Electronic Supplementary Information

Computational Characterization of the Mechanism for the Light-Driven Catalytic Trichloromethylation Of Acylpyridines

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Contents

S.1 *Excited States of all Complexes*

5
ES1 E=387nm f=0.1482
160 -> 162
ES2 E=371nm f=0.0196
160 -> 163
ES3 E=343nm f=0.0604
161 -> 162

4
ES1 E=388nm f=0.0063
161 -> 162
ES2 E=373nm f=0.1704
161 -> 163
ES3 E=356nm f=0.0266
161 -> 164
ES4 E=330nm f=0.0239
159 -> 162

2
ES1 E=445nm f=0.0596
125 -> 126
ES2 E=398nm f=0.0143
125-127
ES3 E=354nm f=0.0075
124 -> 126
ES4 E=351nm f=0.0365
123-126
ES5 E=346nm f=0.1082
124 -> 127

1
ES1 E=348nm f=0.2912
147 -> 148

ES2 E=340nm f=0.0542
147 -> 149

S.2 Components of Single Electron Transfer calculations

Table S1. Components for the estimation of SET steps in kcal.mol^{-1}.

Step	λ_S	λ_N	ΔG	$\Delta G^{\ddagger}$
SET1	40.8	12.4	-40.9	5.1
SET2	45.1	8.9	-23.2	7.4

S.3 Cartesian Coordinates of all species studied

TSmajor_e_gas
Energy (POTENTIAL) = -3227.26777507 Eh

	Atom	X	Y	Z
1	Ir	-1.1930	-0.7062	1.8600
2	N	-2.1685	-2.5182	2.2749
3	C	-2.4039	-2.7145	3.5826
4	C	-2.0460	-1.6076	4.4630
5	C	-1.5630	-0.4654	3.7877
6	C	-1.3365	0.6828	4.5704
7	H	-1.0079	1.6017	4.0940
8	C	-1.5145	0.6695	5.9464
9	C	-1.9420	-0.4919	6.6017
10	H	-2.0721	-0.5001	7.6799
11	C	-2.2199	-1.6255	5.8568
12	H	-2.5753	-2.5161	6.3679
13	C	-4.1600	-0.2382	1.3025
14	H	-4.4001	-1.1616	1.8229
15	C	-5.1739	0.4549	0.6512
16	H	-6.1909	0.0705	0.6758
17	C	-4.8983	1.6388	-0.0401
18	H	-5.6932	2.1719	-0.5535
19	C	-3.6032	2.1353	-0.0556
20	H	-3.4026	3.0654	-0.5804
21	C	-2.5838	1.4411	0.6096
22	C	-1.2157	1.9343	0.7532
23	H	-1.3202	1.5716	6.5216
24	C	-2.6210	-3.4540	1.3592
25	C	-2.4371	-3.2411	-0.0255

26	C	-3.3026	-4.6170	1.7884
27	C	-2.9464	-4.1107	-0.9829
28	H	-1.8774	-2.3515	-0.2961
29	C	-3.8035	-5.5084	0.8183
30	C	-3.6467	-5.2650	-0.5225
31	H	-4.3310	-6.3988	1.1512
32	H	-4.0753	-6.0023	-1.1930
33	C	-2.6991	-3.8309	-2.4782
34	C	-2.8382	0.2263	1.2803
35	N	-0.4159	1.1889	1.5308
36	C	0.7999	1.6980	1.9462
37	C	1.5338	1.0479	2.9694
38	C	1.2773	2.9222	1.4288
39	C	2.6986	1.5890	3.4954
40	H	1.0846	0.1379	3.3392
41	C	2.5073	3.4247	1.8985
42	C	3.1924	2.7878	2.8990
43	H	2.8961	4.3446	1.4697
44	H	4.1229	3.2398	3.2292
45	C	3.4535	0.9797	4.6932
46	C	1.0579	-2.5725	3.0346
47	C	1.2462	-2.1165	0.7570
48	C	2.1282	-3.4477	3.0118
49	H	0.5102	-2.3702	3.9512
50	C	2.3468	-2.9784	0.6719
51	C	2.7919	-3.6430	1.8001
52	H	2.4325	-3.9571	3.9195
53	H	2.8357	-3.1339	-0.2820
54	H	3.6403	-4.3180	1.7371
55	C	0.6297	-1.4159	-0.4022
56	O	-0.5517	-0.8972	-0.1941
57	N	0.6373	-1.9114	1.9463
58	C	1.2680	-1.3298	-1.6115
59	H	2.1690	-1.9053	-1.7858
60	C	0.6303	-0.6448	-2.7812
61	H	0.0448	0.2175	-2.4463
62	H	1.3837	-0.3043	-3.4993
63	H	-0.0582	-1.3074	-3.3232
64	C	3.2796	0.4052	-1.2986
65	Cl	2.6196	1.9485	-1.7492
66	Cl	3.8058	0.2955	0.3518
67	Cl	4.4165	-0.2468	-2.4552
68	C	4.8760	0.5757	4.2513
69	H	5.4650	1.4558	3.9190

70	H	5.4286	0.1003	5.0906
71	H	4.8277	-0.1495	3.4101
72	C	3.5431	2.0217	5.8300
73	H	4.0436	1.5896	6.7236
74	H	4.1289	2.9132	5.5236
75	H	2.5256	2.3568	6.1271
76	C	2.7616	-0.2767	5.2692
77	H	1.7212	-0.0498	5.5888
78	H	2.7506	-1.0888	4.5172
79	H	3.3110	-0.6592	6.1567
80	C	-1.2016	-4.0321	-2.7797
81	H	-0.5759	-3.3855	-2.1345
82	H	-0.9054	-5.0861	-2.5881
83	H	-0.9755	-3.7907	-3.8408
84	C	-3.1111	-2.3809	-2.8277
85	H	-4.1641	-2.1948	-2.5244
86	H	-2.4638	-1.6324	-2.3268
87	H	-3.0248	-2.1975	-3.9206
88	C	-3.5021	-4.7756	-3.4047
89	H	-4.5909	-4.6990	-3.1941
90	H	-3.3416	-4.5110	-4.4726
91	H	-3.1784	-5.8314	-3.2807
92	C	0.4789	3.6227	0.4908
93	C	-0.7595	3.1526	0.1843
94	H	0.8531	4.5454	0.0548
95	H	-1.4064	3.6967	-0.4928
96	C	-3.0281	-3.8991	4.0571
97	C	-3.4725	-4.8354	3.1771
98	H	-3.9712	-5.7376	3.5222
99	H	-3.1723	-4.0317	5.1220

TSminor_e_gas
Energy (POTENTIAL) = -3227.26689477 Eh

	Atom	X	Y	Z
1	Ir	-1.3048	-0.6060	1.7769
2	N	-1.8157	-2.6033	2.0593
3	C	-1.4102	-3.0473	3.2573
4	C	-1.1806	-2.0070	4.2574
5	C	-1.2559	-0.6888	3.7569
6	C	-1.1475	0.3590	4.6816
7	H	-1.2151	1.3888	4.3399
8	C	-0.9406	0.1054	6.0325
9	C	-0.8379	-1.2069	6.5058
10	H	-0.6722	-1.3977	7.5620
11	C	-0.9616	-2.2644	5.6171
12	H	-0.9001	-3.2820	5.9945
13	C	-4.3455	-0.4556	1.8098
14	H	-4.3726	-1.5039	2.0964
15	C	-5.5377	0.2113	1.5602
16	H	-6.4824	-0.3189	1.6545
17	C	-5.5381	1.5620	1.1908
18	H	-6.4737	2.0769	0.9939
19	C	-4.3340	2.2419	1.0967
20	H	-4.3436	3.2958	0.8308
21	C	-3.1299	1.5688	1.3535
22	C	-1.8163	2.2088	1.3654
23	H	-0.8557	0.9348	6.7306
24	C	-2.2184	-3.5037	1.0965
25	C	-2.9168	-3.0470	-0.0478
26	C	-1.9997	-4.8871	1.2717
27	C	-3.3569	-3.9180	-1.0327
28	H	-3.1131	-1.9834	-0.0608
29	C	-2.3580	-5.7606	0.2237
30	C	-2.9953	-5.2936	-0.8969
31	H	-2.1414	-6.8209	0.3265
32	H	-3.2414	-6.0186	-1.6668
33	C	-3.1049	0.1950	1.6892
34	N	-0.7916	1.3971	1.6697
35	C	0.4561	1.9378	1.9278
36	C	1.4851	1.1131	2.4396
37	C	0.6872	3.3227	1.7603
38	C	2.7089	1.6339	2.8324
39	H	1.2391	0.0622	2.5040
40	C	1.9554	3.8403	2.0990
41	C	2.9254	3.0307	2.6318

42	H	2.1425	4.9022	1.9615
43	H	3.8665	3.4991	2.9048
44	C	3.8040	0.7827	3.5049
45	C	-1.5690	-0.0007	-1.3152
46	C	0.0736	-1.5403	-0.7228
47	C	-1.2740	-0.1154	-2.6622
48	H	-2.3593	0.6551	-0.9623
49	C	0.4028	-1.7217	-2.0698
50	C	-0.2733	-1.0082	-3.0442
51	H	-1.8222	0.4743	-3.3888
52	H	1.2088	-2.3917	-2.3427
53	H	-0.0146	-1.1349	-4.0912
54	C	0.7797	-2.1827	0.4197
55	O	0.6120	-1.6108	1.5816
56	C	1.5568	-3.2950	0.2313
57	H	1.5710	-3.7655	-0.7463
58	C	2.1194	-4.0712	1.3809
59	H	1.4118	-4.8507	1.6997
60	H	3.0567	-4.5697	1.1122
61	H	2.2986	-3.4226	2.2421
62	N	-0.9261	-0.7033	-0.3729
63	C	3.7439	-2.0077	-0.5768
64	Cl	3.3362	-0.3155	-0.6528
65	Cl	4.9843	-2.3827	0.5899
66	Cl	4.0391	-2.7326	-2.1499
67	C	4.0562	1.3149	4.9313
68	H	4.8195	0.6977	5.4531
69	H	4.4259	2.3618	4.9146
70	H	3.1172	1.2866	5.5259
71	C	3.4189	-0.7119	3.6210
72	H	2.5078	-0.8416	4.2451
73	H	3.2364	-1.1466	2.6164
74	H	4.2362	-1.2961	4.0970
75	C	5.1114	0.8720	2.6881
76	H	5.5175	1.9047	2.6769
77	H	5.8942	0.2134	3.1230
78	H	4.9356	0.5570	1.6388
79	C	-3.4021	-3.6435	-3.5285
80	H	-3.1225	-4.7059	-3.6912
81	H	-3.9897	-3.3072	-4.4101
82	H	-2.4687	-3.0423	-3.4798
83	C	-4.6708	-1.9964	-2.1340
84	H	-5.2360	-1.8175	-1.1934
85	H	-3.8034	-1.3105	-2.1723

86	H	-5.3337	-1.7290	-2.9854
87	C	-5.4961	-4.3384	-2.3091
88	H	-6.1627	-3.9869	-3.1264
89	H	-5.2623	-5.4028	-2.5175
90	H	-6.0586	-4.2831	-1.3519
91	C	-4.2174	-3.4728	-2.2314
92	C	-1.6145	3.5950	1.1373
93	C	-0.3791	4.1409	1.3119
94	H	-0.2087	5.2020	1.1490
95	H	-2.4544	4.2126	0.8428
96	C	-1.4616	-5.3342	2.5054
97	C	-1.2250	-4.4340	3.4991
98	H	-1.2718	-6.3942	2.6541
99	H	-0.8443	-4.7580	4.4602

5_e_gas
Energy (POTENTIAL) = -1808.69525247 Eh

	Atom	X	Y	Z
1	Ir	-1.2875	-0.7552	1.9372
2	N	-2.2819	-2.5469	2.3195
3	C	-2.5834	-2.7425	3.6131
4	C	-2.2497	-1.6377	4.5076
5	C	-1.6933	-0.5143	3.8555
6	C	-1.4245	0.6148	4.6515
7	H	-1.0265	1.5134	4.1871
8	C	-1.6554	0.6069	6.0203
9	C	-2.1774	-0.5292	6.6512
10	H	-2.3533	-0.5313	7.7229
11	C	-2.4819	-1.6475	5.8922
12	H	-2.9020	-2.5200	6.3858
13	C	-4.2451	-0.1854	1.3951
14	H	-4.5108	-1.0988	1.9216
15	C	-5.2455	0.5545	0.7749
16	H	-6.2779	0.2167	0.8291
17	C	-4.9389	1.7288	0.0799
18	H	-5.7250	2.3010	-0.4042
19	C	-3.6227	2.1634	0.0215
20	H	-3.3933	3.0862	-0.5053
21	C	-2.6173	1.4211	0.6545
22	C	-1.2154	1.8301	0.7143
23	H	-1.4318	1.4934	6.6091
24	C	-2.6579	-3.4941	1.3822
25	C	-2.4106	-3.2682	0.0102
26	C	-3.3158	-4.6824	1.7762
27	C	-2.8063	-4.1650	-0.9723
28	H	-1.8754	-2.3561	-0.2348
29	C	-3.7021	-5.6033	0.7798
30	C	-3.4653	-5.3588	-0.5501
31	H	-4.2057	-6.5182	1.0822
32	H	-3.8064	-6.1214	-1.2426
33	C	-2.5203	-3.8389	-2.4520
34	C	-2.9050	0.2212	1.3408
35	N	-0.4484	1.1043	1.5388
36	C	0.8499	1.4923	1.7871
37	C	1.5678	0.9043	2.8570
38	C	1.4529	2.5127	1.0212
39	C	2.8751	1.2637	3.1457
40	H	1.0006	0.1931	3.4424
41	C	2.8116	2.8107	1.2544

42	C	3.5053	2.1950	2.2643
43	H	3.3019	3.5530	0.6294
44	H	4.5504	2.4642	2.3857
45	C	3.6528	0.7185	4.3595
46	C	0.9309	-2.6317	3.1774
47	C	1.2910	-1.9485	0.9787
48	C	2.0790	-3.4043	3.1880
49	H	0.2861	-2.5573	4.0487
50	C	2.4627	-2.7101	0.9242
51	C	2.8638	-3.4337	2.0349
52	H	2.3473	-3.9663	4.0759
53	H	3.0300	-2.7489	0.0015
54	H	3.7705	-4.0308	2.0002
55	C	0.7210	-1.1696	-0.1579
56	O	-0.5840	-0.9830	-0.0992
57	N	0.5558	-1.9141	2.1103
58	C	1.5219	-0.6786	-1.1327
59	H	2.5907	-0.8711	-1.0913
60	C	1.0009	0.1649	-2.2548
61	H	-0.0661	0.3589	-2.1126
62	H	1.5262	1.1286	-2.3058
63	H	1.1320	-0.3244	-3.2300
64	C	4.8142	-0.1630	3.8588
65	H	5.5250	0.4224	3.2379
66	H	5.3812	-0.5903	4.7141
67	H	4.4241	-1.0023	3.2430
68	C	4.2179	1.8928	5.1913
69	H	4.7240	1.5204	6.1084
70	H	4.9694	2.4781	4.6224
71	H	3.3982	2.5778	5.4988
72	C	2.7735	-0.1313	5.3077
73	H	1.8982	0.4534	5.6656
74	H	2.4161	-1.0483	4.8019
75	H	3.3528	-0.4573	6.1987
76	C	-0.9953	-3.7500	-2.6759
77	H	-0.5458	-2.9232	-2.0903
78	H	-0.5033	-4.6992	-2.3722
79	H	-0.7642	-3.5624	-3.7469
80	C	-3.1734	-2.4885	-2.8242
81	H	-4.2651	-2.5172	-2.6173
82	H	-2.7318	-1.6467	-2.2505
83	H	-3.0276	-2.2640	-3.9031
84	C	-3.0773	-4.9121	-3.4170
85	H	-4.1791	-5.0085	-3.3066

86	H	-2.8684	-4.6385	-4.4743
87	H	-2.6021	-5.8992	-3.2295
88	C	0.6564	3.2027	0.0728
89	C	-0.6676	2.9032	-0.0370
90	H	1.1055	3.9818	-0.5380
91	H	-1.3015	3.4409	-0.7317
92	C	-3.2167	-3.9354	4.0530
93	C	-3.5728	-4.8924	3.1531
94	H	-4.0643	-5.8073	3.4745
95	H	-3.4233	-4.0668	5.1081

7major_tbu_solv
Energy (POTENTIAL) = -4183.24726772 Eh

	Atom	X	Y	Z
1	Ir	-1.5155	-0.6655	2.0607
2	N	-2.5078	-2.4631	1.9992
3	C	-2.5986	-3.0677	3.1695
4	C	-2.1290	-2.3488	4.3324
5	C	-1.6542	-1.0526	4.0192
6	C	-1.2426	-0.2546	5.0901
7	H	-0.8740	0.7520	4.9135
8	C	-1.2877	-0.7334	6.3982
9	C	-1.7466	-2.0227	6.6807
10	H	-1.7754	-2.3825	7.7041
11	C	-2.1725	-2.8372	5.6425
12	H	-2.5400	-3.8393	5.8513
13	C	-4.4991	-0.0699	1.9773
14	H	-4.6921	-1.1283	1.8358
15	C	-5.5791	0.8075	2.0116
16	H	-6.5854	0.4149	1.8940
17	C	-5.3939	2.1808	2.2012
18	H	-6.2469	2.8508	2.2301
19	C	-4.1102	2.6774	2.3544
20	H	-3.9513	3.7429	2.5033
21	C	-3.0253	1.7919	2.3151
22	C	-1.6407	2.1770	2.4375
23	H	-0.9615	-0.0924	7.2127
24	S	-3.3676	-4.6186	3.1141
25	C	-3.1322	-3.1750	0.9799
26	C	-3.3424	-2.7335	-0.3246
27	C	-3.6375	-4.4074	1.4004
28	C	-4.0283	-3.5292	-1.2483
29	H	-2.9730	-1.7460	-0.5706
30	C	-4.2946	-5.2378	0.4995
31	C	-4.4770	-4.7997	-0.8057
32	H	-4.6804	-6.2044	0.8064
33	H	-5.0044	-5.4908	-1.4533
34	C	-4.2735	-2.9929	-2.6717
35	C	-3.1870	0.3991	2.1256
36	N	-0.7273	1.2284	2.3278
37	S	-1.0071	3.7650	2.7100
38	C	0.5670	1.7281	2.4411
39	C	1.7453	0.9917	2.3401
40	C	0.6105	3.1086	2.6563
41	C	2.9917	1.6229	2.4433

42	H	1.6391	-0.0768	2.1883
43	C	1.8304	3.7614	2.7859
44	C	2.9994	3.0209	2.6772
45	H	1.8795	4.8308	2.9627
46	H	3.9160	3.5898	2.7826
47	C	4.2765	0.7939	2.2647
48	C	-1.4349	0.4382	-0.8746
49	C	0.0741	-1.2751	-0.4694
50	C	-0.9581	0.6029	-2.1723
51	H	-2.2462	1.0441	-0.4817
52	C	0.5888	-1.1760	-1.7565
53	C	0.0681	-0.2170	-2.6212
54	H	-1.3950	1.3618	-2.8120
55	H	1.3855	-1.8301	-2.0897
56	H	0.4609	-0.1166	-3.6274
57	C	0.6078	-2.1947	0.5775
58	O	0.2722	-1.9884	1.7414
59	C	1.5634	-3.3477	0.2785
60	C	2.6355	-3.4534	1.3684
61	H	2.1873	-3.4628	2.3629
62	H	3.2249	-4.3619	1.2335
63	H	3.3214	-2.6080	1.2978
64	N	-0.9329	-0.4766	-0.0413
65	H	2.0445	-3.1786	-0.6881
66	C	0.7796	-4.6824	0.0915
67	Cl	0.0329	-5.2223	1.6151
68	Cl	-0.5040	-4.4789	-1.1406
69	Cl	1.9084	-5.9375	-0.4929
70	C	4.3040	-0.3541	3.2985
71	H	4.2551	0.0557	4.3305
72	H	3.4526	-1.0513	3.1645
73	H	5.2380	-0.9492	3.2026
74	C	4.3052	0.2116	0.8351
75	H	4.3430	1.0313	0.0853
76	H	5.1965	-0.4367	0.6904
77	H	3.4012	-0.3943	0.6221
78	C	5.5654	1.6274	2.4597
79	H	6.4680	0.9900	2.3360
80	H	5.6303	2.4430	1.7073
81	H	5.6006	2.0675	3.4799
82	C	-2.9199	-2.7385	-3.3680
83	H	-2.3345	-3.6806	-3.4326
84	H	-3.0733	-2.3526	-4.3990
85	H	-2.3150	-1.9903	-2.8167

86	C	-5.0667	-1.6691	-2.5963
87	H	-6.0204	-1.8208	-2.0459
88	H	-4.4882	-0.8742	-2.0803
89	H	-5.3068	-1.2944	-3.6149
90	C	-5.0802	-3.9767	-3.5516
91	H	-5.2446	-3.5537	-4.5666
92	H	-4.5342	-4.9368	-3.6755
93	H	-6.0785	-4.1777	-3.1059

1

Energy (POTENTIAL) = -440.126977109 Eh

	Atom	X	Y	Z
1	C	0.6176	-1.8658	3.4561
2	C	0.9758	-1.5789	1.2089
3	C	1.8569	-2.4838	3.6330
4	H	-0.0510	-1.7236	4.3018
5	C	2.2297	-2.1851	1.2879
6	C	2.6766	-2.6456	2.5251
7	H	2.1599	-2.8259	4.6176
8	H	2.8556	-2.3022	0.4103
9	H	3.6483	-3.1216	2.6154
10	C	0.4246	-1.0543	-0.0980
11	O	-0.6655	-0.5007	-0.1188
12	N	0.1812	-1.4210	2.2795
13	C	1.2430	-1.2327	-1.3535
14	H	1.4511	-2.3046	-1.4702
15	H	2.2187	-0.7562	-1.1901
16	C	0.5799	-0.6742	-2.6044
17	H	0.4056	0.4034	-2.5168
18	H	1.2267	-0.8441	-3.4712
19	H	-0.3819	-1.1600	-2.7991

2_Me

Energy (POTENTIAL) = -2354.69754347 Eh

	Atom	X	Y	Z
1	Ir	-1.5909	-0.4479	2.0063
2	N	-2.6566	-2.2241	2.0635
3	C	-3.1355	-2.5170	3.2572
4	C	-2.8758	-1.5940	4.3426
5	C	-2.1255	-0.4677	3.9327
6	C	-1.8387	0.4889	4.9149
7	H	-1.2714	1.3812	4.6618
8	C	-2.2695	0.3204	6.2304
9	C	-3.0040	-0.8076	6.6104
10	H	-3.3332	-0.9286	7.6382
11	C	-3.3112	-1.7724	5.6610
12	H	-3.8827	-2.6520	5.9500
13	C	-4.5057	0.2181	1.3262
14	H	-4.7403	-0.8430	1.3547
15	C	-5.5248	1.1216	1.0270
16	H	-6.5277	0.7498	0.8309
17	C	-5.2782	2.4973	0.9769
18	H	-6.0797	3.1913	0.7420
19	C	-3.9982	2.9700	1.2322
20	H	-3.7991	4.0391	1.1961
21	C	-2.9823	2.0554	1.5330
22	C	-1.6113	2.4151	1.8286
23	H	-2.0304	1.0783	6.9723
24	S	-4.0425	-3.9888	3.3305
25	C	-2.9948	-3.1774	1.1057
26	C	-2.6596	-3.1588	-0.2512
27	C	-3.7602	-4.2308	1.6233
28	C	-3.0854	-4.1915	-1.0770
29	H	-2.0756	-2.3412	-0.6528
30	C	-4.1951	-5.2773	0.8095
31	C	-3.8507	-5.2438	-0.5326
32	H	-4.7870	-6.0937	1.2121
33	H	-4.1818	-6.0489	-1.1839
34	C	-2.7447	-4.1928	-2.5445
35	H	-3.6537	-4.1439	-3.1554
36	H	-2.1119	-3.3395	-2.8078
37	H	-2.2146	-5.1107	-2.8235
38	C	-3.2016	0.6595	1.5845
39	N	-0.7600	1.4465	2.1049
40	S	-0.9356	4.0072	1.8791
41	C	0.5165	1.9253	2.3909

42	C	1.6362	1.1676	2.7458
43	C	0.6128	3.3207	2.3093
44	C	2.8428	1.8065	3.0023
45	H	1.5570	0.0913	2.8253
46	C	1.8162	3.9794	2.5621
47	C	2.9183	3.2114	2.9035
48	H	1.8895	5.0607	2.4958
49	H	3.8655	3.7060	3.1040
50	C	4.0684	1.0126	3.3735
51	H	3.8268	-0.0428	3.5325
52	H	4.8254	1.0716	2.5823
53	H	4.5262	1.4013	4.2900
54	N	0.1055	-1.7013	2.4193
55	N	-0.9455	-0.3797	-0.0421
56	C	-0.5277	-0.2035	-1.1017
57	C	0.9128	-2.4913	2.6490
58	C	-0.0085	-0.0110	-2.4418
59	H	0.6949	-0.8145	-2.6767
60	H	-0.8348	-0.0278	-3.1580
61	H	0.5049	0.9527	-2.4999
62	C	1.9490	-3.4626	2.9412
63	H	2.8666	-3.1817	2.4167
64	H	2.1346	-3.4819	4.0186
65	H	1.6254	-4.4526	2.6080

TSmajor_d_gas
Energy (POTENTIAL) = -3868.82516852 Eh

	Atom	X	Y	Z
1	Ir	-1.5359	-0.4431	2.0072
2	N	-2.6312	-2.1906	2.0501
3	C	-3.0566	-2.5163	3.2555
4	C	-2.7851	-1.6089	4.3452
5	C	-2.0829	-0.4515	3.9219
6	C	-1.7990	0.4931	4.9244
7	H	-1.2715	1.4084	4.6698
8	C	-2.1708	0.2822	6.2470
9	C	-2.8531	-0.8792	6.6339
10	H	-3.1357	-1.0310	7.6711
11	C	-3.1647	-1.8295	5.6763
12	H	-3.6984	-2.7348	5.9596
13	C	-4.3817	0.3372	1.1566
14	H	-4.7039	-0.6851	1.3375
15	C	-5.2934	1.2480	0.6328
16	H	-6.3099	0.9257	0.4201
17	C	-4.9255	2.5735	0.3729
18	H	-5.6465	3.2732	-0.0389
19	C	-3.6323	2.9852	0.6529
20	H	-3.3341	4.0140	0.4616
21	C	-2.7229	2.0631	1.1835
22	C	-1.3714	2.3737	1.5862
23	H	-1.9297	1.0326	6.9961
24	S	-3.9287	-4.0161	3.3333
25	C	-3.0100	-3.1185	1.0808
26	C	-2.7711	-3.0247	-0.2930
27	C	-3.7232	-4.1996	1.6098
28	C	-3.2375	-4.0264	-1.1578
29	H	-2.2293	-2.1439	-0.6299
30	C	-4.1801	-5.2140	0.7799
31	C	-3.9327	-5.1204	-0.5816
32	H	-4.7276	-6.0624	1.1780
33	H	-4.3215	-5.9466	-1.1666
34	C	-3.0609	0.7122	1.4403
35	N	-0.6401	1.3985	2.0871
36	S	-0.6109	3.9374	1.6317
37	C	0.5647	1.8520	2.6083
38	C	1.4963	1.0822	3.2992
39	C	0.7618	3.2254	2.4455
40	C	2.6435	1.6657	3.8460
41	H	1.2698	0.0297	3.4041

42	C	1.9141	3.8284	2.9358
43	C	2.8363	3.0526	3.6268
44	H	2.0911	4.8906	2.7997
45	H	3.7055	3.5886	3.9918
46	C	0.5402	-2.4325	3.2792
47	C	0.8432	-1.9722	1.0096
48	C	1.5597	-3.3654	3.2881
49	H	-0.0298	-2.2021	4.1746
50	C	1.8901	-2.9016	0.9587
51	C	2.2514	-3.5977	2.0978
52	H	1.7994	-3.8980	4.2015
53	H	2.4052	-3.0796	0.0231
54	H	3.0587	-4.3229	2.0613
55	C	0.3371	-1.1999	-0.1559
56	O	-0.7845	-0.5506	0.0157
57	N	0.1947	-1.7499	2.1753
58	C	1.0012	-1.1650	-1.3557
59	H	1.8495	-1.8155	-1.5326
60	C	0.3984	-0.4237	-2.5115
61	H	0.6034	0.6536	-2.4573
62	H	0.7842	-0.7904	-3.4669
63	H	-0.6922	-0.5171	-2.4912
64	C	3.0067	0.4645	-0.9677
65	Cl	2.2829	1.9287	-0.3801
66	Cl	4.0712	-0.3173	0.1734
67	Cl	3.6856	0.5949	-2.5723
68	C	-3.0016	-3.8982	-2.6759
69	C	-3.6731	-2.5960	-3.2055
70	C	-3.5912	-5.1022	-3.4809
71	C	-1.4748	-3.8327	-2.9732
72	H	-4.7685	-2.6271	-3.0121
73	H	-3.2739	-1.7011	-2.6808
74	C	-3.4187	-2.4320	-4.7214
75	H	-4.6890	-5.1785	-3.3143
76	H	-3.1250	-6.0559	-3.1469
77	C	-3.3355	-4.9331	-4.9924
78	H	-1.0027	-2.9872	-2.4339
79	H	-0.9773	-4.7620	-2.6168
80	C	-1.2243	-3.6573	-4.4889
81	H	-3.9010	-1.4961	-5.0785
82	C	-4.0111	-3.6357	-5.4813
83	C	-1.9003	-2.3603	-4.9856
84	H	-3.7623	-5.8011	-5.5405
85	C	-1.8160	-4.8606	-5.2502

86	H	-0.1303	-3.6002	-4.6787
87	H	-3.8501	-3.5123	-6.5749
88	H	-5.1091	-3.6898	-5.3119
89	H	-1.4690	-1.4782	-4.4719
90	H	-1.7106	-2.2271	-6.0734
91	H	-1.3269	-5.8015	-4.9146
92	H	-1.6199	-4.7557	-6.3399
93	C	3.6086	0.7967	4.6729
94	C	2.8457	0.1653	5.8777
95	C	4.8147	1.6087	5.2440
96	C	4.1840	-0.3449	3.7846
97	H	2.4395	0.9673	6.5334
98	H	1.9811	-0.4419	5.5331
99	C	3.7849	-0.7480	6.6948
100	H	4.4510	2.4315	5.8991
101	H	5.4014	2.0641	4.4153
102	C	5.7498	0.6953	6.0658
103	H	3.3709	-0.9634	3.3490
104	H	4.7562	0.0921	2.9379
105	C	5.1137	-1.2598	4.6114
106	H	3.2215	-1.1942	7.5431
107	C	4.9639	0.0816	7.2424
108	C	4.3238	-1.8742	5.7869
109	H	6.5994	1.2937	6.4610
110	C	6.2924	-0.4313	5.1622
111	H	5.5043	-2.0736	3.9624
112	H	5.6336	-0.5651	7.8510
113	H	4.5852	0.8873	7.9092
114	H	3.4808	-2.4857	5.4005
115	H	4.9821	-2.5522	6.3733
116	H	6.8780	0.0028	4.3221
117	H	6.9798	-1.0861	5.7416

5_d_solv
Energy (POTENTIAL) = -3229.20057104 Eh

	Atom	X	Y	Z
1	Ir	-1.6770	-0.3696	2.0987
2	N	-2.7153	-2.1330	2.1323
3	C	-3.1202	-2.5150	3.3257
4	C	-2.8396	-1.6352	4.4381
5	C	-2.1520	-0.4601	4.0324
6	C	-1.8435	0.4540	5.0541
7	H	-1.3227	1.3762	4.8075
8	C	-2.1857	0.2054	6.3788
9	C	-2.8588	-0.9673	6.7465
10	H	-3.1196	-1.1478	7.7849
11	C	-3.1885	-1.8932	5.7700
12	H	-3.7128	-2.8082	6.0394
13	C	-4.6055	0.3442	1.5090
14	H	-4.8713	-0.7017	1.6388
15	C	-5.5959	1.2493	1.1435
16	H	-6.6143	0.8975	0.9969
17	C	-5.3050	2.6064	0.9576
18	H	-6.0871	3.3017	0.6682
19	C	-4.0075	3.0527	1.1479
20	H	-3.7672	4.1047	1.0078
21	C	-3.0178	2.1340	1.5183
22	C	-1.6374	2.4694	1.7707
23	H	-1.9297	0.9345	7.1438
24	S	-3.9543	-4.0426	3.3395
25	C	-3.0670	-3.0292	1.1297
26	C	-2.8150	-2.8583	-0.2302
27	C	-3.7450	-4.1542	1.6054
28	C	-3.2187	-3.8358	-1.1461
29	H	-2.2994	-1.9406	-0.5068
30	C	-4.1545	-5.1435	0.7182
31	C	-3.8850	-4.9797	-0.6354
32	H	-4.6780	-6.0287	1.0656
33	H	-4.2296	-5.7891	-1.2703
34	C	-3.2780	0.7553	1.7011
35	N	-0.8178	1.5041	2.1356
36	S	-0.9071	4.0456	1.6887
37	C	0.4655	1.9715	2.3948
38	C	1.5459	1.2080	2.8319
39	C	0.6103	3.3483	2.1990
40	C	2.7950	1.7948	3.0623
41	H	1.3611	0.1528	2.9797

42	C	1.8365	3.9636	2.4212
43	C	2.9104	3.1905	2.8435
44	H	1.9626	5.0310	2.2696
45	H	3.8370	3.7335	2.9941
46	C	0.4664	-2.3670	3.2314
47	C	0.7133	-1.7786	0.9836
48	C	1.4921	-3.2908	3.1646
49	H	-0.0809	-2.1861	4.1517
50	C	1.7439	-2.7181	0.8477
51	C	2.1383	-3.4708	1.9399
52	H	1.7679	-3.8604	4.0452
53	H	2.2114	-2.8615	-0.1190
54	H	2.9359	-4.2013	1.8406
55	C	0.2018	-0.9037	-0.1099
56	O	-1.0138	-0.4188	0.0636
57	N	0.0880	-1.6331	2.1721
58	C	0.9765	-0.6396	-1.1902
59	H	1.9750	-1.0631	-1.2464
60	C	0.5379	0.2581	-2.3050
61	H	1.0964	1.2048	-2.3026
62	H	0.7074	-0.2096	-3.2834
63	H	-0.5252	0.4938	-2.2072
64	C	-2.9354	-3.6192	-2.6437
65	C	-3.6590	-2.3282	-3.1316
66	C	-3.4271	-4.8076	-3.5302
67	C	-1.4021	-3.4561	-2.8741
68	H	-4.7578	-2.4305	-2.9887
69	H	-3.3346	-1.4426	-2.5433
70	C	-3.3517	-2.0662	-4.6224
71	H	-4.5244	-4.9500	-3.4123
72	H	-2.9236	-5.7517	-3.2240
73	C	-3.1223	-4.5421	-5.0201
74	H	-0.9951	-2.6125	-2.2788
75	H	-0.8673	-4.3748	-2.5453
76	C	-1.1044	-3.1858	-4.3650
77	H	-3.8705	-1.1389	-4.9498
78	C	-3.8461	-3.2563	-5.4696
79	C	-1.8292	-1.8969	-4.8109
80	H	-3.4798	-5.4000	-5.6303
81	C	-1.6010	-4.3746	-5.2125
82	H	-0.0086	-3.0618	-4.5069
83	H	-3.6471	-3.0648	-6.5470
84	H	-4.9455	-3.3767	-5.3518
85	H	-1.4697	-1.0308	-4.2150

86	H	-1.5999	-1.6823	-5.8778
87	H	-1.0737	-5.3056	-4.9084
88	H	-1.3705	-4.1986	-6.2863
89	C	3.9691	0.9106	3.5218
90	C	3.6102	0.2126	4.8688
91	C	5.2872	1.7202	3.7388
92	C	4.2534	-0.1813	2.4479
93	H	3.4179	0.9771	5.6540
94	H	2.6850	-0.3953	4.7722
95	C	4.7583	-0.7173	5.3190
96	H	5.1350	2.5061	4.5119
97	H	5.5923	2.2228	2.7940
98	C	6.4323	0.7905	4.1945
99	H	3.3508	-0.7984	2.2627
100	H	4.5256	0.2961	1.4804
101	C	5.3967	-1.1114	2.9091
102	H	4.4811	-1.2113	6.2756
103	C	6.0433	0.1105	5.5231
104	C	5.0044	-1.7922	4.2383
105	H	7.3584	1.3877	4.3422
106	C	6.6816	-0.2839	3.1157
107	H	5.5766	-1.8884	2.1345
108	H	6.8696	-0.5490	5.8689
109	H	5.8803	0.8785	6.3109
110	H	4.0887	-2.4049	4.0969
111	H	5.8143	-2.4807	4.5653
112	H	6.9814	0.1985	2.1594
113	H	7.5165	-0.9494	3.4274

5_d_gas
Energy (POTENTIAL) = -2450.24885820 Eh

	Atom	X	Y	Z
1	Ir	-1.6177	-0.3438	2.1532
2	N	-2.6242	-2.1326	2.0937
3	C	-3.0136	-2.5716	3.2741
4	C	-2.7634	-1.7302	4.4233
5	C	-2.1708	-0.4925	4.0604
6	C	-1.9892	0.4319	5.1027
7	H	-1.5556	1.4049	4.8862
8	C	-2.3365	0.1238	6.4136
9	C	-2.8869	-1.1214	6.7446
10	H	-3.1441	-1.3511	7.7741
11	C	-3.1064	-2.0531	5.7425
12	H	-3.5433	-3.0207	5.9822
13	C	-4.5006	0.2950	1.3235
14	H	-4.6960	-0.7710	1.2445
15	C	-5.5215	1.1842	1.0081
16	H	-6.4843	0.7984	0.6815
17	C	-5.3315	2.5663	1.1012
18	H	-6.1399	3.2509	0.8630
19	C	-4.0932	3.0507	1.4861
20	H	-3.9230	4.1237	1.5496
21	C	-3.0682	2.1453	1.7860
22	C	-1.7030	2.5202	2.0453
23	H	-2.1802	0.8619	7.1968
24	S	-3.9006	-4.0660	3.2265
25	C	-3.0525	-2.9483	1.0493
26	C	-2.8519	-2.6988	-0.3099
27	C	-3.7565	-4.0754	1.4847
28	C	-3.3455	-3.6008	-1.2597
29	H	-2.3150	-1.7839	-0.5415
30	C	-4.2448	-4.9945	0.5633
31	C	-4.0328	-4.7476	-0.7851
32	H	-4.7813	-5.8825	0.8819
33	H	-4.4261	-5.4894	-1.4741
34	C	-3.2398	0.7467	1.7433
35	N	-0.8155	1.5681	2.3071
36	S	-1.0473	4.1231	1.9183
37	C	0.4885	2.0909	2.4044
38	C	1.6632	1.3778	2.6886
39	C	0.5443	3.4828	2.2230
40	C	2.9057	2.0415	2.7386
41	H	1.5258	0.3253	2.8709

42	C	1.7546	4.1614	2.2937
43	C	2.9068	3.4401	2.5350
44	H	1.8023	5.2379	2.1657
45	H	3.8307	4.0096	2.5701
46	C	0.5367	-2.2590	3.4157
47	C	0.7285	-1.8956	1.1132
48	C	1.5154	-3.2350	3.4065
49	H	0.0266	-1.9712	4.3296
50	C	1.6972	-2.9072	1.0349
51	C	2.0935	-3.5754	2.1806
52	H	1.8052	-3.7230	4.3303
53	H	2.1270	-3.1649	0.0749
54	H	2.8472	-4.3551	2.1240
55	C	0.2734	-1.0507	-0.0299
56	O	-0.8145	-0.3352	0.1741
57	N	0.1441	-1.6188	2.3002
58	C	0.9912	-1.0163	-1.1824
59	H	1.9148	-1.5822	-1.2550
60	C	0.6542	-0.1058	-2.3229
61	H	1.4558	0.6260	-2.4933
62	H	0.5262	-0.6568	-3.2644
63	H	-0.2690	0.4408	-2.1131
64	C	-3.1609	-3.3948	-2.7745
65	C	-2.3863	-2.0816	-3.1124
66	C	-4.5516	-3.3192	-3.4725
67	C	-2.3566	-4.5873	-3.3737
68	H	-2.9281	-1.1955	-2.7123
69	H	-1.3786	-2.1091	-2.6460
70	C	-2.2218	-1.9156	-4.6374
71	H	-5.1340	-2.4614	-3.0681
72	H	-5.1466	-4.2373	-3.2794
73	C	-4.3818	-3.1581	-4.9996
74	H	-1.3524	-4.6465	-2.8975
75	H	-2.8678	-5.5539	-3.1773
76	C	-2.1975	-4.4194	-4.9011
77	H	-1.6690	-0.9748	-4.8506
78	C	-3.6135	-1.8546	-5.2991
79	C	-1.4317	-3.1143	-5.2003
80	H	-5.3830	-3.1154	-5.4810
81	C	-3.5929	-4.3615	-5.5602
82	H	-1.6299	-5.2828	-5.3114
83	H	-3.5065	-1.7200	-6.3980
84	H	-4.1815	-0.9803	-4.9116
85	H	-0.4194	-3.1525	-4.7407

86	H	-1.2936	-2.9971	-6.2977
87	H	-4.1468	-5.3053	-5.3616
88	H	-3.4876	-4.2654	-6.6633
89	C	4.2543	1.3339	2.9782
90	C	4.0715	-0.2070	3.1703
91	C	4.9402	1.8951	4.2591
92	C	5.1974	1.5505	1.7569
93	H	3.4124	-0.4134	4.0430
94	H	3.5934	-0.6549	2.2704
95	C	5.4312	-0.8966	3.4043
96	H	4.2857	1.7318	5.1440
97	H	5.1100	2.9897	4.1762
98	C	6.3034	1.2040	4.4862
99	H	4.7277	1.1389	0.8357
100	H	5.3777	2.6316	1.5760
101	C	6.5589	0.8617	1.9980
102	H	5.2742	-1.9893	3.5381
103	C	6.0901	-0.3126	4.6708
104	C	6.3446	-0.6543	2.1856
105	H	6.7833	1.6227	5.3975
106	C	7.2164	1.4508	3.2652
107	H	7.2216	1.0350	1.1224
108	H	7.0652	-0.8139	4.8576
109	H	5.4452	-0.5013	5.5571
110	H	5.8834	-1.0898	1.2718
111	H	7.3231	-1.1610	2.3370
112	H	7.3877	2.5417	3.1327
113	H	8.2091	0.9778	3.4321

TSminor_d_gas
Energy (POTENTIAL) = -3868.82106378 Eh

	Atom	X	Y	Z
1	Ir	-1.4731	-0.4459	2.0730
2	N	-2.2796	-2.3489	2.0918
3	C	-2.1973	-2.9326	3.2715
4	C	-1.7655	-2.1414	4.3979
5	C	-1.4731	-0.8038	4.0393
6	C	-1.1168	0.0545	5.0904
7	H	-0.8909	1.0981	4.8889
8	C	-1.0301	-0.4042	6.4003
9	C	-1.3010	-1.7400	6.7200
10	H	-1.2214	-2.0866	7.7459
11	C	-1.6760	-2.6140	5.7131
12	H	-1.8960	-3.6538	5.9466
13	C	-4.4925	0.0693	1.9740
14	H	-4.6576	-1.0051	1.9522
15	C	-5.5858	0.9232	1.8788
16	H	-6.5848	0.5041	1.7853
17	C	-5.4242	2.3147	1.9030
18	H	-6.2877	2.9691	1.8305
19	C	-4.1513	2.8479	2.0262
20	H	-4.0099	3.9267	2.0510
21	C	-3.0544	1.9814	2.1180
22	C	-1.6782	2.3972	2.2707
23	H	-0.7429	0.2859	7.1898
24	S	-2.7085	-4.5937	3.2937
25	C	-2.8088	-3.1933	1.1220
26	C	-3.0983	-2.8498	-0.1971
27	C	-3.0966	-4.4769	1.5954
28	C	-3.6637	-3.7832	-1.0741
29	H	-2.8755	-1.8308	-0.4889
30	C	-3.6457	-5.4307	0.7472
31	C	-3.9196	-5.0821	-0.5687
32	H	-3.8676	-6.4324	1.1018
33	H	-4.3493	-5.8732	-1.1735
34	C	-3.1839	0.5671	2.0903
35	N	-0.7621	1.4508	2.2989
36	S	-1.0569	3.9986	2.5404
37	C	0.5036	1.9331	2.6130
38	C	1.6314	1.1474	2.8462
39	C	0.5384	3.3196	2.7790
40	C	2.8212	1.7445	3.2781
41	H	1.5129	0.0770	2.6955

42	C	1.7226	3.9447	3.1517
43	C	2.8399	3.1581	3.4011
44	H	1.7767	5.0215	3.2769
45	H	3.7229	3.7079	3.7085
46	C	-1.6865	0.6357	-0.8889
47	C	-0.1226	-1.0521	-0.5097
48	C	-1.3197	0.7499	-2.2193
49	H	-2.4746	1.2466	-0.4588
50	C	0.2858	-0.9948	-1.8452
51	C	-0.3114	-0.0842	-2.7029
52	H	-1.8146	1.4739	-2.8571
53	H	1.0740	-1.6501	-2.1953
54	H	0.0047	-0.0231	-3.7400
55	C	0.4444	-1.9588	0.5239
56	O	0.3760	-1.5252	1.7585
57	C	0.9211	-3.1948	0.1775
58	H	0.7975	-3.5251	-0.8487
59	C	1.2172	-4.2212	1.2280
60	H	0.2813	-4.6191	1.6483
61	H	1.7844	-5.0630	0.8198
62	H	1.7806	-3.7868	2.0592
63	N	-1.1035	-0.2398	-0.0578
64	C	3.3690	-2.8014	-0.6841
65	Cl	3.6607	-1.0899	-0.8675
66	Cl	4.3964	-3.5688	0.4920
67	Cl	3.3042	-3.6581	-2.2158
68	C	4.0239	0.8520	3.6346
69	C	3.6226	-0.1435	4.7660
70	C	5.2569	1.6707	4.1348
71	C	4.4659	0.0384	2.3837
72	H	3.3165	0.4181	5.6766
73	H	2.7546	-0.7676	4.4621
74	C	4.8021	-1.0812	5.1055
75	H	4.9887	2.2581	5.0411
76	H	5.5912	2.3843	3.3490
77	C	6.4329	0.7337	4.4822
78	H	3.6271	-0.5819	2.0024
79	H	4.7660	0.7294	1.5649
80	C	5.6442	-0.8965	2.7342
81	H	4.4942	-1.7886	5.9060
82	C	6.0012	-0.2438	5.5946
83	C	5.2075	-1.8762	3.8451
84	H	7.2966	1.3379	4.8357
85	C	6.8424	-0.0599	3.2255

86	H	5.9458	-1.4679	1.8307
87	H	6.8482	-0.9130	5.8625
88	H	5.7223	0.3213	6.5111
89	H	4.3514	-2.4934	3.4939
90	H	6.0407	-2.5723	4.0863
91	H	7.1728	0.6379	2.4248
92	H	7.7013	-0.7266	3.4597
93	C	-3.9689	-3.3676	-2.5244
94	C	-4.9523	-2.1574	-2.5321
95	C	-4.6162	-4.5148	-3.3638
96	C	-2.6478	-2.9504	-3.2327
97	H	-5.9108	-2.4429	-2.0442
98	H	-4.5393	-1.2989	-1.9604
99	C	-5.2241	-1.6905	-3.9786
100	H	-5.5744	-4.8391	-2.9001
101	H	-3.9379	-5.3961	-3.4024
102	C	-4.8948	-4.0451	-4.8084
103	H	-2.1565	-2.1265	-2.6810
104	H	-1.9347	-3.8045	-3.2495
105	C	-2.9292	-2.4766	-4.6747
106	H	-5.9192	-0.8229	-3.9633
107	C	-5.8610	-2.8432	-4.7812
108	C	-3.8941	-1.2716	-4.6422
109	H	-5.3548	-4.8761	-5.3863
110	C	-3.5689	-3.6274	-5.4777
111	H	-1.9745	-2.1733	-5.1572
112	H	-6.0805	-2.5081	-5.8188
113	H	-6.8271	-3.1415	-4.3176
114	H	-3.4349	-0.4316	-4.0765
115	H	-4.0835	-0.9094	-5.6765
116	H	-2.8736	-4.4945	-5.5198
117	H	-3.7570	-3.3021	-6.5245

TSminor_e_solv
Energy (POTENTIAL) = -3541.76919073 Eh

	Atom	X	Y	Z
1	Ir	-1.3048	-0.6060	1.7769
2	N	-1.8157	-2.6033	2.0593
3	C	-1.4102	-3.0473	3.2573
4	C	-1.1806	-2.0070	4.2574
5	C	-1.2559	-0.6888	3.7569
6	C	-1.1475	0.3590	4.6816
7	H	-1.2151	1.3888	4.3399
8	C	-0.9406	0.1054	6.0325
9	C	-0.8379	-1.2069	6.5058
10	H	-0.6722	-1.3977	7.5620
11	C	-0.9616	-2.2644	5.6171
12	H	-0.9001	-3.2820	5.9945
13	C	-4.3455	-0.4556	1.8098
14	H	-4.3726	-1.5039	2.0964
15	C	-5.5377	0.2113	1.5602
16	H	-6.4824	-0.3189	1.6545
17	C	-5.5381	1.5620	1.1908
18	H	-6.4737	2.0769	0.9939
19	C	-4.3340	2.2419	1.0967
20	H	-4.3436	3.2958	0.8308
21	C	-3.1299	1.5688	1.3535
22	C	-1.8163	2.2088	1.3654
23	H	-0.8557	0.9348	6.7306
24	C	-2.2184	-3.5037	1.0965
25	C	-2.9168	-3.0470	-0.0478
26	C	-1.9997	-4.8871	1.2717
27	C	-3.3569	-3.9180	-1.0327
28	H	-3.1131	-1.9834	-0.0608
29	C	-2.3580	-5.7606	0.2237
30	C	-2.9953	-5.2936	-0.8969
31	H	-2.1414	-6.8209	0.3265
32	H	-3.2414	-6.0186	-1.6668
33	C	-3.1049	0.1950	1.6892
34	N	-0.7916	1.3971	1.6697
35	C	0.4561	1.9378	1.9278
36	C	1.4850	1.1131	2.4396
37	C	0.6872	3.3227	1.7603
38	C	2.7089	1.6339	2.8324
39	H	1.2391	0.0622	2.5040
40	C	1.9554	3.8403	2.0990
41	C	2.9254	3.0307	2.6318

42	H	2.1425	4.9022	1.9615
43	H	3.8665	3.4991	2.9048
44	C	3.8040	0.7827	3.5049
45	C	-1.5690	-0.0007	-1.3152
46	C	0.0736	-1.5403	-0.7228
47	C	-1.2740	-0.1154	-2.6622
48	H	-2.3593	0.6551	-0.9623
49	C	0.4028	-1.7217	-2.0698
50	C	-0.2733	-1.0082	-3.0442
51	H	-1.8222	0.4743	-3.3888
52	H	1.2088	-2.3917	-2.3427
53	H	-0.0146	-1.1349	-4.0912
54	C	0.7797	-2.1827	0.4197
55	O	0.6120	-1.6108	1.5816
56	C	1.5568	-3.2950	0.2313
57	H	1.5710	-3.7655	-0.7463
58	C	2.1194	-4.0712	1.3809
59	H	1.4118	-4.8507	1.6997
60	H	3.0567	-4.5697	1.1122
61	H	2.2986	-3.4226	2.2421
62	N	-0.9261	-0.7033	-0.3729
63	C	3.7439	-2.0077	-0.5768
64	Cl	3.3362	-0.3155	-0.6528
65	Cl	4.9843	-2.3827	0.5899
66	Cl	4.0391	-2.7326	-2.1499
67	C	4.0562	1.3149	4.9313
68	H	4.8195	0.6977	5.4531
69	H	4.4259	2.3618	4.9146
70	H	3.1172	1.2866	5.5259
71	C	3.4189	-0.7119	3.6210
72	H	2.5078	-0.8416	4.2451
73	H	3.2364	-1.1466	2.6164
74	H	4.2362	-1.2961	4.0970
75	C	5.1114	0.8720	2.6881
76	H	5.5175	1.9047	2.6769
77	H	5.8942	0.2134	3.1230
78	H	4.9356	0.5570	1.6388
79	C	-3.4021	-3.6435	-3.5285
80	H	-3.1225	-4.7059	-3.6912
81	H	-3.9897	-3.3072	-4.4101
82	H	-2.4687	-3.0423	-3.4798
83	C	-4.6708	-1.9964	-2.1340
84	H	-5.2360	-1.8175	-1.1934
85	H	-3.8034	-1.3105	-2.1723

86	H	-5.3337	-1.7290	-2.9854
87	C	-5.4961	-4.3384	-2.3091
88	H	-6.1627	-3.9869	-3.1264
89	H	-5.2623	-5.4028	-2.5175
90	H	-6.0586	-4.2831	-1.3519
91	C	-4.2174	-3.4728	-2.2314
92	C	-1.6145	3.5950	1.1373
93	C	-0.3791	4.1409	1.3119
94	H	-0.2087	5.2020	1.1490
95	H	-2.4544	4.2126	0.8428
96	C	-1.4616	-5.3342	2.5054
97	C	-1.2250	-4.4340	3.4991
98	H	-1.2718	-6.3942	2.6541
99	H	-0.8443	-4.7580	4.4602

TSmajor_e_solv
Energy (POTENTIAL) = -3541.77029945 Eh

	Atom	X	Y	Z
1	Ir	-1.1930	-0.7062	1.8600
2	N	-2.1685	-2.5182	2.2749
3	C	-2.4039	-2.7145	3.5826
4	C	-2.0460	-1.6076	4.4630
5	C	-1.5630	-0.4654	3.7877
6	C	-1.3365	0.6828	4.5704
7	H	-1.0079	1.6017	4.0940
8	C	-1.5145	0.6695	5.9464
9	C	-1.9420	-0.4919	6.6017
10	H	-2.0721	-0.5001	7.6799
11	C	-2.2199	-1.6255	5.8568
12	H	-2.5753	-2.5161	6.3679
13	C	-4.1600	-0.2382	1.3025
14	H	-4.4001	-1.1616	1.8229
15	C	-5.1739	0.4549	0.6512
16	H	-6.1909	0.0706	0.6758
17	C	-4.8983	1.6388	-0.0401
18	H	-5.6932	2.1719	-0.5535
19	C	-3.6032	2.1353	-0.0556
20	H	-3.4026	3.0654	-0.5804
21	C	-2.5838	1.4411	0.6096
22	C	-1.2157	1.9343	0.7532
23	H	-1.3202	1.5716	6.5216
24	C	-2.6210	-3.4540	1.3592
25	C	-2.4371	-3.2411	-0.0255
26	C	-3.3026	-4.6170	1.7884
27	C	-2.9464	-4.1107	-0.9829
28	H	-1.8774	-2.3515	-0.2961
29	C	-3.8035	-5.5084	0.8183
30	C	-3.6467	-5.2650	-0.5225
31	H	-4.3310	-6.3988	1.1512
32	H	-4.0753	-6.0023	-1.1930
33	C	-2.6991	-3.8309	-2.4782
34	C	-2.8382	0.2263	1.2803
35	N	-0.4159	1.1889	1.5308
36	C	0.7999	1.6980	1.9462
37	C	1.5338	1.0479	2.9694
38	C	1.2773	2.9222	1.4288
39	C	2.6986	1.5890	3.4954
40	H	1.0846	0.1379	3.3392
41	C	2.5073	3.4247	1.8985

42	C	3.1924	2.7878	2.8990
43	H	2.8961	4.3446	1.4697
44	H	4.1229	3.2398	3.2292
45	C	3.4535	0.9797	4.6932
46	C	1.0579	-2.5725	3.0346
47	C	1.2462	-2.1165	0.7570
48	C	2.1282	-3.4477	3.0118
49	H	0.5102	-2.3702	3.9512
50	C	2.3468	-2.9784	0.6719
51	C	2.7919	-3.6430	1.8001
52	H	2.4325	-3.9571	3.9195
53	H	2.8357	-3.1339	-0.2820
54	H	3.6403	-4.3180	1.7371
55	C	0.6297	-1.4159	-0.4022
56	O	-0.5517	-0.8972	-0.1941
57	N	0.6373	-1.9114	1.9463
58	C	1.2680	-1.3298	-1.6115
59	H	2.1690	-1.9053	-1.7858
60	C	0.6303	-0.6448	-2.7812
61	H	0.0448	0.2175	-2.4463
62	H	1.3837	-0.3043	-3.4993
63	H	-0.0582	-1.3074	-3.3232
64	C	3.2796	0.4052	-1.2986
65	Cl	2.6196	1.9485	-1.7492
66	Cl	3.8058	0.2955	0.3518
67	Cl	4.4165	-0.2468	-2.4552
68	C	4.8760	0.5757	4.2513
69	H	5.4650	1.4558	3.9190
70	H	5.4286	0.1003	5.0906
71	H	4.8277	-0.1495	3.4101
72	C	3.5431	2.0217	5.8300
73	H	4.0436	1.5896	6.7236
74	H	4.1289	2.9132	5.5236
75	H	2.5256	2.3568	6.1271
76	C	2.7616	-0.2767	5.2692
77	H	1.7212	-0.0498	5.5888
78	H	2.7506	-1.0888	4.5172
79	H	3.3110	-0.6592	6.1567
80	C	-1.2016	-4.0321	-2.7797
81	H	-0.5759	-3.3855	-2.1345
82	H	-0.9054	-5.0861	-2.5881
83	H	-0.9755	-3.7907	-3.8408
84	C	-3.1111	-2.3809	-2.8277
85	H	-4.1641	-2.1948	-2.5244

86	H	-2.4638	-1.6324	-2.3268
87	H	-3.0248	-2.1975	-3.9206
88	C	-3.5021	-4.7756	-3.4047
89	H	-4.5909	-4.6990	-3.1941
90	H	-3.3416	-4.5110	-4.4726
91	H	-3.1784	-5.8314	-3.2807
92	C	0.4789	3.6227	0.4908
93	C	-0.7595	3.1526	0.1843
94	H	0.8531	4.5454	0.0548
95	H	-1.4064	3.6967	-0.4928
96	C	-3.0281	-3.8991	4.0571
97	C	-3.4725	-4.8354	3.1771
98	H	-3.9712	-5.7376	3.5222
99	H	-3.1723	-4.0317	5.1220

5_e_solv
Energy (POTENTIAL) = -2123.19469209 Eh

	Atom	X	Y	Z
1	Ir	-1.2875	-0.7552	1.9372
2	N	-2.2819	-2.5469	2.3195
3	C	-2.5834	-2.7425	3.6131
4	C	-2.2497	-1.6377	4.5076
5	C	-1.6933	-0.5143	3.8555
6	C	-1.4245	0.6148	4.6514
7	H	-1.0265	1.5134	4.1871
8	C	-1.6554	0.6069	6.0203
9	C	-2.1774	-0.5292	6.6512
10	H	-2.3533	-0.5313	7.7229
11	C	-2.4819	-1.6475	5.8922
12	H	-2.9020	-2.5200	6.3858
13	C	-4.2451	-0.1854	1.3951
14	H	-4.5108	-1.0988	1.9216
15	C	-5.2455	0.5545	0.7749
16	H	-6.2779	0.2167	0.8291
17	C	-4.9389	1.7288	0.0799
18	H	-5.7250	2.3010	-0.4042
19	C	-3.6227	2.1634	0.0215
20	H	-3.3933	3.0862	-0.5053
21	C	-2.6173	1.4211	0.6545
22	C	-1.2154	1.8301	0.7143
23	H	-1.4318	1.4934	6.6091
24	C	-2.6579	-3.4941	1.3822
25	C	-2.4106	-3.2682	0.0102
26	C	-3.3158	-4.6824	1.7762
27	C	-2.8063	-4.1650	-0.9723
28	H	-1.8754	-2.3561	-0.2348
29	C	-3.7020	-5.6033	0.7798
30	C	-3.4653	-5.3588	-0.5501
31	H	-4.2057	-6.5182	1.0822
32	H	-3.8064	-6.1214	-1.2426
33	C	-2.5203	-3.8389	-2.4520
34	C	-2.9050	0.2212	1.3408
35	N	-0.4484	1.1043	1.5388
36	C	0.8499	1.4923	1.7871
37	C	1.5678	0.9043	2.8570
38	C	1.4529	2.5127	1.0212
39	C	2.8751	1.2637	3.1457
40	H	1.0006	0.1931	3.4424
41	C	2.8116	2.8107	1.2544

42	C	3.5053	2.1950	2.2643
43	H	3.3019	3.5530	0.6294
44	H	4.5504	2.4642	2.3857
45	C	3.6528	0.7185	4.3595
46	C	0.9309	-2.6317	3.1774
47	C	1.2910	-1.9485	0.9787
48	C	2.0790	-3.4043	3.1880
49	H	0.2861	-2.5573	4.0487
50	C	2.4627	-2.7101	0.9242
51	C	2.8638	-3.4337	2.0349
52	H	2.3473	-3.9663	4.0759
53	H	3.0300	-2.7489	0.0015
54	H	3.7705	-4.0308	2.0002
55	C	0.7210	-1.1696	-0.1579
56	O	-0.5840	-0.9830	-0.0992
57	N	0.5558	-1.9141	2.1103
58	C	1.5219	-0.6786	-1.1327
59	H	2.5907	-0.8711	-1.0913
60	C	1.0009	0.1649	-2.2548
61	H	-0.0661	0.3589	-2.1126
62	H	1.5262	1.1286	-2.3058
63	H	1.1320	-0.3244	-3.2300
64	C	4.8142	-0.1630	3.8588
65	H	5.5250	0.4224	3.2379
66	H	5.3812	-0.5903	4.7141
67	H	4.4241	-1.0023	3.2430
68	C	4.2179	1.8928	5.1913
69	H	4.7240	1.5204	6.1084
70	H	4.9694	2.4781	4.6224
71	H	3.3982	2.5778	5.4988
72	C	2.7735	-0.1312	5.3077
73	H	1.8982	0.4534	5.6656
74	H	2.4161	-1.0483	4.8019
75	H	3.3528	-0.4573	6.1987
76	C	-0.9953	-3.7500	-2.6759
77	H	-0.5458	-2.9232	-2.0903
78	H	-0.5033	-4.6992	-2.3722
79	H	-0.7642	-3.5624	-3.7469
80	C	-3.1734	-2.4885	-2.8242
81	H	-4.2651	-2.5172	-2.6173
82	H	-2.7318	-1.6467	-2.2505
83	H	-3.0276	-2.2640	-3.9031
84	C	-3.0773	-4.9121	-3.4170
85	H	-4.1791	-5.0085	-3.3066

86	H	-2.8684	-4.6385	-4.4743
87	H	-2.6021	-5.8992	-3.2295
88	C	0.6564	3.2027	0.0728
89	C	-0.6676	2.9032	-0.0370
90	H	1.1055	3.9818	-0.5380
91	H	-1.3015	3.4409	-0.7317
92	C	-3.2167	-3.9354	4.0530
93	C	-3.5728	-4.8924	3.1531
94	H	-4.0643	-5.8073	3.4745
95	H	-3.4233	-4.0668	5.1081

8_tbu_solv
Energy (POTENTIAL) = -2764.64878255 Eh

	Atom	X	Y	Z
1	Ir	-1.5546	-0.3633	1.9553
2	N	-2.6386	-2.1120	1.9769
3	C	-3.2278	-2.3476	3.1603
4	C	-2.9593	-1.4576	4.2382
5	C	-2.1021	-0.3739	3.8856
6	C	-1.7402	0.5159	4.8989
7	H	-1.0878	1.3552	4.6789
8	C	-2.2009	0.3496	6.2060
9	C	-3.0539	-0.7133	6.5316
10	H	-3.4173	-0.8294	7.5488
11	C	-3.4376	-1.6142	5.5550
12	H	-4.1032	-2.4382	5.8031
13	C	-4.3978	0.3097	1.1084
14	H	-4.5758	-0.7487	0.9397
15	C	-5.4334	1.2159	0.8811
16	H	-6.3972	0.8555	0.5318
17	C	-5.2440	2.5878	1.1088
18	H	-6.0606	3.2834	0.9362
19	C	-4.0231	3.0594	1.5541
20	H	-3.8759	4.1225	1.7299
21	C	-2.9690	2.1462	1.7665
22	C	-1.6495	2.4694	2.1569
23	H	-1.9016	1.0578	6.9736
24	S	-4.1761	-3.8135	3.1881
25	C	-2.9138	-3.0837	1.0312
26	C	-2.4776	-3.0917	-0.2969
27	C	-3.7386	-4.1095	1.5160
28	C	-2.8319	-4.1457	-1.1517
29	H	-1.8917	-2.2323	-0.5997
30	C	-4.1153	-5.1556	0.6878
31	C	-3.6562	-5.1684	-0.6249
32	H	-4.7592	-5.9517	1.0488
33	H	-3.9743	-6.0061	-1.2384
34	C	-2.3711	-4.2205	-2.6206
35	C	-3.1482	0.7493	1.5489
36	N	-0.7392	1.4634	2.2156
37	S	-0.9766	4.0427	2.5047
38	C	0.5323	1.9163	2.5165
39	C	1.6845	1.1356	2.6391
40	C	0.6024	3.3044	2.7093
41	C	2.9219	1.7208	2.9396

42	H	1.5432	0.0756	2.4901
43	C	1.8102	3.9106	3.0162
44	C	2.9521	3.1224	3.1258
45	H	1.8737	4.9839	3.1673
46	H	3.8767	3.6395	3.3643
47	C	4.2222	0.9036	3.0693
48	C	0.4540	-2.4503	3.2616
49	C	0.7966	-2.0000	1.0004
50	C	1.3997	-3.4613	3.2552
51	H	-0.1004	-2.1797	4.1554
52	C	1.7453	-3.0217	0.9194
53	C	2.0516	-3.7525	2.0570
54	H	1.6110	-4.0111	4.1655
55	H	2.2245	-3.2475	-0.0261
56	H	2.7882	-4.5487	2.0104
57	C	0.3917	-1.1071	-0.1167
58	O	-0.7083	-0.4051	0.0835
59	N	0.1667	-1.7408	2.1626
60	C	1.1189	-0.9758	-1.2573
61	H	2.0348	-1.5501	-1.3654
62	C	0.7408	-0.0596	-2.3725
63	H	-0.1997	0.4510	-2.1565
64	H	1.5215	0.6951	-2.5331
65	H	0.6349	-0.6126	-3.3146
66	C	5.2516	1.4053	2.0338
67	H	5.5332	2.4631	2.2177
68	H	6.1832	0.8004	2.0791
69	H	4.8345	1.3282	1.0063
70	C	4.7977	1.0741	4.4914
71	H	5.7152	0.4600	4.6215
72	H	5.0718	2.1302	4.6960
73	H	4.0518	0.7535	5.2507
74	C	4.0086	-0.6101	2.8244
75	H	3.2995	-1.0351	3.5671
76	H	3.6199	-0.7932	1.7994
77	H	4.9665	-1.1656	2.9225
78	C	-1.4544	-3.0409	-3.0233
79	H	-1.9837	-2.0693	-2.9164
80	H	-0.5360	-3.0302	-2.3988
81	H	-1.1363	-3.1315	-4.0846
82	C	-1.5780	-5.5261	-2.8475
83	H	-2.2111	-6.4231	-2.6849
84	H	-1.1923	-5.5773	-3.8889
85	H	-0.7126	-5.5782	-2.1516

86	C	-3.6041	-4.1996	-3.5485
87	H	-3.2940	-4.2141	-4.6160
88	H	-4.2564	-5.0817	-3.3785
89	H	-4.2053	-3.2816	-3.3714

2_tbu_solv
Energy (POTENTIAL) = -2325.04668145 Eh

	Atom	X	Y	Z
1	Ir	-1.7038	-0.3577	2.1189
2	N	-2.6778	-2.1569	2.1042
3	C	-3.0367	-2.5958	3.2953
4	C	-2.7315	-1.7306	4.4216
5	C	-2.1074	-0.5192	4.0392
6	C	-1.7944	0.4145	5.0238
7	H	-1.3277	1.3590	4.7645
8	C	-2.0779	0.1326	6.3623
9	C	-2.6812	-1.0685	6.7314
10	H	-2.8947	-1.2721	7.7754
11	C	-3.0123	-2.0067	5.7592
12	H	-3.4853	-2.9431	6.0436
13	C	-4.4829	0.3227	1.1898
14	H	-4.7601	-0.7169	1.3289
15	C	-5.4244	1.2251	0.6892
16	H	-6.4215	0.8708	0.4452
17	C	-5.1038	2.5686	0.5021
18	H	-5.8462	3.2575	0.1133
19	C	-3.8303	3.0290	0.8206
20	H	-3.5791	4.0770	0.6788
21	C	-2.8871	2.1330	1.3222
22	C	-1.5316	2.4668	1.7242
23	H	-1.8245	0.8639	7.1239
24	S	-3.8488	-4.1166	3.2824
25	C	-3.0482	-3.0185	1.0773
26	C	-2.8337	-2.7985	-0.2840
27	C	-3.7054	-4.1614	1.5386
28	C	-3.2754	-3.7405	-1.2180
29	H	-2.3305	-1.8721	-0.5444
30	C	-4.1482	-5.1212	0.6345
31	C	-3.9271	-4.8985	-0.7161
32	H	-4.6564	-6.0205	0.9657
33	H	-4.2878	-5.6669	-1.3921
34	C	-3.0885	-3.5678	-2.7371
35	C	-3.1993	0.7643	1.5011
36	N	-0.7886	1.4714	2.1687
37	S	-0.7542	4.0055	1.7471
38	C	0.4745	1.8829	2.5806
39	C	1.4584	1.0585	3.1284
40	C	0.6778	3.2552	2.4177
41	C	2.6838	1.6059	3.5205

42	H	1.1998	0.0091	3.2330
43	C	1.8900	3.8273	2.7890
44	C	2.8648	3.0015	3.3279
45	H	2.0763	4.8890	2.6675
46	H	3.7963	3.4829	3.6071
47	C	3.8166	0.7689	4.1442
48	C	5.0756	0.8611	3.2554
49	H	5.4579	1.9015	3.1959
50	H	5.8935	0.2288	3.6641
51	H	4.8470	0.5136	2.2245
52	C	4.1413	1.3097	5.5535
53	H	4.9260	0.6918	6.0416
54	H	4.5174	2.3533	5.5136
55	H	3.2326	1.2902	6.1936
56	C	3.4482	-0.7277	4.2872
57	H	2.5623	-0.8560	4.9464
58	H	3.2340	-1.1792	3.2944
59	H	4.2875	-1.2990	4.7402
60	C	-2.3662	-2.2496	-3.1072
61	H	-2.9480	-1.3684	-2.7596
62	H	-1.3493	-2.2164	-2.6596
63	H	-2.2495	-2.1597	-4.2092
64	C	-2.2459	-4.7375	-3.2894
65	H	-2.7596	-5.7117	-3.1508
66	H	-2.0613	-4.6106	-4.3783
67	H	-1.2634	-4.7842	-2.7716
68	C	-4.4691	-3.5572	-3.4284
69	H	-4.3610	-3.3884	-4.5219
70	H	-5.0012	-4.5218	-3.2923
71	H	-5.1041	-2.7461	-3.0107

7major_tbu_gas
Energy (POTENTIAL) = -3868.70255562 Eh

	Atom	X	Y	Z
1	Ir	-1.5152	-0.6661	2.0612
2	N	-2.5077	-2.4634	1.9994
3	C	-2.5989	-3.0682	3.1695
4	C	-2.1292	-2.3496	4.3326
5	C	-1.6539	-1.0535	4.0194
6	C	-1.2419	-0.2558	5.0903
7	H	-0.8727	0.7506	4.9137
8	C	-1.2869	-0.7348	6.3984
9	C	-1.7463	-2.0239	6.6808
10	H	-1.7751	-2.3837	7.7042
11	C	-2.1727	-2.8382	5.6427
12	H	-2.5405	-3.8402	5.8514
13	C	-4.4990	-0.0712	1.9792
14	H	-4.6920	-1.1298	1.8386
15	C	-5.5793	0.8058	2.0137
16	H	-6.5856	0.4129	1.8971
17	C	-5.3943	2.1793	2.2023
18	H	-6.2475	2.8492	2.2313
19	C	-4.1106	2.6763	2.3544
20	H	-3.9519	3.7420	2.5025
21	C	-3.0256	1.7910	2.3150
22	C	-1.6410	2.1766	2.4364
23	H	-0.9602	-0.0940	7.2129
24	S	-3.3688	-4.6188	3.1136
25	C	-3.1322	-3.1747	0.9798
26	C	-3.3422	-2.7323	-0.3244
27	C	-3.6383	-4.4069	1.3998
28	C	-4.0288	-3.5270	-1.2485
29	H	-2.9723	-1.7449	-0.5697
30	C	-4.2963	-5.2363	0.4985
31	C	-4.4784	-4.7974	-0.8064
32	H	-4.6828	-6.2028	0.8049
33	H	-5.0066	-5.4876	-1.4544
34	C	-4.2744	-2.9894	-2.6714
35	C	-3.1870	0.3982	2.1263
36	N	-0.7272	1.2283	2.3272
37	S	-1.0080	3.7652	2.7066
38	C	0.5669	1.7287	2.4394
39	C	1.7455	0.9928	2.3387
40	C	0.6098	3.1095	2.6530
41	C	2.9916	1.6246	2.4412

42	H	1.6396	-0.0759	2.1881
43	C	1.8294	3.7630	2.7814
44	C	2.9987	3.0230	2.6735
45	H	1.8780	4.8327	2.9569
46	H	3.9150	3.5925	2.7783
47	C	4.2769	0.7957	2.2652
48	C	-1.4337	0.4380	-0.8742
49	C	0.0754	-1.2750	-0.4684
50	C	-0.9562	0.6032	-2.1716
51	H	-2.2455	1.0435	-0.4817
52	C	0.5910	-1.1754	-1.7551
53	C	0.0706	-0.2163	-2.6200
54	H	-1.3930	1.3620	-2.8115
55	H	1.3881	-1.8291	-2.0880
56	H	0.4640	-0.1157	-3.6260
57	C	0.6083	-2.1950	0.5785
58	O	0.2718	-1.9891	1.7422
59	C	1.5638	-3.3481	0.2799
60	C	2.6342	-3.4554	1.3713
61	H	2.1844	-3.4684	2.3650
62	H	3.2252	-4.3626	1.2346
63	H	3.3188	-2.6087	1.3047
64	N	-0.9321	-0.4768	-0.0409
65	H	2.0464	-3.1784	-0.6859
66	C	0.7796	-4.6823	0.0907
67	Cl	0.0309	-5.2234	1.6128
68	Cl	-0.5025	-4.4771	-1.1428
69	Cl	1.9086	-5.9372	-0.4936
70	C	4.3035	-0.3513	3.3002
71	H	4.2547	0.0595	4.3318
72	H	3.4517	-1.0481	3.1669
73	H	5.2371	-0.9471	3.2050
74	C	4.3076	0.2120	0.8363
75	H	4.3448	1.0311	0.0857
76	H	5.2001	-0.4349	0.6929
77	H	3.4047	-0.3956	0.6234
78	C	5.5653	1.6298	2.4611
79	H	6.4683	0.9926	2.3390
80	H	5.6309	2.4447	1.7080
81	H	5.5990	2.0709	3.4808
82	C	-2.9209	-2.7345	-3.3677
83	H	-2.3351	-3.6764	-3.4324
84	H	-3.0745	-2.3486	-4.3987
85	H	-2.3163	-1.9860	-2.8165

86	C	-5.0673	-1.6656	-2.5946
87	H	-6.0210	-1.8176	-2.0444
88	H	-4.4886	-0.8713	-2.0777
89	H	-5.3072	-1.2897	-3.6129
90	C	-5.0813	-3.9723	-3.5520
91	H	-5.2452	-3.5488	-4.5668
92	H	-4.5357	-4.9326	-3.6763
93	H	-6.0798	-4.1731	-3.1067

5_tbu_solv
Energy (POTENTIAL) = -2764.74471620 Eh

	Atom	X	Y	Z
1	Ir	-1.6043	-0.4461	2.0922
2	N	-2.6816	-2.1879	2.0856
3	C	-3.1745	-2.5370	3.2562
4	C	-2.9217	-1.6595	4.3769
5	C	-2.1675	-0.5156	4.0033
6	C	-1.8791	0.3935	5.0353
7	H	-1.3107	1.2932	4.8116
8	C	-2.3055	0.1704	6.3399
9	C	-3.0452	-0.9712	6.6762
10	H	-3.3732	-1.1317	7.6988
11	C	-3.3557	-1.8918	5.6884
12	H	-3.9302	-2.7831	5.9340
13	C	-4.5014	0.3165	1.4073
14	H	-4.7918	-0.7233	1.5330
15	C	-5.4638	1.2379	1.0092
16	H	-6.4841	0.9044	0.8352
17	C	-5.1427	2.5883	0.8258
18	H	-5.9029	3.2967	0.5110
19	C	-3.8431	3.0110	1.0526
20	H	-3.5795	4.0579	0.9158
21	C	-2.8821	2.0762	1.4566
22	C	-1.5049	2.3894	1.7514
23	H	-2.0647	0.8959	7.1133
24	S	-4.0815	-4.0211	3.2343
25	C	-3.0076	-3.0842	1.0724
26	C	-2.6428	-2.9496	-0.2682
27	C	-3.7727	-4.1655	1.5180
28	C	-3.0316	-3.9268	-1.1901
29	H	-2.0653	-2.0569	-0.4991
30	C	-4.1799	-5.1465	0.6202
31	C	-3.8046	-5.0160	-0.7096
32	H	-4.7776	-5.9937	0.9416
33	H	-4.1416	-5.8003	-1.3814
34	C	-2.6539	-3.8555	-2.6820
35	C	-3.1727	0.7037	1.6372
36	N	-0.7131	1.4155	2.1539
37	S	-0.7482	3.9521	1.6728
38	C	0.5701	1.8660	2.4493
39	C	1.6211	1.0866	2.9352
40	C	0.7405	3.2383	2.2383
41	C	2.8686	1.6644	3.1953

42	H	1.3917	0.0416	3.0890
43	C	1.9664	3.8427	2.4898
44	C	3.0077	3.0553	2.9577
45	H	2.1130	4.9058	2.3275
46	H	3.9504	3.5624	3.1403
47	C	4.0718	0.8569	3.7191
48	C	0.4537	-2.4898	3.2923
49	C	0.8134	-1.8759	1.0661
50	C	1.4706	-3.4258	3.2617
51	H	-0.1364	-2.3143	4.1868
52	C	1.8429	-2.8208	0.9690
53	C	2.1744	-3.5946	2.0675
54	H	1.6960	-4.0120	4.1457
55	H	2.3547	-2.9578	0.0240
56	H	2.9671	-4.3336	1.9955
57	C	0.3501	-0.9960	-0.0454
58	O	-0.8697	-0.5072	0.0841
59	N	0.1358	-1.7369	2.2266
60	C	1.1591	-0.7361	-1.1012
61	H	2.1525	-1.1739	-1.1344
62	C	0.7556	0.1629	-2.2283
63	H	-0.2047	0.6373	-2.0088
64	H	1.5042	0.9476	-2.3992
65	H	0.6523	-0.3905	-3.1723
66	C	5.2416	0.9648	2.7169
67	H	5.5990	2.0109	2.6169
68	H	6.1050	0.3495	3.0511
69	H	4.9246	0.6063	1.7135
70	C	4.5125	1.4186	5.0875
71	H	5.3552	0.8252	5.5041
72	H	4.8551	2.4712	5.0046
73	H	3.6684	1.3821	5.8099
74	C	3.7510	-0.6452	3.9053
75	H	2.9315	-0.7889	4.6424
76	H	3.4589	-1.1044	2.9372
77	H	4.6400	-1.1962	4.2820
78	C	-1.7914	-2.6160	-3.0239
79	H	-2.3384	-1.6754	-2.7966
80	H	-0.8378	-2.6312	-2.4537
81	H	-1.5345	-2.5995	-4.1054
82	C	-1.8434	-5.1112	-3.0697
83	H	-2.4435	-6.0374	-2.9519
84	H	-1.5188	-5.0585	-4.1316
85	H	-0.9374	-5.1983	-2.4314

86	C	-3.9382	-3.7880	-3.5351
87	H	-3.6895	-3.6964	-4.6147
88	H	-4.5574	-4.7010	-3.4115
89	H	-4.5509	-2.9082	-3.2417

4_tbu_solv
Energy (POTENTIAL) = -2765.21130896 Eh

	Atom	X	Y	Z
1	Ir	-1.5550	-0.6308	2.1478
2	N	-2.6174	-2.4157	2.1456
3	C	-2.8631	-2.8860	3.3537
4	C	-2.4268	-2.1085	4.4959
5	C	-1.7592	-0.9165	4.1247
6	C	-1.3234	-0.0912	5.1712
7	H	-0.8126	0.8442	4.9555
8	C	-1.5365	-0.4423	6.5035
9	C	-2.1939	-1.6302	6.8408
10	H	-2.3565	-1.8911	7.8825
11	C	-2.6427	-2.4706	5.8313
12	H	-3.1572	-3.3948	6.0866
13	C	-4.4976	0.1431	2.1475
14	H	-4.7562	-0.9105	2.0787
15	C	-5.5204	1.0897	2.1450
16	H	-6.5537	0.7576	2.0769
17	C	-5.2416	2.4587	2.2279
18	H	-6.0486	3.1853	2.2236
19	C	-3.9227	2.8815	2.3158
20	H	-3.6965	3.9438	2.3805
21	C	-2.8990	1.9271	2.3182
22	C	-1.4855	2.2241	2.3995
23	H	-1.1890	0.2202	7.2928
24	S	-3.7049	-4.3990	3.3827
25	C	-3.1021	-3.2513	1.1412
26	C	-3.0277	-3.0395	-0.2392
27	C	-3.7261	-4.4046	1.6354
28	C	-3.5535	-3.9848	-1.1105
29	H	-2.5706	-2.1410	-0.6308
30	C	-4.2616	-5.3646	0.7760
31	C	-4.1631	-5.1444	-0.5888
32	H	-4.7399	-6.2593	1.1631
33	H	-4.5698	-5.8826	-1.2757
34	C	-3.4803	-3.7768	-2.6006
35	C	-3.1529	0.5352	2.2257
36	N	-0.6549	1.2029	2.3681
37	S	-0.7178	3.7673	2.5733
38	C	0.6743	1.5813	2.5126
39	C	1.7752	0.7278	2.5758
40	C	0.8407	2.9692	2.6277
41	C	3.0484	1.2688	2.7310

42	H	1.6308	-0.3456	2.5196
43	C	2.1070	3.5269	2.7837
44	C	3.1969	2.6655	2.8287
45	H	2.2444	4.5998	2.8768
46	H	4.1915	3.0857	2.9532
47	C	4.2475	0.3570	2.7867
48	C	-1.8285	0.4074	-0.7933
49	C	-0.0813	-1.0788	-0.4883
50	C	-1.5134	0.5579	-2.1412
51	H	-2.6691	0.9330	-0.3534
52	C	0.2919	-0.9790	-1.8214
53	C	-0.4410	-0.1474	-2.6658
54	H	-2.1143	1.2175	-2.7577
55	H	1.1386	-1.5397	-2.2006
56	H	-0.1729	-0.0558	-3.7133
57	C	0.6236	-1.9554	0.4884
58	O	0.2087	-1.9854	1.6495
59	C	1.8185	-2.7550	0.0802
60	H	2.5394	-2.0561	-0.3656
61	H	1.5129	-3.4266	-0.7333
62	C	2.4523	-3.5297	1.2263
63	H	1.7535	-4.2554	1.6545
64	H	3.3268	-4.0741	0.8573
65	H	2.7827	-2.8579	2.0253
66	N	-1.1372	-0.3992	0.0155
67	C	4.4776	-0.3277	1.4266
68	H	5.4676	-0.7322	1.3939
69	H	3.7657	-1.1163	1.2993
70	H	4.3593	0.3898	0.6416
71	C	5.5272	1.1331	3.1492
72	H	5.3830	1.6451	4.0776
73	H	6.3448	0.4492	3.2423
74	H	5.7431	1.8444	2.3795
75	C	4.0490	-0.7553	3.8331
76	H	3.7208	-0.3231	4.7553
77	H	3.3130	-1.4481	3.4821
78	H	4.9753	-1.2677	3.9891
79	C	-2.7175	-2.4849	-2.9481
80	H	-3.2321	-1.6441	-2.5322
81	H	-1.7287	-2.5344	-2.5423
82	H	-2.6618	-2.3787	-4.0114
83	C	-2.7660	-4.9558	-3.2872
84	H	-3.3878	-5.8253	-3.2410
85	H	-2.5732	-4.7091	-4.3103

86	H	-1.8406	-5.1522	-2.7871
87	C	-4.8899	-3.6781	-3.2129
88	H	-4.8116	-3.4239	-4.2493
89	H	-5.3888	-4.6194	-3.1132
90	H	-5.4488	-2.9224	-2.7015

TSmajor_tbu_solv
Energy (POTENTIAL) = -4183.31638391 Eh

	Atom	X	Y	Z
1	Ir	-1.5437	-0.5290	2.0727
2	N	-2.4497	-2.3903	2.1089
3	C	-2.3973	-2.9575	3.2988
4	C	-1.9495	-2.1671	4.4199
5	C	-1.5827	-0.8533	4.0441
6	C	-1.2083	0.0076	5.0868
7	H	-0.9283	1.0350	4.8700
8	C	-1.1760	-0.4280	6.4068
9	C	-1.5202	-1.7425	6.7448
10	H	-1.4838	-2.0711	7.7791
11	C	-1.9139	-2.6172	5.7458
12	H	-2.1920	-3.6395	5.9943
13	C	-4.5286	0.1737	2.0021
14	H	-4.7607	-0.8885	2.0163
15	C	-5.5656	1.0940	1.8926
16	H	-6.5912	0.7390	1.8244
17	C	-5.3135	2.4720	1.8698
18	H	-6.1328	3.1793	1.7848
19	C	-4.0069	2.9243	1.9639
20	H	-3.7963	3.9920	1.9534
21	C	-2.9680	1.9916	2.0730
22	C	-1.5668	2.3230	2.2097
23	H	-0.8756	0.2633	7.1905
24	S	-2.9461	-4.6051	3.3412
25	C	-2.9857	-3.2386	1.1432
26	C	-3.2541	-2.9058	-0.1866
27	C	-3.3048	-4.5085	1.6365
28	C	-3.8212	-3.8507	-1.0507
29	H	-3.0106	-1.8903	-0.4708
30	C	-3.8552	-5.4718	0.8005
31	C	-4.0988	-5.1368	-0.5224
32	H	-4.0984	-6.4631	1.1696
33	H	-4.5307	-5.9156	-1.1439
34	C	-3.1891	0.5879	2.0867
35	N	-0.7149	1.3207	2.2742
36	S	-0.8413	3.8886	2.4223
37	C	0.5787	1.7285	2.5848
38	C	1.6426	0.8714	2.8689
39	C	0.7061	3.1158	2.6920
40	C	2.8682	1.4068	3.2790
41	H	1.4273	-0.1874	2.7567

42	C	1.9303	3.6763	3.0403
43	C	2.9845	2.8204	3.3278
44	H	2.0596	4.7511	3.1171
45	H	3.9188	3.2930	3.6168
46	C	4.0562	0.5265	3.7112
47	C	-1.7777	0.4955	-0.8877
48	C	-0.1995	-1.1830	-0.5126
49	C	-1.4416	0.5937	-2.2258
50	H	-2.5551	1.1133	-0.4490
51	C	0.1658	-1.1492	-1.8631
52	C	-0.4498	-0.2544	-2.7207
53	H	-1.9488	1.3116	-2.8608
54	H	0.9535	-1.7981	-2.2244
55	H	-0.1558	-0.2108	-3.7651
56	C	0.4452	-2.0367	0.5211
57	O	0.2462	-1.6880	1.7669
58	C	1.2140	-3.1157	0.1689
59	H	1.2298	-3.4372	-0.8665
60	C	1.7486	-4.0501	1.2103
61	H	0.9400	-4.6617	1.6359
62	H	2.4997	-4.7268	0.7922
63	H	2.1985	-3.5006	2.0431
64	N	-1.1768	-0.3695	-0.0557
65	C	3.4845	-1.9492	-0.6030
66	Cl	3.2279	-0.2366	-0.4148
67	Cl	4.7381	-2.5982	0.4176
68	Cl	3.6365	-2.4592	-2.2771
69	C	4.4333	0.8519	5.1729
70	H	5.2557	0.1915	5.5241
71	H	4.7803	1.9007	5.2812
72	H	3.5568	0.7036	5.8404
73	C	3.7357	-0.9857	3.6372
74	H	2.8952	-1.2459	4.3167
75	H	3.4643	-1.2794	2.6028
76	H	4.6160	-1.5933	3.9402
77	C	5.2684	0.8031	2.7971
78	H	5.6112	1.8554	2.8829
79	H	6.1248	0.1490	3.0703
80	H	5.0076	0.6082	1.7361
81	C	-3.3672	-4.5094	-3.4397
82	H	-3.6609	-5.5665	-3.2719
83	H	-3.5564	-4.2776	-4.5103
84	H	-2.2758	-4.4156	-3.2495
85	C	-3.7924	-2.1031	-2.9360

86	H	-4.3464	-1.3613	-2.3208
87	H	-2.7022	-1.9335	-2.8240
88	H	-4.0518	-1.9173	-4.0009
89	C	-5.6696	-3.7379	-2.7593
90	H	-5.9407	-3.4826	-3.8068
91	H	-5.9817	-4.7883	-2.5821
92	H	-6.2516	-3.0808	-2.0773
93	C	-4.1556	-3.5482	-2.5239

6minor_tbu_solv
Energy (POTENTIAL) = -4183.37587338 Eh

	Atom	X	Y	Z
1	Ir	-1.3984	-0.4880	2.1057
2	N	-2.2208	-2.3822	2.1115
3	C	-2.1670	-2.9704	3.2912
4	C	-1.7138	-2.1995	4.4232
5	C	-1.3756	-0.8717	4.0697
6	C	-0.9855	-0.0315	5.1237
7	H	-0.7239	1.0041	4.9228
8	C	-0.9151	-0.4984	6.4317
9	C	-1.2354	-1.8248	6.7465
10	H	-1.1693	-2.1776	7.7712
11	C	-1.6415	-2.6811	5.7365
12	H	-1.8983	-3.7133	5.9666
13	C	-4.4221	-0.0352	2.1467
14	H	-4.5675	-1.1120	2.1649
15	C	-5.5359	0.7945	2.0804
16	H	-6.5293	0.3536	2.0497
17	C	-5.4022	2.1889	2.0519
18	H	-6.2816	2.8236	1.9998
19	C	-4.1364	2.7496	2.0980
20	H	-4.0162	3.8311	2.0824
21	C	-3.0191	1.9071	2.1658
22	C	-1.6482	2.3532	2.2480
23	H	-0.6036	0.1774	7.2246
24	S	-2.7284	-4.6148	3.3052
25	C	-2.7601	-3.2102	1.1324
26	C	-2.9961	-2.8695	-0.1992
27	C	-3.0922	-4.4844	1.6035
28	C	-3.5618	-3.7960	-1.0849
29	H	-2.7227	-1.8649	-0.4981
30	C	-3.6403	-5.4308	0.7468
31	C	-3.8683	-5.0839	-0.5779
32	H	-3.8937	-6.4252	1.1006
33	H	-4.2991	-5.8682	-1.1909
34	C	-3.8117	-3.3880	-2.5493
35	C	-3.1208	0.4929	2.1817
36	N	-0.7077	1.4320	2.3145
37	S	-1.0657	3.9859	2.3490
38	C	0.5562	1.9724	2.5380
39	C	1.7174	1.2421	2.8031
40	C	0.5555	3.3709	2.5652
41	C	2.9055	1.9223	3.1045

42	H	1.6092	0.1614	2.7719
43	C	1.7343	4.0688	2.7948
44	C	2.8842	3.3400	3.0548
45	H	1.7587	5.1539	2.7948
46	H	3.7851	3.9175	3.2396
47	C	4.2072	1.2030	3.5052
48	C	-1.7289	0.6264	-0.8241
49	C	-0.0241	-0.9638	-0.5064
50	C	-1.4119	0.7960	-2.1589
51	H	-2.5537	1.1688	-0.3703
52	C	0.3465	-0.8221	-1.8729
53	C	-0.3346	0.0527	-2.6833
54	H	-1.9803	1.4878	-2.7697
55	H	1.1980	-1.3703	-2.2604
56	H	-0.0389	0.1746	-3.7213
57	C	0.6170	-1.8033	0.4438
58	O	0.4097	-1.6325	1.7076
59	C	1.3490	-3.0555	-0.0021
60	H	1.3682	-3.0739	-1.0949
61	C	0.5579	-4.2828	0.4772
62	H	-0.4107	-4.2930	-0.0315
63	H	1.0773	-5.2167	0.2456
64	H	0.3816	-4.2244	1.5542
65	N	-1.0745	-0.2165	-0.0144
66	C	2.8421	-3.1152	0.3923
67	Cl	3.6483	-1.5799	-0.0706
68	Cl	3.0878	-3.4268	2.1281
69	Cl	3.6439	-4.4447	-0.5308
70	C	5.2949	1.4863	2.4482
71	H	5.5319	2.5694	2.3907
72	H	6.2355	0.9486	2.6972
73	H	4.9552	1.1502	1.4444
74	C	4.0311	-0.3272	3.6126
75	H	3.2560	-0.5862	4.3663
76	H	3.7389	-0.7471	2.6319
77	H	4.9813	-0.8176	3.9169
78	C	4.6836	1.7108	4.8848
79	H	5.5862	1.1548	5.2197
80	H	4.9540	2.7866	4.8563
81	H	3.8850	1.5702	5.6451
82	C	-4.7188	-2.1379	-2.5949
83	H	-5.6727	-2.3331	-2.0587
84	H	-4.2289	-1.2579	-2.1278
85	H	-4.9579	-1.8621	-3.6449

86	C	-4.5020	-4.5003	-3.3739
87	H	-4.6829	-4.1625	-4.4177
88	H	-3.8651	-5.4097	-3.4261
89	H	-5.4862	-4.7664	-2.9311
90	C	-2.4634	-3.0682	-3.2246
91	H	-1.7849	-3.9473	-3.1741
92	H	-2.6095	-2.7958	-4.2923
93	H	-1.9631	-2.2165	-2.7258

6major_tbu_solv
Energy (POTENTIAL) = -4183.38024263 Eh

	Atom	X	Y	Z
1	Ir	-1.4970	-0.6639	2.0574
2	N	-2.4745	-2.4705	1.9709
3	C	-2.5675	-3.0823	3.1339
4	C	-2.1008	-2.3839	4.3094
5	C	-1.6307	-1.0823	4.0125
6	C	-1.2277	-0.3039	5.1064
7	H	-0.8597	0.7064	4.9457
8	C	-1.2748	-0.8028	6.4048
9	C	-1.7291	-2.1006	6.6652
10	H	-1.7571	-2.4796	7.6823
11	C	-2.1475	-2.8967	5.6106
12	H	-2.5087	-3.9059	5.7986
13	C	-4.4958	-0.0484	1.9634
14	H	-4.6925	-1.1048	1.8045
15	C	-5.5710	0.8308	2.0043
16	H	-6.5796	0.4451	1.8771
17	C	-5.3808	2.2039	2.2092
18	H	-6.2309	2.8785	2.2405
19	C	-4.0948	2.6901	2.3698
20	H	-3.9288	3.7539	2.5273
21	C	-3.0156	1.7969	2.3231
22	C	-1.6298	2.1740	2.4446
23	H	-0.9516	-0.1749	7.2316
24	S	-3.3675	-4.6233	3.0738
25	C	-3.1040	-3.1728	0.9482
26	C	-3.2868	-2.7318	-0.3611
27	C	-3.6400	-4.3943	1.3646
28	C	-4.0006	-3.5064	-1.2826
29	H	-2.8564	-1.7708	-0.6133
30	C	-4.3201	-5.2054	0.4643
31	C	-4.4941	-4.7595	-0.8390
32	H	-4.7276	-6.1635	0.7708
33	H	-5.0429	-5.4349	-1.4864
34	C	-4.2166	-2.9723	-2.7117
35	C	-3.1733	0.4034	2.1197
36	N	-0.7174	1.2274	2.3354
37	S	-0.9914	3.7683	2.7100
38	C	0.5769	1.7281	2.4354
39	C	1.7505	0.9862	2.3188
40	C	0.6245	3.1091	2.6497
41	C	2.9980	1.6187	2.4116

42	H	1.6297	-0.0805	2.1526
43	C	1.8459	3.7599	2.7677
44	C	3.0120	3.0162	2.6482
45	H	1.8978	4.8301	2.9413
46	H	3.9310	3.5843	2.7438
47	C	4.2802	0.7888	2.2196
48	C	-1.4599	0.4509	-0.8746
49	C	0.0589	-1.2923	-0.4190
50	C	-1.0372	0.5651	-2.1852
51	H	-2.2501	1.0829	-0.4772
52	C	0.4976	-1.2425	-1.7708
53	C	-0.0343	-0.3183	-2.6353
54	H	-1.4809	1.3063	-2.8400
55	H	1.2643	-1.9268	-2.1157
56	H	0.3157	-0.2719	-3.6625
57	C	0.5993	-2.1178	0.6059
58	O	0.2686	-1.8979	1.8365
59	C	1.5557	-3.2718	0.3423
60	C	2.6087	-3.3819	1.4516
61	H	2.1388	-3.2970	2.4326
62	H	3.1581	-4.3238	1.3930
63	H	3.3354	-2.5756	1.3414
64	N	-0.9556	-0.4464	-0.0169
65	H	2.0625	-3.1183	-0.6156
66	C	0.8064	-4.6264	0.1494
67	Cl	0.0214	-5.1705	1.6579
68	Cl	-0.4373	-4.5107	-1.1313
69	Cl	1.9805	-5.8950	-0.3768
70	C	4.3210	-0.3511	3.2614
71	H	4.3138	0.0679	4.2909
72	H	3.4514	-1.0308	3.1644
73	H	5.2404	-0.9640	3.1399
74	C	4.2902	0.1994	0.7924
75	H	4.3245	1.0156	0.0386
76	H	5.1765	-0.4541	0.6408
77	H	3.3809	-0.4016	0.5903
78	C	5.5726	1.6223	2.3919
79	H	6.4725	0.9835	2.2568
80	H	5.6263	2.4352	1.6358
81	H	5.6242	2.0661	3.4097
82	C	-2.8519	-2.8180	-3.4128
83	H	-2.3310	-3.7980	-3.4676
84	H	-2.9805	-2.4318	-4.4472
85	H	-2.1992	-2.1088	-2.8670

86	C	-4.9207	-1.5979	-2.6521
87	H	-5.8786	-1.6784	-2.0939
88	H	-4.2882	-0.8342	-2.1529
89	H	-5.1425	-1.2233	-3.6749
90	C	-5.0901	-3.9109	-3.5774
91	H	-5.2404	-3.4839	-4.5929
92	H	-4.6035	-4.9022	-3.7039
93	H	-6.0929	-4.0506	-3.1188

7minor_tbu_solv
Energy (POTENTIAL) = -4183.24481518 Eh

	Atom	X	Y	Z
1	Ir	-1.4297	-0.4870	2.1353
2	N	-2.2576	-2.3784	2.1728
3	C	-2.2168	-2.9466	3.3659
4	C	-1.7909	-2.1405	4.4851
5	C	-1.4380	-0.8234	4.1067
6	C	-1.0626	0.0479	5.1345
7	H	-0.7938	1.0762	4.9111
8	C	-1.0219	-0.3822	6.4586
9	C	-1.3571	-1.6950	6.8043
10	H	-1.3176	-2.0155	7.8403
11	C	-1.7473	-2.5812	5.8133
12	H	-2.0175	-3.6027	6.0711
13	C	-4.4300	-0.0381	2.1919
14	H	-4.5723	-1.1142	2.2230
15	C	-5.5460	0.7931	2.1326
16	H	-6.5384	0.3513	2.1175
17	C	-5.4123	2.1851	2.0971
18	H	-6.2926	2.8182	2.0547
19	C	-4.1472	2.7506	2.1287
20	H	-4.0309	3.8319	2.1125
21	C	-3.0266	1.9132	2.1897
22	C	-1.6532	2.3596	2.2609
23	H	-0.7248	0.3152	7.2369
24	S	-2.7128	-4.6062	3.3885
25	C	-2.7407	-3.2378	1.1923
26	C	-2.9677	-2.9199	-0.1461
27	C	-3.0187	-4.5215	1.6708
28	C	-3.4332	-3.8891	-1.0440
29	H	-2.7858	-1.8937	-0.4411
30	C	-3.4787	-5.5071	0.8056
31	C	-3.6695	-5.1904	-0.5332
32	H	-3.6916	-6.5099	1.1614
33	H	-4.0254	-6.0058	-1.1525
34	C	-3.6628	-3.5065	-2.5180
35	C	-3.1387	0.5013	2.2134
36	N	-0.7214	1.4274	2.3264
37	S	-1.0522	3.9811	2.3356
38	C	0.5514	1.9535	2.5306
39	C	1.7054	1.2147	2.8004
40	C	0.5678	3.3514	2.5306
41	C	2.9107	1.8797	3.0568

42	H	1.5811	0.1372	2.8331
43	C	1.7617	4.0364	2.7236
44	C	2.9076	3.2964	2.9709
45	H	1.8026	5.1205	2.7042
46	H	3.8202	3.8639	3.1224
47	C	4.2093	1.1473	3.4442
48	C	-1.6954	0.6632	-0.7802
49	C	-0.0333	-0.9288	-0.5441
50	C	-1.3081	0.9270	-2.0915
51	H	-2.5352	1.1769	-0.3225
52	C	0.4144	-0.7153	-1.8422
53	C	-0.2280	0.2402	-2.6270
54	H	-1.8503	1.6668	-2.6700
55	H	1.2667	-1.2592	-2.2323
56	H	0.1100	0.4346	-3.6394
57	C	0.5863	-1.9034	0.4001
58	O	0.3952	-1.7544	1.6033
59	C	1.3050	-3.1369	-0.1263
60	H	1.3386	-3.0838	-1.2167
61	C	0.4765	-4.3700	0.2659
62	H	-0.5077	-4.3142	-0.2087
63	H	0.9702	-5.2797	-0.0830
64	H	0.3423	-4.4239	1.3486
65	N	-1.0665	-0.2338	-0.0161
66	C	2.7875	-3.2037	0.3076
67	Cl	3.5582	-1.6254	-0.0904
68	Cl	2.9831	-3.5462	2.0375
69	Cl	3.6047	-4.4807	-0.6375
70	C	5.2738	1.3842	2.3530
71	H	5.5258	2.4615	2.2601
72	H	6.2119	0.8382	2.5927
73	H	4.9033	1.0270	1.3677
74	C	4.0110	-0.3779	3.5971
75	H	3.2565	-0.6029	4.3819
76	H	3.6813	-0.8239	2.6390
77	H	4.9621	-0.8754	3.8867
78	C	4.7294	1.6831	4.7970
79	H	5.6309	1.1206	5.1237
80	H	5.0168	2.7530	4.7326
81	H	3.9484	1.5767	5.5807
82	C	-4.7063	-2.3711	-2.6019
83	H	-5.6571	-2.6838	-2.1185
84	H	-4.3471	-1.4478	-2.1005
85	H	-4.9211	-2.1111	-3.6611

86	C	-4.1796	-4.6885	-3.3717
87	H	-4.3341	-4.3747	-4.4270
88	H	-3.4464	-5.5240	-3.3758
89	H	-5.1548	-5.0577	-2.9867
90	C	-2.3323	-3.0257	-3.1346
91	H	-1.5496	-3.8081	-3.0294
92	H	-2.4567	-2.7945	-4.2148
93	H	-1.9716	-2.1036	-2.6376

9_tbu_solv
Energy (POTENTIAL) = -2764.57369999 Eh

	Atom	X	Y	Z
1	Ir	-1.5766	-0.4295	2.0543
2	N	-2.6567	-2.1764	2.0409
3	C	-3.1294	-2.5347	3.2198
4	C	-2.8765	-1.6496	4.3340
5	C	-2.1494	-0.4937	3.9569
6	C	-1.8647	0.4308	4.9689
7	H	-1.3168	1.3401	4.7396
8	C	-2.2764	0.2053	6.2802
9	C	-2.9895	-0.9463	6.6287
10	H	-3.3056	-1.1057	7.6544
11	C	-3.2926	-1.8803	5.6508
12	H	-3.8497	-2.7784	5.9079
13	C	-4.4651	0.2827	1.3051
14	H	-4.7272	-0.7699	1.3615
15	C	-5.4470	1.1978	0.9329
16	H	-6.4499	0.8434	0.7108
17	C	-5.1663	2.5643	0.8433
18	H	-5.9411	3.2658	0.5518
19	C	-3.8889	3.0160	1.1343
20	H	-3.6598	4.0773	1.0704
21	C	-2.9082	2.0904	1.5096
22	C	-1.5479	2.4298	1.8538
23	H	-2.0434	0.9406	7.0454
24	S	-4.0113	-4.0253	3.2143
25	C	-3.0029	-3.0673	1.0296
26	C	-2.7073	-2.9170	-0.3259
27	C	-3.7382	-4.1620	1.4925
28	C	-3.1178	-3.8903	-1.2431
29	H	-2.1866	-2.0055	-0.5929
30	C	-4.1633	-5.1438	0.6043
31	C	-3.8440	-4.9997	-0.7377
32	H	-4.7370	-6.0007	0.9417
33	H	-4.1950	-5.7838	-1.4010
34	C	-2.8220	-3.7944	-2.7518
35	C	-3.1638	0.7032	1.5986
36	N	-0.7288	1.4512	2.1967
37	S	-0.8408	4.0097	1.8974
38	C	0.5378	1.9164	2.5442
39	C	1.6058	1.1391	2.9955
40	C	0.6661	3.3038	2.4270
41	C	2.8321	1.7358	3.3093

42	H	1.4043	0.0822	3.0976
43	C	1.8699	3.9276	2.7338
44	C	2.9302	3.1427	3.1612
45	H	1.9856	5.0029	2.6463
46	H	3.8534	3.6650	3.3910
47	C	4.0510	0.9339	3.8043
48	C	0.4860	-2.4569	3.2948
49	C	0.8773	-1.9086	1.0735
50	C	1.5116	-3.3939	3.2892
51	H	-0.1078	-2.2639	4.1830
52	C	1.9149	-2.8329	0.9953
53	C	2.2354	-3.5880	2.1186
54	H	1.7301	-3.9566	4.1899
55	H	2.4571	-2.9823	0.0689
56	H	3.0365	-4.3185	2.0766
57	C	0.4153	-1.0595	-0.0628
58	O	-0.6861	-0.4487	0.0733
59	N	0.1758	-1.7316	2.2138
60	C	1.1603	-0.9076	-1.2512
61	H	2.1191	-1.4094	-1.3399
62	C	0.7169	-0.0532	-2.3750
63	H	1.4282	0.7729	-2.5137
64	H	0.7294	-0.6228	-3.3131
65	H	-0.2789	0.3595	-2.2083
66	C	5.2329	1.1390	2.8321
67	H	5.5581	2.1998	2.8021
68	H	6.1101	0.5315	3.1442
69	H	4.9442	0.8328	1.8032
70	C	4.4518	1.4228	5.2123
71	H	5.3051	0.8297	5.6072
72	H	4.7637	2.4881	5.2002
73	H	3.5974	1.3171	5.9155
74	C	3.7741	-0.5861	3.8919
75	H	2.9518	-0.7997	4.6087
76	H	3.5058	-0.9934	2.8937
77	H	4.6751	-1.1328	4.2454
78	C	-2.0025	-2.5350	-3.1230
79	H	-2.5568	-1.6077	-2.8616
80	H	-1.0235	-2.5368	-2.5977
81	H	-1.7973	-2.5041	-4.2151
82	C	-2.0093	-5.0293	-3.1980
83	H	-2.5846	-5.9686	-3.0617
84	H	-1.7419	-4.9574	-4.2746
85	H	-1.0695	-5.1065	-2.6091

86	C	-4.1508	-3.7423	-3.5351
87	H	-3.9614	-3.6329	-4.6251
88	H	-4.7448	-4.6690	-3.3908
89	H	-4.7641	-2.8786	-3.1982

TSminor_tbu_solv
Energy (POTENTIAL) = -4183.32222225 Eh

	Atom	X	Y	Z
1	Ir	-1.5021	-0.4952	2.0171
2	N	-2.6526	-2.2036	2.0711
3	C	-3.1569	-2.4745	3.2588
4	C	-2.8539	-1.5753	4.3466
5	C	-2.0599	-0.4746	3.9318
6	C	-1.7371	0.4573	4.9346
7	H	-1.1410	1.3314	4.6866
8	C	-2.1623	0.2896	6.2474
9	C	-2.9381	-0.8145	6.6247
10	H	-3.2635	-0.9325	7.6538
11	C	-3.2885	-1.7513	5.6672
12	H	-3.8945	-2.6125	5.9428
13	C	-4.3451	0.3422	1.1996
14	H	-4.6903	-0.6712	1.3877
15	C	-5.2423	1.2710	0.6827
16	H	-6.2685	0.9712	0.4840
17	C	-4.8475	2.5863	0.4112
18	H	-5.5573	3.3001	0.0044
19	C	-3.5419	2.9691	0.6737
20	H	-3.2227	3.9901	0.4741
21	C	-2.6474	2.0291	1.1984
22	C	-1.2875	2.3165	1.5907
23	H	-1.8907	1.0304	6.9955
24	S	-4.1667	-3.8885	3.3078
25	C	-3.0522	-3.1196	1.1012
26	C	-2.6939	-3.0912	-0.2459
27	C	-3.8925	-4.1206	1.5979
28	C	-3.1718	-4.0735	-1.1231
29	H	-2.0475	-2.2729	-0.5524
30	C	-4.3862	-5.1048	0.7501
31	C	-4.0251	-5.0730	-0.5906
32	H	-5.0444	-5.8852	1.1189
33	H	-4.4440	-5.8692	-1.1968
34	C	-2.7364	-4.0388	-2.6001
35	C	-3.0127	0.6880	1.4655
36	N	-0.5641	1.3345	2.0902
37	S	-0.5151	3.8740	1.6316
38	C	0.6460	1.7810	2.6148
39	C	1.5656	1.0072	3.3237
40	C	0.8510	3.1534	2.4445
41	C	2.7149	1.5940	3.8653

42	H	1.3120	-0.0390	3.4246
43	C	1.9960	3.7606	2.9450
44	C	2.9036	2.9817	3.6471
45	H	2.1723	4.8231	2.8115
46	H	3.7733	3.4972	4.0430
47	C	3.7454	0.8065	4.6980
48	C	0.5712	-2.4949	3.2506
49	C	0.8911	-1.9824	0.9924
50	C	1.6280	-3.3852	3.2621
51	H	-0.0236	-2.3015	4.1386
52	C	1.9835	-2.8586	0.9488
53	C	2.3549	-3.5582	2.0825
54	H	1.8773	-3.9207	4.1715
55	H	2.5245	-2.9976	0.0212
56	H	3.1973	-4.2427	2.0492
57	C	0.3439	-1.2432	-0.1804
58	O	-0.7998	-0.6331	0.0056
59	N	0.2208	-1.8038	2.1535
60	C	0.9865	-1.2329	-1.3884
61	H	1.8946	-1.8099	-1.5257
62	C	0.3730	-0.5948	-2.5975
63	H	-0.3508	0.1685	-2.2997
64	H	1.1325	-0.1352	-3.2390
65	H	-0.1580	-1.3315	-3.2161
66	C	2.7341	0.7766	-0.9644
67	Cl	1.6758	2.1446	-0.8728
68	Cl	3.5633	0.3883	0.5110
69	Cl	3.7462	0.7310	-2.3832
70	C	5.1485	0.9427	4.0659
71	H	5.5015	1.9946	4.0702
72	H	5.8945	0.3431	4.6313
73	H	5.1382	0.5813	3.0161
74	C	3.7749	1.3690	6.1344
75	H	4.4863	0.7958	6.7678
76	H	4.0954	2.4321	6.1466
77	H	2.7655	1.3041	6.5956
78	C	3.4172	-0.7026	4.7842
79	H	2.4363	-0.8699	5.2796
80	H	3.3998	-1.1547	3.7695
81	H	4.1860	-1.2415	5.3795
82	C	-1.2088	-4.2406	-2.6819
83	H	-0.6667	-3.4604	-2.1114
84	H	-0.9261	-5.2289	-2.2592
85	H	-0.8603	-4.1971	-3.7365

86	C	-3.1139	-2.6765	-3.2243
87	H	-4.2072	-2.4993	-3.1313
88	H	-2.5830	-1.8363	-2.7315
89	H	-2.8456	-2.6486	-4.3027
90	C	-3.4051	-5.1444	-3.4512
91	H	-4.5119	-5.0433	-3.4298
92	H	-3.0804	-5.0747	-4.5123
93	H	-3.1225	-6.1548	-3.0846

4_tbu_gas
Energy (POTENTIAL) = -2450.68384961 Eh

	Atom	X	Y	Z
1	Ir	-1.5584	-0.5906	2.1211
2	N	-2.5554	-2.4060	2.1403
3	C	-2.7045	-2.9132	3.3519
4	C	-2.2551	-2.1315	4.4795
5	C	-1.6918	-0.8935	4.0958
6	C	-1.2494	-0.0574	5.1263
7	H	-0.8105	0.9099	4.8996
8	C	-1.3569	-0.4446	6.4600
9	C	-1.9125	-1.6777	6.8129
10	H	-1.9928	-1.9644	7.8564
11	C	-2.3653	-2.5286	5.8173
12	H	-2.8029	-3.4892	6.0795
13	C	-4.5182	0.1021	2.0774
14	H	-4.7452	-0.9582	2.0177
15	C	-5.5640	1.0215	2.0548
16	H	-6.5867	0.6625	1.9788
17	C	-5.3228	2.3970	2.1343
18	H	-6.1492	3.1001	2.1212
19	C	-4.0188	2.8552	2.2362
20	H	-3.8191	3.9221	2.3043
21	C	-2.9695	1.9285	2.2561
22	C	-1.5676	2.2621	2.3610
23	H	-1.0056	0.2256	7.2399
24	S	-3.4544	-4.4731	3.3953
25	C	-3.0663	-3.2435	1.1506
26	C	-3.1121	-2.9700	-0.2179
27	C	-3.5923	-4.4370	1.6555
28	C	-3.6605	-3.9007	-1.1082
29	H	-2.7269	-2.0041	-0.5141
30	C	-4.1449	-5.3812	0.7979
31	C	-4.1662	-5.1072	-0.5612
32	H	-4.5584	-6.3104	1.1759
33	H	-4.6068	-5.8673	-1.1983
34	C	-3.7426	-3.6601	-2.6277
35	C	-3.1891	0.5313	2.1750
36	N	-0.7066	1.2620	2.3434
37	S	-0.8462	3.8259	2.5448
38	C	0.6072	1.6836	2.5152
39	C	1.7266	0.8590	2.6112
40	C	0.7294	3.0711	2.6277
41	C	3.0006	1.4097	2.7925

42	H	1.5514	-0.2102	2.5697
43	C	1.9812	3.6490	2.8064
44	C	3.0948	2.8223	2.8790
45	H	2.0969	4.7240	2.8976
46	H	4.0392	3.3358	3.0194
47	C	4.2202	0.4738	2.8914
48	C	-1.6917	0.5120	-0.8184
49	C	-0.0361	-1.0687	-0.4708
50	C	-1.2685	0.7212	-2.1285
51	H	-2.5395	1.0456	-0.3995
52	C	0.4349	-0.9212	-1.7693
53	C	-0.1888	-0.0044	-2.6130
54	H	-1.7893	1.4414	-2.7498
55	H	1.2793	-1.5044	-2.1189
56	H	0.1642	0.1351	-3.6294
57	C	0.5844	-1.9901	0.5276
58	O	0.2301	-1.8980	1.7028
59	C	1.6089	-3.0032	0.1100
60	H	2.4541	-2.4701	-0.3471
61	H	1.1677	-3.6042	-0.6973
62	C	2.0828	-3.8899	1.2560
63	H	1.2495	-4.4468	1.6921
64	H	2.8214	-4.6060	0.8872
65	H	2.5431	-3.3002	2.0530
66	N	-1.0907	-0.3620	-0.0063
67	C	4.3502	-0.3371	1.5846
68	H	5.2399	-1.0026	1.6190
69	H	3.4604	-0.9769	1.4172
70	H	4.4556	0.3455	0.7137
71	C	5.5478	1.2382	3.1075
72	H	5.5191	1.8204	4.0539
73	H	6.4031	0.5310	3.1751
74	H	5.7511	1.9269	2.2591
75	C	4.0356	-0.4955	4.0798
76	H	3.8863	0.0735	5.0229
77	H	3.1605	-1.1624	3.9318
78	H	4.9295	-1.1452	4.2011
79	C	-3.1330	-2.3033	-3.0536
80	H	-3.6728	-1.4569	-2.5764
81	H	-2.0583	-2.2555	-2.7783
82	H	-3.2032	-2.1658	-4.1545
83	C	-2.9705	-4.7731	-3.3689
84	H	-3.4244	-5.7710	-3.1949
85	H	-2.9756	-4.5929	-4.4659

86	H	-1.9139	-4.8049	-3.0250
87	C	-5.2204	-3.6743	-3.0728
88	H	-5.3064	-3.4613	-4.1604
89	H	-5.6919	-4.6623	-2.8883
90	H	-5.7980	-2.9030	-2.5187

5_tbu_gas
Energy (POTENTIAL) = -2450.25305125 Eh

	Atom	X	Y	Z
1	Ir	-1.6043	-0.4461	2.0922
2	N	-2.6816	-2.1879	2.0856
3	C	-3.1745	-2.5370	3.2562
4	C	-2.9217	-1.6595	4.3769
5	C	-2.1675	-0.5156	4.0033
6	C	-1.8791	0.3935	5.0353
7	H	-1.3107	1.2932	4.8116
8	C	-2.3055	0.1704	6.3399
9	C	-3.0452	-0.9712	6.6762
10	H	-3.3732	-1.1317	7.6988
11	C	-3.3557	-1.8918	5.6884
12	H	-3.9302	-2.7831	5.9340
13	C	-4.5014	0.3165	1.4073
14	H	-4.7918	-0.7233	1.5330
15	C	-5.4638	1.2379	1.0092
16	H	-6.4841	0.9044	0.8351
17	C	-5.1427	2.5883	0.8258
18	H	-5.9029	3.2967	0.5110
19	C	-3.8431	3.0110	1.0526
20	H	-3.5795	4.0579	0.9158
21	C	-2.8821	2.0762	1.4566
22	C	-1.5049	2.3894	1.7514
23	H	-2.0647	0.8959	7.1133
24	S	-4.0815	-4.0211	3.2343
25	C	-3.0076	-3.0842	1.0724
26	C	-2.6428	-2.9497	-0.2682
27	C	-3.7727	-4.1655	1.5180
28	C	-3.0316	-3.9268	-1.1901
29	H	-2.0653	-2.0569	-0.4991
30	C	-4.1799	-5.1465	0.6202
31	C	-3.8046	-5.0160	-0.7096
32	H	-4.7776	-5.9937	0.9416
33	H	-4.1416	-5.8003	-1.3814
34	C	-2.6539	-3.8555	-2.6820
35	C	-3.1727	0.7037	1.6372
36	N	-0.7131	1.4155	2.1539
37	S	-0.7482	3.9521	1.6728
38	C	0.5701	1.8660	2.4493
39	C	1.6211	1.0866	2.9352
40	C	0.7405	3.2383	2.2383
41	C	2.8686	1.6644	3.1953

42	H	1.3917	0.0416	3.0890
43	C	1.9664	3.8427	2.4898
44	C	3.0077	3.0553	2.9577
45	H	2.1130	4.9058	2.3275
46	H	3.9504	3.5624	3.1403
47	C	4.0718	0.8569	3.7191
48	C	0.4537	-2.4898	3.2923
49	C	0.8134	-1.8759	1.0661
50	C	1.4706	-3.4258	3.2617
51	H	-0.1364	-2.3143	4.1868
52	C	1.8429	-2.8208	0.9690
53	C	2.1744	-3.5946	2.0675
54	H	1.6960	-4.0120	4.1457
55	H	2.3547	-2.9578	0.0240
56	H	2.9671	-4.3336	1.9955
57	C	0.3501	-0.9960	-0.0454
58	O	-0.8697	-0.5072	0.0841
59	N	0.1358	-1.7369	2.2266
60	C	1.1591	-0.7361	-1.1012
61	H	2.1525	-1.1739	-1.1344
62	C	0.7556	0.1629	-2.2283
63	H	-0.2047	0.6373	-2.0088
64	H	1.5042	0.9476	-2.3992
65	H	0.6523	-0.3905	-3.1723
66	C	5.2416	0.9648	2.7169
67	H	5.5990	2.0109	2.6169
68	H	6.1050	0.3495	3.0511
69	H	4.9246	0.6063	1.7135
70	C	4.5125	1.4186	5.0875
71	H	5.3552	0.8252	5.5041
72	H	4.8551	2.4712	5.0046
73	H	3.6684	1.3821	5.8099
74	C	3.7510	-0.6452	3.9053
75	H	2.9315	-0.7889	4.6424
76	H	3.4589	-1.1044	2.9372
77	H	4.6400	-1.1962	4.2820
78	C	-1.7914	-2.6160	-3.0239
79	H	-2.3384	-1.6754	-2.7966
80	H	-0.8378	-2.6312	-2.4537
81	H	-1.5345	-2.5995	-4.1054
82	C	-1.8434	-5.1112	-3.0697
83	H	-2.4435	-6.0374	-2.9519
84	H	-1.5188	-5.0585	-4.1316
85	H	-0.9374	-5.1983	-2.4314

86	C	-3.9382	-3.7880	-3.5351
87	H	-3.6895	-3.6964	-4.6147
88	H	-4.5574	-4.7010	-3.4115
89	H	-4.5509	-2.9082	-3.2417

3
Energy (POTENTIAL) = -1858.15055969 Eh

	Atom	X	Y	Z
1	C	-1.2081	0.7370	-0.6973
2	C	-0.2240	-1.3248	-0.5373
3	C	-1.0798	0.7489	-2.0879
4	H	-1.6602	1.5798	-0.1804
5	C	-0.0446	-1.4032	-1.9170
6	C	-0.4934	-0.3452	-2.7068
7	H	-1.4369	1.5995	-2.6596
8	H	0.4032	-2.2727	-2.3852
9	H	-0.3815	-0.3837	-3.7861
10	C	0.1726	-2.4410	0.3924
11	O	-0.4469	-2.6264	1.4231
12	C	1.4262	-3.2460	0.0468
13	C	2.6163	-2.5304	0.7059
14	H	2.4847	-2.4477	1.7881
15	H	3.5522	-3.0548	0.4953
16	H	2.6976	-1.5215	0.2899
17	N	-0.8033	-0.2749	0.0672
18	H	1.5821	-3.2256	-1.0340
19	C	1.3227	-4.7439	0.3975
20	Cl	1.3858	-5.0843	2.1498
21	Cl	-0.2008	-5.4213	-0.2750
22	Cl	2.6946	-5.6139	-0.3805

2_tbu_gas
Energy (POTENTIAL) = -2010.47528719 Eh

	Atom	X	Y	Z
1	Ir	-1.7038	-0.3577	2.1189
2	N	-2.6778	-2.1569	2.1042
3	C	-3.0367	-2.5958	3.2953
4	C	-2.7315	-1.7306	4.4216
5	C	-2.1074	-0.5192	4.0392
6	C	-1.7944	0.4145	5.0238
7	H	-1.3277	1.3590	4.7645
8	C	-2.0779	0.1326	6.3623
9	C	-2.6812	-1.0685	6.7314
10	H	-2.8947	-1.2721	7.7754
11	C	-3.0123	-2.0067	5.7592
12	H	-3.4853	-2.9431	6.0437
13	C	-4.4829	0.3227	1.1898
14	H	-4.7601	-0.7169	1.3289
15	C	-5.4244	1.2251	0.6892
16	H	-6.4215	0.8708	0.4452
17	C	-5.1038	2.5686	0.5021
18	H	-5.8462	3.2575	0.1133
19	C	-3.8303	3.0290	0.8206
20	H	-3.5791	4.0770	0.6788
21	C	-2.8871	2.1330	1.3222
22	C	-1.5316	2.4668	1.7242
23	H	-1.8245	0.8639	7.1239
24	S	-3.8488	-4.1166	3.2824
25	C	-3.0482	-3.0185	1.0773
26	C	-2.8337	-2.7985	-0.2840
27	C	-3.7054	-4.1614	1.5386
28	C	-3.2754	-3.7405	-1.2180
29	H	-2.3305	-1.8721	-0.5444
30	C	-4.1482	-5.1212	0.6345
31	C	-3.9271	-4.8985	-0.7161
32	H	-4.6564	-6.0205	0.9657
33	H	-4.2878	-5.6669	-1.3921
34	C	-3.0885	-3.5678	-2.7371
35	C	-3.1993	0.7643	1.5011
36	N	-0.7886	1.4714	2.1687
37	S	-0.7542	4.0055	1.7471
38	C	0.4745	1.8829	2.5806
39	C	1.4584	1.0585	3.1284
40	C	0.6778	3.2552	2.4177
41	C	2.6838	1.6059	3.5205

42	H	1.1998	0.0091	3.2330
43	C	1.8900	3.8273	2.7890
44	C	2.8648	3.0015	3.3279
45	H	2.0763	4.8890	2.6675
46	H	3.7963	3.4829	3.6071
47	C	3.8166	0.7689	4.1442
48	C	5.0756	0.8611	3.2554
49	H	5.4579	1.9015	3.1959
50	H	5.8935	0.2288	3.6641
51	H	4.8470	0.5136	2.2245
52	C	4.1413	1.3097	5.5535
53	H	4.9260	0.6918	6.0416
54	H	4.5174	2.3533	5.5136
55	H	3.2326	1.2902	6.1936
56	C	3.4482	-0.7277	4.2872
57	H	2.5623	-0.8560	4.9464
58	H	3.2340	-1.1792	3.2944
59	H	4.2875	-1.2990	4.7402
60	C	-2.3662	-2.2496	-3.1071
61	H	-2.9480	-1.3684	-2.7596
62	H	-1.3493	-2.2164	-2.6596
63	H	-2.2495	-2.1597	-4.2092
64	C	-2.2459	-4.7375	-3.2894
65	H	-2.7596	-5.7117	-3.1508
66	H	-2.0613	-4.6106	-4.3783
67	H	-1.2634	-4.7842	-2.7716
68	C	-4.4691	-3.5572	-3.4284
69	H	-4.3610	-3.3884	-4.5219
70	H	-5.0012	-4.5218	-3.2923
71	H	-5.1041	-2.7461	-3.0107

8_tbu_gas
Energy (POTENTIAL) = -2450.15621155 Eh

	Atom	X	Y	Z
1	Ir	-1.5546	-0.3633	1.9553
2	N	-2.6386	-2.1120	1.9769
3	C	-3.2278	-2.3476	3.1603
4	C	-2.9593	-1.4576	4.2382
5	C	-2.1021	-0.3739	3.8856
6	C	-1.7402	0.5159	4.8989
7	H	-1.0878	1.3552	4.6789
8	C	-2.2009	0.3496	6.2060
9	C	-3.0539	-0.7133	6.5316
10	H	-3.4173	-0.8294	7.5488
11	C	-3.4376	-1.6142	5.5550
12	H	-4.1032	-2.4382	5.8031
13	C	-4.3978	0.3097	1.1084
14	H	-4.5758	-0.7487	0.9397
15	C	-5.4334	1.2159	0.8811
16	H	-6.3972	0.8555	0.5318
17	C	-5.2440	2.5878	1.1088
18	H	-6.0606	3.2834	0.9362
19	C	-4.0231	3.0594	1.5541
20	H	-3.8759	4.1225	1.7299
21	C	-2.9690	2.1462	1.7665
22	C	-1.6495	2.4694	2.1569
23	H	-1.9016	1.0578	6.9736
24	S	-4.1761	-3.8135	3.1881
25	C	-2.9138	-3.0837	1.0312
26	C	-2.4776	-3.0917	-0.2969
27	C	-3.7386	-4.1095	1.5160
28	C	-2.8319	-4.1457	-1.1517
29	H	-1.8917	-2.2323	-0.5997
30	C	-4.1153	-5.1556	0.6878
31	C	-3.6562	-5.1684	-0.6249
32	H	-4.7591	-5.9517	1.0488
33	H	-3.9743	-6.0061	-1.2384
34	C	-2.3711	-4.2205	-2.6206
35	C	-3.1482	0.7493	1.5489
36	N	-0.7392	1.4634	2.2156
37	S	-0.9766	4.0427	2.5047
38	C	0.5323	1.9163	2.5165
39	C	1.6845	1.1356	2.6391
40	C	0.6024	3.3044	2.7093
41	C	2.9219	1.7208	2.9396

42	H	1.5432	0.0756	2.4901
43	C	1.8102	3.9106	3.0162
44	C	2.9521	3.1224	3.1258
45	H	1.8737	4.9839	3.1673
46	H	3.8767	3.6395	3.3643
47	C	4.2222	0.9036	3.0693
48	C	0.4540	-2.4503	3.2616
49	C	0.7966	-2.0000	1.0004
50	C	1.3997	-3.4613	3.2552
51	H	-0.1004	-2.1797	4.1554
52	C	1.7453	-3.0217	0.9194
53	C	2.0516	-3.7525	2.0570
54	H	1.6110	-4.0111	4.1655
55	H	2.2245	-3.2475	-0.0261
56	H	2.7882	-4.5487	2.0104
57	C	0.3917	-1.1071	-0.1167
58	O	-0.7083	-0.4051	0.0835
59	N	0.1667	-1.7408	2.1626
60	C	1.1189	-0.9758	-1.2573
61	H	2.0348	-1.5501	-1.3654
62	C	0.7408	-0.0596	-2.3725
63	H	-0.1997	0.4510	-2.1565
64	H	1.5215	0.6951	-2.5331
65	H	0.6349	-0.6126	-3.3146
66	C	5.2516	1.4053	2.0338
67	H	5.5332	2.4631	2.2177
68	H	6.1832	0.8004	2.0791
69	H	4.8345	1.3282	1.0063
70	C	4.7977	1.0741	4.4914
71	H	5.7152	0.4600	4.6215
72	H	5.0718	2.1302	4.6960
73	H	4.0518	0.7535	5.2507
74	C	4.0086	-0.6101	2.8244
75	H	3.2995	-1.0351	3.5671
76	H	3.6199	-0.7932	1.7994
77	H	4.9665	-1.1656	2.9225
78	C	-1.4544	-3.0409	-3.0233
79	H	-1.9837	-2.0693	-2.9164
80	H	-0.5360	-3.0302	-2.3988
81	H	-1.1363	-3.1315	-4.0846
82	C	-1.5780	-5.5261	-2.8475
83	H	-2.2111	-6.4231	-2.6849
84	H	-1.1923	-5.5773	-3.8889
85	H	-0.7126	-5.5782	-2.1516

86	C	-3.6041	-4.1996	-3.5485
87	H	-3.2940	-4.2141	-4.6160
88	H	-4.2564	-5.0817	-3.3785
89	H	-4.2053	-3.2816	-3.3714

9_tbu_gas
Energy (POTENTIAL) = -2450.03583151 Eh

	Atom	X	Y	Z
1	Ir	-1.5766	-0.4295	2.0543
2	N	-2.6567	-2.1764	2.0409
3	C	-3.1294	-2.5347	3.2198
4	C	-2.8765	-1.6496	4.3340
5	C	-2.1494	-0.4937	3.9569
6	C	-1.8647	0.4308	4.9689
7	H	-1.3168	1.3401	4.7396
8	C	-2.2764	0.2053	6.2802
9	C	-2.9895	-0.9463	6.6287
10	H	-3.3056	-1.1057	7.6544
11	C	-3.2926	-1.8803	5.6508
12	H	-3.8497	-2.7784	5.9079
13	C	-4.4651	0.2827	1.3051
14	H	-4.7272	-0.7699	1.3615
15	C	-5.4470	1.1978	0.9329
16	H	-6.4499	0.8434	0.7108
17	C	-5.1663	2.5643	0.8433
18	H	-5.9411	3.2658	0.5518
19	C	-3.8889	3.0160	1.1343
20	H	-3.6598	4.0773	1.0704
21	C	-2.9082	2.0904	1.5096
22	C	-1.5479	2.4298	1.8538
23	H	-2.0434	0.9406	7.0454
24	S	-4.0113	-4.0253	3.2143
25	C	-3.0029	-3.0673	1.0296
26	C	-2.7073	-2.9170	-0.3259
27	C	-3.7382	-4.1620	1.4925
28	C	-3.1178	-3.8903	-1.2431
29	H	-2.1866	-2.0055	-0.5929
30	C	-4.1633	-5.1438	0.6043
31	C	-3.8440	-4.9997	-0.7377
32	H	-4.7370	-6.0007	0.9417
33	H	-4.1950	-5.7838	-1.4010
34	C	-2.8220	-3.7944	-2.7518
35	C	-3.1638	0.7032	1.5986
36	N	-0.7288	1.4512	2.1967
37	S	-0.8408	4.0097	1.8974
38	C	0.5378	1.9164	2.5442
39	C	1.6058	1.1391	2.9955
40	C	0.6661	3.3038	2.4270
41	C	2.8321	1.7358	3.3093

42	H	1.4043	0.0822	3.0976
43	C	1.8699	3.9276	2.7338
44	C	2.9302	3.1427	3.1612
45	H	1.9856	5.0029	2.6463
46	H	3.8534	3.6650	3.3910
47	C	4.0510	0.9339	3.8043
48	C	0.4860	-2.4569	3.2948
49	C	0.8773	-1.9086	1.0735
50	C	1.5116	-3.3939	3.2892
51	H	-0.1078	-2.2639	4.1830
52	C	1.9149	-2.8329	0.9953
53	C	2.2354	-3.5880	2.1186
54	H	1.7301	-3.9565	4.1899
55	H	2.4571	-2.9823	0.0689
56	H	3.0365	-4.3185	2.0766
57	C	0.4153	-1.0595	-0.0628
58	O	-0.6861	-0.4487	0.0733
59	N	0.1758	-1.7316	2.2138
60	C	1.1603	-0.9076	-1.2512
61	H	2.1191	-1.4094	-1.3399
62	C	0.7169	-0.0532	-2.3750
63	H	1.4282	0.7729	-2.5137
64	H	0.7294	-0.6228	-3.3131
65	H	-0.2789	0.3595	-2.2083
66	C	5.2329	1.1390	2.8321
67	H	5.5581	2.1998	2.8021
68	H	6.1101	0.5315	3.1442
69	H	4.9442	0.8328	1.8032
70	C	4.4518	1.4228	5.2123
71	H	5.3051	0.8297	5.6072
72	H	4.7637	2.4881	5.2002
73	H	3.5974	1.3171	5.9155
74	C	3.7741	-0.5861	3.8919
75	H	2.9518	-0.7997	4.6087
76	H	3.5058	-0.9934	2.8937
77	H	4.6751	-1.1328	4.2454
78	C	-2.0025	-2.5350	-3.1230
79	H	-2.5568	-1.6077	-2.8616
80	H	-1.0235	-2.5368	-2.5977
81	H	-1.7973	-2.5041	-4.2151
82	C	-2.0093	-5.0293	-3.1980
83	H	-2.5846	-5.9686	-3.0617
84	H	-1.7419	-4.9574	-4.2746
85	H	-1.0695	-5.1065	-2.6091

86	C	-4.1508	-3.7423	-3.5351
87	H	-3.9614	-3.6329	-4.6251
88	H	-4.7448	-4.6690	-3.3908
89	H	-4.7641	-2.8786	-3.1982

TSminor_tbu_gas
Energy (POTENTIAL) = -3868.82803667 Eh

	Atom	X	Y	Z
1	Ir	-1.5021	-0.4952	2.0171
2	N	-2.6526	-2.2036	2.0711
3	C	-3.1569	-2.4745	3.2588
4	C	-2.8539	-1.5753	4.3466
5	C	-2.0599	-0.4746	3.9318
6	C	-1.7371	0.4573	4.9346
7	H	-1.1410	1.3314	4.6866
8	C	-2.1623	0.2896	6.2474
9	C	-2.9381	-0.8145	6.6247
10	H	-3.2635	-0.9325	7.6538
11	C	-3.2885	-1.7513	5.6672
12	H	-3.8945	-2.6125	5.9428
13	C	-4.3451	0.3422	1.1996
14	H	-4.6903	-0.6712	1.3877
15	C	-5.2423	1.2710	0.6827
16	H	-6.2685	0.9712	0.4839
17	C	-4.8475	2.5863	0.4112
18	H	-5.5573	3.3001	0.0044
19	C	-3.5419	2.9691	0.6737
20	H	-3.2227	3.9901	0.4741
21	C	-2.6474	2.0291	1.1984
22	C	-1.2875	2.3165	1.5907
23	H	-1.8907	1.0304	6.9955
24	S	-4.1667	-3.8885	3.3078
25	C	-3.0522	-3.1196	1.1012
26	C	-2.6939	-3.0912	-0.2459
27	C	-3.8925	-4.1206	1.5979
28	C	-3.1718	-4.0735	-1.1231
29	H	-2.0475	-2.2729	-0.5524
30	C	-4.3862	-5.1048	0.7501
31	C	-4.0251	-5.0730	-0.5906
32	H	-5.0444	-5.8852	1.1189
33	H	-4.4440	-5.8692	-1.1968
34	C	-2.7364	-4.0388	-2.6001
35	C	-3.0127	0.6880	1.4655
36	N	-0.5641	1.3345	2.0902
37	S	-0.5151	3.8740	1.6316
38	C	0.6460	1.7810	2.6148
39	C	1.5656	1.0072	3.3237
40	C	0.8510	3.1534	2.4445
41	C	2.7149	1.5940	3.8653

42	H	1.3120	-0.0390	3.4246
43	C	1.9960	3.7606	2.9450
44	C	2.9036	2.9817	3.6471
45	H	2.1723	4.8231	2.8115
46	H	3.7733	3.4972	4.0430
47	C	3.7454	0.8065	4.6980
48	C	0.5712	-2.4949	3.2506
49	C	0.8911	-1.9824	0.9924
50	C	1.6280	-3.3852	3.2621
51	H	-0.0236	-2.3015	4.1386
52	C	1.9835	-2.8586	0.9488
53	C	2.3549	-3.5582	2.0825
54	H	1.8773	-3.9207	4.1715
55	H	2.5245	-2.9976	0.0212
56	H	3.1973	-4.2427	2.0492
57	C	0.3439	-1.2432	-0.1804
58	O	-0.7998	-0.6331	0.0056
59	N	0.2208	-1.8038	2.1535
60	C	0.9865	-1.2329	-1.3884
61	H	1.8946	-1.8099	-1.5257
62	C	0.3730	-0.5948	-2.5975
63	H	-0.3508	0.1685	-2.2997
64	H	1.1325	-0.1352	-3.2390
65	H	-0.1580	-1.3315	-3.2161
66	C	2.7341	0.7766	-0.9643
67	Cl	1.6758	2.1446	-0.8728
68	Cl	3.5633	0.3883	0.5110
69	Cl	3.7462	0.7310	-2.3832
70	C	5.1485	0.9427	4.0659
71	H	5.5015	1.9946	4.0702
72	H	5.8945	0.3431	4.6313
73	H	5.1382	0.5813	3.0161
74	C	3.7749	1.3690	6.1344
75	H	4.4863	0.7958	6.7678
76	H	4.0954	2.4321	6.1466
77	H	2.7655	1.3041	6.5956
78	C	3.4172	-0.7026	4.7842
79	H	2.4363	-0.8699	5.2796
80	H	3.3998	-1.1547	3.7695
81	H	4.1860	-1.2415	5.3795
82	C	-1.2088	-4.2406	-2.6819
83	H	-0.6667	-3.4604	-2.1114
84	H	-0.9261	-5.2289	-2.2592
85	H	-0.8603	-4.1971	-3.7365

86	C	-3.1139	-2.6765	-3.2243
87	H	-4.2072	-2.4993	-3.1313
88	H	-2.5830	-1.8363	-2.7315
89	H	-2.8456	-2.6486	-4.3027
90	C	-3.4051	-5.1444	-3.4512
91	H	-4.5119	-5.0433	-3.4298
92	H	-3.0804	-5.0747	-4.5123
93	H	-3.1225	-6.1548	-3.0846

7minor_tbu_gas
Energy (POTENTIAL) = -3868.70246860 Eh

	Atom	X	Y	Z
1	Ir	-1.4297	-0.4870	2.1353
2	N	-2.2576	-2.3784	2.1728
3	C	-2.2168	-2.9466	3.3659
4	C	-1.7909	-2.1405	4.4851
5	C	-1.4380	-0.8234	4.1067
6	C	-1.0626	0.0479	5.1345
7	H	-0.7938	1.0762	4.9111
8	C	-1.0219	-0.3822	6.4586
9	C	-1.3571	-1.6950	6.8043
10	H	-1.3176	-2.0155	7.8403
11	C	-1.7473	-2.5812	5.8133
12	H	-2.0175	-3.6027	6.0711
13	C	-4.4300	-0.0381	2.1919
14	H	-4.5723	-1.1142	2.2230
15	C	-5.5460	0.7931	2.1326
16	H	-6.5384	0.3513	2.1175
17	C	-5.4123	2.1851	2.0971
18	H	-6.2926	2.8182	2.0547
19	C	-4.1472	2.7506	2.1287
20	H	-4.0309	3.8319	2.1125
21	C	-3.0266	1.9132	2.1897
22	C	-1.6532	2.3596	2.2609
23	H	-0.7248	0.3152	7.2369
24	S	-2.7128	-4.6062	3.3885
25	C	-2.7407	-3.2378	1.1923
26	C	-2.9677	-2.9199	-0.1461
27	C	-3.0187	-4.5215	1.6708
28	C	-3.4332	-3.8891	-1.0440
29	H	-2.7858	-1.8937	-0.4411
30	C	-3.4787	-5.5071	0.8056
31	C	-3.6695	-5.1904	-0.5332
32	H	-3.6916	-6.5099	1.1614
33	H	-4.0254	-6.0058	-1.1525
34	C	-3.6628	-3.5065	-2.5180
35	C	-3.1387	0.5013	2.2134
36	N	-0.7214	1.4274	2.3264
37	S	-1.0522	3.9811	2.3356
38	C	0.5514	1.9535	2.5306
39	C	1.7054	1.2147	2.8004
40	C	0.5678	3.3514	2.5306
41	C	2.9107	1.8797	3.0568

42	H	1.5811	0.1372	2.8331
43	C	1.7617	4.0364	2.7236
44	C	2.9076	3.2964	2.9709
45	H	1.8026	5.1205	2.7042
46	H	3.8202	3.8639	3.1224
47	C	4.2093	1.1473	3.4442
48	C	-1.6954	0.6632	-0.7802
49	C	-0.0333	-0.9288	-0.5441
50	C	-1.3081	0.9270	-2.0915
51	H	-2.5352	1.1769	-0.3225
52	C	0.4144	-0.7153	-1.8422
53	C	-0.2280	0.2402	-2.6270
54	H	-1.8503	1.6668	-2.6700
55	H	1.2667	-1.2592	-2.2323
56	H	0.1100	0.4346	-3.6394
57	C	0.5863	-1.9034	0.4001
58	O	0.3952	-1.7544	1.6033
59	C	1.3050	-3.1369	-0.1263
60	H	1.3386	-3.0838	-1.2167
61	C	0.4765	-4.3700	0.2659
62	H	-0.5077	-4.3142	-0.2087
63	H	0.9702	-5.2797	-0.0830
64	H	0.3423	-4.4239	1.3486
65	N	-1.0665	-0.2338	-0.0161
66	C	2.7875	-3.2037	0.3076
67	Cl	3.5582	-1.6254	-0.0904
68	Cl	2.9831	-3.5462	2.0375
69	Cl	3.6047	-4.4807	-0.6375
70	C	5.2738	1.3842	2.3530
71	H	5.5258	2.4615	2.2601
72	H	6.2119	0.8382	2.5927
73	H	4.9033	1.0270	1.3677
74	C	4.0110	-0.3779	3.5971
75	H	3.2565	-0.6029	4.3819
76	H	3.6813	-0.8239	2.6390
77	H	4.9621	-0.8754	3.8867
78	C	4.7294	1.6831	4.7970
79	H	5.6309	1.1206	5.1237
80	H	5.0168	2.7530	4.7326
81	H	3.9484	1.5767	5.5807
82	C	-4.7063	-2.3711	-2.6019
83	H	-5.6571	-2.6838	-2.1185
84	H	-4.3471	-1.4478	-2.1005
85	H	-4.9211	-2.1111	-3.6611

86	C	-4.1796	-4.6885	-3.3717
87	H	-4.3341	-4.3747	-4.4270
88	H	-3.4464	-5.5240	-3.3758
89	H	-5.1548	-5.0577	-2.9867
90	C	-2.3323	-3.0257	-3.1346
91	H	-1.5496	-3.8081	-3.0294
92	H	-2.4567	-2.7945	-4.2148
93	H	-1.9716	-2.1036	-2.6376

6major_tbu_gas
Energy (POTENTIAL) = -3868.88823647 Eh

	Atom	X	Y	Z
1	Ir	-1.4970	-0.6639	2.0574
2	N	-2.4745	-2.4705	1.9709
3	C	-2.5675	-3.0823	3.1339
4	C	-2.1008	-2.3839	4.3094
5	C	-1.6307	-1.0823	4.0125
6	C	-1.2277	-0.3039	5.1064
7	H	-0.8597	0.7064	4.9457
8	C	-1.2748	-0.8028	6.4048
9	C	-1.7291	-2.1006	6.6652
10	H	-1.7571	-2.4796	7.6823
11	C	-2.1475	-2.8967	5.6106
12	H	-2.5087	-3.9059	5.7986
13	C	-4.4958	-0.0484	1.9634
14	H	-4.6925	-1.1048	1.8045
15	C	-5.5710	0.8308	2.0043
16	H	-6.5796	0.4451	1.8771
17	C	-5.3808	2.2039	2.2092
18	H	-6.2309	2.8785	2.2405
19	C	-4.0948	2.6901	2.3698
20	H	-3.9288	3.7539	2.5273
21	C	-3.0156	1.7969	2.3231
22	C	-1.6298	2.1740	2.4446
23	H	-0.9516	-0.1749	7.2316
24	S	-3.3675	-4.6233	3.0738
25	C	-3.1040	-3.1728	0.9482
26	C	-3.2868	-2.7318	-0.3611
27	C	-3.6400	-4.3943	1.3646
28	C	-4.0006	-3.5064	-1.2826
29	H	-2.8564	-1.7708	-0.6133
30	C	-4.3201	-5.2054	0.4643
31	C	-4.4941	-4.7595	-0.8390
32	H	-4.7276	-6.1635	0.7708
33	H	-5.0429	-5.4349	-1.4864
34	C	-4.2166	-2.9723	-2.7117
35	C	-3.1733	0.4034	2.1197
36	N	-0.7174	1.2274	2.3355
37	S	-0.9914	3.7683	2.7100
38	C	0.5769	1.7281	2.4354
39	C	1.7505	0.9862	2.3188
40	C	0.6245	3.1091	2.6497
41	C	2.9980	1.6187	2.4116

42	H	1.6297	-0.0805	2.1526
43	C	1.8459	3.7599	2.7677
44	C	3.0120	3.0162	2.6482
45	H	1.8978	4.8301	2.9413
46	H	3.9310	3.5843	2.7438
47	C	4.2802	0.7888	2.2196
48	C	-1.4599	0.4509	-0.8746
49	C	0.0589	-1.2923	-0.4190
50	C	-1.0372	0.5651	-2.1852
51	H	-2.2501	1.0829	-0.4772
52	C	0.4976	-1.2425	-1.7708
53	C	-0.0343	-0.3183	-2.6353
54	H	-1.4809	1.3063	-2.8400
55	H	1.2643	-1.9268	-2.1157
56	H	0.3157	-0.2719	-3.6625
57	C	0.5993	-2.1178	0.6059
58	O	0.2686	-1.8979	1.8365
59	C	1.5557	-3.2718	0.3423
60	C	2.6087	-3.3819	1.4516
61	H	2.1388	-3.2970	2.4326
62	H	3.1581	-4.3238	1.3930
63	H	3.3354	-2.5756	1.3414
64	N	-0.9556	-0.4464	-0.0169
65	H	2.0625	-3.1183	-0.6156
66	C	0.8064	-4.6264	0.1494
67	Cl	0.0214	-5.1705	1.6579
68	Cl	-0.4373	-4.5107	-1.1313
69	Cl	1.9805	-5.8950	-0.3768
70	C	4.3210	-0.3511	3.2614
71	H	4.3138	0.0679	4.2909
72	H	3.4514	-1.0308	3.1644
73	H	5.2404	-0.9640	3.1399
74	C	4.2902	0.1994	0.7924
75	H	4.3245	1.0156	0.0386
76	H	5.1765	-0.4541	0.6408
77	H	3.3809	-0.4016	0.5903
78	C	5.5726	1.6223	2.3919
79	H	6.4725	0.9835	2.2568
80	H	5.6263	2.4352	1.6358
81	H	5.6242	2.0661	3.4097
82	C	-2.8519	-2.8180	-3.4128
83	H	-2.3310	-3.7980	-3.4676
84	H	-2.9805	-2.4318	-4.4472
85	H	-2.1992	-2.1088	-2.8670

86	C	-4.9207	-1.5979	-2.6521
87	H	-5.8786	-1.6784	-2.0939
88	H	-4.2882	-0.8342	-2.1529
89	H	-5.1425	-1.2233	-3.6749
90	C	-5.0901	-3.9109	-3.5774
91	H	-5.2404	-3.4839	-4.5929
92	H	-4.6035	-4.9022	-3.7039
93	H	-6.0929	-4.0506	-3.1188

6minor_tbu_gas
Energy (POTENTIAL) = -3868.88559260 Eh

	Atom	X	Y	Z
1	Ir	-1.3984	-0.4880	2.1057
2	N	-2.2208	-2.3822	2.1115
3	C	-2.1670	-2.9704	3.2912
4	C	-1.7138	-2.1995	4.4232
5	C	-1.3756	-0.8717	4.0697
6	C	-0.9855	-0.0315	5.1237
7	H	-0.7239	1.0041	4.9228
8	C	-0.9151	-0.4984	6.4317
9	C	-1.2355	-1.8248	6.7465
10	H	-1.1693	-2.1776	7.7712
11	C	-1.6415	-2.6811	5.7365
12	H	-1.8983	-3.7133	5.9666
13	C	-4.4221	-0.0352	2.1467
14	H	-4.5675	-1.1120	2.1649
15	C	-5.5359	0.7945	2.0804
16	H	-6.5293	0.3536	2.0497
17	C	-5.4022	2.1889	2.0519
18	H	-6.2816	2.8236	1.9998
19	C	-4.1364	2.7496	2.0980
20	H	-4.0162	3.8311	2.0824
21	C	-3.0191	1.9071	2.1658
22	C	-1.6482	2.3532	2.2480
23	H	-0.6036	0.1774	7.2246
24	S	-2.7284	-4.6148	3.3052
25	C	-2.7601	-3.2102	1.1324
26	C	-2.9961	-2.8695	-0.1992
27	C	-3.0922	-4.4844	1.6035
28	C	-3.5618	-3.7960	-1.0849
29	H	-2.7227	-1.8649	-0.4981
30	C	-3.6403	-5.4308	0.7468
31	C	-3.8683	-5.0839	-0.5779
32	H	-3.8937	-6.4252	1.1006
33	H	-4.2991	-5.8682	-1.1909
34	C	-3.8117	-3.3880	-2.5493
35	C	-3.1208	0.4929	2.1817
36	N	-0.7077	1.4320	2.3145
37	S	-1.0657	3.9859	2.3489
38	C	0.5562	1.9724	2.5380
39	C	1.7174	1.2421	2.8031
40	C	0.5555	3.3709	2.5652
41	C	2.9055	1.9223	3.1045

42	H	1.6092	0.1614	2.7719
43	C	1.7343	4.0688	2.7948
44	C	2.8842	3.3400	3.0548
45	H	1.7587	5.1539	2.7948
46	H	3.7851	3.9175	3.2396
47	C	4.2072	1.2030	3.5052
48	C	-1.7289	0.6264	-0.8241
49	C	-0.0241	-0.9638	-0.5064
50	C	-1.4119	0.7960	-2.1589
51	H	-2.5537	1.1688	-0.3703
52	C	0.3465	-0.8221	-1.8729
53	C	-0.3346	0.0527	-2.6833
54	H	-1.9803	1.4878	-2.7697
55	H	1.1980	-1.3703	-2.2604
56	H	-0.0389	0.1746	-3.7213
57	C	0.6170	-1.8033	0.4438
58	O	0.4097	-1.6325	1.7076
59	C	1.3490	-3.0555	-0.0021
60	H	1.3682	-3.0739	-1.0949
61	C	0.5579	-4.2828	0.4772
62	H	-0.4107	-4.2930	-0.0315
63	H	1.0773	-5.2167	0.2456
64	H	0.3816	-4.2244	1.5542
65	N	-1.0745	-0.2165	-0.0144
66	C	2.8421	-3.1152	0.3923
67	Cl	3.6483	-1.5799	-0.0706
68	Cl	3.0878	-3.4268	2.1281
69	Cl	3.6439	-4.4447	-0.5308
70	C	5.2949	1.4863	2.4482
71	H	5.5319	2.5694	2.3907
72	H	6.2355	0.9486	2.6972
73	H	4.9552	1.1502	1.4444
74	C	4.0311	-0.3272	3.6126
75	H	3.2560	-0.5862	4.3663
76	H	3.7389	-0.7471	2.6319
77	H	4.9813	-0.8176	3.9169
78	C	4.6836	1.7108	4.8848
79	H	5.5862	1.1548	5.2197
80	H	4.9540	2.7866	4.8563
81	H	3.8849	1.5702	5.6451
82	C	-4.7188	-2.1379	-2.5949
83	H	-5.6727	-2.3331	-2.0587
84	H	-4.2289	-1.2579	-2.1278
85	H	-4.9579	-1.8621	-3.6449

86	C	-4.5020	-4.5003	-3.3739
87	H	-4.6829	-4.1625	-4.4177
88	H	-3.8651	-5.4097	-3.4261
89	H	-5.4862	-4.7664	-2.9311
90	C	-2.4634	-3.0682	-3.2246
91	H	-1.7849	-3.9473	-3.1741
92	H	-2.6095	-2.7958	-4.2923
93	H	-1.9631	-2.2165	-2.7258

TSmajor_tbu_gas
Energy (POTENTIAL) = -3868.82383426 Eh

	Atom	X	Y	Z
1	Ir	-1.5437	-0.5290	2.0727
2	N	-2.4497	-2.3903	2.1089
3	C	-2.3973	-2.9575	3.2988
4	C	-1.9495	-2.1671	4.4199
5	C	-1.5827	-0.8533	4.0441
6	C	-1.2083	0.0076	5.0868
7	H	-0.9283	1.0350	4.8700
8	C	-1.1760	-0.4280	6.4068
9	C	-1.5202	-1.7425	6.7448
10	H	-1.4838	-2.0711	7.7791
11	C	-1.9139	-2.6172	5.7458
12	H	-2.1920	-3.6395	5.9943
13	C	-4.5286	0.1737	2.0021
14	H	-4.7607	-0.8885	2.0163
15	C	-5.5656	1.0940	1.8926
16	H	-6.5912	0.7390	1.8244
17	C	-5.3135	2.4720	1.8698
18	H	-6.1328	3.1793	1.7848
19	C	-4.0069	2.9243	1.9639
20	H	-3.7963	3.9920	1.9534
21	C	-2.9680	1.9916	2.0730
22	C	-1.5668	2.3230	2.2097
23	H	-0.8756	0.2633	7.1905
24	S	-2.9461	-4.6051	3.3412
25	C	-2.9857	-3.2386	1.1432
26	C	-3.2541	-2.9058	-0.1866
27	C	-3.3048	-4.5085	1.6365
28	C	-3.8212	-3.8507	-1.0507
29	H	-3.0106	-1.8903	-0.4708
30	C	-3.8552	-5.4718	0.8005
31	C	-4.0988	-5.1368	-0.5224
32	H	-4.0984	-6.4631	1.1696
33	H	-4.5307	-5.9156	-1.1439
34	C	-3.1891	0.5879	2.0867
35	N	-0.7149	1.3207	2.2742
36	S	-0.8413	3.8886	2.4223
37	C	0.5787	1.7285	2.5848
38	C	1.6426	0.8714	2.8689
39	C	0.7061	3.1158	2.6920
40	C	2.8682	1.4068	3.2790
41	H	1.4273	-0.1874	2.7567

42	C	1.9303	3.6763	3.0403
43	C	2.9845	2.8204	3.3278
44	H	2.0596	4.7511	3.1171
45	H	3.9188	3.2930	3.6168
46	C	4.0562	0.5265	3.7112
47	C	-1.7777	0.4955	-0.8877
48	C	-0.1995	-1.1830	-0.5126
49	C	-1.4416	0.5937	-2.2258
50	H	-2.5551	1.1133	-0.4490
51	C	0.1658	-1.1492	-1.8631
52	C	-0.4498	-0.2544	-2.7207
53	H	-1.9488	1.3116	-2.8608
54	H	0.9535	-1.7981	-2.2244
55	H	-0.1558	-0.2108	-3.7651
56	C	0.4452	-2.0367	0.5211
57	O	0.2462	-1.6880	1.7669
58	C	1.2140	-3.1157	0.1689
59	H	1.2298	-3.4372	-0.8665
60	C	1.7486	-4.0501	1.2103
61	H	0.9400	-4.6617	1.6359
62	H	2.4997	-4.7268	0.7922
63	H	2.1985	-3.5006	2.0431
64	N	-1.1768	-0.3695	-0.0557
65	C	3.4845	-1.9492	-0.6030
66	Cl	3.2279	-0.2366	-0.4148
67	Cl	4.7381	-2.5982	0.4176
68	Cl	3.6365	-2.4592	-2.2771
69	C	4.4333	0.8519	5.1729
70	H	5.2557	0.1915	5.5241
71	H	4.7803	1.9007	5.2812
72	H	3.5568	0.7036	5.8404
73	C	3.7357	-0.9857	3.6372
74	H	2.8952	-1.2459	4.3167
75	H	3.4643	-1.2794	2.6028
76	H	4.6160	-1.5933	3.9402
77	C	5.2684	0.8031	2.7971
78	H	5.6112	1.8554	2.8829
79	H	6.1248	0.1490	3.0703
80	H	5.0076	0.6082	1.7361
81	C	-3.3672	-4.5094	-3.4397
82	H	-3.6609	-5.5665	-3.2719
83	H	-3.5564	-4.2776	-4.5103
84	H	-2.2758	-4.4156	-3.2495
85	C	-3.7924	-2.1031	-2.9360

86	H	-4.3464	-1.3613	-2.3208
87	H	-2.7022	-1.9335	-2.8240
88	H	-4.0518	-1.9173	-4.0009
89	C	-5.6696	-3.7379	-2.7593
90	H	-5.9407	-3.4826	-3.8068
91	H	-5.9817	-4.7883	-2.5821
92	H	-6.2516	-3.0808	-2.0773
93	C	-4.1556	-3.5482	-2.5239

TSmajor_d_solv
Energy (POTENTIAL) = -4647.77621153 Eh

	Atom	X	Y	Z
1	Ir	-1.5359	-0.4431	2.0072
2	N	-2.6312	-2.1906	2.0501
3	C	-3.0566	-2.5163	3.2555
4	C	-2.7851	-1.6089	4.3452
5	C	-2.0829	-0.4515	3.9219
6	C	-1.7990	0.4931	4.9244
7	H	-1.2715	1.4084	4.6698
8	C	-2.1708	0.2822	6.2470
9	C	-2.8531	-0.8792	6.6339
10	H	-3.1357	-1.0310	7.6711
11	C	-3.1647	-1.8295	5.6763
12	H	-3.6984	-2.7348	5.9596
13	C	-4.3817	0.3372	1.1566
14	H	-4.7039	-0.6851	1.3375
15	C	-5.2934	1.2480	0.6328
16	H	-6.3099	0.9257	0.4201
17	C	-4.9255	2.5735	0.3729
18	H	-5.6465	3.2732	-0.0389
19	C	-3.6323	2.9852	0.6529
20	H	-3.3341	4.0140	0.4616
21	C	-2.7229	2.0631	1.1835
22	C	-1.3714	2.3737	1.5862
23	H	-1.9297	1.0326	6.9961
24	S	-3.9287	-4.0161	3.3333
25	C	-3.0100	-3.1185	1.0808
26	C	-2.7711	-3.0247	-0.2930
27	C	-3.7232	-4.1996	1.6098
28	C	-3.2375	-4.0264	-1.1578
29	H	-2.2293	-2.1439	-0.6299
30	C	-4.1801	-5.2140	0.7799
31	C	-3.9327	-5.1204	-0.5816
32	H	-4.7276	-6.0624	1.1780
33	H	-4.3215	-5.9466	-1.1666
34	C	-3.0609	0.7122	1.4403
35	N	-0.6401	1.3985	2.0871
36	S	-0.6109	3.9374	1.6317
37	C	0.5647	1.8520	2.6083
38	C	1.4963	1.0822	3.2992
39	C	0.7618	3.2254	2.4455
40	C	2.6435	1.6657	3.8460
41	H	1.2698	0.0297	3.4041

42	C	1.9141	3.8284	2.9358
43	C	2.8363	3.0526	3.6268
44	H	2.0911	4.8906	2.7997
45	H	3.7055	3.5886	3.9918
46	C	0.5402	-2.4325	3.2792
47	C	0.8432	-1.9722	1.0096
48	C	1.5597	-3.3654	3.2881
49	H	-0.0298	-2.2021	4.1746
50	C	1.8901	-2.9016	0.9587
51	C	2.2514	-3.5977	2.0978
52	H	1.7994	-3.8980	4.2015
53	H	2.4052	-3.0796	0.0231
54	H	3.0587	-4.3229	2.0613
55	C	0.3371	-1.1999	-0.1559
56	O	-0.7845	-0.5506	0.0157
57	N	0.1947	-1.7499	2.1753
58	C	1.0012	-1.1650	-1.3557
59	H	1.8495	-1.8155	-1.5326
60	C	0.3984	-0.4237	-2.5115
61	H	0.6034	0.6536	-2.4573
62	H	0.7842	-0.7904	-3.4669
63	H	-0.6922	-0.5171	-2.4912
64	C	3.0067	0.4645	-0.9677
65	Cl	2.2829	1.9287	-0.3801
66	Cl	4.0712	-0.3173	0.1734
67	Cl	3.6856	0.5949	-2.5723
68	C	-3.0016	-3.8982	-2.6759
69	C	-3.6731	-2.5960	-3.2055
70	C	-3.5912	-5.1022	-3.4809
71	C	-1.4748	-3.8327	-2.9732
72	H	-4.7685	-2.6271	-3.0121
73	H	-3.2739	-1.7011	-2.6808
74	C	-3.4187	-2.4320	-4.7214
75	H	-4.6890	-5.1785	-3.3143
76	H	-3.1250	-6.0559	-3.1469
77	C	-3.3355	-4.9331	-4.9924
78	H	-1.0027	-2.9872	-2.4339
79	H	-0.9773	-4.7620	-2.6168
80	C	-1.2242	-3.6573	-4.4889
81	H	-3.9010	-1.4961	-5.0785
82	C	-4.0111	-3.6357	-5.4813
83	C	-1.9003	-2.3603	-4.9856
84	H	-3.7623	-5.8011	-5.5405
85	C	-1.8160	-4.8606	-5.2502

86	H	-0.1303	-3.6002	-4.6787
87	H	-3.8501	-3.5123	-6.5749
88	H	-5.1091	-3.6898	-5.3119
89	H	-1.4690	-1.4782	-4.4719
90	H	-1.7106	-2.2271	-6.0734
91	H	-1.3269	-5.8015	-4.9146
92	H	-1.6199	-4.7557	-6.3399
93	C	3.6086	0.7967	4.6729
94	C	2.8457	0.1653	5.8777
95	C	4.8147	1.6087	5.2440
96	C	4.1840	-0.3449	3.7846
97	H	2.4395	0.9673	6.5334
98	H	1.9811	-0.4419	5.5331
99	C	3.7849	-0.7480	6.6948
100	H	4.4510	2.4315	5.8991
101	H	5.4014	2.0641	4.4153
102	C	5.7498	0.6953	6.0658
103	H	3.3709	-0.9634	3.3490
104	H	4.7562	0.0921	2.9379
105	C	5.1137	-1.2598	4.6114
106	H	3.2215	-1.1942	7.5431
107	C	4.9639	0.0816	7.2424
108	C	4.3238	-1.8742	5.7869
109	H	6.5994	1.2937	6.4610
110	C	6.2924	-0.4313	5.1622
111	H	5.5043	-2.0736	3.9624
112	H	5.6336	-0.5651	7.8510
113	H	4.5852	0.8873	7.9092
114	H	3.4808	-2.4857	5.4005
115	H	4.9821	-2.5522	6.3733
116	H	6.8780	0.0028	4.3221
117	H	6.9798	-1.0861	5.7416

TSminor_d_solv
Energy (POTENTIAL) = -4647.77025491 Eh

	Atom	X	Y	Z
1	Ir	-1.4731	-0.4459	2.0730
2	N	-2.2796	-2.3489	2.0918
3	C	-2.1973	-2.9326	3.2715
4	C	-1.7655	-2.1414	4.3979
5	C	-1.4731	-0.8038	4.0393
6	C	-1.1168	0.0545	5.0904
7	H	-0.8909	1.0981	4.8889
8	C	-1.0301	-0.4042	6.4003
9	C	-1.3010	-1.7400	6.7200
10	H	-1.2214	-2.0866	7.7459
11	C	-1.6760	-2.6140	5.7131
12	H	-1.8960	-3.6538	5.9466
13	C	-4.4925	0.0693	1.9740
14	H	-4.6576	-1.0051	1.9522
15	C	-5.5858	0.9232	1.8788
16	H	-6.5848	0.5041	1.7853
17	C	-5.4242	2.3147	1.9030
18	H	-6.2877	2.9691	1.8305
19	C	-4.1513	2.8479	2.0262
20	H	-4.0099	3.9267	2.0510
21	C	-3.0544	1.9814	2.1180
22	C	-1.6782	2.3972	2.2707
23	H	-0.7429	0.2859	7.1898
24	S	-2.7085	-4.5937	3.2937
25	C	-2.8088	-3.1933	1.1220
26	C	-3.0983	-2.8498	-0.1971
27	C	-3.0966	-4.4769	1.5954
28	C	-3.6637	-3.7832	-1.0741
29	H	-2.8755	-1.8308	-0.4889
30	C	-3.6457	-5.4307	0.7472
31	C	-3.9196	-5.0821	-0.5687
32	H	-3.8676	-6.4324	1.1018
33	H	-4.3493	-5.8732	-1.1735
34	C	-3.1839	0.5671	2.0903
35	N	-0.7621	1.4508	2.2989
36	S	-1.0569	3.9986	2.5404
37	C	0.5036	1.9331	2.6130
38	C	1.6314	1.1474	2.8462
39	C	0.5384	3.3196	2.7790
40	C	2.8212	1.7445	3.2781
41	H	1.5129	0.0770	2.6955

42	C	1.7226	3.9447	3.1517
43	C	2.8399	3.1581	3.4011
44	H	1.7767	5.0215	3.2769
45	H	3.7229	3.7079	3.7085
46	C	-1.6865	0.6357	-0.8889
47	C	-0.1226	-1.0521	-0.5097
48	C	-1.3197	0.7499	-2.2193
49	H	-2.4746	1.2466	-0.4588
50	C	0.2858	-0.9948	-1.8452
51	C	-0.3114	-0.0842	-2.7029
52	H	-1.8146	1.4739	-2.8571
53	H	1.0740	-1.6501	-2.1953
54	H	0.0047	-0.0231	-3.7400
55	C	0.4444	-1.9588	0.5239
56	O	0.3760	-1.5252	1.7585
57	C	0.9211	-3.1948	0.1775
58	H	0.7975	-3.5251	-0.8487
59	C	1.2172	-4.2212	1.2280
60	H	0.2813	-4.6191	1.6483
61	H	1.7844	-5.0630	0.8198
62	H	1.7806	-3.7868	2.0592
63	N	-1.1035	-0.2398	-0.0578
64	C	3.3690	-2.8014	-0.6841
65	Cl	3.6607	-1.0899	-0.8675
66	Cl	4.3964	-3.5688	0.4920
67	Cl	3.3042	-3.6581	-2.2158
68	C	4.0239	0.8520	3.6346
69	C	3.6226	-0.1435	4.7660
70	C	5.2569	1.6707	4.1348
71	C	4.4659	0.0384	2.3837
72	H	3.3165	0.4181	5.6766
73	H	2.7546	-0.7676	4.4621
74	C	4.8021	-1.0812	5.1055
75	H	4.9887	2.2581	5.0411
76	H	5.5912	2.3843	3.3490
77	C	6.4329	0.7337	4.4822
78	H	3.6270	-0.5819	2.0024
79	H	4.7660	0.7294	1.5649
80	C	5.6442	-0.8965	2.7342
81	H	4.4942	-1.7886	5.9060
82	C	6.0012	-0.2438	5.5946
83	C	5.2075	-1.8762	3.8451
84	H	7.2966	1.3380	4.8357
85	C	6.8424	-0.0599	3.2255

86	H	5.9458	-1.4679	1.8307
87	H	6.8482	-0.9130	5.8625
88	H	5.7223	0.3213	6.5111
89	H	4.3514	-2.4934	3.4939
90	H	6.0407	-2.5723	4.0863
91	H	7.1728	0.6379	2.4248
92	H	7.7013	-0.7266	3.4597
93	C	-3.9689	-3.3676	-2.5244
94	C	-4.9523	-2.1574	-2.5321
95	C	-4.6162	-4.5148	-3.3638
96	C	-2.6478	-2.9504	-3.2327
97	H	-5.9108	-2.4429	-2.0442
98	H	-4.5393	-1.2989	-1.9604
99	C	-5.2241	-1.6905	-3.9786
100	H	-5.5744	-4.8391	-2.9001
101	H	-3.9379	-5.3961	-3.4024
102	C	-4.8948	-4.0451	-4.8084
103	H	-2.1565	-2.1265	-2.6810
104	H	-1.9347	-3.8045	-3.2495
105	C	-2.9292	-2.4766	-4.6747
106	H	-5.9192	-0.8229	-3.9633
107	C	-5.8610	-2.8432	-4.7812
108	C	-3.8941	-1.2716	-4.6422
109	H	-5.3548	-4.8761	-5.3863
110	C	-3.5689	-3.6274	-5.4777
111	H	-1.9745	-2.1733	-5.1572
112	H	-6.0805	-2.5081	-5.8188
113	H	-6.8271	-3.1415	-4.3176
114	H	-3.4349	-0.4316	-4.0765
115	H	-4.0835	-0.9094	-5.6765
116	H	-2.8736	-4.4945	-5.5198
117	H	-3.7570	-3.3021	-6.5245

TSminor_c_phenyl
Energy (POTENTIAL) = -3829.50950985 Eh

	Atom	X	Y	Z
1	Ir	-1.5935	-0.3970	2.1143
2	N	-2.3905	-2.3166	2.1024
3	C	-2.2271	-2.9235	3.2620
4	C	-1.8646	-2.1260	4.4094
5	C	-1.6212	-0.7728	4.0752
6	C	-1.3195	0.0866	5.1412
7	H	-1.1325	1.1407	4.9530
8	C	-1.2398	-0.3855	6.4471
9	C	-1.4600	-1.7357	6.7440
10	H	-1.3859	-2.0922	7.7669
11	C	-1.7770	-2.6124	5.7192
12	H	-1.9585	-3.6632	5.9357
13	C	-4.5888	0.2382	2.0669
14	H	-4.7923	-0.8294	2.0352
15	C	-5.6490	1.1362	2.0106
16	H	-6.6660	0.7590	1.9341
17	C	-5.4314	2.5198	2.0537
18	H	-6.2694	3.2089	2.0122
19	C	-4.1360	3.0008	2.1563
20	H	-3.9522	4.0727	2.1963
21	C	-3.0725	2.0909	2.2105
22	C	-1.6765	2.4478	2.3331
23	H	-0.9975	0.3049	7.2513
24	S	-2.4642	-4.6434	3.2176
25	C	-2.7620	-3.1986	1.0928
26	C	-3.0755	-2.8510	-0.2225
27	C	-2.8223	-4.5307	1.5134
28	C	-3.3963	-3.8438	-1.1550
29	H	-3.0477	-1.7910	-0.4441
30	C	-3.1256	-5.5402	0.6087
31	C	-3.3898	-5.1894	-0.7064
32	H	-3.1507	-6.5813	0.9145
33	H	-3.6054	-6.0067	-1.3879
34	C	-3.2600	0.6828	2.1630
35	N	-0.8068	1.4588	2.3464
36	S	-0.9650	4.0196	2.5455
37	C	0.4956	1.8805	2.5916
38	C	1.5932	1.0368	2.7687
39	C	0.6080	3.2678	2.7131
40	C	2.8428	1.5869	3.0701
41	H	1.3905	-0.0238	2.6542

42	C	1.8478	3.8432	2.9702
43	C	2.9385	3.0015	3.1403
44	H	1.9667	4.9187	3.0540
45	H	3.8887	3.4860	3.3449
46	C	4.0880	0.7203	3.3381
47	C	-1.7209	0.7183	-0.8311
48	C	-0.2416	-1.0468	-0.4663
49	C	-1.3395	0.8339	-2.1574
50	H	-2.4788	1.3626	-0.3956
51	C	0.1660	-1.0008	-1.8015
52	C	-0.3787	-0.0491	-2.6494
53	H	-1.7907	1.5931	-2.7867
54	H	0.9231	-1.6882	-2.1593
55	H	-0.0543	0.0084	-3.6841
56	C	0.2929	-1.9835	0.5710
57	O	0.2111	-1.5384	1.7911
58	C	0.7573	-3.2212	0.1776
59	H	0.5981	-3.4652	-0.8681
60	N	-1.1859	-0.1956	-0.0097
61	C	3.1635	-2.8676	-0.4825
62	Cl	3.4158	-1.1377	-0.6066
63	Cl	4.2197	-3.6252	0.6878
64	Cl	3.2006	-3.6700	-2.0502
65	C	4.6471	1.0364	4.7427
66	H	5.5151	0.3827	4.9778
67	H	4.9958	2.0874	4.8181
68	H	3.8657	0.8710	5.5158
69	C	3.7851	-0.7975	3.2890
70	H	3.0277	-1.0743	4.0542
71	H	3.4109	-1.0958	2.2884
72	H	4.7026	-1.3915	3.4914
73	C	5.1642	1.0276	2.2763
74	H	5.5007	2.0841	2.3343
75	H	6.0573	0.3818	2.4216
76	H	4.7637	0.8466	1.2561
77	C	-2.6780	-4.1932	-3.5395
78	H	-2.6854	-5.2988	-3.4384
79	H	-2.8754	-3.9525	-4.6066
80	H	-1.6608	-3.8263	-3.2802
81	C	-3.7479	-2.0199	-2.9328
82	H	-4.4955	-1.4936	-2.3007
83	H	-2.7465	-1.5786	-2.7585
84	H	-4.0124	-1.8333	-3.9963
85	C	-5.1328	-4.0934	-2.9675

86	H	-5.4165	-3.8349	-4.0108
87	H	-5.1654	-5.1993	-2.8818
88	H	-5.8965	-3.6666	-2.2818
89	C	-3.7337	-3.5354	-2.6259
90	C	0.8982	-4.3590	1.1205
91	C	0.5469	-5.6478	0.6860
92	C	1.3577	-4.1842	2.4404
93	C	0.6231	-6.7351	1.5611
94	H	0.1905	-5.8088	-0.3242
95	C	1.4347	-5.2752	3.3107
96	H	1.6799	-3.2159	2.7971
97	C	1.0628	-6.5484	2.8735
98	H	0.3367	-7.7222	1.2223
99	H	1.7867	-5.1335	4.3243
100	H	1.1205	-7.3912	3.5500

4_Me
Energy (POTENTIAL) = -2529.39739093 Eh

	Atom	X	Y	Z
1	Ir	-1.5550	-0.6308	2.1478
2	N	-2.6174	-2.4157	2.1456
3	C	-2.8631	-2.8860	3.3537
4	C	-2.4268	-2.1085	4.4959
5	C	-1.7592	-0.9165	4.1247
6	C	-1.3234	-0.0912	5.1712
7	H	-0.8126	0.8442	4.9555
8	C	-1.5365	-0.4423	6.5035
9	C	-2.1939	-1.6302	6.8408
10	H	-2.3565	-1.8911	7.8825
11	C	-2.6427	-2.4706	5.8313
12	H	-3.1572	-3.3948	6.0866
13	C	-4.4976	0.1431	2.1475
14	H	-4.7562	-0.9105	2.0787
15	C	-5.5204	1.0897	2.1450
16	H	-6.5537	0.7576	2.0769
17	C	-5.2416	2.4587	2.2279
18	H	-6.0486	3.1853	2.2236
19	C	-3.9227	2.8815	2.3158
20	H	-3.6965	3.9438	2.3805
21	C	-2.8990	1.9271	2.3182
22	C	-1.4855	2.2241	2.3995
23	H	-1.1890	0.2202	7.2928
24	S	-3.7049	-4.3990	3.3827
25	C	-3.1021	-3.2513	1.1412
26	C	-3.0277	-3.0395	-0.2392
27	C	-3.7261	-4.4046	1.6354
28	C	-3.5535	-3.9848	-1.1105
29	H	-2.5706	-2.1410	-0.6308
30	C	-4.2616	-5.3646	0.7760
31	C	-4.1631	-5.1444	-0.5888
32	H	-4.7399	-6.2593	1.1631
33	H	-4.5698	-5.8826	-1.2757
34	C	-3.4803	-3.7768	-2.6006
35	H	-4.4838	-3.7066	-3.0365
36	H	-2.9381	-2.8586	-2.8476
37	H	-2.9719	-4.6160	-3.0893
38	C	-3.1529	0.5352	2.2257
39	N	-0.6549	1.2029	2.3681
40	S	-0.7178	3.7673	2.5733
41	C	0.6743	1.5813	2.5126

42	C	1.7752	0.7277	2.5758
43	C	0.8407	2.9692	2.6277
44	C	3.0484	1.2688	2.7310
45	H	1.6308	-0.3456	2.5196
46	C	2.1070	3.5269	2.7837
47	C	3.1969	2.6655	2.8287
48	H	2.2444	4.5998	2.8768
49	H	4.1915	3.0857	2.9532
50	C	4.2475	0.3570	2.7867
51	H	4.1063	-0.4344	3.5312
52	H	4.4113	-0.1305	1.8183
53	H	5.1568	0.9085	3.0443
54	C	-1.8285	0.4074	-0.7933
55	C	-0.0813	-1.0788	-0.4883
56	C	-1.5134	0.5579	-2.1412
57	H	-2.6691	0.9330	-0.3534
58	C	0.2919	-0.9790	-1.8214
59	C	-0.4410	-0.1474	-2.6658
60	H	-2.1143	1.2175	-2.7577
61	H	1.1386	-1.5397	-2.2006
62	H	-0.1729	-0.0558	-3.7133
63	C	0.6236	-1.9554	0.4884
64	O	0.2087	-1.9854	1.6495
65	C	1.8185	-2.7550	0.0802
66	H	2.5394	-2.0561	-0.3656
67	H	1.5129	-3.4266	-0.7333
68	C	2.4523	-3.5297	1.2263
69	H	1.7535	-4.2554	1.6545
70	H	3.3268	-4.0741	0.8573
71	H	2.7827	-2.8579	2.0253
72	N	-1.1372	-0.3992	0.0155

TSPA
Energy (POTENTIAL) = -2856.21677656 Eh

	Atom	X	Y	Z
1	Ir	-2.0212	-1.9233	1.3297
2	N	-2.4988	-3.7599	0.5028
3	C	-2.6858	-4.7042	1.4056
4	C	-2.7326	-4.3159	2.8012
5	C	-2.5316	-2.9260	2.9899
6	C	-2.6388	-2.4520	4.3063
7	H	-2.5050	-1.3934	4.5168
8	C	-2.9088	-3.3165	5.3657
9	C	-3.0829	-4.6885	5.1508
10	H	-3.2907	-5.3534	5.9841
11	C	-2.9968	-5.1932	3.8605
12	H	-3.1417	-6.2574	3.6859
13	C	-4.9745	-1.7424	0.6040
14	H	-4.9144	-2.7468	0.1925
15	C	-6.1823	-1.0535	0.5243
16	H	-7.0397	-1.5302	0.0549
17	C	-6.3131	0.2416	1.0409
18	H	-7.2613	0.7666	0.9714
19	C	-5.2212	0.8471	1.6459
20	H	-5.3147	1.8514	2.0541
21	C	-4.0094	0.1495	1.7241
22	C	-2.8027	0.6446	2.3502
23	H	-2.9859	-2.9190	6.3751
24	S	-2.9114	-6.2925	0.7520
25	C	-2.5918	-4.2451	-0.8002
26	C	-2.5575	-3.4949	-1.9807
27	C	-2.7883	-5.6310	-0.8611
28	C	-2.6670	-4.1371	-3.2071
29	H	-2.4750	-2.4164	-1.9397
30	C	-2.8982	-6.2939	-2.0839
31	C	-2.8241	-5.5381	-3.2437
32	H	-3.0472	-7.3686	-2.1291
33	H	-2.9092	-6.0367	-4.2061
34	C	-2.6374	-3.3475	-4.4899
35	H	-3.5899	-3.4383	-5.0253
36	H	-2.4536	-2.2856	-4.2988
37	H	-1.8516	-3.7149	-5.1600
38	C	-3.8442	-1.1596	1.1994
39	N	-1.7487	-0.1447	2.3253
40	S	-2.5662	2.1214	3.2296
41	C	-0.6832	0.3517	3.0640

42	C	0.5238	-0.3074	3.3069
43	C	-0.9398	1.6068	3.6289
44	C	1.4820	0.3067	4.1035
45	H	0.6910	-1.2900	2.8775
46	C	0.0189	2.2444	4.4170
47	C	1.2191	1.5848	4.6403
48	H	-0.1695	3.2189	4.8575
49	H	1.9751	2.0615	5.2600
50	C	2.7925	-0.3752	4.3972
51	H	2.8116	-1.3913	3.9923
52	H	3.6312	0.1804	3.9613
53	H	2.9692	-0.4347	5.4772
54	C	-1.7401	-0.0310	-1.1426
55	C	-0.0644	-1.6285	-0.9378
56	C	-1.2182	0.4304	-2.3430
57	H	-2.6365	0.4067	-0.7159
58	C	0.5012	-1.2274	-2.1444
59	C	-0.0856	-0.1878	-2.8585
60	H	-1.7023	1.2529	-2.8582
61	H	1.3938	-1.7104	-2.5244
62	H	0.3452	0.1383	-3.8000
63	C	0.5371	-2.6749	-0.0408
64	O	0.0719	-2.7467	1.1422
65	C	1.6348	-3.4343	-0.4819
66	H	2.6707	-2.4752	-0.6257
67	H	1.6070	-3.6766	-1.5466
68	C	2.1618	-4.5186	0.4307
69	H	1.4179	-5.3055	0.6194
70	H	3.0449	-4.9942	-0.0099
71	H	2.4570	-4.1096	1.4045
72	N	-1.1849	-1.0425	-0.4644
73	C	3.7150	-0.4854	-0.2751
74	C	4.4414	-1.9726	-1.9559
75	C	4.6468	0.4652	-0.6788
76	C	5.3881	-1.0521	-2.3925
77	C	5.4873	0.1771	-1.7487
78	H	4.7063	1.4141	-0.1559
79	H	6.0365	-1.3027	-3.2257
80	H	6.2202	0.9074	-2.0787
81	N	3.6435	-1.6653	-0.9165
82	C	2.7571	-0.2570	0.8533
83	H	1.7536	-0.0453	0.4662
84	H	2.6939	-1.1403	1.4944
85	H	3.0717	0.5974	1.4568

86	C	4.2553	-3.3102	-2.6071
87	H	4.2213	-4.1085	-1.8598
88	H	3.3144	-3.3364	-3.1688
89	H	5.0727	-3.5126	-3.3030

5_Me
Energy (POTENTIAL) = -2528.91819204 Eh

	Atom	X	Y	Z
1	Ir	-1.6115	-0.4217	2.0706
2	N	-2.6842	-2.1756	2.0326
3	C	-3.2021	-2.5278	3.1927
4	C	-2.9942	-1.6396	4.3163
5	C	-2.2246	-0.5001	3.9644
6	C	-1.9796	0.4230	4.9959
7	H	-1.4058	1.3242	4.7900
8	C	-2.4591	0.2127	6.2867
9	C	-3.2081	-0.9280	6.6037
10	H	-3.5766	-1.0806	7.6140
11	C	-3.4782	-1.8605	5.6122
12	H	-4.0596	-2.7497	5.8489
13	C	-4.5117	0.3860	1.4261
14	H	-4.7990	-0.6623	1.4755
15	C	-5.4842	1.3339	1.1143
16	H	-6.5066	1.0129	0.9276
17	C	-5.1666	2.6955	1.0380
18	H	-5.9324	3.4256	0.7925
19	C	-3.8629	3.1048	1.2814
20	H	-3.6105	4.1620	1.2258
21	C	-2.8934	2.1442	1.5967
22	C	-1.5067	2.4382	1.8931
23	H	-2.2510	0.9471	7.0617
24	S	-4.0688	-4.0303	3.1648
25	C	-2.9517	-3.0945	1.0240
26	C	-2.5483	-2.9960	-0.3111
27	C	-3.7027	-4.1931	1.4610
28	C	-2.8897	-4.0095	-1.1981
29	H	-1.9779	-2.1282	-0.6287
30	C	-4.0566	-5.2166	0.5812
31	C	-3.6416	-5.1112	-0.7381
32	H	-4.6380	-6.0706	0.9155
33	H	-3.9053	-5.8995	-1.4391
34	C	-2.4615	-3.9445	-2.6413
35	H	-3.3279	-3.9747	-3.3124
36	H	-1.9036	-3.0261	-2.8476
37	H	-1.8212	-4.7965	-2.8989
38	C	-3.1804	0.7593	1.6729
39	N	-0.7112	1.4349	2.2096
40	S	-0.7455	3.9961	1.8972
41	C	0.5847	1.8568	2.4971

42	C	1.6590	1.0557	2.8978
43	C	0.7596	3.2414	2.3651
44	C	2.8991	1.6361	3.1321
45	H	1.5215	-0.0090	3.0331
46	C	1.9965	3.8421	2.6002
47	C	3.0546	3.0287	2.9753
48	H	2.1301	4.9141	2.4914
49	H	4.0286	3.4768	3.1566
50	C	4.0776	0.7897	3.5377
51	H	3.7834	-0.2522	3.6983
52	H	4.8522	0.8069	2.7617
53	H	4.5343	1.1643	4.4608
54	C	0.4457	-2.4334	3.2859
55	C	0.8261	-1.8564	1.0557
56	C	1.5045	-3.3220	3.2985
57	H	-0.1654	-2.2707	4.1677
58	C	1.9022	-2.7490	1.0031
59	C	2.2472	-3.4797	2.1284
60	H	1.7348	-3.8774	4.2013
61	H	2.4552	-2.8819	0.0807
62	H	3.0804	-4.1755	2.0925
63	C	0.3665	-1.0179	-0.0919
64	O	-0.7975	-0.4037	0.0646
65	N	0.1203	-1.7142	2.1980
66	C	1.0986	-0.9009	-1.2269
67	H	2.0514	-1.4128	-1.3126
68	C	0.6391	-0.0596	-2.3827
69	H	0.4334	0.9767	-2.0783
70	H	1.3955	-0.0323	-3.1735
71	H	-0.2919	-0.4410	-2.8269

8_Me
Energy (POTENTIAL) = -2528.82745763 Eh

	Atom	X	Y	Z
1	Ir	-1.6308	-0.3866	1.9969
2	N	-2.7567	-2.1048	1.9539
3	C	-3.4254	-2.3271	3.0985
4	C	-3.1732	-1.4582	4.1948
5	C	-2.2206	-0.4372	3.8828
6	C	-1.8419	0.4200	4.9236
7	H	-1.1220	1.2137	4.7411
8	C	-2.3708	0.2812	6.2120
9	C	-3.3152	-0.7184	6.4917
10	H	-3.7308	-0.8130	7.4919
11	C	-3.7201	-1.5866	5.4908
12	H	-4.4532	-2.3617	5.7074
13	C	-4.5119	0.3986	1.3015
14	H	-4.7323	-0.6518	1.1218
15	C	-5.5388	1.3365	1.1497
16	H	-6.5316	1.0075	0.8505
17	C	-5.2984	2.6987	1.3879
18	H	-6.1013	3.4230	1.2734
19	C	-4.0353	3.1230	1.7698
20	H	-3.8515	4.1806	1.9516
21	C	-2.9982	2.1749	1.9128
22	C	-1.6443	2.4703	2.2381
23	H	-2.0515	0.9600	6.9994
24	S	-4.4181	-3.7675	3.0663
25	C	-2.9836	-3.0804	1.0042
26	C	-2.4362	-3.1377	-0.2833
27	C	-3.8667	-4.0893	1.4279
28	C	-2.7484	-4.2036	-1.1229
29	H	-1.7793	-2.3441	-0.6215
30	C	-4.1985	-5.1534	0.5956
31	C	-3.6290	-5.2052	-0.6731
32	H	-4.8827	-5.9297	0.9267
33	H	-3.8738	-6.0349	-1.3322
34	C	-2.1564	-4.2880	-2.5072
35	H	-2.9390	-4.2427	-3.2739
36	H	-1.4534	-3.4694	-2.6914
37	H	-1.6211	-5.2344	-2.6478
38	C	-3.2203	0.7827	1.6839
39	N	-0.7485	1.4641	2.2377
40	S	-0.9469	4.0419	2.5581
41	C	0.5361	1.9023	2.5033

42	C	1.6918	1.1170	2.6031
43	C	0.6347	3.2918	2.7001
44	C	2.9221	1.7123	2.8669
45	H	1.6264	0.0434	2.4826
46	C	1.8555	3.9016	2.9710
47	C	2.9940	3.1057	3.0465
48	H	1.9220	4.9757	3.1208
49	H	3.9552	3.5705	3.2519
50	C	4.1714	0.8728	2.9588
51	H	3.9532	-0.1863	2.7881
52	H	4.9124	1.1906	2.2160
53	H	4.6408	0.9694	3.9450
54	C	0.3280	-2.4853	3.2220
55	C	0.8330	-1.9494	1.0251
56	C	1.3135	-3.4648	3.2550
57	H	-0.2904	-2.2778	4.0893
58	C	1.8284	-2.9205	0.9805
59	C	2.0710	-3.6913	2.1134
60	H	1.4721	-4.0339	4.1647
61	H	2.3997	-3.0908	0.0755
62	H	2.8411	-4.4561	2.0990
63	C	0.4937	-1.0501	-0.1154
64	O	-0.5779	-0.3893	-0.0518
65	N	0.0900	-1.7453	2.1345
66	C	1.3496	-0.9042	-1.2381
67	H	2.2921	-1.4404	-1.2631
68	C	1.0002	0.0012	-2.3547
69	H	0.9066	1.0359	-1.9943
70	H	1.7558	-0.0309	-3.1415
71	H	0.0224	-0.2612	-2.7806

9_Me
Energy (POTENTIAL) = -2528.74630347 Eh

	Atom	X	Y	Z
1	Ir	-1.5414	-0.6233	2.1535
2	N	-2.5937	-2.4129	2.1592
3	C	-2.8386	-2.8819	3.3676
4	C	-2.4116	-2.0972	4.5084
5	C	-1.7517	-0.9023	4.1339
6	C	-1.3229	-0.0699	5.1775
7	H	-0.8166	0.8672	4.9587
8	C	-1.5367	-0.4164	6.5108
9	C	-2.1874	-1.6071	6.8517
10	H	-2.3505	-1.8645	7.8941
11	C	-2.6283	-2.4550	5.8449
12	H	-3.1373	-3.3814	6.1031
13	C	-4.4962	0.1207	2.1379
14	H	-4.7430	-0.9347	2.0559
15	C	-5.5303	1.0550	2.1424
16	H	-6.5593	0.7113	2.0665
17	C	-5.2682	2.4261	2.2425
18	H	-6.0837	3.1433	2.2438
19	C	-3.9546	2.8632	2.3390
20	H	-3.7408	3.9273	2.4155
21	C	-2.9201	1.9204	2.3337
22	C	-1.5102	2.2336	2.4157
23	H	-1.1947	0.2514	7.2980
24	S	-3.6668	-4.4026	3.3974
25	C	-3.0686	-3.2537	1.1554
26	C	-2.9932	-3.0404	-0.2245
27	C	-3.6830	-4.4120	1.6499
28	C	-3.5080	-3.9915	-1.0963
29	H	-2.5442	-2.1361	-0.6132
30	C	-4.2074	-5.3774	0.7899
31	C	-4.1073	-5.1568	-0.5749
32	H	-4.6787	-6.2761	1.1761
33	H	-4.5054	-5.8992	-1.2622
34	C	-3.4352	-3.7839	-2.5864
35	H	-4.4390	-3.7153	-3.0219
36	H	-2.8946	-2.8648	-2.8337
37	H	-2.9257	-4.6226	-3.0748
38	C	-3.1561	0.5266	2.2266
39	N	-0.6665	1.2236	2.3711
40	S	-0.7620	3.7856	2.5951
41	C	0.6592	1.6196	2.5013

42	C	1.7725	0.7810	2.5367
43	C	0.8076	3.0087	2.6263
44	C	3.0402	1.3388	2.6779
45	H	1.6405	-0.2935	2.4654
46	C	2.0681	3.5827	2.7691
47	C	3.1704	2.7364	2.7892
48	H	2.1922	4.6565	2.8695
49	H	4.1608	3.1693	2.9027
50	C	4.2533	0.4445	2.7036
51	H	4.1393	-0.3520	3.4475
52	H	4.4029	-0.0374	1.7301
53	H	5.1601	1.0078	2.9439
54	C	-1.7460	0.4607	-0.7715
55	C	-0.0447	-1.0849	-0.4630
56	C	-1.3905	0.6507	-2.1014
57	H	-2.5847	0.9916	-0.3339
58	C	0.3711	-0.9397	-1.7819
59	C	-0.3141	-0.0597	-2.6144
60	H	-1.9567	1.3448	-2.7126
61	H	1.2194	-1.4955	-2.1628
62	H	-0.0063	0.0655	-3.6475
63	C	0.5937	-2.0073	0.5168
64	O	0.1915	-1.9701	1.7126
65	C	1.6201	-2.9156	0.1535
66	H	1.9317	-2.9830	-0.8830
67	C	2.2407	-3.8156	1.1476
68	H	1.5863	-4.6874	1.3100
69	H	3.2040	-4.1884	0.7916
70	H	2.3615	-3.3292	2.1211
71	N	-1.0947	-0.3892	0.0295

TSmajor_Me
Energy (POTENTIAL) = -3947.49754039 Eh

	Atom	X	Y	Z
1	Ir	-1.5454	-0.3975	2.0555
2	N	-2.6406	-2.1415	2.0061
3	C	-3.1660	-2.4878	3.1639
4	C	-2.9777	-1.5886	4.2820
5	C	-2.2069	-0.4493	3.9329
6	C	-1.9880	0.4874	4.9580
7	H	-1.4140	1.3889	4.7545
8	C	-2.4935	0.2895	6.2407
9	C	-3.2420	-0.8520	6.5561
10	H	-3.6309	-0.9947	7.5602
11	C	-3.4862	-1.7976	5.5706
12	H	-4.0679	-2.6869	5.8056
13	C	-4.4058	0.4335	1.2876
14	H	-4.7098	-0.6092	1.3540
15	C	-5.3499	1.3852	0.9076
16	H	-6.3680	1.0731	0.6855
17	C	-5.0094	2.7397	0.8076
18	H	-5.7527	3.4724	0.5071
19	C	-3.7123	3.1388	1.0991
20	H	-3.4426	4.1907	1.0272
21	C	-2.7717	2.1750	1.4837
22	C	-1.3989	2.4583	1.8477
23	H	-2.3063	1.0345	7.0109
24	S	-4.0209	-3.9981	3.1437
25	C	-2.9007	-3.0670	1.0000
26	C	-2.5048	-2.9717	-0.3341
27	C	-3.6434	-4.1717	1.4427
28	C	-2.8295	-3.9975	-1.2175
29	H	-1.9545	-2.0978	-0.6659
30	C	-3.9827	-5.2032	0.5708
31	C	-3.5638	-5.1042	-0.7510
32	H	-4.5553	-6.0617	0.9089
33	H	-3.8155	-5.9038	-1.4429
34	C	-2.3959	-3.9058	-2.6588
35	H	-2.6305	-4.8241	-3.2060
36	H	-2.8976	-3.0729	-3.1657
37	H	-1.3165	-3.7307	-2.7335
38	C	-3.0812	0.7964	1.5806
39	N	-0.6325	1.4488	2.2124
40	S	-0.6316	4.0116	1.9159
41	C	0.6383	1.8622	2.6030

42	C	1.6743	1.0512	3.0726
43	C	0.8288	3.2466	2.4958
44	C	2.8942	1.6221	3.4116
45	H	1.5258	-0.0159	3.1693
46	C	2.0479	3.8374	2.8271
47	C	3.0688	3.0143	3.2781
48	H	2.1973	4.9090	2.7341
49	H	4.0281	3.4554	3.5380
50	C	4.0230	0.7660	3.9230
51	H	3.7951	-0.2992	3.8161
52	H	4.9531	0.9749	3.3828
53	H	4.2135	0.9656	4.9847
54	C	0.4883	-2.3766	3.3682
55	C	0.8279	-1.9747	1.0941
56	C	1.5166	-3.2999	3.4187
57	H	-0.0929	-2.1306	4.2512
58	C	1.8773	-2.8999	1.0816
59	C	2.2265	-3.5619	2.2475
60	H	1.7502	-3.7994	4.3527
61	H	2.4149	-3.1051	0.1641
62	H	3.0399	-4.2814	2.2426
63	C	0.3470	-1.2304	-0.1036
64	O	-0.6822	-0.4327	0.0717
65	N	0.1586	-1.7243	2.2411
66	C	0.9238	-1.3865	-1.3351
67	H	1.7262	-2.1025	-1.4698
68	C	0.3099	-0.7690	-2.5562
69	H	0.2670	0.3266	-2.4928
70	H	0.8683	-1.0351	-3.4583
71	H	-0.7276	-1.1071	-2.6922
72	C	2.8883	0.3726	-1.0471
73	Cl	2.0675	1.8638	-0.6786
74	Cl	3.9235	-0.2016	0.2353
75	Cl	3.6556	0.3583	-2.6204

TSminor_Me
Energy (POTENTIAL) = -3947.49341775 Eh

	Atom	X	Y	Z
1	Ir	-1.4916	-0.4792	2.1185
2	N	-2.3927	-2.3402	2.0802
3	C	-2.4205	-2.9344	3.2571
4	C	-2.0208	-2.1659	4.4186
5	C	-1.6006	-0.8545	4.0837
6	C	-1.2533	-0.0192	5.1576
7	H	-0.9338	1.0036	4.9696
8	C	-1.3048	-0.4731	6.4741
9	C	-1.7053	-1.7814	6.7713
10	H	-1.7376	-2.1256	7.8010
11	C	-2.0676	-2.6344	5.7379
12	H	-2.3854	-3.6509	5.9621
13	C	-4.4892	0.1218	2.1107
14	H	-4.6815	-0.9452	2.0232
15	C	-5.5690	1.0012	2.1279
16	H	-6.5804	0.6081	2.0529
17	C	-5.3744	2.3840	2.2408
18	H	-6.2246	3.0600	2.2530
19	C	-4.0838	2.8841	2.3376
20	H	-3.9231	3.9567	2.4268
21	C	-3.0028	1.9932	2.3180
22	C	-1.6097	2.3734	2.4091
23	H	-1.0280	0.1982	7.2839
24	S	-2.9701	-4.5783	3.2234
25	C	-2.8613	-3.1624	1.0589
26	C	-3.0382	-2.8126	-0.2839
27	C	-3.2014	-4.4495	1.4956
28	C	-3.4997	-3.7625	-1.1857
29	H	-2.8311	-1.8021	-0.6137
30	C	-3.6693	-5.4160	0.6047
31	C	-3.8009	-5.0628	-0.7293
32	H	-3.9247	-6.4156	0.9438
33	H	-4.1586	-5.8036	-1.4404
34	C	-3.6792	-3.4160	-2.6409
35	H	-4.7136	-3.5859	-2.9612
36	H	-3.4290	-2.3680	-2.8339
37	H	-3.0365	-4.0408	-3.2723
38	C	-3.1661	0.5883	2.1990
39	N	-0.7130	1.4082	2.3578
40	S	-0.9426	3.9596	2.6232
41	C	0.5871	1.8719	2.5192

42	C	1.7426	1.0863	2.5646
43	C	0.6618	3.2620	2.6745
44	C	2.9715	1.7045	2.7639
45	H	1.6577	0.0095	2.4472
46	C	1.8895	3.8976	2.8605
47	C	3.0286	3.1076	2.9022
48	H	1.9552	4.9749	2.9805
49	H	3.9943	3.5842	3.0538
50	C	4.2394	0.8950	2.8425
51	H	4.0323	-0.1750	2.7572
52	H	4.9364	1.1735	2.0436
53	H	4.7531	1.0668	3.7958
54	C	-1.6540	0.6005	-0.8201
55	C	-0.1639	-1.1608	-0.4755
56	C	-1.3768	0.6415	-2.1756
57	H	-2.3721	1.2789	-0.3707
58	C	0.1540	-1.1741	-1.8357
59	C	-0.4593	-0.2722	-2.6919
60	H	-1.8728	1.3703	-2.8075
61	H	0.8835	-1.8776	-2.2196
62	H	-0.2184	-0.2752	-3.7508
63	C	0.4187	-2.0792	0.5427
64	O	0.2978	-1.6980	1.7964
65	C	1.0135	-3.2545	0.1760
66	H	1.0033	-3.5413	-0.8701
67	C	1.3915	-4.2999	1.1804
68	H	0.5029	-4.8653	1.5018
69	H	2.1019	-5.0203	0.7606
70	H	1.8345	-3.8663	2.0830
71	N	-1.0743	-0.2849	0.0047
72	C	3.4656	-2.2973	-0.3074
73	Cl	3.3693	-0.5707	-0.5424
74	Cl	4.4044	-2.7540	1.0920
75	Cl	3.8973	-3.1834	-1.7544

6major_Me
Energy (POTENTIAL) = -3947.55722534 Eh

	Atom	X	Y	Z
1	Ir	-1.5717	-0.6498	2.0664
2	N	-2.6069	-2.4391	1.9833
3	C	-2.7183	-3.0399	3.1519
4	C	-2.2711	-2.3273	4.3319
5	C	-1.7274	-1.0545	4.0262
6	C	-1.3197	-0.2747	5.1206
7	H	-0.9021	0.7166	4.9551
8	C	-1.4338	-0.7436	6.4282
9	C	-1.9636	-2.0115	6.6959
10	H	-2.0484	-2.3675	7.7187
11	C	-2.3866	-2.8094	5.6417
12	H	-2.8078	-3.7923	5.8432
13	C	-4.5269	0.1473	2.0497
14	H	-4.7914	-0.9041	1.9619
15	C	-5.5442	1.0985	2.0608
16	H	-6.5800	0.7757	1.9815
17	C	-5.2571	2.4653	2.1727
18	H	-6.0595	3.1973	2.1791
19	C	-3.9359	2.8760	2.2767
20	H	-3.7033	3.9354	2.3665
21	C	-2.9187	1.9131	2.2646
22	C	-1.5048	2.1995	2.3686
23	H	-1.1084	-0.1151	7.2542
24	S	-3.4371	-4.6163	3.0881
25	C	-3.1378	-3.1976	0.9429
26	C	-3.2430	-2.8219	-0.3994
27	C	-3.6199	-4.4460	1.3587
28	C	-3.7818	-3.7097	-1.3210
29	H	-2.9038	-1.8441	-0.7161
30	C	-4.1667	-5.3502	0.4478
31	C	-4.2317	-4.9732	-0.8849
32	H	-4.5340	-6.3198	0.7706
33	H	-4.6474	-5.6679	-1.6110
34	C	-3.8664	-3.3394	-2.7790
35	H	-4.8884	-3.4497	-3.1593
36	H	-3.5482	-2.3051	-2.9443
37	H	-3.2232	-3.9905	-3.3834
38	C	-3.1751	0.5222	2.1433
39	N	-0.6753	1.1764	2.3340
40	S	-0.7343	3.7405	2.5718
41	C	0.6524	1.5532	2.4977

42	C	1.7519	0.6931	2.5591
43	C	0.8203	2.9374	2.6362
44	C	3.0212	1.2295	2.7475
45	H	1.5953	-0.3773	2.4680
46	C	2.0871	3.4905	2.8184
47	C	3.1718	2.6262	2.8695
48	H	2.2250	4.5618	2.9287
49	H	4.1664	3.0397	3.0178
50	C	4.2325	0.3347	2.8052
51	H	3.9596	-0.6895	3.0762
52	H	4.7371	0.2997	1.8316
53	H	4.9599	0.7026	3.5367
54	C	-1.7150	0.4060	-0.8784
55	C	-0.1573	-1.3175	-0.4847
56	C	-1.4431	0.4305	-2.2342
57	H	-2.4530	1.0750	-0.4450
58	C	0.1290	-1.3581	-1.8783
59	C	-0.5082	-0.4951	-2.7378
60	H	-1.9567	1.1341	-2.8801
61	H	0.8492	-2.0675	-2.2695
62	H	-0.2881	-0.5286	-3.8013
63	C	0.4690	-2.1055	0.5170
64	O	0.1460	-1.9456	1.7633
65	C	1.5866	-3.0868	0.2237
66	C	2.7887	-2.8057	1.1322
67	H	2.5402	-2.9292	2.1889
68	H	3.6380	-3.4501	0.8900
69	H	3.0984	-1.7689	0.9712
70	N	-1.1266	-0.4460	-0.0280
71	H	1.9185	-2.9618	-0.8100
72	C	1.1096	-4.5627	0.2852
73	Cl	0.6219	-5.0778	1.9297
74	Cl	-0.2869	-4.8149	-0.8150
75	Cl	2.4359	-5.6568	-0.2676

6minor_Me
Energy (POTENTIAL) = -3947.55526035 Eh

	Atom	X	Y	Z
1	Ir	-1.4224	-0.4399	2.1202
2	N	-2.2701	-2.3248	2.0583
3	C	-2.2605	-2.9447	3.2221
4	C	-1.8666	-2.1882	4.3940
5	C	-1.4959	-0.8562	4.0814
6	C	-1.1612	-0.0333	5.1690
7	H	-0.8794	1.0038	4.9979
8	C	-1.1756	-0.5172	6.4758
9	C	-1.5261	-1.8448	6.7496
10	H	-1.5293	-2.2130	7.7716
11	C	-1.8766	-2.6868	5.7030
12	H	-2.1564	-3.7180	5.9097
13	C	-4.4359	0.0588	2.1639
14	H	-4.5924	-1.0121	2.0561
15	C	-5.5464	0.8975	2.2157
16	H	-6.5438	0.4689	2.1468
17	C	-5.4010	2.2840	2.3548
18	H	-6.2755	2.9272	2.3936
19	C	-4.1282	2.8289	2.4420
20	H	-4.0041	3.9046	2.5502
21	C	-3.0159	1.9786	2.3874
22	C	-1.6367	2.4072	2.4578
23	H	-0.9083	0.1449	7.2963
24	S	-2.7662	-4.6019	3.1612
25	C	-2.7320	-3.1374	1.0270
26	C	-2.9308	-2.7665	-0.3067
27	C	-3.0290	-4.4426	1.4407
28	C	-3.3735	-3.7112	-1.2232
29	H	-2.7514	-1.7446	-0.6164
30	C	-3.4750	-5.4051	0.5344
31	C	-3.6305	-5.0291	-0.7910
32	H	-3.6947	-6.4193	0.8544
33	H	-3.9732	-5.7657	-1.5137
34	C	-3.5811	-3.3401	-2.6686
35	H	-4.6184	-3.5191	-2.9749
36	H	-3.3495	-2.2851	-2.8455
37	H	-2.9403	-3.9438	-3.3220
38	C	-3.1290	0.5711	2.2425
39	N	-0.7119	1.4733	2.3713
40	S	-1.0132	4.0117	2.6752
41	C	0.5772	1.9759	2.4936

42	C	1.7569	1.2264	2.4833
43	C	0.6140	3.3655	2.6647
44	C	2.9737	1.8795	2.6445
45	H	1.7019	0.1487	2.3568
46	C	1.8273	4.0361	2.8171
47	C	2.9914	3.2813	2.8049
48	H	1.8643	5.1129	2.9526
49	H	3.9467	3.7852	2.9311
50	C	4.2697	1.1111	2.6413
51	H	4.0974	0.0402	2.7808
52	H	4.8014	1.2470	1.6916
53	H	4.9352	1.4586	3.4393
54	C	-1.6737	0.6365	-0.8097
55	C	-0.0934	-1.0802	-0.4804
56	C	-1.4595	0.6595	-2.1760
57	H	-2.3971	1.3021	-0.3467
58	C	0.1419	-1.1154	-1.8831
59	C	-0.5361	-0.2570	-2.7160
60	H	-2.0042	1.3583	-2.8014
61	H	0.8665	-1.8060	-2.2997
62	H	-0.3515	-0.2829	-3.7863
63	C	0.5658	-1.8748	0.4951
64	O	0.3664	-1.6508	1.7576
65	C	1.3959	-3.0875	0.1274
66	H	1.3957	-3.2049	-0.9589
67	C	0.7623	-4.3466	0.7351
68	H	-0.2276	-4.4833	0.2879
69	H	1.3516	-5.2434	0.5226
70	H	0.6389	-4.2495	1.8168
71	N	-1.0430	-0.2094	0.0158
72	C	2.8964	-2.9377	0.4808
73	Cl	3.5299	-1.3771	-0.1442
74	Cl	3.2235	-3.0213	2.2382
75	Cl	3.8355	-4.2597	-0.3143

7major_Me
Energy (POTENTIAL) = -3947.42424765 Eh

	Atom	X	Y	Z
1	Ir	-1.5939	-0.6690	2.1038
2	N	-2.6608	-2.4441	2.0311
3	C	-2.8245	-3.0099	3.2112
4	C	-2.4089	-2.2687	4.3861
5	C	-1.8242	-1.0189	4.0677
6	C	-1.4350	-0.2135	5.1467
7	H	-0.9865	0.7611	4.9692
8	C	-1.6087	-0.6404	6.4629
9	C	-2.1781	-1.8857	6.7482
10	H	-2.3083	-2.2069	7.7775
11	C	-2.5824	-2.7070	5.7042
12	H	-3.0322	-3.6741	5.9195
13	C	-4.5225	0.1323	2.0766
14	H	-4.7869	-0.9168	1.9729
15	C	-5.5378	1.0862	2.0978
16	H	-6.5729	0.7648	2.0097
17	C	-5.2496	2.4495	2.2320
18	H	-6.0515	3.1817	2.2467
19	C	-3.9288	2.8592	2.3468
20	H	-3.6956	3.9168	2.4522
21	C	-2.9118	1.8976	2.3248
22	C	-1.4964	2.1774	2.4266
23	H	-1.2976	0.0059	7.2803
24	S	-3.5484	-4.5814	3.1607
25	C	-3.1537	-3.2263	0.9902
26	C	-3.2019	-2.8861	-0.3645
27	C	-3.6599	-4.4595	1.4209
28	C	-3.7091	-3.7959	-1.2827
29	H	-2.8511	-1.9174	-0.6963
30	C	-4.1736	-5.3863	0.5136
31	C	-4.1816	-5.0454	-0.8301
32	H	-4.5583	-6.3453	0.8473
33	H	-4.5713	-5.7576	-1.5536
34	C	-3.7357	-3.4656	-2.7520
35	H	-4.7409	-3.5926	-3.1697
36	H	-3.4169	-2.4344	-2.9333
37	H	-3.0661	-4.1302	-3.3112
38	C	-3.1761	0.5123	2.1823
39	N	-0.6766	1.1474	2.3748
40	S	-0.7110	3.7071	2.6278
41	C	0.6571	1.5091	2.5131

42	C	1.7517	0.6409	2.5396
43	C	0.8379	2.8910	2.6545
44	C	3.0290	1.1680	2.6939
45	H	1.5942	-0.4293	2.4535
46	C	2.1126	3.4352	2.8070
47	C	3.1914	2.5635	2.8211
48	H	2.2601	4.5049	2.9201
49	H	4.1929	2.9686	2.9439
50	C	4.2390	0.2704	2.7119
51	H	3.9646	-0.7689	2.9135
52	H	4.7586	0.3020	1.7463
53	H	4.9543	0.5925	3.4761
54	C	-1.6704	0.4650	-0.8069
55	C	-0.1455	-1.2585	-0.5466
56	C	-1.3719	0.5757	-2.1640
57	H	-2.4143	1.1062	-0.3462
58	C	0.1899	-1.2159	-1.8932
59	C	-0.4396	-0.2850	-2.7184
60	H	-1.8818	1.3231	-2.7619
61	H	0.9254	-1.8910	-2.3132
62	H	-0.1951	-0.2387	-3.7743
63	C	0.4734	-2.1821	0.4390
64	O	0.1143	-2.1179	1.6110
65	C	1.6027	-3.1404	0.0813
66	C	2.8330	-2.7514	0.9091
67	H	2.6422	-2.8440	1.9807
68	H	3.6924	-3.3696	0.6380
69	H	3.0851	-1.7095	0.6903
70	N	-1.0873	-0.4373	-0.0175
71	H	1.8556	-3.0404	-0.9749
72	C	1.1673	-4.6163	0.2449
73	Cl	0.8613	-5.0845	1.9418
74	Cl	-0.3327	-4.9015	-0.6997
75	Cl	2.4542	-5.6821	-0.4103

7minor_Me
Energy (POTENTIAL) = -3947.42294477 Eh

	Atom	X	Y	Z
1	Ir	-1.3984	-0.4492	2.1333
2	N	-2.2493	-2.3353	2.1056
3	C	-2.2736	-2.9185	3.2890
4	C	-1.8956	-2.1287	4.4449
5	C	-1.5051	-0.8104	4.1044
6	C	-1.1808	0.0445	5.1666
7	H	-0.8824	1.0717	4.9708
8	C	-1.2292	-0.3992	6.4876
9	C	-1.6015	-1.7123	6.7943
10	H	-1.6322	-2.0471	7.8270
11	C	-1.9388	-2.5846	5.7680
12	H	-2.2340	-3.6057	6.0009
13	C	-4.4039	-0.0038	2.1903
14	H	-4.5438	-1.0771	2.0940
15	C	-5.5263	0.8209	2.2371
16	H	-6.5166	0.3764	2.1757
17	C	-5.4010	2.2094	2.3619
18	H	-6.2852	2.8392	2.3970
19	C	-4.1369	2.7760	2.4404
20	H	-4.0283	3.8542	2.5381
21	C	-3.0119	1.9443	2.3915
22	C	-1.6381	2.3931	2.4536
23	H	-0.9713	0.2857	7.2919
24	S	-2.8026	-4.5665	3.2667
25	C	-2.7134	-3.1671	1.0906
26	C	-2.8984	-2.8270	-0.2534
27	C	-3.0346	-4.4548	1.5379
28	C	-3.3501	-3.7887	-1.1477
29	H	-2.7142	-1.8145	-0.5903
30	C	-3.4884	-5.4341	0.6539
31	C	-3.6277	-5.0910	-0.6819
32	H	-3.7299	-6.4348	0.9997
33	H	-3.9782	-5.8406	-1.3871
34	C	-3.5508	-3.4516	-2.6020
35	H	-4.5892	-3.6290	-2.9051
36	H	-3.3101	-2.4033	-2.8046
37	H	-2.9148	-4.0774	-3.2390
38	C	-3.1111	0.5353	2.2597
39	N	-0.7079	1.4652	2.3699
40	S	-1.0233	3.9995	2.6591
41	C	0.5789	1.9711	2.4947

42	C	1.7601	1.2248	2.5050
43	C	0.6083	3.3619	2.6532
44	C	2.9738	1.8827	2.6670
45	H	1.7151	0.1445	2.4036
46	C	1.8188	4.0381	2.8048
47	C	2.9850	3.2868	2.8076
48	H	1.8519	5.1162	2.9299
49	H	3.9378	3.7951	2.9339
50	C	4.2713	1.1172	2.6868
51	H	4.1011	0.0494	2.8515
52	H	4.8059	1.2330	1.7360
53	H	4.9331	1.4853	3.4783
54	C	-1.6430	0.6654	-0.7818
55	C	-0.0665	-1.0151	-0.5626
56	C	-1.3771	0.7853	-2.1449
57	H	-2.3960	1.2838	-0.3050
58	C	0.2416	-0.9617	-1.9147
59	C	-0.4277	-0.0422	-2.7213
60	H	-1.9221	1.5175	-2.7306
61	H	0.9957	-1.6093	-2.3460
62	H	-0.2017	0.0208	-3.7806
63	C	0.6035	-1.9157	0.4080
64	O	0.4194	-1.7260	1.6080
65	C	1.4121	-3.1237	-0.0369
66	H	1.4817	-3.1358	-1.1258
67	C	0.6462	-4.3779	0.4067
68	H	-0.3300	-4.3847	-0.0879
69	H	1.1814	-5.2818	0.1047
70	H	0.4901	-4.3911	1.4883
71	N	-1.0108	-0.2160	-0.0067
72	C	2.8755	-3.0602	0.4553
73	Cl	3.5773	-1.4644	0.0119
74	Cl	3.0463	-3.2917	2.2167
75	Cl	3.8251	-4.3371	-0.3732

TSmajor_c_phenyl
Energy (POTENTIAL) = -3829.51665934 Eh

	Atom	X	Y	Z
1	Ir	-1.5025	-0.4679	2.0533
2	N	-2.6278	-2.1881	2.0568
3	C	-3.1612	-2.4826	3.2256
4	C	-2.8851	-1.6003	4.3356
5	C	-2.0973	-0.4831	3.9537
6	C	-1.7959	0.4338	4.9755
7	H	-1.2015	1.3153	4.7488
8	C	-2.2403	0.2397	6.2786
9	C	-3.0123	-0.8774	6.6240
10	H	-3.3535	-1.0154	7.6454
11	C	-3.3381	-1.8024	5.6459
12	H	-3.9383	-2.6746	5.8982
13	C	-4.3618	0.2979	1.2176
14	H	-4.6746	-0.7322	1.3661
15	C	-5.2881	1.2123	0.7269
16	H	-6.3010	0.8825	0.5089
17	C	-4.9392	2.5494	0.5061
18	H	-5.6706	3.2520	0.1186
19	C	-3.6499	2.9680	0.7928
20	H	-3.3656	4.0056	0.6299
21	C	-2.7263	2.0415	1.2904
22	C	-1.3739	2.3602	1.6816
23	H	-1.9872	0.9694	7.0439
24	S	-4.1856	-3.8868	3.2143
25	C	-3.0204	-3.0684	1.0515
26	C	-2.6430	-2.9996	-0.2894
27	C	-3.8835	-4.0714	1.5021
28	C	-3.1268	-3.9395	-1.2081
29	H	-1.9797	-2.1841	-0.5610
30	C	-4.3820	-5.0162	0.6129
31	C	-4.0040	-4.9421	-0.7216
32	H	-5.0585	-5.7975	0.9449
33	H	-4.4289	-5.7079	-1.3617
34	C	-2.6634	-3.8654	-2.6759
35	C	-3.0441	0.6806	1.5066
36	N	-0.6083	1.3894	2.1397
37	S	-0.6503	3.9383	1.7314
38	C	0.6172	1.8585	2.6055
39	C	1.6200	1.0900	3.1973
40	C	0.7709	3.2413	2.4653
41	C	2.7933	1.6948	3.6629

42	H	1.4138	0.0315	3.2693
43	C	1.9280	3.8704	2.9068
44	C	2.9135	3.0978	3.5018
45	H	2.0605	4.9424	2.8010
46	H	3.7931	3.6285	3.8530
47	C	3.9184	0.9100	4.3648
48	C	0.5649	-2.4306	3.3331
49	C	0.9127	-1.9602	1.0695
50	C	1.6029	-3.3432	3.3667
51	H	-0.0308	-2.2088	4.2135
52	C	1.9754	-2.8712	1.0450
53	C	2.3233	-3.5623	2.1927
54	H	1.8374	-3.8647	4.2881
55	H	2.5204	-3.0428	0.1260
56	H	3.1452	-4.2716	2.1727
57	C	0.3944	-1.2040	-0.1181
58	O	-0.7339	-0.5886	0.0702
59	N	0.2345	-1.7544	2.2213
60	C	1.0875	-1.2242	-1.3117
61	H	1.9201	-1.9141	-1.3900
62	C	2.9232	0.5196	-1.0229
63	Cl	2.1640	1.9908	-0.4861
64	Cl	3.9902	-0.1915	0.1720
65	Cl	3.6609	0.6448	-2.6072
66	C	5.2641	1.1577	3.6471
67	H	5.5805	2.2186	3.7199
68	H	6.0722	0.5436	4.1007
69	H	5.1864	0.8907	2.5731
70	C	4.0279	1.3828	5.8292
71	H	4.8136	0.8118	6.3700
72	H	4.2929	2.4597	5.8874
73	H	3.0609	1.2335	6.3570
74	C	3.6669	-0.6168	4.3739
75	H	2.7441	-0.8645	4.9416
76	H	3.5753	-1.0043	3.3364
77	H	4.5087	-1.1541	4.8621
78	C	-1.1459	-4.1333	-2.7378
79	H	-0.5833	-3.3974	-2.1295
80	H	-0.9152	-5.1473	-2.3454
81	H	-0.7757	-4.0689	-3.7840
82	C	-2.9634	-2.4639	-3.2552
83	H	-4.0463	-2.2314	-3.1631
84	H	-2.3905	-1.6711	-2.7328
85	H	-2.6840	-2.4123	-4.3299

86	C	-3.3658	-4.9050	-3.5809
87	H	-4.4678	-4.7603	-3.5643
88	H	-3.0266	-4.8027	-4.6347
89	H	-3.1275	-5.9413	-3.2574
90	C	0.5276	-0.7025	-2.5855
91	C	0.8251	-1.3725	-3.7840
92	C	-0.2706	0.4575	-2.6326
93	C	0.3013	-0.9195	-4.9981
94	H	1.4483	-2.2584	-3.7773
95	C	-0.7892	0.9085	-3.8499
96	H	-0.4785	1.0317	-1.7405
97	C	-0.5091	0.2173	-5.0305
98	H	0.5234	-1.4509	-5.9144
99	H	-1.4045	1.7984	-3.8781
100	H	-0.9134	0.5673	-5.9714

TSminor_d_phenyl
Energy (POTENTIAL) = -3829.50736302 Eh

	Atom	X	Y	Z
1	Ir	-1.5366	-0.3922	2.0775
2	N	-2.3010	-2.3211	2.0927
3	C	-2.1418	-2.9156	3.2590
4	C	-1.7421	-2.1122	4.3890
5	C	-1.5187	-0.7585	4.0417
6	C	-1.1872	0.1052	5.0958
7	H	-1.0133	1.1601	4.9019
8	C	-1.0564	-0.3633	6.3988
9	C	-1.2565	-1.7140	6.7068
10	H	-1.1421	-2.0677	7.7270
11	C	-1.6060	-2.5944	5.6962
12	H	-1.7721	-3.6460	5.9209
13	C	-4.5490	0.1501	1.9980
14	H	-4.7211	-0.9231	1.9731
15	C	-5.6353	1.0146	1.9160
16	H	-6.6388	0.6055	1.8279
17	C	-5.4606	2.4045	1.9475
18	H	-6.3187	3.0670	1.8862
19	C	-4.1821	2.9261	2.0641
20	H	-4.0313	4.0034	2.0950
21	C	-3.0919	2.0502	2.1425
22	C	-1.7097	2.4505	2.2888
23	H	-0.7889	0.3309	7.1916
24	S	-2.4731	-4.6212	3.2532
25	C	-2.7430	-3.2001	1.1107
26	C	-3.0655	-2.8671	-0.2030
27	C	-2.8781	-4.5172	1.5586
28	C	-3.4917	-3.8480	-1.1065
29	H	-2.9710	-1.8213	-0.4717
30	C	-3.2921	-5.5157	0.6860
31	C	-3.5849	-5.1791	-0.6290
32	H	-3.3887	-6.5445	1.0183
33	H	-3.8965	-6.0067	-1.2567
34	C	-3.2359	0.6361	2.1084
35	N	-0.8112	1.4879	2.3088
36	S	-1.0518	4.0382	2.5582
37	C	0.4658	1.9416	2.6150
38	C	1.5744	1.1285	2.8410
39	C	0.5337	3.3263	2.7809
40	C	2.7843	1.6937	3.2545
41	H	1.4294	0.0617	2.6962

42	C	1.7386	3.9209	3.1405
43	C	2.8406	3.1066	3.3749
44	H	1.8217	4.9959	3.2648
45	H	3.7427	3.6328	3.6678
46	C	-1.7156	0.6981	-0.8842
47	C	-0.1654	-0.9995	-0.5002
48	C	-1.3188	0.8328	-2.2049
49	H	-2.5106	1.3048	-0.4608
50	C	0.2726	-0.9232	-1.8238
51	C	-0.3005	0.0067	-2.6789
52	H	-1.7989	1.5673	-2.8420
53	H	1.0646	-1.5768	-2.1682
54	H	0.0408	0.0852	-3.7068
55	C	0.3706	-1.9323	0.5388
56	O	0.3077	-1.4726	1.7547
57	C	0.7838	-3.1937	0.1553
58	H	0.5806	-3.4461	-0.8810
59	N	-1.1504	-0.1890	-0.0542
60	C	3.1496	-3.0983	-0.6065
61	Cl	3.5888	-1.4120	-0.8098
62	Cl	4.1816	-3.9309	0.5369
63	Cl	3.0326	-3.9474	-2.1484
64	C	3.9640	0.7651	3.5950
65	C	3.5541	-0.2059	4.7445
66	C	5.2347	1.5456	4.0583
67	C	4.3493	-0.0760	2.3427
68	H	3.2882	0.3740	5.6562
69	H	2.6584	-0.8024	4.4657
70	C	4.7081	-1.1808	5.0667
71	H	5.0081	2.1495	4.9651
72	H	5.5734	2.2414	3.2585
73	C	6.3858	0.5707	4.3873
74	H	3.4823	-0.6715	1.9865
75	H	4.6540	0.5960	1.5099
76	C	5.5010	-1.0491	2.6751
77	H	4.3945	-1.8693	5.8814
78	C	5.9467	-0.3809	5.5194
79	C	5.0568	-2.0018	3.8061
80	H	7.2781	1.1474	4.7146
81	C	6.7384	-0.2495	3.1297
82	H	5.7585	-1.6409	1.7705
83	H	6.7761	-1.0767	5.7743
84	H	5.7091	0.2019	6.4364
85	H	4.1731	-2.5934	3.4811

86	H	5.8711	-2.7236	4.0357
87	H	7.0740	0.4284	2.3142
88	H	7.5789	-0.9433	3.3513
89	C	-3.8248	-3.4468	-2.5547
90	C	-4.9582	-2.3762	-2.5615
91	C	-4.2999	-4.6517	-3.4275
92	C	-2.5578	-2.8452	-3.2273
93	H	-5.8799	-2.7949	-2.0996
94	H	-4.6721	-1.4833	-1.9653
95	C	-5.2612	-1.9191	-4.0052
96	H	-5.2157	-5.1081	-2.9899
97	H	-3.5110	-5.4355	-3.4672
98	C	-4.6109	-4.1934	-4.8691
99	H	-2.1959	-1.9724	-2.6520
100	H	-1.7356	-3.5951	-3.2410
101	C	-2.8707	-2.3846	-4.6667
102	H	-6.0640	-1.1502	-3.9894
103	C	-5.7264	-3.1286	-4.8414
104	C	-3.9852	-1.3166	-4.6331
105	H	-4.9473	-5.0656	-5.4710
106	C	-3.3388	-3.5930	-5.5027
107	H	-1.9548	-1.9499	-5.1232
108	H	-5.9681	-2.8040	-5.8775
109	H	-6.6538	-3.5597	-4.4042
110	H	-3.6496	-0.4356	-4.0427
111	H	-4.2010	-0.9612	-5.6646
112	H	-2.5351	-4.3608	-5.5447
113	H	-3.5480	-3.2743	-6.5476
114	C	0.8792	-4.3178	1.1206
115	C	0.4484	-5.5943	0.7237
116	C	1.3784	-4.1390	2.4256
117	C	0.4866	-6.6645	1.6219
118	H	0.0605	-5.7573	-0.2745
119	C	1.4175	-5.2130	3.3189
120	H	1.7597	-3.1810	2.7515
121	C	0.9673	-6.4735	2.9195
122	H	0.1388	-7.6417	1.3128
123	H	1.8008	-5.0684	4.3207
124	H	0.9953	-7.3031	3.6138

TSmajor_d_phenyl
Energy (POTENTIAL) = -3829.51572130 Eh

	Atom	X	Y	Z
1	Ir	-1.5407	-0.4603	2.0120
2	N	-2.6510	-2.1876	2.0752
3	C	-3.0263	-2.5426	3.2875
4	C	-2.7298	-1.6391	4.3747
5	C	-2.0526	-0.4698	3.9362
6	C	-1.7631	0.4791	4.9325
7	H	-1.2581	1.4036	4.6665
8	C	-2.0992	0.2606	6.2634
9	C	-2.7512	-0.9128	6.6656
10	H	-3.0054	-1.0702	7.7093
11	C	-3.0723	-1.8665	5.7144
12	H	-3.5864	-2.7797	6.0083
13	C	-4.3694	0.3739	1.1533
14	H	-4.7220	-0.6312	1.3710
15	C	-5.2492	1.2889	0.5837
16	H	-6.2726	0.9884	0.3728
17	C	-4.8390	2.5908	0.2739
18	H	-5.5344	3.2931	-0.1755
19	C	-3.5369	2.9763	0.5515
20	H	-3.2060	3.9870	0.3211
21	C	-2.6596	2.0514	1.1282
22	C	-1.3038	2.3414	1.5361
23	H	-1.8537	1.0149	7.0069
24	S	-3.8607	-4.0662	3.3616
25	C	-3.0576	-3.0930	1.0997
26	C	-2.8944	-2.9245	-0.2766
27	C	-3.7196	-4.2066	1.6247
28	C	-3.3836	-3.8984	-1.1542
29	H	-2.3840	-2.0134	-0.5738
30	C	-4.1791	-5.2081	0.7776
31	C	-3.9982	-5.0453	-0.5880
32	H	-4.6762	-6.0918	1.1647
33	H	-4.3683	-5.8499	-1.2166
34	C	-3.0410	0.7214	1.4333
35	N	-0.6035	1.3613	2.0698
36	S	-0.5108	3.8892	1.5718
37	C	0.5932	1.8013	2.6225
38	C	1.4696	1.0335	3.3840
39	C	0.8242	3.1659	2.4368
40	C	2.5997	1.6086	3.9732
41	H	1.2110	-0.0090	3.5116

42	C	1.9655	3.7579	2.9647
43	C	2.8356	2.9831	3.7217
44	H	2.1709	4.8124	2.8099
45	H	3.6981	3.5105	4.1141
46	C	0.5436	-2.4593	3.2323
47	C	0.8570	-1.9362	0.9755
48	C	1.5863	-3.3664	3.2324
49	H	-0.0402	-2.2628	4.1268
50	C	1.9297	-2.8354	0.9196
51	C	2.2966	-3.5499	2.0462
52	H	1.8318	-3.9117	4.1368
53	H	2.4677	-2.9807	-0.0081
54	H	3.1256	-4.2498	2.0013
55	C	0.3196	-1.1596	-0.1913
56	O	-0.8381	-0.6063	0.0015
57	N	0.1920	-1.7618	2.1401
58	C	1.0620	-1.0775	-1.3566
59	H	1.9270	-1.7272	-1.4257
60	C	2.7621	0.6972	-0.9116
61	Cl	1.9179	2.2157	-0.7200
62	Cl	3.6064	0.2002	0.5412
63	Cl	3.7926	0.6588	-2.3356
64	C	-3.2940	-3.7596	-2.6843
65	C	-4.7224	-3.8268	-3.3057
66	C	-2.4326	-4.9196	-3.2659
67	C	-2.6434	-2.4117	-3.1321
68	H	-5.2360	-4.7734	-3.0341
69	H	-5.3470	-2.9932	-2.9140
70	C	-4.6481	-3.7415	-4.8455
71	H	-2.8566	-5.9087	-2.9888
72	H	-1.4029	-4.8763	-2.8458
73	C	-2.3685	-4.8255	-4.8067
74	H	-3.2288	-1.5485	-2.7435
75	H	-1.6104	-2.3339	-2.7293
76	C	-2.5794	-2.3211	-4.6713
77	H	-5.6738	-3.8025	-5.2700
78	C	-3.7971	-4.9112	-5.3868
79	C	-4.0037	-2.4028	-5.2545
80	H	-1.7567	-5.6644	-5.2038
81	C	-1.7262	-3.4841	-5.2165
82	H	-2.1229	-1.3557	-4.9680
83	H	-3.7584	-4.8699	-6.4976
84	H	-4.2633	-5.8817	-5.1077
85	H	-4.6175	-1.5541	-4.8802

86	H	-3.9660	-2.3216	-6.3632
87	H	-0.6911	-3.4187	-4.8145
88	H	-1.6560	-3.4176	-6.3245
89	C	3.4974	0.7458	4.8792
90	C	2.6526	0.1756	6.0600
91	C	4.6909	1.5471	5.4900
92	C	4.0914	-0.4398	4.0629
93	H	2.2326	1.0096	6.6652
94	H	1.7920	-0.4212	5.6883
95	C	3.5196	-0.7322	6.9583
96	H	4.3134	2.4008	6.0961
97	H	5.3342	1.9591	4.6809
98	C	5.5542	0.6394	6.3934
99	H	3.2875	-1.0514	3.6034
100	H	4.7216	-0.0499	3.2341
101	C	4.9477	-1.3489	4.9713
102	H	2.8981	-1.1344	7.7878
103	C	4.6883	0.0860	7.5436
104	C	4.0763	-1.9024	6.1194
105	H	6.3963	1.2297	6.8159
106	C	6.1157	-0.5315	5.5602
107	H	5.3518	-2.1943	4.3729
108	H	5.3058	-0.5561	8.2095
109	H	4.2952	0.9232	8.1615
110	H	3.2387	-2.5045	5.7056
111	H	4.6817	-2.5769	6.7639
112	H	6.7590	-0.1418	4.7409
113	H	6.7514	-1.1828	6.1994
114	C	0.5610	-0.5001	-2.6333
115	C	1.0657	-1.0012	-3.8458
116	C	-0.3434	0.5807	-2.6684
117	C	0.6761	-0.4385	-5.0645
118	H	1.7681	-1.8256	-3.8491
119	C	-0.7309	1.1387	-3.8902
120	H	-0.7210	1.0299	-1.7614
121	C	-0.2179	0.6338	-5.0866
122	H	1.0698	-0.8327	-5.9923
123	H	-1.4197	1.9734	-3.9082
124	H	-0.5174	1.0696	-6.0309