Conformational Equilibrium of Cinchonidine in C_6D_{12} Solution. An Alternative NMR/DFT Approach

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Supporting Information

Content

1. Mathematical formulation of δ/σ dependence

The results of correlation analysis reported in rows 7, 8, 11 and 12 of Table 3 were obtained assuming the following functional relationship between the chemical shift, δ_{calc}, of a given nucleus and isotropic shielding constants, σ, calculated theoretically for this nucleus in particular cinchonidine conformers:

$$\delta_{calc} = s(\sigma_{ref} - \Sigma_c \Sigma_v p_c p_v \sigma_{av(c,v)})$$

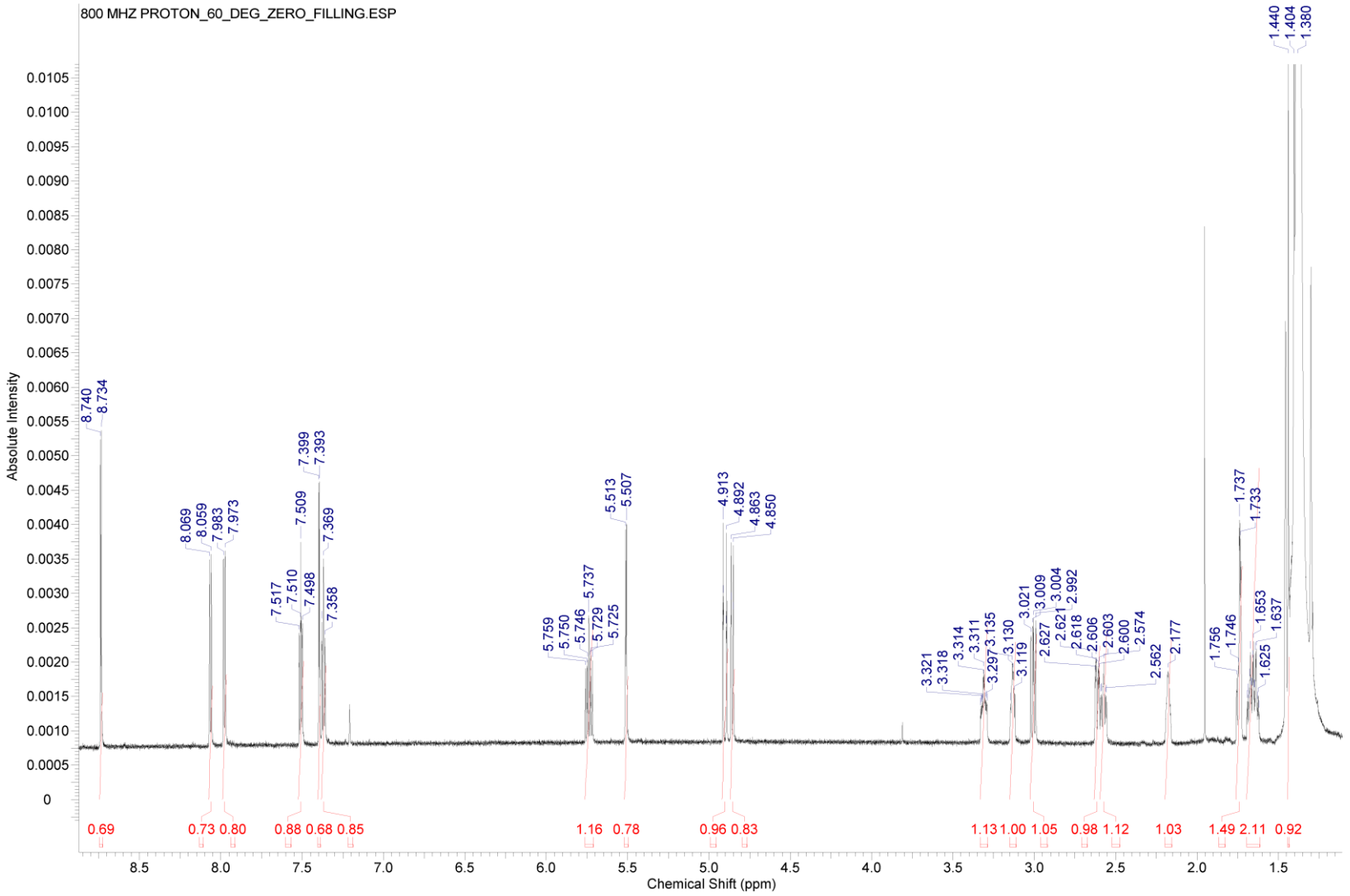
With constrains:

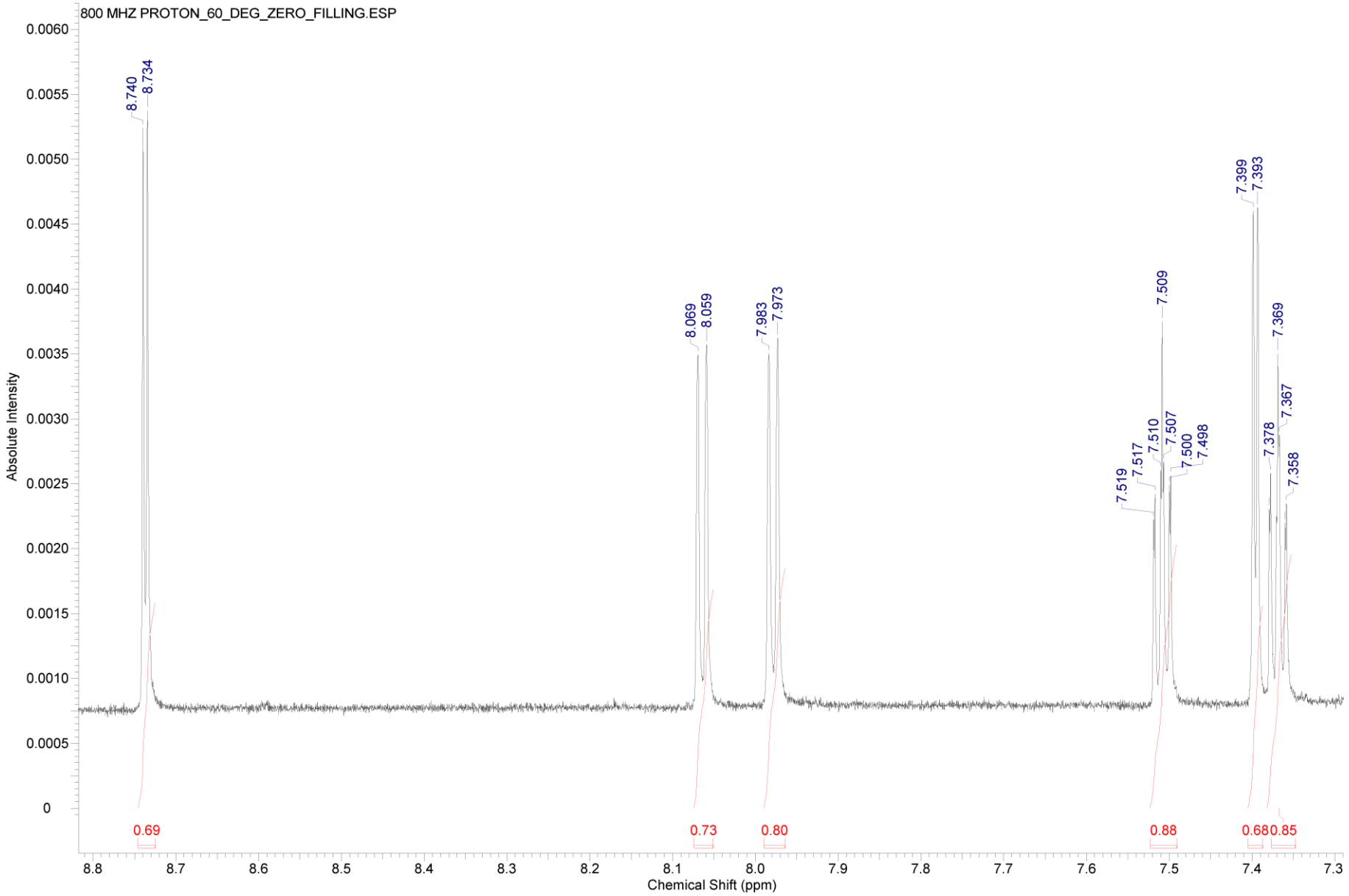
$$\Sigma_c p_c = 1$$
$$\Sigma_v p_v = 1$$

The parameters p_c and p_v denoted populations of the skeletal conformers and populations of particular orientations of the vinyl group, respectively, whereas $\sigma_{av(c,v)}$ were weighted mean values of the shielding constants for c,v-th group of conformers calculated using appropriately normalized Boltzmann factors as the weights. Seven parameters: s, σ_{ref}, three of p_c, and two of p_v were adjusted using non-linear least-squares algorithm.

2. NMR spectra of cinchonidine in C_6D_{12} at 60°C.

2.1. 18.8 T ^{1}H NMR spectrum.

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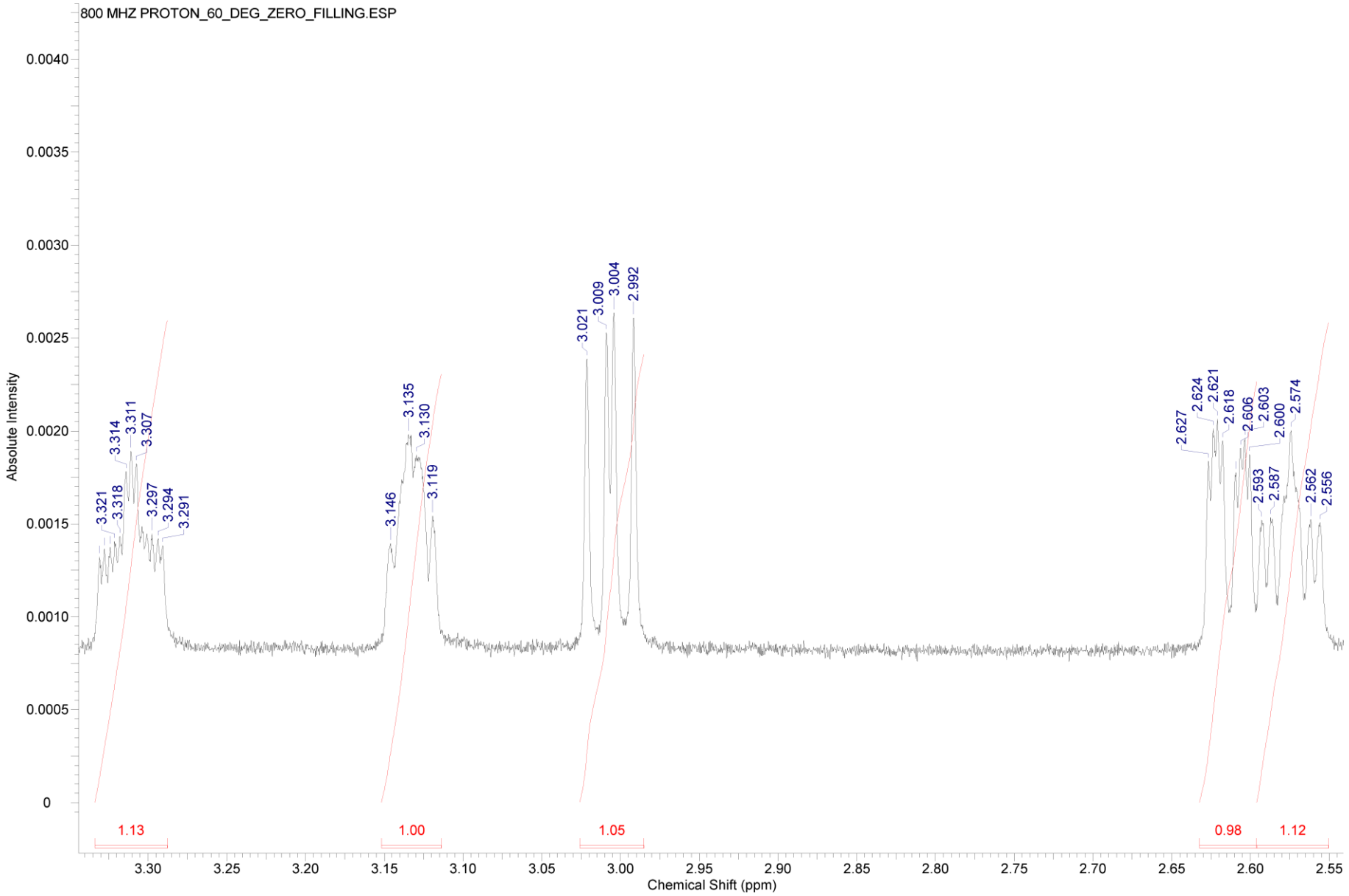
Absolute Intensity
Chemical Shift (ppm)
8.740
8.734
8.069
8.059
7.983
7.973
7.519
7.517
7.510
7.509
7.507
7.500
7.498
7.399
7.393
7.378
7.369
7.367
7.358
0.69
0.73
0.80
0.88
0.68
0.85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Absolute Intensity
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0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0
3.321
3.318
3.314
3.311
3.307
3.297
3.294
3.291
3.146
3.135
3.130
3.119
3.021
3.009
3.004
2.992
2.627
2.624
2.621
2.618
2.606
2.603
2.600
2.593
2.587
2.574
2.562
2.556
1.13
1.00
1.05
0.98
1.12
3.30
3.25
3.20
3.15
3.10
3.05
3.00
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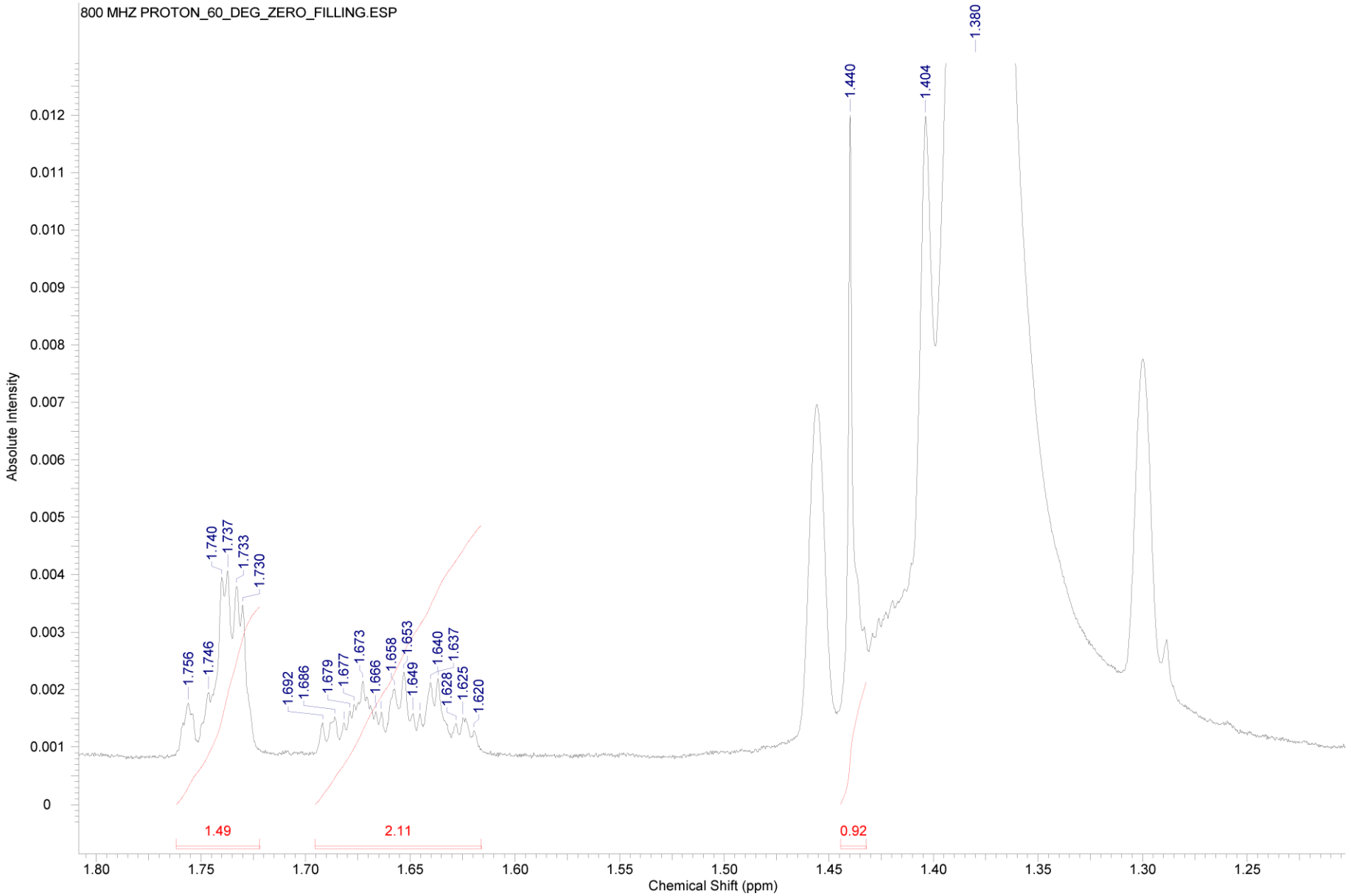
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
Chemical Shift (ppm)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Absolute Intensity
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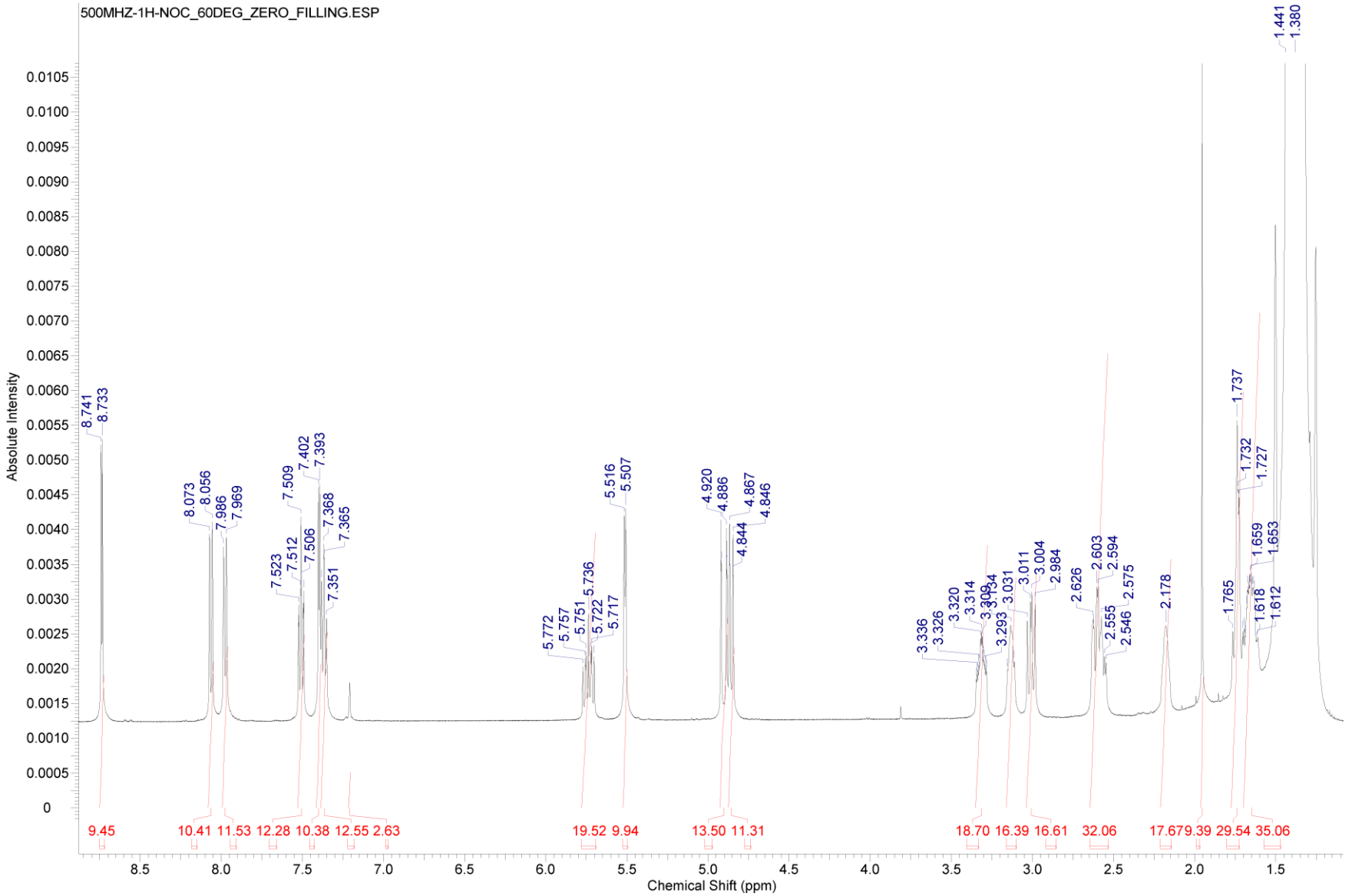
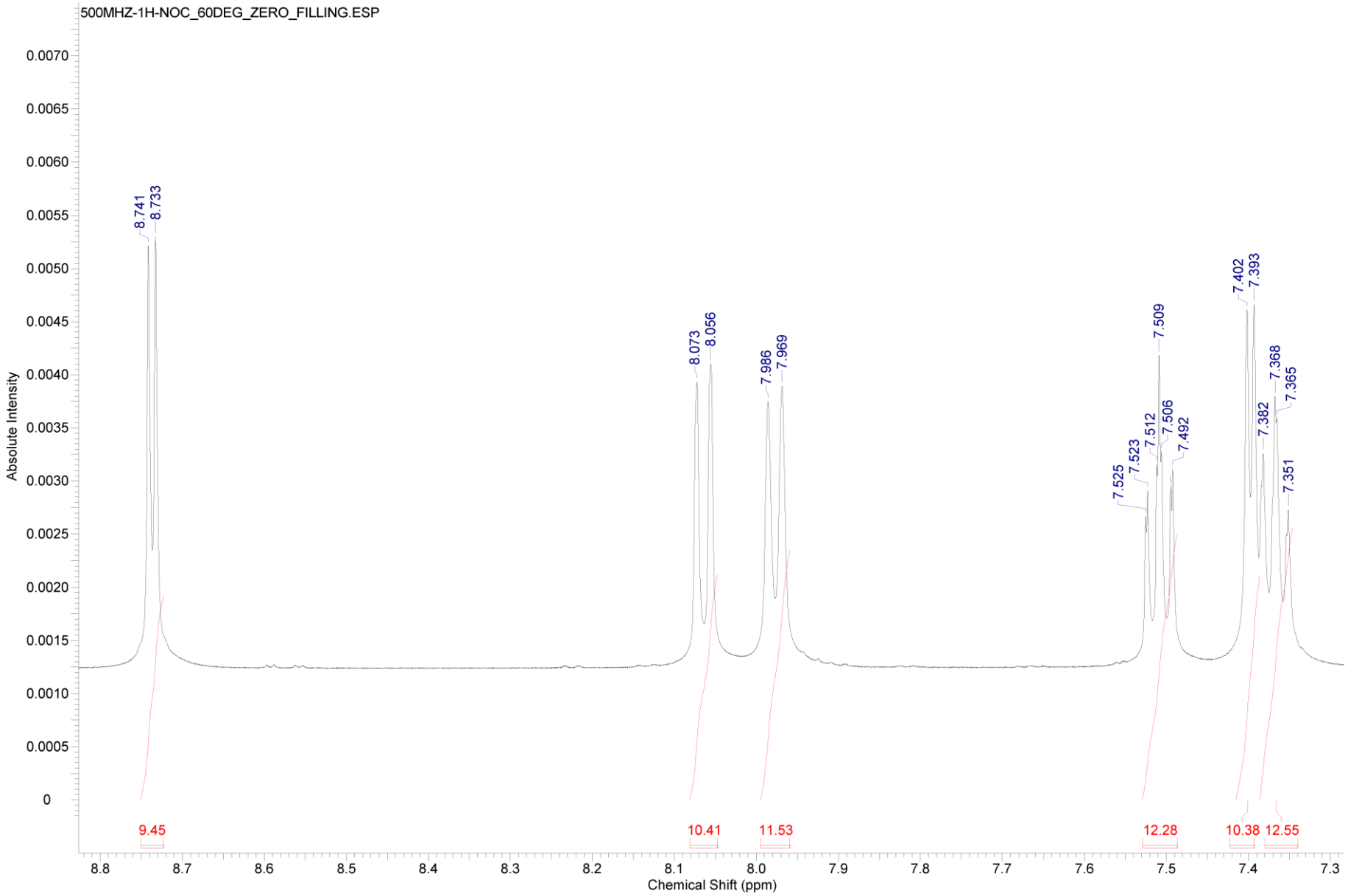
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
1.380
1.440
1.404
1.740
1.737
1.733
1.730
1.756
1.746
1.692
1.686
1.679
1.677
1.673
1.666
1.658
1.653
1.649
1.640
1.637
1.628
1.625
1.620
1.49
2.11
0.92
1.80
1.75
1.70
1.65
1.60
1.55
1.50
1.45
1.40
1.35
1.30
1.25
Chemical Shift (ppm)

2.2. 11.7 T ^{1}H NMR spectrum.




500MHZ-1H-NOC_60DEG_ZERO_FILLING.ESP
Absolute Intensity
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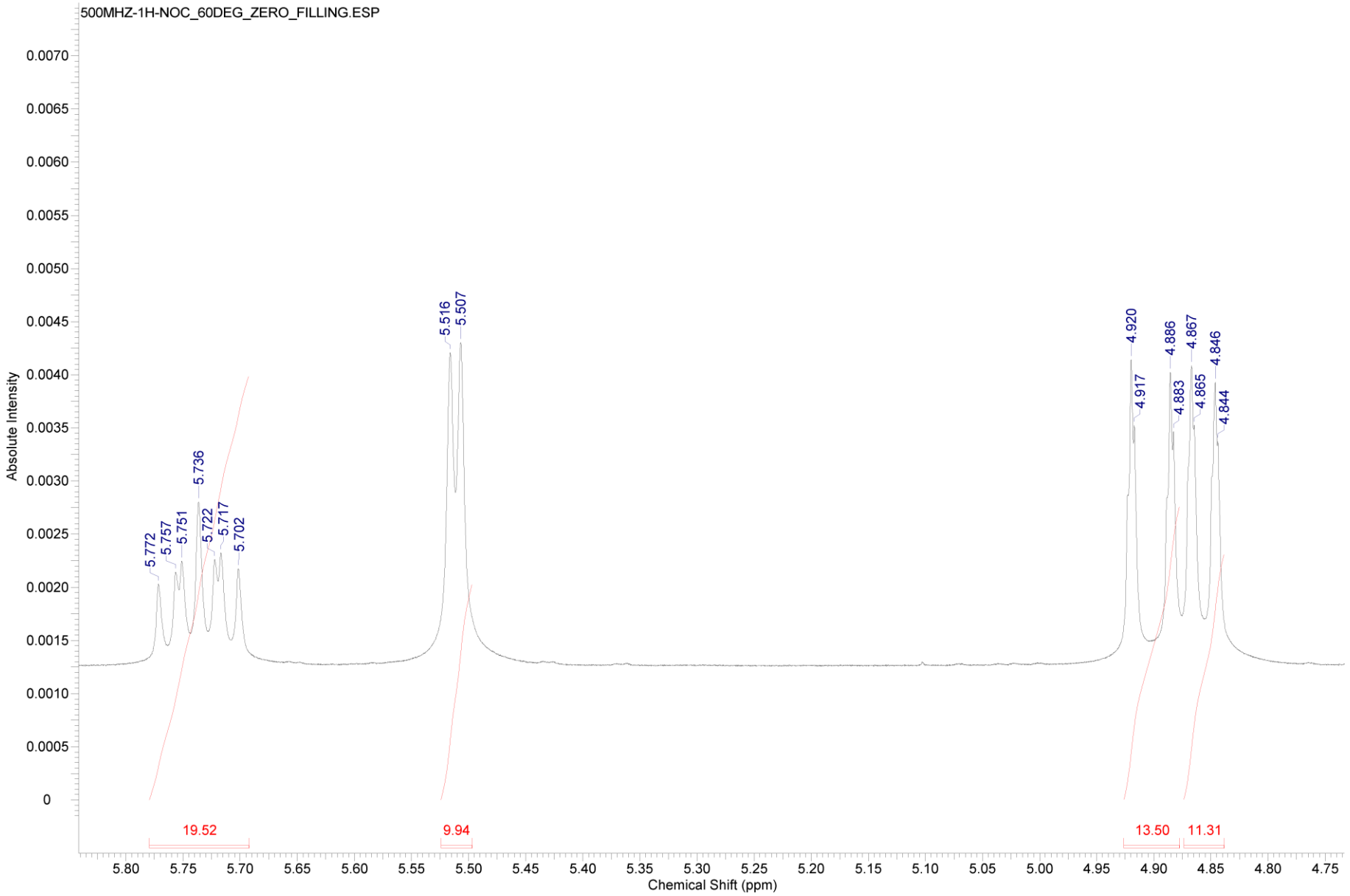
0.0060
0.0055
0.0050
0.0045
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0
8.741
8.733
8.073
8.056
7.986
7.969
7.525
7.523
7.512
7.509
7.506
7.492
7.402
7.393
7.382
7.368
7.365
7.351
9.45
10.41
11.53
12.28
10.38
12.55
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
Chemical Shift (ppm)


500MHZ-1H-NOC_60DEG_ZERO_FILLING.ESP
Absolute Intensity
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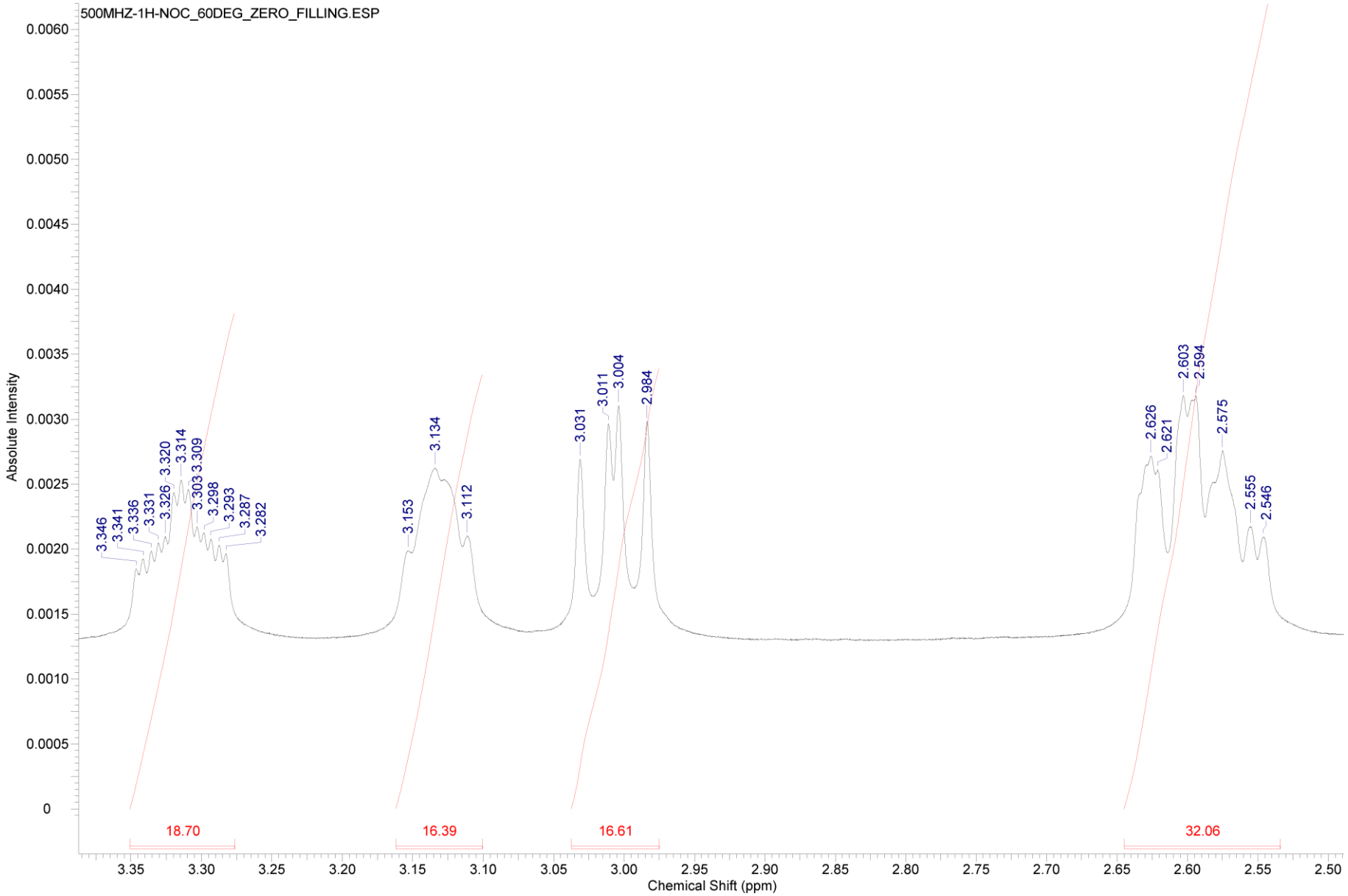
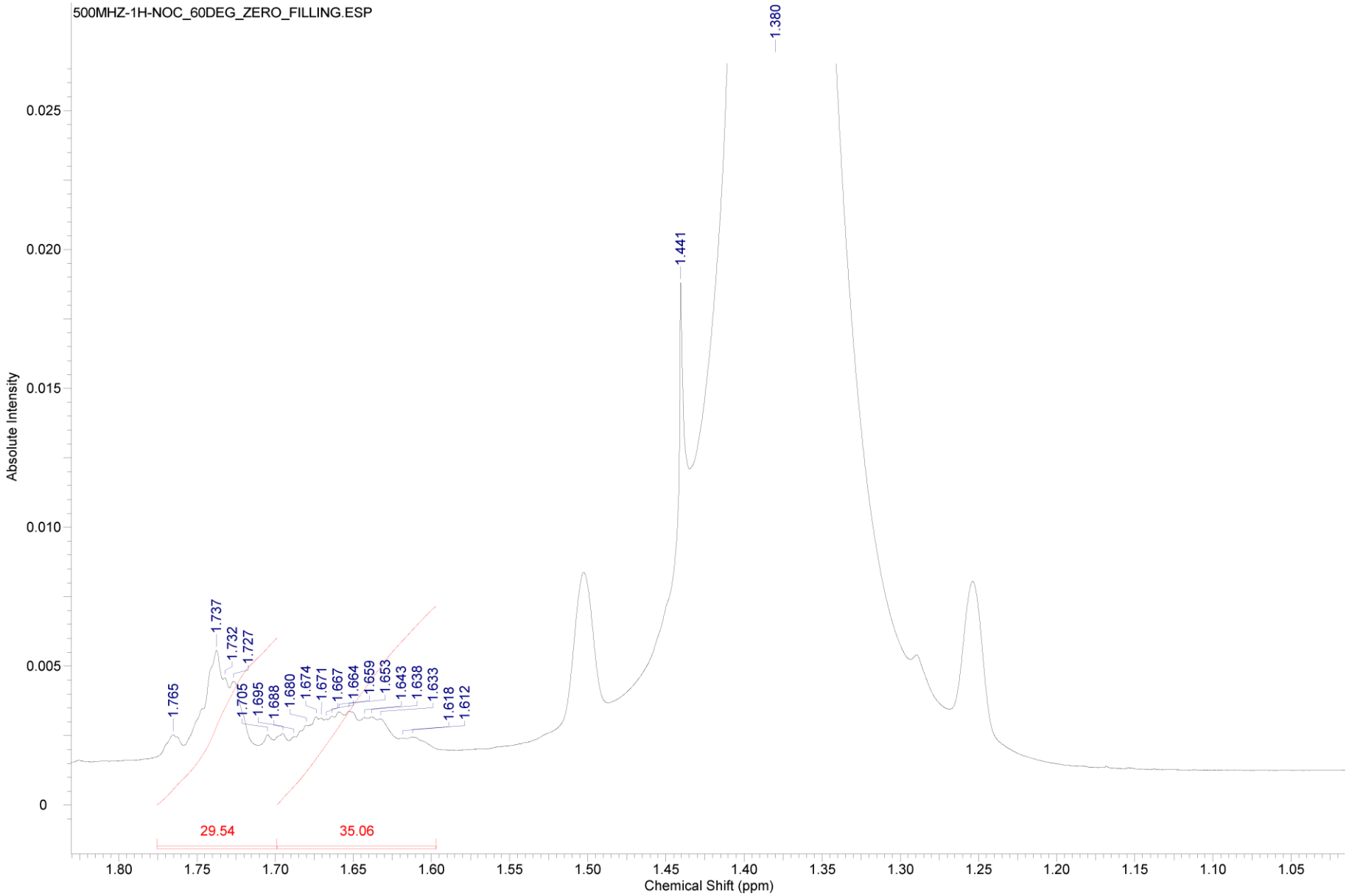
0.0065
0.0060
0.0055
0.0050
0.0045
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0
5.772
5.757
5.751
5.736
5.722
5.717
5.702
5.516
5.507
4.920
4.917
4.886
4.883
4.867
4.865
4.846
4.844
19.52
9.94
13.50
11.31
5.80
5.75
5.70
5.65
5.60
5.55
5.50
5.45
5.40
5.35
5.30
5.25
5.20
5.15
5.10
5.05
5.00
4.95
4.90
4.85
4.80
4.75
Chemical Shift (ppm)


500MHZ-1H-NOC_60DEG_ZERO_FILLING.ESP
Absolute Intensity
0.0060
0.0055
0.0050
0.0045
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0
3.346
3.341
3.336
3.331
3.326
3.320
3.314
3.309
3.303
3.298
3.293
3.287
3.282
3.153
3.134
3.112
3.031
3.011
3.004
2.984
2.626
2.621
2.603
2.594
2.575
2.555
2.546
18.70
16.39
16.61
32.06
3.35
3.30
3.25
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
2.50
Chemical Shift (ppm)


500MHZ-1H-NOC_60DEG_ZERO_FILLING.ESP
Absolute Intensity
0.025
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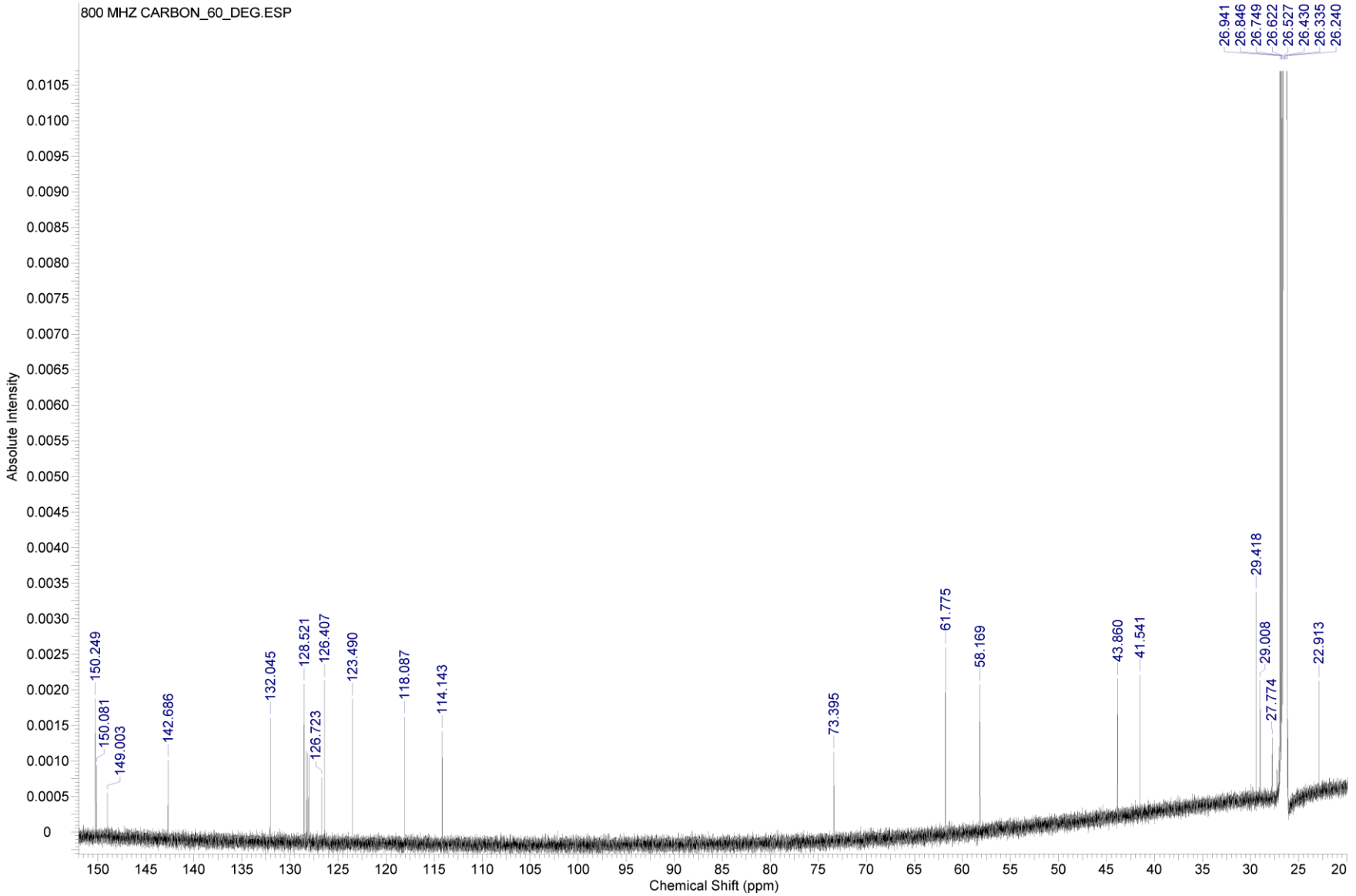
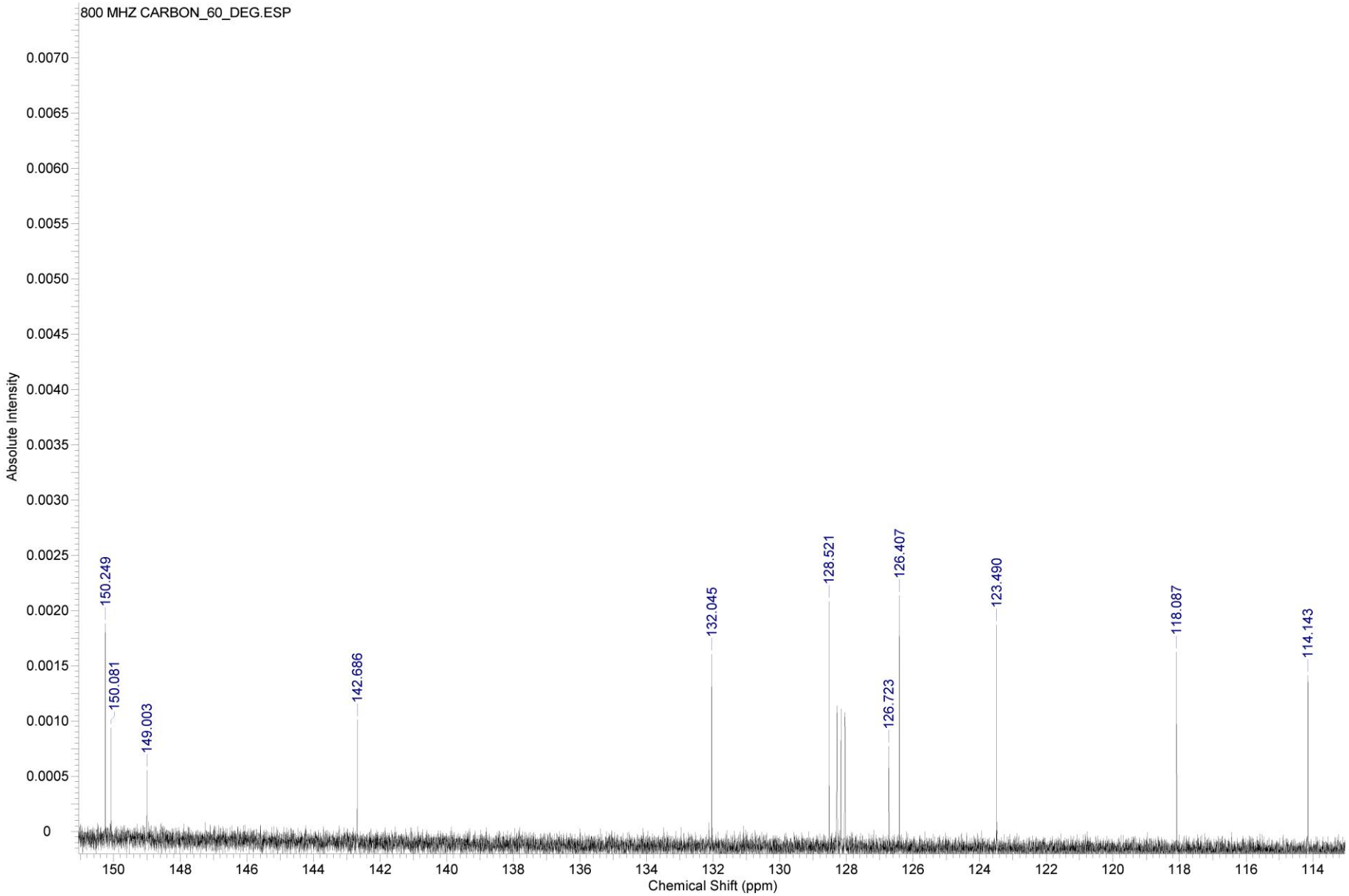
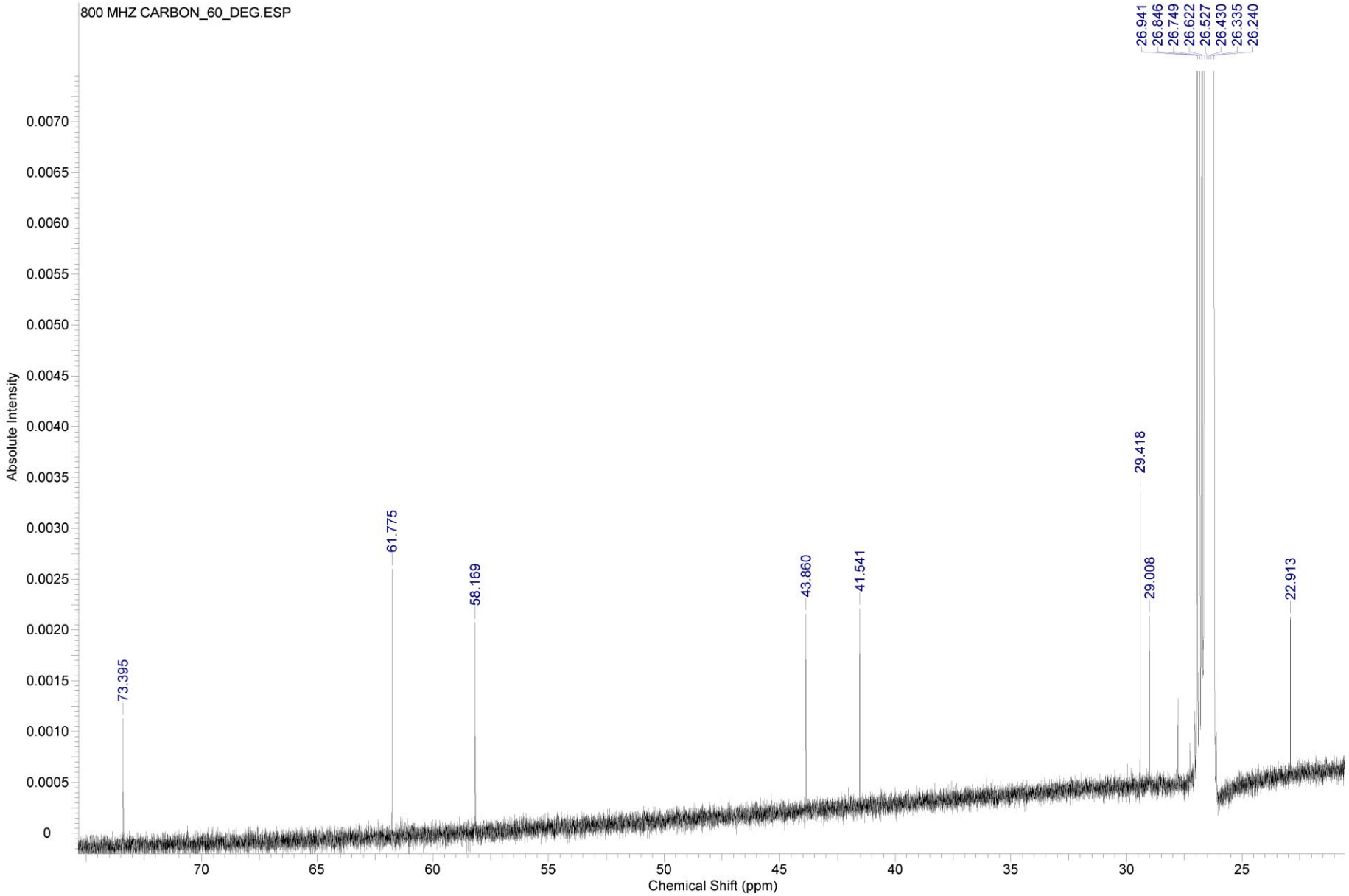
0.015
0.010
0.005
0
1.380
1.441
1.765
1.737
1.732
1.727
1.705
1.695
1.688
1.680
1.674
1.671
1.667
1.664
1.659
1.653
1.643
1.638
1.633
1.618
1.612
29.54
35.06
1.80
1.75
1.70
1.65
1.60
1.55
1.50
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
1.05
Chemical Shift (ppm)

2.3 18.8 T ^{13}C NMR spectrum.




800 MHZ CARBON_60_DEG.ESP
Absolute Intensity
0.0070
0.0065
0.0060
0.0055
0.0050
0.0045
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0
150.249
150.081
149.003
142.686
132.045
128.521
126.723
126.407
123.490
118.087
114.143
150
148
146
144
142
140
138
136
134
132
130
128
126
124
122
120
118
116
114
Chemical Shift (ppm)


800 MHZ CARBON_60_DEG.ESP
26.941
26.846
26.749
26.622
26.527
26.430
26.335
26.240
29.418
29.008
73.395
61.775
58.169
43.860
41.541
22.913
Absolute Intensity
0.0070
0.0065
0.0060
0.0055
0.0050
0.0045
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0
70
65
60
55
50
45
40
35
30
25
Chemical Shift (ppm)

3. Optimised molecular geometries.

Below the optimum molecular geometries of 36 cinchonidine conformers are reported. The labels and ordering of the conformers are the same as in Table 2. Each data segment contains: conformer label, conformer energy in Hartrees, ant the table of the Cartesian coordinates of all atoms, in a Gaussian 03 format. In this format the second column of the table contains information on the kind of the atom (atomic number), its x, y and z coordinates are given in columns 4, 5 and 6, respectively, the numbers in the first column are (nothing more than) row numbers, and the third column is irrelevant for the case in hand.

0-3/γ/1

After PCM corrections, the SCF energy is -922.2249

Number	Number	Type	X	Y	Z
1	7	0	-1.854369	-0.054822	-1.433352
2	6	0	-0.874794	-0.287188	-0.347750
3	6	0	-1.592201	-0.675466	0.978646
4	6	0	-3.107967	-0.492817	0.776854
5	6	0	-3.438661	0.937829	0.271574
6	6	0	-2.647360	1.130524	-1.072999
7	6	0	-3.568233	-1.490978	-0.298652
8	6	0	-2.774882	-1.197789	-1.605760
9	1	0	-0.385641	0.679000	-0.208750
10	6	0	0.253740	-1.252499	-0.774612
11	8	0	-0.202465	-2.601800	-0.650021
12	1	0	0.435356	-3.181131	-1.084866
13	1	0	0.456531	-1.043069	-1.829264
14	1	0	-1.224527	-0.065785	1.806291
15	1	0	-1.395947	-1.717347	1.236164
16	1	0	-3.633725	-0.677168	1.716344
17	1	0	-4.512424	0.968961	0.061497
18	6	0	-3.140937	2.015836	1.269984
19	6	0	-4.045524	2.818462	1.822026
20	1	0	-2.095664	2.147361	1.545278
21	1	0	-3.765920	3.585359	2.534766
22	1	0	-5.100434	2.736604	1.579100
23	1	0	-3.339830	1.338503	-1.891664
24	1	0	-1.970529	1.985461	-0.999192
25	1	0	-4.645327	-1.395442	-0.462875
26	1	0	-3.382473	-2.512456	0.042290
27	1	0	-2.196218	-2.065690	-1.912176
28	1	0	-3.449269	-0.943645	-2.426540
29	7	0	3.856998	-0.599310	1.590429
30	6	0	3.017785	-1.576190	1.838567
31	6	0	1.845780	-1.824011	1.092422
32	6	0	1.520806	-1.012468	0.033771
33	6	0	2.207555	0.975954	-1.344881
34	6	0	3.104725	1.986178	-1.587786
35	6	0	4.248537	2.140413	-0.776446

36	6	0	4.475560	1.277347	0.263984
37	6	0	3.570546	0.224152	0.541316
38	6	0	2.408140	0.063897	-0.275781
39	1	0	1.207028	-2.655509	1.358828
40	1	0	3.260594	-2.223165	2.677940
41	1	0	5.346101	1.371137	0.901402
42	1	0	4.947148	2.943222	-0.980517
43	1	0	2.934085	2.670811	-2.410149
44	1	0	1.336722	0.880197	-1.980145

O-3/γ/2

After PCM corrections, the SCF energy is -922.2229

Number	Number	Type	X	Y	Z
1	7	0	-1.998997	0.064735	-1.356719
2	6	0	-0.974695	-0.239627	-0.330197
3	6	0	-1.637525	-0.657297	1.015250
4	6	0	-3.153252	-0.422140	0.893139
5	6	0	-3.440618	1.042137	0.462755
6	6	0	-2.733284	1.262988	-0.910662
7	6	0	-3.703112	-1.359967	-0.192537
8	6	0	-2.963411	-1.040931	-1.525003
9	1	0	-0.449981	0.705017	-0.175997
10	6	0	0.102121	-1.218475	-0.847019
11	8	0	-0.402960	-2.555400	-0.788090
12	1	0	0.203618	-3.132143	-1.268678
13	1	0	0.284289	-0.954702	-1.893426
14	1	0	-1.219001	-0.076893	1.839396
15	1	0	-1.457015	-1.711744	1.229924
16	1	0	-3.639963	-0.624485	1.851030
17	1	0	-4.526244	1.109576	0.312422
18	6	0	-3.117485	2.022104	1.561732
19	6	0	-2.360598	3.113324	1.515526
20	1	0	-3.597170	1.783678	2.510835
21	1	0	-2.229531	3.732377	2.395074
22	1	0	-1.847276	3.442199	0.619932
23	1	0	-3.465024	1.512811	-1.681877
24	1	0	-2.023041	2.089026	-0.866502
25	1	0	-4.782704	-1.219560	-0.299322
26	1	0	-3.539055	-2.400393	0.098977
27	1	0	-2.428528	-1.913836	-1.890226
28	1	0	-3.668098	-0.735660	-2.301920
29	7	0	3.784025	-0.853619	1.459369
30	6	0	2.912710	-1.811882	1.666022
31	6	0	1.715147	-1.966085	0.935825
32	6	0	1.398335	-1.076861	-0.061235
33	6	0	2.134078	0.965290	-1.331223
34	6	0	3.064441	1.954431	-1.532296
35	6	0	4.230062	2.014595	-0.739817

36	6	0	4.445535	1.079515	0.239054
37	6	0	3.506633	0.045385	0.471511
38	6	0	2.321083	-0.018574	-0.325329
39	1	0	1.049156	-2.787029	1.165180
40	1	0	3.148693	-2.519977	2.456615
41	1	0	5.332435	1.100438	0.860297
42	1	0	4.954747	2.802111	-0.909852
43	1	0	2.903466	2.695022	-2.306764
44	1	0	1.247726	0.941973	-1.951927

O-3/γ/3

After PCM corrections, the SCF energy is -922.2224

Number	Number	Type	X	Y	Z
1	7	0	-1.924119	0.058267	-1.473168
2	6	0	-0.936270	-0.201881	-0.401068
3	6	0	-1.644136	-0.551792	0.938982
4	6	0	-3.156251	-0.304927	0.764930
5	6	0	-3.440669	1.121152	0.243777
6	6	0	-2.659950	1.278903	-1.113632
7	6	0	-3.673016	-1.297867	-0.291152
8	6	0	-2.895583	-1.046009	-1.616889
9	1	0	-0.411351	0.747103	-0.275233
10	6	0	0.150114	-1.208803	-0.837464
11	8	0	-0.364942	-2.538822	-0.731473
12	1	0	0.252398	-3.140477	-1.165605
13	1	0	0.365266	-0.995303	-1.889050
14	1	0	-1.231595	0.049844	1.749114
15	1	0	-1.489962	-1.600479	1.198818
16	1	0	-3.672894	-0.471077	1.712857
17	1	0	-4.512759	1.172566	0.012941
18	6	0	-3.165130	2.258091	1.191553
19	6	0	-2.927328	2.197096	2.497829
20	1	0	-3.191408	3.243284	0.726400
21	1	0	-2.762493	3.098555	3.076102
22	1	0	-2.892126	1.261183	3.042754
23	1	0	-3.348729	1.510077	-1.929329
24	1	0	-1.944040	2.102091	-1.049181
25	1	0	-4.749248	-1.166937	-0.436199
26	1	0	-3.515799	-2.321736	0.056681
27	1	0	-2.360599	-1.939209	-1.929247
28	1	0	-3.576421	-0.768761	-2.424868
29	7	0	3.765851	-0.754729	1.555389
30	6	0	2.880126	-1.694481	1.784718
31	6	0	1.702924	-1.876494	1.028337
32	6	0	1.423230	-1.036520	-0.021100
33	6	0	2.213712	0.933475	-1.370189
34	6	0	3.158532	1.903956	-1.593450
35	6	0	4.301477	1.994915	-0.771436

36	6	0	4.480226	1.108603	0.258795
37	6	0	3.525350	0.095076	0.515749
38	6	0	2.362636	0.000124	-0.311138
39	1	0	1.023294	-2.679949	1.278661
40	1	0	3.086667	-2.363299	2.616663
41	1	0	5.349123	1.153901	0.903724
42	1	0	5.038167	2.766959	-0.959805
43	1	0	3.026564	2.605794	-2.408414
44	1	0	1.345395	0.885983	-2.014459

0-3/α/1

After PCM corrections, the SCF energy is -922.2215

Number	Number	Type	X	Y	Z
1	7	0	-1.813303	-0.054526	-1.414113
2	6	0	-0.836365	-0.305203	-0.332357
3	6	0	-1.562551	-0.663039	1.000326
4	6	0	-3.080414	-0.519654	0.781262
5	6	0	-3.434233	0.904533	0.273150
6	6	0	-2.606507	1.127038	-1.043519
7	6	0	-3.506330	-1.526539	-0.300643
8	6	0	-2.731463	-1.194193	-1.610300
9	1	0	-0.330657	0.650798	-0.191127
10	6	0	0.274929	-1.298448	-0.769157
11	8	0	-0.123225	-2.665299	-0.738499
12	1	0	-0.480990	-2.879050	0.131149
13	1	0	0.461446	-1.104735	-1.827186
14	1	0	-1.213493	-0.020505	1.810489
15	1	0	-1.361096	-1.688308	1.330447
16	1	0	-3.611800	-0.715716	1.715015
17	1	0	-4.501226	0.904016	0.029645
18	6	0	-3.200143	1.985246	1.285529
19	6	0	-4.145744	2.754693	1.815329
20	1	0	-2.167702	2.150472	1.589568
21	1	0	-3.911177	3.526549	2.538774
22	1	0	-5.190022	2.640880	1.541511
23	1	0	-3.274906	1.364208	-1.874031
24	1	0	-1.924792	1.973170	-0.927535
25	1	0	-4.586754	-1.471876	-0.458566
26	1	0	-3.286258	-2.544838	0.032781
27	1	0	-2.156631	-2.050576	-1.955078
28	1	0	-3.418979	-0.916705	-2.412019
29	7	0	3.929259	-0.592101	1.508398
30	6	0	3.163873	-1.636116	1.715116
31	6	0	1.984277	-1.910743	0.990321
32	6	0	1.564943	-1.054507	0.003534
33	6	0	2.110122	1.026785	-1.299053
34	6	0	2.943865	2.095253	-1.516906
35	6	0	4.094312	2.281427	-0.722001

36	6	0	4.396096	1.385891	0.270767
37	6	0	3.560929	0.269118	0.516688
38	6	0	2.384537	0.083556	-0.274145
39	1	0	1.434190	-2.814171	1.218658
40	1	0	3.476119	-2.320244	2.500290
41	1	0	5.277052	1.498589	0.890558
42	1	0	4.741563	3.131119	-0.904368
43	1	0	2.718067	2.800867	-2.307602
44	1	0	1.237349	0.904246	-1.927023

0-3/α/2

After PCM corrections, the SCF energy is -922.2196

Number	Number	Type	X	Y	Z
1	7	0	-1.970189	0.034534	-1.342121
2	6	0	-0.946548	-0.272146	-0.318076
3	6	0	-1.613912	-0.640801	1.041753
4	6	0	-3.130814	-0.415795	0.910785
5	6	0	-3.416114	1.041696	0.456225
6	6	0	-2.691495	1.245206	-0.910268
7	6	0	-3.675265	-1.371465	-0.162432
8	6	0	-2.943840	-1.062512	-1.502871
9	1	0	-0.405401	0.664174	-0.178125
10	6	0	0.110049	-1.286856	-0.829988
11	8	0	-0.343629	-2.637312	-0.844020
12	1	0	-0.688769	-2.870081	0.025872
13	1	0	0.276109	-1.056096	-1.883991
14	1	0	-1.195474	-0.031897	1.844660
15	1	0	-1.441036	-1.683746	1.330857
16	1	0	-3.619563	-0.603326	1.870416
17	1	0	-4.499800	1.101989	0.290879
18	6	0	-3.111632	2.037692	1.546243
19	6	0	-2.349452	3.124963	1.497094
20	1	0	-3.611192	1.816295	2.489124
21	1	0	-2.233434	3.757834	2.368828
22	1	0	-1.817769	3.437678	0.606536
23	1	0	-3.411279	1.501957	-1.690248
24	1	0	-1.969536	2.060621	-0.862254
25	1	0	-4.756098	-1.242379	-0.266088
26	1	0	-3.507805	-2.408552	0.142951
27	1	0	-2.421026	-1.939479	-1.876908
28	1	0	-3.653820	-0.751505	-2.272233
29	7	0	3.839676	-0.829845	1.389952
30	6	0	3.036161	-1.850165	1.567621
31	6	0	1.831978	-2.044406	0.857733
32	6	0	1.428353	-1.129595	-0.082030
33	6	0	2.036626	0.980022	-1.309188
34	6	0	2.909488	2.022354	-1.498729
35	6	0	4.080413	2.128360	-0.719213

36	6	0	4.363144	1.179695	0.228785
37	6	0	3.487772	0.087687	0.443811
38	6	0	2.289854	-0.015783	-0.329609
39	1	0	1.249318	-2.933572	1.058864
40	1	0	3.335090	-2.579906	2.316081
41	1	0	5.258837	1.230779	0.835455
42	1	0	4.758416	2.958484	-0.878638
43	1	0	2.699352	2.768887	-2.255488
44	1	0	1.148911	0.918608	-1.925071

0-3/α/3

After PCM corrections, the SCF energy is -922.2189

Number	Number	Type	X	Y	Z
1	7	0	-1.882179	0.054652	-1.458655
2	6	0	-0.899355	-0.219819	-0.387504
3	6	0	-1.616998	-0.531788	0.959602
4	6	0	-3.133235	-0.329450	0.764002
5	6	0	-3.440996	1.089016	0.236017
6	6	0	-2.619657	1.272145	-1.093515
7	6	0	-3.612042	-1.336572	-0.296845
8	6	0	-2.850286	-1.047806	-1.624789
9	1	0	-0.356002	0.717726	-0.264556
10	6	0	0.166400	-1.259557	-0.825371
11	8	0	-0.295932	-2.606667	-0.802195
12	1	0	-0.662282	-2.806774	0.067119
13	1	0	0.366432	-1.069883	-1.881599
14	1	0	-1.226430	0.110606	1.748754
15	1	0	-1.451802	-1.561086	1.298301
16	1	0	-3.657546	-0.505052	1.705766
17	1	0	-4.505752	1.108273	-0.030179
18	6	0	-3.228930	2.231030	1.193237
19	6	0	-3.015350	2.174135	2.503783
20	1	0	-3.281213	3.215823	0.729781
21	1	0	-2.894649	3.078865	3.087626
22	1	0	-2.958860	1.238650	3.047875
23	1	0	-3.282626	1.528545	-1.922846
24	1	0	-1.899783	2.087453	-0.988454
25	1	0	-4.692776	-1.248890	-0.437336
26	1	0	-3.419634	-2.357060	0.046745
27	1	0	-2.318387	-1.929971	-1.972986
28	1	0	-3.542096	-0.749305	-2.415328
29	7	0	3.835931	-0.748255	1.480822
30	6	0	3.018205	-1.754251	1.674222
31	6	0	1.832045	-1.964641	0.939148
32	6	0	1.462526	-1.081985	-0.044330
33	6	0	2.121346	0.978337	-1.328489
34	6	0	3.009214	2.005184	-1.532412
35	6	0	4.161468	2.127870	-0.727926

36	6	0	4.409878	1.211908	0.260927
37	6	0	3.517867	0.136976	0.492799
38	6	0	2.339822	0.015736	-0.308130
39	1	0	1.236605	-2.841534	1.156078
40	1	0	3.290037	-2.458474	2.456679
41	1	0	5.290832	1.275918	0.887623
42	1	0	4.851550	2.945584	-0.899179
43	1	0	2.825800	2.725940	-2.320446
44	1	0	1.248242	0.904391	-1.963608

O-3/β/1

After PCM corrections, the SCF energy is -922.2212

Number	Number	Type	X	Y	Z
1	7	0	-1.824957	-0.047988	-1.425597
2	6	0	-0.847294	-0.308142	-0.340175
3	6	0	-1.570813	-0.680699	0.986348
4	6	0	-3.085908	-0.504589	0.777838
5	6	0	-3.418828	0.928456	0.279109
6	6	0	-2.603152	1.143436	-1.047020
7	6	0	-3.535944	-1.500739	-0.304749
8	6	0	-2.771933	-1.160818	-1.618823
9	1	0	-0.341594	0.648662	-0.203348
10	6	0	0.271229	-1.298690	-0.767942
11	8	0	-0.062944	-2.679212	-0.605623
12	1	0	-0.912192	-2.848318	-1.024869
13	1	0	0.465421	-1.107476	-1.828901
14	1	0	-1.208552	-0.059947	1.807584
15	1	0	-1.366758	-1.717609	1.261830
16	1	0	-3.617560	-0.698071	1.711828
17	1	0	-4.488628	0.953822	0.048730
18	6	0	-3.148658	1.997932	1.294747
19	6	0	-4.070461	2.786445	1.837959
20	1	0	-2.109927	2.133738	1.591502
21	1	0	-3.811096	3.547133	2.564731
22	1	0	-5.119830	2.699195	1.573763
23	1	0	-3.277673	1.387432	-1.870702
24	1	0	-1.910232	1.980966	-0.939597
25	1	0	-4.616113	-1.434461	-0.458246
26	1	0	-3.324115	-2.521790	0.024600
27	1	0	-2.240667	-2.025578	-2.025112
28	1	0	-3.465350	-0.857078	-2.405678
29	7	0	3.885315	-0.584611	1.549395
30	6	0	3.091961	-1.604110	1.776936
31	6	0	1.919261	-1.878646	1.041813
32	6	0	1.544974	-1.048302	0.014913
33	6	0	2.148372	0.987081	-1.336015
34	6	0	3.003736	2.035916	-1.565600
35	6	0	4.144508	2.221659	-0.756633

36	6	0	4.412270	1.347319	0.264349
37	6	0	3.552528	0.252684	0.525622
38	6	0	2.388664	0.065239	-0.283488
39	1	0	1.324588	-2.747340	1.286068
40	1	0	3.374710	-2.266638	2.591321
41	1	0	5.284424	1.460601	0.896435
42	1	0	4.809431	3.055514	-0.948379
43	1	0	2.803418	2.725545	-2.377066
44	1	0	1.282278	0.864992	-1.973233

O-3/β/2

After PCM corrections, the SCF energy is -922.2192

Number	Number	Type	X	Y	Z
1	7	0	-1.987243	0.047416	-1.355215
2	6	0	-0.953771	-0.265367	-0.335089
3	6	0	-1.607061	-0.647162	1.023953
4	6	0	-3.123203	-0.413799	0.911159
5	6	0	-3.413789	1.045604	0.464556
6	6	0	-2.696239	1.261245	-0.904533
7	6	0	-3.679490	-1.368265	-0.157289
8	6	0	-2.987086	-1.024114	-1.508894
9	1	0	-0.415907	0.674698	-0.205770
10	6	0	0.115340	-1.269517	-0.845592
11	8	0	-0.266743	-2.644362	-0.752701
12	1	0	-1.132130	-2.756913	-1.157425
13	1	0	0.293533	-1.025511	-1.898659
14	1	0	-1.180754	-0.047880	1.829997
15	1	0	-1.420645	-1.695701	1.265788
16	1	0	-3.604266	-0.605867	1.873572
17	1	0	-4.498403	1.107544	0.304371
18	6	0	-3.103775	2.036419	1.557515
19	6	0	-2.353455	3.131644	1.504785
20	1	0	-3.588375	1.803841	2.505369
21	1	0	-2.231649	3.759887	2.379020
22	1	0	-1.836569	3.455204	0.609385
23	1	0	-3.417637	1.535272	-1.677209
24	1	0	-1.964560	2.066946	-0.850607
25	1	0	-4.763923	-1.258398	-0.241067
26	1	0	-3.485740	-2.403581	0.136584
27	1	0	-2.521538	-1.898836	-1.970037
28	1	0	-3.717598	-0.674458	-2.241485
29	7	0	3.793072	-0.829733	1.440680
30	6	0	2.956348	-1.821441	1.632480
31	6	0	1.762370	-2.006354	0.904195
32	6	0	1.412401	-1.112117	-0.076701
33	6	0	2.092468	0.954742	-1.340736
34	6	0	2.992707	1.972764	-1.534627
35	6	0	4.151412	2.067593	-0.735503

36	6	0	4.391707	1.134497	0.239232
37	6	0	3.485515	0.069363	0.462312
38	6	0	2.303146	-0.025808	-0.336011
39	1	0	1.131316	-2.857769	1.115575
40	1	0	3.218895	-2.533422	2.411110
41	1	0	5.275904	1.178310	0.863164
42	1	0	4.852187	2.877763	-0.899188
43	1	0	2.813908	2.708352	-2.310009
44	1	0	1.213815	0.902070	-1.970388

O-3/β/3

After PCM corrections, the SCF energy is -922.2186

Number	Number	Type	X	Y	Z
1	7	0	-1.862937	0.141013	-1.470711
2	6	0	-0.889715	-0.180119	-0.396457
3	6	0	-1.619304	-0.546239	0.928217
4	6	0	-3.136616	-0.378313	0.713782
5	6	0	-3.481092	1.050438	0.239208
6	6	0	-2.616510	1.331252	-1.044027
7	6	0	-3.567022	-1.355324	-0.395521
8	6	0	-2.831297	-0.945587	-1.705635
9	1	0	-0.343326	0.751874	-0.245755
10	6	0	0.183797	-1.208319	-0.849989
11	8	0	-0.217168	-2.576266	-0.736498
12	1	0	-1.065779	-2.692069	-1.174364
13	1	0	0.398905	-0.991100	-1.901961
14	1	0	-1.264403	0.089163	1.739692
15	1	0	-1.412752	-1.580160	1.212692
16	1	0	-3.673049	-0.611552	1.635866
17	1	0	-4.534535	1.043765	-0.070068
18	6	0	-3.351995	2.154430	1.254071
19	6	0	-3.163323	2.045239	2.564893
20	1	0	-3.445733	3.156345	0.835966
21	1	0	-3.102777	2.925793	3.193356
22	1	0	-3.066576	1.088778	3.064759
23	1	0	-3.250347	1.650627	-1.874478
24	1	0	-1.899820	2.133132	-0.853849
25	1	0	-4.650479	-1.322844	-0.536232
26	1	0	-3.316297	-2.378056	-0.100235
27	1	0	-2.325170	-1.789534	-2.181854
28	1	0	-3.540935	-0.583678	-2.452727
29	7	0	3.794951	-0.761928	1.537719
30	6	0	2.937563	-1.735856	1.729251
31	6	0	1.763724	-1.922315	0.969292
32	6	0	1.457655	-1.048537	-0.044148
33	6	0	2.202944	0.978924	-1.334528
34	6	0	3.123913	1.978707	-1.526174
35	6	0	4.261037	2.075181	-0.696832

36	6	0	4.459014	1.162588	0.306483
37	6	0	3.530394	0.116808	0.528707
38	6	0	2.370763	0.019199	-0.302012
39	1	0	1.113532	-2.758711	1.182594
40	1	0	3.165867	-2.431728	2.532833
41	1	0	5.325620	1.208634	0.954432
42	1	0	4.978774	2.870548	-0.859689
43	1	0	2.978227	2.698585	-2.322921
44	1	0	1.340727	0.925776	-1.986618

C-1/γ/1

After PCM corrections, the SCF energy is -922.2230

Number	Number	Type	X	Y	Z
1	7	0	-1.210984	-0.707639	-0.799533
2	6	0	-0.950821	-0.204572	0.564275
3	6	0	-2.256594	-0.212401	1.410000
4	6	0	-3.444677	-0.453608	0.460522
5	6	0	-3.414330	0.530556	-0.740097
6	6	0	-2.053201	0.279648	-1.489629
7	6	0	-3.316846	-1.879623	-0.098621
8	6	0	-1.922424	-1.999654	-0.780648
9	1	0	-0.618697	0.827019	0.435271
10	6	0	0.205888	-0.953700	1.252465
11	8	0	0.343880	-0.352232	2.546576
12	1	0	1.035830	-0.819273	3.030755
13	1	0	-0.090120	-2.001372	1.384378
14	1	0	-2.363726	0.722228	1.962291
15	1	0	-2.227874	-1.008161	2.159743
16	1	0	-4.387148	-0.339258	1.000335
17	1	0	-4.241412	0.260709	-1.404190
18	6	0	-3.597301	1.966299	-0.348820
19	6	0	-4.613331	2.737214	-0.723478
20	1	0	-2.821869	2.400905	0.279710
21	1	0	-4.685200	3.773329	-0.414345
22	1	0	-5.410315	2.358494	-1.355892
23	1	0	-2.242025	-0.082319	-2.502723
24	1	0	-1.486296	1.208996	-1.580353
25	1	0	-4.121021	-2.080427	-0.811983
26	1	0	-3.418555	-2.607247	0.711291
27	1	0	-1.300262	-2.737577	-0.273137
28	1	0	-2.017087	-2.333122	-1.816191
29	7	0	3.847045	-1.125193	-1.133329
30	6	0	3.090132	-2.169430	-0.897638
31	6	0	1.919263	-2.128883	-0.114053
32	6	0	1.500748	-0.951453	0.456631
33	6	0	2.043605	1.487244	0.803874
34	6	0	2.861521	2.556985	0.539483
35	6	0	3.996546	2.409665	-0.285515

36	6	0	4.298075	1.186681	-0.824181
37	6	0	3.476462	0.061000	-0.570974
38	6	0	2.312258	0.207282	0.249356
39	1	0	1.345816	-3.038792	0.020484
40	1	0	3.402249	-3.109494	-1.345890
41	1	0	5.167181	1.039833	-1.453446
42	1	0	4.631588	3.264848	-0.485133
43	1	0	2.637647	3.524013	0.974501
44	1	0	1.197990	1.608863	1.464244

C-1/γ/2

After PCM corrections, the SCF energy is -922.2210

Number	Number	Type	X	Y	Z
1	7	0	-1.307367	-0.699464	-0.823588
2	6	0	-1.048195	-0.177803	0.533926
3	6	0	-2.364846	-0.115729	1.359748
4	6	0	-3.544068	-0.328371	0.394364
5	6	0	-3.437378	0.639235	-0.817000
6	6	0	-2.098036	0.309363	-1.549390
7	6	0	-3.471711	-1.767926	-0.136460
8	6	0	-2.070969	-1.959805	-0.789218
9	1	0	-0.677746	0.838040	0.390290
10	6	0	0.068812	-0.957787	1.252577
11	8	0	0.207466	-0.344686	2.541328
12	1	0	0.876422	-0.828460	3.041149
13	1	0	-0.265500	-1.992772	1.393046
14	1	0	-2.443030	0.839737	1.879831
15	1	0	-2.379568	-0.892770	2.129128
16	1	0	-4.491309	-0.162117	0.914089
17	1	0	-4.272369	0.388001	-1.484249
18	6	0	-3.657017	2.073406	-0.406219
19	6	0	-2.911445	3.141920	-0.666742
20	1	0	-4.570429	2.225920	0.168412
21	1	0	-3.208816	4.122209	-0.313609
22	1	0	-1.991666	3.098685	-1.237282
23	1	0	-2.296265	-0.078054	-2.551011
24	1	0	-1.475143	1.195553	-1.669449
25	1	0	-4.270025	-1.945486	-0.862671
26	1	0	-3.620899	-2.476315	0.683074
27	1	0	-1.489495	-2.710367	-0.252804
28	1	0	-2.161356	-2.314182	-1.818238
29	7	0	3.747182	-1.290371	-1.059130
30	6	0	2.948661	-2.303748	-0.825875
31	6	0	1.764576	-2.211390	-0.066897
32	6	0	1.376772	-1.012368	0.480105
33	6	0	1.997263	1.410703	0.804383
34	6	0	2.858212	2.447144	0.544017
35	6	0	4.005032	2.248219	-0.253411

36	6	0	4.274086	1.008094	-0.769700
37	6	0	3.407643	-0.084279	-0.519917
38	6	0	2.232651	0.114263	0.273558
39	1	0	1.157189	-3.098932	0.068167
40	1	0	3.235866	-3.260194	-1.255803
41	1	0	5.150642	0.822133	-1.377968
42	1	0	4.674508	3.077485	-0.449964
43	1	0	2.659059	3.427506	0.960826
44	1	0	1.141244	1.571862	1.442348

C-1/γ/3

After PCM corrections, the SCF energy is -922.2204

Number	Number	Type	X	Y	Z
1	7	0	-1.191206	-0.776522	-0.821999
2	6	0	-0.998025	-0.115956	0.483679
3	6	0	-2.344014	-0.015588	1.253384
4	6	0	-3.486603	-0.355236	0.275740
5	6	0	-3.377686	0.464308	-1.030410
6	6	0	-1.979358	0.126383	-1.670289
7	6	0	-3.346961	-1.841003	-0.099486
8	6	0	-1.920420	-2.051520	-0.688196
9	1	0	-0.651580	0.892403	0.251890
10	6	0	0.114227	-0.782469	1.315476
11	8	0	0.205757	-0.018997	2.525655
12	1	0	0.860869	-0.432440	3.101140
13	1	0	-0.205298	-1.800612	1.569070
14	1	0	-2.458506	0.978506	1.683345
15	1	0	-2.366969	-0.721436	2.089116
16	1	0	-4.454551	-0.182852	0.751573
17	1	0	-4.149213	0.086574	-1.714031
18	6	0	-3.612340	1.947800	-0.920006
19	6	0	-4.145092	2.619805	0.095437
20	1	0	-3.323257	2.512499	-1.806012
21	1	0	-4.283400	3.693190	0.040635
22	1	0	-4.468273	2.138021	1.010602
23	1	0	-2.106696	-0.351167	-2.644404
24	1	0	-1.398964	1.038169	-1.828827
25	1	0	-4.115223	-2.122333	-0.825303
26	1	0	-3.498587	-2.464972	0.785478
27	1	0	-1.335580	-2.727528	-0.063693
28	1	0	-1.966034	-2.506416	-1.679900
29	7	0	3.848797	-1.303643	-0.867014
30	6	0	3.069512	-2.300694	-0.524057
31	6	0	1.868928	-2.146060	0.198022
32	6	0	1.442823	-0.899079	0.586349
33	6	0	2.007273	1.558272	0.632782
34	6	0	2.850432	2.576485	0.264582
35	6	0	4.014000	2.311405	-0.488053

36	6	0	4.319080	1.025384	-0.848865
37	6	0	3.472673	-0.049839	-0.483078
38	6	0	2.279189	0.214318	0.262059
39	1	0	1.278793	-3.025388	0.429199
40	1	0	3.386595	-3.294876	-0.829340
41	1	0	5.209977	0.789404	-1.417685
42	1	0	4.668588	3.126964	-0.772501
43	1	0	2.624026	3.594124	0.560578
44	1	0	1.138252	1.772994	1.236502

C-1/β/1

After PCM corrections, the SCF energy is -922.2207

Number	Number	Type	X	Y	Z
1	7	0	-1.217607	-0.742578	-0.794861
2	6	0	-0.946511	-0.218831	0.558534
3	6	0	-2.255353	-0.197198	1.402771
4	6	0	-3.448486	-0.417684	0.452950
5	6	0	-3.385833	0.554607	-0.756067
6	6	0	-2.038153	0.246412	-1.507852
7	6	0	-3.354751	-1.851818	-0.092300
8	6	0	-1.953016	-2.019815	-0.749304
9	1	0	-0.605049	0.807418	0.413144
10	6	0	0.208520	-0.963994	1.266271
11	8	0	0.458758	-0.379295	2.553549
12	1	0	-0.294607	-0.563137	3.126755
13	1	0	-0.080933	-2.011021	1.410149
14	1	0	-2.350652	0.740354	1.953762
15	1	0	-2.260636	-1.002100	2.148492
16	1	0	-4.388470	-0.272577	0.989244
17	1	0	-4.225348	0.308126	-1.413358
18	6	0	-3.516673	1.999642	-0.376958
19	6	0	-4.512829	2.798638	-0.745802
20	1	0	-2.718233	2.416561	0.234523
21	1	0	-4.546745	3.839844	-0.447590
22	1	0	-5.330475	2.438913	-1.362613
23	1	0	-2.244469	-0.139971	-2.508394
24	1	0	-1.448036	1.157389	-1.629479
25	1	0	-4.152778	-2.031331	-0.817785
26	1	0	-3.493943	-2.570577	0.720092
27	1	0	-1.352746	-2.753107	-0.209751
28	1	0	-2.039674	-2.383549	-1.775175
29	7	0	3.817734	-1.127523	-1.158356
30	6	0	3.063440	-2.172586	-0.918076
31	6	0	1.905177	-2.137325	-0.116228
32	6	0	1.499126	-0.964718	0.471044
33	6	0	2.052848	1.468112	0.835048
34	6	0	2.868273	2.538885	0.568480
35	6	0	3.988925	2.397977	-0.277168

36	6	0	4.278535	1.180199	-0.833594
37	6	0	3.458665	0.053548	-0.578676
38	6	0	2.308816	0.193670	0.262468
39	1	0	1.334058	-3.048073	0.020155
40	1	0	3.366881	-3.109476	-1.378739
41	1	0	5.137399	1.037819	-1.477780
42	1	0	4.623044	3.253689	-0.477678
43	1	0	2.655491	3.501120	1.019477
44	1	0	1.220648	1.582413	1.513437

C-1/β/2

After PCM corrections, the SCF energy is -922.2188

Number	Number	Type	X	Y	Z
1	7	0	-1.320060	-0.728194	-0.816037
2	6	0	-1.043950	-0.181839	0.527412
3	6	0	-2.361508	-0.074126	1.350943
4	6	0	-3.547295	-0.270758	0.388178
5	6	0	-3.408790	0.672022	-0.839676
6	6	0	-2.083468	0.282036	-1.567724
7	6	0	-3.514328	-1.721217	-0.116603
8	6	0	-2.113072	-1.968132	-0.750073
9	1	0	-0.657049	0.824367	0.361984
10	6	0	0.065739	-0.962494	1.268612
11	8	0	0.316954	-0.371817	2.552916
12	1	0	-0.459281	-0.505020	3.109344
13	1	0	-0.267624	-1.995253	1.420194
14	1	0	-2.421523	0.889633	1.859417
15	1	0	-2.415236	-0.850243	2.125055
16	1	0	-4.489082	-0.067565	0.904251
17	1	0	-4.253845	0.437850	-1.499952
18	6	0	-3.577916	2.119691	-0.452029
19	6	0	-2.777466	3.150937	-0.699423
20	1	0	-4.500279	2.318696	0.093381
21	1	0	-3.041320	4.147183	-0.364873
22	1	0	-1.843551	3.060668	-1.240743
23	1	0	-2.298688	-0.128246	-2.556626
24	1	0	-1.436392	1.145889	-1.716536
25	1	0	-4.310050	-1.883623	-0.848791
26	1	0	-3.696316	-2.411506	0.711826
27	1	0	-1.554519	-2.714122	-0.183869
28	1	0	-2.204045	-2.354342	-1.767375
29	7	0	3.710204	-1.306547	-1.084808
30	6	0	2.908264	-2.316101	-0.846739
31	6	0	1.737808	-2.222726	-0.067559
32	6	0	1.370052	-1.027088	0.498319
33	6	0	2.014148	1.386768	0.837826
34	6	0	2.877691	2.419720	0.573392
35	6	0	4.009000	2.220913	-0.246069

36	6	0	4.259542	0.984455	-0.779883
37	6	0	3.389144	-0.104165	-0.527077
38	6	0	2.229937	0.094574	0.289185
39	1	0	1.126671	-3.107249	0.067957
40	1	0	3.180536	-3.270528	-1.290613
41	1	0	5.124500	0.798108	-1.404454
42	1	0	4.681759	3.047005	-0.444948
43	1	0	2.694567	3.396378	1.006036
44	1	0	1.172937	1.544808	1.495850

C-1/β/3

After PCM corrections, the SCF energy is -922.2183

Number	Number	Type	X	Y	Z
1	7	0	-1.196356	-0.802300	-0.814631
2	6	0	-0.990140	-0.121418	0.477605
3	6	0	-2.337892	0.008886	1.244423
4	6	0	-3.486204	-0.329696	0.271776
5	6	0	-3.361355	0.471716	-1.043785
6	6	0	-1.971561	0.094495	-1.680951
7	6	0	-3.367892	-1.822518	-0.081882
8	6	0	-1.940277	-2.065183	-0.655893
9	1	0	-0.634244	0.879511	0.229161
10	6	0	0.118927	-0.779558	1.330446
11	8	0	0.320017	-0.032110	2.539711
12	1	0	-0.467930	-0.119829	3.088756
13	1	0	-0.196048	-1.794629	1.598134
14	1	0	-2.446167	1.010621	1.660216
15	1	0	-2.387432	-0.695378	2.085191
16	1	0	-4.450995	-0.135284	0.745069
17	1	0	-4.142678	0.102656	-1.720674
18	6	0	-3.563293	1.961205	-0.948638
19	6	0	-4.093535	2.653745	0.054256
20	1	0	-3.250782	2.511259	-1.835664
21	1	0	-4.207129	3.729354	-0.011221
22	1	0	-4.441134	2.187437	0.968671
23	1	0	-2.111656	-0.403414	-2.642960
24	1	0	-1.376257	0.992054	-1.862813
25	1	0	-4.135397	-2.098468	-0.810173
26	1	0	-3.538726	-2.433012	0.809133
27	1	0	-1.367451	-2.732045	-0.010822
28	1	0	-1.985788	-2.544307	-1.635991
29	7	0	3.827309	-1.313827	-0.882464
30	6	0	3.046685	-2.307763	-0.533658
31	6	0	1.856323	-2.149912	0.203844
32	6	0	1.444391	-0.903127	0.604993
33	6	0	2.021441	1.550518	0.654152
34	6	0	2.864204	2.566112	0.278797
35	6	0	4.016666	2.298331	-0.489975

36	6	0	4.310383	1.012318	-0.859605
37	6	0	3.463173	-0.060227	-0.487521
38	6	0	2.281213	0.206775	0.274879
39	1	0	1.265477	-3.027370	0.438778
40	1	0	3.354018	-3.302575	-0.846766
41	1	0	5.193026	0.773911	-1.440178
42	1	0	4.671924	3.111656	-0.779364
43	1	0	2.647633	3.583493	0.582998
44	1	0	1.163374	1.765920	1.272909

C-1/α/1

After PCM corrections, the SCF energy is -922.2193

Number	Number	Type	X	Y	Z
1	7	0	-1.203267	-0.620822	-0.834464
2	6	0	-0.953752	-0.191933	0.557464
3	6	0	-2.258002	-0.278590	1.402707
4	6	0	-3.437504	-0.539855	0.447958
5	6	0	-3.467282	0.497789	-0.706748
6	6	0	-2.091737	0.368350	-1.460772
7	6	0	-3.240155	-1.931003	-0.176027
8	6	0	-1.856965	-1.941894	-0.891036
9	1	0	-0.653772	0.854056	0.482093
10	6	0	0.214326	-0.967543	1.204161
11	8	0	0.389260	-0.560620	2.570887
12	1	0	1.015707	0.169626	2.616540
13	1	0	-0.084376	-2.014631	1.284341
14	1	0	-2.405522	0.633950	1.982295
15	1	0	-2.195331	-1.092927	2.129981
16	1	0	-4.381015	-0.500062	0.996393
17	1	0	-4.274379	0.206366	-1.385940
18	6	0	-3.741986	1.900087	-0.252757
19	6	0	-4.800304	2.624081	-0.603153
20	1	0	-3.000156	2.352331	0.403498
21	1	0	-4.938339	3.638579	-0.248221
22	1	0	-5.567492	2.226587	-1.260404
23	1	0	-2.256981	0.071202	-2.498775
24	1	0	-1.572442	1.329145	-1.480201
25	1	0	-4.046997	-2.147164	-0.881613
26	1	0	-3.282710	-2.696299	0.603690
27	1	0	-1.191994	-2.685050	-0.450209
28	1	0	-1.959964	-2.206998	-1.945250
29	7	0	3.953593	-1.098438	-1.032224
30	6	0	3.203170	-2.151761	-0.819260
31	6	0	1.991344	-2.119831	-0.100169
32	6	0	1.514778	-0.941378	0.418616
33	6	0	1.972414	1.530400	0.689427
34	6	0	2.789945	2.608745	0.459108
35	6	0	3.987817	2.457868	-0.268641

36	6	0	4.343619	1.225217	-0.749102
37	6	0	3.524713	0.091803	-0.524455
38	6	0	2.303532	0.234096	0.209886
39	1	0	1.441332	-3.042739	0.040311
40	1	0	3.558220	-3.094896	-1.226950
41	1	0	5.255849	1.075837	-1.313217
42	1	0	4.622994	3.317633	-0.444931
43	1	0	2.509385	3.585030	0.836025
44	1	0	1.053779	1.692317	1.237018

C-1/α/2

After PCM corrections, the SCF energy is -922.2173

Number	Number	Type	X	Y	Z
1	7	0	-1.269281	-0.594395	-0.859400
2	6	0	-1.044595	-0.169951	0.538111
3	6	0	-2.369515	-0.228054	1.353673
4	6	0	-3.525579	-0.487064	0.372501
5	6	0	-3.505969	0.555608	-0.778474
6	6	0	-2.130961	0.410275	-1.505749
7	6	0	-3.332138	-1.882091	-0.240684
8	6	0	-1.936534	-1.906560	-0.931391
9	1	0	-0.724889	0.870621	0.470703
10	6	0	0.092286	-0.968635	1.211343
11	8	0	0.260293	-0.560902	2.577228
12	1	0	0.788917	0.243697	2.615437
13	1	0	-0.234397	-2.006478	1.299602
14	1	0	-2.522090	0.701727	1.903957
15	1	0	-2.333895	-1.028318	2.098151
16	1	0	-4.482868	-0.433960	0.897718
17	1	0	-4.302791	0.259289	-1.473460
18	6	0	-3.877125	1.933962	-0.293499
19	6	0	-3.251346	3.088425	-0.497193
20	1	0	-4.801419	1.958566	0.283381
21	1	0	-3.652298	4.012083	-0.096915
22	1	0	-2.333711	3.173616	-1.067066
23	1	0	-2.276551	0.110124	-2.545656
24	1	0	-1.583339	1.352528	-1.519666
25	1	0	-4.128055	-2.093832	-0.960165
26	1	0	-3.395733	-2.644113	0.540966
27	1	0	-1.288011	-2.658972	-0.481632
28	1	0	-2.025216	-2.167685	-1.988015
29	7	0	3.865798	-1.237027	-0.956825
30	6	0	3.084145	-2.266095	-0.737312
31	6	0	1.861499	-2.188228	-0.040479
32	6	0	1.406819	-0.987799	0.446958
33	6	0	1.925697	1.475479	0.678522
34	6	0	2.775631	2.527375	0.443894
35	6	0	3.982199	2.330814	-0.258118

36	6	0	4.312751	1.080389	-0.709729
37	6	0	3.459500	-0.026323	-0.479385
38	6	0	2.230038	0.161889	0.230314
39	1	0	1.285165	-3.093779	0.108228
40	1	0	3.422076	-3.226005	-1.119749
41	1	0	5.231382	0.895973	-1.252803
42	1	0	4.643277	3.170006	-0.438749
43	1	0	2.514817	3.517578	0.798133
44	1	0	1.000851	1.674018	1.203544

C-1/α/3

After PCM corrections, the SCF energy is -922.2167

Number	Number	Type	X	Y	Z
1	7	0	-1.185835	-0.680266	-0.872701
2	6	0	-0.998579	-0.100644	0.473735
3	6	0	-2.342762	-0.072691	1.255526
4	6	0	-3.480430	-0.435330	0.280594
5	6	0	-3.441225	0.441829	-0.990697
6	6	0	-2.025212	0.241183	-1.648696
7	6	0	-3.265505	-1.894210	-0.157845
8	6	0	-1.857014	-1.992634	-0.816110
9	1	0	-0.678777	0.927271	0.297547
10	6	0	0.124569	-0.813416	1.258202
11	8	0	0.252232	-0.263353	2.577707
12	1	0	0.794573	0.532385	2.549202
13	1	0	-0.196197	-1.840073	1.444779
14	1	0	-2.497159	0.906342	1.708073
15	1	0	-2.328575	-0.795977	2.075651
16	1	0	-4.447912	-0.337219	0.777749
17	1	0	-4.185485	0.033798	-1.686980
18	6	0	-3.787153	1.897224	-0.820426
19	6	0	-4.338460	2.490177	0.233734
20	1	0	-3.568869	2.512827	-1.692732
21	1	0	-4.560275	3.550847	0.222883
22	1	0	-4.596941	1.952483	1.138304
23	1	0	-2.122605	-0.158131	-2.660873
24	1	0	-1.499386	1.195675	-1.725689
25	1	0	-4.046777	-2.198895	-0.859828
26	1	0	-3.337826	-2.556652	0.708978
27	1	0	-1.219255	-2.694101	-0.277584
28	1	0	-1.926623	-2.363485	-1.840858
29	7	0	3.949442	-1.260851	-0.787669
30	6	0	3.170847	-2.270451	-0.483599
31	6	0	1.932997	-2.135982	0.176872
32	6	0	1.458273	-0.897507	0.532236
33	6	0	1.953765	1.581647	0.529281
34	6	0	2.801546	2.613131	0.211003
35	6	0	4.025025	2.359414	-0.441508

36	6	0	4.374223	1.073725	-0.760771
37	6	0	3.524060	-0.012880	-0.440677
38	6	0	2.277748	0.233017	0.220294
39	1	0	1.360261	-3.027953	0.401617
40	1	0	3.523964	-3.260090	-0.762508
41	1	0	5.306015	0.845442	-1.263208
42	1	0	4.684231	3.182761	-0.689430
43	1	0	2.525268	3.630965	0.459347
44	1	0	1.014960	1.822797	1.009617

O-10/α/1

After PCM corrections, the SCF energy is -922.2228

Number	Number	Type	X	Y	Z
1	7	0	-1.890819	-1.370864	-0.245718
2	6	0	-1.143630	-0.234032	-0.842311
3	6	0	-1.113724	0.959937	0.139573
4	6	0	-2.221080	0.734785	1.190884
5	6	0	-3.570354	0.341547	0.529103
6	6	0	-3.319152	-1.006050	-0.241384
7	6	0	-1.782179	-0.439514	2.079339
8	6	0	-1.473648	-1.645491	1.148060
9	6	0	0.189871	-0.724316	-1.504413
10	8	0	-0.093475	-1.961869	-2.138645
11	6	0	-4.148875	1.412413	-0.348899
12	6	0	-5.299374	2.039688	-0.127324
13	7	0	3.773230	-1.106833	0.963442
14	6	0	3.003010	-2.126805	0.664047
15	6	0	1.842750	-2.036292	-0.130211
16	6	0	1.438616	-0.823466	-0.633906
17	6	0	2.046262	1.607448	-0.893741
18	6	0	2.895782	2.646421	-0.608910
19	6	0	4.020317	2.446658	0.219731
20	6	0	4.281092	1.203698	0.733273
21	6	0	3.431977	0.106496	0.446106
22	6	0	2.274194	0.306412	-0.371854
23	1	0	-1.745746	0.051919	-1.708747
24	1	0	-1.256391	1.899979	-0.397865
25	1	0	-0.156797	1.038359	0.658064
26	1	0	-2.358570	1.637856	1.788591
27	1	0	-4.285199	0.157587	1.336716
28	1	0	-3.876088	-1.820893	0.225823
29	1	0	-3.660961	-0.930577	-1.275662
30	1	0	-2.570969	-0.686233	2.795010
31	1	0	-0.897403	-0.164450	2.658825
32	1	0	-0.411547	-1.877133	1.151020
33	1	0	-1.998927	-2.545302	1.474214
34	1	0	0.412071	-0.008560	-2.301455
35	1	0	-0.868633	-2.314111	-1.658105

36	1	0	-3.578778	1.678777	-1.237206
37	1	0	-5.669331	2.803053	-0.801549
38	1	0	-5.914014	1.811314	0.737797
39	1	0	3.298832	-3.092567	1.066419
40	1	0	1.280471	-2.931883	-0.357063
41	1	0	1.191510	1.791254	-1.530441
42	1	0	2.703328	3.628382	-1.024744
43	1	0	4.680033	3.277520	0.440314
44	1	0	5.142905	1.017307	1.362162

O-10/α/2

After PCM corrections, the SCF energy is -922.2211

Number	Number	Type	X	Y	Z
1	7	0	-1.977164	-1.266659	-0.199584
2	6	0	-1.223040	-0.094567	-0.716948
3	6	0	-1.102580	0.989177	0.378257
4	6	0	-2.174892	0.691729	1.447208
5	6	0	-3.554900	0.414095	0.789828
6	6	0	-3.394761	-0.865285	-0.090719
7	6	0	-1.748478	-0.577366	2.197894
8	6	0	-1.502257	-1.686745	1.138119
9	6	0	0.055500	-0.554946	-1.497961
10	8	0	-0.304197	-1.713422	-2.234401
11	6	0	-4.113033	1.644054	0.118050
12	6	0	-4.603601	1.779466	-1.109139
13	7	0	3.744941	-1.289619	0.722048
14	6	0	2.925816	-2.251377	0.364636
15	6	0	1.731109	-2.047757	-0.353694
16	6	0	1.343988	-0.778992	-0.712495
17	6	0	2.019689	1.646569	-0.761496
18	6	0	2.917484	2.626803	-0.422178
19	6	0	4.075380	2.312303	0.320468
20	6	0	4.319542	1.017014	0.694010
21	6	0	3.420071	-0.020938	0.346140
22	6	0	2.229942	0.293732	-0.384524
23	1	0	-1.859773	0.301894	-1.510509
24	1	0	-1.240161	1.981446	-0.056141
25	1	0	-0.121645	0.983391	0.856341
26	1	0	-2.259827	1.534431	2.137429
27	1	0	-4.243605	0.184791	1.613071
28	1	0	-3.946481	-1.701592	0.343144
29	1	0	-3.783218	-0.716072	-1.097559
30	1	0	-2.526116	-0.875554	2.906347
31	1	0	-0.840970	-0.389298	2.776885
32	1	0	-0.444757	-1.928736	1.067341
33	1	0	-2.025895	-2.608769	1.398407
34	1	0	0.260863	0.230287	-2.231467
35	1	0	-1.065302	-2.087613	-1.747249

36	1	0	-4.120319	2.522859	0.762180
37	1	0	-4.989996	2.733615	-1.447030
38	1	0	-4.652841	0.965736	-1.823007
39	1	0	3.208213	-3.260843	0.653366
40	1	0	1.127615	-2.899226	-0.637474
41	1	0	1.140713	1.917347	-1.330311
42	1	0	2.737886	3.650521	-0.728620
43	1	0	4.773405	3.097345	0.586332
44	1	0	5.205471	0.743545	1.253748

O-10/α/3

After PCM corrections, the SCF energy is -922.2206

Number	Number	Type	X	Y	Z
1	7	0	-1.951835	-1.387655	-0.227982
2	6	0	-1.217322	-0.227908	-0.796640
3	6	0	-1.161774	0.920953	0.231360
4	6	0	-2.295726	0.685155	1.254935
5	6	0	-3.627223	0.312487	0.560572
6	6	0	-3.382571	-1.036405	-0.209682
7	6	0	-1.880611	-0.517044	2.120256
8	6	0	-1.528363	-1.686948	1.159350
9	6	0	0.098632	-0.694519	-1.507477
10	8	0	-0.204005	-1.903049	-2.187373
11	6	0	-4.248095	1.372530	-0.313478
12	6	0	-3.995107	2.677188	-0.315322
13	7	0	3.721455	-1.196746	0.880017
14	6	0	2.938732	-2.199168	0.554760
15	6	0	1.765606	-2.070501	-0.215070
16	6	0	1.362124	-0.836445	-0.664782
17	6	0	1.979057	1.599330	-0.836137
18	6	0	2.839098	2.621816	-0.524456
19	6	0	3.977258	2.382708	0.274586
20	6	0	4.240085	1.118597	0.732676
21	6	0	3.379436	0.038293	0.417177
22	6	0	2.209260	0.277137	-0.371959
23	1	0	-1.840526	0.099811	-1.632759
24	1	0	-1.263518	1.882123	-0.273720
25	1	0	-0.211617	0.942511	0.768376
26	1	0	-2.428803	1.569232	1.881289
27	1	0	-4.357834	0.106483	1.353178
28	1	0	-3.923068	-1.858286	0.264302
29	1	0	-3.735658	-0.964180	-1.240682
30	1	0	-2.693392	-0.793535	2.797517
31	1	0	-1.019483	-0.257958	2.740991
32	1	0	-0.458203	-1.879121	1.157400
33	1	0	-2.020641	-2.613376	1.461672
34	1	0	0.308660	0.052811	-2.278467
35	1	0	-0.961450	-2.278074	-1.695827

36	1	0	-5.017180	1.003245	-0.991062
37	1	0	-4.535277	3.347497	-0.973303
38	1	0	-3.256026	3.130745	0.334600
39	1	0	3.234540	-3.181748	0.914214
40	1	0	1.192515	-2.952877	-0.465408
41	1	0	1.114018	1.812381	-1.449252
42	1	0	2.644897	3.620792	-0.896671
43	1	0	4.645766	3.200509	0.516560
44	1	0	5.111999	0.902679	1.337774

C-2/γ/1

After PCM corrections, the SCF energy is -922.2226

Number	Number	Type	X	Y	Z
1	7	0	1.049790	0.559204	-0.601690
2	6	0	1.119603	-0.304561	0.592635
3	6	0	2.388267	0.019680	1.430107
4	6	0	3.323674	0.888138	0.567834
5	6	0	3.548464	0.257479	-0.833696
6	6	0	2.131699	0.153395	-1.511053
7	6	0	2.640149	2.248468	0.360282
8	6	0	1.236362	1.981990	-0.256812
9	1	0	1.202403	-1.326432	0.213489
10	6	0	-0.183533	-0.276665	1.412067
11	8	0	0.069270	-1.116110	2.548487
12	1	0	-0.730272	-1.152934	3.087571
13	1	0	-0.366856	0.741288	1.764209
14	1	0	2.875485	-0.898758	1.759231
15	1	0	2.125347	0.567478	2.339526
16	1	0	4.286154	1.016509	1.067467
17	1	0	4.165904	0.954074	-1.409146
18	6	0	4.267882	-1.057912	-0.795163
19	6	0	5.460420	-1.290960	-1.333973
20	1	0	3.756709	-1.878614	-0.294928
21	1	0	5.928277	-2.266846	-1.280019
22	1	0	6.012107	-0.511299	-1.849887
23	1	0	2.089309	0.790960	-2.396860
24	1	0	1.936737	-0.869276	-1.840908
25	1	0	3.244581	2.879249	-0.297282
26	1	0	2.551504	2.773613	1.315076
27	1	0	0.446659	2.281954	0.431484
28	1	0	1.088379	2.562052	-1.169815
29	7	0	-3.528444	-1.892763	-0.865390
30	6	0	-2.534609	-2.629129	-0.424816
31	6	0	-1.449731	-2.124568	0.316081
32	6	0	-1.377014	-0.784175	0.616450
33	6	0	-2.537849	1.444375	0.430799
34	6	0	-3.598680	2.183223	-0.026765
35	6	0	-4.629611	1.573131	-0.772751

36	6	0	-4.580893	0.230345	-1.037674
37	6	0	-3.502257	-0.562708	-0.573778
38	6	0	-2.445246	0.051245	0.173804
39	1	0	-0.676925	-2.803450	0.653913
40	1	0	-2.573736	-3.689607	-0.660884
41	1	0	-5.359022	-0.267021	-1.603292
42	1	0	-5.459585	2.170241	-1.131533
43	1	0	-3.646060	3.244796	0.185138
44	1	0	-1.763270	1.941075	0.997637

C-2/γ/2

After PCM corrections, the SCF energy is -922.2204

Number	Number	Type	X	Y	Z
1	7	0	-1.079034	-0.612470	-0.637625
2	6	0	-1.202105	0.213145	0.580722
3	6	0	-2.489533	-0.158659	1.366194
4	6	0	-3.385493	-0.998316	0.437004
5	6	0	-3.555990	-0.298294	-0.939384
6	6	0	-2.133406	-0.187354	-1.575572
7	6	0	-2.691243	-2.346717	0.198111
8	6	0	-1.262812	-2.046016	-0.342888
9	1	0	-1.297742	1.244207	0.232640
10	6	0	0.077890	0.181215	1.435545
11	8	0	-0.218479	0.980769	2.589092
12	1	0	0.558513	0.995137	3.161062
13	1	0	0.271169	-0.843722	1.761481
14	1	0	-2.999333	0.743770	1.704650
15	1	0	-2.250003	-0.736862	2.263307
16	1	0	-4.366359	-1.150429	0.894716
17	1	0	-4.161913	-0.976310	-1.554757
18	6	0	-4.355930	0.974982	-0.824047
19	6	0	-4.070156	2.188368	-1.283848
20	1	0	-5.302030	0.846622	-0.298599
21	1	0	-4.758130	3.011982	-1.134323
22	1	0	-3.158758	2.419429	-1.822014
23	1	0	-2.063257	-0.815989	-2.465716
24	1	0	-1.909296	0.831932	-1.888994
25	1	0	-3.262667	-2.946302	-0.515996
26	1	0	-2.642727	-2.916512	1.129978
27	1	0	-0.504384	-2.356606	0.375398
28	1	0	-1.063443	-2.598896	-1.263108
29	7	0	3.449010	1.929831	-0.703270
30	6	0	2.446530	2.637493	-0.236309
31	6	0	1.353608	2.089559	0.461208
32	6	0	1.282127	0.734490	0.686468
33	6	0	2.452982	-1.476795	0.393105
34	6	0	3.522567	-2.186384	-0.089708
35	6	0	4.561708	-1.532938	-0.786568

36	6	0	4.511783	-0.177676	-0.977951
37	6	0	3.424012	0.585613	-0.485947
38	6	0	2.358934	-0.071776	0.211736
39	1	0	0.573352	2.745856	0.825662
40	1	0	2.484466	3.709607	-0.413038
41	1	0	5.296298	0.352269	-1.503955
42	1	0	5.398422	-2.107140	-1.166698
43	1	0	3.571132	-3.257985	0.063793
44	1	0	1.671851	-2.005377	0.920829

C-2/γ/3

After PCM corrections, the SCF energy is -922.2199

Number	Number	Type	X	Y	Z
1	7	0	1.031822	0.599423	-0.695905
2	6	0	1.173989	-0.321687	0.449071
3	6	0	2.464281	-0.003742	1.251986
4	6	0	3.345720	0.928387	0.396439
5	6	0	3.521390	0.384698	-1.040055
6	6	0	2.081875	0.270528	-1.668853
7	6	0	2.618615	2.279170	0.288759
8	6	0	1.197431	2.007048	-0.286050
9	1	0	1.271917	-1.320611	0.016395
10	6	0	-0.092014	-0.372318	1.322164
11	8	0	0.217722	-1.297511	2.374696
12	1	0	-0.550071	-1.371450	2.954558
13	1	0	-0.265255	0.612033	1.763432
14	1	0	2.979316	-0.926368	1.515417
15	1	0	2.223064	0.497242	2.194409
16	1	0	4.320271	1.067042	0.869510
17	1	0	4.066562	1.148421	-1.609760
18	6	0	4.313636	-0.887056	-1.190682
19	6	0	5.095890	-1.475447	-0.291802
20	1	0	4.239953	-1.344733	-2.176830
21	1	0	5.637550	-2.382164	-0.533873
22	1	0	5.234288	-1.082863	0.708438
23	1	0	1.977802	0.947635	-2.519578
24	1	0	1.901820	-0.742314	-2.035954
25	1	0	3.178459	2.961250	-0.357132
26	1	0	2.555673	2.750224	1.273278
27	1	0	0.427996	2.251489	0.445810
28	1	0	0.999549	2.628325	-1.161858
29	7	0	-3.533097	-1.839255	-0.912838
30	6	0	-2.508669	-2.594533	-0.589918
31	6	0	-1.391860	-2.138566	0.135009
32	6	0	-1.317522	-0.827574	0.544149
33	6	0	-2.512365	1.389854	0.612937
34	6	0	-3.606560	2.146951	0.280961
35	6	0	-4.669792	1.586097	-0.458379

36	6	0	-4.618982	0.272479	-0.842246
37	6	0	-3.506628	-0.539232	-0.508501
38	6	0	-2.416841	0.025844	0.230566
39	1	0	-0.595945	-2.832285	0.375052
40	1	0	-2.548023	-3.631249	-0.914860
41	1	0	-5.421045	-0.187213	-1.406376
42	1	0	-5.526372	2.197375	-0.716815
43	1	0	-3.655117	3.185330	0.586820
44	1	0	-1.714797	1.848385	1.180221

C-2/β/1

After PCM corrections, the SCF energy is -922.2205

Number	Number	Type	X	Y	Z
1	7	0	1.029836	0.563147	-0.587491
2	6	0	1.108635	-0.320312	0.591286
3	6	0	2.387798	-0.003146	1.421430
4	6	0	3.312048	0.885469	0.565975
5	6	0	3.526730	0.275138	-0.845890
6	6	0	2.104835	0.177699	-1.513338
7	6	0	2.619217	2.244724	0.386190
8	6	0	1.210443	1.980637	-0.221157
9	1	0	1.195432	-1.335903	0.197128
10	6	0	-0.188683	-0.319440	1.430285
11	8	0	-0.044894	-1.220044	2.539953
12	1	0	0.655219	-0.890336	3.115711
13	1	0	-0.376713	0.684931	1.816723
14	1	0	2.890089	-0.921988	1.729848
15	1	0	2.142591	0.545161	2.340176
16	1	0	4.277799	1.009544	1.060142
17	1	0	4.138363	0.982910	-1.413751
18	6	0	4.249735	-1.038923	-0.832901
19	6	0	5.445136	-1.256758	-1.371681
20	1	0	3.737604	-1.872848	-0.355683
21	1	0	5.914642	-2.232798	-1.338651
22	1	0	5.997009	-0.464528	-1.867998
23	1	0	2.052509	0.830405	-2.387552
24	1	0	1.911151	-0.839901	-1.859195
25	1	0	3.215041	2.887094	-0.267724
26	1	0	2.538941	2.756197	1.349404
27	1	0	0.425754	2.264889	0.479234
28	1	0	1.050991	2.575187	-1.122792
29	7	0	-3.521506	-1.871094	-0.897769
30	6	0	-2.544438	-2.624121	-0.448558
31	6	0	-1.464186	-2.141316	0.313727
32	6	0	-1.382059	-0.806316	0.630145
33	6	0	-2.521056	1.434699	0.467692
34	6	0	-3.567606	2.191146	0.006114
35	6	0	-4.590114	1.603807	-0.769300

36	6	0	-4.548102	0.265369	-1.056610
37	6	0	-3.485137	-0.545577	-0.587417
38	6	0	-2.434619	0.046177	0.186304
39	1	0	-0.706722	-2.834068	0.656720
40	1	0	-2.593279	-3.681751	-0.695573
41	1	0	-5.321478	-0.215720	-1.642612
42	1	0	-5.409251	2.214204	-1.130835
43	1	0	-3.611348	3.248500	0.239266
44	1	0	-1.754971	1.913063	1.061444

C-2/β/2

After PCM corrections, the SCF energy is -922.2186

Number	Number	Type	X	Y	Z
1	7	0	-1.065991	-0.619477	-0.631954
2	6	0	-1.190972	0.217717	0.577220
3	6	0	-2.490348	-0.143677	1.354491
4	6	0	-3.380396	-0.994468	0.428311
5	6	0	-3.539820	-0.305770	-0.955071
6	6	0	-2.112314	-0.200629	-1.581054
7	6	0	-2.683422	-2.344584	0.209342
8	6	0	-1.251751	-2.049914	-0.326573
9	1	0	-1.283700	1.245738	0.220416
10	6	0	0.083619	0.198084	1.450280
11	8	0	-0.102744	1.039957	2.598659
12	1	0	-0.837642	0.693126	3.118064
13	1	0	0.281637	-0.820677	1.792288
14	1	0	-3.009581	0.760653	1.676580
15	1	0	-2.272133	-0.729492	2.256913
16	1	0	-4.363932	-1.140857	0.881807
17	1	0	-4.140636	-0.990801	-1.567331
18	6	0	-4.342124	0.967383	-0.856112
19	6	0	-4.042816	2.182475	-1.302348
20	1	0	-5.303511	0.837272	-0.359604
21	1	0	-4.734657	3.005584	-1.168807
22	1	0	-3.118640	2.414556	-1.817663
23	1	0	-2.036305	-0.836058	-2.465942
24	1	0	-1.884947	0.815852	-1.900838
25	1	0	-3.251736	-2.950960	-0.501184
26	1	0	-2.641794	-2.905037	1.147439
27	1	0	-0.496794	-2.355592	0.397342
28	1	0	-1.049038	-2.610729	-1.241153
29	7	0	3.440883	1.922181	-0.716500
30	6	0	2.449579	2.636885	-0.236536
31	6	0	1.361685	2.097719	0.475372
32	6	0	1.286940	0.744592	0.705018
33	6	0	2.448106	-1.472069	0.418151
34	6	0	3.508563	-2.189215	-0.073369
35	6	0	4.538340	-1.545431	-0.792364

36	6	0	4.489201	-0.191666	-0.994129
37	6	0	3.411572	0.579210	-0.491875
38	6	0	2.354081	-0.069116	0.224848
39	1	0	0.591885	2.760018	0.849433
40	1	0	2.492747	3.708535	-0.414670
41	1	0	5.267590	0.332014	-1.535284
42	1	0	5.368599	-2.125028	-1.178433
43	1	0	3.557704	-3.259060	0.091921
44	1	0	1.676256	-1.992792	0.967012

C-2/β/3

After PCM corrections, the SCF energy is -922.2180

Number	Number	Type	X	Y	Z
1	7	0	0.995887	0.666456	-0.632665
2	6	0	1.155508	-0.318218	0.453935
3	6	0	2.472514	-0.050537	1.236309
4	6	0	3.352696	0.893927	0.390049
5	6	0	3.463581	0.403750	-1.072364
6	6	0	2.002982	0.371202	-1.659837
7	6	0	2.656599	2.265334	0.360955
8	6	0	1.203754	2.045730	-0.152808
9	1	0	1.239442	-1.292887	-0.033187
10	6	0	-0.093402	-0.416532	1.358638
11	8	0	0.124030	-1.405678	2.375874
12	1	0	0.868853	-1.126614	2.921397
13	1	0	-0.276144	0.546942	1.840922
14	1	0	2.983178	-0.988120	1.456305
15	1	0	2.272413	0.442041	2.196841
16	1	0	4.345156	0.986858	0.835455
17	1	0	4.021259	1.170302	-1.625670
18	6	0	4.202700	-0.889672	-1.295230
19	6	0	5.005396	-1.529677	-0.450985
20	1	0	4.068600	-1.315061	-2.289249
21	1	0	5.504276	-2.445802	-0.744068
22	1	0	5.207500	-1.170698	0.551366
23	1	0	1.893149	1.105354	-2.460968
24	1	0	1.781075	-0.609889	-2.085288
25	1	0	3.204411	2.951919	-0.290228
26	1	0	2.652423	2.707894	1.360755
27	1	0	0.480023	2.255335	0.634332
28	1	0	0.969197	2.721007	-0.977907
29	7	0	-3.520522	-1.824530	-0.923938
30	6	0	-2.520510	-2.599664	-0.574016
31	6	0	-1.409664	-2.164544	0.173172
32	6	0	-1.320079	-0.855177	0.581439
33	6	0	-2.474516	1.383089	0.628306
34	6	0	-3.543726	2.162640	0.268357
35	6	0	-4.597468	1.624273	-0.500842

36	6	0	-4.562706	0.309922	-0.884063
37	6	0	-3.476515	-0.524432	-0.520836
38	6	0	-2.395062	0.018624	0.245750
39	1	0	-0.633710	-2.873259	0.431721
40	1	0	-2.574838	-3.637079	-0.894712
41	1	0	-5.359159	-0.133948	-1.468534
42	1	0	-5.434153	2.252960	-0.781950
43	1	0	-3.581143	3.200649	0.577287
44	1	0	-1.684090	1.823807	1.219017

C-7/α/1

After PCM corrections, the SCF energy is -922.2223

Number	Number	Type	X	Y	Z
1	7	0	1.476943	0.452584	0.843114
2	6	0	1.184691	-0.102513	-0.494474
3	6	0	2.230395	-1.197088	-0.871718
4	6	0	3.329389	-1.217154	0.204943
5	6	0	3.951721	0.192029	0.395624
6	6	0	2.767638	1.150958	0.781748
7	6	0	2.683651	-1.632374	1.537682
8	6	0	1.558332	-0.606750	1.865500
9	6	0	-0.256484	-0.625157	-0.626395
10	8	0	-0.439702	-1.181844	-1.939525
11	6	0	4.719504	0.682144	-0.794964
12	6	0	6.020611	0.954351	-0.806766
13	7	0	-3.476597	2.201120	0.188955
14	6	0	-2.239899	2.592698	-0.001127
15	6	0	-1.159726	1.718841	-0.250487
16	6	0	-1.371026	0.364052	-0.321034
17	6	0	-3.082717	-1.473230	-0.193037
18	6	0	-4.383288	-1.858240	0.014812
19	6	0	-5.382590	-0.899069	0.285607
20	6	0	-5.060841	0.431857	0.339572
21	6	0	-3.727687	0.861714	0.130547
22	6	0	-2.709116	-0.105694	-0.133427
23	1	0	1.287508	0.734115	-1.193783
24	1	0	2.647336	-1.010737	-1.862694
25	1	0	1.756540	-2.180630	-0.923173
26	1	0	4.112222	-1.925945	-0.073443
27	1	0	4.649049	0.131293	1.236986
28	1	0	2.955057	1.609362	1.755389
29	1	0	2.681374	1.963697	0.055650
30	1	0	3.435275	-1.653842	2.331505
31	1	0	2.278220	-2.644368	1.453439
32	1	0	0.586770	-1.095000	1.949328
33	1	0	1.740321	-0.116033	2.823849
34	1	0	-0.369766	-1.484670	0.037814
35	1	0	-0.560776	-0.455745	-2.565254

36	1	0	4.150003	0.836298	-1.710040
37	1	0	6.518003	1.315219	-1.699331
38	1	0	6.635356	0.826249	0.078658
39	1	0	-2.055974	3.663041	0.049434
40	1	0	-0.168536	2.135655	-0.350615
41	1	0	-2.337812	-2.220970	-0.427831
42	1	0	-4.648221	-2.907766	-0.036375
43	1	0	-6.405109	-1.219585	0.447058
44	1	0	-5.806999	1.190942	0.539509

C-7/α/2

After PCM corrections, the SCF energy is -922.2202

Number	Number	Type	X	Y	Z
1	7	0	-1.526028	0.409154	-0.867245
2	6	0	-1.243562	-0.066731	0.503296
3	6	0	-2.292080	-1.139553	0.939354
4	6	0	-3.299256	-1.329823	-0.205680
5	6	0	-3.989086	0.018201	-0.546578
6	6	0	-2.856961	1.038849	-0.872194
7	6	0	-2.535503	-1.809667	-1.450004
8	6	0	-1.518409	-0.696897	-1.841108
9	6	0	0.197472	-0.579595	0.676327
10	8	0	0.378128	-1.037783	2.027255
11	6	0	-4.986346	0.429030	0.506008
12	6	0	-5.101408	1.595129	1.133010
13	7	0	3.419046	2.183036	-0.329223
14	6	0	2.183010	2.587019	-0.162139
15	6	0	1.102988	1.732149	0.146076
16	6	0	1.313609	0.384579	0.303883
17	6	0	3.025526	-1.457410	0.300217
18	6	0	4.326040	-1.855446	0.117841
19	6	0	5.324568	-0.917105	-0.220412
20	6	0	5.002518	0.407089	-0.364156
21	6	0	3.669822	0.850305	-0.182099
22	6	0	2.651426	-0.097250	0.147310
23	1	0	-1.351835	0.808845	1.151720
24	1	0	-2.801287	-0.828815	1.853296
25	1	0	-1.802772	-2.090157	1.163169
26	1	0	-4.054134	-2.066793	0.080920
27	1	0	-4.575027	-0.158078	-1.458721
28	1	0	-3.015190	1.492503	-1.853131
29	1	0	-2.835744	1.850318	-0.143557
30	1	0	-3.229086	-2.009415	-2.271301
31	1	0	-2.023323	-2.750335	-1.228773
32	1	0	-0.505665	-1.092928	-1.926497
33	1	0	-1.763002	-0.267111	-2.814728
34	1	0	0.311735	-1.485859	0.077880
35	1	0	0.479476	-0.266580	2.600391

36	1	0	-5.709727	-0.348415	0.750259
37	1	0	-5.886905	1.756204	1.861770
38	1	0	-4.439483	2.433519	0.951029
39	1	0	1.999395	3.651899	-0.282097
40	1	0	0.111932	2.154230	0.221107
41	1	0	2.281490	-2.187305	0.587938
42	1	0	4.591435	-2.898962	0.240210
43	1	0	6.347071	-1.247673	-0.360289
44	1	0	5.748279	1.150603	-0.617081

C-7/α/3

After PCM corrections, the SCF energy is -922.2197

Number	Number	Type	X	Y	Z
1	7	0	1.463326	0.597152	0.869061
2	6	0	1.228310	-0.006942	-0.457973
3	6	0	2.322904	-1.070173	-0.778695
4	6	0	3.358920	-1.072452	0.361130
5	6	0	3.955421	0.334219	0.582003
6	6	0	2.746461	1.309656	0.830579
7	6	0	2.632631	-1.478649	1.655573
8	6	0	1.518792	-0.424834	1.931217
9	6	0	-0.189203	-0.586516	-0.608222
10	8	0	-0.323572	-1.183787	-1.909959
11	6	0	4.890602	0.852624	-0.477179
12	6	0	5.437300	0.183039	-1.486848
13	7	0	-3.529848	2.137015	0.056998
14	6	0	-2.310085	2.570832	-0.151710
15	6	0	-1.192836	1.732359	-0.353911
16	6	0	-1.345886	0.367721	-0.354334
17	6	0	-2.980414	-1.531395	-0.145561
18	6	0	-4.264312	-1.960812	0.078670
19	6	0	-5.303506	-1.032921	0.304457
20	6	0	-5.038192	0.311458	0.294560
21	6	0	-3.723822	0.787004	0.065426
22	6	0	-2.664181	-0.148233	-0.148591
23	1	0	1.319403	0.812454	-1.178444
24	1	0	2.791286	-0.855689	-1.739068
25	1	0	1.878915	-2.064964	-0.865950
26	1	0	4.152697	-1.790431	0.143632
27	1	0	4.540365	0.295907	1.510307
28	1	0	2.869401	1.843991	1.775571
29	1	0	2.692798	2.059592	0.036919
30	1	0	3.338324	-1.526070	2.489400
31	1	0	2.205546	-2.478675	1.541083
32	1	0	0.539064	-0.894744	2.024993
33	1	0	1.698890	0.100296	2.871595
34	1	0	-0.285937	-1.432466	0.075254
35	1	0	-0.455732	-0.479034	-2.557382

36	1	0	5.149401	1.905501	-0.366940
37	1	0	6.115968	0.671493	-2.176102
38	1	0	5.240610	-0.867319	-1.666260
39	1	0	-2.172122	3.649275	-0.156200
40	1	0	-0.220544	2.186314	-0.477375
41	1	0	-2.204694	-2.257411	-0.346495
42	1	0	-4.484474	-3.021872	0.077185
43	1	0	-6.312152	-1.387979	0.480253
44	1	0	-5.816205	1.047042	0.457719

C-7/γ/1

After PCM corrections, the SCF energy is -922.2212

Number	Number	Type	X	Y	Z
1	7	0	-1.448027	0.395926	-0.854817
2	6	0	-1.188919	-0.066374	0.522616
3	6	0	-2.237811	-1.141324	0.947059
4	6	0	-3.314092	-1.232019	-0.148648
5	6	0	-3.931406	0.161729	-0.443595
6	6	0	-2.739817	1.095107	-0.867634
7	6	0	-2.640023	-1.731127	-1.438043
8	6	0	-1.507687	-0.727467	-1.806964
9	6	0	0.246759	-0.566302	0.722017
10	8	0	0.332039	-0.890046	2.123129
11	6	0	-4.721220	0.727845	0.697949
12	6	0	-6.023192	0.994589	0.668702
13	7	0	3.484497	2.186974	-0.245917
14	6	0	2.255741	2.600738	-0.043409
15	6	0	1.169818	1.750339	0.249584
16	6	0	1.360892	0.394445	0.340823
17	6	0	3.040639	-1.475341	0.184459
18	6	0	4.334131	-1.882872	-0.026559
19	6	0	5.345162	-0.941200	-0.312581
20	6	0	5.040465	0.393056	-0.382323
21	6	0	3.716258	0.846858	-0.166754
22	6	0	2.684787	-0.101216	0.123346
23	1	0	-1.307149	0.809169	1.166118
24	1	0	-2.671459	-0.894721	1.917116
25	1	0	-1.761780	-2.118452	1.065702
26	1	0	-4.103347	-1.921808	0.158103
27	1	0	-4.612682	0.045263	-1.292304
28	1	0	-2.906394	1.486839	-1.873635
29	1	0	-2.669628	1.954162	-0.195383
30	1	0	-3.374506	-1.804654	-2.244720
31	1	0	-2.236833	-2.735290	-1.280114
32	1	0	-0.534565	-1.219188	-1.835556
33	1	0	-1.667778	-0.301723	-2.799708
34	1	0	0.368507	-1.487744	0.142055
35	1	0	1.249108	-1.089972	2.344531

36	1	0	-4.167493	0.945151	1.609859
37	1	0	-6.537412	1.412751	1.526035
38	1	0	-6.621960	0.804255	-0.216629
39	1	0	2.087363	3.672439	-0.113279
40	1	0	0.190191	2.185487	0.382247
41	1	0	2.285420	-2.222308	0.395259
42	1	0	4.581065	-2.936734	0.023748
43	1	0	6.361670	-1.277932	-0.478015
44	1	0	5.795142	1.138296	-0.601590

C-7/γ/2

After PCM corrections, the SCF energy is -922.2190

Number	Number	Type	X	Y	Z
1	7	0	-1.474920	0.274195	-0.909081
2	6	0	-1.254885	-0.014649	0.521880
3	6	0	-2.309258	-1.039890	1.046611
4	6	0	-3.294215	-1.349597	-0.092006
5	6	0	-3.952980	-0.039574	-0.602480
6	6	0	-2.796619	0.906901	-1.051799
7	6	0	-2.511116	-1.981800	-1.253907
8	6	0	-1.443106	-0.951558	-1.725366
9	6	0	0.177663	-0.474216	0.819388
10	8	0	0.234370	-0.604381	2.253040
11	6	0	-4.942824	0.517530	0.388283
12	6	0	-5.036586	1.751423	0.872454
13	7	0	3.421616	2.156219	-0.427133
14	6	0	2.199344	2.595719	-0.239354
15	6	0	1.113359	1.780984	0.139051
16	6	0	1.295907	0.435218	0.337330
17	6	0	2.964163	-1.453293	0.319635
18	6	0	4.251566	-1.886168	0.122972
19	6	0	5.262613	-0.979679	-0.260101
20	6	0	4.964010	0.345755	-0.438164
21	6	0	3.646092	0.825586	-0.240406
22	6	0	2.613554	-0.087326	0.145088
23	1	0	-1.397425	0.930351	1.051325
24	1	0	-2.831328	-0.637735	1.915876
25	1	0	-1.823546	-1.962780	1.373656
26	1	0	-4.068463	-2.036457	0.259908
27	1	0	-4.541851	-0.316536	-1.487217
28	1	0	-2.921256	1.196691	-2.097391
29	1	0	-2.783652	1.825871	-0.464811
30	1	0	-3.188217	-2.242709	-2.071916
31	1	0	-2.040189	-2.910448	-0.919679
32	1	0	-0.438691	-1.375555	-1.692687
33	1	0	-1.617634	-0.652310	-2.760974
34	1	0	0.315344	-1.465135	0.374477
35	1	0	1.140881	-0.803699	2.514710

36	1	0	-5.681946	-0.210655	0.721295
37	1	0	-5.819929	2.011358	1.574422
38	1	0	-4.358068	2.549909	0.597912
39	1	0	2.037405	3.659480	-0.394175
40	1	0	0.139649	2.233815	0.255746
41	1	0	2.209791	-2.174294	0.608121
42	1	0	4.493910	-2.933263	0.260806
43	1	0	6.274209	-1.336437	-0.413160
44	1	0	5.719092	1.064489	-0.731713

C-7/γ/3

After PCM corrections, the SCF energy is -922.2185

Number	Number	Type	X	Y	Z
1	7	0	-1.424643	0.516062	-0.896657
2	6	0	-1.234901	0.047279	0.489449
3	6	0	-2.334575	-0.989795	0.875802
4	6	0	-3.331195	-1.108382	-0.292798
5	6	0	-3.924654	0.267474	-0.665735
6	6	0	-2.710535	1.221063	-0.969743
7	6	0	-2.560947	-1.631269	-1.518633
8	6	0	-1.441166	-0.602205	-1.856767
9	6	0	0.174567	-0.501240	0.740747
10	8	0	0.206979	-0.806279	2.148085
11	6	0	-4.893433	0.879581	0.310165
12	6	0	-5.468853	0.308469	1.363469
13	7	0	3.539605	2.118087	-0.164160
14	6	0	2.332500	2.584262	0.054822
15	6	0	1.208507	1.778528	0.328596
16	6	0	1.334584	0.412737	0.380788
17	6	0	2.927249	-1.529019	0.178002
18	6	0	4.199880	-1.990975	-0.046946
19	6	0	5.252632	-1.090711	-0.315524
20	6	0	5.009790	0.257428	-0.352157
21	6	0	3.708455	0.767045	-0.120832
22	6	0	2.633933	-0.138885	0.148486
23	1	0	-1.348791	0.926744	1.127682
24	1	0	-2.832508	-0.685722	1.795804
25	1	0	-1.890115	-1.969352	1.070818
26	1	0	-4.129702	-1.807205	-0.034317
27	1	0	-4.481151	0.137484	-1.603204
28	1	0	-2.803593	1.657991	-1.966703
29	1	0	-2.684082	2.045926	-0.253163
30	1	0	-3.238469	-1.762417	-2.366633
31	1	0	-2.135066	-2.613424	-1.295498
32	1	0	-0.457905	-1.073855	-1.869652
33	1	0	-1.589732	-0.171808	-2.849302
34	1	0	0.278176	-1.435321	0.178915
35	1	0	1.103254	-1.064096	2.393235

36	1	0	-5.152133	1.915144	0.090020
37	1	0	-6.169243	0.858459	1.980871
38	1	0	-5.275453	-0.718136	1.651014
39	1	0	2.215126	3.664340	0.015260
40	1	0	0.251813	2.257195	0.479878
41	1	0	2.139979	-2.245140	0.377201
42	1	0	4.398128	-3.055947	-0.020140
43	1	0	6.252087	-1.470010	-0.492514
44	1	0	5.797781	0.972044	-0.555669

C-7/β/1

After PCM corrections, the SCF energy is -922.2200

Number	Number	Type	X	Y	Z
1	7	0	1.469779	0.438260	0.859098
2	6	0	1.180808	-0.118028	-0.477123
3	6	0	2.230694	-1.215728	-0.842525
4	6	0	3.342524	-1.208007	0.222586
5	6	0	3.942802	0.213471	0.389403
6	6	0	2.750338	1.154514	0.793841
7	6	0	2.715049	-1.618571	1.565225
8	6	0	1.565541	-0.616701	1.883664
9	6	0	-0.260510	-0.635487	-0.623927
10	8	0	-0.472905	-1.081714	-1.975406
11	6	0	4.678288	0.706593	-0.820788
12	6	0	5.977331	0.984833	-0.863735
13	7	0	-3.464012	2.206135	0.186833
14	6	0	-2.225701	2.591080	-0.008515
15	6	0	-1.152003	1.712330	-0.265011
16	6	0	-1.370844	0.360211	-0.335346
17	6	0	-3.091573	-1.467910	-0.204158
18	6	0	-4.393293	-1.847182	0.005435
19	6	0	-5.387022	-0.883303	0.280766
20	6	0	-5.057224	0.445331	0.336828
21	6	0	-3.722121	0.868890	0.125279
22	6	0	-2.708923	-0.103046	-0.143500
23	1	0	1.287626	0.709037	-1.183688
24	1	0	2.636458	-1.052864	-1.842581
25	1	0	1.775417	-2.213935	-0.846823
26	1	0	4.133293	-1.906992	-0.057600
27	1	0	4.658413	0.168683	1.216192
28	1	0	2.939724	1.605604	1.770439
29	1	0	2.648567	1.972555	0.076174
30	1	0	3.472730	-1.608083	2.353203
31	1	0	2.335776	-2.642314	1.501002
32	1	0	0.604143	-1.125818	1.958697
33	1	0	1.729675	-0.122708	2.843446
34	1	0	-0.391636	-1.488289	0.053185
35	1	0	0.098992	-1.840060	-2.146095

36	1	0	4.086058	0.858784	-1.721712
37	1	0	6.451390	1.348379	-1.767777
38	1	0	6.613640	0.860204	0.006877
39	1	0	-2.035699	3.660357	0.041796
40	1	0	-0.161179	2.125982	-0.378191
41	1	0	-2.351849	-2.219960	-0.441176
42	1	0	-4.663970	-2.895232	-0.047301
43	1	0	-6.411114	-1.198384	0.442966
44	1	0	-5.798546	1.208246	0.540307

C-7/β/2

After PCM corrections, the SCF energy is -922.2178

Number	Number	Type	X	Y	Z
1	7	0	1.517754	0.348343	0.910275
2	6	0	1.245134	-0.105711	-0.467823
3	6	0	2.292493	-1.183815	-0.899679
4	6	0	3.347888	-1.313366	0.212252
5	6	0	3.985408	0.069472	0.511777
6	6	0	2.824163	1.026480	0.923868
7	6	0	2.648560	-1.811786	1.486483
8	6	0	1.550222	-0.773442	1.863371
9	6	0	-0.198280	-0.597602	-0.673318
10	8	0	-0.401899	-0.918200	-2.061099
11	6	0	4.883836	0.529731	-0.607974
12	6	0	4.906576	1.703257	-1.230612
13	7	0	-3.389911	2.182307	0.366190
14	6	0	-2.149523	2.575995	0.203828
15	6	0	-1.080144	1.716349	-0.124504
16	6	0	-1.305526	0.375755	-0.306945
17	6	0	-3.036587	-1.447078	-0.337606
18	6	0	-4.340910	-1.835398	-0.163777
19	6	0	-5.329684	-0.893248	0.192807
20	6	0	-4.992715	0.423777	0.363578
21	6	0	-3.655007	0.856514	0.190811
22	6	0	-2.646490	-0.094671	-0.158473
23	1	0	1.370419	0.769622	-1.109560
24	1	0	2.758195	-0.912967	-1.848790
25	1	0	1.822574	-2.165198	-1.040303
26	1	0	4.125734	-2.017890	-0.093266
27	1	0	4.641617	-0.078665	1.379508
28	1	0	2.989168	1.420301	1.929044
29	1	0	2.756985	1.883049	0.252199
30	1	0	3.374408	-1.924858	2.296223
31	1	0	2.212224	-2.798965	1.309562
32	1	0	0.563117	-1.235303	1.902865
33	1	0	1.733696	-0.351548	2.853600
34	1	0	-0.341153	-1.507295	-0.077343
35	1	0	0.185996	-1.644570	-2.302012

36	1	0	5.619175	-0.215223	-0.911195
37	1	0	5.629985	1.899912	-2.012864
38	1	0	4.227046	2.513246	-0.994704
39	1	0	-1.954147	3.636190	0.344621
40	1	0	-0.086911	2.131864	-0.202450
41	1	0	-2.300587	-2.179815	-0.638352
42	1	0	-4.617573	-2.873247	-0.307991
43	1	0	-6.355857	-1.215312	0.325519
44	1	0	-5.730308	1.170448	0.630837

C-7/β/3

After PCM corrections, the SCF energy is -922.2174

Number	Number	Type	X	Y	Z
1	7	0	1.460269	0.541968	0.922082
2	6	0	1.226458	-0.043453	-0.412090
3	6	0	2.319537	-1.109985	-0.733458
4	6	0	3.401116	-1.056527	0.363517
5	6	0	3.948167	0.376626	0.540494
6	6	0	2.718011	1.297255	0.880421
7	6	0	2.740242	-1.473045	1.689486
8	6	0	1.560636	-0.493295	1.966703
9	6	0	-0.193220	-0.609703	-0.583406
10	8	0	-0.359464	-1.098055	-1.926491
11	6	0	4.778346	0.929632	-0.587207
12	6	0	5.305536	0.272618	-1.615117
13	7	0	-3.502544	2.149533	0.071323
14	6	0	-2.275562	2.569031	-0.124890
15	6	0	-1.169027	1.718558	-0.332006
16	6	0	-1.340304	0.357956	-0.348947
17	6	0	-2.999419	-1.521799	-0.169168
18	6	0	-4.290101	-1.937716	0.038814
19	6	0	-5.319770	-0.998919	0.264496
20	6	0	-5.036558	0.341559	0.272407
21	6	0	-3.714027	0.802860	0.060533
22	6	0	-2.664492	-0.143118	-0.156483
23	1	0	1.328100	0.774946	-1.128879
24	1	0	2.745216	-0.938428	-1.722148
25	1	0	1.896643	-2.122627	-0.736661
26	1	0	4.213420	-1.745401	0.122413
27	1	0	4.602179	0.365147	1.421974
28	1	0	2.855225	1.781453	1.849929
29	1	0	2.614496	2.088320	0.133242
30	1	0	3.471554	-1.444048	2.501586
31	1	0	2.383161	-2.504193	1.618501
32	1	0	0.610350	-1.024122	2.031688
33	1	0	1.693216	0.021093	2.920642
34	1	0	-0.315405	-1.448020	0.113087
35	1	0	0.260276	-1.823469	-2.071948

36	1	0	4.973874	1.999044	-0.514093
37	1	0	5.906460	0.787156	-2.355494
38	1	0	5.170582	-0.792820	-1.759844
39	1	0	-2.123025	3.645445	-0.115733
40	1	0	-0.192165	2.162462	-0.453723
41	1	0	-2.230926	-2.256096	-0.367576
42	1	0	-4.523975	-2.995789	0.023563
43	1	0	-6.334654	-1.342779	0.426125
44	1	0	-5.806375	1.085454	0.436859

4. Full reference 25.

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