Supplementary Material

Identification of local benzenoid aromaticity and global aromaticity of polycyclic aromatic hydrocarbons (PAHs) *via* the corresponding ring current effects in ^{1}H NMR spectroscopy

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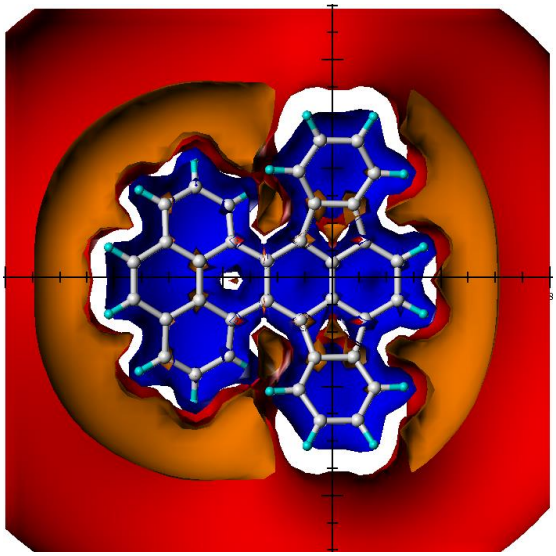

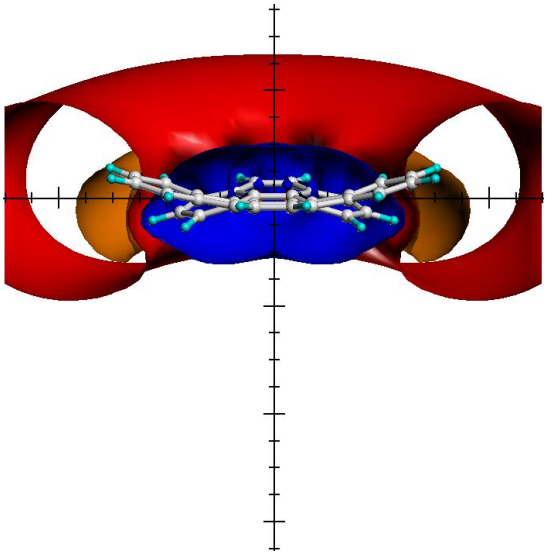

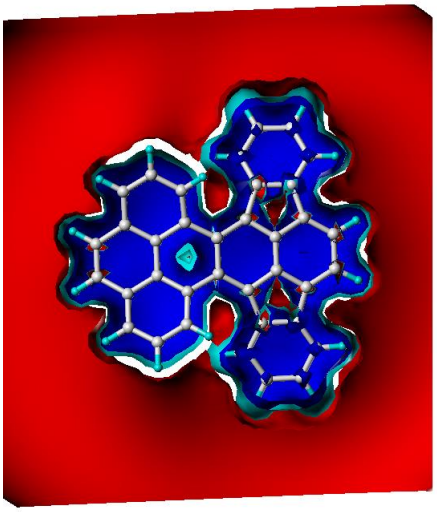

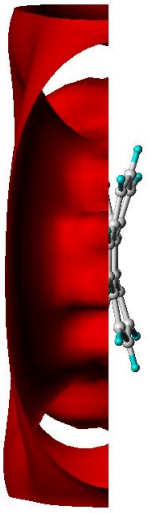

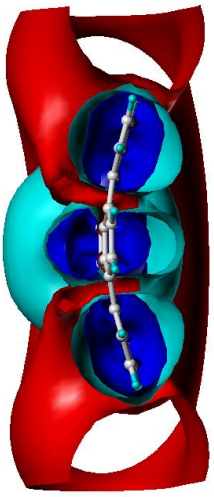

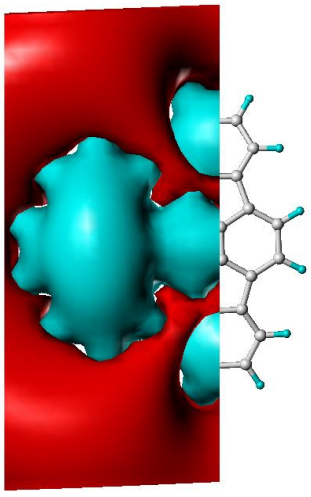

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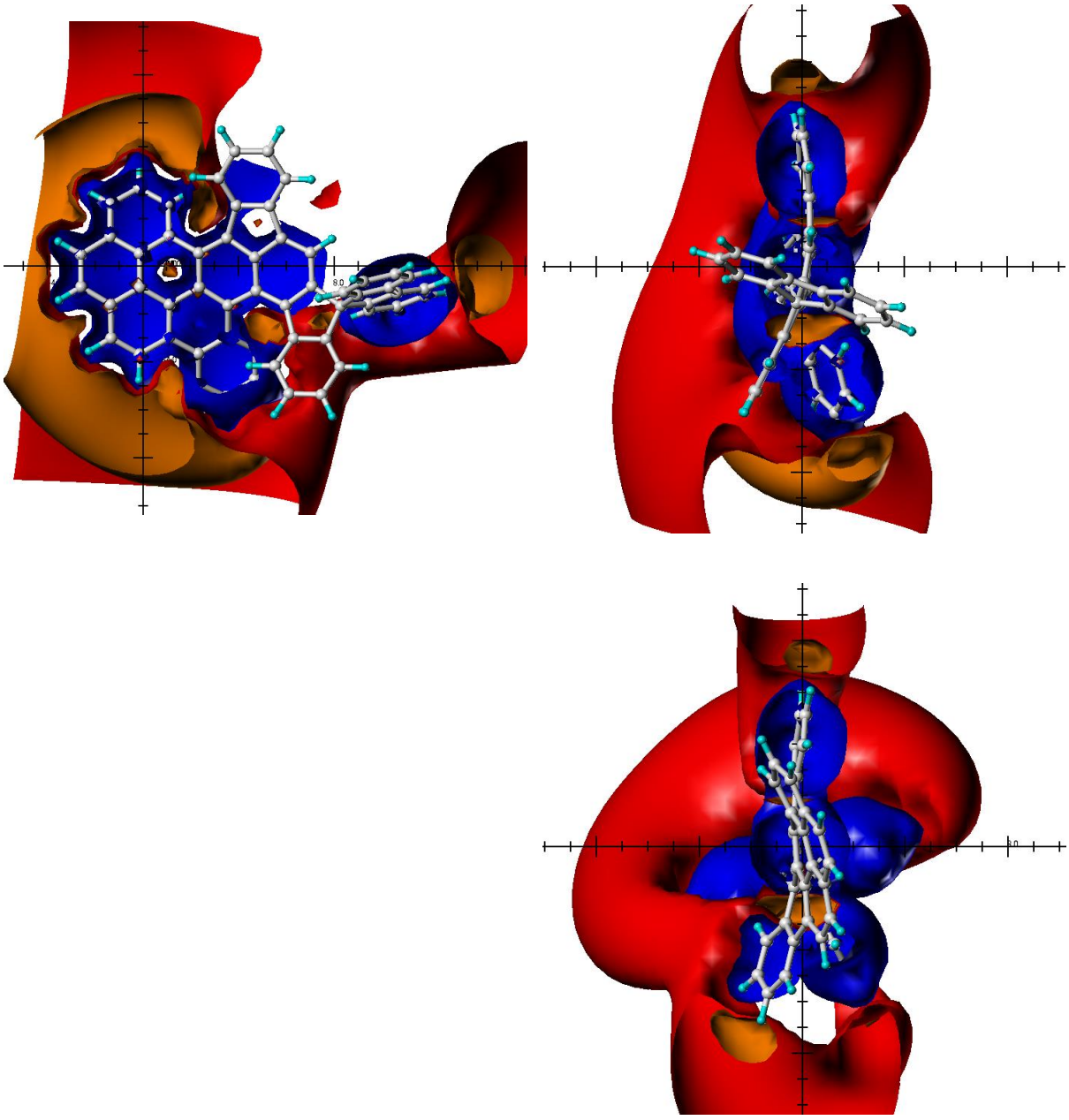

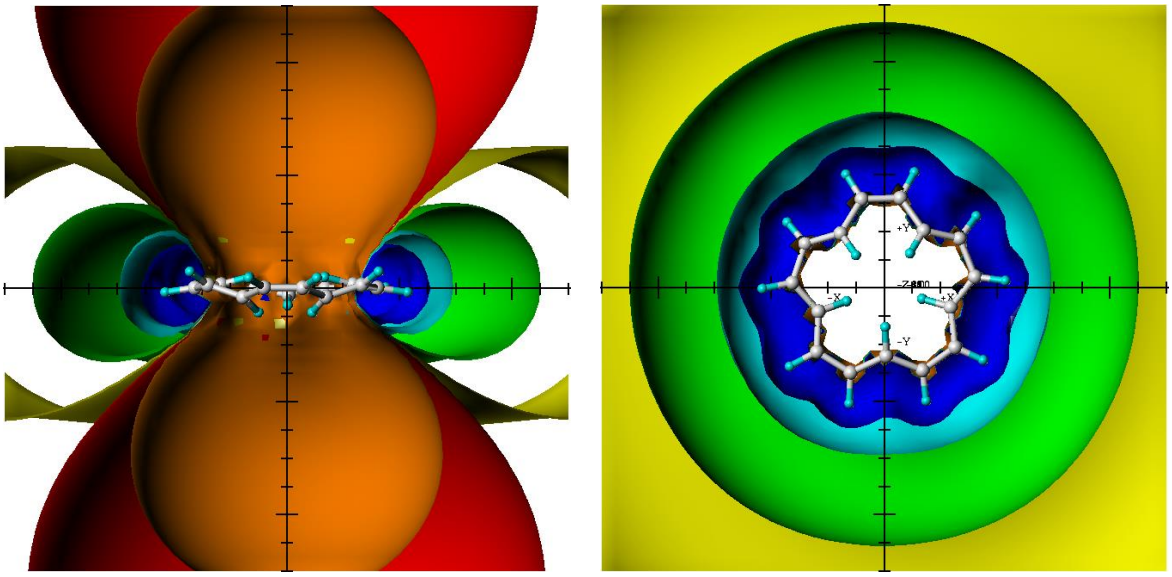

Table S1: Coordinates and absolute energies of the Compounds **1–8** studied at the B3LYP/6-311G(d,p) level of theory.

1

HF=-3224.6169485 a.u.

1	6	0.910963	2.735172	1.016692
2	6	-0.246141	3.419410	0.714934
3	6	-1.288370	2.805029	0.012062
4	6	-1.230713	1.404127	-0.166770
5	6	-0.020146	0.709366	0.111283
6	6	1.125026	1.409268	0.586749
7	6	0.020118	-0.709251	-0.111249
8	6	1.230663	-1.404019	0.166887
9	6	2.434835	-0.683153	0.517949
10	6	2.440512	0.738224	0.607978
11	6	1.288300	-2.804937	-0.011824
12	6	2.383299	-3.543971	0.592604
13	6	3.523491	-2.830534	1.023520
14	6	3.639743	-1.407158	0.685483
15	1	1.666258	3.252272	1.579179
16	1	-0.337762	4.453501	1.022919
17	6	-2.383405	3.544099	-0.592251
18	6	-2.434871	0.683261	-0.517879
19	6	-1.125044	-1.409161	-0.586733
20	6	3.692655	1.407142	0.667324
21	6	0.246079	-3.419354	-0.714673
22	6	2.277994	-4.918358	0.886377
23	6	4.452078	-3.487237	1.855780
24	6	4.887496	-0.754332	0.551535
25	6	-3.523605	2.830681	-1.023184
26	6	-3.639799	1.407259	-0.685315
27	6	-2.440524	-0.738106	-0.608042
28	6	-0.910992	-2.735109	-1.016543
29	6	3.239094	-5.559378	1.645089
30	6	4.316841	-4.828680	2.161355
31	6	4.927208	0.702339	0.576512
32	6	3.752274	2.899409	0.763398
33	6	4.120036	3.517859	1.962773
34	6	4.188449	4.906530	2.052759
35	6	3.897146	5.695296	0.941085
36	6	3.535896	5.086686	-0.261033
37	6	3.462416	3.699585	-0.348337
38	6	6.254848	1.394871	0.493249
39	6	7.352785	0.569506	0.642023
40	6	7.288998	-0.854457	0.527871
41	6	6.120080	-1.532934	0.296945
42	6	8.674896	0.954499	0.306866
43	6	9.416454	-0.207668	-0.013000
44	6	8.552823	-1.318896	0.100456
45	6	9.010615	2.196693	-0.200875
46	6	7.919683	3.123596	-0.212230
47	6	6.622505	2.742326	0.101812
48	6	10.287329	2.260177	-0.875244
49	6	11.011780	1.121008	-1.176014
50	6	10.528379	-0.197524	-0.834881
51	6	10.852484	-1.477195	-1.422337
52	6	8.733863	-2.478851	-0.632804
53	6	7.536316	-3.254256	-0.805264
54	6	6.298298	-2.800074	-0.376381

55	6	-2.278133	4.918517	-0.885896
56	6	-3.239281	5.559600	-1.644491
57	6	-4.317041	4.828935	-2.160776
58	6	-4.452238	3.487458	-1.855338
59	6	-4.887533	0.754378	-0.551432
60	6	-4.927231	-0.702288	-0.576731
61	6	-3.692646	-1.407032	-0.667612
62	6	-3.752189	-2.899279	-0.764008
63	6	-3.462763	-3.699647	0.347699
64	6	-3.536149	-5.086737	0.260103
65	6	-3.896856	-5.695135	-0.942284
66	6	-4.187710	-4.906171	-2.053939
67	6	-4.119395	-3.517517	-1.963662
68	6	-6.120105	1.532917	-0.296589
69	6	-7.289027	0.854487	-0.527594
70	6	-7.352817	-0.569447	-0.642092
71	6	-6.254871	-1.394854	-0.493602
72	6	-8.552830	1.318828	-0.100014
73	6	-9.416452	0.207575	0.013224
74	6	-8.674911	-0.954515	-0.306950
75	6	-6.622538	-2.742413	-0.102507
76	6	-7.919704	-3.123754	0.211508
77	6	-9.010625	-2.196836	0.200479
78	6	-6.298284	2.799906	0.377034
79	6	-7.536281	3.253991	0.806080
80	6	-8.733837	2.478620	0.633510
81	6	-9.995651	2.560534	1.332131
82	6	-10.852433	1.476784	1.422890
83	6	-10.528350	0.197242	0.835138
84	6	-11.011743	-1.121372	1.175966
85	6	-10.287311	-2.260472	0.874889
86	6	9.995702	-2.560924	-1.331362
87	1	10.648856	3.217076	-1.238100
88	1	0.337675	-4.453478	-1.022560
89	1	1.400952	-5.466109	0.564894
90	1	5.280183	-2.929367	2.270885
91	1	-1.666275	-3.252256	-1.579000
92	1	3.132530	-6.612797	1.878080
93	1	5.039750	-5.308359	2.811077
94	1	4.352874	2.905677	2.826725
95	1	4.474429	5.371753	2.989485
96	1	3.954248	6.775795	1.009539
97	1	3.312700	5.693116	-1.131814
98	1	3.180953	3.228304	-1.282961
99	1	8.076551	4.138697	-0.563267
100	1	5.868677	3.496647	-0.031834
101	1	11.918759	1.221347	-1.763784
102	1	-1.401076	5.466243	-0.564414
103	1	-3.132741	6.613042	-1.877390
104	1	11.745192	-1.571827	-2.032510
105	1	7.573658	-4.180182	-1.370302
106	1	5.433805	-3.397700	-0.628769
107	1	-5.039994	5.308668	-2.810410
108	1	-5.280343	2.929621	-2.270483
109	1	-3.181722	-3.228530	1.282532
110	1	-3.313297	-5.693320	1.130866
111	1	-3.953882	-6.775622	-1.010972
112	1	-4.473265	-5.371231	-2.990875
113	1	-4.351882	-2.905180	-2.827600
114	1	-5.868732	-3.496794	0.030892
115	1	-8.076555	-4.138953	0.562265
116	1	-5.433775	3.397484	0.629487
117	1	-7.573598	4.179795	1.371319

118	1	-10.244408	3.465511	1.877266
119	1	-11.745117	1.571283	2.033119
120	1	-11.918703	-1.221854	1.763743
121	1	-10.648839	-3.217457	1.237516
122	1	10.244475	-3.466028	-1.876281

2

HF=-2150.1535249 a.u.

1	6	-5.960165	-1.421024	-0.354138
2	6	-7.111766	-0.716241	-0.663479
3	6	-7.111757	0.716332	-0.663494
4	6	-5.960146	1.421109	-0.354172
5	6	-3.653882	1.448809	0.209839
6	6	-2.488392	0.736453	0.557228
7	6	-2.488396	-0.736391	0.557174
8	6	-3.653901	-1.448727	0.209834
9	6	-4.816309	-0.683321	0.015389
10	6	-4.816297	0.683409	0.015372
11	6	-5.494338	-2.816682	-0.424053
12	1	-8.021732	-1.228754	-0.956511
13	1	-8.021716	1.228848	-0.956540
14	6	-5.494306	2.816759	-0.424123
15	6	-4.087891	2.845589	-0.130328
16	6	-1.230548	1.404981	0.911020
17	6	-1.230555	-1.404985	0.910823
18	6	-4.087927	-2.845517	-0.130248
19	6	-6.170710	-3.968782	-0.796557
20	6	0.000002	-0.721723	0.739435
21	6	0.000008	0.721738	0.739547
22	6	1.230553	-1.404996	0.910803
23	6	2.488396	-0.736404	0.557153
24	6	2.488410	0.736438	0.557229
25	6	1.230571	1.404975	0.911018
26	6	-1.205380	-2.670059	1.508470
27	6	0.000005	-3.278914	1.837216
28	6	1.205387	-2.670083	1.508422
29	6	-1.205368	2.669918	1.508956
30	6	0.000018	3.278675	1.837871
31	6	1.205400	2.669917	1.508940
32	6	-5.465782	-5.169334	-0.919810
33	6	-4.093373	-5.196946	-0.695439
34	6	-3.401460	-4.044121	-0.305270
35	6	-6.170673	3.968845	-0.796679
36	6	-5.465740	5.169383	-0.920010
37	6	-4.093326	5.196988	-0.695680
38	6	-3.401418	4.044179	-0.305459
39	1	-7.233552	-3.935140	-1.010052
40	6	3.653884	-1.448752	0.209804
41	6	3.653913	1.448781	0.209862
42	1	-2.136981	-3.146653	1.777719
43	1	0.000005	-4.228238	2.360538
44	1	2.136995	-3.146698	1.777620
45	1	-2.136964	3.146436	1.778346
46	1	0.000023	4.227859	2.361446
47	1	2.136999	3.146437	1.778318
48	1	-5.986349	-6.074623	-1.210643
49	1	-3.544973	-6.123087	-0.825669
50	1	-2.332072	-4.099954	-0.161985
51	1	-7.233517	3.935199	-1.010166

52	1	-5.986303	6.074659	-1.210889
53	1	-3.544916	6.123113	-0.825989
54	1	-2.332025	4.100010	-0.162231
55	6	4.816313	0.683365	0.015363
56	6	4.816299	-0.683365	0.015336
57	6	5.960169	1.421053	-0.354186
58	6	7.111753	0.716257	-0.663569
59	6	7.111736	-0.716316	-0.663588
60	6	5.960130	-1.421085	-0.354228
61	6	4.087950	2.845567	-0.130250
62	6	5.494357	2.816714	-0.424081
63	6	4.087880	-2.845551	-0.130257
64	6	5.494278	-2.816738	-0.424125
65	6	6.170741	3.968802	-0.796604
66	6	5.465831	5.169361	-0.919869
67	6	4.093423	5.196988	-0.695501
68	6	3.401499	4.044178	-0.305310
69	6	3.401384	-4.044147	-0.305210
70	6	4.093260	-5.196988	-0.695396
71	6	5.465657	-5.169395	-0.919851
72	6	6.170611	-3.968853	-0.796654
73	1	8.021716	1.228764	-0.956622
74	1	8.021687	-1.228840	-0.956648
75	1	7.233580	3.935140	-1.010113
76	1	5.986407	6.074638	-1.210720
77	1	3.545031	6.123130	-0.825755
78	1	2.332110	4.100028	-0.162048
79	1	2.332003	-4.099958	-0.161848
80	1	3.544841	-6.123125	-0.825573
81	1	5.986195	-6.074696	-1.210698
82	1	7.233443	-3.935232	-1.010202

3

HF=-1383.0260836 a.u.

1	6	3.214667	1.416253	0.308861
2	6	4.406882	0.713435	0.340348
3	6	4.406100	-0.718196	0.340233
4	6	3.213104	-1.419670	0.308440
5	6	0.840412	-1.448791	0.195185
6	6	-0.381531	-0.738609	0.250338
7	6	-0.380753	0.739140	0.250198
8	6	0.841980	1.448004	0.195314
9	6	2.009802	0.682830	0.353248
10	6	2.009065	-0.684880	0.352893
11	6	2.796021	2.805122	0.065773
12	1	5.361835	1.226841	0.308421
13	1	5.360494	-1.232641	0.308337
14	6	2.792859	-2.808075	0.065410
15	6	1.362649	-2.836593	-0.068772
16	6	-1.682098	-1.421508	0.273675
17	6	-1.680654	1.423318	0.273150
18	6	1.365875	2.835275	-0.068681
19	6	3.563046	3.941334	-0.145870
20	6	-2.869196	0.716779	-0.062187
21	6	-2.869930	-0.713929	-0.061920
22	6	-4.099321	1.418307	-0.216136
23	6	-5.284811	0.680893	-0.546885
24	6	-5.285495	-0.675841	-0.546641
25	6	-4.100744	-1.414299	-0.215593
26	6	-1.811347	2.757341	0.664724

27	6	-3.022438	3.441869	0.541065
28	6	-4.143234	2.797572	0.049126
29	6	-1.814063	-2.755248	0.665814
30	6	-3.025863	-3.438594	0.542557
31	6	-4.146026	-2.793389	0.050350
32	6	2.939319	5.127398	-0.540701
33	6	1.564735	5.150396	-0.750635
34	6	0.778586	4.014931	-0.522041
35	6	3.558590	-3.945073	-0.146721
36	6	2.933454	-5.130376	-0.541594
37	6	1.558778	-5.151815	-0.751174
38	6	0.773953	-4.015529	-0.522226
39	1	4.640838	3.902543	-0.030851
40	1	-6.198255	1.233127	-0.740501
41	1	-6.199482	-1.227222	-0.740123
42	1	-0.961344	3.268304	1.089557
43	1	-3.078890	4.483109	0.838052
44	1	-5.080370	3.330852	-0.068841
45	1	-0.964500	-3.266918	1.090691
46	1	-3.083406	-4.479620	0.840081
47	1	-5.083687	-3.325804	-0.067363
48	1	3.530181	6.020509	-0.709025
49	1	1.087942	6.059253	-1.100081
50	1	-0.280728	4.069068	-0.724570
51	1	4.636458	-3.907462	-0.032021
52	1	3.523271	-6.024120	-0.710217
53	1	1.080903	-6.060092	-1.100653
54	1	-0.285493	-4.068428	-0.724434

4

HF=-1730.9344139 a.u.

1	6	-2.564981	0.237307	0.027044
2	6	-3.306706	1.422740	0.144508
3	6	-2.711098	2.683827	0.305592
4	6	-1.335106	2.750296	0.276771
5	6	0.823488	1.846046	0.209031
6	6	1.721907	0.777542	0.224039
7	6	1.174610	-0.564296	0.201727
8	6	-0.208481	-0.822459	0.376599
9	6	-1.140746	0.265180	0.248848
10	6	-0.572303	1.555103	0.257594
11	6	-0.588997	-2.164826	0.794111
12	6	-4.798193	1.173099	-0.049428
13	1	-3.321125	3.578924	0.360895
14	6	-0.395775	3.862310	0.169274
15	6	0.920028	3.327580	0.058536
16	6	3.183149	0.907427	0.300696
17	6	2.052166	-1.682180	-0.075378
18	6	-0.131186	-4.555110	0.912377
19	6	-1.288473	-4.756458	1.639051
20	6	3.420814	-1.449418	-0.402986
21	6	3.997793	-0.166021	-0.153424
22	6	4.241372	-2.510993	-0.856493
23	6	5.631069	-2.268822	-1.096553
24	6	6.195865	-1.070949	-0.788421
25	6	5.408893	0.000509	-0.255292
26	6	1.558938	-3.004851	-0.094604
27	6	2.379258	-4.036690	-0.610245
28	6	3.672064	-3.795770	-1.002463
29	6	3.818650	2.014630	0.862588

30	6	5.209577	2.155309	0.820489
31	6	5.993924	1.189453	0.217717
32	6	-2.080815	-3.660315	2.004542
33	6	-1.735194	-2.391242	1.586147
34	6	-3.485580	-0.804264	-0.482535
35	6	-0.638195	5.226796	0.057341
36	6	0.423945	6.084864	-0.222198
37	6	1.702819	5.565508	-0.419698
38	6	1.955950	4.198437	-0.286937
39	6	-4.792344	-0.276992	-0.500944
40	1	6.238194	-3.080663	-1.482880
41	1	7.261469	-0.914341	-0.917930
42	6	0.262008	-3.263252	0.504773
43	1	1.979679	-5.038611	-0.700352
44	1	4.283961	-4.603302	-1.390021
45	1	3.227884	2.772474	1.354945
46	1	5.669085	3.033456	1.260025
47	1	7.069258	1.314551	0.149593
48	6	-3.256919	-2.074034	-1.024191
49	6	-4.332162	-2.817070	-1.507403
50	6	-5.631637	-2.313639	-1.457567
51	1	-1.645451	5.616738	0.156782
52	1	0.250823	7.150963	-0.315643
53	1	2.518050	6.229682	-0.684031
54	1	2.955145	3.834886	-0.474112
55	6	-5.863271	-1.029844	-0.960746
56	6	-5.408077	2.091166	-1.129474
57	6	-5.557633	1.353875	1.286185
58	1	-5.361046	3.139810	-0.823356
59	1	-6.459381	1.842454	-1.296325
60	1	-4.877657	1.986244	-2.078235
61	1	-5.146210	0.704766	2.062128
62	1	-6.615821	1.108386	1.160129
63	1	-5.489631	2.388489	1.634232
64	1	0.512065	-5.400509	0.704934
65	1	-1.558401	-5.755993	1.960549
66	1	-2.959579	-3.804127	2.622332
67	1	-2.340274	-1.548067	1.888508
68	1	-2.259636	-2.483679	-1.086320
69	1	-4.151144	-3.799917	-1.927868
70	1	-6.458553	-2.909097	-1.828100
71	1	-6.868180	-0.620543	-0.961475

5

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1	6	1.311506	-0.587333	0.071447
2	6	2.333279	0.360892	-0.076829
3	6	2.097745	1.724086	-0.312677
4	6	0.786824	2.144126	-0.333604
5	6	-1.534010	1.835489	-0.294722
6	6	-2.680305	1.038110	-0.286809
7	6	-2.503892	-0.396100	-0.179622
8	6	-1.233613	-1.014802	-0.297300
9	6	-0.052032	-0.201553	-0.195582
10	6	-0.262306	1.189687	-0.284160
11	6	-1.210528	-2.431744	-0.632981
12	6	3.706499	-0.253959	0.182034
13	1	2.927998	2.417781	-0.381702

14	6	0.167668	3.465698	-0.309058
15	6	-1.243653	3.297389	-0.217653
16	6	-4.054833	1.539321	-0.417848
17	6	-3.648102	-1.229323	0.125790
18	6	-2.274065	-4.623795	-0.640494
19	6	-1.197570	-5.161024	-1.319185
20	6	-4.913946	-0.629919	0.395997
21	6	-5.130310	0.742724	0.062574
22	6	-5.991831	-1.413413	0.875856
23	6	-7.274075	-0.804655	1.057001
24	6	-7.500024	0.478943	0.669494
25	6	-6.450344	1.276204	0.108980
26	6	-3.518223	-2.631282	0.229381
27	6	-4.589066	-3.382480	0.770116
28	6	-5.780996	-2.791266	1.106354
29	6	-4.367631	2.739773	-1.055471
30	6	-5.673871	3.239568	-1.066920
31	6	-6.694893	2.547164	-0.442739
32	6	-0.141078	-4.331509	-1.717370
33	6	-0.150937	-2.994000	-1.376713
34	6	1.922004	-1.802189	0.662061
35	6	0.756258	4.723972	-0.252757
36	6	-0.050747	5.842005	-0.049872
37	6	-1.424743	5.684076	0.127924
38	6	-2.023454	4.424701	0.050970
39	6	3.319361	-1.630759	0.702766
40	1	-8.079510	-1.406833	1.463904
41	1	-8.489809	0.914551	0.755355
42	6	-2.323561	-3.252556	-0.313671
43	1	-4.467154	-4.446828	0.924778
44	1	-6.589854	-3.387987	1.514252
45	1	-3.589781	3.288482	-1.565040
46	1	-5.879197	4.180367	-1.565106
47	1	-7.701139	2.951418	-0.416871
48	6	1.364536	-2.939352	1.257165
49	6	2.203972	-3.902599	1.813489
50	6	3.590345	-3.750316	1.786552
51	1	1.832184	4.832038	-0.335818
52	1	0.392774	6.829969	-0.000500
53	1	-2.043534	6.550538	0.332778
54	1	-3.086576	4.344018	0.220725
55	6	4.155347	-2.599128	1.236932
56	6	4.591177	-0.279631	-1.071695
57	6	5.795449	0.407083	-0.840696
58	6	5.789214	0.919043	0.536099
59	6	4.581570	0.545103	1.149747
60	6	6.738587	1.657846	1.242049
61	6	6.467426	2.016291	2.561401
62	6	5.265990	1.642592	3.168219
63	6	4.314093	0.902560	2.463692
64	6	4.335833	-0.866355	-2.302385
65	6	5.296677	-0.765781	-3.310766
66	6	6.495006	-0.084968	-3.084758
67	6	6.753540	0.506121	-1.849221
68	1	-3.118787	-5.259734	-0.409136
69	1	-1.192432	-6.213506	-1.578984
70	1	0.679537	-4.734571	-2.299342
71	1	0.656831	-2.354893	-1.704524
72	1	0.294623	-3.077862	1.303591
73	1	1.768154	-4.781802	2.274568
74	1	4.228257	-4.514418	2.216225
75	1	5.229229	-2.449748	1.252564
76	1	7.673548	1.950715	0.776964

77	1	7.195840	2.590536	3.122963
78	1	5.070900	1.929248	4.195398
79	1	3.382864	0.612870	2.937699
80	1	3.406499	-1.395344	-2.481846
81	1	5.110437	-1.219322	-4.277708
82	1	7.230425	-0.015679	-3.878452
83	1	7.686072	1.033332	-1.679894

6

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1	6	-5.086467	2.830928	-1.269896
2	6	-4.057197	3.513821	-0.670369
3	6	-2.948238	2.836304	-0.106603
4	6	-2.892745	1.430935	-0.215896
5	6	-3.987819	0.713891	-0.779083
6	6	-5.094671	1.417642	-1.319293
7	6	-3.987799	-0.713957	-0.779087
8	6	-5.094624	-1.417738	-1.319308
9	6	-6.177377	-0.681881	-1.887511
10	6	-6.177399	0.681755	-1.887504
11	6	-5.086371	-2.831025	-1.269935
12	6	-0.744126	-2.788761	1.041988
13	1	-7.010472	-1.231068	-2.313265
14	1	-7.010513	1.230918	-2.313254
15	1	-5.919592	3.375749	-1.701148
16	1	-4.096150	4.594857	-0.640999
17	6	-1.907144	3.510968	0.651620
18	6	-1.714510	0.712229	0.187082
19	6	-2.892704	-1.430974	-0.215905
20	1	-5.919475	-3.375866	-1.701204
21	6	-4.057085	-3.513892	-0.670410
22	6	0.147979	-3.396523	1.954834
23	6	-2.058404	-4.842980	1.096881
24	6	-0.039592	-4.689155	2.396949
25	6	-0.744197	2.788781	1.041981
26	6	-0.564498	1.410482	0.600832
27	6	-1.714493	-0.712234	0.187088
28	6	-2.948152	-2.836345	-0.106625
29	6	-1.139727	-5.430311	1.941758
30	1	0.987491	-2.826246	2.327690
31	1	-2.937735	-5.405031	0.811027
32	1	0.655466	-5.123172	3.106446
33	1	-1.290489	-6.448481	2.282095
34	6	-2.058542	4.842952	1.096925
35	6	-1.139875	5.430294	1.941807
36	6	-0.039711	4.689169	2.396973
37	6	0.147900	3.396551	1.954827
38	6	0.696256	0.723364	0.566990
39	6	0.696273	-0.723306	0.567016
40	6	-0.564468	-1.410457	0.600857
41	6	1.963474	1.459903	0.385420
42	6	3.111823	0.713668	0.539338
43	6	3.111833	-0.713575	0.539371
44	6	1.963495	-1.459833	0.385489
45	6	4.381587	1.143968	0.081457
46	6	5.172582	0.000037	-0.179436
47	6	4.381595	-1.143885	0.081497
48	6	2.188476	-2.770046	-0.186532
49	6	3.431966	-3.196374	-0.623051

50	6	4.589790	-2.346209	-0.571867
51	6	2.188451	2.770100	-0.186651
52	6	3.431939	3.196413	-0.623191
53	6	4.589766	2.346257	-0.571972
54	6	5.812165	2.421030	-1.337937
55	6	6.594788	1.304826	-1.574340
56	6	6.225861	0.000021	-1.076698
57	6	6.594799	-1.304799	-1.574282
58	6	5.812186	-2.421002	-1.337828
59	1	-4.095990	-4.594931	-0.641066
60	6	-1.907047	-3.510982	0.651604
61	1	-2.937890	5.404985	0.811093
62	1	-1.290668	6.448453	2.282164
63	1	0.655334	5.123199	3.106473
64	1	0.987434	2.826294	2.327661
65	1	1.349456	-3.429217	-0.357121
66	1	3.499443	-4.164266	-1.109574
67	1	1.349432	3.429265	-0.357265
68	1	3.499419	4.164289	-1.109746
69	1	6.080146	3.355360	-1.820864
70	1	7.452572	1.401236	-2.232372
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72	1	6.080183	-3.355351	-1.820710

7

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1	6	-5.335533	2.825703	-1.468186
2	6	-4.331084	3.515068	-0.836229
3	6	-3.267453	2.847295	-0.184861
4	6	-3.227880	1.434530	-0.225129
5	6	-4.288282	0.713938	-0.850761
6	6	-5.352004	1.414709	-1.479782
7	6	-4.288405	-0.713606	-0.850699
8	6	-5.352269	-1.414235	-1.479629
9	6	-6.400243	-0.680596	-2.111301
10	6	-6.400114	0.681199	-2.111378
11	6	-5.336053	-2.825230	-1.467904
12	6	-1.133474	-2.853056	1.086569
13	1	-7.201200	-1.231987	-2.592192
14	1	-7.200965	1.232688	-2.592335
15	1	-6.135666	3.364792	-1.964112
16	1	-4.356264	4.596253	-0.851122
17	6	-2.250373	3.562777	0.571305
18	6	-2.100274	0.713348	0.307205
19	6	-3.228108	-1.434337	-0.225032
20	1	-6.136294	-3.364217	-1.963768
21	6	-4.331708	-3.514721	-0.835921
22	6	-0.254613	-3.526358	1.963061
23	6	-2.377986	-4.936015	0.875926
24	6	-0.411245	-4.865162	2.258534
25	6	-1.133244	2.852954	1.086717
26	6	-0.978366	1.432255	0.797429
27	6	-2.100352	-0.713313	0.307193
28	6	-3.267924	-2.847089	-0.184638
29	6	-1.471810	-5.583451	1.690305
30	1	0.544026	-2.972765	2.435096
31	1	-3.224302	-5.493479	0.497931
32	1	0.273679	-5.351298	2.943838
33	1	-1.602728	-6.635578	1.916472
34	6	6.054205	1.449473	-1.299482

35	6	5.503353	2.775801	-1.445996
36	6	6.054089	-1.449594	-1.299802
37	6	5.503131	-2.775847	-1.446606
38	6	6.821912	-0.690546	-2.261972
39	6	6.821971	0.690574	-2.261816
40	1	5.907845	3.437528	-2.205332
41	1	5.907582	-3.437441	-2.206080
42	1	7.328736	-1.211883	-3.067771
43	1	7.328835	1.212049	-3.067501
44	1	1.711813	-3.202918	0.219720
45	1	1.712068	3.202787	0.220326
46	1	3.935615	4.140992	-0.992664
47	1	3.935292	-4.141018	-0.993573
48	6	-2.377246	4.936162	0.875578
49	6	-1.471183	5.583434	1.690218
50	6	-0.410998	4.864929	2.258887
51	6	-0.254541	3.526081	1.963499
52	6	-0.978480	-1.432357	0.797323
53	6	0.226645	0.712310	0.962607
54	6	0.226574	-0.712511	0.962493
55	6	1.642351	1.189413	0.980682
56	6	2.409458	-0.000192	1.161358
57	6	1.642288	-1.189716	0.980523
58	6	2.287062	-2.330959	0.507632
59	6	2.287226	2.330715	0.508079
60	6	3.701584	2.307161	0.183679
61	6	4.414376	1.154648	0.506691
62	6	3.760339	-0.000222	0.996192
63	6	4.414288	-1.155041	0.506439
64	6	3.701400	-2.307433	0.183186
65	1	-4.357075	-4.595897	-0.850760
66	6	-2.250870	-3.562684	0.571464
67	1	-3.223280	5.493818	0.497219
68	1	-1.601916	6.635617	1.916233
69	1	0.273757	5.350934	2.944453
70	1	0.543822	2.972310	2.435802
71	6	4.378063	3.180188	-0.749453
72	6	5.536746	0.713038	-0.246929
73	6	5.536683	-0.713348	-0.247092
74	6	4.377808	-3.180298	-0.750156

8

HF=-2817.7640288 a.u.

1	6	7.497047	1.016762	0.368995
2	6	7.617774	2.294550	0.884429
3	6	6.465517	3.005204	1.238758
4	6	5.210105	2.475642	1.008179
5	6	5.038074	1.206048	0.402275
6	6	6.221061	0.449271	0.159613
7	6	3.747181	0.601540	0.112761
8	6	3.693028	-0.801761	-0.067934
9	6	4.900388	-1.523404	-0.278704
10	6	6.120898	-0.912250	-0.234273
11	6	2.516830	1.361271	-0.011236
12	6	1.268551	0.678704	-0.019234
13	6	1.219426	-0.747180	0.007362
14	6	2.419195	-1.495749	-0.047239
15	6	8.735143	0.250288	0.064632
16	1	8.607973	2.703275	1.039900

17	1	6.554904	3.975641	1.711932
18	1	4.350659	3.033182	1.348275
19	1	4.884589	-2.577017	-0.519513
20	6	7.336648	-1.712620	-0.534642
21	6	2.495951	2.764572	-0.216991
22	6	0.044602	1.410396	-0.050151
23	6	-0.043246	-1.410579	0.049217
24	6	2.338651	-2.908341	-0.001178
25	7	8.567464	-1.068703	-0.385881
26	8	7.285487	-2.873866	-0.893399
27	8	9.842183	0.735569	0.194180
28	6	9.762792	-1.862863	-0.699878
29	6	1.129223	-3.555863	0.102375
30	6	-0.076938	-2.820544	0.120009
31	6	-1.267503	-0.678929	0.018395
32	6	-1.218350	0.747055	-0.008082
33	6	0.078533	2.820358	-0.120877
34	6	1.321091	3.479086	-0.248433
35	6	-1.127938	3.554566	-0.102481
36	6	-2.337684	2.908293	0.001173
37	6	-2.418267	1.495598	0.046893
38	6	1.380566	4.955054	-0.419970
39	7	0.154756	5.635827	-0.385622
40	6	-1.101466	5.035329	-0.219981
41	8	2.432875	5.547264	-0.567322
42	8	-2.108122	5.715646	-0.189311
43	6	0.160378	7.098942	-0.525547
44	6	-1.319780	-3.478132	0.247176
45	6	-2.495059	-2.764899	0.215779
46	6	-2.515992	-1.361436	0.010436
47	6	-3.746232	-0.601625	-0.113275
48	6	-3.691986	0.801618	0.067749
49	6	-4.899267	1.523290	0.278987
50	6	-6.119817	0.912236	0.234803
51	6	-6.220162	-0.449196	-0.159401
52	6	-5.037291	-1.205973	-0.402581
53	6	-5.209586	-2.475344	-1.008833
54	6	-6.465096	-3.004791	-1.239205
55	6	-7.617205	-2.294188	-0.884334
56	6	-7.496240	-1.016540	-0.368587
57	6	-7.335424	1.712597	0.535758
58	7	-8.566314	1.068791	0.387188
59	6	-8.734199	-0.250048	-0.063715
60	8	-9.841304	-0.735217	-0.193146
61	6	-9.761490	1.862931	0.701812
62	8	-7.284096	2.873736	0.894837
63	6	1.110075	-5.038713	0.219571
64	8	2.126543	-5.703761	0.186787
65	7	-0.150618	-5.636167	0.384831
66	6	-1.371906	-4.952524	0.417928
67	8	-2.415350	-5.560604	0.565162
68	6	-0.219156	-7.097131	0.530251
69	1	3.407373	3.316615	-0.383765
70	1	3.226259	-3.524974	-0.007172
71	1	10.629367	-1.222568	-0.570539
72	1	9.701101	-2.227095	-1.725321
73	1	9.821562	-2.723830	-0.032948
74	1	-3.224984	3.525529	0.007536
75	1	-0.438498	7.388080	-1.389372
76	1	1.190442	7.416254	-0.651467
77	1	-0.276245	7.555732	0.362923
78	1	-3.406205	-3.317712	0.382084
79	1	-4.883290	2.576845	0.520024

80	1	-4.350255	-3.032743	-1.349434
81	1	-6.554674	-3.975088	-1.712633
82	1	-8.607474	-2.702804	-1.039636
83	1	-9.700273	2.225515	1.727884
84	1	-10.628250	1.223177	0.571051
85	1	-9.819490	2.724959	0.036210
86	1	-0.683326	-7.350522	1.483560
87	1	0.794026	-7.482984	0.483765
88	1	-0.826724	-7.519305	-0.270623

9

HF=-916.1080888 a.u.

1	6	-3.414813	-1.553383	-0.007608
2	6	-3.745406	-0.214172	0.008182
3	6	-2.739487	0.792442	-0.020998
4	6	-1.369480	0.396144	0.016155
5	6	-1.027805	-0.987943	-0.016383
6	6	-2.056003	-1.976247	0.020967
7	6	0.341677	-1.384071	0.016690
8	6	0.683474	-2.768653	-0.020942
9	6	-0.362134	-3.733981	0.007665
10	6	-1.687206	-3.350689	-0.008463
11	6	1.369474	-0.396145	-0.016886
12	6	2.739445	-0.792434	0.020972
13	6	3.052637	-2.180611	-0.007748
14	6	2.058164	-3.136499	0.008499
15	1	-4.197910	-2.309218	0.008288
16	1	-4.790277	0.090436	-0.007447
17	6	-3.052673	2.180638	0.007636
18	6	-0.341654	1.384081	-0.016230
19	1	-0.099102	-4.790084	-0.007791
20	1	-2.473439	-4.103278	0.006730
21	6	1.027821	0.987921	0.016690
22	6	3.745374	0.214151	-0.008207
23	1	4.098770	-2.480860	0.007512
24	1	2.316798	-4.193693	-0.006460
25	6	2.056009	1.976212	-0.020992
26	6	3.414802	1.553347	0.007549
27	6	-2.058170	3.136544	-0.008031
28	6	-0.683454	2.768684	0.020982
29	6	0.362169	3.733994	-0.007684
30	6	1.687242	3.350672	0.008167
31	1	-4.098798	2.480900	-0.008204
32	1	4.790236	-0.090470	0.007442
33	1	4.197895	2.309184	-0.008313
34	1	-2.316810	4.193728	0.007705
35	1	0.099144	4.790098	0.007949
36	1	2.473478	4.103248	-0.007296

10

HF=-768.3151487 a.u.

1	1	3.657529	-2.144445	-0.622881
2	1	1.889755	-3.795097	-0.623741
3	6	2.677898	-1.852005	-0.258286
4	6	1.664873	-2.797879	-0.258962
5	6	0.304351	-2.462392	0.097159
6	6	0.147756	-1.195193	0.627235
7	6	1.182313	-0.228920	0.627196

8	6	2.435965	-0.471728	0.097307
9	6	-1.091095	-0.509775	0.627189
10	6	-0.822007	0.880156	0.627038
11	6	0.583011	1.053798	0.626955
12	6	-2.247889	-1.050316	0.097371
13	6	-2.146466	-2.448235	-0.258119
14	6	-0.933980	-3.119135	-0.258120
15	6	-3.254983	-0.075665	-0.258270
16	6	-2.991629	1.284908	-0.258445
17	6	-1.693573	1.813348	0.097069
18	6	-1.077848	3.072349	-0.258448
19	6	1.201204	2.171068	0.097239
20	6	2.588986	1.974381	-0.258187
21	6	3.175577	0.718935	-0.258111
22	6	0.297515	3.242299	-0.258328
23	1	-4.219346	-0.414941	-0.623028
24	1	-3.025484	-2.970165	-0.622897
25	1	-0.909210	-4.141056	-0.623057
26	1	-3.759766	1.959488	-0.623205
27	1	-1.698488	3.884686	-0.623218
28	1	3.169872	2.815644	-0.622863
29	1	4.193487	0.624614	-0.622935
30	1	0.701777	4.181280	-0.623084

11

HF=-692.0690675 a.u.

1	6	-1.627853	-3.422032	0.027221
2	6	-2.770265	-2.592136	0.054120
3	6	-2.725425	-1.199723	-0.052756
4	6	-3.795070	-0.304222	0.026871
5	6	-3.644019	1.099286	-0.016872
6	6	-2.406833	1.745495	0.046782
7	6	-2.155648	3.116156	-0.055117
8	1	-1.780202	-4.501616	0.054098
9	6	-0.863552	3.685918	-0.036536
10	6	1.627898	3.422147	0.027037
11	6	2.770281	2.592248	0.053861
12	6	2.725309	1.199768	-0.052335
13	6	3.794988	0.304250	0.027117
14	6	3.644005	-1.099301	-0.016822
15	6	2.406853	-1.745663	0.046982
16	6	2.155680	-3.116247	-0.055394
17	6	0.863567	-3.685970	-0.036728
18	6	-0.316795	-2.939968	0.006454
19	6	0.316892	2.939996	0.006179
20	1	-3.745369	-3.070287	0.154532
21	1	-1.744935	-0.759993	-0.220459
22	1	-4.805210	-0.709474	0.097280
23	1	-4.545382	1.710987	-0.070782
24	1	-1.540430	1.105167	0.195289
25	1	-3.007686	3.790009	-0.152408
26	1	-0.785028	4.772674	-0.083635
27	1	1.780249	4.501726	0.054119
28	1	3.745430	3.070415	0.153792
29	1	1.744725	0.759962	-0.219291
30	1	4.805116	0.709609	0.097060
31	1	4.545353	-1.710977	-0.071224
32	1	1.540497	-1.105406	0.196062
33	1	3.007666	-3.790105	-0.153171
34	1	0.784978	-4.772713	-0.084083
35	1	-0.202470	-1.858877	0.026575

36	1	0.202624	1.858880	0.025863

12

HF=-576.4994295 a.u.

1	1	3.521718	2.453958	0.080783
2	1	4.302673	0.092873	-0.202445
3	6	2.797932	1.642297	0.020339
4	6	3.249563	0.301825	-0.019039
5	6	2.337424	-0.742126	0.199178
6	1	1.391473	-0.415479	0.617854
7	1	0.827236	1.061992	-0.391060
8	6	1.426799	1.919214	-0.104841
9	1	-0.000424	-1.290125	-0.001121
10	1	1.397026	-4.021384	-0.104888
11	1	3.391330	-2.563849	-0.298979
12	6	-0.000792	-2.371814	-0.000403
13	6	1.276052	-2.942253	-0.023065
14	6	2.430633	-2.114848	-0.050143
15	6	-1.278052	-2.941361	0.023368
16	6	-2.431999	-2.113156	0.050411
17	6	-2.338093	-0.740629	-0.199940
18	6	-3.249303	0.303885	0.019376
19	6	-1.425428	1.920016	0.104137
20	6	-0.709376	3.112790	-0.024581
21	6	0.711459	3.112309	0.024811
22	6	-2.796845	1.644090	-0.020012
23	1	-1.399671	-4.020319	0.106487
24	1	-3.392839	-2.561212	0.300407
25	1	-1.392400	-0.414752	-0.619831
26	1	-4.302324	0.095553	0.204010
27	1	-0.826205	1.062142	0.389075
28	1	-1.234228	4.061916	-0.124802
29	1	1.236920	4.060985	0.126153
30	1	-3.520145	2.456273	-0.079220

13

HF=-576.7114877 a.u.

1	1	2.534309	-3.266847	-0.597269
2	1	0.254630	-4.294273	0.132588
3	6	1.744722	-2.674764	-0.123171
4	6	0.394836	-3.223424	-0.021908
5	6	-0.677496	-2.365814	-0.142478
6	1	-0.381003	-1.350837	-0.404629
7	1	1.222787	-0.916078	0.846458
8	6	2.024065	-1.404672	0.300610
9	1	-1.378450	-0.044911	0.595425
10	1	-3.983716	-1.490381	-0.155063
11	1	-2.546368	-3.507515	-0.033717
12	6	-2.400661	-0.078366	0.233390
13	6	-2.904014	-1.371495	-0.007913
14	6	-2.093161	-2.516448	-0.045440
15	6	-2.987437	1.179143	-0.007923
16	6	-2.253071	2.374567	-0.045558
17	6	-0.830551	2.316589	-0.142718
18	6	0.183545	3.242263	-0.021813
19	6	1.927860	1.533628	0.300659
20	6	3.134012	0.787377	-0.027983

21	6	3.178851	-0.581169	-0.028018
22	6	1.566328	2.782813	-0.123120
23	1	-4.072612	1.227317	-0.154948
24	1	-2.769982	3.333945	-0.033717
25	1	-0.468543	1.323201	-0.405294
26	1	-0.026269	4.301604	0.133182
27	1	1.160135	0.993810	0.846474
28	1	4.006510	1.343415	-0.375946
29	1	4.085890	-1.078837	-0.376024
30	1	2.315711	3.425030	-0.597213

