

## Electronic Supplementary Information

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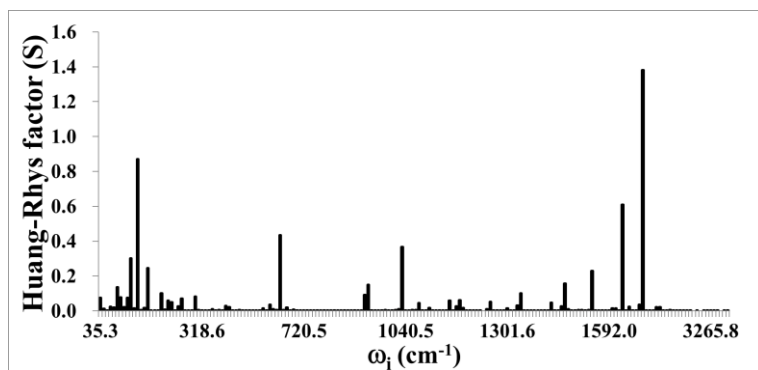
**Fig. S1.** Huang-Rhys factors for Ir(III) and Pt(II) phosphorescent materials.

**Table S1.** The calculated  $T_1$  and  $^3MC$  energies of Ir(III) and Pt(II) phosphorescent materials by B3LYP/LANL2DZ with 6-311G\*\* and 6-311+G\*\* (with GD3).

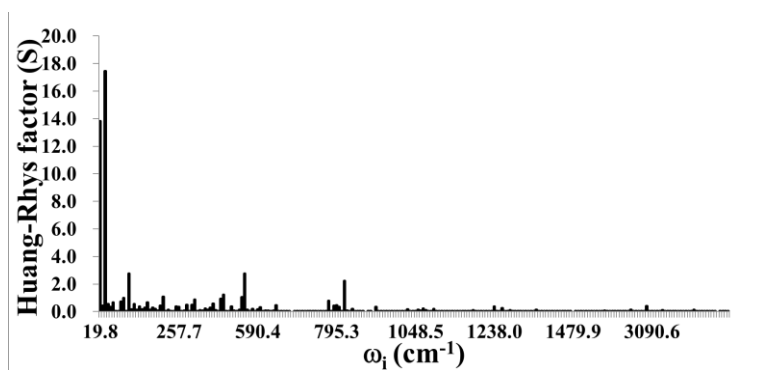
**Table S2.** The cartesian coordinates of optimized structures in  $S_0$ ,  $T_1$ , and  $^3MC$  state of Ir(III) and Pt(II) phosphorescent materials.

**Fig S1.** Huang-Rhys factors for Ir(III) and Pt(II) phosphorescent materials.

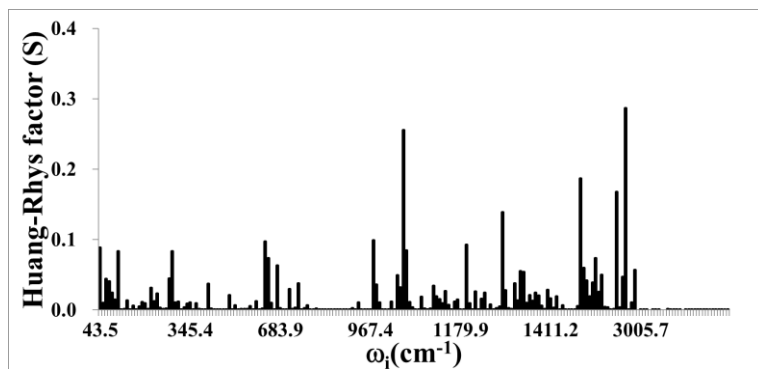
*fac*-Ir(pmi)<sub>3</sub>



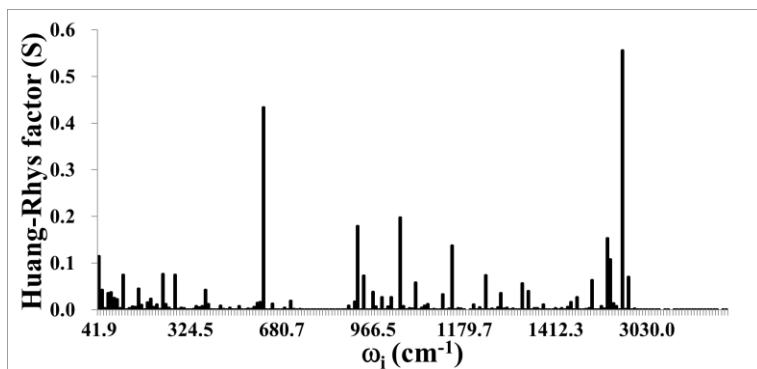
*fac* -Ir(pmb)<sub>3</sub>



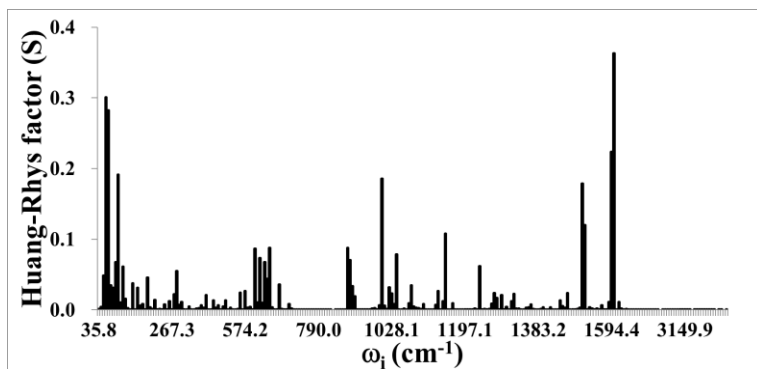
**Ir-C**



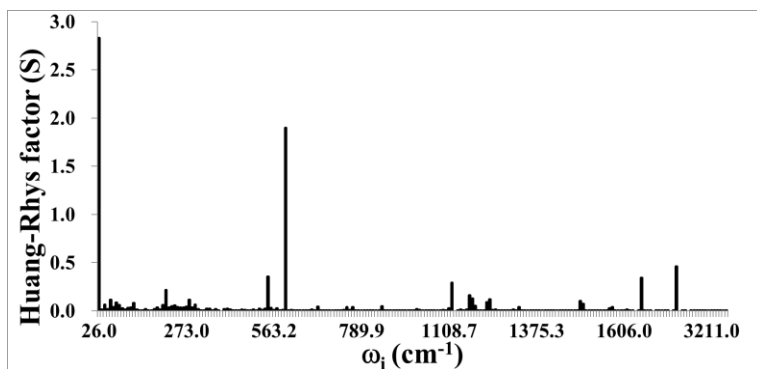
### Ir-N



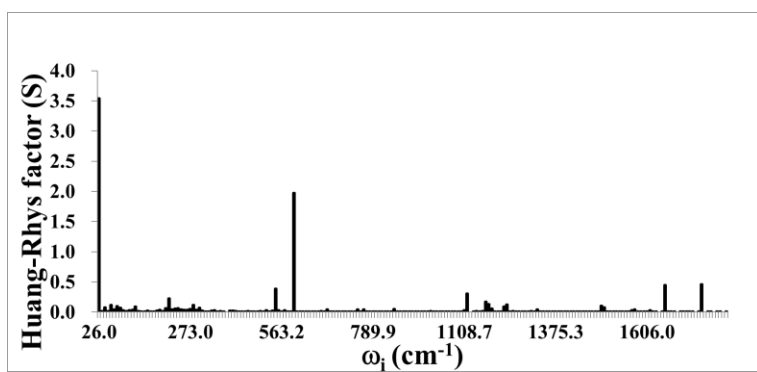
### Ir-Ph



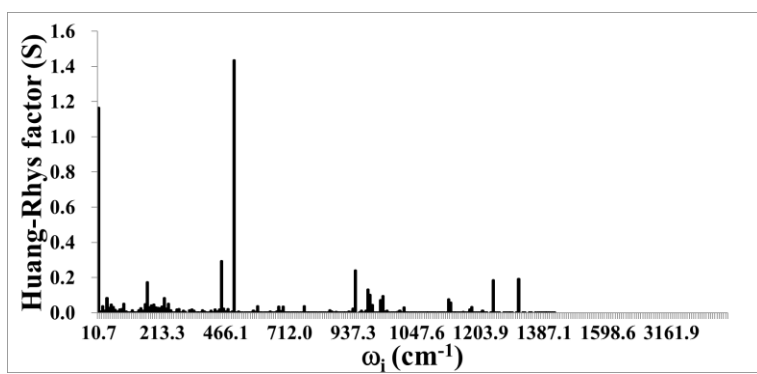
### Ir-N-CN



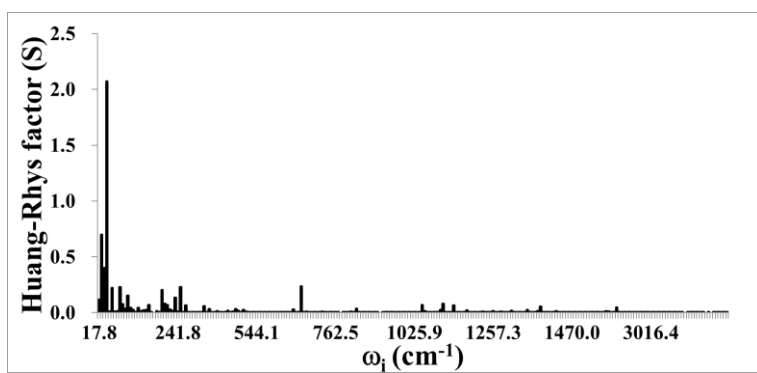
### Ir-N-F



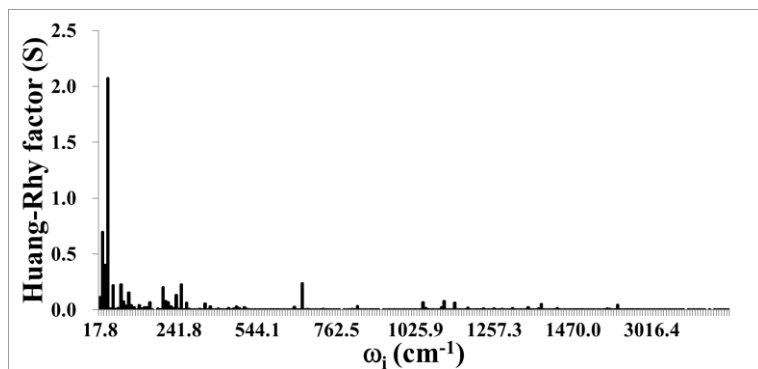
### Ir-N-Ph



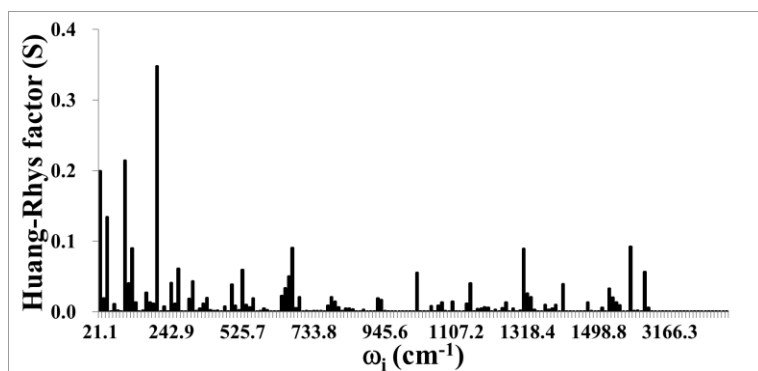
### HB-*fac*-Ir(pmi)<sub>3</sub>



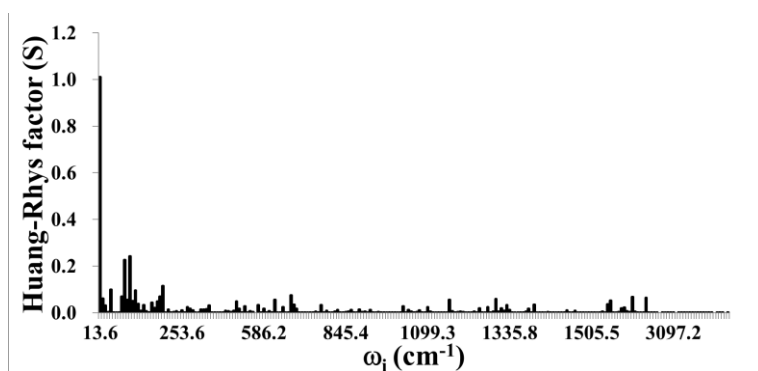
### HB-*fac*-Ir(pmiCN)<sub>3</sub>



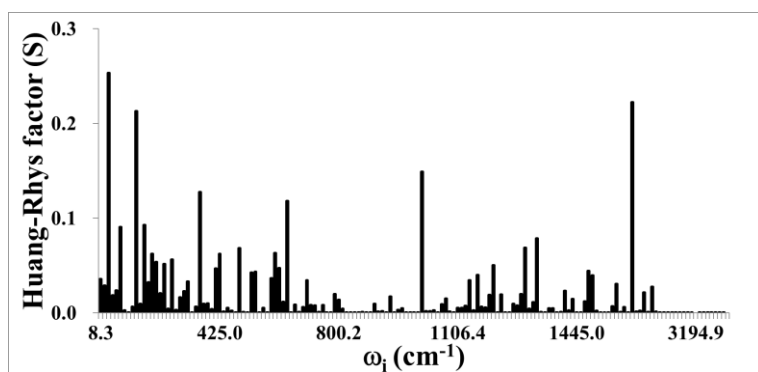
### Pt[*pti*-O-CbPy]



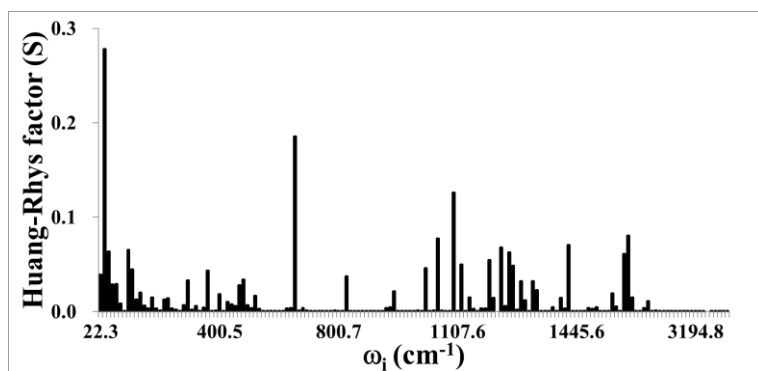
### Pt-IP



### Pt[*pti*-O-InPy]



### Pt-In-H



**Table S1.** The calculated  $T_1$  and  $^3MC$  energies of Ir(III) and Pt(II) phosphorescent materials by B3LYP/LANL2DZ with 6-311G\*\* and 6-311+G\*\* (with GD3).

	6-311G**		6-311+G** with GD3	
	$T_1$ (eV)	$^3MC$ (kcal/mol)	$T_1$ (eV)	$^3MC$ (kcal/mol)
<i>fac</i> -Ir(pmi) <sub>3</sub>	3.28	1.88	3.26	1.77
<i>fac</i> -Ir(pmb) <sub>3</sub>	3.15	3.28	3.09	3.72
Ir-N	3.26	8.00	3.26	11.14
Ir-C	3.26	8.10	3.26	7.11
Ir-Ph	3.19	11.12	3.23	18.04
Ir-N-CN	2.80	19.5	2.76	22.26
Ir-N-F	2.80	18.70	3.33	9.75
Ir-N-Ph	2.79	19.70	2.73	18.62
HB- <i>fac</i> -Ir(pmi) <sub>3</sub>	3.26	6.70	3.44	5.92
HB- <i>fac</i> -Ir(pmiCN) <sub>3</sub>	2.90	12.60	3.17	11.10
Pt[ <i>pti</i> -O-CbPy]	2.70	7.90	2.66	9.89
Pt-IP	2.70	12.60	2.68	11.77
Pt[ <i>pti</i> -O-InPy]	2.51	11.50	2.50	14.75
Pt-In-H	2.57	23.30	2.55	22.86

**Table S2.** The cartesian coordinates of optimized structures in S<sub>0</sub>, T<sub>1</sub>, and <sup>3</sup>MC state of Ir(III) and Pt(II) phosphorescent materials.

**S<sub>0</sub> state**

**Irpmi**

Ir	0.005199	0.007904	-0.05773
C	0.377944	1.853966	-0.87232
N	-0.14946	2.681558	-1.81467
N	1.379532	2.587277	-0.29716
C	0.50583	3.911101	-1.81667
C	-1.33336	2.366304	-2.60012
C	2.082279	1.988416	0.789402
C	1.470367	3.848149	-0.86484
H	0.230344	4.709361	-2.48429
H	-2.23431	2.480384	-1.99387
H	-1.27651	1.334911	-2.94392
C	1.595124	0.712063	1.134977
C	3.134883	2.62569	1.439072
H	2.189991	4.583566	-0.55274
C	2.24695	0.091962	2.20887
C	3.751975	1.970882	2.504815
H	3.473575	3.611153	1.136584
C	3.303726	0.706025	2.886395
H	1.914687	-0.8906	2.525863
H	4.571894	2.447446	3.030143
H	3.779597	0.196515	3.718403
C	1.386113	-1.14718	-1.04125
N	2.321104	-1.01319	-2.02021
N	1.553671	-2.42534	-0.58286
C	3.065242	-2.18313	-2.15811
C	2.587199	0.233101	-2.72267
C	0.72846	-2.84007	0.503578
C	2.577659	-3.07175	-1.25646
H	3.864239	-2.27691	-2.87342
H	3.187461	0.902245	-2.10261
H	1.643458	0.726205	-2.94879
C	-0.12908	-1.82526	0.973571
C	0.791037	-4.12184	1.041356



H	2.87511	-4.08301	-1.04441
C	-0.94664	-2.18354	2.053008
C	-0.04003	-4.43242	2.117559
H	1.470407	-4.86921	0.644896
C	-0.9053	-3.46015	2.620181
H	-1.6236	-1.44293	2.464565
H	-0.00713	-5.42273	2.557471
H	-1.54921	-3.69765	3.461135
C	-1.72038	-0.51301	-1.03514
N	-2.10684	-1.29657	-2.0775
N	-2.89288	-0.05616	-0.49821
C	-3.49588	-1.33349	-2.18071
C	-1.18432	-2.09132	-2.87436
C	-2.79873	0.757599	0.66892
C	-3.98834	-0.54906	-1.18922
H	-4.00253	-1.90788	-2.93713
H	-0.83616	-2.95464	-2.30395
H	-0.32104	-1.48418	-3.14247
C	-1.47564	0.936419	1.120036
C	-3.91729	1.300254	1.293782
H	-5.00424	-0.31546	-0.92562
C	-1.33578	1.713949	2.27669
C	-3.72956	2.067275	2.443565
H	-4.91766	1.133993	0.907821
C	-2.43824	2.269486	2.931613
H	-0.34168	1.880763	2.676953
H	-4.58509	2.498186	2.951227
H	-2.29044	2.861747	3.82919
H	-1.68961	-2.42896	-3.77945
H	3.119271	0.017661	-3.64978
H	-1.38339	3.035598	-3.45943

Irpmb

C	1.875664	2.947431	3.074968
C	1.529254	1.739731	2.464763
C	0.613674	1.679872	1.408827
C	0.053924	2.907988	1.001933
C	0.402311	4.129462	1.575564
C	1.320593	4.143273	2.62577
H	2.583655	2.95495	3.8974

H	1.978356	0.819309	2.820426
H	1.596223	5.086601	3.08345
c	-1.80651	3.665966	-0.63294
c	-2.52757	2.915058	-1.58181
c	-1.03741	1.516846	-0.59952
N	-2.01646	1.62005	-1.54094
N	-0.89233	2.77621	-0.06271
Ir	0.008122	0.000523	0.293183
C	-1.73643	-0.30316	1.434015
C	-2.52316	-1.40956	1.054098
C	-2.22916	0.470394	2.490262
C	-3.73869	-1.72123	1.660409
C	-3.43434	0.168109	3.128237
H	-1.65424	1.32673	2.824353
C	-4.19277	-0.92266	2.710458
H	-3.78274	0.786503	3.949145
H	-5.13495	-1.15768	3.192528
C	-2.30053	-3.38874	-0.6046
C	-1.30729	-3.63928	-1.5715
N	-0.42186	-2.56608	-1.52579
N	-1.95546	-2.16827	-0.01745
C	-0.79554	-1.67155	-0.5689
C	1.157133	-1.33716	1.444828
C	2.503545	-1.47072	1.04841
C	0.748656	-2.13428	2.519184
C	3.388929	-2.36092	1.652814
C	1.622426	-3.01727	3.158018
H	-0.27596	-2.05969	2.86584
C	2.939548	-3.13728	2.721385
H	1.272909	-3.61537	3.993364
H	3.620043	-3.83075	3.202397
C	4.08869	-0.29326	-0.63061
C	3.79658	0.679112	-1.60719
C	1.845765	0.129454	-0.5924
N	2.42182	0.894712	-1.56066
N	2.863708	-0.61365	-0.03881
C	4.781786	1.252912	-2.40108
C	5.406035	-0.70447	-0.43131
C	-3.33034	-4.3092	-0.41238
C	-1.31059	-4.78224	-2.36095

C	-2.11393	5.010637	-0.42934
C	-3.54713	3.469783	-2.34554
C	6.094993	0.829222	-2.20095
H	6.891045	1.256406	-2.79896
C	6.396964	-0.1317	-1.2295
H	7.426529	-0.4372	-1.08503
H	5.674059	-1.42945	0.320649
H	4.541879	2.009754	-3.13741
C	-3.84065	4.817802	-2.14319
H	-4.63163	5.284061	-2.7183
C	-3.13527	5.570448	-1.19744
H	-3.3905	6.613035	-1.04885
H	-1.60288	5.611333	0.306167
H	-4.10285	2.875935	-3.06028
C	-2.34871	-5.69282	-2.16773
H	-2.38397	-6.59723	-2.76321
C	-3.3381	-5.45636	-1.20677
H	-4.12971	-6.18322	-1.06788
H	-4.09921	-4.16497	0.329928
H	-0.53092	-4.96505	-3.08991
C	1.725691	1.882556	-2.36638
H	0.66883	1.631677	-2.38213
H	1.848673	2.882922	-1.94371
H	2.118245	1.867226	-3.38477
C	-2.55273	0.508032	-2.30631
H	-1.79378	-0.26656	-2.37099
H	-3.44023	0.09667	-1.81905
H	-2.81155	0.846408	-3.31093
C	0.786985	-2.47818	-2.32559
H	1.128427	-1.44733	-2.31981
H	1.57149	-3.11646	-1.91131
H	0.572378	-2.78517	-3.3511
H	-4.34159	-2.55562	1.334904
H	-0.00791	5.06356	1.221755
H	4.406668	-2.47476	1.310528
Ir-N			
Ir	-0.33609	-0.00085	-0.00067
C	0.636136	1.238165	1.315319

N	1.713811	2.071943	1.349249
N	0.111354	1.312096	2.578788
C	1.861346	2.638427	2.615272
C	2.624949	2.311948	0.239571
C	-1.05282	0.533262	2.850002
C	0.850805	2.161964	3.384172
H	2.645368	3.339787	2.844687
H	2.933491	3.361266	0.279228
H	2.071312	2.160814	-0.683
C	-1.48976	-0.22359	1.745124
C	-1.68263	0.542204	4.090732
H	0.597392	2.370277	4.408166
C	-2.63636	-0.99844	1.965604
C	-2.82114	-0.24441	4.263802
H	-1.31022	1.147388	4.910705
C	-3.29369	-1.01193	3.198499
H	-3.02723	-1.59828	1.15094
H	-3.33217	-0.25271	5.219908
H	-4.18183	-1.62224	3.329342
C	0.650247	-1.75238	0.414928
N	1.729046	-2.19185	1.122223
N	0.132954	-2.8874	-0.1522
C	1.885242	-3.57071	0.981292
C	2.636646	-1.34565	1.882971
C	-1.03155	-2.7413	-0.96302
C	0.878954	-4.00502	0.182544
H	2.671928	-4.11481	1.475564
H	2.948914	-1.90254	2.771906
H	2.079838	-0.47305	2.213604
C	-1.4788	-1.40945	-1.06599
C	-1.65332	-3.82514	-1.57516
H	0.632317	-4.99775	-0.14896
C	-2.62652	-1.22183	-1.84771
C	-2.7935	-3.59054	-2.34294
H	-1.2735	-4.83505	-1.46054
C	-3.27578	-2.28787	-2.47556
H	-3.02441	-0.21936	-1.96059
H	-3.29841	-4.41843	-2.82772
H	-4.16508	-2.10285	-3.06993
C	0.643939	0.523276	-1.72586

N	1.724933	0.137966	-2.46081
N	0.119129	1.578882	-2.42427
C	1.875546	0.951547	-3.58368
C	2.636995	-0.94101	-2.11032
C	-1.04972	2.199126	-1.89128
C	0.863214	1.853723	-3.55943
H	2.662893	0.801064	-4.30245
H	2.949521	-1.43147	-3.03747
H	2.082809	-1.66502	-1.51898
C	-1.49159	1.618226	-0.68629
C	-1.67952	3.267339	-2.52248
H	0.611286	2.636095	-4.25273
C	-2.64332	2.192742	-0.1321
C	-2.82294	3.806622	-1.93401
H	-1.30339	3.676477	-3.4544
C	-3.30066	3.265441	-0.73989
H	-3.03865	1.78498	0.791644
H	-3.33397	4.637349	-2.40739
H	-4.19282	3.680561	-0.28154
C	3.879956	1.422544	0.268784
H	4.582667	1.839811	-0.46705
H	4.353941	1.535003	1.250944
C	3.887942	-0.92347	1.094484
H	4.362608	-1.82955	0.700089
C	3.887987	-0.46619	-1.35083
H	4.359823	0.330408	-1.938
H	4.592196	-0.49186	1.820561
H	4.594673	-1.3086	-1.34147
N	3.664453	0.010118	0.00374

Ir-C

Ir	-0.38809	0.000582	-0.00104
C	0.623872	0.859894	-1.56339
N	1.765814	0.662099	-2.28014
N	0.110969	2.03088	-2.05176
C	1.957137	1.695858	-3.19622
C	2.664076	-0.47716	-2.12988
C	-1.07779	2.528538	-1.43908
C	0.917298	2.554601	-3.0489
H	2.792305	1.717275	-3.87521

H	2.831518	-0.8866	-3.13067
H	2.130157	-1.23082	-1.56432
C	-1.53972	1.725341	-0.37772
C	-1.70296	3.695195	-1.86824
H	0.687627	3.465902	-3.57127
C	-2.70677	2.179827	0.251573
C	-2.862	4.108484	-1.21232
H	-1.3108	4.27532	-2.69709
C	-3.35902	3.347462	-0.15375
H	-3.1176	1.6028	1.072488
H	-3.36936	5.012754	-1.52909
H	-4.26256	3.665255	0.35706
C	0.616537	0.922724	1.528701
N	1.761396	1.636531	1.723476
N	0.095683	0.761657	2.784485
C	1.946614	1.910634	3.078103
C	2.664353	2.076874	0.665374
C	-1.09695	-0.01361	2.901485
C	0.900091	1.358296	3.74157
H	2.782598	2.483555	3.441332
H	2.832609	3.147808	0.814232
H	2.133341	1.966334	-0.27224
C	-1.55081	-0.53178	1.671935
C	-1.73295	-0.22226	4.121579
H	0.664461	1.35484	4.790716
C	-2.72029	-1.30116	1.742819
C	-2.89395	-0.99461	4.143059
H	-1.34786	0.206001	5.041226
C	-3.38273	-1.53134	2.951392
H	-3.12419	-1.72361	0.829568
H	-3.40952	-1.17021	5.080532
H	-4.28755	-2.13095	2.964622
C	0.613545	-1.78689	0.036278
N	1.753292	-2.31321	0.566434
N	0.09643	-2.7942	-0.73176
C	1.938252	-3.62565	0.133315
C	2.651041	-1.61282	1.477838
C	-1.09189	-2.50704	-1.46789
C	0.896777	-3.92388	-0.68368
H	2.770221	-4.22794	0.455671

H	2.810803	-2.26989	2.337888
H	2.118528	-0.74132	1.837719
C	-1.54517	-1.18236	-1.30555
C	-1.7247	-3.45999	-2.25997
H	0.662661	-4.83183	-1.20991
C	-2.71156	-0.85931	-2.01202
C	-2.88281	-3.09258	-2.94425
H	-1.33966	-4.4708	-2.34614
C	-3.37144	-1.79183	-2.81672
H	-3.11578	0.143	-1.9241
H	-3.39627	-3.81716	-3.56615
H	-4.27429	-1.5039	-3.34617
C	4.041506	-0.17762	-1.51534
H	4.673154	-1.01685	-1.83073
H	4.455974	0.703452	-2.02053
C	4.309088	-0.00914	0.006836
C	4.041613	1.393984	0.620729
H	4.45437	1.391239	1.636847
C	4.032426	-1.24034	0.915225
H	4.443764	-2.12186	0.408297
H	4.674289	2.086215	0.052115
H	4.661948	-1.09485	1.801417
H	5.408549	-0.0124	0.009264

Ir-Ph

Ir	-0.86487	0.090389	0.03748
C	0.301535	0.521777	1.692496
N	1.285464	1.405079	2.033148
N	-0.14945	0.038159	2.89278
C	1.426075	1.475759	3.417015
C	1.837132	2.365777	1.074934
C	-1.36399	-0.70733	2.881679
C	0.532329	0.611808	3.955576
H	2.139547	2.12115	3.897063
H	1.113996	3.176676	0.954613
H	1.893114	1.840888	0.124747
C	-1.98832	-0.74745	1.619345
C	-1.88238	-1.30014	4.029286
H	0.323326	0.375235	4.983438
C	-3.21671	-1.42098	1.581292

C	-3.10779	-1.96028	3.943076
H	-1.35434	-1.25301	4.976124
C	-3.77361	-2.01255	2.718265
H	-3.75303	-1.48051	0.640747
H	-3.53474	-2.42552	4.824424
H	-4.73209	-2.51733	2.648757
C	-0.49754	-1.91427	-0.3696
N	0.254019	-2.94591	0.10175
N	-1.39844	-2.51454	-1.21033
C	-0.18728	-4.16178	-0.41604
C	1.389802	-2.79462	1.007164
C	-2.38585	-1.69226	-1.82267
C	-1.22556	-3.88734	-1.24217
H	0.26852	-5.10141	-0.15884
H	1.079816	-3.05086	2.024924
H	1.63446	-1.73323	0.998728
C	-2.35144	-0.35544	-1.38498
C	-3.2949	-2.18763	-2.75287
H	-1.84659	-4.54512	-1.82316
C	-3.31883	0.485401	-1.95125
C	-4.24193	-1.31502	-3.28794
H	-3.27847	-3.22756	-3.06151
C	-4.25009	0.019829	-2.88321
H	-3.35502	1.525623	-1.64793
H	-4.96383	-1.67755	-4.01102
H	-4.9898	0.700872	-3.29219
C	0.11829	1.067009	-1.48525
N	0.929636	0.773647	-2.5395
N	-0.20071	2.387927	-1.6569
C	1.086365	1.885902	-3.36429
C	1.406733	-0.58343	-2.8122
C	-1.07971	2.974664	-0.70178
C	0.384433	2.901898	-2.80242
H	1.673443	1.865122	-4.26488
H	0.625672	-1.124	-3.35579
H	1.509669	-1.06021	-1.8393
C	-1.55752	2.058191	0.256965
C	-1.41664	4.324506	-0.72452
H	0.252646	3.918883	-3.12596
C	-2.42263	2.590889	1.220555



C	-2.28311	4.811088	0.254799
H	-1.02108	4.992749	-1.4823
C	-2.78357	3.941111	1.224202
H	-2.83057	1.929966	1.978002
H	-2.56332	5.858382	0.256027
H	-3.46125	4.316726	1.984398
C	3.201855	2.941794	1.448915
C	2.585749	-3.65126	0.55689
C	2.720672	-0.66008	-3.59302
C	4.108874	-1.45668	-0.9616
C	4.147385	-1.67623	0.41696
C	4.236574	-0.57389	1.267096
C	4.2938	0.72699	0.76842
C	4.234976	0.914658	-0.61445
C	4.119807	-0.16416	-1.49163
H	4.015434	-2.30554	-1.63201
H	4.221093	-0.72915	2.3416
H	4.230527	1.922488	-1.01789
C	3.928748	0.078191	-2.97381
C	3.947526	-3.06725	0.978679
C	4.313075	1.902916	1.717607
H	4.222093	1.522603	2.737915
H	5.282135	2.411975	1.667373
H	3.116657	3.604717	2.316077
H	3.490733	3.588419	0.614421
H	4.022942	-3.03743	2.070061
H	4.738517	-3.73912	0.628546
H	2.491027	-4.67231	0.939798
H	2.561795	-3.72628	-0.53368
H	4.827201	-0.22445	-3.52393
H	3.819615	1.153394	-3.13619
H	2.577595	-0.30016	-4.61747
H	2.949551	-1.72615	-3.68954

Ir-N-F

Ir	0.010428	0.001743	-0.36818
C	1.7806	-0.20264	0.647247
N	2.273546	-0.85196	1.733218
N	2.853151	0.506675	0.144104
C	3.625485	-0.55124	1.938315

C	1.503156	-1.71047	2.622094
C	2.626892	1.299582	-1.02934
C	3.958023	0.290513	0.934188
H	4.220819	-0.97359	2.72748
H	2.155034	-2.52769	2.945559
H	0.691122	-2.14093	2.042588
C	1.296192	1.232833	-1.48714
C	3.631964	2.042596	-1.64504
C	1.019774	1.983003	-2.63779
C	3.306521	2.771624	-2.78791
H	4.642191	2.055481	-1.25872
C	2.002062	2.739305	-3.28045
H	0.014867	1.966438	-3.04425
H	4.070902	3.355864	-3.28745
H	1.749776	3.303846	-4.17252
C	-0.73403	1.654736	0.592084
N	-0.45813	2.426858	1.674459
N	-1.86632	2.218133	0.037387
C	-1.40271	3.448824	1.827678
C	0.633222	2.202916	2.611744
C	-2.39855	1.602705	-1.14353
C	-2.26109	3.296321	0.794622
H	-1.36385	4.189774	2.60556
H	1.005717	3.180855	2.931682
H	1.432186	1.700342	2.074048
C	-1.65771	0.477707	-1.5557
C	-3.52425	2.086447	-1.80697
C	-2.12726	-0.15932	-2.71182
C	-3.95165	1.417721	-2.95319
H	-4.05634	2.959444	-1.45389
C	-3.25175	0.297874	-3.40206
H	-1.59406	-1.02719	-3.08327
H	-4.82344	1.775234	-3.48921
H	-3.58266	-0.2202	-4.29662
C	-1.08649	-1.44964	0.581594
N	-1.93876	-1.5744	1.631003
N	-0.99062	-2.72221	0.05326
C	-2.36298	-2.89903	1.790941
C	-2.32554	-0.5	2.534011
C	-0.14754	-2.89899	-1.09315

C	-1.76149	-3.58683	0.794812
H	-3.05749	-3.21909	2.546461
H	-3.37152	-0.65759	2.814144
H	-2.26381	0.43315	1.981553
C	0.473228	-1.70381	-1.50614
C	0.019457	-4.12896	-1.72625
C	1.302422	-1.81638	-2.62989
C	0.854771	-4.18868	-2.8407
H	-0.4852	-5.01861	-1.37447
C	1.492774	-3.03246	-3.28925
H	1.802161	-0.92927	-3.00194
H	0.99963	-5.13315	-3.35272
H	2.139698	-3.07814	-4.15962
C	0.95976	-0.98161	3.863326
H	0.600828	-1.75631	4.555852
H	1.800507	-0.48466	4.361107
C	0.220023	1.392737	3.852097
H	-0.64934	1.883377	4.304851
C	-1.46686	-0.43397	3.808219
H	-1.47494	-1.42561	4.27509
H	1.041125	1.480219	4.578112
H	-1.97945	0.244136	4.505441
N	-0.09071	-0.00751	3.61722
F	-3.32291	4.030324	0.479622
F	-1.85881	-4.87844	0.498648
F	5.134938	0.848125	0.670631

Ir-N-CN

Ir	-0.002	0.000052	-0.36533
C	-1.79812	0.209638	0.589461
N	-2.30878	0.888891	1.664022
N	-2.86472	-0.4693	0.064434
C	-3.65181	0.630755	1.818935
C	-1.53505	1.735618	2.565758
C	-2.61109	-1.27309	-1.09816
C	-4.01741	-0.22368	0.817193
H	-4.25437	1.071383	2.594957
H	-2.17881	2.560887	2.882544
H	-0.71094	2.153007	1.99478
C	-1.26673	-1.22366	-1.51541

C	-3.60049	-2.01095	-1.74415
C	-0.95666	-1.98329	-2.65046
C	-3.24409	-2.74985	-2.87042
H	-4.6257	-2.0202	-1.40037
C	-1.92387	-2.73417	-3.32014
H	0.06152	-1.97778	-3.02252
H	-3.99787	-3.32975	-3.38996
H	-1.64794	-3.30704	-4.19947
C	0.718802	-1.66404	0.580117
N	0.387745	-2.45173	1.651184
N	1.83977	-2.24427	0.050739
C	1.283834	-3.48577	1.799404
C	-0.72951	-2.20996	2.557987
C	2.405983	-1.61672	-1.11035
C	2.205569	-3.36879	0.797353
H	1.204967	-4.23223	2.571391
H	-1.12067	-3.18177	2.871527
H	-1.50561	-1.70266	1.992641
C	1.688307	-0.47679	-1.52193
C	3.539777	-2.09999	-1.75964
C	2.187516	0.175777	-2.65625
C	3.998516	-1.417	-2.88411
H	4.061883	-2.98411	-1.42047
C	3.32156	-0.28167	-3.32902
H	1.670989	1.053992	-3.02598
H	4.877143	-1.77659	-3.40671
H	3.677289	0.247252	-4.20722
C	1.085855	1.450093	0.581872
N	1.936777	1.551304	1.65084
N	1.027899	2.713317	0.058246
C	2.388383	2.842776	1.80177
C	2.288519	0.45922	2.552481
C	0.193942	2.897071	-1.09635
C	1.824774	3.587487	0.804221
H	3.077612	3.143105	2.57257
H	3.325509	0.607781	2.866244
H	2.241108	-0.46513	1.983698
C	-0.44011	1.709108	-1.50937
C	0.0444	4.123721	-1.73941
C	-1.26265	1.822194	-2.63727

C	-0.784	4.186511	-2.85795
H	0.553219	5.015447	-1.39997
C	-1.43497	3.036337	-3.30357
H	-1.76968	0.938455	-3.00712
H	-0.91296	5.129882	-3.37549
H	-2.07669	3.085425	-4.17725
C	-1.01861	0.993602	3.810327
H	-0.64712	1.761948	4.502479
H	-1.87507	0.52011	4.304203
C	-0.33908	-1.39878	3.805112
H	0.501792	-1.90658	4.291657
C	1.393045	0.385667	3.801443
H	1.414306	1.36618	4.291089
H	-1.18668	-1.46455	4.50124
H	1.875823	-0.31757	4.494058
N	0.01086	-0.00622	3.576351
C	2.021671	4.967291	0.582906
N	2.208444	6.100718	0.450657
C	3.302964	-4.22694	0.571433
N	4.192076	-4.95346	0.434727
C	-5.31101	-0.74323	0.597028
N	-6.38547	-1.14925	0.464873

Ir-N-Ph

Ir	-0.01073	0.02193	-0.38275
C	0.453877	-1.72392	0.576537
N	-0.02521	-2.46211	1.612674
N	1.504614	-2.45632	0.077424
C	0.708924	-3.63348	1.760731
C	-1.13904	-2.0869	2.47188
C	2.254112	-1.84021	-0.98355
C	1.661447	-3.65303	0.789313
H	0.448973	-4.39454	2.476746
H	-1.66669	-3.00375	2.752498
H	-1.82007	-1.47408	1.887003
C	1.685511	-0.62987	-1.43489
C	3.449457	-2.35676	-1.48092
C	2.361747	0.007104	-2.48388
C	4.092379	-1.68186	-2.51824
H	3.889316	-3.25746	-1.07855

C	3.539142	-0.50852	-3.02864
H	1.954901	0.931259	-2.87929
H	5.019881	-2.07595	-2.91845
H	4.032157	0.011338	-3.84437
C	1.201065	1.32159	0.63038
N	1.999093	1.305645	1.731299
N	1.359696	2.57929	0.09835
C	2.64726	2.525984	1.884636
C	2.154799	0.183386	2.645639
C	0.530564	2.893329	-1.03374
C	2.270706	3.329785	0.853423
H	3.383196	2.70033	2.6511
H	3.188193	0.187809	3.005747
H	2.000421	-0.73157	2.08046
C	-0.21175	1.788234	-1.50136
C	0.424414	4.171949	-1.57891
C	-1.03104	2.028538	-2.61225
C	-0.41112	4.365344	-2.6787
H	0.964733	5.010962	-1.16578
C	-1.12676	3.289824	-3.20291
H	-1.60923	1.20577	-3.01871
H	-0.49916	5.35373	-3.11581
H	-1.76884	3.437325	-4.06588
C	-1.81105	0.449527	0.491751
N	-2.27865	1.18676	1.534392
N	-2.93709	-0.06495	-0.10711
C	-3.66688	1.135809	1.588526
C	-1.45792	1.915381	2.490817
C	-2.71244	-0.97611	-1.19609
C	-4.0959	0.369369	0.549569
H	-4.24152	1.710776	2.294685
H	-2.00601	2.817044	2.781121
H	-0.5484	2.225114	1.983581
C	-1.35476	-1.07277	-1.5679
C	-3.72345	-1.73255	-1.78712
C	-1.07413	-1.93699	-2.63459
C	-3.39471	-2.587	-2.83911
H	-4.74632	-1.67803	-1.44458
C	-2.07225	-2.67672	-3.27113
H	-0.04709	-2.03252	-2.96973

H	-4.17212	-3.17707	-3.31151
H	-1.81724	-3.33282	-4.09772
C	-0.70924	-1.34922	3.7522
H	-1.58389	-1.3334	4.418768
H	0.053644	-1.95656	4.253452
C	1.205322	0.236955	3.85513
H	1.314293	1.219623	4.328656
C	-1.12367	1.104871	3.754798
H	-2.06302	0.72272	4.171185
H	1.572487	-0.50318	4.581383
H	-0.72004	1.814169	4.492235
N	-0.19951	-0.00071	3.57109
C	-5.48852	0.195804	0.104791
C	-5.88301	0.630774	-1.16884
C	-6.44999	-0.33857	0.969253
C	-7.21046	0.523626	-1.56782
H	-5.14078	1.044522	-1.84135
C	-7.7824	-0.43772	0.569732
H	-6.14607	-0.68701	1.949858
C	-8.16499	-0.01034	-0.69973
H	-7.50258	0.861125	-2.55575
H	-8.51766	-0.85719	1.247288
H	-9.19948	-0.09294	-1.01323
C	2.544542	-4.78103	0.449287
C	3.431498	-5.301	1.398163
C	2.456854	-5.39247	-0.80977
C	4.218715	-6.41158	1.0955
H	3.510101	-4.82281	2.367996
C	3.247822	-6.49515	-1.11169
H	1.772103	-4.99112	-1.54757
C	4.131233	-7.00876	-0.16
H	4.905472	-6.80298	1.837665
H	3.172865	-6.95785	-2.08922
H	4.747335	-7.86846	-0.39797
C	2.84757	4.638975	0.506484
C	3.503553	4.819567	-0.71993
C	2.812618	5.696643	1.421714
C	4.10249	6.036861	-1.02355
H	3.532039	4.002725	-1.43142
C	3.420967	6.91422	1.118177

H	2.29552	5.563896	2.365316
C	4.063889	7.088183	-0.10537
H	4.604256	6.165287	-1.97591
H	3.38349	7.727889	1.833816
H	4.531262	8.03662	-0.34478

HB-Ir

C	-2.30534	2.577287	3.163893
C	-1.21717	1.922837	2.57301
C	-1.38777	1.128062	1.439242
C	-2.71783	1.070488	0.978544
C	-3.56527	2.428867	2.60454
H	-2.17663	3.192683	4.046575
H	-0.22863	2.029196	3.006363
H	-4.43968	2.913314	3.024341
C	-4.0631	-0.10355	-0.8923
C	-3.60836	-0.96799	-1.89891
C	-1.78689	-0.32975	-0.69541
N	-2.21975	-1.0696	-1.7457
N	-2.90862	0.264529	-0.17152
Ir	-0.02268	0.001373	0.325504
C	-0.4286	-1.74599	1.402231
C	0.308105	-2.87621	0.997985
C	-1.30141	-1.99116	2.462627
C	-1.39353	-3.26383	3.040193
H	-1.91314	-1.18288	2.848192
C	-0.60441	-4.28856	2.540753
H	-2.06794	-3.45642	3.866312
H	-0.63835	-5.29114	2.952049
C	2.148789	-3.46678	-0.71928
C	2.777237	-2.63944	-1.66135
N	2.181961	-1.37653	-1.54914
N	1.204302	-2.64213	-0.07455
C	1.228364	-1.36753	-0.58498
C	1.585288	0.51561	1.562685
C	2.244295	1.709715	1.21043
C	2.124264	-0.11629	2.683904
C	3.219216	0.433027	3.363052
H	1.685774	-1.04333	3.037253
C	3.770639	1.619494	2.904198



H	3.63808	-0.05382	4.235955
H	4.618977	2.08464	3.393554
C	2.023654	3.588308	-0.55208
C	1.086615	3.724086	-1.58658
C	0.631779	1.761636	-0.52893
N	0.264664	2.591176	-1.53724
N	1.704159	2.368145	0.077954
C	1.06476	4.810828	-2.45363
C	3.01215	4.569145	-0.3465
C	2.516333	-4.81981	-0.59455
C	3.785934	-3.08394	-2.50894
C	-5.42947	0.21721	-0.78551
C	-4.45397	-1.55778	-2.8318
C	2.045078	5.780553	-2.24495
H	2.076512	6.651509	-2.88916
C	2.98968	5.662282	-1.2246
H	3.743091	6.426421	-1.07865
H	0.327103	4.901836	-3.23948
C	-5.80708	-1.23916	-2.71992
H	-6.51403	-1.67163	-3.41831
C	-6.27945	-0.37775	-1.72891
H	-7.33422	-0.14266	-1.65842
H	-4.086	-2.23033	-3.59482
C	4.14841	-4.42436	-2.37951
H	4.930752	-4.82672	-3.01241
C	3.531691	-5.26578	-1.45275
H	3.827246	-6.30413	-1.36747
H	4.267218	-2.42777	-3.22153
C	-0.85333	2.385965	-2.44167
H	-1.23168	1.378509	-2.30405
H	-1.65004	3.103087	-2.23039
H	-0.52131	2.51389	-3.47438
C	-1.38499	-1.90074	-2.59583
H	-0.34535	-1.64882	-2.41339
H	-1.54506	-2.95861	-2.37426
H	-1.6271	-1.71331	-3.64401
C	2.587917	-0.2345	-2.35018
H	3.563726	0.134214	-2.0252
H	2.646617	-0.5256	-3.40095
H	1.849949	0.552301	-2.2335

O	1.970058	-5.68876	0.267544
H	1.279106	-5.2159	0.819469
N	0.246481	-4.09647	1.517896
O	-5.9574	1.035718	0.13543
H	-5.22854	1.367258	0.739088
O	3.952112	4.525086	0.607997
H	3.822008	3.698187	1.16047
N	-3.77315	1.676214	1.510256
N	3.284659	2.258876	1.82609

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CN

C	1.87185	-2.84123	3.521247
C	0.890757	-2.06248	2.896175
C	1.198782	-1.27967	1.782465
C	2.544251	-1.36741	1.381515
C	3.164285	-2.83073	3.017783
H	1.636807	-3.44769	4.38781
H	-0.1211	-2.06329	3.286324
H	3.959365	-3.41589	3.465405
C	4.088832	-0.32908	-0.4106
C	3.778434	0.593677	-1.42173
C	1.848623	0.150435	-0.30795
N	2.406737	0.850708	-1.32669
N	2.874813	-0.57194	0.253449
Ir	0.015758	0.000687	0.621876
C	0.548161	1.675592	1.756658
C	-0.04995	2.881509	1.349434
C	1.389027	1.80825	2.862838
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H	1.895167	0.934107	3.257271
C	0.922906	4.162425	2.967919
H	2.22802	3.157171	4.338176
H	1.036768	5.147206	3.40624
C	-1.76049	3.682917	-0.41227
C	-2.43327	2.94198	-1.39638
N	-1.96214	1.627757	-1.30509
N	-0.91777	2.761281	0.232169
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C	-1.68827	-0.36241	1.784503
C	-2.44061	-1.4858	1.398771

C	-2.20772	0.312069	2.890874
C	-3.37356	-0.13614	3.523158
H	-1.69799	1.191722	3.268739
C	-4.0157	-1.2642	3.033848
H	-3.77829	0.382474	4.384075
H	-4.92117	-1.65091	3.487152
C	-2.33061	-3.35943	-0.37612
C	-1.38057	-3.56756	-1.3879
C	-0.77661	-1.67362	-0.28734
N	-0.4587	-2.51939	-1.29903
N	-1.92076	-2.18553	0.27849
C	-1.43055	-4.63487	-2.27096
C	-3.41031	-4.24918	-0.20723
C	-2.00378	5.062175	-0.25646
C	-3.36842	3.494383	-2.25796
C	5.404178	-0.80702	-0.24948
C	4.718717	1.095305	-2.30822
C	-2.50642	-5.51812	-2.10174
C	-3.46786	-5.32824	-1.0976
H	-4.28848	-6.02501	-0.98862
H	-0.68968	-4.7892	-3.04238
C	6.027372	0.619095	-2.14524
C	6.358055	-0.30681	-1.14407
H	7.376005	-0.65839	-1.04033
H	4.471057	1.813256	-3.07688
C	-3.6114	4.866018	-2.0984
C	-2.94546	5.626441	-1.12534
H	-3.15115	6.683795	-1.02378
H	-3.8887	2.912663	-3.00523
C	0.690241	-2.39963	-2.18206
H	1.170898	-1.44477	-1.99604
H	1.400703	-3.20739	-1.99189
H	0.363178	-2.44685	-3.22329
C	1.707957	1.783462	-2.19635
H	0.64008	1.64464	-2.06174
H	1.974803	2.812731	-1.94606
H	1.972689	1.585644	-3.23678
C	-2.45026	0.547861	-2.1481
H	-1.79151	-0.30641	-2.03126
H	-3.46491	0.265656	-1.85796

H	-2.45006	0.866821	-3.19221
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O	5.793357	-1.68691	0.6767
H	5.005105	-1.94418	1.245158
O	-4.3624	-4.13392	0.721928
H	-4.17843	-3.32433	1.289272
N	3.501603	-2.09377	1.945668
N	-3.54981	-1.93982	1.969625
C	-2.6263	-6.6427	-2.97881
N	-2.71629	-7.54684	-3.69285
C	-4.56503	5.506467	-2.95204
N	-5.33571	6.015947	-3.64617
C	7.051927	1.090527	-3.02623
N	7.872072	1.475151	-3.74369

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C	-2.18145	-1.96567	-0.03851
C	-1.99234	-3.33936	0.099248
C	-3.50891	-1.53743	-0.2398
N	-3.61592	-0.11959	-0.36873
C	-3.07362	-4.23275	0.04535
C	-4.59977	-2.38976	-0.29829
C	-4.36314	-3.76087	-0.15253
H	-2.87465	-5.29164	0.15863
H	-5.60681	-2.01699	-0.44264
H	-5.19156	-4.45808	-0.19376
Pt	-0.80807	-0.54295	0.215146
C	0.658221	-1.94124	0.268793
C	0.454098	-3.32733	0.208574
C	1.996542	-1.56572	0.120832
C	1.495056	-4.2554	0.018982
C	3.054529	-2.453	-0.14816
C	2.795788	-3.82568	-0.17779
H	1.241834	-5.308	-0.0148
H	3.589168	-4.53802	-0.37204
O	-0.77952	-3.94215	0.302041
C	0.121803	1.953669	1.659721
C	1.979795	0.829312	0.836287

C	0.884722	2.897036	2.312657
H	-0.95611	1.980769	1.713136
C	2.819715	1.732308	1.520487
C	2.273789	2.771478	2.245077
H	0.403864	3.688421	2.871454
H	3.886682	1.574785	1.512433
H	2.922314	3.457357	2.778304
N	0.634722	0.946656	0.91578
C	-4.67112	0.683189	-0.76726
C	-4.1829	1.943539	-0.86861
H	-4.6533	2.862943	-1.16958
H	-5.65827	0.302212	-0.95892
N	2.520501	-0.22978	0.112623
C	4.234905	-1.66744	-0.42893
C	3.876603	-0.3076	-0.29172
C	5.519631	-2.00695	-0.85755
C	6.423647	-0.99437	-1.16451
C	6.042637	0.350044	-1.07072
C	4.764892	0.70849	-0.64127
H	4.475593	1.750795	-0.61078
H	6.744401	1.128381	-1.34762
H	7.423132	-1.24585	-1.50024
H	5.799438	-3.04868	-0.96602
N	-2.82747	1.879587	-0.53325
C	-2.46965	0.604585	-0.20762
C	-1.90789	2.966444	-0.62344
C	-0.71817	2.799981	-1.33139
C	-2.18218	4.172671	0.015263
C	0.208568	3.834402	-1.36293
H	-0.51742	1.8547	-1.81907
C	-1.2494	5.205874	-0.03802
H	-3.10526	4.291232	0.571298
C	-0.03465	5.04993	-0.71281
H	1.139219	3.692285	-1.90219
H	-1.46484	6.140829	0.468348
C	1.003815	6.143779	-0.71604
H	0.568259	7.11313	-0.46499
H	1.78828	5.931048	0.018405
H	1.487139	6.230572	-1.69241

## Pt-Iso

C	-3.55156	-0.45766	0.103221
C	-4.15171	-1.68476	0.383386
C	-4.42031	0.626459	-0.13975
N	-3.71932	1.84369	-0.40801
C	-5.54877	-1.81583	0.417762
C	-5.80218	0.531594	-0.11214
C	-6.36266	-0.71915	0.170536
H	-5.9714	-2.78866	0.638615
H	-6.43582	1.391818	-0.29294
H	-7.44	-0.83195	0.198534
Pt	-1.60769	-0.03737	0.205482
C	-1.17612	-2.01029	0.375222
C	-2.11413	-3.04288	0.494118
C	0.125451	-2.45774	0.146305
C	-1.76677	-4.40602	0.429728
C	0.511032	-3.80036	0.011694
C	-0.45939	-4.79355	0.180914
H	-2.55519	-5.14119	0.537037
H	-0.20536	-5.84352	0.092028
O	-3.47301	-2.84546	0.656744
C	0.672259	1.54928	1.465696
C	1.476744	-0.4623	0.661384
C	1.864992	1.8603	2.077918
H	-0.17213	2.220714	1.522263
C	2.695741	-0.2361	1.323197
C	2.917785	0.933114	2.028398
H	1.960672	2.801788	2.602599
H	3.45729	-1.00193	1.28003
N	0.460087	0.417548	0.756608
C	-4.14858	3.064649	-0.90214
C	-3.03551	3.805026	-1.13279
H	-2.91585	4.796271	-1.53342
H	-5.18569	3.300726	-1.06163
N	1.275053	-1.62793	-0.0817
C	1.902197	-3.82296	-0.39517
C	2.333273	-2.47793	-0.50542
C	2.759802	-4.86079	-0.75689
C	4.022058	-4.5408	-1.24786
C	4.395243	-3.20693	-1.43722

C	3.553217	-2.13616	-1.1054
H	5.354125	-2.99605	-1.89709
H	4.709355	-5.33066	-1.52949
H	2.439083	-5.89293	-0.67544
N	-1.94136	3.010849	-0.77634
C	-2.35827	1.799266	-0.31354
C	-0.56584	3.331133	-0.98622
C	0.241173	2.431692	-1.67979
C	-0.02224	4.503666	-0.46528
C	1.600063	2.69301	-1.81601
H	-0.19196	1.521591	-2.07394
C	1.33713	4.758952	-0.62278
H	-0.65384	5.194146	0.08227
C	2.173448	3.852064	-1.28508
H	2.222888	1.978822	-2.34381
H	1.757204	5.669265	-0.20761
C	3.656143	4.106866	-1.3943
H	3.867312	5.157753	-1.60782
H	4.159489	3.854566	-0.45577
H	4.107523	3.502057	-2.18362
C	4.244706	1.190828	2.714393
C	4.069862	1.460554	4.218342
C	4.996228	2.343704	2.023699
H	4.84934	0.284232	2.603741
H	3.543303	0.638202	4.708423
H	5.045005	1.578973	4.698553
H	3.499203	2.377063	4.392916
H	5.162535	2.125446	0.966282
H	4.428933	3.276648	2.094051
H	5.968602	2.504838	2.497271
C	3.909438	-0.71877	-1.54284
C	3.802836	-0.60177	-3.07565
C	5.29207	-0.25974	-1.05257
H	3.174446	-0.03079	-1.12606
H	2.804936	-0.88432	-3.41995
H	4.000992	0.426027	-3.39824
H	4.525817	-1.25493	-3.57177
H	5.374732	-0.32565	0.034592
H	6.091821	-0.86644	-1.48524
H	5.472339	0.779676	-1.34335

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C	2.213011	-1.42258	0.035266
C	3.55535	-1.04896	0.062956
C	1.954754	-2.80783	0.029327
N	0.560232	-3.10781	-0.02546
C	4.57899	-2.00943	0.098498
C	2.938136	-3.78322	0.065557
C	4.271743	-3.36197	0.10077
H	5.606616	-1.66709	0.121336
H	2.693359	-4.83865	0.073266
H	5.068448	-4.09585	0.128711
Pt	0.634085	-0.21516	0.18992
C	1.82988	1.408181	0.01608
C	3.224534	1.372038	-0.11416
C	1.281102	2.676147	-0.2133
C	4.002327	2.494737	-0.45923
C	2.016355	3.812314	-0.61697
C	3.408051	3.713685	-0.7276
H	5.074689	2.364821	-0.54101
H	4.004376	4.567809	-1.02705
O	4.002824	0.242529	0.062168
C	-2.00149	0.51965	1.49627
C	-1.11913	2.422807	0.501839
C	-3.11754	1.179831	1.959253
H	-1.85139	-0.52737	1.710685
C	-2.23636	3.163223	0.951304
C	-3.23851	2.539512	1.662871
H	-3.86225	0.645621	2.533021
H	-4.08966	3.112778	2.012272
N	-1.03118	1.095926	0.747973
C	-0.10169	-4.29721	-0.27835
C	-1.41343	-3.98865	-0.41847
H	-2.26575	-4.6045	-0.64531
H	0.402201	-5.24419	-0.35401
N	-0.08703	3.064204	-0.16848
C	1.08189	4.875518	-0.86802
C	-0.16024	4.40679	-0.59391
N	-1.52274	-2.60462	-0.25296
C	-0.30264	-2.04989	0.005811



C	-2.71423	-1.8529	-0.47649
C	-2.68225	-0.76232	-1.34527
C	-3.89385	-2.19412	0.178843
C	-3.82794	0.002035	-1.52459
H	-1.7555	-0.50838	-1.84394
C	-5.03861	-1.42574	-0.02227
H	-3.90834	-3.03738	0.860004
C	-5.02207	-0.30944	-0.86343
H	-3.79182	0.858617	-2.18944
H	-5.95296	-1.69137	0.497741
C	-6.24215	0.560548	-1.03519
H	-7.14769	0.057516	-0.68995
H	-6.13659	1.488252	-0.46238
H	-6.38668	0.8401	-2.08197
H	-2.28264	4.227151	0.780042
H	-1.10901	4.900877	-0.70431
H	1.310245	5.862583	-1.24086

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C	2.511945	-1.1133	0.038683
C	3.767764	-0.51078	0.030619
C	2.499773	-2.52294	0.054674
N	1.179354	-3.06318	0.016116
C	4.945394	-1.27316	0.060523
C	3.640791	-3.30738	0.087435
C	4.880324	-2.65815	0.091461
H	5.89703	-0.75553	0.055965
H	3.586012	-4.38908	0.114399
H	5.793684	-3.24037	0.116529
Pt	0.749619	-0.20158	0.202351
C	1.647786	1.592813	0.001887
C	3.018083	1.812116	-0.15016
C	0.880085	2.747806	-0.20346
C	3.581242	3.070695	-0.48541
C	1.39463	4.006924	-0.58251
C	2.784925	4.168898	-0.71644
H	4.658498	3.130782	-0.58093
H	3.214517	5.122248	-0.99937
O	3.98452	0.844068	-0.01005
C	-1.99397	0.06095	1.472287

C	-1.48103	2.073991	0.424821
C	-3.25118	0.495001	1.828254
H	-1.63597	-0.91841	1.746553
C	-2.79033	2.574566	0.708437
C	-3.66083	1.758026	1.416679
H	-3.90347	-0.15126	2.39971
H	-4.64306	2.15097	1.649092
N	-1.13588	0.812463	0.745039
C	0.735452	-4.34977	-0.24069
C	-0.60863	-4.27207	-0.39209
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H	1.396254	-5.19528	-0.31082
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C	0.14417	-2.17199	0.03915
C	-2.25958	-2.39251	-0.47079
C	-2.40307	-1.30914	-1.3375
C	-3.37043	-2.92923	0.17238
C	-3.65705	-0.74218	-1.52051
H	-1.52843	-0.89992	-1.82683
C	-4.62509	-2.35916	-0.03418
H	-3.24994	-3.76509	0.852178
C	-4.78686	-1.24807	-0.86669
H	-3.75817	0.116632	-2.17544
H	-5.48602	-2.77331	0.479816
C	-6.1274	-0.57776	-1.02986
H	-6.94104	-1.2079	-0.66511
H	-6.15299	0.362726	-0.46888
H	-6.3267	-0.33564	-2.07697
H	0.220487	5.880325	-1.05466
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H	-2.46703	4.264197	-0.08917
N	-0.85372	4.198318	-0.49917

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Ir	-0.00709	-0.01405	-0.03524
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C	-2.8724	-0.44381	0.71094
C	-3.44914	-2.18674	-1.07267
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H	0.111173	-3.50795	-2.45011
H	0.466675	-1.79274	-2.71832
C	-1.74178	0.285664	1.125552
C	-4.11536	-0.3763	1.333669
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C	-1.93414	1.115372	2.237132
C	-4.26016	0.46071	2.439617
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C	1.084984	2.693531	0.621318
C	-0.23811	4.037515	-1.11663
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H	-2.99094	1.068058	-2.01062
H	-1.68331	0.569221	-3.09659
C	1.161754	1.354687	1.053667
C	1.793217	3.742075	1.200027
H	0.127538	5.019051	-0.87419
C	2.011444	1.122543	2.14243
C	2.631429	3.462854	2.279003
H	1.699355	4.75854	0.832449
C	2.735251	2.15275	2.747613
H	2.09594	0.114197	2.533482
H	3.19121	4.263187	2.749441
H	3.38023	1.934388	3.592819
C	1.710586	-0.5326	-1.04033
N	2.535209	-0.07312	-2.02988

N	2.408458	-1.63703	-0.4949
C	3.674536	-0.84688	-2.13456
C	2.288639	1.159668	-2.75683
C	1.887111	-2.24446	0.59104
C	3.607926	-1.83873	-1.19713
H	4.43962	-0.63764	-2.86322
H	2.45161	2.02319	-2.10765
H	1.254491	1.181577	-3.10414
C	0.619684	-1.62408	1.091763
C	2.490523	-3.39039	1.227661
H	4.301052	-2.62431	-0.96009
C	0.067449	-2.21459	2.215431
C	1.869993	-3.90619	2.325869
H	3.410575	-3.8202	0.850021
C	0.652318	-3.33376	2.84352
H	-0.84427	-1.7979	2.627713
H	2.301874	-4.76485	2.829981
H	0.196079	-3.77177	3.723128
H	2.960509	1.213403	-3.61368
H	-2.64391	2.017961	-3.47843
H	-0.61236	-2.66311	-3.84415

Irpmb

C	-1.50981	2.67814	3.417653
C	-0.70323	1.850259	2.635291
C	-1.21371	1.166456	1.526288
C	-2.57134	1.366504	1.229591
C	-3.38879	2.213841	1.976331
C	-2.84939	2.867208	3.083692
H	-1.09122	3.18085	4.283417
H	0.340352	1.722637	2.899764
H	-3.47687	3.524629	3.674618
C	-4.29245	0.388638	-0.42637
C	-4.08938	-0.45488	-1.5323
C	-2.05642	-0.02555	-0.63969
N	-2.71858	-0.67627	-1.62929
N	-3.01597	0.645646	0.082971
Ir	-0.1156	-0.06768	0.199247
C	-0.77573	-1.91718	0.947092
C	-0.1625	-3.02485	0.323679

C	-1.733	-2.19456	1.925811
C	-0.48781	-4.34504	0.643428
C	-2.05426	-3.50797	2.281451
H	-2.22341	-1.36951	2.432265
C	-1.43605	-4.58142	1.637438
H	-2.78699	-3.69548	3.05961
H	-1.69796	-5.60074	1.898873
C	2.083361	-3.17727	-0.77482
C	2.810659	-2.2426	-1.56135
N	1.964475	-1.2169	-1.88193
N	0.798763	-2.68758	-0.65505
C	0.703041	-1.36604	-1.24321
C	1.651406	-0.12528	1.249575
C	2.55282	0.940613	0.996307
C	2.108854	-1.13326	2.11358
C	3.838034	0.98081	1.524102
C	3.38687	-1.10231	2.667847
H	1.446335	-1.95796	2.346983
C	4.251687	-0.05151	2.369105
H	3.713108	-1.90169	3.324014
H	5.252638	-0.02941	2.784757
C	2.478885	3.194519	-0.27695
C	1.466575	3.712634	-1.10745
C	0.786267	1.669206	-0.41622
N	0.460007	2.751329	-1.16577
N	2.024734	1.933927	0.123062
C	1.560878	4.96614	-1.69841
C	3.620119	3.949878	-0.01368
C	2.713641	-4.30561	-0.25023
C	4.15992	-2.43921	-1.85435
C	-5.58627	0.753145	-0.05416
C	-5.14046	-0.93442	-2.30473
C	2.710143	5.711515	-1.43813
H	2.820209	6.69461	-1.87984
C	3.717905	5.209352	-0.60683
H	4.59693	5.812389	-0.41277
H	4.406686	3.597219	0.634771
H	0.769311	5.351568	-2.32895
C	-6.42922	-0.55429	-1.93601
H	-7.27624	-0.91085	-2.5098

C	-6.64379	0.271395	-0.82525
H	-7.65682	0.540343	-0.55027
H	-5.78571	1.370108	0.807624
H	-4.96304	-1.58729	-3.15005
C	4.772086	-3.59368	-1.35074
H	5.816981	-3.77878	-1.57215
C	4.065103	-4.50357	-0.55876
H	4.572074	-5.3794	-0.17098
H	2.181523	-4.99909	0.384905
H	4.716009	-1.71714	-2.43893
C	-0.79536	2.930862	-1.87357
H	-1.32828	1.984321	-1.86512
H	-1.40451	3.691212	-1.379
H	-0.60119	3.234239	-2.90482
C	-2.12929	-1.55552	-2.62845
H	-1.04556	-1.54516	-2.4878
H	-2.50455	-2.57223	-2.49001
H	-2.38894	-1.20378	-3.63021
C	2.35585	-0.05689	-2.64232
H	1.468085	0.534933	-2.85663
H	3.068689	0.564414	-2.08776
H	2.817134	-0.35962	-3.58769
H	-0.03178	-5.17186	0.112309
H	-4.41952	2.392325	1.708658
H	4.528802	1.77515	1.284434

Ir-N

Ir	-0.35373	-0.01189	-0.00286
C	0.662969	0.007463	-1.80415
N	1.74964	-0.56782	-2.38702
N	0.16408	0.845092	-2.76365
C	1.930681	-0.0816	-3.68151
C	2.652489	-1.50892	-1.73903
C	-1.00348	1.597445	-2.43648
C	0.930054	0.80315	-3.91681
H	2.728892	-0.42263	-4.31845
H	2.977276	-2.23414	-2.49156
H	2.087456	-2.04482	-0.98074
C	-1.47109	1.367898	-1.12836

C	-1.60905	2.462679	-3.34233
H	0.70023	1.377092	-4.7965
C	-2.62422	2.07829	-0.77003
C	-2.75153	3.153285	-2.93992
H	-1.21485	2.601481	-4.34355
C	-3.25507	2.957146	-1.65342
H	-3.04447	1.927666	0.218504
H	-3.24316	3.831844	-3.62774
H	-4.14793	3.488603	-1.33948
C	0.64944	1.540744	0.900392
N	1.717009	2.374734	0.716783
N	0.074003	1.982662	2.116823
C	1.841929	3.272801	1.763155
C	2.652247	2.287869	-0.39328
C	-1.04555	1.36863	2.555792
C	0.826185	3.042758	2.647648
H	2.622584	4.014492	1.785866
H	2.984313	3.303015	-0.63257
H	2.115062	1.902634	-1.25673
C	-1.52983	0.264338	1.667257
C	-1.71598	1.721871	3.785491
H	0.561182	3.551668	3.555661
C	-2.67299	-0.38954	2.091577
C	-2.83461	1.019826	4.120463
H	-1.34793	2.523861	4.414003
C	-3.33914	-0.04334	3.286655
H	-3.06992	-1.19321	1.482295
H	-3.36515	1.265332	5.035017
H	-4.23556	-0.57067	3.589996
C	0.637355	-1.57865	0.910625
N	1.708113	-1.80009	1.719271
N	0.117466	-2.82389	0.681284
C	1.859512	-3.16166	1.975375
C	2.61119	-0.77079	2.217755
C	-1.03888	-2.91474	-0.15181
C	0.855786	-3.80256	1.324947
H	2.640491	-3.54506	2.609701
H	2.910108	-1.04976	3.232738
H	2.053427	0.160941	2.272261
C	-1.48145	-1.67054	-0.64108

C	-1.65549	-4.1296	-0.43563
H	0.607396	-4.848	1.286393
C	-2.61337	-1.71677	-1.46488
C	-2.78135	-4.12738	-1.25818
H	-1.28388	-5.06327	-0.02655
C	-3.25587	-2.91922	-1.77038
H	-3.00621	-0.7892	-1.86689
H	-3.28205	-5.06033	-1.49094
H	-4.13458	-2.9146	-2.40763
C	3.893775	-0.84057	-1.12218
H	4.596341	-1.64794	-0.86896
H	4.377415	-0.24005	-1.90151
C	3.889474	1.423678	-0.09493
H	4.34795	1.800591	0.826294
C	3.869253	-0.59673	1.351759
H	4.338506	-1.58011	1.229282
H	4.611571	1.609319	-0.90392
H	4.573905	0.016891	1.931074
N	3.652321	-0.00491	0.041879

#### Ir-C

Ir	-0.4023	0.008127	0.001166
C	0.62612	-0.01531	1.792257
N	1.768528	0.494365	2.327597
N	0.121982	-0.82902	2.767524
C	1.9684	0.00519	3.6176
C	2.670871	1.421318	1.652554
C	-1.06696	-1.55666	2.462059
C	0.932711	-0.82755	3.890556
H	2.806242	0.302839	4.224411
H	2.835974	2.259405	2.335902
H	2.141226	1.813091	0.792774
C	-1.53393	-1.34366	1.150536
C	-1.68942	-2.38667	3.388859
H	0.709591	-1.39417	4.776755
C	-2.7045	-2.03483	0.811863
C	-2.84873	-3.05957	3.005202
H	-1.29512	-2.51091	4.391962
C	-3.35153	-2.8804	1.716009
H	-3.12583	-1.89533	-0.17774



H	-3.35355	-3.71127	3.709226
H	-4.25665	-3.39895	1.415942
C	0.629982	-1.52677	-0.89677
N	1.773681	-2.26114	-0.7533
N	0.071442	-1.98771	-2.11058
C	1.939183	-3.14541	-1.80538
C	2.686651	-2.14411	0.376221
C	-1.0698	-1.4119	-2.54636
C	0.885611	-2.99077	-2.66195
H	2.772215	-3.82627	-1.85262
H	2.862068	-3.15621	0.753064
H	2.161228	-1.60439	1.155007
C	-1.57396	-0.30457	-1.66825
C	-1.74211	-1.80112	-3.76397
H	0.648397	-3.49936	-3.57787
C	-2.73211	0.318747	-2.09735
C	-2.87663	-1.12854	-4.1028
H	-1.36426	-2.61016	-4.37741
C	-3.39606	-0.05882	-3.28387
H	-3.14313	1.123628	-1.49903
H	-3.41032	-1.40237	-5.00735
H	-4.30282	0.447488	-3.59217
C	0.614838	1.56473	-0.89172
N	1.756853	1.777764	-1.59854
N	0.089791	2.812337	-0.69803
C	1.938008	3.137372	-1.84221
C	2.661464	0.726519	-2.05551
C	-1.09728	2.911146	0.089623
C	0.889344	3.785443	-1.27377
H	2.772066	3.516436	-2.40754
H	2.813838	0.88009	-3.12758
H	2.132091	-0.21193	-1.93656
C	-1.54713	1.673553	0.590154
C	-1.72968	4.127214	0.32879
H	0.651571	4.833739	-1.24587
C	-2.70293	1.729546	1.37939
C	-2.87929	4.134491	1.11784
H	-1.35155	5.054274	-0.08925
C	-3.36067	2.934173	1.641551
H	-3.10175	0.808206	1.789383

H	-3.39226	5.06866	1.316503
H	-4.25661	2.937081	2.254333
C	4.04867	0.858017	1.264024
H	4.691701	1.741331	1.171471
H	4.444295	0.299844	2.121358
C	4.324867	0.013024	-0.01213
C	4.060299	-1.51631	0.081179
H	4.455736	-1.97618	-0.83258
C	4.043324	0.692208	-1.38178
H	4.427807	1.718341	-1.329
H	4.708041	-1.87381	0.890798
H	4.690745	0.17607	-2.10014
H	5.424256	0.020239	-0.01346

Ir-Ph

Ir	-0.87182	0.086923	0.048151
C	0.306396	0.495488	1.720771
N	1.266514	1.391878	2.082717
N	-0.14205	-0.02437	2.905213
C	1.397035	1.438534	3.467284
C	1.809766	2.377235	1.144686
C	-1.3403	-0.79731	2.874517
C	0.518576	0.544278	3.983154
H	2.09236	2.091371	3.963877
H	1.089951	3.196997	1.059878
H	1.844743	1.880352	0.177502
C	-1.9701	-0.81712	1.615318
C	-1.83916	-1.43609	4.00625
H	0.305873	0.285875	5.004962
C	-3.17979	-1.52131	1.559935
C	-3.04779	-2.1239	3.904705
H	-1.3088	-1.40357	4.952345
C	-3.71725	-2.15875	2.681057
H	-3.71713	-1.56619	0.618894
H	-3.45966	-2.6243	4.773823
H	-4.66296	-2.68539	2.600824
C	-0.4987	-1.91632	-0.43942
N	0.241506	-2.96668	0.000453
N	-1.3872	-2.47186	-1.31848

C	-0.19238	-4.15668	-0.57886
C	1.364007	-2.85318	0.928902
C	-2.37114	-1.62079	-1.89786
C	-1.21714	-3.84296	-1.40855
H	0.259755	-5.10733	-0.3579
H	1.039388	-3.16027	1.927679
H	1.60224	-1.79145	0.975189
C	-2.34684	-0.30758	-1.39422
C	-3.26986	-2.07053	-2.86084
H	-1.82984	-4.47182	-2.029
C	-3.31778	0.555615	-1.91814
C	-4.21423	-1.17461	-3.35983
H	-3.24701	-3.09325	-3.22182
C	-4.23506	0.136925	-2.88422
H	-3.36909	1.574623	-1.55045
H	-4.92751	-1.50186	-4.10776
H	-4.97588	0.834308	-3.26204
C	0.155429	1.088682	-1.43004
N	0.969663	0.848891	-2.50526
N	-0.19987	2.453117	-1.56198
C	1.134315	1.985942	-3.26924
C	1.430839	-0.49705	-2.83708
C	-1.07091	2.974866	-0.67124
C	0.4333	3.004754	-2.68345
H	1.73555	1.999741	-4.16128
H	0.644922	-1.0099	-3.40166
H	1.530391	-1.01665	-1.88503
C	-1.59003	1.995011	0.325046
C	-1.44484	4.369398	-0.64502
H	0.307459	4.028316	-2.9845
C	-2.46065	2.498098	1.273872
C	-2.30658	4.778273	0.331251
H	-1.06174	5.064682	-1.38227
C	-2.83368	3.860681	1.304453
H	-2.87703	1.820024	2.010698
H	-2.60929	5.819765	0.373457
H	-3.5234	4.225306	2.056188
C	3.184228	2.928507	1.519129
C	2.574021	-3.67728	0.456235
C	2.74641	-0.5582	-3.61635

C	4.104599	-1.43094	-0.98653
C	4.119663	-1.68313	0.387035
C	4.191567	-0.60049	1.264113
C	4.254345	0.712188	0.796659
C	4.214665	0.932223	-0.58205
C	4.120342	-0.12627	-1.48582
H	4.029248	-2.26345	-1.67943
H	4.163844	-0.7808	2.33453
H	4.213029	1.948861	-0.96245
C	3.957959	0.14772	-2.9656
C	3.92386	-3.08989	0.910986
C	4.27588	1.866284	1.772908
H	4.168656	1.463923	2.783233
H	5.252742	2.362086	1.745089
H	3.113721	3.581133	2.395468
H	3.48075	3.580659	0.69179
H	3.984224	-3.08779	2.003778
H	4.726117	-3.74505	0.554891
H	2.489554	-4.71283	0.800632
H	2.559946	-3.71164	-0.63648
H	4.859859	-0.16101	-3.50682
H	3.869672	1.227265	-3.10863
H	2.610622	-0.1604	-4.62756
H	2.966876	-1.62225	-3.74948

#### Ir-N-CN

Ir	-0.03205	-0.05585	-0.35989
C	0.944867	1.522185	0.546415
N	1.853606	1.700605	1.551199
N	0.686451	2.773138	0.068141
C	2.151362	3.035003	1.707548
C	2.392819	0.649446	2.412985
C	-0.26342	2.879703	-1.00418
C	1.424245	3.725283	0.779649
H	2.855123	3.401469	2.435337
H	3.41751	0.929032	2.67079
H	2.438567	-0.26601	1.833013
C	-0.79225	1.637369	-1.39811
C	-0.6098	4.094194	-1.5917
C	-1.72625	1.678128	-2.44021

C	-1.54146	4.085469	-2.62728
H	-0.17383	5.030561	-1.27251
C	-2.09804	2.87853	-3.04767
H	-2.1616	0.751391	-2.79449
H	-1.82297	5.01856	-3.10079
H	-2.81993	2.87101	-3.85758
C	-1.77818	-0.07695	0.730495
N	-2.29779	0.526066	1.840537
N	-2.79471	-0.84259	0.232033
C	-3.60226	0.1363	2.046335
C	-1.57478	1.442952	2.718861
C	-2.53308	-1.55738	-0.98478
C	-3.93145	-0.72567	1.03902
H	-4.20577	0.496823	2.861847
H	-2.29801	2.164842	3.10757
H	-0.85724	1.985323	2.109431
C	-1.23772	-1.33451	-1.49265
C	-3.46976	-2.38191	-1.60166
C	-0.9235	-1.98649	-2.69035
C	-3.11127	-3.01701	-2.78956
H	-4.45724	-2.53663	-1.18962
C	-1.84133	-2.81867	-3.33104
H	0.055419	-1.83293	-3.12896
H	-3.82763	-3.66022	-3.2869
H	-1.56742	-3.31217	-4.25739
C	0.972196	-1.56959	0.480558
N	0.81979	-2.40865	1.535085
N	2.192117	-1.92168	-0.12158
C	1.917613	-3.25853	1.713417
C	-0.26249	-2.35886	2.504511
C	2.53224	-1.23432	-1.30464
C	2.830001	-2.94248	0.584155
H	1.762623	-4.24804	2.12867
H	-0.48286	-3.38799	2.806306
H	-1.14446	-1.95919	2.013422
C	1.600335	-0.23264	-1.66601
C	3.681368	-1.51687	-2.0502
C	1.884971	0.489831	-2.82452
C	3.922	-0.77184	-3.20099
H	4.370709	-2.29517	-1.75432

C	3.028466	0.228284	-3.587
H	1.199103	1.264565	-3.14662
H	4.805936	-0.97686	-3.79364
H	3.21984	0.80431	-4.48625
C	1.584413	0.450712	3.706252
H	2.189404	-0.19637	4.355302
H	1.511909	1.420156	4.21264
C	-0.87621	0.740912	3.894842
H	-1.62589	0.145977	4.428922
C	0.098517	-1.54126	3.755723
H	1.032433	-1.94842	4.157582
H	-0.55693	1.531438	4.587849
H	-0.67976	-1.73178	4.506899
N	0.250741	-0.10716	3.543585
C	-5.17832	-1.36057	0.855149
N	-6.21428	-1.86287	0.749932
C	4.075734	-3.47489	0.368282
N	5.12622	-3.98535	0.238043
C	1.428865	5.123212	0.586019
N	1.460735	6.273442	0.474351

Ir-N-F

Ir	0.081614	0.038705	-0.39318
C	-0.59225	1.702575	0.574827
N	-0.38067	2.422402	1.73862
N	-1.63344	2.390988	-0.0938
C	-1.24421	3.50091	1.808028
C	0.650657	2.130679	2.716332
C	-2.10822	1.865775	-1.30025
C	-1.9978	3.469769	0.677391
H	-1.23971	4.219788	2.608726
H	1.063712	3.078729	3.077945
H	1.447906	1.595625	2.205948
C	-1.46592	0.648849	-1.67715
C	-3.14078	2.448982	-2.05805
C	-1.93765	0.032163	-2.834
C	-3.55785	1.801393	-3.21283
H	-3.59785	3.382	-1.75724
C	-2.96577	0.592868	-3.60491
H	-1.47856	-0.89596	-3.15663

H	-4.34735	2.240533	-3.81296
H	-3.29546	0.098968	-4.51255
C	-1.31188	-1.27703	0.516858
N	-2.26155	-1.26072	1.480212
N	-1.36412	-2.54385	-0.01483
C	-2.90363	-2.4984	1.581019
C	-2.51057	-0.17153	2.418787
C	-0.43819	-2.86962	-1.05771
C	-2.33124	-3.27534	0.635197
H	-3.70577	-2.70116	2.267563
H	-3.57989	-0.17277	2.648763
H	-2.26896	0.760362	1.916013
C	0.395874	-1.79596	-1.40876
C	-0.37818	-4.13047	-1.64819
C	1.336044	-2.06129	-2.41347
C	0.569113	-4.34687	-2.64669
H	-1.04757	-4.92556	-1.34987
C	1.423318	-3.31204	-3.02601
H	1.999861	-1.26711	-2.73453
H	0.633095	-5.31803	-3.12378
H	2.157191	-3.47787	-3.80807
C	1.740733	-0.35512	0.765192
N	2.111288	-1.06345	1.866316
N	2.905463	0.269163	0.323636
C	3.472171	-0.89932	2.135431
C	1.209795	-1.86532	2.679344
C	2.833339	0.997944	-0.87229
C	3.945585	-0.08511	1.16417
H	3.978916	-1.37367	2.956601
H	1.758936	-2.74792	3.023469
H	0.402675	-2.20531	2.033102
C	1.508016	1.018753	-1.45088
C	3.927475	1.635012	-1.46806
C	1.371215	1.730846	-2.6564
C	3.722501	2.325336	-2.65605
H	4.91114	1.596128	-1.02011
C	2.444244	2.387619	-3.25079
H	0.396865	1.756403	-3.12925
H	4.56335	2.819053	-3.13105
H	2.306363	2.937659	-4.17445

C	0.149549	1.313794	3.918328
H	0.96629	1.291781	4.654215
H	-0.67797	1.86245	4.384685
C	-1.70803	-0.31376	3.723632
H	-1.85177	-1.33248	4.102152
C	0.639841	-1.12674	3.904119
H	1.4808	-0.73965	4.490613
H	-2.1691	0.362494	4.458395
H	0.147161	-1.8868	4.528269
N	-0.28464	-0.04164	3.61553
F	-2.60519	-4.53331	0.310354
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F	-2.94841	4.32181	0.298432

Ir-N-Ph

Ir	-0.00698	-0.06296	-0.29754
C	-0.20854	1.764314	0.622387
N	0.353196	2.442018	1.655737
N	-1.08002	2.653675	0.044884
C	-0.15696	3.734018	1.726616
C	1.363525	1.914837	2.565143
C	-1.85914	2.153857	-1.0546
C	-1.04476	3.88809	0.707636
H	0.202004	4.461692	2.434358
H	2.016817	2.745225	2.849106
H	1.960775	1.192027	2.01601
C	-1.4883	0.854836	-1.45893
C	-2.91439	2.855359	-1.63479
C	-2.19318	0.314591	-2.53985
C	-3.59918	2.27446	-2.70182
H	-3.21475	3.827416	-1.27268
C	-3.22983	1.011423	-3.1621
H	-1.92633	-0.67543	-2.89201
H	-4.41955	2.811478	-3.16447
H	-3.75958	0.563973	-3.99688
C	-1.40245	-1.13656	0.665423
N	-2.21633	-0.98107	1.755774
N	-1.72672	-2.37431	0.130104
C	-2.99466	-2.10629	1.988703
C	-2.22525	0.171653	2.641323



C	-0.86077	-2.84877	-0.89808
C	-2.83024	-2.95027	0.783904
H	-3.90177	-2.02197	2.570045
H	-3.25996	0.335703	2.959687
H	-1.90797	1.038793	2.068883
C	0.030615	-1.86682	-1.37868
C	-0.82225	-4.17991	-1.31396
C	0.899289	-2.26763	-2.39795
C	0.072645	-4.54108	-2.32115
H	-1.46642	-4.92483	-0.86611
C	0.914468	-3.58062	-2.87974
H	1.58765	-1.54116	-2.81609
H	0.106056	-5.56964	-2.66283
H	1.596786	-3.85762	-3.67727
C	1.699283	-0.74336	0.629982
N	2.010311	-1.52914	1.6911
N	2.901635	-0.42421	0.055006
C	3.386593	-1.70591	1.777806
C	1.060089	-2.09648	2.639184
C	2.852543	0.496742	-1.04771
C	3.959236	-1.03364	0.743231
H	3.84225	-2.35518	2.505854
H	1.448904	-3.06821	2.956867
H	0.124357	-2.26837	2.114944
C	1.539772	0.807503	-1.45428
C	3.987239	1.068915	-1.62036
C	1.426931	1.695525	-2.53136
C	3.826614	1.953283	-2.6862
H	4.978909	0.84905	-1.25362
C	2.547083	2.255051	-3.14866
H	0.438468	1.954838	-2.89328
H	4.700537	2.40151	-3.14531
H	2.42094	2.934557	-3.98574
C	0.783836	1.274682	3.837908
H	1.622236	1.14357	4.537599
H	0.100683	1.995879	4.301414
C	-1.34296	-0.0107	3.888539
H	-1.61569	-0.96398	4.354426
C	0.832431	-1.21473	3.879081
H	1.810961	-0.96915	4.307524

H	-1.62076	0.780758	4.599675
H	0.311843	-1.83753	4.620683
N	0.090097	0.013172	3.649863
C	5.371493	-1.0862	0.329977
C	5.720642	-1.61903	-0.91925
C	6.383654	-0.66936	1.20081
C	7.056807	-1.72094	-1.28956
H	4.938489	-1.94426	-1.59533
C	7.723433	-0.77964	0.830002
H	6.115292	-0.24754	2.162791
C	8.062455	-1.3018	-0.41618
H	7.315286	-2.13207	-2.25873
H	8.49956	-0.44984	1.511404
H	9.103532	-1.38226	-0.70751
C	-1.69843	5.139286	0.287412
C	-2.55129	5.824409	1.159127
C	-1.42251	5.690258	-0.97225
C	-3.12214	7.038648	0.778809
H	-2.77529	5.395122	2.129067
C	-1.99872	6.89723	-1.35197
H	-0.76237	5.161734	-1.65005
C	-2.85033	7.575387	-0.47758
H	-3.78527	7.558604	1.460967
H	-1.78069	7.312123	-2.32945
H	-3.29899	8.516021	-0.77605
C	-3.78386	-3.84582	0.298817
C	-3.92947	-4.20345	-1.08831
C	-4.75281	-4.39629	1.216067
C	-4.91888	-5.06861	-1.49408
H	-3.27981	-3.75123	-1.82356
C	-5.72857	-5.27035	0.7827
H	-4.68788	-4.15118	2.269393
C	-5.82517	-5.63026	-0.5707
H	-5.0142	-5.30464	-2.54862
H	-6.42983	-5.68322	1.50028
H	-6.59693	-6.313	-0.90478

HB-Ir

C	-0.05245	-3.4138	3.224698
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C	1.054377	-4.0989	2.733624
H	-0.57627	-3.79668	4.092067
H	-1.30804	-1.66588	2.972711
H	1.400931	-5.01294	3.204997
C	3.128998	-2.58103	-0.75252
C	3.341948	-1.67647	-1.81537
C	1.537761	-0.92931	-0.65597
N	2.354152	-0.70165	-1.72463
N	2.007938	-2.09493	-0.06043
Ir	-0.02245	-0.02791	0.352666
C	1.384586	0.958606	1.488841
C	1.671455	2.278899	1.053337
C	2.10777	0.526774	2.605763
C	3.074219	1.376678	3.179979
H	1.918987	-0.45176	3.027926
C	3.258629	2.652601	2.657531
H	3.658781	1.063184	4.036413
H	3.976596	3.33655	3.098806
C	0.811178	3.975045	-0.66103
C	-0.23002	3.839859	-1.60006
N	-0.68969	2.526864	-1.50948
N	0.925542	2.716058	-0.04121
C	0.003734	1.826807	-0.57229
C	-1.62265	0.667468	1.51042
C	-2.89445	0.223117	1.108178
C	-1.63584	1.503083	2.628145
C	-2.84214	1.840165	3.253262
H	-0.6995	1.883293	3.021439
C	-4.02943	1.329308	2.748916
H	-2.86005	2.484153	4.124511
H	-4.98811	1.557386	3.201029
C	-3.92457	-1.32867	-0.6843
C	-3.28168	-2.07229	-1.68532
C	-1.67241	-0.92198	-0.57312
N	-1.91372	-1.79468	-1.57787
N	-2.89354	-0.63373	-0.02111
C	-3.9608	-2.8979	-2.574

C	-5.32382	-1.38845	-0.5328
C	1.503386	5.196358	-0.52096
C	-0.63525	4.880276	-2.42765
C	3.978184	-3.69591	-0.57103
C	4.38309	-1.82242	-2.72438
C	-5.34535	-2.95358	-2.41946
H	-5.92878	-3.58268	-3.08151
C	-6.00547	-2.22139	-1.43098
H	-7.08187	-2.27977	-1.32769
H	-3.44462	-3.46676	-3.33549
C	5.215425	-2.92962	-2.54033
H	6.04368	-3.0851	-3.2221
C	5.020702	-3.83931	-1.50232
H	5.68134	-4.68759	-1.37616
H	4.550344	-1.11282	-3.52328
C	0.055148	6.086774	-2.28558
H	-0.2248	6.931191	-2.90482
C	1.091134	6.241593	-1.36603
H	1.610612	7.186594	-1.26966
H	-1.44643	4.767711	-3.13425
C	-0.91062	-2.41515	-2.42768
H	0.062711	-2.01518	-2.16169
H	-0.91204	-3.49687	-2.27739
H	-1.12481	-2.19885	-3.47706
C	2.303428	0.479045	-2.56762
H	1.311165	0.917577	-2.49388
H	3.041258	1.218394	-2.24422
H	2.50278	0.200614	-3.60385
C	-1.78504	1.998905	-2.30253
H	-1.77225	0.914535	-2.23528
H	-2.7446	2.369405	-1.93309
H	-1.66313	2.297775	-3.3457
O	2.501851	5.414254	0.334762
H	2.640702	4.586781	0.908064
N	2.564666	3.130056	1.611862
O	3.855335	-4.59595	0.403142
H	3.060305	-4.35477	0.989858
O	-6.02649	-0.71485	0.387079
H	-5.39677	-0.18933	0.964656
N	1.760695	-3.68446	1.67303

N	-4.05843	0.518699	1.677755
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HB-Ir-  
CN

C	2.124429	-2.66891	3.54436
C	1.086978	-1.9644	2.922991
C	1.330995	-1.17446	1.798932
C	2.673759	-1.17464	1.382703
C	3.408171	-2.57511	3.026685
H	1.940816	-3.27978	4.420152
H	0.081489	-2.02471	3.324962
H	4.245934	-3.09892	3.472423
C	4.13312	-0.05214	-0.43
C	3.756593	0.839823	-1.44663
C	1.869249	0.27817	-0.3206
N	2.372153	1.007266	-1.34451
N	2.940732	-0.37333	0.239762
Ir	0.048738	0.007746	0.639329
C	0.434466	1.694878	1.746837
C	-0.31049	2.870161	1.304516
C	1.259924	1.896765	2.841907
C	1.34336	3.185686	3.4312
H	1.839871	1.077107	3.245474
C	0.574487	4.247385	2.911401
H	1.985645	3.374623	4.282118
H	0.633388	5.231145	3.3691
C	-2.03681	3.508368	-0.43115
C	-2.64334	2.701319	-1.42488
N	-2.06581	1.442031	-1.34135
N	-1.11865	2.677536	0.231994
C	-1.12908	1.385897	-0.35112
C	-1.63849	-0.44159	1.792403
C	-2.34134	-1.59317	1.398015
C	-2.19076	0.208084	2.897828
C	-3.348	-0.28254	3.513217
H	-1.71147	1.099097	3.289316
C	-3.9433	-1.43178	3.013726
H	-3.78019	0.217868	4.371491
H	-4.83928	-1.85211	3.455732
C	-2.1288	-3.47581	-0.35814
C	-1.14687	-3.66282	-1.34315

C	-0.64429	-1.7331	-0.2587
N	-0.26798	-2.57846	-1.24778
N	-1.77949	-2.27743	0.287753
C	-1.13485	-4.74441	-2.21008
C	-3.17969	-4.40165	-0.20254
C	-2.40546	4.863223	-0.26949
C	-3.6204	3.182977	-2.27683
C	5.480075	-0.43554	-0.27046
C	4.655767	1.398422	-2.3416
C	-2.18151	-5.66399	-2.05358
C	-3.17481	-5.49493	-1.07708
H	-3.97153	-6.22016	-0.9777
H	-0.36883	-4.88301	-2.95952
C	5.994742	1.016638	-2.17953
C	6.392946	0.124381	-1.17202
H	7.433542	-0.1534	-1.0692
H	4.354351	2.089094	-3.11602
C	-3.9826	4.534302	-2.11587
C	-3.39341	5.352899	-1.14366
H	-3.69153	6.386841	-1.03731
H	-4.09744	2.566541	-3.02523
C	0.906283	-2.43334	-2.09379
H	1.325351	-1.44471	-1.93885
H	1.653443	-3.1881	-1.83905
H	0.622502	-2.54786	-3.1419
C	1.609362	1.897912	-2.20541
H	0.55538	1.769615	-1.97623
H	1.89742	2.935533	-2.02309
H	1.794617	1.651561	-3.25305
C	-2.45943	0.299706	-2.14858
H	-1.60596	-0.36657	-2.24996
H	-3.28249	-0.24479	-1.67869
H	-2.767	0.637282	-3.13814
O	-1.89314	5.687573	0.630185
H	-1.20239	5.19045	1.206461
N	-0.2479	4.139107	1.879846
O	5.933154	-1.27902	0.659569
H	5.166915	-1.58324	1.235943
O	-4.15912	-4.30672	0.699514
H	-4.01451	-3.48641	1.263178

N	3.683917	-1.82834	1.944259
N	-3.43882	-2.08965	1.956216
C	-2.23664	-6.80562	-2.91509
N	-2.27378	-7.72306	-3.61643
C	-4.98676	5.080762	-2.97484
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C	6.98175	1.551741	-3.06725
N	7.771614	1.98737	-3.78927

Pt-Ref

C	-2.16439	-1.96632	-0.0432
C	-1.98436	-3.34411	0.068333
C	-3.4982	-1.53674	-0.23827
N	-3.59945	-0.13221	-0.36531
C	-3.05272	-4.25217	0.018303
C	-4.58352	-2.40411	-0.29121
C	-4.34555	-3.77523	-0.15854
H	-2.84679	-5.3109	0.113362
H	-5.5936	-2.03551	-0.42522
H	-5.17513	-4.47083	-0.19683
Pt	-0.79236	-0.54829	0.23266
C	0.663109	-1.92395	0.28323
C	0.462863	-3.34613	0.19095
C	1.998171	-1.55286	0.165615
C	1.516923	-4.28245	-0.00127
C	3.057883	-2.44233	-0.14543
C	2.79972	-3.85031	-0.19745
H	1.257486	-5.33284	-0.04743
H	3.600643	-4.54827	-0.40644
O	-0.7523	-3.93855	0.219298
C	0.074527	1.970471	1.684595
C	1.956853	0.841533	0.896928
C	0.834734	2.908302	2.332927
H	-1.00341	2.005208	1.731697
C	2.780565	1.721025	1.592796
C	2.236917	2.786615	2.309728
H	0.341316	3.705986	2.873514
H	3.846726	1.549445	1.601027
H	2.875877	3.461876	2.863818
N	0.590735	0.934488	0.944987

C	-4.65212	0.6759	-0.76368
C	-4.15371	1.932289	-0.87966
H	-4.6234	2.84963	-1.18859
H	-5.64263	0.301144	-0.95013
N	2.512419	-0.22888	0.165751
C	4.203412	-1.66817	-0.43715
C	3.833723	-0.29203	-0.28334
C	5.499288	-1.99725	-0.8931
C	6.376765	-0.9789	-1.20445
C	5.981742	0.375158	-1.09395
C	4.714661	0.729273	-0.6382
H	4.42071	1.768702	-0.58221
H	6.675342	1.155795	-1.38383
H	7.37431	-1.21241	-1.55818
H	5.788112	-3.03572	-1.00709
N	-2.80096	1.872934	-0.55324
C	-2.4451	0.597427	-0.20595
C	-1.88884	2.964323	-0.65115
C	-0.68809	2.798202	-1.33986
C	-2.18001	4.17669	-0.03098
C	0.228078	3.840551	-1.37665
H	-0.47034	1.847445	-1.80885
C	-1.25886	5.220395	-0.09447
H	-3.10768	4.293585	0.517749
C	-0.03603	5.066144	-0.75202
H	1.168429	3.698004	-1.89859
H	-1.48849	6.159773	0.39725
C	0.994462	6.167254	-0.75968
H	0.556268	7.130475	-0.49003
H	1.791814	5.949868	-0.04116
H	1.460519	6.269058	-1.7434

Pt-Iso

C	-3.55624	0.343698	-0.08535
C	-4.21488	1.546044	-0.33633
C	-4.38125	-0.77543	0.166293
N	-3.63362	-1.9545	0.420257
C	-5.61475	1.640663	-0.35212
C	-5.77099	-0.72148	0.155625
C	-6.38182	0.507808	-0.10729



H	-6.07323	2.60105	-0.55241
H	-6.37172	-1.60464	0.338045
H	-7.46285	0.578495	-0.1201
Pt	-1.60018	-0.00135	-0.2327
C	-1.23663	1.960503	-0.40979
C	-2.24165	2.995843	-0.50556
C	0.038499	2.453298	-0.22707
C	-1.9381	4.383816	-0.46414
C	0.38061	3.826994	-0.08344
C	-0.65662	4.817187	-0.24553
H	-2.76051	5.08283	-0.55807
H	-0.42731	5.871787	-0.16355
O	-3.57006	2.740461	-0.58435
C	0.70028	-1.56311	-1.47678
C	1.46102	0.488586	-0.71
C	1.913545	-1.87244	-2.03413
H	-0.13179	-2.24869	-1.5449
C	2.693536	0.26458	-1.33022
C	2.961807	-0.92648	-1.98946
H	2.037112	-2.83098	-2.52134
H	3.439256	1.046882	-1.28961
N	0.441806	-0.40675	-0.80308
C	-4.00659	-3.19226	0.921677
C	-2.86023	-3.88266	1.148279
H	-2.69927	-4.86602	1.554262
H	-5.03099	-3.47204	1.092091
N	1.218076	1.679451	-0.01272
C	1.727016	3.905067	0.311858
C	2.221967	2.556836	0.445302
C	2.552213	4.994706	0.691433
C	3.795108	4.718845	1.219382
C	4.216506	3.388083	1.43457
C	3.427936	2.273939	1.086592
H	5.166031	3.221299	1.929502
H	4.449455	5.530802	1.516692
H	2.198963	6.013273	0.583818
N	-1.80063	-3.05232	0.78379
C	-2.26924	-1.85966	0.307196
C	-0.41543	-3.3245	0.992992
C	0.366304	-2.39103	1.672686

C	0.165521	-4.48087	0.477104
C	1.731782	-2.60646	1.805012
H	-0.09358	-1.48898	2.054988
C	1.534357	-4.69164	0.633621
H	-0.44269	-5.19183	-0.07065
C	2.341471	-3.75486	1.285697
H	2.335114	-1.86422	2.316559
H	1.983257	-5.58662	0.215591
C	3.825336	-3.97433	1.443757
H	4.222231	-4.61471	0.65311
H	4.368119	-3.02672	1.414334
H	4.050305	-4.45284	2.403033
C	4.307952	-1.19184	-2.62865
C	4.183815	-1.50219	-4.13079
C	5.048566	-2.32294	-1.88931
H	4.904957	-0.27872	-2.52438
H	3.675356	-0.69208	-4.65914
H	5.172899	-1.63796	-4.57791
H	3.613846	-2.42079	-4.29758
H	5.190323	-2.07513	-0.83495
H	4.481855	-3.25749	-1.94052
H	6.031404	-2.49905	-2.33651
C	3.828934	0.880757	1.5574
C	3.725004	0.7931	3.09294
C	5.227634	0.457541	1.08016
H	3.116318	0.163477	1.151338
H	2.719495	1.054962	3.43154
H	3.949411	-0.22292	3.434585
H	4.430431	1.472644	3.578779
H	5.30689	0.48585	-0.00837
H	6.003374	1.110061	1.489756
H	5.448621	-0.5629	1.407896

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C	2.202384	-1.42477	0.044002
C	3.54672	-1.06783	0.075822
C	1.94174	-2.81185	0.031785
N	0.554266	-3.10159	-0.0411
C	4.578408	-2.01476	0.123313
C	2.932479	-3.78461	0.080348

C	4.26568	-3.36868	0.129058
H	5.605153	-1.67137	0.150158
H	2.687771	-4.84015	0.0862
H	5.059141	-4.10513	0.167784
Pt	0.626368	-0.20863	0.19975
C	1.8106	1.404114	0.034756
C	3.244145	1.359194	-0.10492
C	1.284792	2.665595	-0.19021
C	4.038952	2.486339	-0.45764
C	2.029915	3.795131	-0.65534
C	3.456083	3.684568	-0.75965
H	5.110126	2.343087	-0.52835
H	4.048524	4.532458	-1.08095
O	3.98803	0.239421	0.045455
C	-2.01315	0.498503	1.524199
C	-1.12074	2.416696	0.541624
C	-3.10593	1.171962	1.996225
H	-1.8866	-0.55292	1.735426
C	-2.19114	3.166054	1.032159
C	-3.21656	2.562393	1.745789
H	-3.85135	0.635403	2.56865
H	-4.03143	3.150075	2.147854
N	-1.01793	1.058124	0.763261
C	-0.11455	-4.28568	-0.30325
C	-1.42192	-3.96346	-0.46209
H	-2.275	-4.57353	-0.70179
H	0.381451	-5.23717	-0.37426
N	-0.08046	3.057994	-0.15765
C	1.128386	4.810075	-0.9686
C	-0.16031	4.324567	-0.6816
N	-1.52795	-2.58283	-0.29697
C	-0.30832	-2.03597	-0.0147
C	-2.72135	-1.83027	-0.51415
C	-2.68981	-0.72311	-1.36005
C	-3.90035	-2.18711	0.133587
C	-3.83681	0.041136	-1.52579
H	-1.76267	-0.45342	-1.84884
C	-5.04818	-1.42096	-0.05814
H	-3.91246	-3.03976	0.803017
C	-5.03207	-0.28765	-0.87489

H	-3.8002	0.915185	-2.16721
H	-5.96162	-1.69721	0.457812
C	-6.24945	0.590169	-1.02115
H	-7.15782	0.07667	-0.69907
H	-6.14127	1.493676	-0.41192
H	-6.38798	0.90972	-2.05739
H	-2.19665	4.238564	0.894042
H	-1.10964	4.813335	-0.8128
H	1.348099	5.779575	-1.38836

Pt-HB

C	2.531294	-1.08647	0.045606
C	3.782183	-0.47705	0.064919
C	2.531662	-2.49432	0.027454
N	1.218151	-3.04254	-0.03541
C	4.969766	-1.22141	0.09618
C	3.684236	-3.26844	0.057011
C	4.915617	-2.60894	0.095289
H	5.915417	-0.69392	0.116953
H	3.639962	-4.35083	0.05621
H	5.833737	-3.18338	0.120685
Pt	0.753309	-0.1858	0.215738
C	1.597968	1.607048	0.016573
C	3.029019	1.848535	-0.12649
C	0.830306	2.741686	-0.19914
C	3.562871	3.103336	-0.46128
C	1.325216	4.012578	-0.61381
C	2.746492	4.185669	-0.72252
H	4.639955	3.188119	-0.5408
H	3.164406	5.141591	-1.01127
O	3.97412	0.885187	0.049887
C	-1.97531	0.027569	1.516245
C	-1.51266	2.03535	0.418333
C	-3.23655	0.446085	1.873209
H	-1.60767	-0.94516	1.805318
C	-2.83243	2.51242	0.705394
C	-3.68621	1.696418	1.436654
H	-3.86822	-0.20319	2.464259
H	-4.67382	2.072744	1.670422
N	-1.12874	0.772218	0.763624

C	0.784648	-4.32785	-0.31005
C	-0.56176	-4.2571	-0.46079
H	-1.286	-5.01426	-0.70473
H	1.451513	-5.16733	-0.39377
N	-0.57264	2.879707	-0.15626
C	0.220806	4.80984	-0.8408
N	-0.92342	-2.9229	-0.27841
C	0.172113	-2.16304	0.005159
C	-2.23418	-2.39534	-0.49402
C	-2.39745	-1.29707	-1.33777
C	-3.33098	-2.956	0.151825
C	-3.65839	-0.73933	-1.49518
H	-1.53344	-0.86936	-1.82981
C	-4.59369	-2.39534	-0.03054
H	-3.19414	-3.8022	0.815539
C	-4.77554	-1.26996	-0.83876
H	-3.77527	0.132661	-2.12952
H	-5.44418	-2.8266	0.486547
C	-6.12309	-0.60801	-0.97322
H	-6.92429	-1.2401	-0.58514
H	-6.13799	0.335592	-0.41757
H	-6.34867	-0.37323	-2.01679
H	0.162621	5.829577	-1.18679
O	-3.27266	3.717725	0.322967
H	-2.50864	4.180793	-0.13393
N	-0.94632	4.12671	-0.58343

### **<sup>3</sup>MC state**

#### Irpmi

Ir	-0.4834	0.199668	-0.03968
C	0.854616	0.372084	-1.54852
N	1.160572	-0.24048	-2.73103
N	1.731576	1.431408	-1.47247
C	2.202778	0.41716	-3.36237
C	0.580853	-1.49922	-3.16905
C	1.668125	2.240622	-0.30719
C	2.558556	1.468138	-2.57463
H	2.593743	0.09438	-4.31224
H	0.730191	-1.60888	-4.24347
H	-0.48469	-1.49761	-2.9471

C	0.662645	1.824506	0.58736
C	2.543271	3.292187	-0.0645
H	3.309829	2.223597	-2.72107
C	0.596797	2.534877	1.792324
C	2.436256	3.977574	1.146347
H	3.302548	3.57506	-0.78595
C	1.466432	3.592615	2.073854
H	-0.14532	2.247193	2.530152
H	3.107593	4.800945	1.3619
H	1.389344	4.118823	3.019901
C	-1.77226	-1.31934	-0.59668
N	-1.7767	-2.66926	-0.73723
N	-3.08312	-0.95215	-0.76027
C	-3.06529	-3.13353	-0.98583
C	-0.62218	-3.53296	-0.51081
C	-3.39644	0.413455	-0.53481
C	-3.88789	-2.05509	-1.00077
H	-3.28009	-4.17922	-1.12544
H	-0.746	-4.0762	0.428452
H	0.285031	-2.9322	-0.44246
C	-2.29094	1.194461	-0.11657
C	-4.67361	0.932619	-0.69921
H	-4.95003	-1.98825	-1.15518
C	-2.54648	2.552086	0.131775
C	-4.88665	2.28736	-0.43666
H	-5.49622	0.305687	-1.02589
C	-3.8239	3.091781	-0.0224
H	-1.73154	3.190898	0.449152
H	-5.8783	2.707922	-0.55825
H	-3.99182	4.14447	0.179604
H	-0.5291	-4.24582	-1.33351
H	1.055941	-2.32642	-2.63698
C	-0.06697	-0.84902	1.712743
C	1.20252	-1.35926	2.015931
C	-1.08105	-1.07977	2.659336
N	2.300608	-1.18413	1.099742
C	1.45747	-2.05273	3.199332
C	-0.83491	-1.76155	3.849859
H	-2.08221	-0.71003	2.463394
C	2.519138	-1.97827	0.005866

C	3.262182	-0.19032	1.242925
C	0.440125	-2.25374	4.127062
H	2.456343	-2.43625	3.377663
H	-1.64231	-1.91114	4.559668
N	3.657531	-1.43962	-0.51812
C	4.128153	-0.35274	0.215756
H	3.21398	0.552433	2.02037
H	0.638453	-2.79179	5.04694
C	4.320655	-1.96477	-1.69817
H	5.006703	0.20692	-0.0579
H	4.411293	-1.18808	-2.4615
H	3.716663	-2.78401	-2.08432
H	5.316207	-2.34252	-1.44895

Irpmb

C	2.226847	-3.61714	1.485956
C	1.079816	-2.95381	1.042215
C	1.001188	-1.55814	1.008528
C	2.156328	-0.85906	1.413428
C	3.30784	-1.49263	1.868204
C	3.335432	-2.88712	1.906586
H	2.254641	-4.7019	1.502596
H	0.223178	-3.53455	0.715202
H	4.2286	-3.39328	2.254429
C	2.857264	1.626972	1.536845
C	2.089209	2.789268	1.306477
C	0.757447	1.006737	0.9034
N	0.819693	2.373259	0.941456
N	2.002704	0.554762	1.310532
Ir	-0.61044	-0.38654	0.406225
C	-1.99563	-1.13316	1.734144
C	-3.30266	-0.59021	1.628768
C	-1.76301	-2.02948	2.787599
C	-4.31191	-0.90825	2.530273
C	-2.77278	-2.37273	3.686447
H	-0.77539	-2.45615	2.906428
C	-4.0421	-1.8112	3.561171
H	-2.56565	-3.07044	4.490831
H	-4.82608	-2.06422	4.265781
C	-4.58647	0.885644	-0.06474

C	-4.08982	1.575214	-1.18817
N	-2.71149	1.381768	-1.21044
N	-3.4657	0.312006	0.542777
C	-2.32024	0.607203	-0.16692
C	-0.6073	-1.33161	-1.44984
C	0.429063	-1.19512	-2.38483
C	-1.67607	-2.17224	-1.8063
C	0.409528	-1.87317	-3.60501
C	-1.6974	-2.86168	-3.01705
H	-2.49995	-2.3024	-1.11282
C	-0.65046	-2.71459	-3.92614
H	-2.53456	-3.51173	-3.24992
H	-0.66157	-3.24067	-4.87376
C	2.837637	-0.86416	-1.81777
C	3.661064	0.256586	-1.65259
C	1.551412	1.010469	-2.15667
N	2.839137	1.362955	-1.86583
N	1.569988	-0.35933	-2.11799
C	5.006839	0.128138	-1.32137
C	3.325	-2.15561	-1.65515
C	-5.95408	0.87593	0.202501
C	-4.92187	2.272139	-2.05539
C	4.209044	1.737307	1.862386
C	2.629771	4.066202	1.417785
C	5.50011	-1.16659	-1.16324
H	6.542206	-1.31005	-0.90137
C	4.671304	-2.28786	-1.32638
H	5.083142	-3.27827	-1.17392
H	2.672804	-3.01285	-1.75183
H	5.640891	0.99545	-1.18449
C	3.977923	4.166105	1.757883
H	4.434363	5.144455	1.84904
C	4.752041	3.017953	1.969947
H	5.801282	3.122695	2.21962
H	4.833629	0.870344	2.00638
H	2.03143	4.948298	1.228134
C	-6.28792	2.266456	-1.77621
H	-6.96879	2.797583	-2.43052
C	-6.79132	1.576377	-0.66713
H	-7.85821	1.57957	-0.4777



H	-6.37256	0.341103	1.040996
H	-4.52329	2.789797	-2.91886
C	3.326534	2.730403	-1.867
H	2.469972	3.393508	-1.96774
H	3.847726	2.951796	-0.93384
H	4.009513	2.893296	-2.70628
C	-0.24406	3.27018	0.534132
H	-1.18842	2.737611	0.598229
H	-0.27163	4.131977	1.203043
H	-0.08595	3.605486	-0.49412
C	-1.84359	1.841068	-2.28587
H	-0.80487	1.606368	-2.05353
H	-2.1139	1.336896	-3.2168
H	-1.95711	2.920612	-2.41506
H	-5.29233	-0.46034	2.461517
H	4.177368	-0.93902	2.18824
H	1.233072	-1.73026	-4.29636

Ir-N

Ir	0.724065	0.02185	-0.03395
C	-2.75437	-0.90671	1.914624
N	-3.57378	-1.20948	0.868249
N	-1.65948	-1.68228	1.667971
C	-3.01045	-2.14272	-0.00117
C	-4.76931	-0.42965	0.613784
C	-0.44696	-1.52548	2.42911
C	-1.79478	-2.4468	0.512733
H	-3.5064	-2.50396	-0.88669
C	0.608243	-0.75907	1.913343
C	-0.39898	-2.09217	3.702036
H	-1.0235	-3.11088	0.165058
C	1.719879	-0.57582	2.754772
C	0.718032	-1.90551	4.509458
H	-1.25157	-2.66404	4.050283
C	1.778011	-1.13829	4.029588
H	2.558336	0.017759	2.406744
H	0.755784	-2.34524	5.499536
H	2.65473	-0.97236	4.647687
C	0.235388	1.964095	0.505748
N	-0.80998	2.695326	0.980943

N	1.226936	2.887973	0.290345
C	-0.47411	4.046224	1.045519
C	-2.05108	2.139867	1.523033
C	2.47746	2.399309	-0.17409
C	0.804513	4.168377	0.611219
H	-1.16044	4.78946	1.413725
H	-2.22627	2.632566	2.484174
H	-1.89698	1.082901	1.731295
C	2.51348	0.998173	-0.37018
C	3.568251	3.225314	-0.41045
H	1.431665	5.037283	0.521599
C	3.726352	0.460932	-0.82545
C	4.759786	2.650794	-0.85842
H	3.508934	4.296567	-0.25164
C	4.836657	1.272594	-1.06294
H	3.797106	-0.60659	-0.99589
H	5.621447	3.281516	-1.04493
H	5.764189	0.830635	-1.41141
C	-0.45863	-0.24791	-1.65426
N	-1.31642	0.477915	-2.43793
N	-0.31596	-1.44484	-2.32257
C	-1.71367	-0.26652	-3.53824
C	-1.67819	1.873072	-2.23085
C	0.62431	-2.37196	-1.80128
C	-1.08667	-1.47036	-3.46509
H	-2.38351	0.124196	-4.28542
H	-1.51931	2.412503	-3.17064
H	-0.99092	2.27794	-1.49517
C	1.304629	-1.88309	-0.66744
C	0.826211	-3.63374	-2.3508
H	-1.11747	-2.31148	-4.13465
C	2.230164	-2.76632	-0.09637
C	1.765186	-4.47488	-1.75364
H	0.271424	-3.96804	-3.22116
C	2.463902	-4.03762	-0.62719
H	2.767967	-2.45927	0.794346
H	1.943016	-5.4626	-2.16313
H	3.187793	-4.69439	-0.15577
C	-4.61487	0.565645	-0.54765
H	-4.54783	-0.01166	-1.47306

H	-5.55368	1.150214	-0.60039
C	-3.31368	2.308257	0.661164
H	-3.40751	3.359252	0.347525
C	-3.13	2.046669	-1.78097
H	-3.78002	1.618481	-2.54964
H	-4.15215	2.1189	1.33699
H	-3.3486	3.12665	-1.76563
H	-4.998	0.079082	1.549894
H	-5.61298	-1.08827	0.380386
N	-3.42656	1.419977	-0.49952

Ir-C

Ir	0.709712	0.066264	-0.13437
C	-0.77265	-0.39733	-1.43208
N	-1.85099	0.199158	-2.03465
N	-0.71551	-1.65275	-2.00026
C	-2.42368	-0.66225	-2.95989
C	-2.17423	1.619693	-1.94439
C	0.325332	-2.51416	-1.57087
C	-1.71959	-1.82379	-2.92825
H	-3.26601	-0.3783	-3.56704
H	-1.96045	2.056393	-2.92573
H	-1.46717	2.055682	-1.24853
C	1.190956	-1.90131	-0.64444
C	0.444379	-3.83166	-1.99951
H	-1.85292	-2.73188	-3.4888
C	2.211851	-2.71976	-0.14379
C	1.483763	-4.60553	-1.48354
H	-0.25347	-4.26117	-2.71054
C	2.363057	-4.04682	-0.55393
H	2.893793	-2.3147	0.596675
H	1.599505	-5.63554	-1.80102
H	3.165073	-4.65111	-0.14241
C	-2.27737	-0.71864	1.511682
N	-3.14548	-1.30248	0.651222
N	-1.34343	-1.69049	1.716529
C	-2.77577	-2.60993	0.332775
C	-4.3269	-0.63558	0.096528
C	-0.1307	-1.41397	2.439451
C	-1.62527	-2.85243	1.007814

H	-3.33747	-3.23243	-0.34347
H	-5.19305	-1.25856	0.340915
H	-4.23798	-0.63753	-0.99225
C	0.822489	-0.56513	1.859053
C	0.040891	-1.9698	3.704397
H	-0.97425	-3.70952	1.012169
C	1.954267	-0.26321	2.632175
C	1.187235	-1.67904	4.440237
H	-0.73164	-2.61558	4.108179
C	2.138442	-0.81461	3.900982
H	2.715397	0.394674	2.227014
H	1.326713	-2.10919	5.425413
H	3.031104	-0.56816	4.467267
C	0.359883	2.064021	0.309086
N	-0.60405	2.87509	0.822824
N	1.397396	2.910803	0.012423
C	-0.16916	4.198397	0.845475
C	-1.85729	2.412837	1.430857
C	2.572808	2.330493	-0.53193
C	1.086231	4.222562	0.334031
H	-0.78026	4.995432	1.232692
H	-1.81572	2.712037	2.481434
H	-1.85214	1.317985	1.427613
C	2.501552	0.926019	-0.69782
C	3.694308	3.077487	-0.86776
H	1.764759	5.043514	0.185799
C	3.634248	0.305295	-1.24538
C	4.804932	2.419521	-1.40006
H	3.717985	4.152158	-0.72383
C	4.771836	1.037283	-1.58808
H	3.621936	-0.7658	-1.40381
H	5.688248	2.988543	-1.66669
H	5.634494	0.529302	-2.00624
C	-3.62043	1.968724	-1.56736
H	-3.78284	2.966219	-1.99102
H	-4.31262	1.316267	-2.11124
C	-4.06097	2.071896	-0.08576
C	-4.59288	0.780302	0.637743
H	-4.28063	0.797954	1.682861
C	-3.14984	2.975699	0.79416

H	-2.91379	3.880801	0.220761
H	-5.683	0.871583	0.645993
H	-3.78236	3.315519	1.620311
H	-4.96506	2.685903	-0.1725

Ir-Ph

Ir	1.281856	0.050537	-0.14449
C	0.306342	-1.31066	-1.37987
N	-0.78615	-1.36306	-2.18527
N	1.017171	-2.44236	-1.68635
C	-0.75242	-2.50006	-2.98366
C	-1.69833	-0.21357	-2.30458
C	2.325358	-2.53988	-1.14213
C	0.377228	-3.18441	-2.66934
H	-1.52308	-2.72805	-3.69772
H	-1.15015	0.585101	-2.80129
H	-1.89434	0.128954	-1.29175
C	2.74248	-1.3891	-0.43021
C	3.131075	-3.65892	-1.30607
H	0.767412	-4.10689	-3.06084
C	4.039525	-1.41445	0.101666
C	4.417847	-3.64449	-0.76257
H	2.777162	-4.5311	-1.84517
C	4.87008	-2.52417	-0.064
H	4.397894	-0.55074	0.649791
H	5.061488	-4.50778	-0.8878
H	5.872129	-2.51683	0.351782
C	0.74011	-0.40655	1.775716
N	0.144501	-1.4514	2.429822
N	1.408557	0.279289	2.765457
C	0.457633	-1.41971	3.779132
C	-0.61005	-2.50707	1.751748
C	2.269721	1.333146	2.363353
C	1.24387	-0.331	3.990137
H	0.107952	-2.15977	4.476412
H	0.095639	-3.23421	1.337677
H	-1.10596	-2.02441	0.910957
C	2.410115	1.419915	0.964464
C	2.902094	2.177579	3.271038
H	1.699091	0.032822	4.893992

C	3.265559	2.435723	0.512773
C	3.746672	3.16941	2.775047
H	2.746117	2.076949	4.33998
C	3.927139	3.292009	1.39593
H	3.413424	2.565068	-0.55349
H	4.253313	3.840401	3.459185
H	4.582656	4.064479	1.006938
C	-2.32459	2.643291	-0.97428
N	-2.93972	2.87305	0.222142
N	-0.99724	2.664895	-0.63763
C	-2.02736	3.059772	1.262093
C	-4.38979	3.033803	0.286302
C	0.042363	2.562029	-1.62735
C	-0.79442	2.911347	0.71791
H	-2.31786	3.28056	2.275336
C	1.01295	1.552663	-1.58478
C	-0.00417	3.493774	-2.66959
H	0.187885	2.959509	1.155637
C	1.937855	1.528413	-2.64655
C	0.9168	3.440163	-3.70821
H	-0.78384	4.245723	-2.65495
C	1.894685	2.446903	-3.69343
H	2.708963	0.76439	-2.65809
H	0.872678	4.164144	-4.51385
H	2.62462	2.383723	-4.49411
C	-3.00739	-0.43338	-3.05199
C	-1.63006	-3.19168	2.673582
C	-5.1376	2.277799	1.410252
C	-3.90902	-1.39476	1.829013
C	-3.52548	-2.55118	1.156153
C	-3.60086	-2.56209	-0.23696
C	-4.04058	-1.44656	-0.94641
C	-4.39875	-0.28797	-0.24274
C	-4.31813	-0.24114	1.14883
H	-3.83352	-1.35612	2.912163
H	-3.26617	-3.44019	-0.78112
H	-4.67974	0.594861	-0.80169
C	-4.52383	0.999935	1.997057
C	-2.87185	-3.69182	1.907157
C	-3.9936	-1.46423	-2.45659

H	-3.72757	-2.47374	-2.78165
H	-4.98771	-1.26378	-2.87078
H	-2.81856	-0.67701	-4.10327
H	-3.47019	0.557567	-3.04921
H	-2.59042	-4.48228	1.204599
H	-3.56797	-4.14056	2.623586
H	-1.16533	-4.02042	3.216762
H	-1.96643	-2.47321	3.424402
H	-3.54508	1.247278	2.421256
H	-5.14527	0.717237	2.85461
H	-6.14585	2.066223	1.038075
H	-5.2723	2.960274	2.255845
H	-4.73773	2.72385	-0.69741
H	-4.62153	4.100665	0.375195

Ir-N-CN

Ir	0.371644	-0.56939	-0.03521
C	-1.40588	1.65718	2.306058
N	-2.28026	2.434747	1.602655
N	-1.92144	0.412579	2.185068
C	-3.32601	1.705577	1.068742
C	-2.04971	3.865591	1.459555
C	-1.18214	-0.73229	2.660791
C	-3.11472	0.410029	1.444922
H	-4.14088	2.135177	0.509817
C	-0.0626	-1.15687	1.934482
C	-1.56664	-1.32125	3.861738
C	0.705508	-2.18173	2.511053
C	-0.81022	-2.36214	4.391491
H	-2.44687	-0.95298	4.376671
C	0.336555	-2.77798	3.717359
H	1.591707	-2.53728	1.997492
H	-1.10404	-2.8295	5.323872
H	0.947729	-3.57564	4.126957
C	2.069412	0.532042	0.415021
N	2.430204	1.699207	1.036792
N	3.243108	0.023233	-0.08091
C	3.782088	1.919898	0.917574
C	1.544597	2.525022	1.864791
C	3.162604	-1.23268	-0.75861

C	4.312745	0.875415	0.214606
H	4.278431	2.773139	1.347835
H	2.094781	2.765534	2.779362
H	0.674524	1.9249	2.138349
C	1.848599	-1.75652	-0.82875
C	4.263147	-1.88631	-1.29861
C	1.693434	-2.98803	-1.48276
C	4.065227	-3.11272	-1.93648
H	5.260173	-1.47283	-1.23531
C	2.786247	-3.66061	-2.02772
H	0.70353	-3.41836	-1.56342
H	4.916587	-3.63289	-2.35956
H	2.640327	-4.61274	-2.52627
C	-0.57921	0.624231	-1.35708
N	-0.29183	1.763066	-2.08226
N	-1.75335	0.148387	-1.90688
C	-1.26756	2.008729	-3.00878
C	0.926469	2.554968	-1.96384
C	-2.16532	-1.15628	-1.501
C	-2.19611	1.006706	-2.91092
H	-1.24597	2.851147	-3.67958
H	1.302033	2.760784	-2.97067
H	1.659496	1.938314	-1.45395
C	-1.26671	-1.73926	-0.58642
C	-3.30954	-1.78968	-1.97857
C	-1.59241	-3.03159	-0.15621
C	-3.58234	-3.07971	-1.53278
H	-3.98532	-1.30709	-2.67119
C	-2.72466	-3.69754	-0.62375
H	-0.95073	-3.52293	0.566873
H	-4.47391	-3.58741	-1.87988
H	-2.95119	-4.69509	-0.2634
C	-1.21293	4.272925	0.239921
H	-1.77365	3.995684	-0.65695
H	-1.16174	5.378672	0.256903
C	1.049054	3.833191	1.22917
H	1.905607	4.449976	0.919513
C	0.691311	3.864326	-1.20941
H	0.034497	4.503517	-1.81022
H	0.562395	4.383204	2.039956



H	1.652396	4.392305	-1.14991
H	-1.57843	4.192942	2.385963
H	-3.01323	4.377567	1.386893
N	0.114486	3.666207	0.115078
C	5.66707	0.699866	-0.13832
N	6.785477	0.596023	-0.41389
C	-3.37556	0.88887	-3.67542
N	-4.33565	0.84519	-4.31907
C	-3.96209	-0.70824	1.29069
N	-4.69432	-1.5992	1.214823

Ir-N-F

Ir	0.522088	-0.47102	0.001177
C	-2.18388	1.394031	2.157283
N	-3.13505	1.770622	1.265112
N	-2.15144	0.030905	2.021256
C	-3.70245	0.69221	0.578516
C	-3.38266	3.175057	0.997094
C	-1.12462	-0.76374	2.652304
C	-3.07174	-0.3929	1.084695
H	-4.49535	0.77034	-0.14435
C	0.10541	-0.94393	2.005276
C	-1.37771	-1.25558	3.930788
C	1.097102	-1.62528	2.733243
C	-0.38557	-1.94536	4.619281
H	-2.34824	-1.07688	4.379866
C	0.858471	-2.11945	4.015145
H	2.070667	-1.78572	2.283259
H	-0.57756	-2.33001	5.614165
H	1.649899	-2.64386	4.54117
C	1.676106	1.21429	0.385746
N	1.565973	2.485659	0.847879
N	3.001853	1.094287	0.004793
C	2.782015	3.169656	0.751665
C	0.391012	3.046275	1.515881
C	3.429279	-0.17098	-0.49711
C	3.656606	2.283992	0.226975
H	2.922946	4.183128	1.081183
H	0.747958	3.542254	2.423883
H	-0.25864	2.227057	1.827451

C	2.394439	-1.13426	-0.55934
C	4.738118	-0.43634	-0.88278
C	2.748524	-2.40205	-1.0442
C	5.047664	-1.71448	-1.35273
H	5.506734	0.321905	-0.82147
C	4.056541	-2.69231	-1.43208
H	1.986007	-3.16732	-1.11746
H	6.064266	-1.93825	-1.65505
H	4.303079	-3.68279	-1.79962
C	-0.6613	0.180168	-1.50318
N	-0.76971	1.272681	-2.31857
N	-1.52313	-0.75942	-2.05763
C	-1.69523	1.049494	-3.33409
C	0.044185	2.476529	-2.24057
C	-1.47888	-2.08156	-1.5218
C	-2.14293	-0.21574	-3.14863
H	-1.93944	1.773156	-4.09092
H	0.430122	2.69519	-3.24182
H	0.890367	2.252215	-1.59919
C	-0.52726	-2.20767	-0.4929
C	-2.29437	-3.11716	-1.96838
C	-0.4348	-3.47879	0.087226
C	-2.15764	-4.36662	-1.36617
H	-3.01844	-2.96546	-2.75749
C	-1.22906	-4.5439	-0.34031
H	0.264266	-3.63539	0.901706
H	-2.77919	-5.1916	-1.69477
H	-1.13019	-5.51479	0.134325
C	-2.70192	3.706313	-0.27203
H	-3.15575	3.203747	-1.13012
H	-2.96734	4.778673	-0.34956
C	-0.43175	4.056709	0.70043
H	0.233248	4.831188	0.290297
C	-0.74173	3.678171	-1.71387
H	-1.57364	3.873101	-2.39769
H	-1.07409	4.567195	1.42407
H	-0.08691	4.560971	-1.77342
H	-3.04197	3.709675	1.88373
H	-4.45891	3.35149	0.899939
N	-1.25811	3.484351	-0.36521

F	-3.03018	-0.89445	-3.86665
F	-3.28046	-1.67949	0.850194
F	4.946494	2.442494	-0.05182

Ir-N-Ph

Ir	0.643033	-0.61838	-0.12693
C	-0.93029	0.968379	2.813241
N	-1.80509	1.982747	2.589443
N	-1.60735	-0.1337	2.398747
C	-3.01164	1.528828	2.078609
C	-1.45696	3.358713	2.902999
C	-0.93607	-1.41027	2.477704
C	-2.91878	0.168472	1.978306
H	-3.83062	2.183714	1.832466
C	0.133105	-1.69418	1.612367
C	-1.33147	-2.28902	3.485248
C	0.812392	-2.90412	1.842223
C	-0.66116	-3.49328	3.667542
H	-2.16471	-2.0155	4.123264
C	0.425685	-3.79068	2.846544
H	1.6507	-3.16935	1.20641
H	-0.97185	-4.17896	4.447419
H	0.97347	-4.71787	2.982272
C	2.382756	0.344104	0.519322
N	2.794371	1.299176	1.399331
N	3.532091	-0.01919	-0.154
C	4.158467	1.521184	1.278825
C	1.994595	1.906148	2.462908
C	3.376253	-0.94524	-1.23216
C	4.643266	0.690657	0.319102
H	4.692742	2.187058	1.935005
H	2.598947	1.868537	3.375358
H	1.098778	1.299054	2.622768
C	2.066816	-1.47156	-1.36293
C	4.395747	-1.25508	-2.12753
C	1.856737	-2.375	-2.41731
C	4.14351	-2.15911	-3.16044
H	5.372459	-0.80263	-2.04687
C	2.878518	-2.72682	-3.29762
H	0.870242	-2.79453	-2.5625

H	4.937146	-2.40553	-3.85677
H	2.681231	-3.42764	-4.10219
C	-0.46162	0.868426	-0.91986
N	-0.29277	2.188456	-1.23024
N	-1.71715	0.548921	-1.40425
C	-1.43899	2.694156	-1.81543
C	0.953553	2.928299	-1.09095
C	-1.98226	-0.85203	-1.5326
C	-2.35166	1.683028	-1.91058
H	-1.55007	3.735458	-2.06612
H	1.219544	3.348469	-2.06707
H	1.717173	2.207469	-0.81445
C	-0.96934	-1.64569	-0.95816
C	-3.06177	-1.38327	-2.23424
C	-1.14642	-3.03178	-1.05688
C	-3.17977	-2.76794	-2.33491
H	-3.79909	-0.75044	-2.70497
C	-2.23012	-3.59269	-1.73397
H	-0.41309	-3.6864	-0.59807
H	-4.01763	-3.19334	-2.87525
H	-2.32888	-4.67163	-1.7996
C	-0.7687	4.127137	1.76836
H	-1.46604	4.17482	0.928078
H	-0.62512	5.164586	2.130789
C	1.56512	3.363216	2.222389
H	2.435372	3.963025	1.917513
C	0.856972	4.039636	-0.04557
H	0.132049	4.787079	-0.38574
H	1.261595	3.754678	3.199323
H	1.827894	4.554941	-0.01224
H	-0.82211	3.325223	3.788997
H	-2.36571	3.903535	3.175312
N	0.471792	3.544203	1.266496
C	6.060318	0.480052	-0.02344
C	6.666515	-0.76757	0.183077
C	6.837304	1.543254	-0.49624
C	8.018358	-0.94616	-0.08842
H	6.068919	-1.59432	0.549002
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C	-5.3272	-0.38077	1.81012
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C	-6.37521	-1.21812	1.446198
H	-5.54711	0.581245	2.258382
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H	-4.56441	-3.8586	0.324083
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C	-4.16794	2.53642	-3.39102
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C	-6.10056	1.405482	-1.73103
H	-4.45468	0.659475	-0.57399
C	-6.49074	2.145769	-2.84865
H	-5.81684	3.27824	-4.5512
H	-6.84328	0.95413	-1.08292
H	-7.54266	2.274667	-3.07716

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C	2.622187	-2.44652	2.424516
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C	1.042485	-0.89709	1.417177
C	2.105809	0.020499	1.506046
C	3.577296	-1.44097	2.447258
H	2.874855	-3.43701	2.782471
H	0.608	-2.95566	1.860536
H	4.579725	-1.61289	2.821042
C	2.546203	2.4781	0.869504
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C	0.549062	1.448253	0.42506
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H	-2.88315	-1.672	5.021427
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C	-4.67887	0.59799	-0.51624
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H	3.531345	1.947452	-3.40973
C	-0.65755	3.376628	-0.62281
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CN

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C	-5.25616	1.4425	-2.2087
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H	5.579765	-3.48068	-1.03609
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H	5.373887	3.9492	1.201642
H	1.39836	5.194111	0.04129
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C	-7.04119	1.007798	-0.58284
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H	3.238375	2.008333	-3.35976
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H	-2.25492	2.156361	-2.73054
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H	2.207659	-3.99788	-1.78936
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C	1.431506	-3.00513	-0.18952
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C	2.692766	-3.61573	-0.38273
C	3.741959	-1.46801	-0.23563
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O	0.448832	-3.95793	-0.14347
C	0.855336	3.501704	0.834266
C	1.734663	1.396791	0.76177
C	0.019141	3.188513	1.897462
H	0.848227	4.497589	0.403321
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C	0.089098	1.901903	2.431809
H	-0.6598	3.931883	2.295453
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C	-4.75567	-0.75668	0.079929
C	-4.70186	0.592404	-0.05662
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H	-5.60233	-1.41079	0.189673
N	2.664462	0.499359	0.178655
C	4.718268	-0.41476	-0.24485
C	4.020786	0.793526	0.01383
C	6.105437	-0.39358	-0.43448
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C	6.071388	2.007421	-0.07972
C	4.694911	2.015295	0.105944
H	4.153925	2.931713	0.289083

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C	-2.5668	-0.17051	-0.12141
C	-2.86946	2.260946	-0.39417
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C	-3.3954	3.319475	0.343796
C	-1.41592	3.787085	-1.54834
H	-1.46632	1.661099	-1.90413
C	-2.92985	4.611707	0.120295
H	-4.14959	3.131832	1.099401
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H	-0.63444	3.955863	-2.28091
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H	1.078196	-0.0108	2.264519

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C	-2.39494	-3.46486	-0.04373
C	-3.84197	-1.57692	0.105746
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H	-3.31391	-5.39147	0.283043
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C	0.051684	-3.52572	-0.4142
C	1.776357	-1.90357	-0.30302
C	1.015341	-4.54462	-0.60584
C	2.74736	-2.89715	-0.49691
C	2.353065	-4.23529	-0.67497
H	0.66549	-5.5661	-0.68398

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C	1.044752	0.310492	1.616543
C	0.361684	1.396248	2.154212
H	-0.04869	3.499323	1.80429
H	1.019031	-0.6579	2.098882
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H	6.29381	2.150708	-1.16975
H	5.833796	3.361015	0.036564
H	6.949312	2.073478	0.474948
H	3.688084	1.113566	2.152516
H	5.428699	1.280237	2.406345
H	4.438074	2.710144	2.059192
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H	-0.63034	3.321395	4.027892
H	-0.8646	2.15021	5.32501

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C	1.966413	-1.78862	0.067969
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C	4.276232	1.737855	-1.00622
C	2.626665	3.46573	-0.8654
C	3.930445	3.049255	-1.21232

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C	-0.31435	1.981156	1.887157
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H	-1.2368	1.085131	3.605602
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H	-0.1023	5.244153	-0.29109
H	2.361929	5.646271	-1.33525
H	0.665699	1.569444	2.07098

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C	2.101157	-1.73664	-0.0461
C	3.460059	-1.48337	-0.07874
C	1.685464	-3.05941	0.168282
N	0.263057	-3.19874	0.15486
C	4.403362	-2.50933	0.092353
C	2.577221	-4.10029	0.356153
C	3.951557	-3.80277	0.311969
H	5.462067	-2.28166	0.051404
H	2.250172	-5.11898	0.531376
H	4.670072	-4.60171	0.45153
Pt	0.587897	-0.32863	-0.18171
C	1.927504	1.186529	-0.22771
C	3.331506	0.967501	-0.37765
C	1.607838	2.569868	-0.22586
C	4.266955	2.008045	-0.63751
C	2.510995	3.621084	-0.48997
C	3.871174	3.319629	-0.71488
H	5.303299	1.725327	-0.77233
H	4.589415	4.103832	-0.92383
O	3.977897	-0.23254	-0.29845
C	-3.10547	2.502464	0.255964
C	-0.83838	2.63169	0.481676
C	-3.24385	1.842861	1.474454
H	-3.97246	2.729183	-0.35523
C	-0.86388	1.981509	1.733094
C	-2.10398	1.581675	2.222903
H	-4.22141	1.533618	1.82326
H	-2.14293	1.072745	3.178056
N	-1.92656	2.889339	-0.22982
C	-0.53108	-4.32218	0.278229
C	-1.81633	-3.90533	0.145641
H	-2.73843	-4.45958	0.143891
H	-0.13328	-5.30945	0.43207
N	0.386448	3.180921	-0.01062
C	1.729316	4.801662	-0.43653
N	-1.77946	-2.52776	-0.05374
C	-0.49901	-2.07075	-0.04054
C	-2.92285	-1.71061	-0.30882
C	-2.89224	-0.7884	-1.35257
C	-4.06688	-1.85431	0.471913

C	-4.01783	-0.01405	-1.60997
H	-1.99657	-0.68167	-1.95013
C	-5.1872	-1.07494	0.197069
H	-4.07535	-2.55694	1.297202
C	-5.18084	-0.14133	-0.84426
H	-3.98384	0.707935	-2.41822
H	-6.07459	-1.18796	0.810996
C	-6.37578	0.742222	-1.10048
H	-7.3096	0.246211	-0.82617
H	-6.30831	1.663268	-0.51006
H	-6.43941	1.033655	-2.15111
H	2.034494	5.826797	-0.58893
O	0.229	1.776542	2.51387
H	1.009258	1.613656	1.964356
N	0.470123	4.531211	-0.1359



