54
Complex 2 ==
Ir	0.55828	−0.27399	−0.02879
N	−1.47969	1.29515	1.38723
C	−1.38588	0.23867	0.50470
N	0.71897	1.81413	−0.43739
C	2.49406	−0.73093	−1.01092
N	−2.69745	−0.06288	0.20395
C	0.51977	−2.46190	0.00962
C	0.47558	4.07653	0.37741
C	1.69291	−3.13170	−0.71223
C	−4.62302	−0.81071	−1.19801
C	−0.29924	2.08335	1.77787
C	−3.18929	−1.14562	−0.73387
C	0.57438	−1.94925	1.33968
C	−2.27547	−1.18092	−1.97511
C	−3.56362	0.77819	0.90896
C	2.47539	−2.13193	−1.59786
C	0.99611	4.58841	−0.82079
C	2.74230	−0.40387	0.34575
C	−3.20991	−2.48140	0.04025
C	−2.80096	1.64018	1.64361
C	0.33407	2.69300	0.53954
C	3.08094	−1.42038	1.43775
C	1.82278	−1.90282	2.20706
C	1.18997	2.31696	−1.61091
C	1.34064	3.68863	−1.83757
H	1.62290	−1.21872	3.05079
H	2.00370	−2.89859	2.65962
H	3.61612	−2.27566	0.99347
H	3.78586	−0.95911	2.14954
H	3.06895	0.62508	0.55045
H	2.69781	0.06045	−1.74662
H	−0.36338	−1.95100	1.91329
H	−0.46329	−2.79185	−0.34442
H	1.30538	−3.95028	−1.34169
H	2.36100	−3.60905	0.02402
H	1.99842	−2.07333	−2.59213
H	3.50860	−2.49219	−1.77402
H	0.41768	1.42016	2.29277
H	−0.62565	2.87122	2.47344
H	0.17196	4.74584	1.18755
H	1.11424	5.66669	−0.96028
H	1.72612	4.03342	−2.80046
H	1.44563	1.58363	−2.37845
H	−3.08209	2.44110	2.32246
H	−4.64252	0.70259	0.83413
H	−3.54721	−3.29482	−0.62271
H	−3.90816	−2.42434	0.89193
H	−2.21696	−2.74588	0.43329
H	−4.68636	0.19634	−1.64219
H	−5.36565	−0.89896	−0.38805
H	−4.91093	−1.53779	−1.97372
H	−2.55533	−2.03729	−2.60992

H	−2.39740	−0.25878	−2.56779
H	−1.20901	−1.27173	−1.70375
59			
[Ir(C8H13)(py−ItBu’)(ClCH2Cl)]+	==========	==========	==========
C	−0.19656	3.58486	1.75626
C	1.13276	3.51914	1.42153
C	−2.22452	2.12430	1.17283
C	3.10741	2.83238	−0.88972
C	−0.90661	1.01123	−2.03967
C	−2.36367	0.57627	−2.29520
C	−3.51934	0.45487	2.53752
C	−2.55417	0.69124	1.54521
C	0.13827	1.65081	0.61974
C	−0.00964	0.83168	−3.28497
C	−2.54531	−0.80117	−2.95262
C	2.50895	1.75955	0.04260
C	−3.87969	−0.85548	2.87443
C	3.53171	1.34273	1.11984
C	1.98985	0.51808	−0.77750
C	0.53620	−0.61540	−3.43994
C	−2.05721	−1.98626	−2.09680
C	−3.23400	−1.90332	2.20799
C	−2.27521	−1.59719	1.23856
C	0.51237	−1.39809	−2.12352
C	−0.64592	−1.93407	−1.52004
H	−0.75694	4.33914	2.30295
H	−2.75517	2.80957	1.84972
H	−2.57299	2.33209	0.14360
H	1.94498	4.20914	1.63214
H	−0.90969	2.08128	−1.76000
H	3.47358	3.71010	−0.32876
H	−2.95305	0.61972	−1.36096
H	−3.98692	1.30658	3.04013
H	2.36509	3.17489	−1.62967
H	−0.57347	1.13392	−4.18949
H	−3.61836	−0.95769	−3.16363
H	3.96713	2.40625	−1.43196
H	0.83960	1.53019	−3.21461
H	−2.05085	−0.80495	−3.93797
H	3.85440	2.20686	1.72681
H	−4.63564	−1.04982	3.64038
H	2.19004	0.70028	−1.84417
H	−0.03145	−1.17751	−4.20211
H	3.10535	0.58109	1.79188
H	4.42757	0.91761	0.63921
H	−2.77073	−2.12911	−1.26326
H	1.57422	−0.58098	−3.81007
H	−2.13091	−2.91592	−2.69746
H	2.59016	−0.36296	−0.48679
H	−3.45997	−2.94992	2.42794
H	−1.74160	−2.39337	0.72000
H	1.46600	−1.86475	−1.84416
H	−0.45189	−2.76333	−0.81916
Ir	−0.04340	−0.04047	−0.41779

N	−0.79237	2.42491	1.25208
N	1.31089	2.33073	0.71844
N	−1.93190	−0.33002	0.87921
H	−2.80861	1.33768	−2.96988
Cl	1.05780	−1.65662	1.85651
C	2.01730	−3.13897	1.39544
Cl	3.75265	−2.81068	1.17419
H	1.60117	−3.51247	0.45156
H	1.88872	−3.85581	2.21597

64

[Ir(C8H13)(py−ItBu’){kO−(CH3)2SO}]+ ==========

C	−1.45735	−2.40396	2.86036
C	−2.60677	−1.75484	2.48698
C	0.91457	−2.46946	1.88099
C	−4.35482	−0.76361	0.11303
C	−0.16356	−1.91371	−1.51910
C	1.24867	−2.44393	−1.85648
C	3.03822	−1.36227	2.64659
C	1.95587	−1.37439	1.75147
C	−0.94509	−1.02974	1.12915
C	−1.01983	−1.71368	−2.79237
C	2.01273	−1.66760	−2.94196
C	−3.09019	−0.01666	0.57849
C	4.03683	−0.38816	2.53271
C	−3.46626	1.21475	1.42903
C	−2.17786	0.37238	−0.64391
C	−0.77472	−0.33941	−3.47535
C	2.33050	−0.20272	−2.58467
C	3.90216	0.56896	1.52054
C	2.79254	0.50615	0.67315
C	−0.15298	0.68702	−2.52352
C	1.19390	0.69173	−2.10106
H	−1.27420	−3.13667	3.64203
H	1.13328	−3.08012	2.76915
H	0.95484	−3.13298	0.99698
H	−3.61216	−1.81729	2.89367
H	−0.66336	−2.67387	−0.88855
H	−5.00915	−1.04143	0.95783
H	1.87287	−2.50721	−0.94476
H	3.09075	−2.12563	3.42841
H	−4.09105	−1.67942	−0.44138
H	−0.82919	−2.54071	−3.50455
H	2.97113	−2.18057	−3.14139
H	−4.93924	−0.11148	−0.55631
H	−2.08544	−1.79323	−2.52092
H	1.45391	−1.71888	−3.89153
H	−4.05775	0.92899	2.31592
H	4.88900	−0.37567	3.21817
H	−2.60740	−0.07325	−1.55396
H	−0.12593	−0.44526	−4.36301
H	−2.55518	1.73232	1.76966
H	−4.07806	1.91034	0.83044
H	3.12900	−0.19622	−1.81831
H	−1.72942	0.06378	−3.85304

H	2.78166	0.29006	-3.47059
H	-2.22693	1.46745	-0.77073
H	4.64462	1.35875	1.37702
H	2.65360	1.24954	-0.11081
H	-0.67568	1.65177	-2.48387
H	1.55287	1.67285	-1.75029
Ir	-0.10558	-0.10704	-0.41927
N	-0.44606	-1.94361	2.01124
N	-2.26897	-0.92739	1.41853
N	1.82754	-0.44916	0.75161
H	1.12823	-3.48925	-2.21149
O	0.05872	1.97212	0.91640
S	-0.02526	3.51627	1.00387
C	1.51178	4.21937	0.27042
H	2.35057	3.87326	0.89141
H	1.44840	5.31846	0.32035
H	1.63497	3.88438	-0.77152
C	-1.17073	4.14326	-0.29348
H	-1.14093	5.24466	-0.27041
H	-2.18110	3.79690	-0.03415
H	-0.87712	3.76454	-1.28474

64

[Ir(C8H13)(py-ItBu')(kS-(CH3)2SO)]+ ==========

C	1.36005	-2.70369	2.42837
C	2.54232	-2.31469	1.85616
C	-0.99236	-1.72307	2.38876
C	4.00553	0.37618	1.29929
C	0.10884	1.70477	1.57242
C	-1.31145	2.09886	2.03804
C	-3.22962	-2.35651	1.45547
C	-2.06841	-1.57346	1.33179
C	0.90642	-1.03800	0.95813
C	0.96843	2.95876	1.27646
C	-2.02139	3.14488	1.16159
C	3.14306	-0.35104	0.24397
C	-4.29819	-2.18600	0.56790
C	4.03944	-1.13680	-0.73230
C	2.20185	0.66113	-0.50559
C	0.78564	3.49398	-0.17173
C	-2.30705	2.69810	-0.28625
C	-4.15723	-1.23154	-0.44571
C	-2.96660	-0.50351	-0.52331
C	0.17287	2.45888	-1.11737
C	-1.18302	2.07746	-1.11150
H	1.14145	-3.47340	3.16401
H	-1.22802	-2.59109	3.02175
H	-1.00028	-0.82601	3.03818
H	3.55054	-2.69384	1.99656
H	0.59005	1.15517	2.40382
H	4.64477	-0.32888	1.85762
H	-1.95383	1.20466	2.14443
H	-3.28888	-3.09437	2.26083
H	3.37678	0.92154	2.02259
H	0.73768	3.75333	2.01310

H	−2.98901	3.40784	1.62590
H	4.66805	1.09953	0.79661
H	2.03095	2.71438	1.43397
H	−1.43553	4.07949	1.16600
H	4.70233	−1.83746	−0.19487
H	−5.20862	−2.78435	0.66449
H	2.52933	1.67876	−0.25540
H	0.15225	4.39887	−0.18722
H	3.42387	−1.70032	−1.44967
H	4.68497	−0.43182	−1.28192
H	−3.16161	1.99693	−0.26700
H	1.75950	3.81132	−0.58105
H	−2.67523	3.57142	−0.86330
H	2.37231	0.54576	−1.58971
H	−4.94916	−1.04656	−1.17645
H	−2.82089	0.22668	−1.31862
H	0.71719	2.30924	−2.05835
H	−1.54420	1.65830	−2.06516
Ir	0.08541	0.41584	−0.13895
N	0.36032	−1.90308	1.86230
N	2.23991	−1.28682	0.96672
N	−1.92566	−0.63869	0.34268
H	−1.22044	2.52737	3.05811
S	0.22450	−1.08188	−2.21722
C	0.60940	−0.10955	−3.73509
H	−0.18416	0.63330	−3.91520
H	0.69475	−0.81070	−4.57907
H	1.57172	0.39547	−3.57090
C	−1.29477	−1.89053	−2.87672
H	−2.03947	−1.14453	−3.19262
H	−1.69833	−2.53350	−2.08284
H	−0.97114	−2.50722	−3.72912
O	1.25591	−2.19034	−2.09664

60

Complex 4 ==========

C	1.47049	−2.71931	2.30032
C	2.63240	−2.33234	1.68245
C	−0.93635	−1.83103	2.22753
C	4.39656	−0.04195	0.56524
C	0.04155	1.54923	1.58557
C	−1.40470	1.84433	2.06297
C	−3.01778	−2.69224	1.10475
C	−1.95058	−1.77801	1.09858
C	0.95499	−1.07847	0.82368
C	0.83153	2.87196	1.40456
C	−2.17051	2.89233	1.23714
C	3.10927	−0.49927	−0.14666
C	−3.99652	−2.64079	0.10492
C	3.45330	−1.36619	−1.37595
C	2.20727	0.73311	−0.51802
C	0.65018	3.50086	−0.00594
C	−2.41676	2.49777	−0.23037
C	−3.86156	−1.67123	−0.89560
C	−2.76951	−0.79987	−0.84709

C	0.09587	2.51313	-1.03475
C	-1.23388	2.04784	-1.07851
H	1.28542	-3.46869	3.06556
H	-1.14580	-2.70327	2.86386
H	-1.03002	-0.92494	2.85489
H	3.64925	-2.69293	1.80901
H	0.53858	0.98076	2.39620
H	5.06002	-0.88957	0.81125
H	-2.00670	0.91630	2.10799
H	-3.07516	-3.43923	1.90193
H	4.16394	0.50467	1.49383
H	0.53971	3.59660	2.19003
H	-3.15484	3.07208	1.70658
H	4.95964	0.63306	-0.09951
H	1.90419	2.68098	1.57456
H	-1.64304	3.85973	1.29051
H	4.04015	-2.25497	-1.08730
H	-4.83538	-3.34267	0.10644
H	2.54973	1.59888	0.06660
H	-0.01973	4.37888	0.03347
H	2.53488	-1.70403	-1.88077
H	4.05517	-0.78031	-2.08992
H	-3.18484	1.70126	-0.25530
H	1.61710	3.88257	-0.37426
H	-2.88109	3.35512	-0.76034
H	2.36964	0.96809	-1.58360
H	-4.58757	-1.57941	-1.70790
H	-2.62914	-0.04458	-1.62146
H	0.65373	2.45548	-1.97829
H	-1.54388	1.66219	-2.06271
Ir	0.10540	0.40198	-0.20580
N	0.44742	-1.93416	1.75602
N	2.29138	-1.31877	0.78930
N	-1.82444	-0.82131	0.13021
H	-1.34639	2.21901	3.10612
N	0.11001	-0.54953	-2.14600
C	0.09407	-0.95170	-3.24894
C	0.08877	-1.45749	-4.61759
H	-0.46242	-2.41092	-4.67068
H	-0.39212	-0.73141	-5.29377
H	1.12206	-1.62837	-4.96255

54

[Ir(C8H13)(py-ItBu')]+ ==========

C	-1.67055	3.03644	1.48583
C	-2.78526	2.50866	0.87854
C	0.78217	2.24623	1.64280
C	-4.47016	0.05892	-0.09426
C	0.10330	-1.34082	1.57666
C	1.58374	-1.44545	1.98017
C	2.71728	3.11913	0.28374
C	1.76647	2.10834	0.49356
C	-1.04283	1.14635	0.40738
C	-0.62164	-2.70204	1.55915
C	2.40837	-2.52176	1.25526

C	-3.07660	0.38065	-0.65955
C	3.63179	3.01952	-0.77269
C	-3.18282	1.02038	-2.06128
C	-2.15267	-0.88742	-0.68376
C	-0.40167	-3.49932	0.24458
C	2.56851	-2.29575	-0.26207
C	3.54966	1.90033	-1.60892
C	2.58132	0.92751	-1.34223
C	0.03151	-2.60743	-0.92045
C	1.31394	-2.04224	-1.09096
H	-1.54929	3.92427	2.10123
H	0.93379	3.21242	2.14552
H	0.94893	1.44846	2.38952
H	-3.81162	2.86476	0.86606
H	-0.41546	-0.66368	2.27933
H	-5.13822	0.93779	-0.11213
H	2.08273	-0.46362	1.88416
H	2.73284	3.98450	0.95290
H	-4.40455	-0.31352	0.94126
H	-0.29290	-3.29439	2.43616
H	3.41871	-2.55360	1.70097
H	-4.94172	-0.72249	-0.71169
H	-1.69999	-2.52830	1.70182
H	1.97146	-3.51458	1.45425
H	-3.75009	1.96600	-2.03277
H	4.37821	3.80078	-0.94195
H	-2.53668	-1.62140	0.04390
H	0.34303	-4.30268	0.38376
H	-2.17920	1.22982	-2.47047
H	-3.70117	0.33335	-2.74980
H	3.26749	-1.45203	-0.41817
H	-1.33885	-4.00841	-0.03411
H	3.08050	-3.17589	-0.70143
H	-2.24832	-1.34888	-1.68338
H	4.22340	1.76750	-2.45943
H	2.49399	0.04685	-1.98016
H	-0.56218	-2.72220	-1.83584
H	1.54460	-1.76871	-2.13470
Ir	-0.09421	-0.43924	-0.33423
N	-0.60897	2.17961	1.18345
N	-2.37599	1.34629	0.23409
N	1.70097	0.99666	-0.30535
H	1.58966	-1.68023	3.06633

56

Complex 5 ==========

C	1.47091	-3.09560	1.65000
C	2.63668	-2.61349	1.10983
C	-0.93333	-2.19581	1.73159
C	4.43714	-0.20004	0.37383
C	-0.02283	1.20695	1.69564
C	-1.48504	1.41796	2.16547
C	-3.02508	-2.86571	0.50363
C	-1.95714	-1.96180	0.63369
C	0.96967	-1.22875	0.48178

C	0.78172	2.52607	1.80028
C	-2.21187	2.61841	1.53562
C	3.12324	-0.48988	-0.37754
C	-4.01141	-2.65672	-0.46791
C	3.42489	-1.10156	-1.76164
C	2.24713	0.80572	-0.45647
C	0.66953	3.41529	0.52834
C	-2.40738	2.52036	0.01303
C	-3.89045	-1.53886	-1.30116
C	-2.79997	-0.68209	-1.12231
C	0.12670	2.67403	-0.69306
C	-1.20316	2.24965	-0.87480
H	1.28134	-3.96524	2.27384
H	-1.13945	-3.15873	2.22089
H	-1.02030	-1.40326	2.49733
H	3.65164	-2.99526	1.17330
H	0.43936	0.48861	2.40100
H	5.09415	-1.08610	0.41201
H	-2.08979	0.50762	1.99399
H	-3.07474	-3.73293	1.16845
H	4.24398	0.14351	1.40322
H	0.46132	3.09662	2.69434
H	-3.21177	2.71619	1.99564
H	4.98966	0.59272	-0.15592
H	1.84505	2.29591	1.98047
H	-1.68115	3.55023	1.79490
H	4.01043	-2.03086	-1.66164
H	-4.84593	-3.35551	-0.57553
H	2.51610	1.46687	0.37800
H	0.02206	4.29258	0.71050
H	2.50438	-1.33718	-2.31733
H	4.01853	-0.39188	-2.36042
H	-3.17681	1.75454	-0.19898
H	1.65866	3.82808	0.26952
H	-2.84875	3.46852	-0.35832
H	2.48371	1.33121	-1.39504
H	-4.61953	-1.32470	-2.08684
H	-2.66963	0.18786	-1.76826
H	0.71274	2.79792	-1.61275
H	-1.48539	2.08346	-1.92497
Ir	0.12320	0.40135	-0.33150
N	0.45185	-2.22407	1.24891
N	2.30284	-1.45889	0.40588
N	-1.84744	-0.86237	-0.16983
H	-1.47320	1.57432	3.26393
C	0.16624	-0.11732	-2.20798
O	0.11615	-0.32531	-3.35543
6			
CH3CN	==========	==========	==========
N	-1.45060	0.00000	0.00002
C	-0.27711	-0.00002	-0.00003
C	1.18502	0.00000	0.00001
H	1.56890	-0.25949	1.00012
H	1.56895	-0.73635	-0.72477

```
H                1.56888            0.99588           -0.27530
2
CO ============================================================
C                0.00000            0.00000           -0.65714
O                0.00000            0.00000            0.49286
5
CH2Cl2 ========================================================
C                0.00000            0.00000            0.76745
H               -0.90778            0.00000            1.38252
H                0.90778            0.00000            1.38252
Cl               0.00000            1.50375           -0.21676
Cl               0.00000           -1.50375           -0.21676
10
(CH3)2SO ======================================================
S                0.25860            0.43671            0.00000
O               -1.09768            1.12982            0.00000
C                0.25860           -0.81506            1.36819
H               -0.62952           -1.46033            1.27718
H                1.18586           -1.40920            1.32906
H                0.21406           -0.25303            2.31276
C                0.25860           -0.81506           -1.36819
H               -0.62952           -1.46033           -1.27718
H                0.21406           -0.25303           -2.31276
H                1.18586           -1.40920           -1.32906
54
Complex 8 =====================================================
Rh               0.59679           -0.38725           -0.05085
N               -1.23968            1.35479            1.40742
C               -1.26677            0.30139            0.52053
N                0.94617            1.68796           -0.47681
C                2.38553           -1.11161           -1.14091
N               -2.60333            0.13891            0.23189
C                0.33417           -2.53965            0.20228
C                0.95388            3.95006            0.37432
C                1.34929           -3.37982           -0.57469
C               -4.55786           -0.32012           -1.24609
C                0.02268            2.01795            1.76806
C               -3.21522           -0.87019           -0.71656
C                0.57644           -1.92633            1.45934
C               -2.26846           -1.06789           -1.91626
C               -3.37193            1.06088            0.95157
C                2.14665           -2.53849           -1.60320
C                1.50088            4.42373           -0.82817
C                2.79877           -0.71553            0.14272
C               -3.47247           -2.17780            0.06260
C               -2.51567            1.83591            1.67981
C                0.67654            2.58464            0.51824
C                3.12348           -1.67360            1.28487
C                1.90082           -1.92753            2.20509
C                1.44808            2.15647           -1.64806
C                1.73651            3.50914           -1.86254
H                1.85536           -1.14238            2.98136
H                2.02120           -2.88431            2.75358
H                3.50156           -2.62438            0.87449
```

H	3.94742	-1.25249	1.88507
H	3.21016	0.29769	0.24103
H	2.54645	-0.39295	-1.95774
H	-0.29716	-1.75628	2.10422
H	-0.71193	-2.76794	-0.02863
H	0.81512	-4.18545	-1.10593
H	2.03133	-3.88679	0.12904
H	1.58449	-2.49523	-2.55252
H	3.11044	-3.03072	-1.84412
H	0.68800	1.27454	2.24135
H	-0.19761	2.81732	2.49163
H	0.73720	4.63476	1.19954
H	1.72489	5.48662	-0.95625
H	2.14086	3.82738	-2.82688
H	1.61775	1.41210	-2.42964
H	-2.70454	2.66017	2.36280
H	-4.45389	1.09665	0.88920
H	-3.92034	-2.93161	-0.60520
H	-4.17278	-2.00285	0.89639
H	-2.54536	-2.59643	0.48334
H	-4.44137	0.68271	-1.68907
H	-5.34192	-0.28576	-0.47203
H	-4.92078	-0.99717	-2.03549
H	-2.66499	-1.86610	-2.56469
H	-2.20170	-0.14209	-2.51209
H	-1.24773	-1.34435	-1.59996

60

[Rh(C8H13)(py-ItBu')(NCMe)]+ ==========

C	-1.42800	-2.67011	-2.28961
C	-2.59523	-2.31929	-1.66040
C	0.96002	-1.74589	-2.22606
C	-4.41505	-0.08792	-0.48998
C	-0.11363	1.61063	-1.55290
C	1.33006	1.92267	-2.01521
C	3.04454	-2.60837	-1.10371
C	1.97332	-1.69842	-1.09538
C	-0.94647	-1.01310	-0.81740
C	-0.93139	2.90862	-1.35793
C	2.08370	2.98831	-1.20104
C	-3.09985	-0.51700	0.18859
C	4.01492	-2.55705	-0.09530
C	-3.39339	-1.41310	1.41031
C	-2.22581	0.73050	0.55859
C	-0.73888	3.55431	0.04411
C	2.34750	2.60076	0.26484
C	3.86833	-1.59484	0.91075
C	2.77131	-0.72818	0.85740
C	-0.15199	2.59039	1.07436
C	1.17375	2.15651	1.12270
H	-1.22769	-3.41305	-3.05746
H	1.16918	-2.61394	-2.86830
H	1.05205	-0.83698	-2.84919
H	-3.60209	-2.71014	-1.77680
H	-0.59850	1.02337	-2.35534

H	−5.05530	−0.95269	−0.73808
H	1.94530	1.00428	−2.05485
H	3.11207	−3.35028	−1.90500
H	−4.21933	0.48195	−1.41306
H	−0.66948	3.63454	−2.15390
H	3.06126	3.17885	−1.67999
H	−4.98628	0.55631	0.19790
H	−2.00136	2.69138	−1.50953
H	1.54223	3.94775	−1.25482
H	−3.96545	−2.31053	1.11864
H	4.85746	−3.25469	−0.09456
H	−2.58517	1.59847	−0.01099
H	−0.08751	4.44468	−0.01731
H	−2.45513	−1.73733	1.88648
H	−3.99240	−0.85528	2.14883
H	3.11619	1.80527	0.28566
H	−1.70740	3.92229	0.42177
H	2.81646	3.46072	0.78703
H	−2.35504	0.94703	1.63179
H	4.58871	−1.50585	1.72847
H	2.62291	0.02348	1.63496
H	−0.72874	2.47586	2.00050
H	1.48251	1.72577	2.08732
Rh	−0.13362	0.45909	0.21914
N	−0.42400	−1.85451	−1.75569
N	−2.27426	−1.29493	−0.77267
N	1.83501	−0.74951	−0.12506
N	−0.09088	−0.51129	2.19612
C	−0.06677	−0.89573	3.30411
C	−0.05269	−1.37392	4.68303
H	0.38446	−2.38488	4.73273
H	0.54335	−0.69656	5.31685
H	−1.08106	−1.41326	5.07909
H	1.26565	2.28763	−3.06233

54

[Rh(C8H13)(py−ItBu’)]+ ==========

C	1.03099	−3.31268	1.25037
C	2.21650	−2.99097	0.63704
C	−1.19994	−2.07409	1.54456
C	4.04369	−0.38511	0.37173
C	0.45157	1.36045	1.44028
C	−0.90594	1.78111	2.02345
C	−3.33695	−2.51297	0.27591
C	−2.20365	−1.70646	0.46609
C	0.76650	−1.29192	0.25595
C	1.45979	2.50702	1.25856
C	−1.57371	3.01648	1.39820
C	2.97877	−0.83391	−0.65037
C	−4.27151	−2.18368	−0.71503
C	3.64036	−1.56764	−1.83488
C	2.10451	0.36363	−1.14357
C	1.20408	3.37297	−0.00465
C	−1.99185	2.84499	−0.07598
C	−4.02748	−1.05081	−1.49960

C	−2.87819	−0.29253	−1.24853
C	0.42562	2.62167	−1.08207
C	−0.94634	2.36193	−1.07040
H	0.74265	−4.18964	1.82458
H	−1.50122	−3.01339	2.03052
H	−1.16962	−1.28830	2.32164
H	3.14934	−3.54499	0.57912
H	0.89556	0.58368	2.08741
H	4.62052	−1.24347	0.75562
H	−1.60974	0.92737	2.00597
H	−3.48023	−3.39631	0.90538
H	3.58047	0.13003	1.22899
H	1.45922	3.13909	2.17057
H	−2.48177	3.25853	1.97885
H	4.75302	0.30692	−0.11057
H	2.47041	2.07457	1.19113
H	−0.91203	3.89077	1.51475
H	4.26365	−2.41271	−1.49444
H	−5.15996	−2.80193	−0.87261
H	2.68964	1.29231	−1.05936
H	0.66435	4.30174	0.25034
H	2.88193	−1.95058	−2.53751
H	4.29726	−0.87116	−2.38034
H	−2.85826	2.15887	−0.11891
H	2.16929	3.69883	−0.42663
H	−2.37677	3.81467	−0.45344
H	1.85832	0.22023	−2.21895
H	−4.71201	−0.74543	−2.29535
H	−2.66748	0.59618	−1.84658
H	0.92093	2.54192	−2.05802
H	−1.36638	2.10203	−2.05522
Rh	0.13786	0.45286	−0.42116
N	0.15360	−2.25327	1.00711
N	2.02910	−1.74923	0.03744
N	−1.97120	−0.58588	−0.27979
H	−0.72631	1.99514	3.09948