Cartesian coordinates are listed in xyz format (Angström).

Energies are listed in Hartree.

All given structures were optimized with the PBE0

functional (grid m3) and dhf-TZVP basis sets.

For computational details see Supporting Information (PDF).

2-Ferrocenyl-1,10-phenanthroline

41

Energy = -2220.291442125

N	0.6464617	0.1881133	-0.8755112
N	0.4687933	-1.7223149	-2.8295525
Fe	-0.0060567	-0.2549096	2.7561553
C	-1.4572411	-1.5494571	2.1436711
H	-1.3244030	-2.2736000	1.3550046
C	-1.1734434	-1.7450788	3.5221554
H	-0.7974696	-2.6522850	3.9695793
C	-1.4265063	-0.5233822	4.2015669
H	-1.2808277	-0.3418916	5.2553863
C	-1.8686883	0.4274881	3.2428625
H	-2.1175177	1.4588999	3.4402105
C	-1.8876452	-0.2076658	1.9726316
H	-2.1354285	0.2599045	1.0315663
C	1.6474162	-0.6995504	1.6520356
C	1.9523351	-0.7905160	3.0310217
H	2.2886066	-1.6762188	3.5479429
C	1.6969925	0.4741707	3.6272932
H	1.8067115	0.7180248	4.6728300
C	1.2350249	1.3520478	2.6146339
H	0.9335553	2.3771223	2.7657980

C 1.2039030 0.6289844 1.3823762

C 0.7279683 1.0929700 0.0810981

C 0.3710974 2.4411399 -0.1283777

H 0.4633223 3.1606666 0.6748192

C -0.0851837 2.8193770 -1.3589335

H -0.3675216 3.8487471 -1.5549285

C -0.1888727 1.8690972 -2.3873450

C 0.1997236 0.5458734 -2.0822004

C -0.6588837 2.2037472 -3.6883767

H -0.9472874 3.2307149 -3.8867060

C -0.7443218 1.2639382 -4.6571708

H -1.1020836 1.5196104 -5.6487191

C -0.3660075 -0.0852283 -4.3965062

C 0.1063375 -0.4631918 -3.1185723

C -0.4456003 -1.0815279 -5.3811573

H -0.8036971 -0.8228858 -6.3722890

C -0.0703042 -2.3623110 -5.0748344

H -0.1174693 -3.1571909 -5.8090839

C 0.3813167 -2.6277502 -3.7749463

H 0.6843277 -3.6366258 -3.5046147

H 1.6995831 -1.4824485 0.9124270

Monolithiated 2-ferrocenyl-9,10-dihydro-9-n-butyl-1,10-phenanthroline

(Lithium at N)

55

Energy = -2385.563776088

N -0.1601263 -0.0058256 -0.4130939

N -1.4033873 -0.6215298 -2.7400030

Fe -0.5155154 -0.5553218 3.6102798

C -2.2539176 0.4754511 3.9080449

H	-3.1361096	0.3883364	3.2925919
C	-1.9483628	-0.3151310	5.0479301
H	-2.5583777	-1.1082737	5.4519703
C	-0.6815878	0.0966769	5.5399435
H	-0.1597742	-0.3282807	6.3835201
C	-0.2046182	1.1406844	4.7027351
H	0.7429050	1.6477091	4.8006843
C	-1.1764042	1.3744438	3.6941833
H	-1.0900807	2.0782498	2.8802175
C	-0.7741784	-1.6904018	1.9424065
C	-0.5117561	-2.5231783	3.0618181
H	-1.1743770	-3.2741175	3.4637793
C	0.7543523	-2.1577269	3.5890314
H	1.2292308	-2.5911455	4.4555364
C	1.2720712	-1.0985441	2.8007697
H	2.2172440	-0.6001042	2.9505721
C	0.3319880	-0.8032370	1.7690332
C	0.4570583	0.2201298	0.7314870
C	1.2002972	1.3979516	0.9392964
H	1.6940749	1.5593414	1.8890632
C	1.2547039	2.3327016	-0.0551837
H	1.8104037	3.2539825	0.0886395
C	0.5835389	2.1299700	-1.2778308
C	-0.1185301	0.9033325	-1.4145280
C	0.5819275	3.0646963	-2.3267726
H	1.1189790	3.9990257	-2.2185318
C	-0.1261255	2.7697120	-3.4681381
H	-0.1646332	3.4956405	-4.2758010
C	-0.8104322	1.5643147	-3.6458990
C	-0.8041207	0.5646183	-2.6427813
C	-1.6247660	1.2959383	-4.8058877
H	-1.7871024	2.0968839	-5.5217613

C -2.2073796 0.1067586 -4.9675148

H -2.8580759 -0.0817483 -5.8159889

C -1.9567570 -1.0309034 -4.0212431

H -1.6981683 -1.6638298 1.3823270

C -1.0688529 -2.1039418 -4.6805469

C 0.3362403 -1.6366528 -5.0082238

H -1.5660421 -2.4589749 -5.5928757

H -1.0192540 -2.9657092 -4.0004526

C 1.2008619 -2.7227295 -5.6269109

H 0.8140325 -1.2669203 -4.0944071

H 0.2830505 -0.7799951 -5.6887763

C 2.6074540 -2.2468625 -5.9467859

H 0.7210496 -3.0924799 -6.5408233

H 1.2496464 -3.5811869 -4.9457489

H 2.5870873 -1.4105063 -6.6508987

H 3.2131202 -3.0411647 -6.3899255

H 3.1188757 -1.9002101 -5.0444987

H -2.9211626 -1.5276937 -3.8292151

Li -1.0903471 -1.5292219 -1.1444725

Dilithiated 2-ferrocenyl-9,10-dihydro-9-n-butyl-1,10-phenanthroline,

second Li at substituted ring, not in proximity to N atoms

55

Energy = -2392.448894876

N 0.0146206 0.2446888 0.4254907

N -1.2381138 -0.3875065 -1.8804597

Fe -0.3571306 -0.3597573 4.4171446

C -2.0753276 0.7249594 4.6958906

H -2.9670289 0.6682261 4.0903360

C -1.7905040 -0.0600406 5.8545223

H	-2.4988753	-0.6979112	6.3780213
C	-0.5067625	0.3302831	6.3428435
H	-0.0027211	-0.0774155	7.2056623
C	-0.0110284	1.3470148	5.4900875
H	0.9481898	1.8323713	5.5810761
C	-0.9763105	1.5892876	4.4760666
H	-0.8711133	2.2779307	3.6516953
C	-0.5751621	-1.4884736	2.7351705
C	-0.3785079	-2.3806262	3.8386573
Li	-1.7555051	-2.4183954	5.1959144
C	0.8986391	-1.9760850	4.3598368
H	1.3828925	-2.4021269	5.2295539
C	1.4397654	-0.8851813	3.6250113
H	2.3768941	-0.3799897	3.8091410
C	0.5173021	-0.5725220	2.5876374
C	0.6372912	0.4672629	1.5675771
C	1.3708719	1.6528650	1.7718066
H	1.8790892	1.8125206	2.7144474
C	1.4044831	2.5937161	0.7811635
H	1.9536801	3.5192990	0.9236176
C	0.7228822	2.3907975	-0.4364389
C	0.0367613	1.1564923	-0.5708157
C	0.6956484	3.3283343	-1.4838972
H	1.2203718	4.2703092	-1.3805827
C	-0.0214134	3.0251790	-2.6175938
H	-0.0801352	3.7526960	-3.4227452
C	-0.6902007	1.8096226	-2.7918504
C	-0.6566239	0.8080751	-1.7912595
C	-1.5179963	1.5316122	-3.9396510
H	-1.7079198	2.3324648	-4.6489633
C	-2.0815001	0.3320787	-4.0962264
H	-2.7438427	0.1350235	-4.9337402

C -1.7896369 -0.8048376 -3.1599691

H -1.4869236 -1.4177557 2.1500945

C -0.8761438 -1.8467390 -3.8344871

C 0.5115951 -1.3359720 -4.1716967

H -1.3708884 -2.2098422 -4.7451966

H -0.7947298 -2.7106296 -3.1604564

C 1.4006282 -2.3899994 -4.8107108

H 0.9882138 -0.9623803 -3.2589740

H 0.4266616 -0.4745008 -4.8427259

C 2.7883937 -1.8687621 -5.1423729

H 0.9213230 -2.7654765 -5.7226634

H 1.4834313 -3.2525855 -4.1382989

H 2.7343046 -1.0270883 -5.8383605

H 3.4128851 -2.6402498 -5.5996455

H 3.2993772 -1.5146979 -4.2427363

H -2.7371072 -1.3315413 -2.9633217

Li -0.9070433 -1.2940212 -0.2726262

Dilithiated 2-ferrocenyl-9,10-dihydro-9-n-butyl-1,10-phenanthroline,

second Li at substituted ring, in spacial proximity to N atoms

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55

Energy = -2392.481732541

N 0.6800272 0.2326135 -0.2562154

N -1.0542704 -0.5191259 -1.9479892

Fe -0.4967933 -0.6705665 2.9129427

C -2.2981328 0.1016087 2.2918367

H -2.8256117 0.0760447 1.3433944

C -2.4902517 -0.8151224 3.3657054

H -3.0764115 -1.7201380 3.3301825

C -1.7645348 -0.3314611 4.4825410

H	-1.6902725	-0.8148778	5.4442897
C	-1.1155924	0.8740776	4.1018484
H	-0.4636651	1.4669543	4.7245396
C	-1.4435315	1.1450339	2.7499439
H	-1.0929594	1.9831245	2.1658440
C	0.3549458	-1.7725993	1.3485468
C	0.2370884	-2.5505414	2.5371315
H	-0.3470064	-3.4566854	2.6292176
C	0.9289352	-1.9480896	3.6276650
H	0.9666651	-2.3087169	4.6457889
C	1.5247401	-0.7524428	3.1527210
H	2.0915481	-0.0477737	3.7441480
C	1.1850368	-0.6428174	1.7758990
C	1.3658039	0.4727170	0.8397705
C	2.0282478	1.7128861	0.9537330
H	2.6265708	1.9429024	1.8268281
C	1.8887362	2.6398349	-0.0597887
H	2.3953066	3.5962686	0.0264861
C	1.0693338	2.4025062	-1.1904821
C	0.4699858	1.1310292	-1.2108232
C	0.7509242	3.2844113	-2.2465679
H	1.1932983	4.2718166	-2.2952812
C	-0.1629356	2.8709763	-3.1924003
H	-0.4357189	3.5584468	-3.9881748
C	-0.8027968	1.6136675	-3.1776614
C	-0.4913583	0.6906491	-2.1710915
C	-1.8817089	1.2318539	-4.0587595
H	-2.2676912	1.9558386	-4.7702173
C	-2.4345259	0.0200797	-3.9497301
H	-3.2782659	-0.2544557	-4.5758205
C	-1.9134563	-1.0373507	-3.0108781
Li	-1.1306209	-0.6328794	0.2247159

C -1.2036447 -2.1540684 -3.7973417

C 0.0554891 -1.7129614 -4.5196722

H -1.9110435 -2.5828594 -4.5193149

H -0.9638404 -2.9619111 -3.0913924

C 0.7532787 -2.8448424 -5.2557472

H 0.7523603 -1.2624800 -3.8020366

H -0.1945134 -0.9153396 -5.2269098

C 2.0155636 -2.3963847 -5.9715403

H 0.0582991 -3.2878250 -5.9786974

H 0.9966715 -3.6456660 -4.5470848

H 1.7929827 -1.6218549 -6.7101567

H 2.5006082 -3.2248872 -6.4928397

H 2.7394920 -1.9767920 -5.2672101

H -2.7821630 -1.5207745 -2.5400511

Li 0.4012479 -1.6480509 -0.8435037

Dilithiated 2-ferrocenyl-9,10-dihydro-9-n-butyl-1,10-phenanthroline,

second Li at unsubstituted ring, in spacial proximity to N atoms

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55

Energy = -2392.499395002

N 0.6076563 0.3545468 -0.1195141

N -1.4140906 0.1077491 -1.8560176

Fe -0.5391048 -0.9507583 2.7451326

C -2.1382657 -0.4696829 1.4525399

Li -2.5669020 0.4801328 -0.3285385

C -2.4241607 -1.6199948 2.2641297

H -2.6390198 -2.6120101 1.8867684

C -2.3377803 -1.3093452 3.6493807

H -2.4689154 -1.9951455 4.4739464

C -1.9937126 0.0614226 3.7508673

H	-1.8192897	0.6086165	4.6660248
C	-1.8677373	0.5598802	2.4238902
H	-1.5481125	1.5708726	2.1962928
C	0.9969142	-1.8607373	1.7541780
C	0.8096609	-2.4691715	3.0219515
H	0.5619454	-3.5045861	3.1977711
C	0.9843687	-1.4706393	4.0141816
H	0.8698029	-1.6082996	5.0783594
C	1.2897171	-0.2459669	3.3641087
H	1.4299702	0.7108539	3.8439924
C	1.2996014	-0.4779377	1.9620468
C	1.4463118	0.5032483	0.8830243
C	2.3975522	1.5409202	0.8810992
H	3.0890910	1.6400545	1.7084953
C	2.4535280	2.3852338	-0.1976232
H	3.1976375	3.1746360	-0.2341878
C	1.5465427	2.2539739	-1.2681693
C	0.5971840	1.2109934	-1.1531455
C	1.5184987	3.0866057	-2.4064714
H	2.2491117	3.8792315	-2.5146273
C	0.5485350	2.8801542	-3.3523410
H	0.5083551	3.5239864	-4.2260839
C	-0.4362087	1.8818382	-3.2292908
C	-0.4494996	1.0282117	-2.1160808
C	-1.5472150	1.7620868	-4.1439821
H	-1.6778108	2.5218024	-4.9090725
C	-2.4197313	0.7579563	-4.0197630
H	-3.2757652	0.6796719	-4.6826425
C	-2.2159017	-0.3277151	-2.9987802
H	0.9915582	-2.3655375	0.7976111
C	-1.6521977	-1.6057577	-3.6433391
C	-0.2399209	-1.4807400	-4.1838134

H -2.3302448 -1.9143152 -4.4505621

H -1.6859098 -2.4041532 -2.8894888

C 0.2605028 -2.7586828 -4.8367698

H 0.4389971 -1.2022592 -3.3706016

H -0.1966705 -0.6611007 -4.9094359

C 1.6810855 -2.6348919 -5.3599817

H -0.4120192 -3.0337041 -5.6577336

H 0.2048715 -3.5821880 -4.1144835

H 1.7561580 -1.8385360 -6.1057492

H 2.0222607 -3.5617036 -5.8269407

H 2.3771795 -2.3918900 -4.5524299

H -3.2087922 -0.6201382 -2.6185251

Li -0.8197491 -0.9440916 -0.1592663

Lithiated 2-ferrocenyl-9,10-dihydro-9-n-butyl-10-(4-ethylbenzyl)-1,10-phenanthroline, Li at substituted ring, in spacial proximity to N atoms

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74

Energy = -2734.236344597

Fe -1.0266708 -2.7468588 -0.6871935

C -2.0483932 -2.9575951 -2.4461117

H -1.6193891 -3.2874824 -3.3798996

C -2.6135083 -3.7921991 -1.4438764

H -2.6847619 -4.8684719 -1.4798452

C -3.0315229 -2.9643834 -0.3678661

H -3.4694475 -3.3026116 0.5585156

C -2.7297272 -1.6174533 -0.7053913

H -2.8983362 -0.7554554 -0.0787503

C -2.1207371 -1.6144271 -1.9882694

H -1.7389438 -0.7477316 -2.5077849

C 0.9036282 -3.2565580 -1.0067230

C	0.3553924	-4.0855228	-0.0006453
H	0.2515218	-5.1601405	-0.0578444
C	-0.0753388	-3.2377270	1.0670418
H	-0.5850245	-3.6086172	1.9479561
C	0.1827406	-1.8659705	0.7925773
Li	0.1092802	0.1116245	1.1564842
C	0.8033752	-1.9074122	-0.5179954
H	1.3019292	-3.5941548	-1.9530376
N	0.8553108	0.4498605	-0.6473060
N	0.3434306	2.7373178	0.7674101
C	1.0715542	-0.6974907	-1.2736846
C	1.4883275	-0.7099827	-2.6324217
H	1.6953064	-1.6562100	-3.1142549
C	1.5714947	0.4597123	-3.3225300
H	1.8556434	0.4653249	-4.3699573
C	1.2571228	1.6841214	-2.6899618
C	0.9294580	1.6175378	-1.3151359
C	1.2171142	2.9234401	-3.3547225
H	1.4682473	2.9666766	-4.4088400
C	0.8373965	4.0510035	-2.6812343
H	0.7787993	5.0036488	-3.1964503
C	0.5189514	4.0046424	-1.3080527
C	0.5992403	2.8058343	-0.6214268
C	0.0827362	5.1834242	-0.5833991
H	0.1885960	6.1529376	-1.0587370
C	-0.4697369	5.0617244	0.6230289
H	-0.8232423	5.9306715	1.1682428
C	-0.6296664	3.7141305	1.2654640
C	-2.0638062	3.1842712	1.1733137
C	-2.5317909	2.7797776	-0.2140178
H	-2.7352391	3.9543177	1.5735678
H	-2.1438513	2.3217071	1.8463530

C	-3.9866896	2.3394274	-0.2323118
H	-1.9074756	1.9625261	-0.5897329
H	-2.3958030	3.6147647	-0.9097157
C	-4.4515580	1.9026116	-1.6104784
H	-4.6176128	3.1601627	0.1292210
H	-4.1259998	1.5169808	0.4795698
H	-4.3383922	2.7122554	-2.3368058
H	-5.5022452	1.6050272	-1.6028684
H	-3.8708765	1.0497007	-1.9704243
H	-0.4137768	3.8368915	2.3312886
C	1.4873152	-0.8434206	4.1589118
C	2.4719854	-0.6872118	3.1911567
C	2.5080570	0.4359943	2.3824111
C	1.5634494	1.4494955	2.5168695
C	0.5810595	1.3003930	3.4959850
C	0.5465225	0.1705361	4.2995826
H	3.1982277	-1.4774994	3.0354617
H	3.2611754	0.5144738	1.6056865
H	-0.1724010	2.0684733	3.6330182
H	-0.2372178	0.0690260	5.0432068
C	1.4431985	-2.0725623	5.0154903
C	2.4580322	-2.0303268	6.1530900
H	0.4361933	-2.1912826	5.4246099
H	3.4751525	-1.9316704	5.7666482
H	2.2712234	-1.1792013	6.8120691
C	1.5726997	2.6216930	1.5731685
H	2.4206246	2.5150586	0.8948517
H	1.7326298	3.5572631	2.1228016
H	1.6295350	-2.9480690	4.3866964
H	2.4119669	-2.9417668	6.7532255

Lithiated 2-ferrocenyl-9,10-dihydro-9-n-butyl-10-(4-ethylbenzyl)-1,10-phenanthroline, Li at unsubstituted ring, in spacial proximity to N atoms

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74

Energy = -2734.243807767

Fe	-1.0590343	-2.4723581	0.1600777
C	-2.5322419	-1.2092664	-0.4690822
H	-2.5140362	-0.7202308	-1.4366785
C	-3.0535807	-2.5201952	-0.2676223
H	-3.4995904	-3.1650977	-1.0118207
C	-2.8330154	-2.8451224	1.0949631
H	-3.0802507	-3.7824085	1.5738312
C	-2.1839321	-1.7221027	1.6893139
H	-1.8380485	-1.7123200	2.7162273
C	-1.9686516	-0.6701661	0.7383939
Li	-0.3290731	0.4867593	0.6153094
C	0.0362912	-3.3342836	-1.3442199
C	-0.0458832	-4.2167458	-0.2402764
H	-0.4874551	-5.2013650	-0.2502323
C	0.5139093	-3.5658120	0.8911037
H	0.5826147	-3.9760098	1.8860102
C	0.9333666	-2.2711209	0.4991129
H	1.4087821	-1.5333735	1.1287114
C	0.6467194	-2.1215520	-0.8961241
H	-0.3432296	-3.5229974	-2.3370939
N	0.7673207	0.2461650	-1.0346440
N	0.4819633	2.5357757	0.3986965
C	0.8322978	-0.9074535	-1.6730423
C	1.0489276	-0.9573577	-3.0733528
H	1.1253912	-1.9206245	-3.5603617
C	1.1585424	0.2025963	-3.7804265

H	1.3174643	0.1836953	-4.8536496
C	1.0472839	1.4456148	-3.1229834
C	0.8575044	1.4035607	-1.7218898
C	1.0675183	2.6907416	-3.7806762
H	1.2178400	2.7195188	-4.8541195
C	0.8736246	3.8432086	-3.0728120
H	0.8701330	4.8020176	-3.5796868
C	0.6631233	3.8169756	-1.6771746
C	0.6720149	2.6097764	-1.0073737
C	0.4102627	5.0261387	-0.9145332
H	0.5911479	5.9853261	-1.3877100
C	-0.0672314	4.9441673	0.3260820
H	-0.2841895	5.8368950	0.9028201
C	-0.3516775	3.6148891	0.9602552
C	-1.8402342	3.2573507	0.9298525
C	-2.4305812	2.9515609	-0.4350933
H	-2.3925396	4.0855127	1.3904402
H	-1.9963991	2.3795843	1.5675121
C	-3.9041409	2.5914362	-0.3443524
H	-1.9032492	2.1024607	-0.8814701
H	-2.2915712	3.8028250	-1.1108915
C	-4.5091361	2.2607230	-1.6966292
H	-4.4555110	3.4199084	0.1166810
H	-4.0088640	1.7302867	0.3235864
H	-4.4260674	3.1052879	-2.3870928
H	-5.5669896	2.0030522	-1.6097275
H	-3.9985566	1.4077131	-2.1508588
H	-0.0673459	3.6872113	2.0146014
C	1.6855433	-0.6604137	4.2331591
C	0.5491923	0.0835186	3.9461657
C	0.5558853	1.0551682	2.9562943
C	1.7012768	1.3017431	2.2061426

C 2.8412603 0.5545404 2.4913066

C 2.8344964 -0.4038315 3.4888594

H -0.3643066 -0.0967033 4.5030283

H -0.3573235 1.6085675 2.7697125

H 3.7450290 0.7195403 1.9132213

H 3.7355212 -0.9761274 3.6854058

C 1.6573417 -1.7448548 5.2688165

C 1.2429934 -3.0898494 4.6808646

H 2.6453923 -1.8347156 5.7298716

H 0.2532913 -3.0250302 4.2229583

H 1.9456422 -3.4072711 3.9069861

C 1.7559467 2.3337650 1.1096618

H 2.5016544 2.0151239 0.3804505

H 2.1098540 3.2938456 1.5085208

H 0.9625560 -1.4656316 6.0661464

H 1.2134794 -3.8631609 5.4518193

Model Complex I

93

Energy = -3076.034126960

Fe -2.0086629 -0.4106221 3.8444063

C -2.1958758 -1.3003571 2.0189339

H -3.0424506 -1.1672445 1.3631614

C -2.0832558 -2.2875768 3.0308450

H -2.8212623 -3.0390848 3.2665772

C -0.8468694 -2.0898131 3.7022429

H -0.4800719 -2.6683995 4.5362150

C -0.1982511 -0.9771969 3.1129546

H 0.7434595 -0.5438252 3.4074734

C -1.0273832 -0.4812528 2.0634605

N	0.1740811	1.5308093	1.7256372
N	2.2018882	3.2399641	2.7026838
C	-0.7544027	0.7197922	1.2735293
C	-1.4813022	0.9953877	0.0928478
H	-2.2048884	0.2813031	-0.2788767
C	-1.2575997	2.1730740	-0.5549855
H	-1.8136985	2.4275928	-1.4515125
C	-0.3114465	3.0910140	-0.0574724
C	0.4273406	2.6902158	1.0890221
C	-0.1275316	4.3687653	-0.6166718
H	-0.6991327	4.6566620	-1.4914123
C	0.7401125	5.2370498	-0.0192015
H	0.8706248	6.2385954	-0.4160355
C	1.4949089	4.8710354	1.1087274
C	1.4022376	3.5825109	1.6418961
C	2.3939996	5.8095012	1.7420858
H	2.5997856	6.7461909	1.2339087
C	2.9368425	5.5418789	2.9288834
H	3.6032369	6.2466765	3.4142023
C	2.6520407	4.2579108	3.6417752
C	1.6978004	4.4257620	4.8325228
C	0.2683956	4.7780681	4.4631579
H	2.1140566	5.2003658	5.4896158
H	1.7053979	3.4962459	5.4142277
C	-0.6140210	5.0053096	5.6795163
H	-0.1566329	3.9727172	3.8543923
H	0.2604593	5.6755577	3.8344386
C	-2.0530039	5.3258354	5.3161315
H	-0.1952125	5.8199475	6.2824240
H	-0.5888596	4.1141496	6.3176315
H	-2.1099901	6.2180880	4.6865364
H	-2.6614727	5.5054815	6.2054600

H	-2.5109442	4.5008274	4.7647006
H	3.6039553	3.8955351	4.0457210
C	7.0477788	1.7751511	2.8073775
C	6.3361977	1.1363601	3.8151939
C	4.9505844	1.1920548	3.8558969
C	4.2366472	1.8817994	2.8865427
C	4.9450384	2.5274922	1.8777875
C	6.3265869	2.4738597	1.8412418
H	6.8745996	0.5969148	4.5883260
H	4.4151725	0.6970526	4.6604583
H	4.4038307	3.0916113	1.1255959
H	6.8610743	2.9881559	1.0483518
C	8.5437943	1.6809587	2.7349826
C	9.0088448	0.5069452	1.8789489
H	8.9481289	2.6119122	2.3264579
H	8.6399250	-0.4385594	2.2829942
H	8.6326751	0.5973252	0.8572986
C	2.7293505	1.9104312	2.9080785
H	2.3701644	1.4853934	3.8536175
H	2.3384223	1.2655229	2.1253566
H	8.9516716	1.5792636	3.7451568
H	10.0994326	0.4571027	1.8366050
C	-7.1592028	-0.1208655	8.8614798
C	-7.1194587	-1.4268401	8.3790580
C	-6.2342348	-1.7917635	7.3810581
C	-5.3548903	-0.8657921	6.8260350
C	-5.3934782	0.4372170	7.3028421
C	-6.2826300	0.8007950	8.3044483
H	-7.7968452	-2.1684089	8.7916812
H	-6.2264471	-2.8162793	7.0206817
H	-4.7228108	1.1793985	6.8854769
H	-6.2953328	1.8274431	8.6575567

C -8.0846895 0.2613913 9.9795507

C -7.4750792 0.0000146 11.3531036

H -8.3430267 1.3208279 9.8912701

H -7.2288286 -1.0575639 11.4748018

H -6.5519646 0.5697114 11.4827788

C -4.4081367 -1.3036343 5.7322587

H -4.9950223 -1.6713022 4.8838612

H -3.8311733 -2.1627279 6.0909911

H -9.0205997 -0.2976527 9.8852564

H -8.1649546 0.2821415 12.1521030

C -1.6469206 1.1575078 5.0922168

H -0.6716119 1.5946587 5.2405009

C -2.5769854 1.5298158 4.0872403

H -2.4252214 2.2911682 3.3373145

C -3.7019193 0.6704627 4.1928526

H -4.5735446 0.6825434 3.5553628

C -3.4727229 -0.2461137 5.2580458

C -2.2011752 0.0679107 5.8159195

H -1.7299115 -0.4607957 6.6311270

Model Complex II

96

Energy = -4123.733498101

Fe -0.7547402 -0.6669600 3.8217688

C -2.2774668 0.6709053 3.5024722

H -2.4500610 1.2211955 2.5893215

C -2.7984549 -0.6073293 3.8302396

H -3.4359409 -1.2118029 3.2033327

C -2.3033512 -0.9665063 5.1121131

H -2.5002615 -1.8903800 5.6355200

C	-1.4664842	0.0849107	5.5806457
C	-1.4612367	1.0964747	4.5800204
H	-0.9263939	2.0323845	4.6310439
C	-0.1737162	-1.9445307	2.3419896
H	-0.8509993	-2.4224203	1.6510695
C	0.2148019	-2.4596352	3.6025849
H	-0.1117598	-3.3953609	4.0293894
C	1.0706691	-1.5102636	4.2230434
H	1.5139107	-1.6018414	5.2030445
C	1.2092792	-0.4022425	3.3556873
H	1.7824830	0.4908734	3.5388467
C	0.4428474	-0.6646300	2.1788161
N	0.6157851	1.5212789	1.2819897
N	1.1037303	4.3847370	1.8751831
C	0.2432179	0.2707089	1.0813402
C	-0.3389322	-0.1405849	-0.1352682
H	-0.6208925	-1.1749241	-0.2800712
C	-0.5229539	0.7832552	-1.1209241
H	-0.9588297	0.5012335	-2.0731267
C	-0.1583147	2.1241029	-0.9136498
C	0.4016735	2.4464858	0.3467017
C	-0.3509860	3.1094363	-1.9080562
H	-0.7888539	2.8177004	-2.8554603
C	0.0048414	4.3941922	-1.6756544
H	-0.1304823	5.1558609	-2.4332083
C	0.5416409	4.7925274	-0.4260518
C	0.7105700	3.8401820	0.6187777
C	1.0694535	6.1354177	-0.2764061
H	0.8487869	6.8511205	-1.0591246
C	1.8439463	6.4468494	0.7558488
H	2.3002667	7.4254704	0.8430444
C	2.1242020	5.4742937	1.8462579

C	2.2756042	6.2039267	3.1796003
C	1.0609634	6.9866922	3.6396766
H	3.1218568	6.8858569	3.0354722
H	2.6012248	5.5047230	3.9522590
C	1.2857597	7.6729100	4.9765693
H	0.1889772	6.3319975	3.7210418
H	0.7935103	7.7349897	2.8848452
C	0.0626915	8.4443901	5.4403671
H	2.1496996	8.3453434	4.9083822
H	1.5489622	6.9178456	5.7267874
H	-0.1943428	9.2353773	4.7308054
H	0.2266794	8.9107018	6.4144988
H	-0.8045883	7.7846337	5.5206753
H	3.0890980	4.9839986	1.6441146
C	4.8664120	1.5582225	4.0796913
C	4.0235107	2.0706693	5.0608575
C	2.8693577	2.7554284	4.7209622
C	2.5107083	2.9358686	3.3894069
C	3.3581388	2.4402893	2.4065268
C	4.5196549	1.7680662	2.7493288
H	4.2772116	1.9345881	6.1074059
H	2.2258817	3.1463124	5.5033717
H	3.1028466	2.5534594	1.3598614
H	5.1642637	1.3843599	1.9650780
C	6.0784331	0.7548280	4.4464759
C	5.7455985	-0.7220686	4.6372408
H	6.8371284	0.8609342	3.6656444
H	5.0095416	-0.8548352	5.4335327
H	5.3220613	-1.1469132	3.7244654
C	1.1818852	3.5599351	3.0905800
H	0.8732977	4.2048152	3.9130778
H	0.4345195	2.7775133	2.9973358

H	6.5164972	1.1526082	5.3665150
H	6.6372586	-1.2958057	4.8999660
C	-3.1517408	1.7026413	10.1417209
C	-2.3964026	0.5466418	10.2961320
C	-1.6377621	0.0442769	9.2494262
C	-1.6072685	0.6818799	8.0160390
C	-2.3690335	1.8357957	7.8556749
C	-3.1252139	2.3353733	8.9015948
H	-2.4076839	0.0249381	11.2481727
H	-1.0624534	-0.8652451	9.3929599
H	-2.3839113	2.3427287	6.8971045
H	-3.7156381	3.2336146	8.7490338
C	-3.9387446	2.2764075	11.2837445
C	-3.1648464	3.3517629	12.0397154
H	-4.8734034	2.7006450	10.9047278
H	-2.2384757	2.9455765	12.4525929
H	-2.8964740	4.1767709	11.3758236
C	-0.7575419	0.1391043	6.8933871
H	-0.4096660	-0.8607765	7.1653666
H	0.1401369	0.7584019	6.7838010
H	-4.2157188	1.4737864	11.9733768
H	-3.7561169	3.7579135	12.8640276
Pd	-1.0160168	4.7847328	1.4449164
Cl	-1.9888903	5.0170253	3.4880216
Cl	-2.9566558	4.6817069	0.3152713