

Addressing the stereochemistry of complex organic molecules by DFT-NMR: vannusal B in retrospective

Supporting Information

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- 1. Complete refs. 21 and 22**
- 2. Tables of calculated (M06/pcS-2) and experimental ¹³C chemical shifts**
- 3. Correlation graphs**
- 4. Cartesian coordinates**

1. Complete refs. 21 and 22

(21) Gaussian 03, Revision D.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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

2. Tables of calculated (M06/pcS-2) and experimental ^{13}C chemical shifts for the compounds of Figure 1

2-1

C	δ_{exp}	δ_{calc}
32	20.917	23.6608
16	22.086	26.4435
20	21.832	27.1022
30	24.017	27.3425
15	25.017	28.2598
24	28.947	30.2931
5	28.972	30.5968
4	26.756	33.2572
9	31.436	34.5286
8	31.04	34.6104
23	30.014	34.8918
19	37.242	40.676
7	45.358	50.6556
21	50.975	52.573
6	48.229	53.3483
3	52.214	56.0976
18	56.581	59.0668
10	52.823	61.399
17	51.868	61.936
14	57.735	64.7792
13	69.472	78.0019
28	73.198	78.9325
29	78.515	82.3969
22	73.395	84.0094
26	76.792	86.136
25	79.005	91.6937
1	111.513	123.843
12	113.759	125.595
2	144.688	162.454
11	158.199	184.619
31	172.152	188.179
27	198.918	217.73

2-2

C	δ_{exp}	δ_{calc}
32	20.952	23.5019
16	21.633	26.0016
30	24.008	26.3849
15	24.236	28.2586
20	22.049	29.2304
4	26.636	29.3307
24	28.969	31.8074
23	30.029	33.3004
5	28.999	33.5597
9	33.706	36.0127
8	31.018	36.5782
19	37.127	44.3612
7	45.28	48.6624
6	50.65	55.2369
3	52.124	56.6108
21	51.00	57.5673
10	52.429	60.4519
18	56.542	60.5397
17	51.496	61.5135
14	57.326	62.9301
13	68.864	76.6904
22	73.274	78.0103
28	71.121	78.7182
29	78.03	82.0264
25	79.015	93.8086
26	76.72	93.9079
1	111.467	124.528
12	114.319	126.534
2	144.748	162.59
11	157.541	184.743
31	172.052	188.45
27	200.249	218.464

3-1

C	δ_{exp}	δ_{calc}
24	27.482	24.7434
20	23.356	25.0578
32	20.919	25.2158
16	23.139	26.332
30	24.019	27.7165
15	25.316	28.8016
5	28.987	31.0378
4	26.75	32.9958
23	28.079	33.1082
8	31.052	34.986
9	31.435	35.2871
19	40.311	47.9452
7	45.285	50.1819
6	48.295	53.1089
18	53.357	54.041
3	52.093	56.9039
21	57.181	58.6066
10	53.049	60.1298
14	58.572	63.9853
17	55.127	65.5417
13	70.641	77.8206
22	73.326	78.9755
28	73.345	81.4635
29	78.561	82.4491
25	83.024	92.9225
26	81.468	95.4221
1	111.49	124.996
12	113.772	125.779
2	144.724	161.872
11	157.992	184.282
31	172.159	188.296
27	200.354	216.102

3-2

C	δ_{exp}	δ_{calc}
32	20.954	23.177
20	22.876	23.229
16	23.355	28.4897
30	24.003	26.4486
15	24.512	27.4305
4	26.634	28.8649
24	27.47	30.5584
5	28.996	33.7531
23	28.996	25.4463
8	30.988	36.2956
9	33.69	36.5219
19	40.403	40.5353
7	45.216	49.2272
6	50.72	55.3799
3	52.132	56.9781
10	52.607	60.2593
18	53.364	59.755
17	54.736	60.9591
21	57.189	53.9065
14	58.22	63.0944
13	70.047	76.2812
28	71.261	78.1707
22	73.345	81.5771
29	78.056	81.912
26	81.452	86.0982
25	82.975	90.9876
1	111.458	124.516
12	114.329	125.976
2	144.771	162.6
11	157.472	184.949
31	172.115	188.803
27	201.585	217.869

4-1

C	δ_{exp}	δ_{calc}
24	29.625	22.9293
32	20.919	24.8608
30	24.016	27.2539
16	24.334	27.5192
20	23.225	28.3765
15	24.987	29.1228
4	26.741	31.6626
5	28.965	31.835
8	31.038	35.0419
9	31.434	35.4198
23	29.927	36.2929
19	40.227	41.3459
7	45.219	49.0544
6	48.271	52.5882
3	52.097	56.8304
21	51.812	56.8685
17	52.582	59.2358
10	53.107	60.0732
18	58.578	62.8759
14	58.96	63.3839
13	69.246	76.4332
28	73.262	81.4131
29	78.561	82.4611
26	77.643	83.5851
25	78.157	86.2246
22	73.599	86.3226
1	111.489	125.171
12	114.284	127.29
2	144.725	161.829
11	157.703	183.219
31	172.177	187.994
27	200.979	217.493

4-2

C	δ_{exp}	δ_{calc}
32	20.965	22.2274
24	29.643	23.5378
30	24.016	26.3629
20	23.225	26.697
16	24.048	26.7542
15	24.232	27.8293
4	26.632	28.8663
5	28.995	33.156
8	31.009	36.4062
23	29.941	36.8024
9	33.683	37.1631
19	40.315	45.1187
7	45.18	49.6993
6	50.723	55.7333
3	52.126	56.7232
10	52.639	59.7373
17	52.214	60.7131
21	51.778	61.7451
18	58.211	62.8227
14	58.914	63.313
13	68.627	75.1909
28	71.224	78.311
29	78.141	81.9541
22	73.572	83.2847
25	78.042	85.5891
26	77.625	87.608
1	111.459	124.531
12	114.787	126.915
2	144.753	162.627
11	157.206	183.912
31	172.075	189.465
27	202.091	219.232

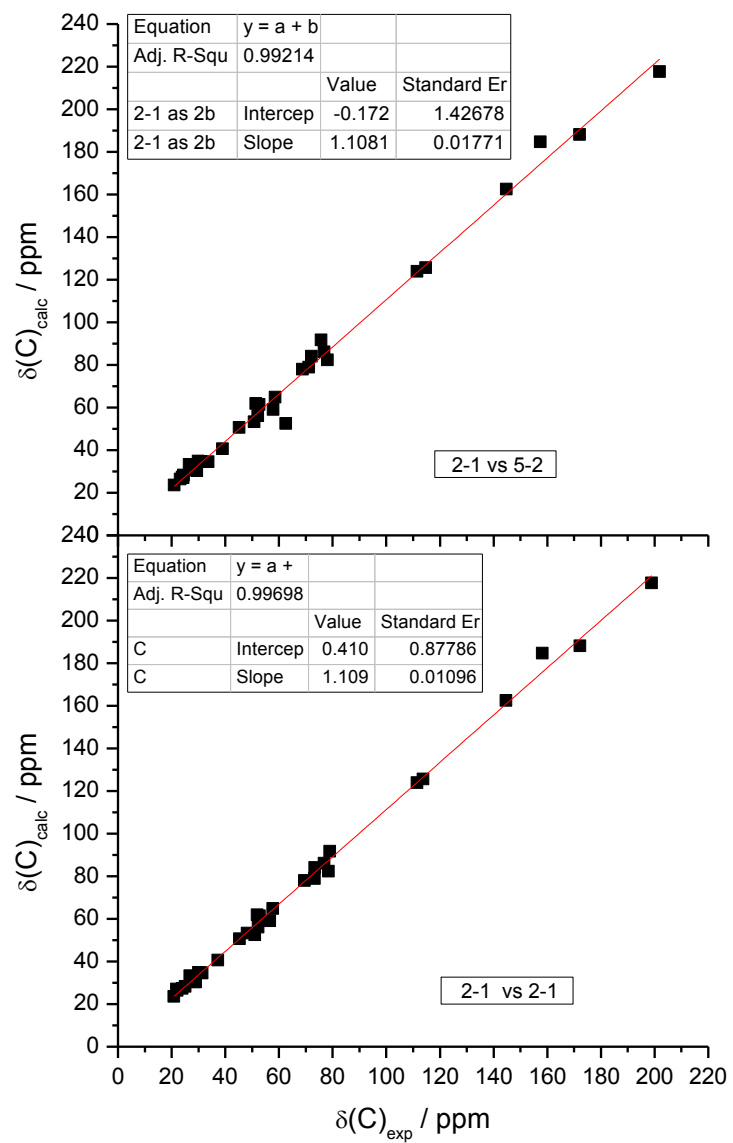
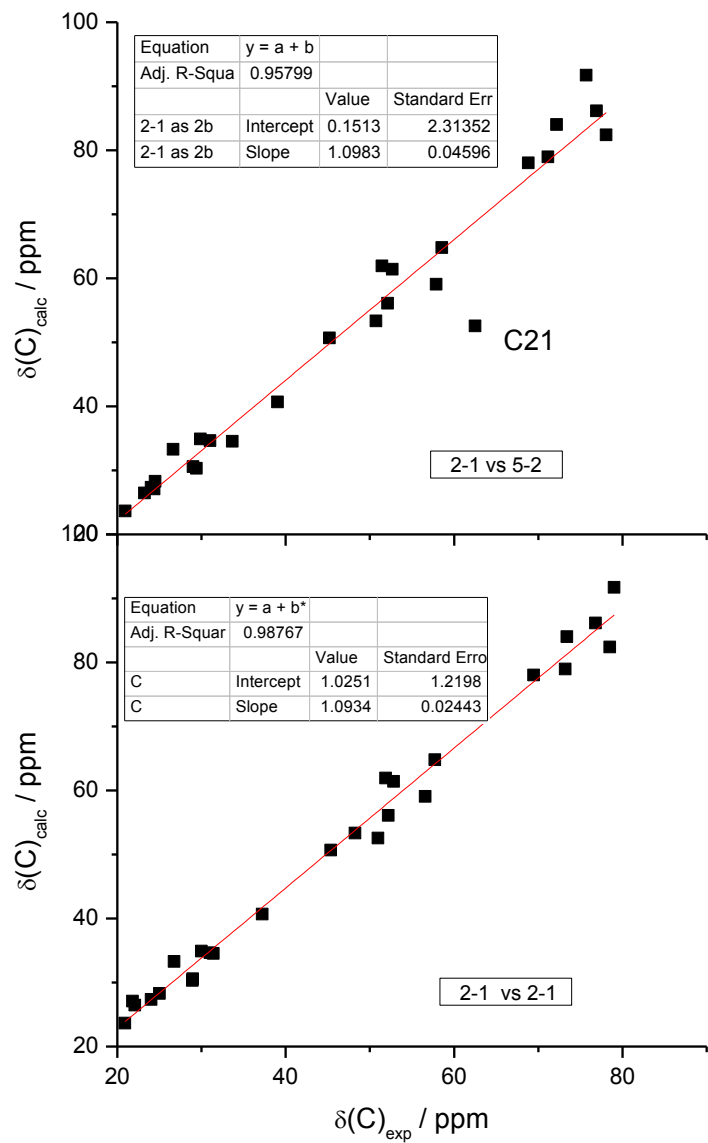
5-1

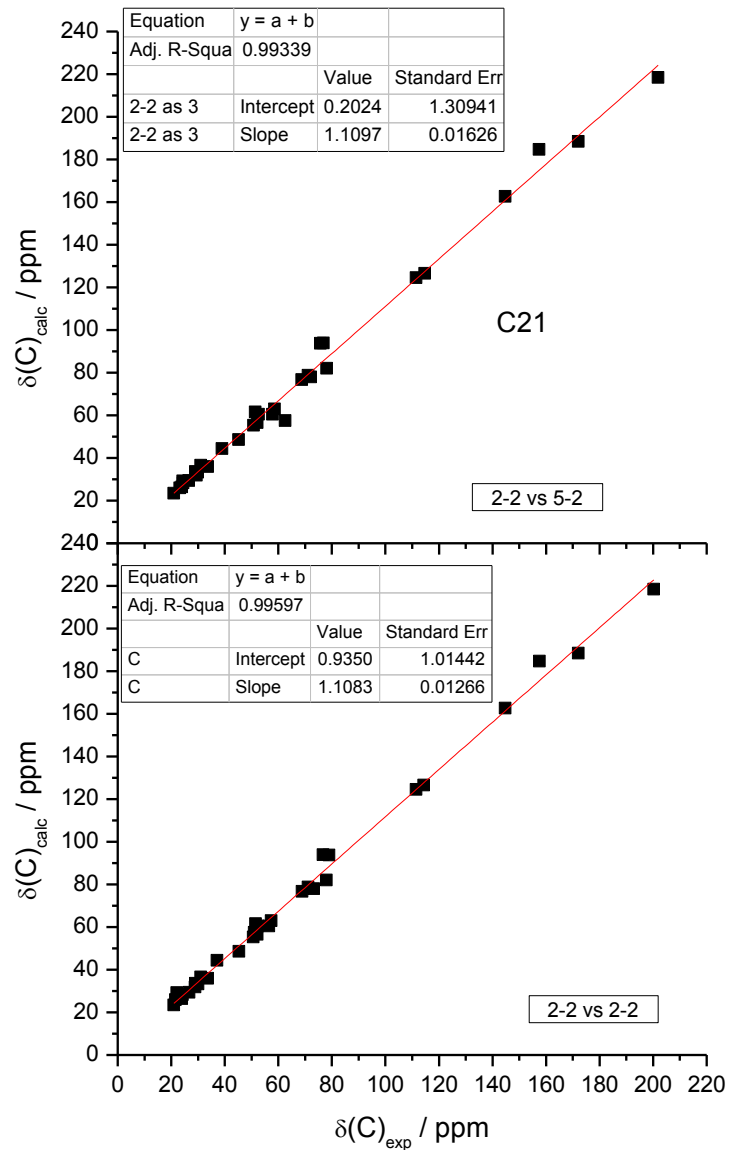
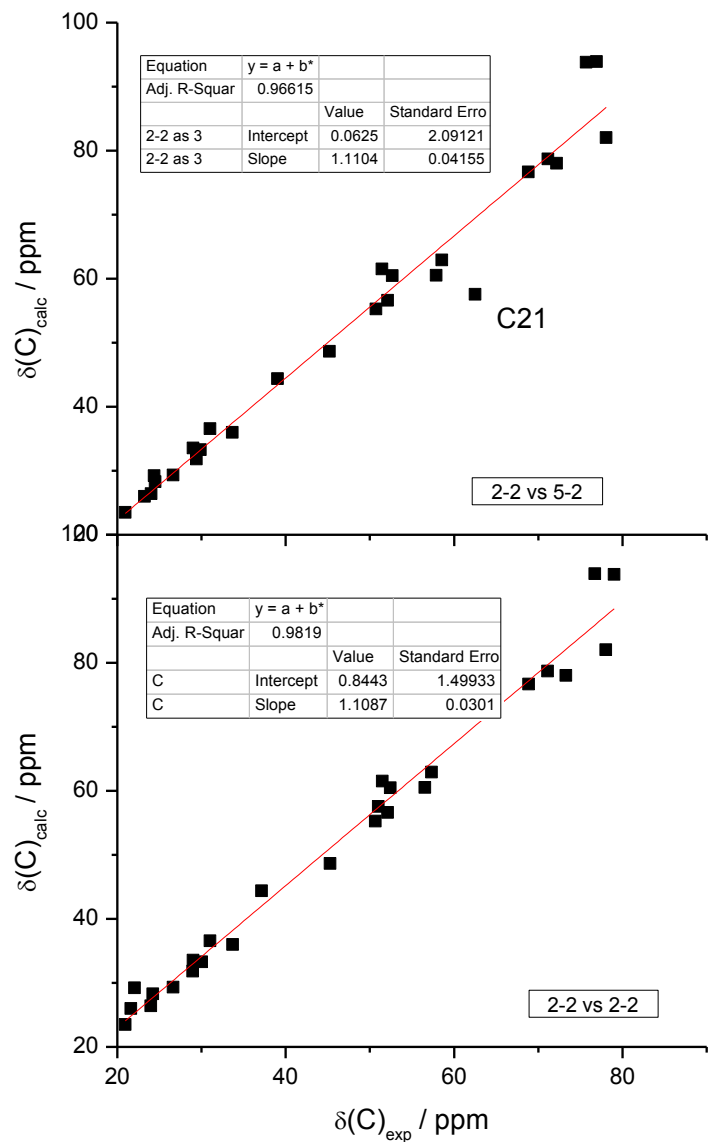
C	δ_{exp}	δ_{calc}
32	20.917	24.9927
20	24.489	26.9322
16	23.536	26.9628
30	24.017	27.4325
15	25.085	27.5552
5	28.95	30.821
24	29.408	31.6969
4	26.74	32.6228
23	29.888	33.3669
9	31.432	34.6399
8	31.021	34.8304
19	38.886	43.5317
7	45.209	50.3993
6	48.254	53.2853
3	52.075	56.0424
17	51.754	59.2098
10	53.174	61.7466
18	58.195	64.1876
14	58.588	64.6448
21	62.495	68.1201
13	69.426	77.2086
28	73.087	79.3946
22	72.162	81.4322
26	76.848	81.4369
25	75.969	82.231
29	78.553	82.5902
1	111.491	124.474
12	114.195	126.367
2	144.733	162.36
11	157.884	183.909
31	172.161	188.451
27	200.765	217.928

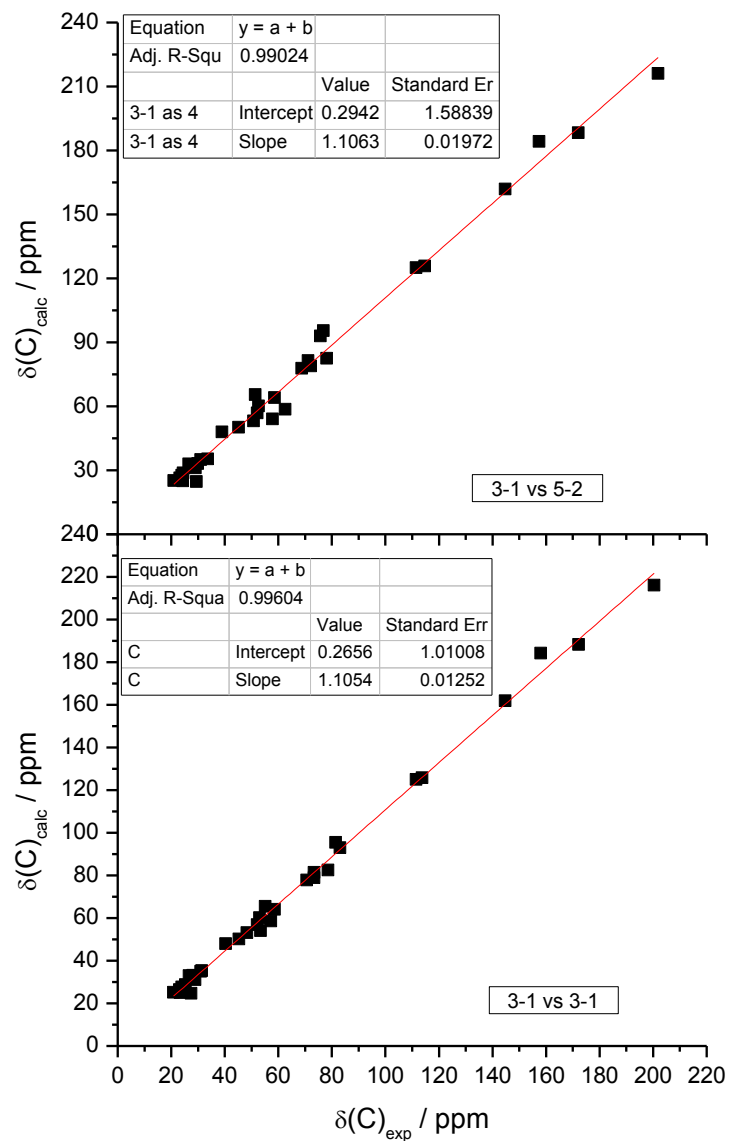
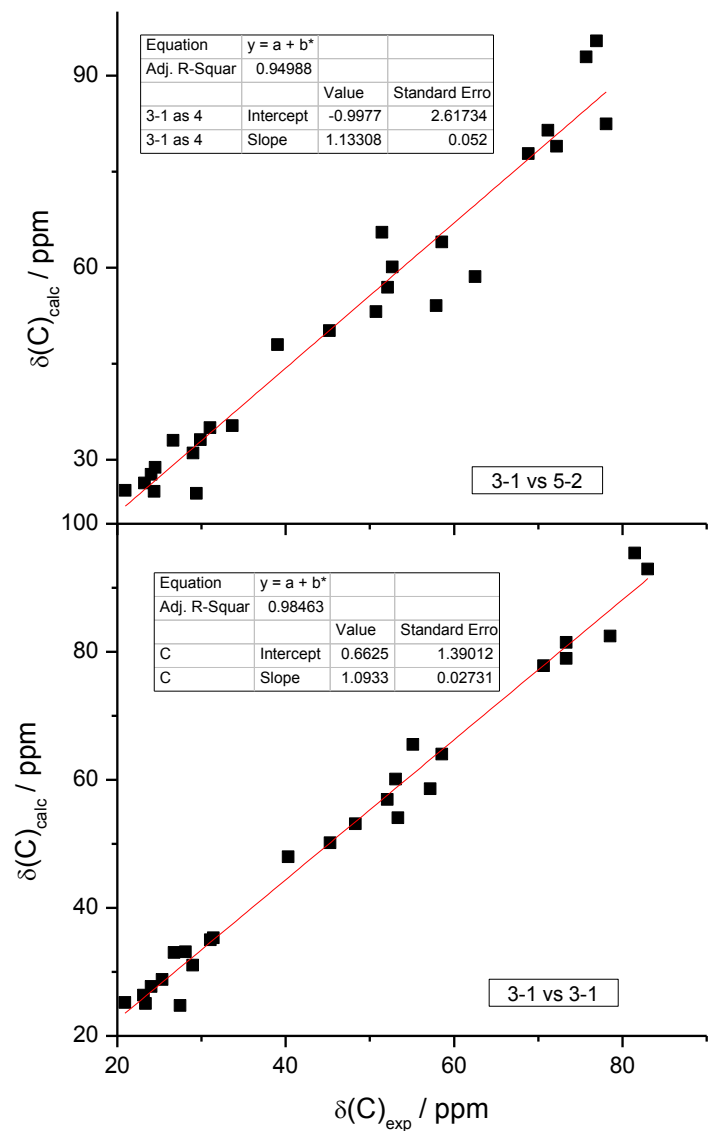
5-2

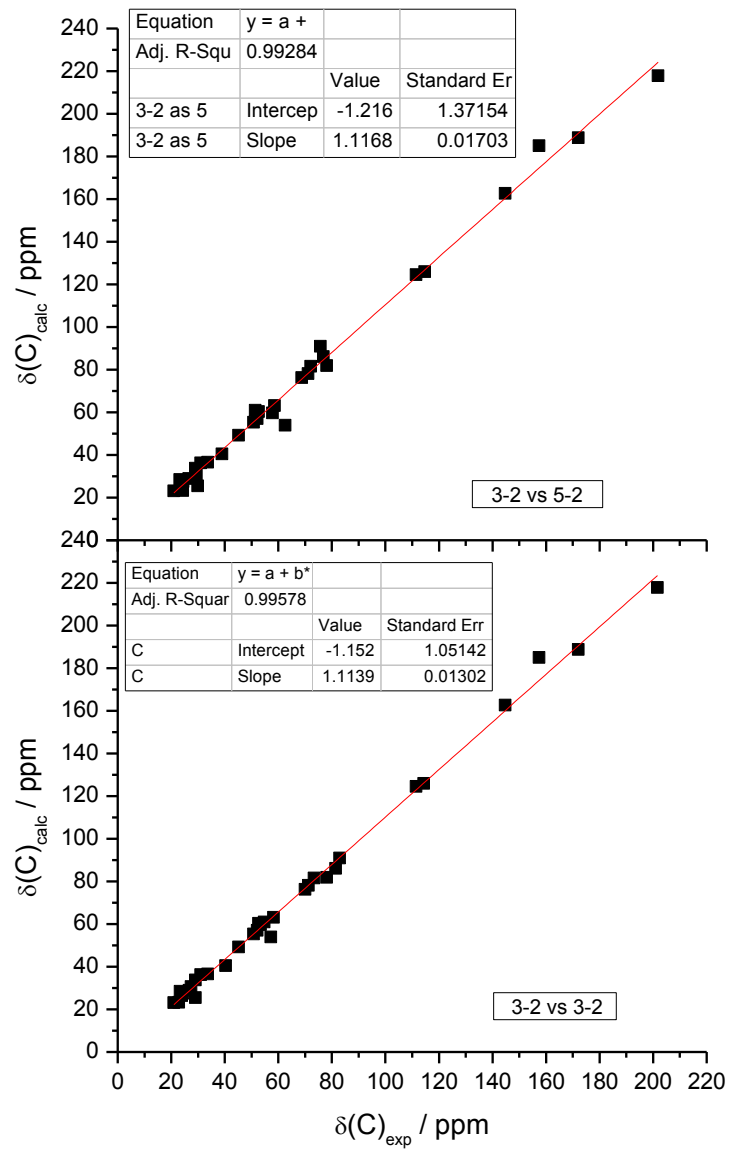
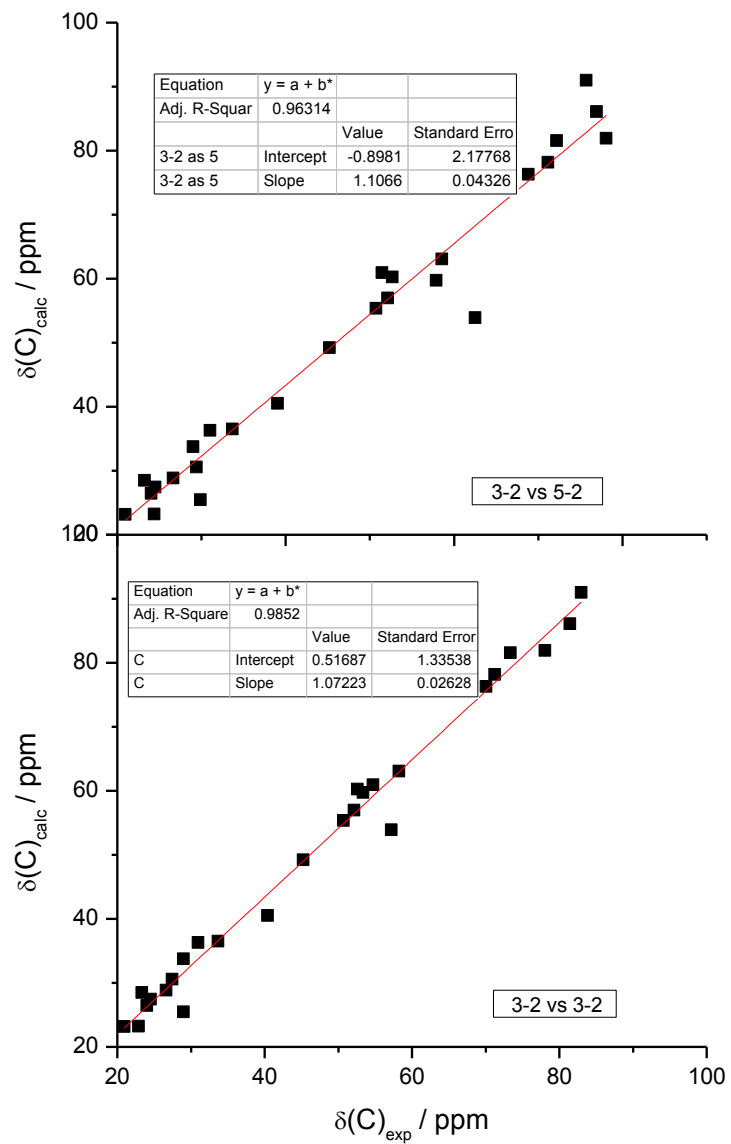
C	δ_{exp}	δ_{calc}
32	20.951	23.5491
16	23.245	25.9001
30	24.014	25.9463
20	24.371	26.3789
15	24.494	28.4143
24	29.414	29.4743
23	29.884	30.3499
4	26.63	30.4449
5	28.995	32.3715
9	33.659	36.2941
8	31.014	36.587
19	39.041	41.913
7	45.219	48.3366
6	50.74	55.481
3	52.125	56.1384
17	51.443	58.4137
10	52.668	60.2379
18	57.879	62.7218
14	58.573	63.3384
21	62.517	69.5276
13	68.843	75.6095
22	72.17	77.7301
28	71.168	78.6153
29	78.071	82.329
25	75.694	83.1121
26	76.911	86.0899
1	111.443	124.086
12	114.762	127.202
2	144.785	162.577
11	157.397	183.793
31	172.106	188.044
27	201.91	218.775

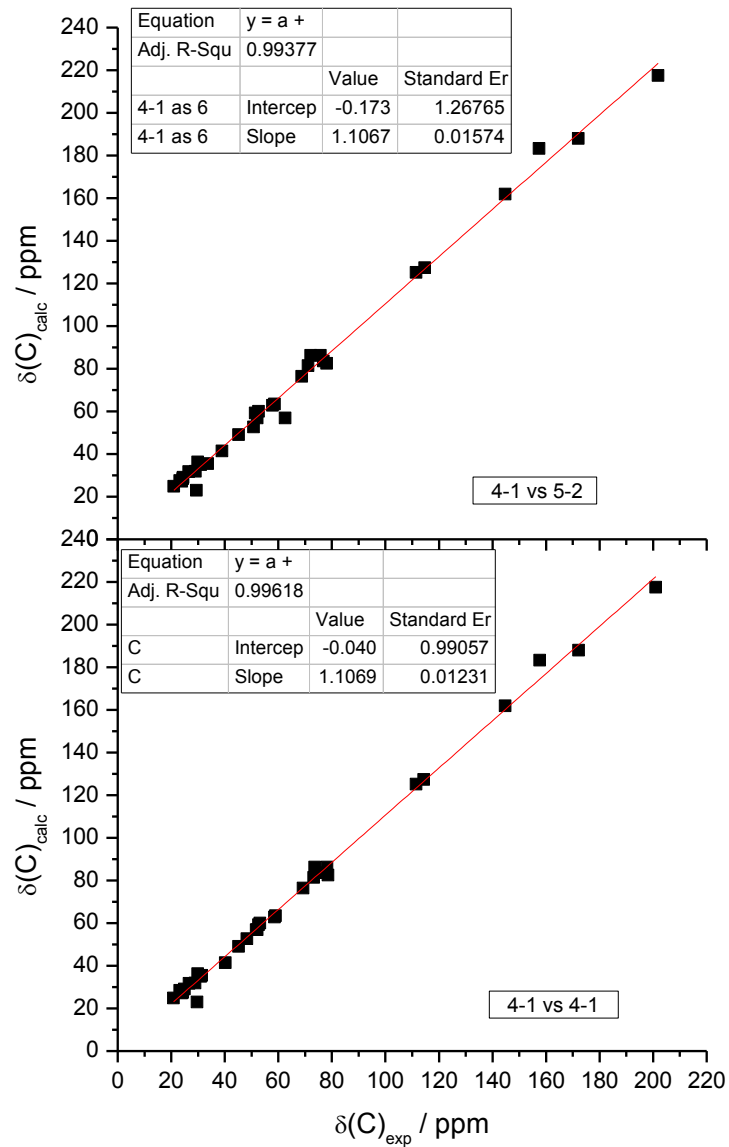
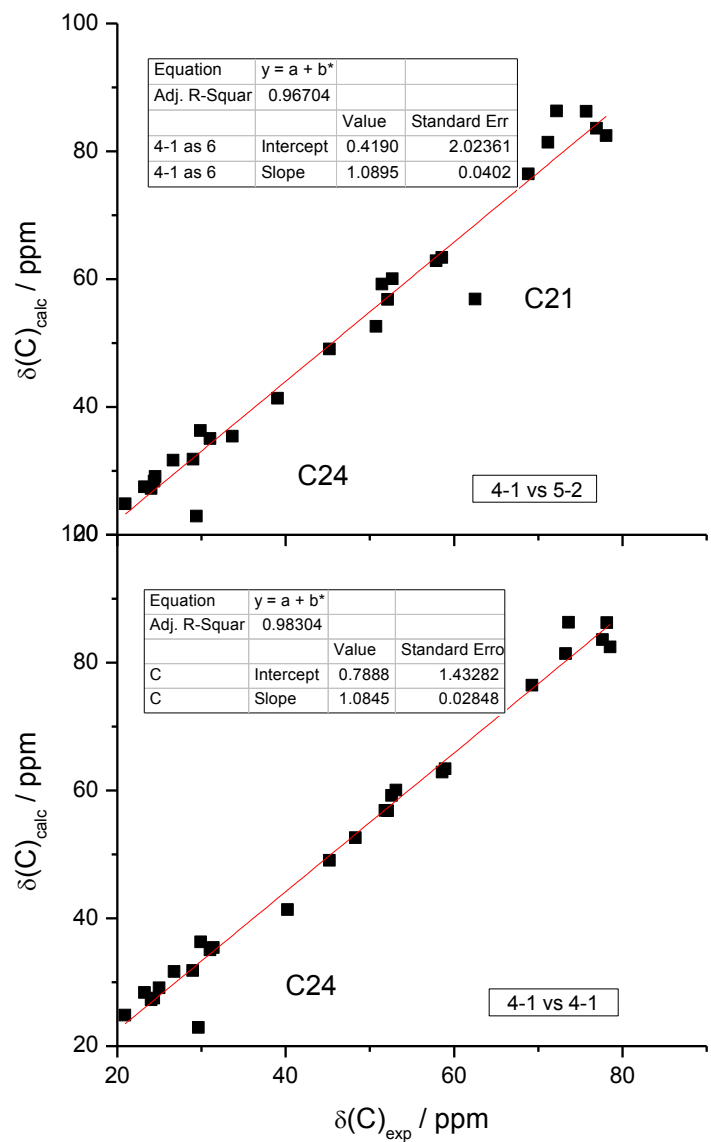
3. Correlation graphs

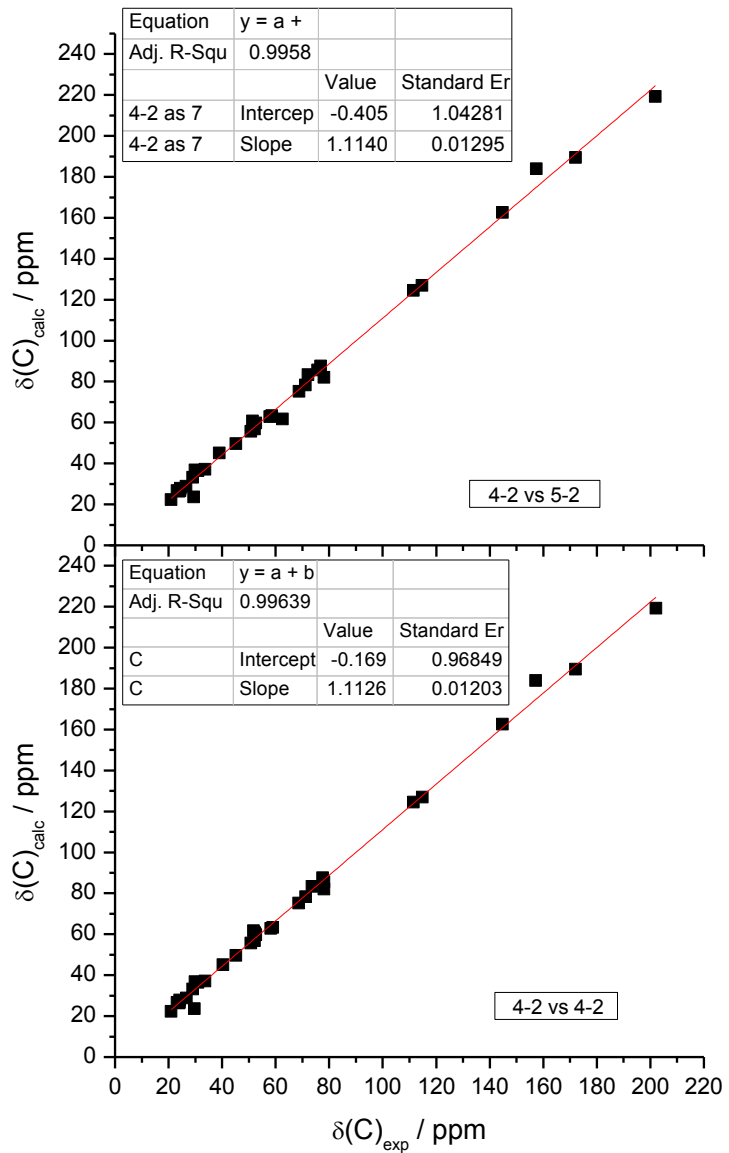
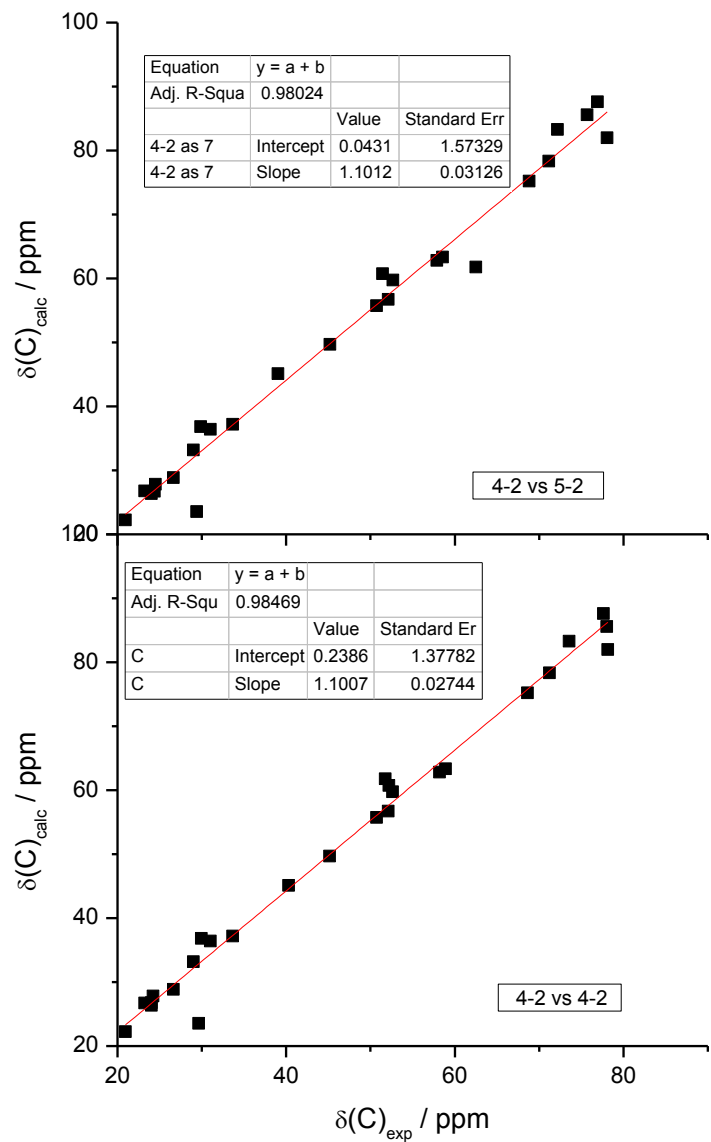


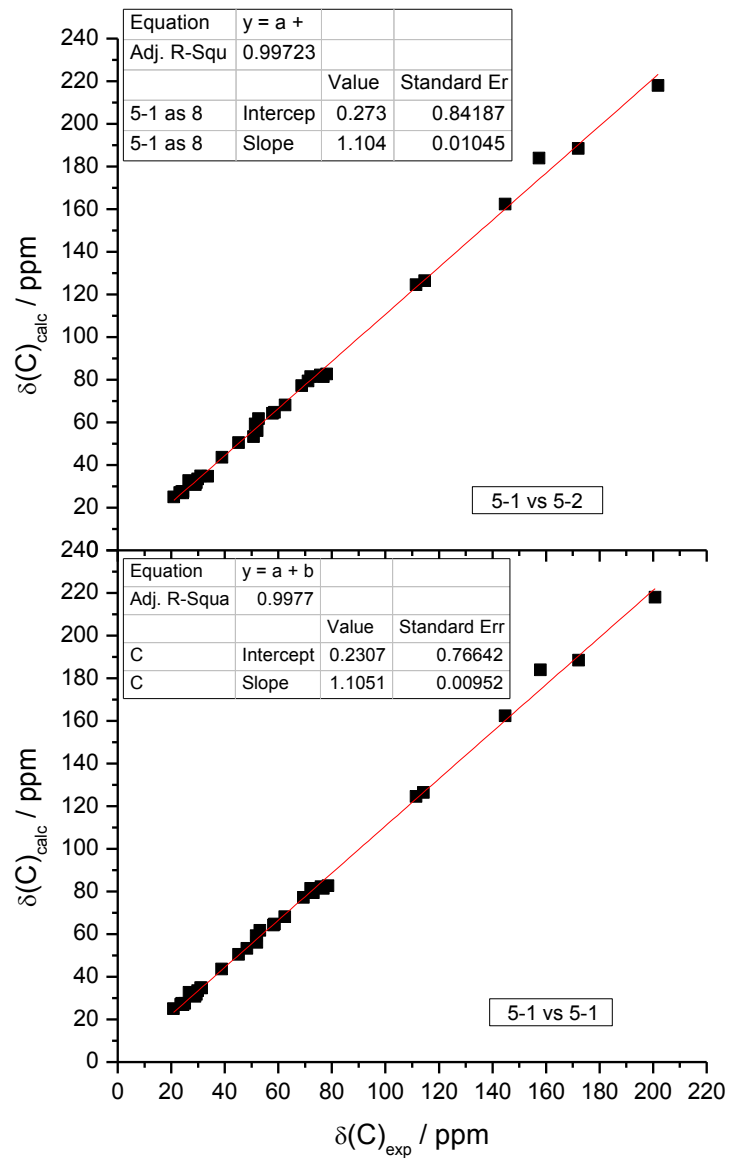
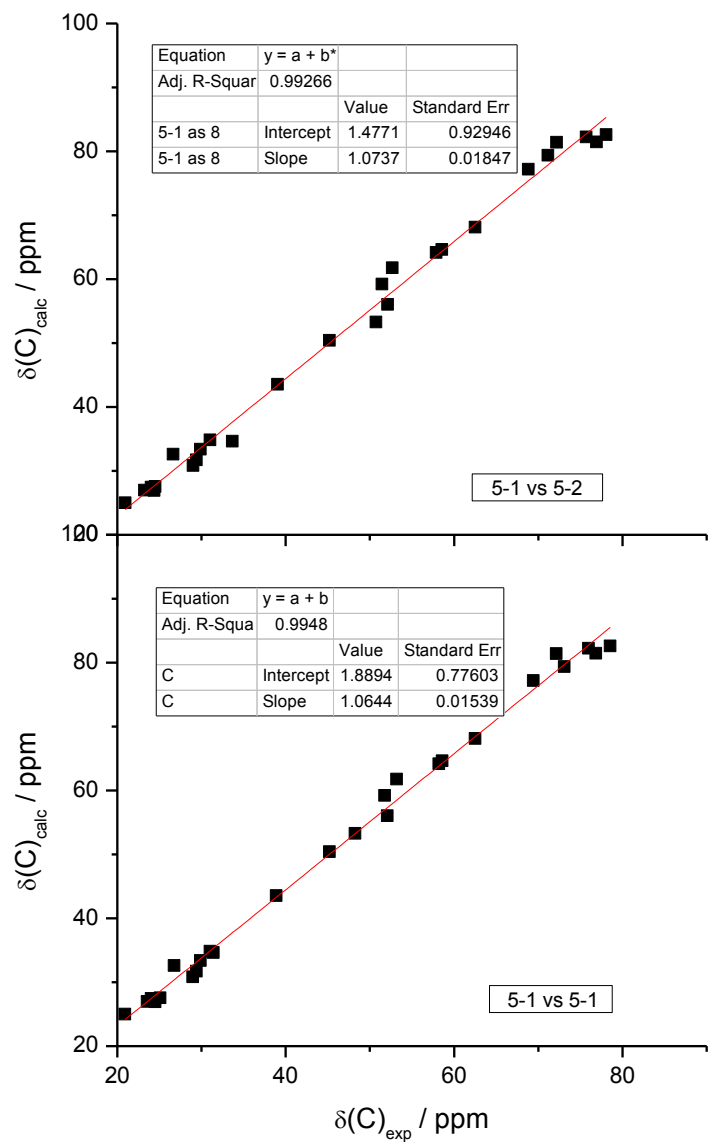


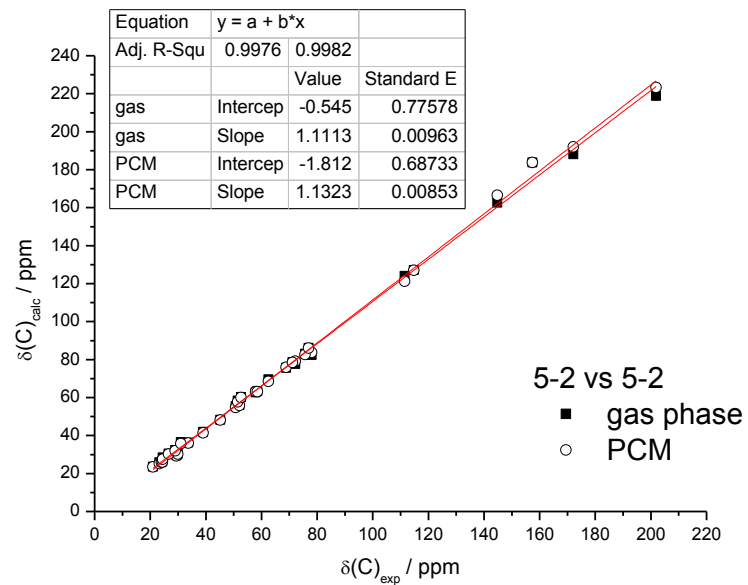
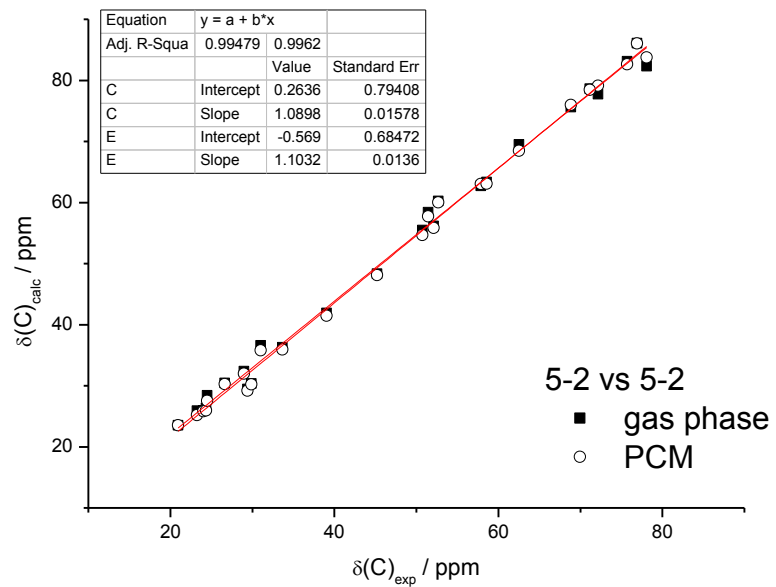












4. Cartesian coordinates and SCF energy in hartrees (B3LYP/6-31G**)

2-1 (E = -1773.687646)

C	4.806831	0.383485	-0.457304
C	3.291633	0.293500	-0.175979
C	3.063659	1.376635	0.918766
C	4.273242	2.347081	0.835734
C	5.070375	1.898047	-0.417159
C	2.753936	-1.118508	0.166405
C	1.225256	-1.149654	0.263664
C	0.656180	-2.010899	-0.858122
C	1.817258	-2.129573	-1.858743
C	3.049591	-2.171440	-0.940820
C	-0.758165	-1.645088	-1.419680
C	-1.448130	-0.594475	-0.524521
C	-1.076340	-0.663301	0.987901
C	0.432646	-0.561329	1.172050
C	-2.995472	-0.622851	-0.468774
C	-3.340959	0.206781	0.849397
C	-1.920450	0.588942	1.374039
C	-4.316971	1.417185	0.644877
C	-5.793908	0.850655	0.832804
C	-5.588791	-0.599772	1.331314
C	-4.150014	-0.643333	1.856026
C	-1.028010	0.868699	-0.861291
C	-1.271476	1.653657	0.460142
C	-4.070193	2.210587	-0.498603
O	-6.798743	0.960511	-0.340036
O	-6.243813	0.198686	-1.446238
C	-1.380511	-1.942103	1.733426
H	-1.294425	-1.852514	2.837519
O	-3.531612	-0.112590	-1.690464
O	-1.526359	-2.824386	-1.608646
C	6.500754	2.397353	-0.513712
C	7.521539	1.645261	-0.938456
O	5.514981	-0.244735	0.648229
C	6.354081	-1.272040	0.385375
C	7.023598	-1.745735	1.652820
C	6.697263	3.856198	-0.171755
O	6.552203	-1.733037	-0.719453
C	-8.140606	0.313296	0.047202
C	-7.042898	2.412022	-0.777327
H	0.518242	-3.008866	-0.413720
H	0.824441	-0.006997	2.020461
H	1.728213	-3.007713	-2.504144
H	1.847776	-1.246532	-2.511128
H	3.995467	-2.004836	-1.459300
H	3.115842	-3.163849	-0.478346
H	3.205617	-1.413636	1.120615
H	2.804004	0.628334	-1.101581
H	2.112329	1.892927	0.770454
H	3.021670	0.911076	1.908598
H	5.118540	-0.095511	-1.384365
H	4.539906	2.302593	-1.295131
H	4.904319	2.243764	1.723849
H	3.966621	3.394608	0.774631
H	7.591391	-2.652383	1.447039
H	7.697789	-0.964635	2.017852
H	6.281781	-1.930202	2.434125
H	8.517905	2.068620	-1.033151
H	7.413730	0.603609	-1.219198
H	6.038757	4.496273	-0.773855
H	6.456358	4.061992	0.877786
H	7.728759	4.170197	-0.350347
H	-1.665636	-3.190178	-0.716880
H	-0.648170	-1.218492	-2.422767
H	-3.334187	-1.656651	-0.351192
H	-1.920265	0.857108	2.437132
H	0.020296	0.908659	-1.166082
H	-1.622961	1.247392	-1.693315
H	-0.328337	1.994088	0.899457
H	-1.912521	2.522491	0.313304
H	-4.146910	2.089447	1.496192
H	-4.095716	-0.177667	2.849774
H	-3.791403	-1.669901	1.959806
H	-6.250487	1.436544	1.639873
H	-6.317657	-0.898638	2.090393
H	-5.693992	-1.297778	0.493107
O	-1.609165	-3.036856	1.238705
H	-4.494586	-0.275341	-1.700198

H	-3.889186	1.577908	-1.221417
H	-8.854350	0.404887	-0.780309
H	-8.023241	-0.748441	0.274474
H	-8.582735	0.809559	0.917065
H	-6.839309	0.286311	-2.201998
H	-7.758849	2.439869	-1.608683
H	-7.479954	2.987944	0.045338
H	-6.111592	2.887967	-1.079568

2-2 (E = -1773.686792)

C	-3.483022	-1.810661	0.085122
C	-3.687290	-0.401071	-0.536265
C	-5.181851	-0.122337	-0.273003
C	-5.837297	-1.474931	-0.596285
C	-4.883756	-2.486333	0.099381
C	-2.734207	0.718446	-0.077055
C	-1.253042	0.517703	-0.416065
C	-0.732960	1.744560	-1.160483
C	-1.736858	2.845477	-0.771369
C	-3.073704	2.097483	-0.710002
C	0.780677	2.100720	-1.005989
C	1.552146	0.989773	-0.274103
C	1.008672	-0.452135	-0.462938
C	-0.462735	-0.516534	-0.088054
C	1.503057	1.143006	1.272411
C	1.718800	-0.298520	1.807823
C	2.037349	-1.090834	0.519559
C	3.419391	-0.621143	-0.053491
C	3.027704	0.783691	-0.689436
C	3.997951	-1.531488	-1.169304
C	5.493336	-1.195653	-1.178428
C	5.842710	-1.258330	0.315141
C	4.574167	-0.655075	1.029202
C	0.986327	-1.000955	-1.873573
H	0.806105	-2.094725	-1.935521
H	0.859646	3.018870	-0.412152
O	-5.344336	0.138212	1.151036
C	-5.906640	1.301931	1.547624
O	-6.259120	2.186955	0.795708
C	-7.319199	-1.656517	-0.323409
C	-7.818530	-3.080557	-0.405234
C	-6.055626	1.333305	3.049610
C	-8.161726	-0.642352	-0.100619
H	-0.833811	-1.388864	0.441212
H	-1.478399	3.248257	0.217192
H	-1.738615	3.682029	-1.475866
H	-3.447388	1.943408	-1.731284
H	-3.854134	2.630975	-0.163816
H	-2.817933	0.799657	1.016035
H	-3.589014	-0.485731	-1.627605
H	-2.752415	-2.391167	-0.483540
H	-3.099722	-1.721370	1.106637
H	-5.585524	0.722941	-0.829627
H	-5.704779	-1.604506	-1.683065
H	-5.214072	-2.652029	1.129071
H	-4.883578	-3.457780	-0.401896
H	-6.357721	2.331568	3.364259
H	-6.819822	0.608825	3.348465
H	-5.121430	1.044863	3.537871
H	-9.223301	-0.826929	0.040204
H	-7.845806	0.394158	-0.064175
H	-7.559234	-3.535727	-1.370292
H	-7.368131	-3.713203	0.368675
H	-8.904324	-3.127348	-0.290793
O	1.365590	2.443450	-2.260637
O	1.054694	-0.344331	-2.902797
H	3.080768	0.684059	-1.775037
O	3.885104	1.869862	-0.329422
H	1.978490	-2.178426	0.637160
H	2.519521	-0.348892	2.546310
H	0.809947	-0.689335	2.275773
H	2.283136	1.831009	1.605502
H	0.542994	1.555095	1.593465
H	3.516629	-1.385385	-2.140036
H	3.865269	-2.587744	-0.896421
H	5.663620	-0.180048	-1.555778
H	6.076027	-1.887143	-1.793582
H	5.859369	-2.323473	0.589696
C	7.222982	-0.685658	0.738458
O	4.780955	0.574321	1.730565
H	4.269961	-1.363533	1.807611
H	-0.869007	1.539302	-2.233723
H	1.326698	1.629709	-2.795753

H	3.645366	2.617056	-0.896040
H	4.560345	1.300190	1.117030
C	8.342452	-1.294491	-0.113755
O	7.287379	0.722359	0.494284
C	7.493956	-0.972117	2.228311
H	6.607287	1.097971	1.074204
H	9.310346	-0.921761	0.234011
H	8.346290	-2.387301	-0.046152
H	8.231136	-1.007484	-1.162275
H	8.464774	-0.552258	2.508606
H	6.728760	-0.515821	2.861586
H	7.514140	-2.049000	2.431265

H	-3.733679	-0.863793	2.554751
H	-4.273672	-1.958704	1.297438
C	-7.001393	1.358954	0.066321
H	-5.701856	0.453873	2.424160
H	-6.398694	-1.048954	1.827278
H	-3.257106	-1.558928	-2.500405
H	-4.106462	0.875397	-1.844569
H	-5.925123	-0.389006	-0.511890
C	-8.327768	0.615860	0.259171
C	-6.948646	2.588659	0.992421
O	-7.012773	1.803074	-1.295858
H	-6.096546	2.052865	-1.507863
H	-9.156005	1.272595	-0.022898
H	-8.366342	-0.269556	-0.382791
H	-8.471260	0.304376	1.298323
H	-7.817000	3.221254	0.788612
H	-6.966114	2.317133	2.053505
H	-6.054374	3.191714	0.806503

3-1 (E = -1773.691561)

C	-1.450325	1.500296	0.089302
C	-2.040916	0.454568	1.059190
C	-1.060365	-0.736333	0.827025
C	-1.352258	-0.823691	-0.697499
C	-1.087963	0.640334	-1.151401
C	0.423193	-0.507256	1.072657
C	1.297649	-1.144682	0.278233
C	0.837496	-2.147442	-0.776600
C	-0.517608	-1.852448	-1.486502
C	2.077534	-2.352276	-1.662380
C	3.234227	-2.233552	-0.657439
C	2.825654	-1.056203	0.274977
C	-3.393976	-0.103868	0.493428
C	-2.882311	-1.053259	-0.665103
C	-4.214362	-0.901417	1.570807
C	-5.637286	-0.291734	1.622938
C	-5.806150	0.387081	0.257872
C	-4.409464	1.009475	0.062401
C	3.335523	0.319670	-0.222298
C	4.865180	0.441367	-0.389545
C	5.071242	1.957006	-0.545973
C	4.149900	2.540544	0.557659
C	2.975309	1.532104	0.685287
O	5.495566	0.009854	0.848673
C	6.376776	-1.015819	0.807519
O	6.668632	-1.630676	-0.196985
C	6.487938	2.500670	-0.592800
C	6.607548	4.000597	-0.453852
O	-1.231378	-3.060772	-1.749129
C	-1.318295	-1.989359	1.638713
O	-1.475834	-3.115147	1.188877
O	-3.536347	-0.836422	-1.919437
O	-4.206561	1.612541	-1.214199
C	7.565625	1.740725	-0.814258
C	6.961644	-1.267109	2.176166
H	-1.267626	-1.842103	2.737865
H	0.668936	-3.090087	-0.232641
H	0.736549	0.152392	1.877178
H	2.062333	-3.306590	-2.195572
H	2.138493	-1.557062	-2.417236
H	4.213224	-2.101801	-1.121279
H	3.289731	-3.154503	-0.064310
H	3.218923	-1.200346	1.287658
H	2.916972	0.498782	-1.222117
H	2.019880	1.974181	0.392445
H	2.870145	1.207605	1.725425
H	5.274127	-0.147293	-1.209453
H	4.608696	2.209215	-1.514660
H	4.703474	2.599044	1.499808
H	3.809745	3.551155	0.317201
H	7.543988	-2.187625	2.159233
H	7.610389	-0.428604	2.448549
H	6.171675	-1.328714	2.928854
H	8.552907	2.189020	-0.885328
H	7.516276	0.665828	-0.947482
H	5.989559	4.518026	-1.199596
H	6.264370	4.345671	0.528584
H	7.641390	4.329490	-0.585408
H	-1.417121	-3.447646	-0.875414
H	-0.312028	-1.438641	-2.480533
H	-3.075363	-2.086784	-0.375631
H	-2.132848	0.806932	2.092259
H	-0.043372	0.771983	-1.445410
H	-1.707601	0.880251	-2.017845
H	-0.559895	1.959078	0.531196
H	-2.153021	2.297891	-0.151580
H	-4.299230	1.832604	0.780934

3-2 (E = -1773.677476)

C	4.620951	-0.567545	0.922870
C	3.421300	-0.529674	-0.074030
C	4.013546	-1.454999	-1.172713
C	5.515366	-1.091096	-1.283186
C	5.875882	-0.379607	0.046462
C	3.034492	0.887661	-0.664663
C	1.547908	1.051531	-0.254991
C	1.020288	-0.385913	-0.507933
C	2.044605	-1.052833	0.464780
C	-0.453210	-0.484796	-0.146791
C	-1.253306	0.558301	-0.417301
C	-0.747921	1.827567	-1.095504
C	0.766729	2.183117	-0.942406
C	-1.755031	2.897624	-0.635326
C	-3.087182	2.138604	-0.608480
C	-2.734590	0.727529	-0.059647
C	1.657862	-0.378229	1.770074
C	1.505433	1.143119	1.300746
C	-3.682988	-0.371257	-0.574767
C	-3.457989	-1.812997	-0.038781
C	-4.852849	-2.500093	-0.038751
C	-5.823488	-1.462904	-0.668940
C	-5.177149	-0.122868	-0.280710
O	-5.326987	0.059905	1.156730
C	-5.897844	1.194595	1.619739
C	-6.030032	1.145847	3.122869
C	-7.300440	-1.673749	-0.389069
C	-8.150589	-0.680532	-0.108480
O	1.334264	2.565443	-2.192860
C	1.015236	-0.885689	-1.936273
O	1.075835	-0.195111	-2.943083
O	3.864456	1.955621	-0.236809
O	4.656512	0.387714	1.992631
O	-6.269143	2.113411	0.919273
C	-7.785884	-3.097588	-0.533354
H	0.853221	-1.979972	-2.035646
H	0.850435	3.082113	-0.320994
H	-0.818520	-1.389066	0.330773
H	-1.491321	3.244218	0.372976
H	-1.767368	3.773643	-1.290062
H	-3.467057	2.042583	-1.634627
H	-3.866998	2.634159	-0.026673
H	-2.810985	0.744707	1.036847
H	-3.595619	-0.391011	-1.670105
H	-2.733272	-2.353329	-0.652774
H	-3.056908	-1.779652	0.979284
H	-5.595166	0.746640	-0.787161
H	-5.702084	-1.533133	-1.762503
H	-5.167148	-2.719337	0.985991
H	-4.852703	-3.445477	-0.587649
H	-6.338909	2.122987	3.492478
H	-6.783248	0.398451	3.391671
H	-5.087341	0.842829	3.585309
H	-9.208523	-0.882859	0.035259
H	-7.844422	0.356216	-0.025451
H	-7.531107	-3.503878	-1.521128
H	-7.321466	-3.761097	0.205674
H	-8.869961	-3.161467	-0.411094
H	3.090167	0.822045	-1.755252
H	2.000664	-2.145777	0.530830
H	2.384334	-0.460495	2.574028

H	0.710487	-0.724607	2.149011	H	7.576375	-0.293982	2.509159
H	2.328967	1.774849	1.640666	H	6.146473	-1.194356	3.014092
H	0.568585	1.583153	1.652956	H	8.557131	2.115486	-0.996142
H	3.498035	-1.366865	-2.132320	H	7.521948	0.590061	-0.964025
H	3.907928	-2.499013	-0.851047	H	5.993054	4.416192	-1.467049
H	5.699393	-0.428250	-2.133409	H	6.261228	4.355205	0.269426
H	6.116653	-1.988936	-1.452997	H	7.642892	4.269372	-0.835773
C	7.219865	-0.775123	0.714400	H	-1.435454	-3.460222	-0.735119
H	4.621844	-1.580059	1.354773	H	-0.286131	-1.566772	-2.444292
H	-0.896228	1.682013	-2.176897	H	-3.111665	-2.048158	-0.377758
H	1.309102	1.763680	-2.746538	H	-2.139930	0.935632	1.986764
H	3.654500	2.692304	-0.831014	H	0.000749	0.699268	-1.522675
H	4.205618	0.012289	2.757590	H	-1.658203	0.785301	-2.114967
H	5.939518	0.698316	-0.134156	H	-0.507559	1.971223	0.398258
O	7.453185	0.082244	1.840434	H	-2.088884	2.327139	-0.282255
C	7.260972	-2.237190	1.196956	O	-4.317292	2.169480	0.737236
C	8.383514	-0.510588	-0.250165	H	-4.412419	-0.054874	2.294371
H	6.582919	0.356169	2.174353	H	-3.901364	-1.673161	1.794126
H	8.246186	-2.446750	1.623070	H	-6.472506	-0.969063	1.394109
H	6.523464	-2.416959	1.985451	H	-5.628003	-1.800652	0.101879
H	7.081699	-2.952975	0.386696	H	-3.215757	-1.589830	-2.515590
H	9.330312	-0.646491	0.281022	H	-5.815957	-0.012641	-1.275606
H	8.369812	-1.188668	-1.109341	H	-6.528096	2.421613	-1.577113
H	8.346794	0.520600	-0.613817	H	-9.073913	1.350592	-0.519424
				H	-8.065605	0.557458	-1.747980
				H	-8.448242	-0.288738	-0.244595
				H	-8.008323	2.417873	1.487354
				H	-7.645555	0.760879	1.985461
				H	-6.353374	1.975906	1.963172
				H	-4.986726	2.780993	0.385350

4-1 (E = -1773.685666)

C	2.974475	1.551753	0.594237
C	3.336962	0.288544	-0.239505
C	4.867243	0.398702	-0.406699
C	5.074475	1.902136	-0.653530
C	4.149510	2.551293	0.410027
C	2.819510	-1.055390	0.331558
C	1.291045	-1.138988	0.322895
C	0.838900	-2.188428	-0.689213
C	2.089838	-2.446109	-1.545036
C	3.233089	-2.283027	-0.530409
C	-0.505974	-1.921636	-1.430529
C	-1.338294	-0.843757	-0.708195
C	-1.072755	-0.686964	0.814354
C	0.409704	-0.461984	1.075471
C	-1.047303	0.593410	-1.229282
C	-1.405726	1.515994	-0.031794
C	-2.034671	0.531363	0.977079
C	-2.877004	-1.032462	-0.707854
C	-3.378994	-0.018106	0.395477
C	-4.342521	1.060090	-0.162029
C	-5.736727	0.354850	-0.246311
C	-5.635040	-0.881783	0.697230
C	-4.291824	-0.718104	1.430715
C	-1.361244	-1.893480	1.681163
O	-1.501340	-3.044009	1.290137
O	-1.225310	-3.138261	-1.629693
O	-3.478871	-0.825030	-1.982977
C	-6.959595	1.289773	-0.016028
O	-6.685753	2.579802	-0.635173
H	-4.034626	1.388760	-1.161268
O	5.492344	0.042660	0.858273
C	6.374016	-0.982502	0.883184
C	6.945684	-1.155835	2.269539
C	6.490867	2.442512	-0.730370
C	7.570057	1.671323	-0.899795
O	6.675615	-1.653491	-0.081893
C	6.608815	3.948333	-0.687442
C	-8.213013	0.692400	-0.669779
C	-7.251443	1.628814	1.451519
H	-1.356232	-1.684641	2.771855
H	0.655768	-3.102021	-0.102643
H	0.715441	0.233270	1.852773
H	2.075748	-3.426805	-2.028218
H	2.168001	-1.691854	-2.339390
H	4.219999	-2.182933	-0.985632
H	3.271484	-3.171615	0.111479
H	3.203064	-1.143190	1.354463
H	2.924717	0.411420	-1.250473
H	2.019543	1.975304	0.274040
H	2.866355	1.288712	1.651183
H	5.279997	-0.238469	-1.187554
H	4.614591	2.095002	-1.637057
H	4.699819	2.666631	1.348884
H	3.810127	3.545524	0.107890
H	7.542502	-2.066477	2.305338

4-2 (E = -1773.679401)

C	-5.177221	-0.087324	-0.292402
C	-3.679156	-0.311401	-0.586214
C	-3.453712	-1.783158	-0.139659
C	-4.845154	-2.474232	-0.199431
C	-5.813702	-1.430236	-0.772021
C	-2.739542	0.756136	0.005084
C	-1.255775	0.614302	-0.354951
C	-0.747844	1.928472	-0.939825
C	-1.765241	2.961702	-0.421813
C	-3.093817	2.197140	-0.457423
C	0.762021	2.280387	-0.737210
C	1.546392	1.095961	-0.146327
C	1.016930	-0.315945	-0.515897
C	-0.454004	-0.443427	-0.156312
C	2.049327	-1.064730	0.381729
C	3.416798	-0.514252	-0.147320
C	3.032441	0.964086	-0.565695
C	3.991261	-1.337328	-1.356995
C	5.534361	-1.423452	-1.166246
C	5.833307	-0.447369	-0.009564
C	4.582548	-0.577429	0.882236
C	1.727681	-0.441544	1.757017
C	1.497472	1.054446	1.408349
H	4.539023	0.218315	1.623342
C	7.223190	-0.501066	0.673447
C	8.317618	-0.129204	-0.343434
O	3.877745	1.951624	0.022763
C	1.015005	-0.688959	-1.982557
O	1.113507	0.082230	-2.926129
O	1.337540	2.783859	-1.940543
C	-7.292391	-1.635901	-0.520988
C	-7.770359	-3.050120	-0.755709
O	-5.343398	0.002565	1.151953
C	-5.921221	1.104403	1.680510
O	-6.287254	2.065661	1.036316
C	-6.067309	0.959591	3.176131
C	-8.149657	-0.664920	-0.188800
O	7.235920	0.461607	1.743598
C	7.567869	-1.832958	1.347556
H	0.825955	-1.765777	-2.178176
H	0.828591	3.118921	-0.033955
H	-0.815257	-1.377324	0.263372
H	-1.513291	3.241261	0.610067
H	-1.775267	3.879104	-1.017278
H	-3.462390	2.164018	-1.491723
H	-3.882093	2.651956	0.146044
H	-2.823784	0.703988	1.099954
H	-3.581602	-0.261435	-1.679893
H	-2.719699	-2.280856	-0.778061

H	-3.063742	-1.811625	0.882722
H	-5.593364	0.811378	-0.746821
H	-5.680580	-1.401824	-1.866441
H	-5.169395	-2.760917	0.805355
H	-4.834721	-3.382030	-0.808432
H	-6.395096	1.906802	3.602891
H	-6.810000	0.184556	3.390166
H	-5.123804	0.643485	3.628218
H	-9.208001	-0.879720	-0.067897
H	-7.848656	0.365863	-0.039048
H	-7.504918	-3.395692	-1.763656
H	-7.310081	-3.755324	-0.053643
H	-8.855257	-3.125099	-0.647688
H	3.104903	1.055120	-1.651899
H	1.991820	-2.156855	0.368874
H	2.526594	-0.611057	2.478185
H	0.819254	-0.893265	2.168465
H	2.272911	1.710079	1.811400
H	0.534325	1.412419	1.781829
H	3.742736	-0.867969	-2.312269
H	3.549915	-2.340682	-1.386931
H	6.076735	-1.167659	-2.080194
H	5.837640	-2.446016	-0.908295
O	4.530461	-1.794144	1.637923
H	-0.877949	1.855772	-2.030823
H	1.324859	2.037018	-2.566314
H	3.663576	2.779125	-0.431524
H	5.756981	0.566460	-0.426736
H	6.954037	1.310213	1.373566
H	8.554992	-1.754321	1.812656
H	6.833367	-2.071148	2.116642
H	7.603395	-2.649540	0.619243
H	9.282779	-0.056989	0.166099
H	8.405263	-0.872747	-1.142620
H	8.105994	0.840400	-0.810476
H	4.668411	-2.535020	1.033058

5-1 (E = -1773.683527)

C	-1.311226	1.643896	0.273794
C	-1.947126	0.631351	1.255987
C	-1.089454	-0.631865	0.949667
C	-1.437860	-0.655769	-0.568368
C	-1.017443	0.784149	-0.987930
C	0.415794	-0.505720	1.150634
C	1.224959	-1.145982	0.293528
C	0.675465	-2.082351	-0.776450
C	-0.728312	-1.754004	-1.387487
C	1.854949	-2.272716	-1.744017
C	3.070825	-2.244880	-0.803093
C	2.754214	-1.111950	0.215492
C	-3.355724	0.200018	0.745692
C	-2.989399	-0.669882	-0.551553
C	-4.171714	-0.629422	1.768753
C	-5.596561	-0.621940	1.205067
C	-5.784110	0.815716	0.664856
C	-4.333587	1.362858	0.426111
C	3.289791	0.270950	-0.232621
C	4.811241	0.350197	-0.480944
C	5.062852	1.864586	-0.570816
C	4.224610	2.419903	0.611216
C	3.026679	1.442143	0.757770
O	5.493250	-0.169419	0.695225
C	6.340091	-1.213207	0.549223
O	6.571962	-1.769352	-0.504090
C	6.491967	2.366458	-0.670759
C	6.667700	3.853145	-0.464646
O	-1.487128	-2.946708	-1.524825
C	-1.392616	-1.868246	1.764283
O	-1.599737	-2.993401	1.331906
O	-3.467609	-0.173173	-1.785784
H	-4.185256	1.695420	-0.604839
C	-6.773942	0.933280	-0.516096
C	-6.882222	2.376551	-1.031822
O	-6.254752	0.086973	-1.570029
C	-8.164521	0.415175	-0.117806
C	7.531285	1.587735	-0.989063
C	6.972103	-1.571094	1.872839
H	-1.326764	-1.712571	2.862556
H	0.526235	-3.046497	-0.266216
H	0.790926	0.105539	1.967056
H	1.777740	-3.196108	-2.324566
H	1.897763	-1.440328	-2.459215
H	4.026123	-2.115692	-1.315219

H	3.128868	-3.199829	-0.266581
H	3.194441	-1.327571	1.195968
H	2.824294	0.520215	-1.195901
H	2.070517	1.927574	0.549122
H	2.973599	1.063645	1.783411
H	5.152775	-0.206535	-1.352327
H	4.556578	2.181938	-1.497542
H	4.831772	2.415719	1.521787
H	3.905210	3.451150	0.438870
H	7.546627	-2.490295	1.764334
H	7.634461	-0.758616	2.187599
H	6.207533	-1.688953	2.645016
H	8.527072	2.010487	-1.092555
H	7.440070	0.523046	-1.172103
H	6.024975	4.426086	-1.146220
H	6.391735	4.156601	0.552152
H	7.702429	4.158532	-0.639694
H	-1.650733	-3.255389	-0.615882
H	-0.598368	-1.385413	-2.4111038
H	-3.343534	-1.696734	-0.405593
H	-1.952981	0.970778	2.295551
H	0.040583	0.816994	-1.258841
H	-1.595581	1.094695	-1.858469
H	-0.389206	2.049568	0.703293
H	-1.972803	2.489466	0.086129
O	-4.060046	2.439507	1.338271
H	-4.149818	-0.121681	2.741644
H	-3.803359	-1.646973	1.916009
H	-6.195214	1.436201	1.470427
H	-6.346413	-0.892957	1.954340
H	-5.680434	-1.344132	0.385887
H	-4.438529	-0.241069	-1.799066
H	-8.857862	0.488738	-0.964304
H	-8.118304	-0.631319	0.191248
H	-8.584475	1.003034	0.704661
H	-6.837250	0.155446	-2.338054
H	-7.598320	2.436418	-1.860061
H	-7.240636	3.049025	-0.245075
H	-5.920036	2.743683	-1.397842
H	-4.586227	3.198765	1.056107

5-2 (E = -1773.688368)

C	4.592202	-0.780871	1.136048
C	3.418809	-0.804300	0.113743
C	3.960274	-1.790189	-0.952727
C	5.433552	-1.397970	-1.105818
C	5.903747	-1.096746	0.336093
C	3.108543	0.609474	-0.527945
C	1.625953	0.871624	-0.167897
C	1.037089	-0.555513	-0.324659
C	2.021755	-1.203000	0.698605
C	-0.443319	-0.559352	0.021243
C	-1.191583	0.488610	-0.357195
C	-0.614458	1.675759	-1.122209
C	0.907645	1.986018	-0.948391
C	-1.586874	2.819976	-0.781201
C	-2.950400	2.120403	-0.734386
C	-2.674766	0.743114	-0.066577
C	1.712088	-0.357038	1.953103
C	1.546872	1.073672	1.372500
C	-3.646516	-0.353659	-0.541919
C	-3.511302	-1.759125	0.106161
C	-4.931305	-2.392496	0.068462
C	-5.825817	-1.358481	-0.671548
C	-5.139912	-0.023911	-0.337344
O	-5.345748	0.256684	1.077621
C	-5.881384	1.442396	1.443321
C	-6.080149	1.494109	2.939088
C	-7.321334	-1.491774	-0.452261
C	-8.139130	-0.451532	-0.259214
O	1.523806	2.273195	-2.200862
C	1.020870	-1.140451	-1.720327
O	1.135788	-0.515617	-2.765351
O	3.975188	1.658584	-0.070984
C	7.058736	-0.057399	0.427568
C	7.397748	0.271694	1.895244
H	4.639030	0.185373	1.647354
O	-6.178216	2.330930	0.671686
C	-7.863003	-2.899359	-0.551807
C	8.312518	-0.609480	-0.265660
O	6.745395	1.145527	-0.272475
H	0.797728	-2.227456	-1.756671
H	1.005020	2.918152	-0.379285

H	-0.855396	-1.402499	0.567477
H	-1.335988	3.235963	0.203876
H	-1.543203	3.639490	-1.504196
H	-3.305966	1.958836	-1.760978
H	-3.723636	2.692326	-0.217432
H	-2.792412	0.844726	1.021597
H	-3.512009	-0.458515	-1.627688
H	-2.774189	-2.368969	-0.421857
H	-3.169719	-1.665744	1.142009
H	-5.495488	0.827817	-0.916323
H	-5.657350	-1.503440	-1.751354
H	-5.307429	-2.540469	1.085022
H	-4.940586	-3.367149	-0.426449
H	-6.364628	2.503601	3.233700
H	-6.873254	0.793601	3.219088
H	-5.170947	1.185623	3.461225
H	-9.210283	-0.603039	-0.156150
H	-7.792963	0.574821	-0.212139
H	-7.586294	-3.362743	-1.508116
H	-7.459530	-3.546316	0.236068
H	-8.952984	-2.911030	-0.473925
H	3.216289	0.535942	-1.612522
H	1.920116	-2.279699	0.854042
H	2.499411	-0.444730	2.700300
H	0.782501	-0.702681	2.416679
H	2.334807	1.759240	1.692989
H	0.589408	1.517284	1.657525
H	3.421289	-1.758956	-1.903620
H	3.882025	-2.810449	-0.557416
H	5.532263	-0.490695	-1.711745
H	6.026267	-2.178789	-1.590728
H	6.284561	-2.027471	0.775861
O	4.336848	-1.819721	2.096029
H	-0.737364	1.446978	-2.192193
H	1.471562	1.443857	-2.710129
H	3.803829	2.411271	-0.656841
H	5.825398	1.396086	-0.071685
H	9.107977	0.140661	-0.231808
H	8.671690	-1.519991	0.224987
H	8.109327	-0.833053	-1.315796
H	8.245610	0.961785	1.928243
H	6.560619	0.759504	2.404393
H	7.669099	-0.628058	2.461483
H	5.078427	-1.822905	2.715249