0.769861	2.847256	0.282079
29	1	0	2.730751	0.421259	2.266305
30	1	0	1.511740	-0.857959	2.118289
31	1	0	3.237710	-1.263719	2.017503
32	6	0	3.788640	0.280040	-0.217573
33	6	0	3.978206	1.410168	-0.895616
34	1	0	-4.440843	0.205182	0.096944
35	1	0	3.146575	2.044942	-1.182186
36	1	0	4.975357	1.731299	-1.184095
37	1	0	4.641428	-0.341775	0.055982

Conf. 9e

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.80089200

1	6	0	-2.581807	-0.216692	-0.047047
2	6	0	-2.160828	1.120956	0.010125
3	6	0	-1.672016	-1.280974	-0.098232
4	6	0	-0.291227	-1.002591	-0.123348
5	6	0	0.130660	0.332581	-0.046062
6	6	0	-0.786433	1.397659	0.030701
7	6	0	0.738977	-2.112066	-0.229599
8	6	0	2.127164	-1.567977	-0.582852
9	6	0	2.457014	-0.298943	0.224779
10	8	0	1.463414	0.696882	-0.068244
11	6	0	-2.208964	-2.697054	-0.121082
12	6	0	-3.182308	2.233672	0.058023
13	6	0	-0.285678	2.820644	0.118649
14	6	0	2.487236	-0.551591	1.744325
15	8	0	-3.943745	-0.441817	-0.034508
16	1	0	0.788563	-2.677354	0.712690
17	1	0	0.440838	-2.836510	-0.996807
18	1	0	2.894965	-2.332223	-0.415071
19	1	0	2.164506	-1.297380	-1.644324
20	1	0	-2.937178	-2.861234	0.685789
21	1	0	-2.710730	-2.940294	-1.070604
22	1	0	-1.422285	-3.440226	0.016663
23	1	0	-3.228403	2.696466	1.053536
24	1	0	-2.937137	3.030930	-0.652920
25	1	0	-4.179061	1.858044	-0.177180
26	1	0	-0.881827	3.410456	0.822976
27	1	0	0.756340	2.846415	0.440345
28	1	0	-0.342995	3.329559	-0.854045
29	1	0	3.237099	-1.309757	1.998021
30	1	0	2.742044	0.375730	2.265906
31	1	0	1.513966	-0.893255	2.108926
32	6	0	3.790634	0.255602	-0.222116
33	6	0	3.983826	1.398391	-0.877512
34	1	0	-4.109790	-1.375146	-0.228582
35	1	0	3.154542	2.044843	-1.143904
36	1	0	4.981368	1.718634	-1.165619
37	1	0	4.640322	-0.377923	0.033711

Conf. 9f

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.80074300

1	6	0	2.479986	-0.517807	0.063115
2	6	0	2.312634	0.874874	0.096482
3	6	0	1.400315	-1.391891	-0.122013
4	6	0	0.109484	-0.858787	-0.304168
5	6	0	-0.061934	0.531085	-0.244519
6	6	0	1.021854	1.405338	-0.043544
7	6	0	-1.086246	-1.757850	-0.558490
8	6	0	-2.318788	-0.969003	-1.014743
9	6	0	-2.480218	0.331405	-0.217597
10	8	0	-1.295678	1.132843	-0.418531
11	6	0	1.661865	-2.883836	-0.116934
12	6	0	3.507829	1.778541	0.291651
13	6	0	0.796571	2.898448	0.006283
14	6	0	-3.617575	1.195760	-0.776681

15	8	0	3.763853	-0.995106	0.233634
16	1	0	-1.326909	-2.320907	0.353078
17	1	0	-0.844127	-2.504320	-1.324768
18	1	0	-2.215165	-0.689419	-2.070030
19	1	0	-3.221483	-1.584968	-0.934924
20	1	0	0.738816	-3.465085	-0.105620
21	1	0	2.232245	-3.212521	-0.999538
22	1	0	2.231011	-3.187903	0.773247
23	1	0	4.439786	1.217814	0.209336
24	1	0	3.523516	2.584564	-0.451471
25	1	0	3.493268	2.258137	1.280114
26	1	0	1.339343	3.354887	0.841840
27	1	0	1.152540	3.389647	-0.910087
28	1	0	-0.263791	3.129539	0.112809
29	1	0	-3.689608	2.138269	-0.224418
30	1	0	-3.428967	1.427430	-1.830350
31	1	0	-4.572747	0.669142	-0.688750
32	6	0	-2.682715	0.131192	1.276736
33	6	0	-3.313887	-0.881609	1.870360
34	1	0	3.768577	-1.948743	0.069800
35	1	0	-3.720935	-1.724742	1.316971
36	1	0	-3.453965	-0.903794	2.947651
37	1	0	-2.301842	0.955933	1.878659

Conf. 9g

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.79981600

1	6	0	-2.623527	-0.328586	0.030847
2	6	0	-2.287586	1.036223	-0.003250
3	6	0	-1.651107	-1.332036	-0.026772
4	6	0	-0.299516	-0.956527	-0.130497
5	6	0	0.042258	0.402973	-0.140932
6	6	0	-0.937048	1.412737	-0.075984
7	6	0	0.784137	-2.011317	-0.221992
8	6	0	2.126797	-1.419456	-0.663487
9	6	0	2.421979	-0.088468	0.055025
10	8	0	1.349557	0.838409	-0.245579
11	6	0	-2.054116	-2.787616	0.015198
12	6	0	-3.404542	2.057499	0.043740
13	6	0	-0.517505	2.867146	-0.092696
14	6	0	2.532179	-0.250674	1.575532
15	8	0	-3.939836	-0.735291	0.112636
16	1	0	0.486470	-2.796407	-0.927783
17	1	0	0.898024	-2.518312	0.747753
18	1	0	2.944666	-2.125094	-0.481046
19	1	0	2.106109	-1.220487	-1.742113
20	1	0	-3.111049	-2.891338	0.263982
21	1	0	-1.890355	-3.281735	-0.952570
22	1	0	-1.470790	-3.344401	0.758678
23	1	0	-3.033056	3.077026	-0.064756
24	1	0	-4.132668	1.899118	-0.765141
25	1	0	-3.957847	2.023034	0.994965
26	1	0	-0.861275	3.378738	-1.001395
27	1	0	-0.928603	3.416576	0.762860
28	1	0	0.568500	2.951789	-0.056315
29	1	0	2.784331	0.707876	2.037874
30	1	0	1.582274	-0.591583	1.996047
31	1	0	3.303322	-0.982304	1.840121
32	6	0	3.639876	0.555620	-0.571457

33	6	0	4.848828	0.682219	-0.026704
34	1	0	-4.501265	0.042720	0.238400
35	1	0	5.076879	0.348010	0.981562
36	1	0	5.668234	1.131706	-0.580827
37	1	0	3.463689	0.911702	-1.586173

Conf. 9h

Imaginary frequencies = 0

Sum of electronic and thermal Enthalpies (Hartree) = -733.79966300

1	6	0	-2.629575	-0.297646	0.024083
2	6	0	-2.281621	1.061485	-0.004358
3	6	0	-1.664894	-1.312498	-0.026839
4	6	0	-0.304864	-0.961462	-0.134702
5	6	0	0.045737	0.396418	-0.140491
6	6	0	-0.925752	1.412745	-0.071406
7	6	0	0.779579	-2.018390	-0.239714
8	6	0	2.123284	-1.424247	-0.676953
9	6	0	2.422918	-0.101509	0.053142
10	8	0	1.354141	0.828412	-0.244943
11	6	0	-2.122261	-2.754928	0.042537
12	6	0	-3.357366	2.120854	0.049223
13	6	0	-0.509828	2.865327	-0.084767
14	6	0	2.529196	-0.276161	1.572626
15	8	0	-3.974243	-0.595051	0.119857
16	1	0	0.898959	-2.537146	0.722807
17	1	0	0.488277	-2.791668	-0.960569
18	1	0	2.937957	-2.135587	-0.502580
19	1	0	2.101534	-1.214587	-1.753462
20	1	0	-2.777194	-2.926434	0.908824
21	1	0	-2.680213	-3.060944	-0.856060
22	1	0	-1.287641	-3.450118	0.143986
23	1	0	-3.351343	2.651738	1.011158
24	1	0	-3.211225	2.877424	-0.730761
25	1	0	-4.346813	1.680403	-0.080190
26	1	0	-1.018820	3.432432	0.703362
27	1	0	0.566648	2.964327	0.056846
28	1	0	-0.767117	3.347135	-1.038277
29	1	0	3.296478	-1.013284	1.833292
30	1	0	2.784747	0.677666	2.042683
31	1	0	1.576701	-0.615378	1.988764
32	6	0	3.644786	0.542437	-0.565803
33	6	0	4.853673	0.658022	-0.018535
34	1	0	-4.094250	-1.547707	0.000218
35	1	0	5.079128	0.313652	0.986918
36	1	0	5.675661	1.109186	-0.567424
37	1	0	3.471257	0.909313	-1.577107

Compound 10

Conf. *P*-

Imaginary frequencies = 0

1	8	0	-0.347314	0.796006	-0.023839

2	8	0	-5.714224	-0.515269	-0.181873
3	6	0	0.672578	-0.164779	0.343205
4	6	0	0.414111	-1.453784	-0.447915
5	6	0	-0.974360	-2.031125	-0.148518
6	6	0	-2.044359	-0.955613	-0.111924
7	6	0	-3.415032	-1.279508	-0.135526
8	6	0	-4.360373	-0.245363	-0.147443
9	6	0	-3.984703	1.106102	-0.110706
10	6	0	-2.621741	1.429123	-0.043662
11	6	0	-1.667310	0.394130	-0.050440
12	6	0	0.619469	-0.380892	1.863350
13	6	0	-5.040193	2.187105	-0.132105
14	6	0	-2.176710	2.871522	0.021086
15	6	0	1.977138	0.529491	-0.090343
16	1	0	1.185174	-2.200149	-0.228173
17	1	0	-0.950468	-2.574901	0.807479
18	1	0	-1.214624	-2.781354	-0.911342
19	1	0	1.328728	-1.152946	2.180775
20	1	0	0.866444	0.550578	2.383596
21	1	0	-0.380951	-0.687185	2.182361
22	1	0	-6.019154	1.772761	-0.376614
23	1	0	-5.124216	2.687753	0.842416
24	1	0	-4.800157	2.963639	-0.867753
25	1	0	-1.124267	2.941605	0.297387
26	1	0	-2.299394	3.374756	-0.948238
27	1	0	-2.767414	3.438464	0.749677
28	1	0	1.900372	0.736638	-1.165921
29	1	0	0.491038	-1.211106	-1.515344
30	6	0	-3.904025	-2.713113	-0.143708
31	1	0	-4.653207	-2.884764	0.642314
32	1	0	-4.365358	-2.993608	-1.103399
33	1	0	-3.098384	-3.426286	0.036667
34	1	0	-5.841797	-1.459966	-0.347867
35	6	0	3.280198	-0.230242	0.194002
36	1	0	3.368560	-0.440693	1.268497
37	1	0	3.266485	-1.206303	-0.310421
38	6	0	4.523995	0.545813	-0.262622
39	1	0	4.441302	0.765258	-1.337306
40	6	0	5.838502	-0.198589	0.003692
41	1	0	5.816011	-1.171822	-0.509310
42	1	0	2.007962	1.507619	0.408242
43	1	0	4.548606	1.521417	0.244773
44	6	0	7.084802	0.577441	-0.441609
45	1	0	7.005269	0.804965	-1.514190
46	1	0	7.109474	1.548266	0.073437
47	1	0	5.917833	-0.424513	1.077727
48	6	0	8.392376	-0.175370	-0.175200
49	1	0	9.262629	0.403704	-0.504689
50	1	0	8.517995	-0.385939	0.894114
51	1	0	8.411635	-1.135879	-0.704884

Conf. *M*-
Imaginary frequencies = 0

1	8	0	0.341122	1.096639	1.311108
2	8	0	4.134230	-2.117239	-1.107943
3	6	0	-0.321629	2.173495	0.608839
4	6	0	0.747606	2.988242	-0.134848
5	6	0	1.541046	2.128689	-1.124927
6	6	0	1.907431	0.778144	-0.536552
7	6	0	2.861145	-0.056061	-1.152359
8	6	0	3.198661	-1.272639	-0.544658
9	6	0	2.600139	-1.696794	0.651346
10	6	0	1.625565	-0.883766	1.247422
11	6	0	1.288649	0.343716	0.645485
12	6	0	-0.957561	3.016485	1.715949
13	6	0	2.997382	-3.013844	1.275646
14	6	0	0.954036	-1.316445	2.529891
15	6	0	-1.376564	1.595516	-0.363332
16	6	0	-2.477986	0.740247	0.277736
17	6	0	-3.401388	0.090939	-0.762452
18	6	0	-4.495893	-0.786655	-0.142140
19	6	0	-5.426150	-1.432201	-1.177238
20	6	0	-6.507661	-2.317233	-0.549374
21	1	0	1.429954	3.403100	0.617447
22	1	0	0.965190	1.996360	-2.052451
23	1	0	-1.547608	3.833327	1.285259
24	1	0	-1.613351	2.409380	2.345913
25	1	0	-0.180993	3.447925	2.355637
26	1	0	3.836656	-3.462834	0.743404
27	1	0	3.284896	-2.886265	2.326594
28	1	0	2.166324	-3.731971	1.261076
29	1	0	0.153090	-0.629846	2.803725
30	1	0	0.531709	-2.324840	2.438161
31	1	0	1.668704	-1.349621	3.363502
32	1	0	-0.860320	0.983037	-1.112674
33	1	0	-1.829994	2.435131	-0.910044
34	1	0	-3.085983	1.350057	0.959267
35	1	0	-2.012703	-0.041085	0.892023
36	1	0	-2.799270	-0.516719	-1.454266
37	1	0	-3.869449	0.875146	-1.376742
38	1	0	-5.095336	-0.183502	0.556307
39	1	0	-4.826932	-2.029255	-1.879377
40	1	0	-5.901503	-0.643913	-1.778474
41	1	0	-7.144113	-1.741456	0.134098
42	1	0	-6.062582	-3.137484	0.027371
43	1	0	0.282773	3.836662	-0.651110
44	1	0	2.447170	2.674570	-1.414033
45	1	0	4.554952	-1.666806	-1.853808
46	6	0	3.533913	0.314784	-2.457812
47	1	0	3.444217	-0.492744	-3.198698
48	1	0	3.092968	1.202135	-2.914151
49	1	0	4.607222	0.525092	-2.330682
50	1	0	-4.026788	-1.575205	0.464999
51	1	0	-7.156161	-2.761291	-1.313329

Compound 11

Conf. *P*-
Imaginary frequencies = 0

1	8	0	0.401165	-1.312252	-0.161185
2	8	0	5.102762	1.590231	-0.071900
3	6	0	-0.863201	-0.757366	0.312912
4	6	0	-1.019034	0.632597	-0.321816
5	6	0	0.133564	1.562465	0.064816
6	6	0	1.479640	0.869342	-0.007168
7	6	0	2.682070	1.599826	0.031430
8	6	0	3.895779	0.912356	-0.084722
9	6	0	3.955582	-0.481879	-0.211846
10	6	0	2.759280	-1.214058	-0.204392
11	6	0	1.536091	-0.527189	-0.108833
12	6	0	-0.828496	-0.726963	1.849996
13	6	0	5.289129	-1.180314	-0.344129
14	6	0	2.781579	-2.720383	-0.314284
15	6	0	-1.890515	-1.749860	-0.204489
16	1	0	-1.972977	1.076012	-0.032615
17	1	0	-0.028602	1.959065	1.074394
18	1	0	0.121279	2.428891	-0.601758
19	1	0	-1.750310	-0.300840	2.250061
20	1	0	-0.723688	-1.742583	2.236820
21	1	0	0.010602	-0.131738	2.216195
22	1	0	6.089032	-0.467408	-0.534881
23	1	0	5.544496	-1.730623	0.568778
24	1	0	5.275805	-1.907299	-1.160477
25	1	0	1.832358	-3.148772	0.001822
26	1	0	2.961758	-3.043432	-1.346769
27	1	0	3.577696	-3.150885	0.297559
28	1	0	-1.043132	0.497580	-1.407315
29	6	0	2.699010	3.104685	0.189257
30	1	0	3.400916	3.417683	0.970718
31	1	0	2.991124	3.612588	-0.738211
32	1	0	1.725744	3.497325	0.475807
33	1	0	4.945495	2.540063	-0.053549
34	6	0	-3.223039	-1.731279	-0.101602
35	1	0	-3.747577	-2.569792	-0.558521
36	6	0	-4.133637	-0.721780	0.542955
37	1	0	-4.700926	-1.226179	1.336844
38	6	0	-5.136076	-0.112411	-0.454846
39	1	0	-5.685384	-0.921615	-0.951961
40	1	0	-1.436020	-2.589550	-0.723230
41	1	0	-3.572640	0.078931	1.028828
42	6	0	-6.132783	0.850021	0.200387
43	1	0	-6.681407	0.318450	0.987403
44	1	0	-5.581897	1.655149	0.701461
45	1	0	-4.583428	0.413529	-1.242847
46	6	0	-7.126725	1.455353	-0.795142
47	1	0	-7.828039	2.130437	-0.296604
48	1	0	-6.609340	2.027369	-1.571954

49	1	0	-7.711658	0.674842	-1.292212

Conf. *M*-

Imaginary frequencies = 0

1	8	0	1.234324	0.111739	2.222268
2	8	0	5.658396	-1.712870	4.995562
3	6	0	1.235224	1.392402	1.535680
4	6	0	1.807427	2.439960	2.498270
5	6	0	3.240903	2.090313	2.899791
6	6	0	3.384700	0.623263	3.254240
7	6	0	4.518171	0.146862	3.939509
8	6	0	4.574369	-1.204222	4.300114
9	6	0	3.545451	-2.101709	3.986615
10	6	0	2.426455	-1.632633	3.282264
11	6	0	2.368316	-0.278059	2.909645
12	6	0	-0.239777	1.673230	1.234010
13	6	0	3.638647	-3.551616	4.400687
14	6	0	1.298238	-2.578289	2.942916
15	6	0	2.049310	1.356738	0.245915
16	6	0	2.157159	0.384767	-0.665498
17	6	0	1.518423	-0.975759	-0.693468
18	6	0	0.730364	-1.220454	-1.993463
19	6	0	0.122859	-2.625180	-2.075692
20	6	0	-0.658405	-2.867058	-3.370620
21	1	0	1.165406	2.469763	3.384114
22	1	0	3.928928	2.346469	2.084926
23	1	0	-0.338492	2.618805	0.696105
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25	1	0	-0.811296	1.737968	2.163780
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28	1	0	3.489971	-4.218568	3.546079
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38	1	0	0.924047	-3.369002	-1.987172
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46	1	0	5.622609	2.008755	3.777959
47	1	0	5.697079	1.279730	5.376704
48	1	0	-0.068649	-0.473465	-2.077424
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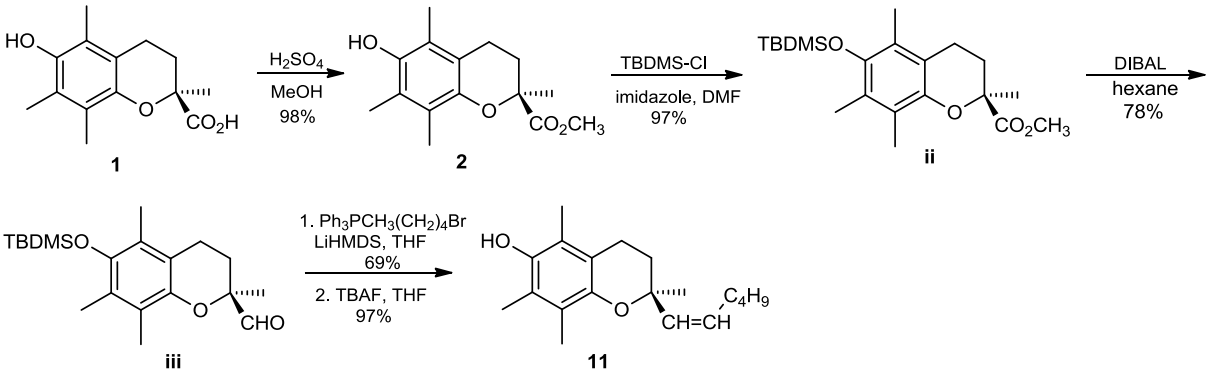
Synthesis of Compound 11.

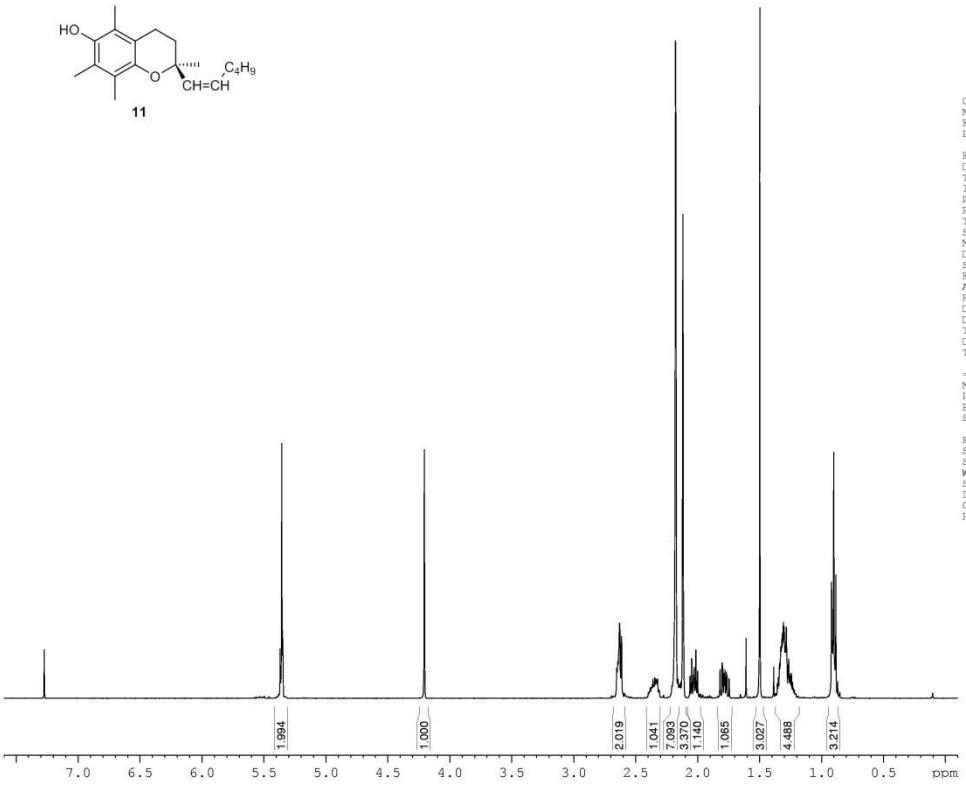


Scheme S1. Synthesis of (*S*)-2-(Z-hex-1-enyl)-6-hydroxy-2,5,7,8-tetramethylchromane (**11**).

n-Pentyltriphenylphosphonium bromide (198 mg, 0.48 mmol) was dissolved in anhydrous THF (12 mL) under argon and a solution of LiHMDS (solution in THF, 1.0 M, 0.65 mL, 0.65 mmol) was added dropwise at room temperature. After stirring for 1 h, a solution of **iii** (150 mg, 0.43 mmol) in anhydrous THF (6 mL) was added and stirred for 6 h at room temperature. The reaction was quenched with saturated ammonium chloride and extracted with dichloromethane. The crude product was purified by flash chromatography over silica gel (hexane/dichloromethane v/v 3:1) to afford product (120 mg, 0.30 mmol, 69%) as oil. A solution of (*S*)-*tert*-butyldimethylsilyloxy-2-[(Z)-hex-1-enyl]-2,5,7,8-tetramethylchromane (100 mg, 0.25 mmol) in anhydrous THF (8 mL) was added dropwise *via* syringe to a stirred solution of TBAF (0.28 mL of a 1 M solution in 2 mL of THF). The mixture was stirred at room temperature until starting material was no longer detected by TLC. The reaction was diluted with ether, washed with water, dried and evaporated to afford light yellow oil. The crude product was purified by flash chromatography on silica gel (hexane/dichloromethane v/v 2:1) and provided 70 mg (97%) of **11** ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.37-5.37 (m, 2H), 4.21 (s, 1H), 2.65-2.62 (m, 2H), 2.36-2.33 (m, 1H), 2.18-2.13 (m, 1H), 2.18 (s, 6H), 2.12 (s, 3H), 2.05-2.00 (m, 1H), 1.82-1.75 (m, 1H), 1.50 (s, 3H), 1.31-1.28 (m, 4H), 0.92-0.89 (m, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.7, 144.7, 133.2, 132.7, 122.4, 121.0, 118.5,

117.7, 75.5, 33.4, 32.2, 27.8, 27.1, 22.5, 21.2, 14.0, 12.2, 12.0, 11.3 ppm; IR (ATR) ν_{max}/cm^{-1}: 3501, 2927, 1639, 1449; MS(+EI): 164 (100), 288 (M^+, 63), HRMS (EI) calculated for $C_{19}H_{28}O_2$: 288.2089, found: 288.2082.

Copies of ^{1}H and ^{13}C NMR, IR and MS spectra for Compound 11.

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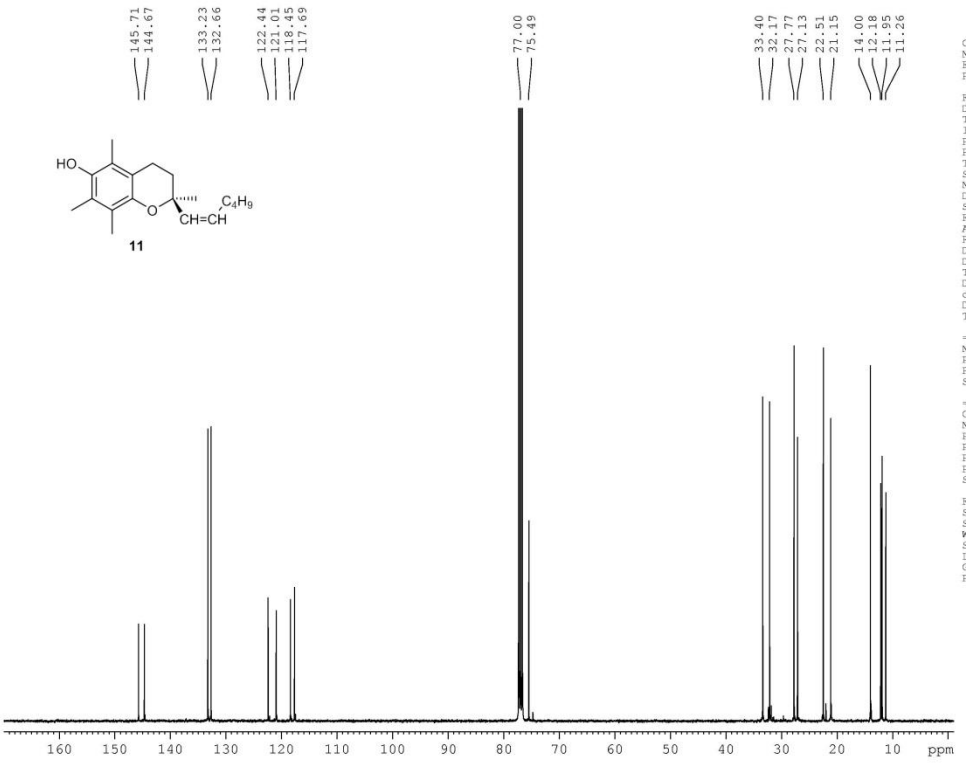


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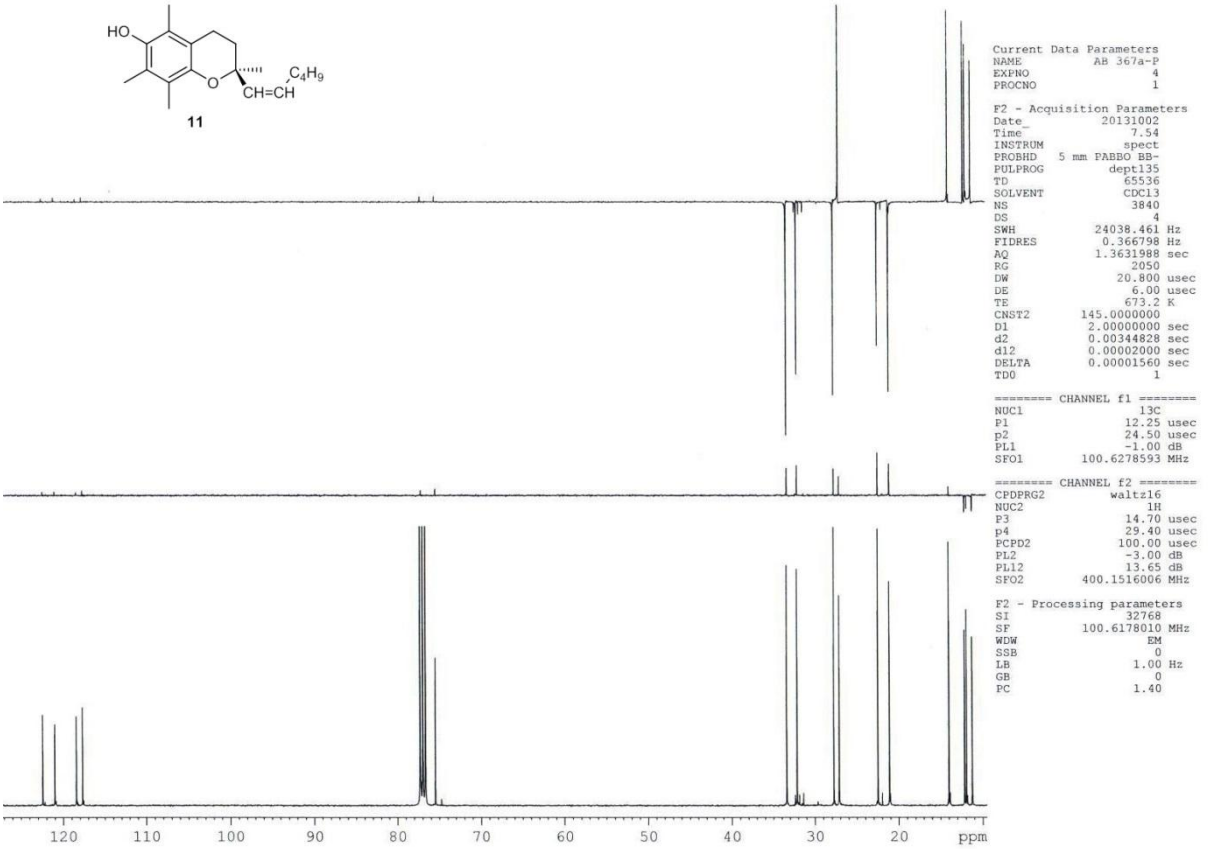


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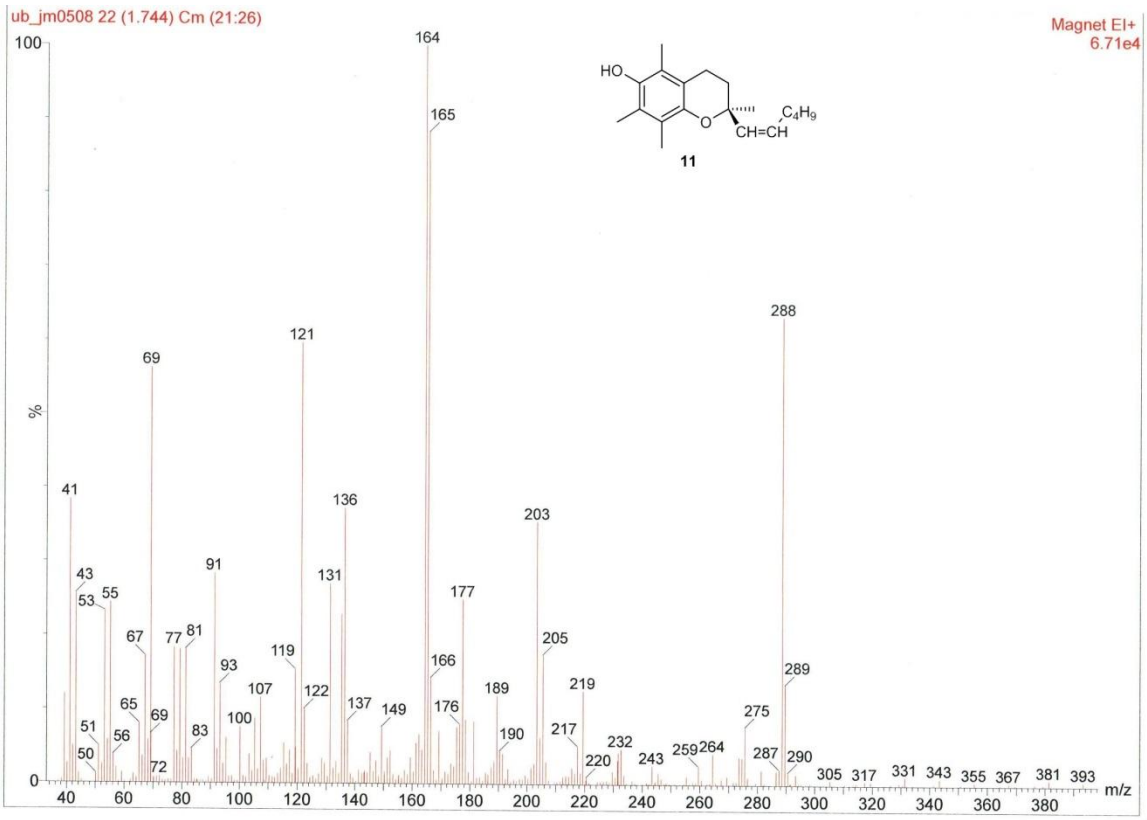
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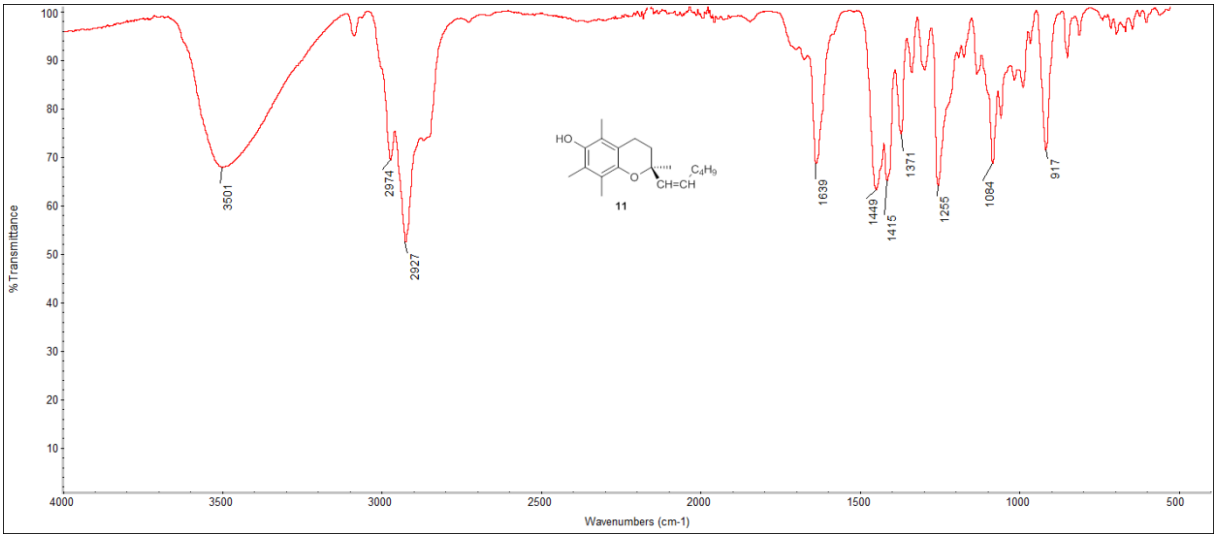
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1639
1449
1415
1371
1255
1084
917
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

X-ray crystallographic data of (*S*)–Trolox methyl ester (2)

$C_{15}H_{20}O_4$, colorless crystal, temperature T=100K, formula weight M=264.31, monoclinic, $P2_1$ space group, a=7.1858(3) Å, b=21.2747(8) Å, c=8.7923(4) Å, β=97.085(4)°, V=1333.87(10) $Å^3$, Z=4, D_x= 1.316 Mgm^{-3}, absorption coefficient μ=0.094 mm^{-1}, F(000)= 568, crystal size = 0.15x0.12x0.11. The collected data range was 1.91<Θ<25.04 deg.(-8<h<8, -25<k<25, -10<l<10), 12743 reflections collected, 2429 reflections unique [R(int) = 0.0359], Data/restraints/parameters 2429/1/361, Goodness-of-fit on F^2=1.120, Final R indices [I>2σ(I)] R1=0.0458, wR^2=0.1211, R indices (all data) R1=0.0504, wR^2=0.1246, maximum and minimum difference electron densities were 0.415 and -0.273 e. $Å^{-3}$.

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(compiled Jul 11 2012,15:38:31)
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H21G H 0.3745 0.3214 0.0739 0.031 Uiso 1 1 calc R . .
C3B C 0.4303(5) 0.45793(17) 0.2421(4) 0.0148(7) Uani 1 1 d . . .
C4B C 0.4241(5) 0.48448(17) 0.3874(4) 0.0152(8) Uani 1 1 d . . .
C5B C 0.4905(5) 0.57855(16) 0.5282(4) 0.0174(8) Uani 1 1 d . . .
C51B C 0.7035(5) 0.57142(15) 0.5312(4) 0.0165(7) Uani 1 1 d . . .
C52B C 0.4448(6) 0.64884(17) 0.5144(5) 0.0230(9) Uani 1 1 d . . .
H52E H 0.4596 0.6633 0.4107 0.034 Uiso 1 1 calc R . .
H52G H 0.5303 0.6723 0.5892 0.034 Uiso 1 1 calc R . .
H52F H 0.3152 0.6559 0.5343 0.034 Uiso 1 1 calc R . .
C53B C 0.9576(5) 0.5785(2) 0.3863(5) 0.0272(9) Uani 1 1 d . . .
H53F H 1.0188 0.6099 0.4574 0.041 Uiso 1 1 calc R . .
H53E H 0.9829 0.5883 0.2818 0.041 Uiso 1 1 calc R . .

H53G H 1.0068 0.5367 0.4152 0.041 Uiso 1 1 calc R . .
C6B C 0.4201(6) 0.54955(17) 0.6686(4) 0.0193(8) Uani 1 1 d . . .
H62B H 0.2848 0.5589 0.6663 0.023 Uiso 1 1 calc R . .
H61B H 0.4868 0.5692 0.7619 0.023 Uiso 1 1 calc R . .
C7B C 0.4491(5) 0.47825(17) 0.6774(4) 0.0173(8) Uani 1 1 d . . .
H72B H 0.5734 0.4692 0.7352 0.021 Uiso 1 1 calc R . .
H71B H 0.3524 0.4594 0.7343 0.021 Uiso 1 1 calc R . .
C8B C 0.4380(5) 0.44797(17) 0.5198(4) 0.0145(7) Uani 1 1 d . . .
C9B C 0.4509(5) 0.38241(17) 0.5080(4) 0.0153(8) Uani 1 1 d . . .
C91B C 0.4633(5) 0.34130(18) 0.6489(4) 0.0178(8) Uani 1 1 d . . .
H91E H 0.5682 0.3553 0.7231 0.027 Uiso 1 1 calc R . .
H91G H 0.4836 0.2976 0.6201 0.027 Uiso 1 1 calc R . .
H91F H 0.3463 0.3444 0.6950 0.027 Uiso 1 1 calc R . .
H1B H 0.482(8) 0.276(3) 0.265(7) 0.057(17) Uiso 1 1 d . . .

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O3A 0.0196(13) 0.0293(15) 0.0184(13) -0.0027(11) 0.0027(10) -0.0017(11)
O4A 0.0279(15) 0.0177(14) 0.0246(14) 0.0007(11) 0.0122(12) 0.0016(11)
C1A 0.0159(19) 0.0093(17) 0.0227(19) -0.0005(14) -0.0006(15) -0.0021(13)
C2A 0.0111(18) 0.0124(17) 0.0193(19) 0.0028(14) 0.0015(14) -0.0009(13)
C21A 0.022(2) 0.0196(19) 0.0202(19) 0.0031(16) 0.0037(16) 0.0006(16)
C3A 0.0133(19) 0.0144(17) 0.0166(18) 0.0000(14) 0.0015(14) -0.0007(13)
C31A 0.023(2) 0.0172(19) 0.0174(18) 0.0011(14) 0.0039(15) -0.0016(15)
C4A 0.018(2) 0.0083(16) 0.0190(18) 0.0033(14) 0.0022(15) -0.0017(14)
C5A 0.0239(19) 0.0138(18) 0.0158(17) 0.0035(14) 0.0065(15) -0.0001(15)
C51A 0.0256(19) 0.0063(16) 0.0179(18) 0.0015(14) 0.0062(15) -0.0017(14)
C52A 0.026(2) 0.016(2) 0.026(2) 0.0015(16) 0.0089(17) 0.0031(16)
C53A 0.0190(19) 0.026(2) 0.027(2) -0.0045(17) 0.0004(16) -0.0035(17)
C6A 0.024(2) 0.0191(19) 0.0179(19) 0.0060(15) 0.0008(15) 0.0007(16)
C7A 0.020(2) 0.0191(18) 0.0174(18) 0.0009(16) 0.0032(15) -0.0022(15)
C8A 0.0145(19) 0.0156(19) 0.0169(19) 0.0001(14) 0.0005(14) -0.0029(14)
C9A 0.0138(18) 0.0165(18) 0.0176(18) -0.0023(15) 0.0001(15) -0.0010(14)
C91A 0.0213(19) 0.0161(18) 0.0211(19) -0.0027(16) 0.0032(15) -0.0018(15)
O1B 0.0358(17) 0.0115(13) 0.0239(15) -0.0010(12) 0.0098(13) 0.0021(12)
O2B 0.0195(13) 0.0152(13) 0.0143(13) -0.0014(10) 0.0005(10) 0.0013(10)
O3B 0.0229(14) 0.0270(15) 0.0165(13) 0.0018(11) 0.0043(10) 0.0004(12)
C31B 0.023(2) 0.0172(19) 0.0163(18) 0.0008(15) 0.0002(15) 0.0046(15)
O4B 0.0268(14) 0.0184(13) 0.0207(14) 0.0038(11) -0.0036(11) -0.0016(11)
C1B 0.019(2) 0.0127(18) 0.021(2) -0.0019(15) 0.0057(16) -0.0002(14)
C2B 0.0128(18) 0.0182(19) 0.0162(19) -0.0035(15) 0.0015(14) 0.0010(14)
C21B 0.028(2) 0.0150(18) 0.0191(19) -0.0043(16) 0.0017(16) 0.0030(15)
C3B 0.0101(17) 0.0188(19) 0.0154(18) 0.0021(14) 0.0015(13) 0.0013(14)
C4B 0.0153(18) 0.0112(17) 0.0192(18) -0.0016(14) 0.0024(15) 0.0018(14)
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C51B 0.030(2) 0.0046(15) 0.0151(17) 0.0002(13) 0.0011(15) -0.0023(15)
C52B 0.033(2) 0.0114(19) 0.025(2) -0.0044(16) 0.0073(17) 0.0023(16)
C53B 0.025(2) 0.031(2) 0.026(2) 0.0040(18) 0.0049(16) -0.0009(18)
C6B 0.025(2) 0.0175(19) 0.0164(18) -0.0037(15) 0.0047(15) 0.0010(15)
C7B 0.022(2) 0.0140(18) 0.0158(18) -0.0010(15) 0.0010(15) -0.0025(15)

C8B 0.0126(17) 0.0171(19) 0.0141(17) -0.0018(15) 0.0029(13) -0.0013(14)
C9B 0.0117(18) 0.0157(18) 0.0187(19) -0.0006(15) 0.0032(15) 0.0006(14)
C91B 0.0197(19) 0.0139(18) 0.0205(19) -0.0009(15) 0.0049(15) -0.0005(15)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C2A C3A 1.404(5) . ?
C2A C21A 1.508(5) . ?
C21A H21C 0.9800 . ?
C21A H21A 0.9800 . ?
C21A H21B 0.9800 . ?
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C6A C7A 1.526(5) . ?
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C91A H91B 0.9800 . ?
O1B C1B 1.383(5) . ?
O1B H1B 0.91(6) . ?
O2B C4B 1.396(4) . ?
O2B C5B 1.430(4) . ?
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C1B C9B 1.400(5) . ?
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C1A C2A C3A 119.1(3) . . ?

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C3A C2A C21A 119.8(3) . . ?
C2A C21A H21C 109.5 . . ?
C2A C21A H21A 109.5 . . ?
H21C C21A H21A 109.5 . . ?
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H21C C21A H21B 109.5 . . ?
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H31C C31A H31B 109.5 . . ?
C8A C4A C3A 122.4(3) . . ?
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H52A C52A H52B 109.5 . . ?
H52C C52A H52B 109.5 . . ?
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C8A C7A C6A 111.9(3) . . ?
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C3B C31B H31E 109.5 . . ?
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H31F C31B H31G 109.5 . . ?
H31E C31B H31G 109.5 . . ?
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O1B C1B C2B 122.1(3) . . ?
C9B C1B C2B 122.2(3) . . ?
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O2B C4B C3B 116.5(3) . . ?
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C5B C52B H52E 109.5 . . ?
C5B C52B H52G 109.5 . . ?
H52E C52B H52G 109.5 . . ?
C5B C52B H52F 109.5 . . ?
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H52G C52B H52F 109.5 . . ?
O3B C53B H53F 109.5 . . ?
O3B C53B H53E 109.5 . . ?
H53F C53B H53E 109.5 . . ?
O3B C53B H53G 109.5 . . ?
H53F C53B H53G 109.5 . . ?
H53E C53B H53G 109.5 . . ?
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C8B C7B H71B 109.1 . . ?
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H72B C7B H71B 107.9 . . ?
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C9B C91B H91G 109.5 . . ?
H91E C91B H91G 109.5 . . ?
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H91G C91B H91F 109.5 . . ?

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O2A C5A C51A O3A 37.7(4) . . . . ?
C6A C5A C51A O3A 159.4(3) . . . . ?
C52A C5A C51A O3A -77.0(4) . . . . ?

O2A C5A C6A C7A 60.0(4) . . . . ?
C52A C5A C6A C7A 177.6(3) . . . . ?
C51A C5A C6A C7A -61.9(4) . . . . ?
C5A C6A C7A C8A -36.7(4) . . . . ?
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O2A C4A C8A C9A -179.3(3) . . . . ?
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O1A C1A C9A C91A 2.8(5) . . . . ?
C2A C1A C9A C91A -179.2(3) . . . . ?
O1B C1B C2B C3B 179.1(3) . . . . ?
C9B C1B C2B C3B -0.8(5) . . . . ?
O1B C1B C2B C21B -1.0(5) . . . . ?
C9B C1B C2B C21B 179.1(3) . . . . ?
C1B C2B C3B C4B -2.3(5) . . . . ?
C21B C2B C3B C4B 177.9(3) . . . . ?
C1B C2B C3B C31B 178.2(3) . . . . ?
C21B C2B C3B C31B -1.7(6) . . . . ?
C5B O2B C4B C8B 33.8(5) . . . . ?
C5B O2B C4B C3B -147.5(3) . . . . ?
C2B C3B C4B C8B 4.1(5) . . . . ?
C31B C3B C4B C8B -176.4(3) . . . . ?
C2B C3B C4B O2B -174.6(3) . . . . ?
C31B C3B C4B O2B 5.0(5) . . . . ?
C4B O2B C5B C6B -58.0(4) . . . . ?
C4B O2B C5B C52B -179.1(3) . . . . ?
C4B O2B C5B C51B 65.1(4) . . . . ?
C53B O3B C51B O4B -0.7(5) . . . . ?
C53B O3B C51B C5B 175.5(3) . . . . ?
O2B C5B C51B O4B -143.7(3) . . . . ?
C6B C5B C51B O4B -22.0(5) . . . . ?
C52B C5B C51B O4B 101.2(4) . . . . ?
O2B C5B C51B O3B 40.1(4) . . . . ?
C6B C5B C51B O3B 161.8(3) . . . . ?
C52B C5B C51B O3B -75.0(3) . . . . ?
O2B C5B C6B C7B 57.2(4) . . . . ?
C52B C5B C6B C7B 175.1(3) . . . . ?
C51B C5B C6B C7B -64.1(4) . . . . ?
C5B C6B C7B C8B -31.2(5) . . . . ?
O2B C4B C8B C9B 175.8(3) . . . . ?
C3B C4B C8B C9B -2.7(5) . . . . ?
O2B C4B C8B C7B -7.1(5) . . . . ?
C3B C4B C8B C7B 174.3(3) . . . . ?
C6B C7B C8B C4B 6.7(5) . . . . ?
C6B C7B C8B C9B -176.3(3) . . . . ?
O1B C1B C9B C8B -177.8(3) . . . . ?
C2B C1B C9B C8B 2.1(5) . . . . ?
O1B C1B C9B C91B 0.9(5) . . . . ?
C2B C1B C9B C91B -179.2(3) . . . . ?
C4B C8B C9B C1B -0.4(5) . . . . ?

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C7B C8B C9B C1B -177.4(3) . . . . ?
C4B C8B C9B C91B -179.1(3) . . . . ?
C7B C8B C9B C91B 3.9(5) . . . . ?

loop_
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 _geom_hbond_atom_site_label_H
 _geom_hbond_atom_site_label_A
 _geom_hbond_distance_DH
 _geom_hbond_distance_HA
 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
O1A H1A O4B  0.81(5) 2.08(5) 2.796(4) 148(5) .

_diffrn_measured_fraction_theta_max    0.997
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.997
_refine_diff_density_max    0.415
_refine_diff_density_min   -0.273
_refine_diff_density_rms    0.065
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