SUPPORTING INFORMATION FOR

*Steric effects determine the mechanisms of reactions between bis(*N*-heterocyclic carbene)-nickel(0) complexes and aryl halides*

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CONTENTS

COMPUTATIONAL DETAILS

- All calculations in this manuscript were carried out using Gaussian 09 (Revision D. 01).[1]
- The nature of all stationary points was verified using frequency calculations.
- The B3LYP density functional[2-4] was used with Grimme's D3 dispersion corrections.[5] This is the same functional that was used during our previous study, and was shown to be appropriate to model the processes that are under investigation.[6] The inclusion of dispersion corrections renders this level of theory appropriate for the study of transition metal complexes.[7]
- The 6-31G(d) basis set was used for H/C/N/Cl atoms during optimisation and frequency calculations. The 6-311+G(d,p) basis set was used for H/C/N/Cl when refining the energies using single point calculations.
- Throughout this work, LANL2TZ(f) was used for Ni, and LANL2DZ(dp) was used for Br and I.[8-10]
- All calculations were carried out in THF solvent using the SMD model.[11]
- Energies for open shell singlet structures were corrected using Yamaguchi's equation (see Supporting Information) to account for spin contamination when $\langle S^2 \rangle_{OSS} \neq 0$.[12-16]
    - $E_{singlet} = (2E_{oss} - E_{triplet} \cdot \langle S^2 \rangle_{OSS}) / (2 - \langle S^2 \rangle_{OSS})$

FORMATION OF $[Ni(NHC)_2]$ FROM $[Ni(COD)_2]$

Table S1. Formation of $[Ni(ITMe)_2]$ (**A-1**), $[Ni(IMes)_2]$ (**B-1**), $[Ni(IXy)_2]$ (**C-1**), and $[Ni(IPhen)_2]$ (**D-1**) from $[Ni(COD)_2]$. Energies are in kcal mol^{-1} in THF solution, relative to $[Ni(NHC)_2]$.

NHC	$[Ni(COD)_2$		[Ni(COD)(NHC)]		$[Ni(NHC)_2]$		
	H_{rel}	G_{rel}	H_{rel}	G_{rel}	Complex	H_{rel}	G_{rel}
ITMe	0.2	5.1	17.8	14.6	**A-1**	0.0	0.0
IMes	17.1	15.7	8.4	10.1	**B-1**	0.0	0.0
IXy	15.8	15.8	16.5	13.8	**C-1**	0.0	0.0
IPhen	9.7	11.0	12.1	11.2	**D-1**	0.0	0.0

ENTHALPIES FOR ALL STRUCTURES

Table S2. Enthalpies of the species considered in this work. Enthalpies are in kcal mol^{-1} in THF solution, relative to $[Ni(NHC)_2]$.

Structure	H_{rel} (kcal mol^{-1})			
	ITMe (A)	IMes (B)	IXy (C)	IPhen (D)
X-1	0.0	0.0	0.0	0.0
X-2-Cl	-16.8	7.3	7.1	-11.1
X-2-Br	-17.8	7.4	- [a]	- [a]
X-2-I	- [b]	5.7	- [a]	- [a]
TS-X-2-3-Cl	-16.6	9.9	9.7	-11.4
TS-X-2-3-Br	- [b]	7.9	- [a]	- [a]
TS-X-2-3-I	- [b]	- [b]	- [a]	- [a]
X-3-Cl	-60.5	-29.5	-28.7	-50.4
X-3-Br	-59.5	-28.5	- [a]	- [a]
X-3-I	-63.3	-31.8	- [a]	- [a]
X-4-Cl	-64.9	-54.5	-53.6	-59.6
X-4-Br	-64.4	-51.2	- [a]	- [a]
X-4-I	-68.8	-51.9	- [a]	- [a]
X-5-Cl	-2.3	-3.4	-3.8	0.3
X-5-Br	-3.1	-4.5	- [a]	- [a]
X-5-I	-9.7	-10.9	- [a]	- [a]
TS-X-5-6-Cl	0.7	2.8	2.8	7.1
TS-X-5-6-Br	-1.5	-5.4	- [a]	- [a]
TS-X-5-6-I	-10.6	1.0	- [a]	- [a]
X-6-Cl	-8.9	-6.7	-5.4	-3.3
X-6-Br	-7.9	-5.7	- [a]	- [a]
X-6-I	-14.0	-11.5	- [a]	- [a]
X-7-Cl	-29.1	-26.9	-25.7	-23.5
X-7-Br	-28.2	-25.9	- [a]	- [a]
X-7-I	-34.3	-31.1	- [a]	- [a]
X-2'	- [a]	26.2	- [a]	- [a]
TS-X-2'-3'	- [a]	31.4	- [a]	- [a]
X-3'	- [a]	-16.1	- [a]	- [a]

a) Not studied. b) Could not be located.

ELECTRONIC ENERGIES FOR THE DISTORTION OF [Ni(IMes)$_2$] (B-1)

Table S3. Electronic energies of the [Ni(IMes)$_2$] fragment, relative to [Ni(IMes)$_2$] (**B-1**).

Ni(IMes)$_2$ Fragment From	**Electronic Energy (kcal mol^{-1})**
[Ni(IMes)$_2$] (**B-1**)	0.0
[Ni(IMes)$_2$(η^2-PhCl) (**B-2-Cl**)	38.0
[Ni(IMes)$_2$(η^2-PhBr) (**B-2-Br**)	39.4
[Ni(IMes)$_2$(η^2-PhI) (**B-2-I**)	40.1

FREE ENERGY PROFILES FOR THE REACTIONS OF [Ni(IXy)$_2$] (C-1)

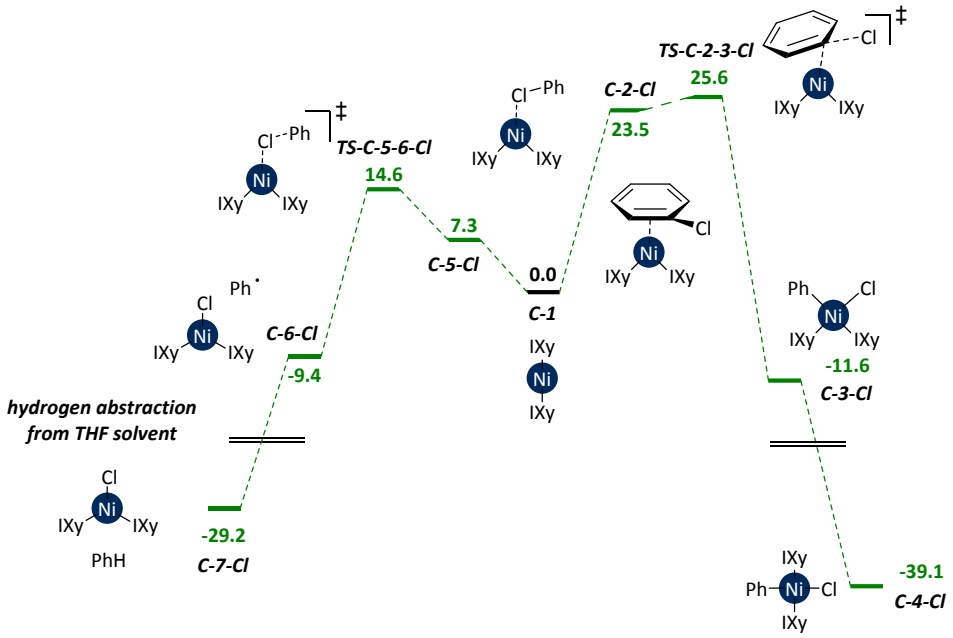

Figure S1. Free energy profiles for the reactions of [Ni(IXy)$_2$] (**C-1**) with PhCl. Energies are free energies in kcal mol^{-1} in THF solution, relative to **C-1**.

CARTESIAN COORDINATES AND POTENTIAL ENERGIES FOR ALL STRUCTURES

large_basis_TS-C-2-3-Cl_NiIXy2_OA_PhCl_bb

Energy (POTENTIAL) = -2552.99075166 Eh

	Atom	X	Y	Z
1	C	1.6848	2.2360	0.0365
2	C	2.6691	2.5005	-0.8429
3	C	2.3783	0.2065	-0.8238
4	N	1.5004	0.8528	0.0338
5	N	3.0829	1.2714	-1.3564
6	Ni	2.6684	-1.6711	-1.3305
7	C	4.3223	-2.9146	-1.2155
8	N	5.0569	-3.2226	-0.0907
9	N	4.7695	-3.8695	-2.1118
10	C	5.9002	-4.3155	-0.2806
11	C	5.7201	-4.7209	-1.5556
12	H	6.5472	-4.6785	0.5029
13	H	6.1719	-5.5181	-2.1252
14	H	1.0898	2.8844	0.6599
15	H	3.1154	3.4295	-1.1606
16	C	4.4764	-3.9539	-3.5166
17	C	3.7868	-5.0744	-4.0091
18	C	5.0001	-2.9609	-4.3618
19	C	3.5690	-5.1502	-5.3919
20	C	4.7441	-3.0659	-5.7334
21	C	4.0292	-4.1493	-6.2462
22	H	3.0244	-6.0012	-5.7931
23	H	5.1302	-2.3015	-6.4028
24	C	5.2075	-2.4247	1.0976
25	C	6.1143	-1.3513	1.0446
26	C	4.5915	-2.8347	2.2886
27	C	6.3351	-0.6223	2.2188
28	C	4.8618	-2.0950	3.4478
29	C	5.7106	-0.9897	3.4120
30	H	7.0232	0.2188	2.1988
31	H	4.3909	-2.3890	4.3821
32	C	0.4041	0.3103	0.7931
33	C	-0.9049	0.6842	0.4299
34	C	0.6652	-0.4732	1.9257
35	C	-1.9640	0.2112	1.2160
36	C	-0.4203	-0.9190	2.6869
37	C	-1.7270	-0.5862	2.3345
38	H	-2.9821	0.4752	0.9411
39	H	-0.2312	-1.5348	3.5625
40	C	4.0852	1.2529	-2.3871
41	C	5.3910	1.6534	-2.0502
42	C	3.6944	1.0125	-3.7180
43	C	6.3308	1.7665	-3.0840
44	C	4.6608	1.1565	-4.7198
45	C	5.9684	1.5290	-4.4086
46	H	7.3485	2.0617	-2.8412
47	H	4.3784	0.9729	-5.7532
48	C	5.8609	-1.8559	-3.8089
49	H	5.2793	-1.1683	-3.1910

50	H	6.6582	-2.2639	-3.1760
51	H	6.3223	-1.2828	-4.6152
52	C	3.2978	-6.1786	-3.1017
53	H	4.0672	-6.9505	-2.9682
54	H	3.0356	-5.8131	-2.1045
55	H	2.4158	-6.6658	-3.5295
56	C	3.6575	-4.0164	2.3148
57	H	4.1404	-4.9222	1.9290
58	H	3.3164	-4.2210	3.3343
59	H	2.7777	-3.8318	1.6877
60	C	6.8713	-1.0481	-0.2234
61	H	7.4325	-1.9284	-0.5607
62	H	6.1977	-0.7680	-1.0374
63	H	7.5832	-0.2340	-0.0681
64	C	5.7678	2.0124	-0.6326
65	H	5.4282	3.0247	-0.3796
66	H	5.3205	1.3320	0.0974
67	H	6.8537	1.9932	-0.5057
68	C	2.2815	0.6220	-4.0571
69	H	1.5554	1.3157	-3.6169
70	H	2.1304	0.6044	-5.1406
71	H	2.0522	-0.3705	-3.6616
72	C	-1.1956	1.5695	-0.7617
73	H	-0.4877	1.4049	-1.5789
74	H	-2.2045	1.3768	-1.1411
75	H	-1.1441	2.6324	-0.4933
76	C	2.0738	-0.8213	2.3029
77	H	2.6881	0.0751	2.4535
78	H	2.0993	-1.4134	3.2210
79	H	2.5466	-1.3981	1.5054
80	C	0.9066	-2.2221	-1.7824
81	C	-0.2381	-1.4415	-2.1133
82	C	1.4555	-3.0738	-2.7821
83	C	-0.6387	-1.3303	-3.4314
84	H	-0.7667	-0.9274	-1.3248
85	C	1.0348	-2.9312	-4.1218
86	H	2.0608	-3.9176	-2.4946
87	C	0.0153	-2.0517	-4.4582
88	H	-1.4741	-0.6771	-3.6769
89	H	1.4894	-3.5620	-4.8802
90	H	-0.3172	-1.9586	-5.4888
91	Cl	0.6722	-3.2541	-0.0011
92	H	-2.5607	-0.9448	2.9327
93	H	6.7065	1.6318	-5.1999
94	H	3.8414	-4.2194	-7.3144
95	H	5.9008	-0.4233	4.3201

large_basis_TS-B-5-6-Cl_NiIMes2_ossts_PhCl_t_bb
Energy (POTENTIAL) = -2710.30413986 Eh

	Atom	X	Y	Z
1	C	-0.5099	1.0261	0.0647
2	C	0.5237	1.8105	-0.3262
3	C	1.2463	-0.3637	-0.4250
4	N	-0.0564	-0.2896	0.0016
5	N	1.5808	0.9512	-0.6206
6	Ni	2.3399	-1.8916	-0.6853
7	C	3.4367	-3.3434	-1.2191
8	N	4.7224	-3.6484	-0.8444
9	N	3.1149	-4.3657	-2.0730
10	C	5.1757	-4.8199	-1.4471
11	C	4.1612	-5.2745	-2.2219
12	H	6.1670	-5.2070	-1.2695
13	H	4.0780	-6.1433	-2.8564
14	H	-1.5144	1.2699	0.3743
15	H	0.6126	2.8816	-0.4234
16	C	1.8393	-4.5201	-2.7145
17	C	0.7954	-5.1374	-2.0069
18	C	1.6904	-4.0878	-4.0412
19	C	-0.4095	-5.3545	-2.6817
20	C	0.4597	-4.3116	-4.6689
21	C	-0.5960	-4.9509	-4.0089
22	H	-1.2251	-5.8423	-2.1534
23	H	0.3252	-3.9802	-5.6963
24	C	5.5124	-2.8580	0.0578
25	C	6.0318	-1.6326	-0.3889
26	C	5.7604	-3.3455	1.3508
27	C	6.7943	-0.8782	0.5091
28	C	6.5296	-2.5547	2.2120
29	C	7.0446	-1.3156	1.8145
30	H	7.2000	0.0744	0.1779
31	H	6.7238	-2.9150	3.2199
32	C	-0.8612	-1.4297	0.3396
33	C	-1.3564	-2.2413	-0.6926
34	C	-1.1433	-1.6866	1.6914
35	C	-2.1371	-3.3474	-0.3383
36	C	-1.9287	-2.8037	1.9950
37	C	-2.4254	-3.6504	0.9966
38	H	-2.5257	-3.9860	-1.1275
39	H	-2.1515	-3.0202	3.0377
40	C	2.8808	1.4055	-1.0295
41	C	3.8797	1.5565	-0.0558
42	C	3.0986	1.7199	-2.3804
43	C	5.1163	2.0676	-0.4639
44	C	4.3552	2.2154	-2.7428
45	C	5.3719	2.4033	-1.7979
46	H	5.8996	2.1972	0.2788
47	H	4.5434	2.4605	-3.7860
48	C	2.8163	-3.3777	-4.7511
49	H	3.0777	-2.4482	-4.2293

50	H	3.7268	-3.9879	-4.7853
51	H	2.5359	-3.1260	-5.7786
52	C	0.9598	-5.5021	-0.5547
53	H	1.8604	-6.1045	-0.3844
54	H	1.0665	-4.5921	0.0485
55	H	0.0944	-6.0627	-0.1888
56	C	-1.9304	-5.1498	-4.6869
57	H	-2.4088	-6.0821	-4.3662
58	H	-2.6194	-4.3306	-4.4375
59	H	-1.8320	-5.1719	-5.7777
60	C	5.2075	-4.6725	1.8076
61	H	5.7250	-5.5132	1.3279
62	H	5.3169	-4.7869	2.8900
63	H	4.1446	-4.7550	1.5625
64	C	5.7571	-1.1288	-1.7822
65	H	5.8971	-1.9165	-2.5317
66	H	4.7177	-0.7883	-1.8626
67	H	6.4125	-0.2904	-2.0315
68	C	7.8253	-0.4539	2.7784
69	H	7.1715	0.2879	3.2573
70	H	8.2801	-1.0510	3.5763
71	H	8.6225	0.0998	2.2688
72	C	3.6308	1.1414	1.3710
73	H	2.7454	1.6378	1.7874
74	H	3.4452	0.0618	1.4240
75	H	4.4893	1.3788	2.0061
76	C	2.0139	1.5005	-3.4056
77	H	1.1163	2.0896	-3.1811
78	H	2.3588	1.7756	-4.4070
79	H	1.7055	0.4477	-3.4250
80	C	6.7335	2.9007	-2.2207
81	H	6.6615	3.6509	-3.0166
82	H	7.2786	3.3448	-1.3807
83	H	7.3471	2.0761	-2.6097
84	C	-1.0339	-1.9541	-2.1361
85	H	-1.1239	-0.8866	-2.3672
86	H	0.0004	-2.2466	-2.3562
87	H	-1.6963	-2.5114	-2.8035
88	C	-0.6070	-0.7966	2.7845
89	H	-1.0963	0.1857	2.7836
90	H	-0.7662	-1.2493	3.7675
91	H	0.4669	-0.6313	2.6567
92	C	-3.2268	-4.8795	1.3537
93	H	-2.5689	-5.7487	1.4905
94	H	-3.7802	-4.7423	2.2894
95	H	-3.9440	-5.1357	0.5658
96	C	2.2979	-3.1134	3.7016
97	C	1.1611	-3.7110	4.2313
98	C	3.4232	-2.8626	4.4768
99	C	1.1519	-4.0709	5.5861
100	H	0.2918	-3.8940	3.6020
101	C	3.4105	-3.2255	5.8306
102	H	4.3012	-2.3953	4.0347

103	C	2.2754	-3.8282	6.3846
104	H	0.2693	-4.5398	6.0178
105	H	4.2846	-3.0372	6.4516
106	H	2.2664	-4.1082	7.4350
107	Cl	2.3141	-2.5660	1.7064

large_basis_THF_THF_bb
Energy (POTENTIAL) = -232.533030898 Eh

	Atom	X	Y	Z
1	C	0.6701	0.6052	0.8900
2	O	1.7199	-0.1900	0.3188
3	C	2.4914	0.6124	-0.5897
4	C	2.0440	2.0628	-0.3776
5	C	0.5770	1.8715	0.0347
6	H	-0.2542	0.0149	0.8954
7	H	0.9214	0.8529	1.9338
8	H	3.5576	0.4551	-0.3846
9	H	2.2918	0.2850	-1.6220
10	H	2.6105	2.5224	0.4416
11	H	2.1731	2.6790	-1.2726
12	H	0.1592	2.7225	0.5817
13	H	-0.0462	1.6888	-0.8494

large_basis_B-5-Br_NiIMes2_BrPh_bb
Energy (POTENTIAL) = -2263.28686329 Eh

	Atom	X	Y	Z
1	C	-0.0388	-0.0133	-0.1505
2	C	1.0120	0.7370	-0.5602
3	C	1.6727	-1.4650	-0.6568
4	N	0.3725	-1.3431	-0.2129
5	N	2.0404	-0.1541	-0.8630
6	Ni	2.6947	-3.0035	-0.9323
7	C	3.7111	-4.5114	-1.3575
8	N	5.0066	-4.8336	-1.0075
9	N	3.3331	-5.5917	-2.1218
10	C	5.4048	-6.0585	-1.5396
11	C	4.3509	-6.5367	-2.2429
12	H	6.3909	-6.4617	-1.3680
13	H	4.2229	-7.4448	-2.8120
14	H	-1.0299	0.2638	0.1741
15	H	1.1302	1.8045	-0.6666
16	C	2.0438	-5.7530	-2.7312
17	C	1.0069	-6.3388	-1.9878
18	C	1.8760	-5.3726	-4.0716
19	C	-0.2095	-6.5750	-2.6353
20	C	0.6364	-5.6152	-4.6736
21	C	-0.4130	-6.2233	-3.9749
22	H	-1.0193	-7.0387	-2.0771
23	H	0.4893	-5.3233	-5.7112
24	C	5.8579	-4.0140	-0.1945
25	C	6.3798	-2.8282	-0.7358
26	C	6.1678	-4.4333	1.1114
27	C	7.2112	-2.0471	0.0753
28	C	6.9964	-3.6148	1.8847
29	C	7.5238	-2.4169	1.3870
30	H	7.6182	-1.1247	-0.3304
31	H	7.2303	-3.9191	2.9033
32	C	-0.4621	-2.4496	0.1565
33	C	-0.9850	-3.2759	-0.8537
34	C	-0.7530	-2.6611	1.5130
35	C	-1.7967	-4.3464	-0.4687
36	C	-1.5670	-3.7498	1.8492
37	C	-2.0903	-4.6064	0.8760
38	H	-2.2056	-4.9956	-1.2385
39	H	-1.7894	-3.9331	2.8984
40	C	3.3391	0.2689	-1.3041
41	C	4.3619	0.4140	-0.3542
42	C	3.5336	0.5742	-2.6610
43	C	5.5966	0.9049	-0.7908
44	C	4.7894	1.0484	-3.0535
45	C	5.8294	1.2267	-2.1324
46	H	6.3977	1.0269	-0.0658
47	H	4.9592	1.2839	-4.1021
48	C	2.9943	-4.6911	-4.8190
49	H	3.2643	-3.7497	-4.3236
50	H	3.9019	-5.3064	-4.8465
51	H	2.7011	-4.4675	-5.8495

52	C	1.1951	-6.6504	-0.5264
53	H	2.0805	-7.2744	-0.3532
54	H	1.3472	-5.7203	0.0346
55	H	0.3224	-7.1676	-0.1161
56	C	-1.7565	-6.4446	-4.6278
57	H	-1.6721	-6.5055	-5.7183
58	H	-2.2313	-7.3648	-4.2685
59	H	-2.4424	-5.6168	-4.3995
60	C	5.6378	-5.7297	1.6745
61	H	6.2874	-6.5750	1.4087
62	H	5.5865	-5.6836	2.7669
63	H	4.6368	-5.9511	1.2975
64	C	6.0299	-2.3849	-2.1324
65	H	6.0798	-3.2159	-2.8455
66	H	4.9996	-2.0072	-2.1562
67	H	6.6997	-1.5904	-2.4728
68	C	8.4230	-1.5582	2.2451
69	H	9.4106	-2.0208	2.3763
70	H	8.5780	-0.5694	1.7998
71	H	8.0007	-1.4156	3.2472
72	C	4.1389	0.0051	1.0782
73	H	3.2730	0.5173	1.5162
74	H	3.9324	-1.0705	1.1295
75	H	5.0173	0.2223	1.6934
76	C	2.4241	0.3655	-3.6612
77	H	1.5422	0.9731	-3.4238
78	H	2.7525	0.6239	-4.6728
79	H	2.0974	-0.6820	-3.6611
80	C	7.1901	1.6985	-2.5864
81	H	7.1153	2.4346	-3.3950
82	H	7.7541	2.1512	-1.7635
83	H	7.7871	0.8587	-2.9686
84	C	-0.6581	-3.0338	-2.3043
85	H	-0.7836	-1.9787	-2.5757
86	H	0.3907	-3.2908	-2.5005
87	H	-1.2920	-3.6402	-2.9565
88	C	-0.2164	-1.7457	2.5861
89	H	-0.8326	-0.8420	2.6868
90	H	-0.2070	-2.2510	3.5567
91	H	0.8034	-1.4254	2.3590
92	C	-2.9303	-5.8026	1.2560
93	H	-3.2874	-5.7341	2.2891
94	H	-3.8029	-5.9057	0.5997
95	H	-2.3518	-6.7324	1.1683
96	Br	2.6993	-3.6976	1.8251
97	C	2.6875	-4.1471	3.7541
98	C	2.7328	-5.4857	4.1522
99	C	2.6300	-3.1232	4.7032
100	C	2.7190	-5.7992	5.5151
101	H	2.7797	-6.2751	3.4073
102	C	2.6166	-3.4464	6.0638
103	H	2.5932	-2.0851	4.3847
104	C	2.6604	-4.7825	6.4727
105	H	2.7542	-6.8407	5.8257
106	H	2.5713	-2.6505	6.8035

107	H	2.6494	-5.0297	7.5308

large_basis_TS-A-5-6-I_NiITMe2_IPh_ossts_t_bb
Energy (POTENTIAL) = -1179.64172017 Eh

	Atom	X	Y	Z
1	C	-0.9927	1.7727	0.1472
2	C	0.0286	2.5877	-0.2508
3	C	0.7618	0.4238	-0.4532
4	N	-0.5243	0.4664	0.0110
5	N	1.0803	1.7449	-0.6105
6	Ni	1.8537	-1.1003	-0.7579
7	C	2.8962	-2.6008	-1.2834
8	N	4.2191	-2.8604	-1.0528
9	N	2.4692	-3.7211	-1.9434
10	C	4.6039	-4.1091	-1.5394
11	C	3.4900	-4.6567	-2.1095
12	C	2.2763	-2.1725	4.1708
13	C	2.2468	-3.5036	4.5970
14	C	2.4463	-1.1476	5.1064
15	C	2.3851	-3.8091	5.9564
16	H	2.1170	-4.3067	3.8736
17	C	2.5852	-1.4540	6.4658
18	H	2.4720	-0.1086	4.7822
19	C	2.5545	-2.7849	6.8929
20	H	2.3611	-4.8471	6.2825
21	H	2.7170	-0.6524	7.1900
22	H	2.6624	-3.0223	7.9483
23	I	2.0641	-1.6791	1.9503
24	C	-1.3048	-0.7118	0.3569
25	H	-2.2467	-0.7225	-0.2009
26	H	-0.7165	-1.5929	0.0976
27	H	-1.5221	-0.7294	1.4297
28	C	2.3704	2.2174	-1.0884
29	H	2.8410	2.8678	-0.3441
30	H	3.0032	1.3438	-1.2579
31	H	2.2558	2.7714	-2.0260
32	C	0.1259	4.0737	-0.3346
33	H	-0.8125	4.5361	-0.0155
34	H	0.9270	4.4646	0.3060
35	H	0.3348	4.4094	-1.3586
36	C	-2.3657	2.0857	0.6377
37	H	-3.1378	1.6625	-0.0181
38	H	-2.5369	1.6835	1.6444
39	H	-2.5182	3.1677	0.6782
40	C	5.1126	-1.9632	-0.3367
41	H	6.0054	-1.7575	-0.9358
42	H	4.5756	-1.0329	-0.1480
43	H	5.4129	-2.4020	0.6202
44	C	1.0991	-3.9344	-2.3829
45	H	0.5275	-3.0344	-2.1471
46	H	1.0646	-4.1159	-3.4621
47	H	0.6575	-4.7902	-1.8614
48	C	3.2824	-5.9592	-2.8056
49	H	4.2085	-6.5409	-2.8083
50	H	2.5073	-6.5629	-2.3164
51	H	2.9735	-5.8171	-3.8495

52	C	5.9938	-4.6318	-1.4030
53	H	6.7217	-3.9969	-1.9247
54	H	6.3033	-4.6851	-0.3514
55	H	6.0648	-5.6383	-1.8245

large_basis_TS-D-5-6-Cl_NiIPhen2_ossts_PhCl_t_oss_bb
Energy (POTENTIAL) = -2238.33779493 Eh

	Atom	X	Y	Z
1	C	-0.2933	1.1673	0.5594
2	C	0.7123	1.8786	-0.0016
3	C	1.2008	-0.3461	-0.3015
4	N	0.0089	-0.1803	0.3616
5	N	1.6050	0.9499	-0.5312
6	Ni	2.2523	-1.8840	-0.6960
7	C	3.4867	-3.1882	-1.3216
8	N	4.7835	-3.3811	-0.9090
9	N	3.3277	-4.1469	-2.2939
10	C	5.3998	-4.4231	-1.6007
11	C	4.4867	-4.9010	-2.4781
12	H	6.4232	-4.7091	-1.4142
13	H	4.5409	-5.7076	-3.1925
14	H	-1.2030	1.4862	1.0435
15	H	0.8627	2.9423	-0.1022
16	C	2.1100	-4.3674	-3.0050
17	C	0.8984	-4.4070	-2.3055
18	C	2.1383	-4.5468	-4.3906
19	C	-0.2909	-4.6083	-3.0068
20	C	0.9428	-4.7618	-5.0809
21	C	-0.2734	-4.7868	-4.3936
22	H	-1.2320	-4.6362	-2.4643
23	H	0.9648	-4.8984	-6.1586
24	C	5.4239	-2.6271	0.1226
25	C	5.3476	-1.2311	0.1199
26	C	6.1212	-3.2995	1.1297
27	C	5.9590	-0.5095	1.1454
28	C	6.7421	-2.5672	2.1444
29	C	6.6575	-1.1724	2.1587
30	H	5.8926	0.5747	1.1416
31	H	7.2794	-3.0915	2.9299
32	C	-0.8229	-1.2488	0.8104
33	C	-1.0635	-2.3400	-0.0290
34	C	-1.3951	-1.1912	2.0837
35	C	-1.8668	-3.3871	0.4203
36	C	-2.2107	-2.2374	2.5192
37	C	-2.4446	-3.3399	1.6930
38	H	-2.0469	-4.2395	-0.2291
39	H	-2.6492	-2.1950	3.5124
40	C	2.8293	1.2876	-1.1795
41	C	3.6943	2.2132	-0.5905
42	C	3.1660	0.6660	-2.3876
43	C	4.9094	2.5117	-1.2125
44	C	4.3878	0.9612	-2.9943
45	C	5.2621	1.8823	-2.4093
46	H	5.5852	3.2262	-0.7510
47	H	4.6520	0.4722	-3.9278
48	C	2.1202	-3.5693	3.5566
49	C	0.9164	-3.9306	4.1488
50	C	3.3162	-3.5716	4.2639
51	C	0.9126	-4.3144	5.4971

52	H	-0.0077	-3.9116	3.5746
53	C	3.3069	-3.9562	5.6116
54	H	4.2443	-3.2768	3.7773
55	C	2.1063	-4.3274	6.2273
56	H	-0.0213	-4.6018	5.9771
57	H	4.2354	-3.9653	6.1800
58	H	2.1006	-4.6241	7.2733
59	Cl	2.1356	-2.9196	1.5793
60	H	3.4280	2.6720	0.3570
61	H	6.2120	2.1094	-2.8850
62	H	2.4772	-0.0441	-2.8330
63	H	7.1342	-0.6059	2.9540
64	H	-1.1811	-0.3498	2.7357
65	H	-3.0738	-4.1559	2.0377
66	H	-0.6084	-2.3649	-1.0123
67	H	3.0840	-4.5014	-4.9228
68	H	-1.2018	-4.9484	-4.9345
69	H	0.9008	-4.2765	-1.2291
70	H	6.1540	-4.3849	1.1317
71	H	4.8132	-0.7240	-0.6745

large_basis_TS-A-5-6-Cl_NiITMe2_ossts_PhCl_t_bb
Energy (POTENTIAL) = -1628.46336906 Eh

	Atom	X	Y	Z
1	C	-0.5129	1.0025	0.0796
2	C	0.5044	1.8031	-0.3546
3	C	1.2534	-0.3643	-0.4424
4	N	-0.0341	-0.3062	0.0135
5	N	1.5637	0.9493	-0.6653
6	Ni	2.3567	-1.9036	-0.6893
7	C	3.4530	-3.3653	-1.2441
8	N	4.6948	-3.7260	-0.7996
9	N	3.1615	-4.3311	-2.1689
10	C	5.1624	-4.8841	-1.4206
11	C	4.1859	-5.2701	-2.2934
12	C	2.2804	-3.0883	3.7539
13	C	1.0773	-3.3755	4.3870
14	C	3.4881	-3.1009	4.4411
15	C	1.0849	-3.6881	5.7532
16	H	0.1416	-3.3584	3.8309
17	C	3.4914	-3.4137	5.8070
18	H	4.4189	-2.8696	3.9262
19	C	2.2907	-3.7068	6.4624
20	H	0.1504	-3.9154	6.2630
21	H	4.4300	-3.4276	6.3579
22	H	2.2945	-3.9487	7.5223
23	Cl	2.2817	-2.5959	1.7561
24	C	-1.8901	1.3286	0.5495
25	H	-2.0475	2.4107	0.5493
26	H	-2.6572	0.8776	-0.0936
27	H	-2.0653	0.9633	1.5696
28	C	0.5939	3.2833	-0.5149
29	H	1.3933	3.7111	0.1040
30	H	0.8011	3.5664	-1.5552
31	H	-0.3467	3.7572	-0.2202
32	C	-0.8109	-1.4720	0.4047
33	H	-1.7562	-1.5015	-0.1469
34	H	-0.2222	-2.3600	0.1737
35	H	-1.0233	-1.4525	1.4786
36	C	2.8540	1.4064	-1.1572
37	H	3.3247	2.0806	-0.4342
38	H	3.4877	0.5281	-1.2978
39	H	2.7399	1.9304	-2.1122
40	C	5.4395	-2.9965	0.2150
41	H	4.8682	-2.1056	0.4754
42	H	5.5734	-3.6101	1.1116
43	H	6.4225	-2.7060	-0.1701
44	C	1.9185	-4.3874	-2.9223
45	H	1.3637	-5.3011	-2.6840
46	H	1.3182	-3.5186	-2.6436
47	H	2.1194	-4.3625	-3.9985
48	C	4.1102	-6.4216	-3.2383
49	H	5.0156	-7.0312	-3.1698
50	H	3.2516	-7.0700	-3.0208
51	H	4.0100	-6.0861	-4.2789

52	C	6.4904	-5.4850	-1.1054
53	H	7.3122	-4.7871	-1.3119
54	H	6.5642	-5.7715	-0.0483
55	H	6.6549	-6.3826	-1.7078

large_basis_B-6-I_NiIIMes2_bb
Energy (POTENTIAL) = -2029.87272324 Eh

	Atom	X	Y	Z
1	C	0.0306	0.0548	0.0376
2	C	1.1687	0.7748	-0.1128
3	C	1.7171	-1.4263	-0.4006
4	N	0.3817	-1.2800	-0.1404
5	N	2.1832	-0.1430	-0.3787
6	Ni	2.7143	-3.0820	-0.6968
7	C	3.7092	-4.6330	-1.3536
8	N	5.0517	-4.8760	-1.2586
9	N	3.2303	-5.7521	-1.9726
10	C	5.3947	-6.1118	-1.7994
11	C	4.2439	-6.6663	-2.2514
12	H	6.4132	-6.4673	-1.8101
13	H	4.0434	-7.6081	-2.7386
14	H	-0.9838	0.3544	0.2498
15	H	1.3604	1.8351	-0.0566
16	C	1.8618	-5.9729	-2.3519
17	C	1.0556	-6.7919	-1.5465
18	C	1.3988	-5.4127	-3.5517
19	C	-0.2409	-7.0680	-1.9922
20	C	0.0946	-5.7169	-3.9553
21	C	-0.7329	-6.5528	-3.1969
22	H	-0.8823	-7.6979	-1.3799
23	H	-0.2815	-5.2907	-4.8826
24	C	6.0114	-3.9467	-0.7294
25	C	6.3522	-2.8259	-1.5038
26	C	6.6086	-4.2072	0.5128
27	C	7.3035	-1.9422	-0.9900
28	C	7.5422	-3.2813	0.9935
29	C	7.8949	-2.1417	0.2631
30	H	7.5821	-1.0743	-1.5791
31	H	8.0027	-3.4590	1.9628
32	C	-0.5655	-2.3600	-0.1179
33	C	-0.9654	-2.9219	-1.3415
34	C	-1.0922	-2.7860	1.1098
35	C	-1.8995	-3.9593	-1.3086
36	C	-2.0106	-3.8427	1.0916
37	C	-2.4186	-4.4454	-0.1024
38	H	-2.2273	-4.3986	-2.2458
39	H	-2.4179	-4.1975	2.0357
40	C	3.5373	0.2607	-0.6437
41	C	4.3887	0.5358	0.4352
42	C	3.9371	0.4347	-1.9789
43	C	5.6642	1.0363	0.1465
44	C	5.2215	0.9302	-2.2169
45	C	6.0915	1.2529	-1.1668
46	H	6.3375	1.2598	0.9706
47	H	5.5497	1.0718	-3.2445
48	C	2.2800	-4.4996	-4.3676
49	H	2.5853	-3.6235	-3.7824
50	H	3.2016	-5.0053	-4.6818
51	H	1.7586	-4.1495	-5.2635

52	C	1.5734	-7.3449	-0.2434
53	H	2.4182	-8.0271	-0.4011
54	H	1.9294	-6.5381	0.4082
55	H	0.7883	-7.8925	0.2867
56	C	-2.1278	-6.8923	-3.6647
57	H	-2.1333	-7.8263	-4.2431
58	H	-2.8100	-7.0311	-2.8191
59	H	-2.5381	-6.1081	-4.3104
60	C	6.2899	-5.4599	1.2902
61	H	6.8517	-6.3193	0.8995
62	H	6.5566	-5.3412	2.3449
63	H	5.2266	-5.7071	1.2349
64	C	5.7125	-2.5854	-2.8484
65	H	5.7670	-3.4764	-3.4856
66	H	4.6519	-2.3381	-2.7319
67	H	6.1991	-1.7561	-3.3694
68	C	8.8625	-1.1274	0.8231
69	H	9.5796	-1.5881	1.5114
70	H	9.4239	-0.6251	0.0274
71	H	8.3247	-0.3508	1.3833
72	C	3.9488	0.2839	1.8544
73	H	3.0349	0.8371	2.1023
74	H	3.7299	-0.7802	2.0079
75	H	4.7297	0.5777	2.5623
76	C	3.0066	0.0829	-3.1129
77	H	2.0824	0.6731	-3.0741
78	H	3.4841	0.2578	-4.0817
79	H	2.7077	-0.9713	-3.0627
80	C	7.4623	1.8157	-1.4577
81	H	7.3932	2.8348	-1.8607
82	H	8.0805	1.8568	-0.5552
83	H	7.9924	1.2136	-2.2057
84	C	-0.4095	-2.4116	-2.6478
85	H	-0.5248	-1.3239	-2.7341
86	H	0.6617	-2.6274	-2.7249
87	H	-0.9137	-2.8811	-3.4969
88	C	-0.7191	-2.1073	2.4037
89	H	-1.2449	-1.1489	2.5119
90	H	-0.9873	-2.7326	3.2607
91	H	0.3542	-1.9056	2.4552
92	C	-3.3754	-5.6130	-0.0969
93	H	-3.9772	-5.6392	0.8179
94	H	-4.0575	-5.5797	-0.9543
95	H	-2.8258	-6.5622	-0.1551
96	I	2.7324	-3.8975	2.0445

large_basis_TS-A-5-6-Cl_NiITMe2_ossts_PhCl_t_oss_bb
Energy (POTENTIAL) = -1628.48697466 Eh

	Atom	X	Y	Z
1	C	-0.5129	1.0025	0.0796
2	C	0.5044	1.8031	-0.3546
3	C	1.2534	-0.3643	-0.4424
4	N	-0.0341	-0.3062	0.0135
5	N	1.5637	0.9493	-0.6653
6	Ni	2.3567	-1.9036	-0.6893
7	C	3.4530	-3.3653	-1.2441
8	N	4.6948	-3.7260	-0.7996
9	N	3.1615	-4.3311	-2.1689
10	C	5.1624	-4.8841	-1.4206
11	C	4.1859	-5.2701	-2.2934
12	C	2.2804	-3.0883	3.7539
13	C	1.0773	-3.3755	4.3870
14	C	3.4881	-3.1009	4.4411
15	C	1.0849	-3.6881	5.7532
16	H	0.1416	-3.3584	3.8309
17	C	3.4914	-3.4137	5.8070
18	H	4.4189	-2.8696	3.9262
19	C	2.2907	-3.7068	6.4624
20	H	0.1504	-3.9154	6.2630
21	H	4.4300	-3.4276	6.3579
22	H	2.2945	-3.9487	7.5223
23	Cl	2.2817	-2.5959	1.7561
24	C	-1.8901	1.3286	0.5495
25	H	-2.0475	2.4107	0.5493
26	H	-2.6572	0.8776	-0.0936
27	H	-2.0653	0.9633	1.5696
28	C	0.5939	3.2833	-0.5149
29	H	1.3933	3.7111	0.1040
30	H	0.8011	3.5664	-1.5552
31	H	-0.3467	3.7572	-0.2202
32	C	-0.8109	-1.4720	0.4047
33	H	-1.7562	-1.5015	-0.1469
34	H	-0.2222	-2.3600	0.1737
35	H	-1.0233	-1.4525	1.4786
36	C	2.8540	1.4064	-1.1572
37	H	3.3247	2.0806	-0.4342
38	H	3.4877	0.5281	-1.2978
39	H	2.7399	1.9304	-2.1122
40	C	5.4395	-2.9965	0.2150
41	H	4.8682	-2.1056	0.4754
42	H	5.5734	-3.6101	1.1116
43	H	6.4225	-2.7060	-0.1701
44	C	1.9185	-4.3874	-2.9223
45	H	1.3637	-5.3011	-2.6840
46	H	1.3182	-3.5186	-2.6436
47	H	2.1194	-4.3625	-3.9985
48	C	4.1102	-6.4216	-3.2383
49	H	5.0156	-7.0312	-3.1698
50	H	3.2516	-7.0700	-3.0208
51	H	4.0100	-6.0861	-4.2789

52	C	6.4904	-5.4850	-1.1054
53	H	7.3122	-4.7871	-1.3119
54	H	6.5642	-5.7715	-0.0483
55	H	6.6549	-6.3826	-1.7078

large_basis_B-1_NiIMes2_bb
Energy (POTENTIAL) = -2018.38016785 Eh

	Atom	X	Y	Z
1	C	1.2518	0.9098	0.0000
2	C	2.3492	1.6683	-0.2485
3	C	2.9535	-0.5249	-0.5697
4	N	1.6314	-0.4165	-0.2001
5	N	3.3728	0.7865	-0.5906
6	Ni	3.9284	-2.0390	-0.9724
7	C	4.9133	-3.5418	-1.3891
8	N	6.2448	-3.7934	-1.1394
9	N	4.4994	-4.6935	-2.0192
10	C	6.6332	-5.0517	-1.5959
11	C	5.5327	-5.6189	-2.1519
12	H	7.6422	-5.4175	-1.4810
13	H	5.3858	-6.5789	-2.6229
14	H	0.2502	1.1816	0.2967
15	H	2.5003	2.7365	-0.2153
16	C	3.1500	-4.8975	-2.4639
17	C	2.2460	-5.5498	-1.6140
18	C	2.7711	-4.4230	-3.7307
19	C	0.9413	-5.7572	-2.0763
20	C	1.4541	-4.6384	-4.1447
21	C	0.5284	-5.3103	-3.3351
22	H	0.2273	-6.2579	-1.4269
23	H	1.1406	-4.2689	-5.1192
24	C	7.1097	-2.8551	-0.4817
25	C	7.9674	-2.0593	-1.2562
26	C	7.0615	-2.7486	0.9188
27	C	8.8096	-1.1607	-0.5923
28	C	7.9119	-1.8279	1.5374
29	C	8.7966	-1.0309	0.7997
30	H	9.4724	-0.5306	-1.1807
31	H	7.8782	-1.7256	2.6204
32	C	0.7596	-1.5488	-0.0583
33	C	-0.0685	-1.9109	-1.1303
34	C	0.7738	-2.2704	1.1475
35	C	-0.9259	-3.0037	-0.9582
36	C	-0.0889	-3.3627	1.2689
37	C	-0.9515	-3.7387	0.2307
38	H	-1.5710	-3.2989	-1.7821
39	H	-0.0846	-3.9384	2.1926
40	C	4.7062	1.1774	-0.9519
41	C	5.6334	1.4611	0.0620
42	C	5.0485	1.2504	-2.3126
43	C	6.9198	1.8601	-0.3159
44	C	6.3511	1.6365	-2.6425
45	C	7.2969	1.9536	-1.6596
46	H	7.6514	2.0747	0.4596
47	H	6.6357	1.6845	-3.6917
48	C	3.7508	-3.6575	-4.5819
49	H	4.0575	-2.7410	-4.0612
50	H	4.6636	-4.2349	-4.7734
51	H	3.3084	-3.3817	-5.5443

52	C	2.6592	-5.9530	-0.2219
53	H	3.5163	-6.6375	-0.2293
54	H	2.9610	-5.0658	0.3490
55	H	1.8349	-6.4397	0.3084
56	C	-0.8887	-5.5215	-3.8125
57	H	-0.9173	-6.1303	-4.7257
58	H	-1.4978	-6.0259	-3.0553
59	H	-1.3732	-4.5667	-4.0529
60	C	6.0741	-3.5605	1.7165
61	H	6.1382	-4.6296	1.4810
62	H	6.2325	-3.4315	2.7919
63	H	5.0523	-3.2413	1.4689
64	C	7.9318	-2.1258	-2.7620
65	H	8.1445	-3.1341	-3.1367
66	H	6.9349	-1.8510	-3.1279
67	H	8.6591	-1.4360	-3.2015
68	C	9.7091	-0.0514	1.4985
69	H	10.5337	-0.5693	2.0073
70	H	10.1522	0.6600	0.7935
71	H	9.1709	0.5198	2.2644
72	C	5.2729	1.2684	1.5130
73	H	4.3946	1.8566	1.8040
74	H	5.0321	0.2151	1.7041
75	H	6.1061	1.5503	2.1644
76	C	4.0524	0.8630	-3.3745
77	H	3.1056	1.4052	-3.2631
78	H	4.4465	1.0550	-4.3774
79	H	3.8183	-0.2069	-3.2856
80	C	8.6918	2.3840	-2.0461
81	H	8.7184	3.4485	-2.3172
82	H	9.3996	2.2386	-1.2229
83	H	9.0566	1.8223	-2.9138
84	C	0.0138	-1.1846	-2.4484
85	H	-0.1560	-0.1070	-2.3381
86	H	1.0137	-1.3089	-2.8829
87	H	-0.7193	-1.5766	-3.1603
88	C	1.7427	-1.9056	2.2422
89	H	1.6577	-0.8506	2.5292
90	H	1.5849	-2.5213	3.1333
91	H	2.7710	-2.0565	1.8869
92	C	-1.8689	-4.9270	0.3949
93	H	-2.5925	-4.7644	1.2044
94	H	-2.4334	-5.1299	-0.5212
95	H	-1.3044	-5.8324	0.6510

large_basis_B-4-Br_transNiBrPhIMes2_bb
Energy (POTENTIAL) = -2263.36317372 Eh

	Atom	X	Y	Z
1	C	-0.5590	1.5191	0.1476
2	C	0.5459	2.2924	0.1719
3	C	1.2304	0.1494	-0.2639
4	N	-0.1353	0.2153	-0.1030
5	N	1.6279	1.4504	-0.0806
6	Ni	2.3274	-1.4388	-0.6368
7	C	3.3608	-3.0887	-0.9459
8	N	4.6820	-3.3461	-0.6829
9	N	2.8651	-4.3209	-1.2889
10	C	4.9839	-4.6993	-0.8307
11	C	3.8419	-5.3110	-1.2160
12	H	5.9789	-5.0778	-0.6557
13	H	3.6219	-6.3411	-1.4490
14	H	-1.6012	1.7561	0.2907
15	H	0.6798	3.3484	0.3456
16	C	1.5504	-4.6045	-1.8045
17	C	0.5952	-5.2320	-0.9929
18	C	1.3127	-4.3554	-3.1713
19	C	-0.6607	-5.5025	-1.5547
20	C	0.0461	-4.6431	-3.6827
21	C	-0.9607	-5.2023	-2.8838
22	H	-1.4203	-5.9642	-0.9277
23	H	-0.1560	-4.4397	-4.7324
24	C	5.7267	-2.3772	-0.4636
25	C	6.5058	-1.9969	-1.5720
26	C	5.9829	-1.8936	0.8256
27	C	7.5233	-1.0632	-1.3676
28	C	7.0000	-0.9401	0.9751
29	C	7.7734	-0.5087	-0.1058
30	H	8.1222	-0.7444	-2.2181
31	H	7.1986	-0.5408	1.9670
32	C	-1.0882	-0.8661	-0.0240
33	C	-1.4590	-1.5671	-1.1779
34	C	-1.6857	-1.1330	1.2225
35	C	-2.4331	-2.5644	-1.0638
36	C	-2.6502	-2.1430	1.2869
37	C	-3.0312	-2.8775	0.1584
38	H	-2.7238	-3.1109	-1.9563
39	H	-3.1072	-2.3671	2.2486
40	C	2.9659	1.9849	-0.0703
41	C	3.8126	1.7114	1.0135
42	C	3.3538	2.8342	-1.1208
43	C	5.0917	2.2826	1.0049
44	C	4.6289	3.4012	-1.0699
45	C	5.5167	3.1301	-0.0218
46	H	5.7658	2.0641	1.8295
47	H	4.9487	4.0464	-1.8854
48	C	2.4188	-3.8808	-4.0800
49	H	2.9762	-3.0481	-3.6506
50	H	3.1360	-4.6926	-4.2643
51	H	2.0213	-3.5611	-5.0481

52	C	0.8968	-5.7042	0.4064
53	H	1.1217	-6.7803	0.3961
54	H	1.7404	-5.1758	0.8482
55	H	0.0315	-5.5541	1.0599
56	C	-2.3253	-5.4894	-3.4621
57	H	-2.2786	-6.2871	-4.2153
58	H	-3.0326	-5.8026	-2.6872
59	H	-2.7394	-4.6052	-3.9621
60	C	5.2370	-2.4189	2.0226
61	H	5.5027	-3.4687	2.2096
62	H	5.4856	-1.8466	2.9219
63	H	4.1542	-2.3892	1.8775
64	C	6.2245	-2.5450	-2.9485
65	H	6.3839	-3.6291	-2.9955
66	H	5.1853	-2.3548	-3.2352
67	H	6.8718	-2.0736	-3.6935
68	C	8.8653	0.5191	0.0701
69	H	9.8481	0.1007	-0.1830
70	H	8.7048	1.3810	-0.5884
71	H	8.9126	0.8856	1.1007
72	C	3.3725	0.8398	2.1592
73	H	2.4613	1.2328	2.6284
74	H	3.1341	-0.1744	1.8284
75	H	4.1517	0.7829	2.9254
76	C	2.4512	3.0743	-2.3043
77	H	1.5679	3.6670	-2.0373
78	H	2.9854	3.6071	-3.0961
79	H	2.0947	2.1229	-2.7134
80	C	6.8901	3.7573	-0.0010
81	H	6.8286	4.8363	0.1954
82	H	7.5236	3.3146	0.7737
83	H	7.3979	3.6379	-0.9658
84	C	-0.7995	-1.3083	-2.5026
85	H	-0.5693	-0.2493	-2.6532
86	H	0.1444	-1.8585	-2.5427
87	H	-1.4255	-1.6546	-3.3312
88	C	-1.3101	-0.3722	2.4705
89	H	-1.8082	0.6047	2.5183
90	H	-1.6043	-0.9353	3.3620
91	H	-0.2310	-0.2048	2.5182
92	C	-4.0306	-4.0046	0.2590
93	H	-4.7227	-3.8603	1.0962
94	H	-4.6207	-4.1025	-0.6593
95	H	-3.5198	-4.9639	0.4203
96	C	3.0682	-0.5983	-2.2010
97	C	2.4879	-0.5995	-3.4852
98	C	4.3006	0.0697	-2.0847
99	C	3.0996	0.0141	-4.5861
100	H	1.5441	-1.1039	-3.6518
101	C	4.9254	0.6822	-3.1755
102	H	4.7913	0.1224	-1.1204
103	C	4.3292	0.6604	-4.4380
104	H	2.6119	-0.0178	-5.5592
105	H	5.8810	1.1813	-3.0298
106	H	4.8115	1.1376	-5.2884

107	Br	1.5457	-2.4354	1.5223

large_basis_D-6-Cl_NiClIPhen2_bb
Energy (POTENTIAL) = -2006.71966450 Eh

	Atom	X	Y	Z
1	C	0.0556	0.0766	0.1182
2	C	1.1240	0.7710	-0.3398
3	C	1.6297	-1.4553	-0.5184
4	N	0.3727	-1.2754	-0.0088
5	N	2.0659	-0.1752	-0.7386
6	Ni	2.6996	-3.0886	-0.6799
7	C	3.8087	-4.5341	-1.4014
8	N	5.1017	-4.8756	-1.1094
9	N	3.3968	-5.5421	-2.2320
10	C	5.4676	-6.0765	-1.7172
11	C	4.3923	-6.4979	-2.4236
12	H	6.4578	-6.4927	-1.6190
13	H	4.2495	-7.3582	-3.0589
14	H	-0.9018	0.4104	0.4865
15	H	1.2922	1.8312	-0.4473
16	C	2.0879	-5.6177	-2.7978
17	C	1.3556	-6.8029	-2.6970
18	C	1.5495	-4.4990	-3.4416
19	C	0.0703	-6.8636	-3.2399
20	C	0.2600	-4.5654	-3.9711
21	C	-0.4825	-5.7461	-3.8715
22	H	-0.5020	-7.7832	-3.1560
23	H	-0.1615	-3.6942	-4.4646
24	C	5.9718	-4.1141	-0.2689
25	C	5.9916	-2.7198	-0.3670
26	C	6.8062	-4.7741	0.6375
27	C	6.8436	-1.9847	0.4571
28	C	7.6650	-4.0299	1.4482
29	C	7.6849	-2.6354	1.3634
30	H	6.8490	-0.9013	0.3787
31	H	8.3089	-4.5440	2.1565
32	C	-0.5214	-2.3364	0.3326
33	C	-0.6367	-3.4418	-0.5150
34	C	-1.2885	-2.2492	1.4970
35	C	-1.5137	-4.4737	-0.1835
36	C	-2.1732	-3.2816	1.8137
37	C	-2.2860	-4.3966	0.9789
38	H	-1.5922	-5.3336	-0.8427
39	H	-2.7639	-3.2176	2.7233
40	C	3.3383	0.1398	-1.3050
41	C	4.1615	1.0852	-0.6893
42	C	3.7483	-0.5118	-2.4729
43	C	5.4090	1.3743	-1.2472
44	C	5.0012	-0.2252	-3.0160
45	C	5.8337	0.7178	-2.4057
46	H	6.0529	2.1055	-0.7666
47	H	5.3229	-0.7367	-3.9188
48	Cl	2.6527	-3.8034	1.6260
49	H	6.8080	0.9402	-2.8314
50	H	8.3503	-2.0601	2.0013
51	H	6.7656	-5.8555	0.7252

52	H	5.3429	-2.2207	-1.0766
53	H	3.8359	1.5696	0.2262
54	H	3.0876	-1.2359	-2.9391
55	H	-1.1746	-1.3969	2.1598
56	H	-0.0397	-3.4911	-1.4177
57	H	-2.9705	-5.2009	1.2340
58	H	-1.4855	-5.7950	-4.2859
59	H	2.1396	-3.5914	-3.5185
60	H	1.7804	-7.6573	-2.1791

large_basis_TS-B-5-6-Br_NiIMes2_ossts_PhBr_t_bb
Energy (POTENTIAL) = -2263.26214208 Eh

	Atom	X	Y	Z
1	C	-3.7678	3.3353	0.0322
2	C	-2.6772	4.0902	-0.2432
3	C	-2.0410	1.8920	-0.4108
4	N	-3.3676	2.0046	-0.0721
5	N	-1.6385	3.1997	-0.5096
6	Ni	-0.9671	0.3535	-0.6419
7	C	0.1454	-1.1177	-1.1102
8	N	1.4134	-1.4427	-0.6902
9	N	-0.1521	-2.1248	-1.9918
10	C	1.8776	-2.6089	-1.2935
11	C	0.8901	-3.0416	-2.1145
12	H	2.8561	-3.0107	-1.0814
13	H	0.8247	-3.8992	-2.7661
14	H	-4.7796	3.6092	0.2872
15	H	-2.5360	5.1595	-0.2785
16	C	-1.3961	-2.2439	-2.6994
17	C	-2.5008	-2.8071	-2.0443
18	C	-1.4542	-1.8244	-4.0393
19	C	-3.6764	-2.9832	-2.7830
20	C	-2.6548	-2.0063	-4.7310
21	C	-3.7727	-2.5922	-4.1219
22	H	-4.5394	-3.4256	-2.2922
23	H	-2.7208	-1.6817	-5.7676
24	C	2.1735	-0.6790	0.2602
25	C	2.6897	0.5643	-0.1272
26	C	2.3678	-1.1978	1.5521
27	C	3.3775	1.3170	0.8334
28	C	3.0663	-0.4144	2.4731
29	C	3.5633	0.8516	2.1379
30	H	3.7694	2.2908	0.5514
31	H	3.1996	-0.7881	3.4859
32	C	-4.2592	0.8963	0.1213
33	C	-4.6837	0.1627	-0.9998
34	C	-4.7149	0.6056	1.4169
35	C	-5.5752	-0.8933	-0.7911
36	C	-5.6022	-0.4661	1.5747
37	C	-6.0376	-1.2297	0.4869
38	H	-5.9176	-1.4655	-1.6496
39	H	-5.9571	-0.7089	2.5741
40	C	-0.3223	3.6290	-0.8936
41	C	0.6330	3.8851	0.1037
42	C	-0.0507	3.8241	-2.2555
43	C	1.8755	4.3842	-0.2971
44	C	1.2102	4.3190	-2.6095
45	C	2.1790	4.6155	-1.6453
46	H	2.6277	4.5893	0.4615
47	H	1.4384	4.4725	-3.6619
48	C	-0.2596	-1.1742	-4.6919
49	H	0.0825	-0.3132	-4.1044
50	H	0.5894	-1.8646	-4.7668
51	H	-0.5042	-0.8279	-5.7008

52	C	-2.4354	-3.1572	-0.5806
53	H	-1.5886	-3.8175	-0.3564
54	H	-2.2946	-2.2456	0.0149
55	H	-3.3547	-3.6511	-0.2518
56	C	-5.0675	-2.7446	-4.8838
57	H	-4.9011	-3.1690	-5.8812
58	H	-5.7733	-3.3913	-4.3519
59	H	-5.5545	-1.7705	-5.0273
60	C	1.8222	-2.5474	1.9455
61	H	2.4024	-3.3652	1.4982
62	H	1.8450	-2.6726	3.0314
63	H	0.7859	-2.6594	1.6134
64	C	2.4894	1.0945	-1.5236
65	H	2.6703	0.3203	-2.2785
66	H	1.4572	1.4394	-1.6558
67	H	3.1586	1.9350	-1.7226
68	C	4.2754	1.6868	3.1754
69	H	5.1767	1.1823	3.5472
70	H	4.5775	2.6596	2.7728
71	H	3.6290	1.8666	4.0440
72	C	0.3286	3.5951	1.5509
73	H	-0.5414	4.1634	1.9029
74	H	0.0916	2.5332	1.6855
75	H	1.1821	3.8435	2.1892
76	C	-1.0777	3.4658	-3.2998
77	H	-2.0242	3.9960	-3.1395
78	H	-0.7177	3.7039	-4.3054
79	H	-1.3034	2.3925	-3.2576
80	C	3.5353	5.1510	-2.0384
81	H	3.6553	5.1862	-3.1261
82	H	3.6903	6.1662	-1.6505
83	H	4.3418	4.5286	-1.6308
84	C	-4.1852	0.4883	-2.3843
85	H	-4.1807	1.5684	-2.5698
86	H	-3.1540	0.1356	-2.5066
87	H	-4.8039	0.0062	-3.1458
88	C	-4.2759	1.4256	2.6045
89	H	-4.7874	2.3966	2.6343
90	H	-4.5007	0.9035	3.5399
91	H	-3.1995	1.6164	2.5712
92	C	-6.9734	-2.4004	0.6752
93	H	-7.4444	-2.3870	1.6637
94	H	-7.7675	-2.4026	-0.0812
95	H	-6.4358	-3.3535	0.5786
96	Br	-0.9439	-0.1569	1.9382
97	C	-0.3732	-0.4884	4.0078
98	C	-0.5254	-1.7396	4.6027
99	C	0.3212	0.5292	4.6613
100	C	0.0208	-1.9736	5.8721
101	H	-1.0536	-2.5358	4.0812
102	C	0.8643	0.2950	5.9306
103	H	0.4521	1.4959	4.1784
104	C	0.7172	-0.9580	6.5359
105	H	-0.0957	-2.9490	6.3410
106	H	1.4055	1.0880	6.4438

107	H	1.1439	-1.1424	7.5188

large_basis_B-4-I_transNiIPhIMes2_bb
Energy (POTENTIAL) = -2261.57557418 Eh

	Atom	X	Y	Z
1	C	-0.1132	0.0467	-0.3154
2	C	1.0000	0.8015	-0.2276
3	C	1.6761	-1.3559	-0.6067
4	N	0.3023	-1.2662	-0.5295
5	N	2.0823	-0.0579	-0.4077
6	Ni	2.7755	-2.9514	-0.9592
7	C	3.8275	-4.5992	-1.2858
8	N	5.1681	-4.8304	-1.0969
9	N	3.3473	-5.8417	-1.6259
10	C	5.4964	-6.1703	-1.2926
11	C	4.3531	-6.8039	-1.6312
12	H	6.5082	-6.5258	-1.1760
13	H	4.1476	-7.8352	-1.8716
14	H	-1.1578	0.3010	-0.2342
15	H	1.1392	1.8556	-0.0486
16	C	2.0038	-6.1833	-2.0188
17	C	1.1969	-6.9386	-1.1497
18	C	1.5887	-5.8724	-3.3251
19	C	-0.0953	-7.2647	-1.5762
20	C	0.2894	-6.2232	-3.7049
21	C	-0.5732	-6.9029	-2.8388
22	H	-0.7384	-7.8278	-0.9030
23	H	-0.0496	-5.9707	-4.7073
24	C	6.2106	-3.8588	-0.8790
25	C	6.9711	-3.4595	-1.9934
26	C	6.4919	-3.4025	0.4147
27	C	7.9952	-2.5334	-1.7886
28	C	7.5098	-2.4497	0.5641
29	C	8.2654	-1.9998	-0.5219
30	H	8.5787	-2.1988	-2.6436
31	H	7.7257	-2.0691	1.5596
32	C	-0.6838	-2.3214	-0.4854
33	C	-1.0009	-3.0440	-1.6437
34	C	-1.3839	-2.5236	0.7195
35	C	-2.0234	-3.9953	-1.5757
36	C	-2.3945	-3.4897	0.7390
37	C	-2.7252	-4.2417	-0.3930
38	H	-2.2740	-4.5547	-2.4725
39	H	-2.9316	-3.6621	1.6693
40	C	3.4207	0.4725	-0.3344
41	C	4.2407	0.1563	0.7578
42	C	3.8377	1.3637	-1.3402
43	C	5.5191	0.7280	0.8062
44	C	5.1105	1.9265	-1.2333
45	C	5.9715	1.6138	-0.1742
46	H	6.1716	0.4734	1.6379
47	H	5.4527	2.6006	-2.0157
48	C	2.5391	-5.2800	-4.3348
49	H	3.2094	-4.5410	-3.8972
50	H	3.1656	-6.0719	-4.7690
51	H	1.9948	-4.8041	-5.1562

52	C	1.7058	-7.5004	0.1558
53	H	2.0280	-8.5412	0.0103
54	H	2.5504	-6.9390	0.5553
55	H	0.9154	-7.5045	0.9125
56	C	-1.9687	-7.2834	-3.2721
57	H	-1.9977	-8.3173	-3.6425
58	H	-2.6774	-7.2183	-2.4396
59	H	-2.3298	-6.6379	-4.0802
60	C	5.7821	-3.9623	1.6184
61	H	6.1287	-4.9842	1.8255
62	H	5.9781	-3.3564	2.5083
63	H	4.7020	-4.0184	1.4722
64	C	6.6578	-3.9745	-3.3757
65	H	6.8476	-5.0513	-3.4627
66	H	5.6034	-3.8071	-3.6201
67	H	7.2651	-3.4625	-4.1273
68	C	9.3556	-0.9699	-0.3477
69	H	10.3316	-1.3694	-0.6520
70	H	9.1642	-0.0857	-0.9676
71	H	9.4369	-0.6400	0.6930
72	C	3.8004	-0.7975	1.8334
73	H	2.7581	-0.6338	2.1259
74	H	3.8636	-1.8299	1.4797
75	H	4.4303	-0.7014	2.7234
76	C	2.9742	1.6490	-2.5435
77	H	2.1166	2.2865	-2.2968
78	H	3.5534	2.1559	-3.3204
79	H	2.5801	0.7182	-2.9652
80	C	7.3465	2.2332	-0.0977
81	H	7.2873	3.2973	0.1679
82	H	7.9706	1.7376	0.6525
83	H	7.8630	2.1737	-1.0631
84	C	-0.2516	-2.8253	-2.9251
85	H	-0.0560	-1.7642	-3.1098
86	H	0.7149	-3.3312	-2.8650
87	H	-0.7961	-3.2385	-3.7795
88	C	-1.0876	-1.7376	1.9754
89	H	-1.6498	-0.7951	2.0027
90	H	-1.3743	-2.3164	2.8592
91	H	-0.0263	-1.4937	2.0646
92	C	-3.7884	-5.3115	-0.3298
93	H	-4.5622	-5.0685	0.4072
94	H	-4.2742	-5.4545	-1.3012
95	H	-3.3520	-6.2756	-0.0362
96	I	1.8481	-4.0670	1.3706
97	C	3.5580	-2.0642	-2.4810
98	C	3.0013	-2.0140	-3.7745
99	C	4.7849	-1.3997	-2.3144
100	C	3.6371	-1.3649	-4.8403
101	H	2.0557	-2.4971	-3.9783
102	C	5.4310	-0.7479	-3.3701
103	H	5.2560	-1.3781	-1.3401
104	C	4.8641	-0.7271	-4.6450
105	H	3.1669	-1.3596	-5.8224
106	H	6.3817	-0.2531	-3.1851

107	H	5.3646	-0.2211	-5.4676

large_basis_A-1_NiITMe2_bb
Energy (POTENTIAL) = -936.542798241 Eh

	Atom	X	Y	Z
1	C	-0.7942	2.1848	0.7712
2	C	0.4851	2.1643	0.2953
3	C	-0.1566	4.3710	0.4338
4	N	-1.1609	3.5286	0.8478
5	N	0.8493	3.4964	0.0974
6	C	-2.4602	3.9870	1.3106
7	H	-2.4543	5.0791	1.2839
8	H	-3.2589	3.6122	0.6610
9	H	-2.6475	3.6489	2.3357
10	C	2.1457	3.9135	-0.4108
11	H	2.3202	3.5029	-1.4114
12	H	2.1457	5.0047	-0.4604
13	H	2.9495	3.5806	0.2549
14	C	1.4069	1.0290	0.0024
15	H	1.6986	1.0050	-1.0558
16	H	2.3310	1.0932	0.5916
17	H	0.9262	0.0752	0.2380
18	C	-1.7117	1.0780	1.1683
19	H	-1.2225	0.1092	1.0326
20	H	-2.0117	1.1573	2.2215
21	H	-2.6315	1.0755	0.5688
22	Ni	-0.1587	6.2415	0.3380
23	C	-0.1717	8.1097	0.2216
24	N	0.1851	8.9030	-0.8429
25	N	-0.5563	9.0311	1.1667
26	C	0.0252	10.2619	-0.5719
27	C	0.6700	8.3837	-2.1108
28	C	-0.4448	10.3435	0.7071
29	C	-1.0256	8.6773	2.4961
30	C	0.3422	11.3213	-1.5730
31	H	0.7028	7.2948	-2.0315
32	H	-0.0004	8.6669	-2.9296
33	H	1.6748	8.7638	-2.3260
34	C	-0.8143	11.5210	1.5448
35	H	-1.0320	7.5872	2.5654
36	H	-0.3600	9.0857	3.2646
37	H	-2.0384	9.0597	2.6637
38	H	0.1284	12.3123	-1.1626
39	H	1.4002	11.3007	-1.8659
40	H	-0.2498	11.2026	-2.4900
41	H	-1.8740	11.4982	1.8314
42	H	-0.2282	11.5618	2.4722
43	H	-0.6372	12.4509	0.9969

large_basis_TS-B-5-6-Cl_NiIMes2_ossts_PhCl_t_oss_bb
Energy (POTENTIAL) = -2710.32684219 Eh

	Atom	X	Y	Z
1	C	-0.5099	1.0261	0.0647
2	C	0.5237	1.8105	-0.3262
3	C	1.2463	-0.3637	-0.4250
4	N	-0.0564	-0.2896	0.0016
5	N	1.5808	0.9512	-0.6206
6	Ni	2.3399	-1.8916	-0.6853
7	C	3.4367	-3.3434	-1.2191
8	N	4.7224	-3.6484	-0.8444
9	N	3.1149	-4.3657	-2.0730
10	C	5.1757	-4.8199	-1.4471
11	C	4.1612	-5.2745	-2.2219
12	H	6.1670	-5.2070	-1.2695
13	H	4.0780	-6.1433	-2.8564
14	H	-1.5144	1.2699	0.3743
15	H	0.6126	2.8816	-0.4234
16	C	1.8393	-4.5201	-2.7145
17	C	0.7954	-5.1374	-2.0069
18	C	1.6904	-4.0878	-4.0412
19	C	-0.4095	-5.3545	-2.6817
20	C	0.4597	-4.3116	-4.6689
21	C	-0.5960	-4.9509	-4.0089
22	H	-1.2251	-5.8423	-2.1534
23	H	0.3252	-3.9802	-5.6963
24	C	5.5124	-2.8580	0.0578
25	C	6.0318	-1.6326	-0.3889
26	C	5.7604	-3.3455	1.3508
27	C	6.7943	-0.8782	0.5091
28	C	6.5296	-2.5547	2.2120
29	C	7.0446	-1.3156	1.8145
30	H	7.2000	0.0744	0.1779
31	H	6.7238	-2.9150	3.2199
32	C	-0.8612	-1.4297	0.3396
33	C	-1.3564	-2.2413	-0.6926
34	C	-1.1433	-1.6866	1.6914
35	C	-2.1371	-3.3474	-0.3383
36	C	-1.9287	-2.8037	1.9950
37	C	-2.4254	-3.6504	0.9966
38	H	-2.5257	-3.9860	-1.1275
39	H	-2.1515	-3.0202	3.0377
40	C	2.8808	1.4055	-1.0295
41	C	3.8797	1.5565	-0.0558
42	C	3.0986	1.7199	-2.3804
43	C	5.1163	2.0676	-0.4639
44	C	4.3552	2.2154	-2.7428
45	C	5.3719	2.4033	-1.7979
46	H	5.8996	2.1972	0.2788
47	H	4.5434	2.4605	-3.7860
48	C	2.8163	-3.3777	-4.7511
49	H	3.0777	-2.4482	-4.2293
50	H	3.7268	-3.9879	-4.7853
51	H	2.5359	-3.1260	-5.7786

52	C	0.9598	-5.5021	-0.5547
53	H	1.8604	-6.1045	-0.3844
54	H	1.0665	-4.5921	0.0485
55	H	0.0944	-6.0627	-0.1888
56	C	-1.9304	-5.1498	-4.6869
57	H	-2.4088	-6.0821	-4.3662
58	H	-2.6194	-4.3306	-4.4375
59	H	-1.8320	-5.1719	-5.7777
60	C	5.2075	-4.6725	1.8076
61	H	5.7250	-5.5132	1.3279
62	H	5.3169	-4.7869	2.8900
63	H	4.1446	-4.7550	1.5625
64	C	5.7571	-1.1288	-1.7822
65	H	5.8971	-1.9165	-2.5317
66	H	4.7177	-0.7883	-1.8626
67	H	6.4125	-0.2904	-2.0315
68	C	7.8253	-0.4539	2.7784
69	H	7.1715	0.2879	3.2573
70	H	8.2801	-1.0510	3.5763
71	H	8.6225	0.0998	2.2688
72	C	3.6308	1.1414	1.3710
73	H	2.7454	1.6378	1.7874
74	H	3.4452	0.0618	1.4240
75	H	4.4893	1.3788	2.0061
76	C	2.0139	1.5005	-3.4056
77	H	1.1163	2.0896	-3.1811
78	H	2.3588	1.7756	-4.4070
79	H	1.7055	0.4477	-3.4250
80	C	6.7335	2.9007	-2.2207
81	H	6.6615	3.6509	-3.0166
82	H	7.2786	3.3448	-1.3807
83	H	7.3471	2.0761	-2.6097
84	C	-1.0339	-1.9541	-2.1361
85	H	-1.1239	-0.8866	-2.3672
86	H	0.0004	-2.2466	-2.3562
87	H	-1.6963	-2.5114	-2.8035
88	C	-0.6070	-0.7966	2.7845
89	H	-1.0963	0.1857	2.7836
90	H	-0.7662	-1.2493	3.7675
91	H	0.4669	-0.6313	2.6567
92	C	-3.2268	-4.8795	1.3537
93	H	-2.5689	-5.7487	1.4905
94	H	-3.7802	-4.7423	2.2894
95	H	-3.9440	-5.1357	0.5658
96	C	2.2979	-3.1134	3.7016
97	C	1.1611	-3.7110	4.2313
98	C	3.4232	-2.8626	4.4768
99	C	1.1519	-4.0709	5.5861
100	H	0.2918	-3.8940	3.6020
101	C	3.4105	-3.2255	5.8306
102	H	4.3012	-2.3953	4.0347
103	C	2.2754	-3.8282	6.3846
104	H	0.2693	-4.5398	6.0178
105	H	4.2846	-3.0372	6.4516
106	H	2.2664	-4.1082	7.4350

107	Cl	2.3141	-2.5660	1.7064

large_basis_B-5-I_NiIMes2_IPh_bb
Energy (POTENTIAL) = -2261.50773286 Eh

	Atom	X	Y	Z
1	C	-0.3880	0.2257	-0.0064
2	C	0.7325	0.9663	-0.1811
3	C	1.2991	-1.2231	-0.5817
4	N	-0.0308	-1.0981	-0.2486
5	N	1.7468	0.0741	-0.5244
6	Ni	2.2832	-2.7768	-1.0021
7	C	3.2588	-4.3068	-1.5119
8	N	4.5992	-4.5765	-1.3512
9	N	2.7983	-5.4378	-2.1409
10	C	4.9494	-5.8211	-1.8678
11	C	3.8136	-6.3653	-2.3669
12	H	5.9627	-6.1902	-1.8307
13	H	3.6257	-7.3086	-2.8564
14	H	-1.3950	0.5052	0.2621
15	H	0.9104	2.0274	-0.0975
16	C	1.4411	-5.6648	-2.5503
17	C	0.6221	-6.4863	-1.7603
18	C	0.9969	-5.1117	-3.7611
19	C	-0.6649	-6.7703	-2.2287
20	C	-0.2994	-5.4190	-4.1859
21	C	-1.1392	-6.2545	-3.4398
22	H	-1.3147	-7.4012	-1.6263
23	H	-0.6622	-4.9924	-5.1186
24	C	5.5453	-3.6708	-0.7635
25	C	5.9616	-2.5574	-1.5157
26	C	6.0626	-3.9409	0.5122
27	C	6.8916	-1.6889	-0.9421
28	C	6.9798	-3.0292	1.0520
29	C	7.3969	-1.8965	0.3479
30	H	7.2237	-0.8263	-1.5123
31	H	7.3754	-3.2146	2.0486
32	C	-0.9656	-2.1867	-0.1997
33	C	-1.4248	-2.7293	-1.4133
34	C	-1.4357	-2.6412	1.0419
35	C	-2.3484	-3.7739	-1.3568
36	C	-2.3465	-3.7060	1.0464
37	C	-2.8077	-4.2881	-0.1374
38	H	-2.7140	-4.2010	-2.2860
39	H	-2.7056	-4.0817	2.0024
40	C	3.0867	0.5022	-0.8135
41	C	3.9444	0.8200	0.2518
42	C	3.4750	0.6523	-2.1535
43	C	5.2123	1.3219	-0.0574
44	C	4.7560	1.1504	-2.4133
45	C	5.6321	1.5019	-1.3804
46	H	5.8915	1.5682	0.7559
47	H	5.0756	1.2645	-3.4467
48	C	1.8864	-4.1883	-4.5539
49	H	2.1736	-3.3213	-3.9449
50	H	2.8177	-4.6846	-4.8553
51	H	1.3798	-3.8308	-5.4556

52	C	1.1100	-7.0210	-0.4375
53	H	1.9978	-7.6542	-0.5562
54	H	1.3901	-6.1982	0.2316
55	H	0.3325	-7.6131	0.0549
56	C	-2.5276	-6.5870	-3.9315
57	H	-2.5093	-7.4403	-4.6235
58	H	-3.1939	-6.8514	-3.1036
59	H	-2.9734	-5.7443	-4.4721
60	C	5.6912	-5.1857	1.2817
61	H	6.4097	-5.9940	1.0865
62	H	5.6981	-4.9918	2.3591
63	H	4.6988	-5.5500	1.0106
64	C	5.4166	-2.3131	-2.8996
65	H	5.5222	-3.2017	-3.5344
66	H	4.3467	-2.0801	-2.8499
67	H	5.9313	-1.4780	-3.3828
68	C	8.3428	-0.8971	0.9691
69	H	8.9518	-1.3522	1.7580
70	H	9.0186	-0.4636	0.2228
71	H	7.7849	-0.0672	1.4238
72	C	3.5217	0.5956	1.6817
73	H	2.6283	1.1765	1.9412
74	H	3.2779	-0.4602	1.8510
75	H	4.3228	0.8759	2.3726
76	C	2.5453	0.2540	-3.2711
77	H	1.6003	0.8101	-3.2283
78	H	3.0047	0.4295	-4.2488
79	H	2.2884	-0.8102	-3.1905
80	C	7.0013	2.0630	-1.6826
81	H	6.9868	3.1617	-1.6883
82	H	7.7352	1.7539	-0.9300
83	H	7.3621	1.7384	-2.6649
84	C	-0.9233	-2.2025	-2.7336
85	H	-1.0261	-1.1121	-2.7970
86	H	0.1424	-2.4315	-2.8505
87	H	-1.4687	-2.6524	-3.5679
88	C	-1.0251	-1.9911	2.3414
89	H	-1.7362	-1.2019	2.6227
90	H	-1.0095	-2.7246	3.1537
91	H	-0.0337	-1.5388	2.2760
92	C	-3.7522	-5.4656	-0.1119
93	H	-4.3270	-5.5047	0.8199
94	H	-4.4597	-5.4331	-0.9486
95	H	-3.1966	-6.4097	-0.1934
96	I	2.3517	-3.5327	1.7049
97	C	2.3914	-4.1174	3.8794
98	C	2.8741	-5.3729	4.2628
99	C	1.9291	-3.2235	4.8510
100	C	2.8931	-5.7328	5.6156
101	H	3.2363	-6.0723	3.5121
102	C	1.9498	-3.5855	6.2030
103	H	1.5516	-2.2460	4.5581
104	C	2.4316	-4.8403	6.5877
105	H	3.2690	-6.7110	5.9087
106	H	1.5886	-2.8864	6.9545

107	H	2.4470	-5.1207	7.6379

large_basis_COD_COD_bb
Energy (POTENTIAL) = -312.138936653 Eh

	Atom	X	Y	Z
1	C	3.0277	0.4876	0.0000
2	C	3.9215	-0.0010	1.1537
3	C	0.8237	1.8349	1.5305
4	C	3.6220	0.3692	2.5908
5	C	1.2920	1.6038	2.9783
6	C	2.6347	0.9711	3.2762
7	H	3.0322	1.5842	-0.0140
8	H	4.9517	0.3290	0.9487
9	H	1.5383	2.4978	1.0283
10	H	0.5337	0.9963	3.4988
11	H	3.4944	0.1619	-0.9382
12	H	3.9704	-1.1015	1.1154
13	H	-0.1284	2.3787	1.5754
14	H	4.4396	0.0251	3.2298
15	H	1.2749	2.5737	3.4994
16	H	2.8220	1.0107	4.3525
17	C	1.6212	-0.0442	0.0766
18	H	1.4285	-0.9977	-0.4155
19	C	0.6399	0.5562	0.7576
20	H	-0.3414	0.0845	0.8136

large_basis_A-6-Cl_NiClITMe2_bb
Energy (POTENTIAL) = -1396.87288804 Eh

	Atom	X	Y	Z
1	C	-0.4769	2.1496	1.2138
2	C	-0.1489	2.1627	-0.1123
3	C	-0.0375	4.3204	0.6432
4	N	-0.4008	3.4736	1.6460
5	N	0.1106	3.4958	-0.4327
6	C	-0.6804	3.8993	3.0100
7	H	-0.4589	4.9638	3.0839
8	H	-1.7305	3.7144	3.2605
9	H	-0.0436	3.3556	3.7142
10	C	0.5148	3.9454	-1.7568
11	H	-0.2649	3.7245	-2.4929
12	H	0.6790	5.0241	-1.7129
13	H	1.4435	3.4523	-2.0604
14	C	-0.0386	1.0615	-1.1125
15	H	-0.7038	1.2239	-1.9703
16	H	0.9830	0.9728	-1.5042
17	H	-0.3061	0.1039	-0.6576
18	C	-0.8581	1.0313	2.1232
19	H	-0.8626	0.0822	1.5804
20	H	-0.1577	0.9351	2.9626
21	H	-1.8589	1.1799	2.5491
22	C	0.0245	8.1739	0.3035
23	N	0.9702	9.0684	-0.0966
24	N	-1.1116	8.9240	0.3810
25	C	0.4441	10.3494	-0.2633
26	C	2.3644	8.7262	-0.3375
27	C	-0.8839	10.2585	0.0433
28	C	-2.4075	8.4049	0.7926
29	C	1.2780	11.5090	-0.6924
30	H	2.5153	7.6901	-0.0354
31	H	2.6106	8.8494	-1.3977
32	H	3.0197	9.3677	0.2591
33	C	-1.9651	11.2855	0.0606
34	H	-3.1458	8.5370	-0.0050
35	H	-2.2924	7.3408	1.0094
36	H	-2.7569	8.9196	1.6931
37	H	0.6628	12.4085	-0.7838
38	H	2.0776	11.7209	0.0288
39	H	1.7546	11.3273	-1.6643
40	H	-2.7838	11.0245	-0.6222
41	H	-2.3997	11.3990	1.0622
42	H	-1.5716	12.2588	-0.2452
43	Ni	0.2399	6.2648	0.7219
44	Cl	1.9573	6.3948	2.4466

large_basis_PhI_PhI_bb
Energy (POTENTIAL) = -243.107614001 Eh

	Atom	X	Y	Z
1	C	-2.2276	0.0432	0.0000
2	C	-0.8296	0.0336	0.0006
3	C	-0.1443	1.2514	0.0000
4	C	-0.8295	2.4693	-0.0010
5	C	-2.2275	2.4599	-0.0015
6	C	-2.9282	1.2516	-0.0010
7	H	-2.7647	-0.9016	0.0005
8	H	-0.2890	-0.9070	0.0014
9	H	-0.2888	3.4099	-0.0014
10	H	-2.7645	3.4047	-0.0023
11	H	-4.0146	1.2516	-0.0014
12	I	1.9845	1.2514	0.0008

large_basis_C-3-Cl_tetNiClPhIXy2_bb
Energy (POTENTIAL) = -2553.05536121 Eh

	Atom	X	Y	Z
1	C	0.4475	0.3962	-0.1598
2	C	0.6541	1.4417	-0.9864
3	C	2.2127	-0.1624	-1.5170
4	N	1.3894	-0.5765	-0.5034
5	N	1.7207	1.0924	-1.8061
6	Ni	3.9762	-0.7009	-2.4450
7	C	3.9612	-2.5273	-3.0203
8	N	4.7982	-3.4580	-2.4362
9	N	3.6033	-3.1151	-4.2083
10	C	4.9805	-4.5606	-3.2740
11	C	4.2315	-4.3490	-4.3776
12	H	5.6062	-5.3899	-2.9833
13	H	4.0654	-4.9500	-5.2579
14	H	-0.2689	0.2359	0.6300
15	H	0.1554	2.3937	-1.0775
16	C	2.5031	-2.7402	-5.0691
17	C	1.2187	-3.1532	-4.6587
18	C	2.7234	-2.1213	-6.3102
19	C	0.1308	-2.8645	-5.4880
20	C	1.6036	-1.8646	-7.1162
21	C	0.3204	-2.2195	-6.7102
22	H	-0.8659	-3.1670	-5.1774
23	H	1.7538	-1.3806	-8.0777
24	C	5.2229	-3.5513	-1.0479
25	C	6.4051	-2.9416	-0.5877
26	C	4.4671	-4.4116	-0.2235
27	C	6.7828	-3.1671	0.7439
28	C	4.9061	-4.6339	1.0867
29	C	6.0486	-4.0070	1.5762
30	H	7.6851	-2.6891	1.1157
31	H	4.3339	-5.3008	1.7248
32	C	1.3232	-1.8493	0.1681
33	C	0.1952	-2.6558	-0.0808
34	C	2.2628	-2.1537	1.1659
35	C	0.0311	-3.8089	0.6969
36	C	2.0413	-3.3014	1.9370
37	C	0.9379	-4.1217	1.7084
38	H	-0.8272	-4.4505	0.5149
39	H	2.7479	-3.5476	2.7234
40	C	2.1570	1.9815	-2.8523
41	C	2.8087	3.1799	-2.5135
42	C	1.8172	1.6591	-4.1771
43	C	3.2082	4.0181	-3.5637
44	C	2.2322	2.5257	-5.1938
45	C	2.9364	3.6910	-4.8917
46	H	3.7354	4.9390	-3.3283
47	H	1.9937	2.2823	-6.2258
48	C	4.0912	-1.7259	-6.7973
49	H	4.3771	-0.7452	-6.4038
50	H	4.8604	-2.4310	-6.4775
51	H	4.1038	-1.6692	-7.8908

52	C	1.0261	-3.9125	-3.3732
53	H	-0.0251	-4.1731	-3.2280
54	H	1.6106	-4.8400	-3.3701
55	H	1.3559	-3.3263	-2.5126
56	C	3.2052	-5.0777	-0.7094
57	H	3.3689	-5.6659	-1.6182
58	H	2.8032	-5.7435	0.0575
59	H	2.4390	-4.3322	-0.9363
60	C	7.2893	-2.0985	-1.4630
61	H	8.1681	-1.7631	-0.9036
62	H	7.6401	-2.6622	-2.3336
63	H	6.7582	-1.2176	-1.8269
64	C	3.0325	3.5963	-1.0818
65	H	3.2693	2.7410	-0.4474
66	H	3.8602	4.3092	-1.0147
67	H	2.1382	4.0897	-0.6771
68	C	1.0125	0.4270	-4.4861
69	H	0.0905	0.3952	-3.8922
70	H	0.7410	0.3923	-5.5427
71	H	1.5777	-0.4769	-4.2516
72	C	-0.8505	-2.2785	-1.1040
73	H	-0.4154	-1.8089	-1.9899
74	H	-1.4097	-3.1628	-1.4239
75	H	-1.5741	-1.5680	-0.6846
76	C	3.4515	-1.2643	1.4126
77	H	3.1375	-0.2513	1.6944
78	H	4.0772	-1.6661	2.2140
79	H	4.0649	-1.1564	0.5138
80	C	5.3368	-0.4431	-3.8129
81	C	5.2801	0.8690	-4.3274
82	C	6.2771	-1.2993	-4.4099
83	C	6.0960	1.2929	-5.3823
84	H	4.6001	1.5873	-3.8870
85	C	7.1250	-0.8784	-5.4408
86	H	6.3603	-2.3293	-4.0834
87	C	7.0343	0.4211	-5.9428
88	H	6.0058	2.3134	-5.7510
89	H	7.8445	-1.5776	-5.8640
90	H	7.6824	0.7498	-6.7521
91	Cl	5.0734	0.8545	-1.0823
92	H	6.3718	-4.1810	2.5992
93	H	-0.5313	-2.0064	-7.3508
94	H	3.2615	4.3524	-5.6906
95	H	0.7869	-5.0097	2.3167

large_basis_C-4-Cl_transNiClPhIXy2_bb
Energy (POTENTIAL) = -2553.09435403 Eh

	Atom	X	Y	Z
1	C	-0.3099	1.5578	0.7002
2	C	0.7902	2.3218	0.5150
3	C	1.3621	0.1728	-0.0217
4	N	0.0500	0.2548	0.3657
5	N	1.7965	1.4673	0.0652
6	Ni	2.4268	-1.4273	-0.4082
7	C	3.4795	-3.0468	-0.7469
8	N	4.7416	-3.3559	-0.3116
9	N	3.0571	-4.2074	-1.3357
10	C	5.0807	-4.6745	-0.6041
11	C	4.0186	-5.2134	-1.2447
12	H	6.0384	-5.0883	-0.3295
13	H	3.8466	-6.1995	-1.6472
14	H	-1.3067	1.8033	1.0321
15	H	0.9639	3.3775	0.6535
16	C	1.8428	-4.3885	-2.0895
17	C	0.6401	-4.6444	-1.4150
18	C	1.9331	-4.3399	-3.4918
19	C	-0.5125	-4.8247	-2.1918
20	C	0.7599	-4.5378	-4.2280
21	C	-0.4556	-4.7703	-3.5839
22	H	-1.4580	-5.0132	-1.6920
23	H	0.8022	-4.4910	-5.3130
24	C	5.6849	-2.4272	0.2563
25	C	6.4361	-1.6308	-0.6291
26	C	5.8926	-2.4056	1.6451
27	C	7.3192	-0.6951	-0.0791
28	C	6.7911	-1.4562	2.1518
29	C	7.4809	-0.5932	1.3028
30	H	7.8911	-0.0541	-0.7448
31	H	6.9516	-1.4060	3.2259
32	C	-0.9080	-0.8204	0.3357
33	C	-1.5651	-1.0840	-0.8813
34	C	-1.2278	-1.4987	1.5231
35	C	-2.4663	-2.1538	-0.9201
36	C	-2.1379	-2.5617	1.4383
37	C	-2.7352	-2.9021	0.2263
38	H	-2.9688	-2.3877	-1.8549
39	H	-2.3822	-3.1170	2.3406
40	C	3.0757	1.9700	-0.3660
41	C	4.1985	1.8147	0.4598
42	C	3.1290	2.6360	-1.6037
43	C	5.4178	2.3320	0.0001
44	C	4.3639	3.1466	-2.0175
45	C	5.5020	2.9908	-1.2256
46	H	6.3038	2.2141	0.6170
47	H	4.4321	3.6527	-2.9768
48	C	3.2393	-4.0311	-4.1789
49	H	3.6401	-3.0742	-3.8266
50	H	3.9988	-4.7966	-3.9809
51	H	3.1013	-3.9628	-5.2618

52	C	0.5888	-4.7259	0.0869
53	H	1.3459	-5.4200	0.4728
54	H	0.7977	-3.7525	0.5411
55	H	-0.3943	-5.0639	0.4258
56	C	5.2655	-3.4179	2.5700
57	H	5.9500	-4.2659	2.7138
58	H	5.0764	-2.9794	3.5548
59	H	4.3195	-3.7970	2.1856
60	C	6.3931	-1.8526	-2.1211
61	H	7.0395	-2.6998	-2.3897
62	H	5.3913	-2.0792	-2.4867
63	H	6.7608	-0.9735	-2.6588
64	C	4.1075	1.1073	1.7854
65	H	3.2519	1.4632	2.3714
66	H	3.9628	0.0316	1.6454
67	H	5.0180	1.2602	2.3715
68	C	1.9101	2.7477	-2.4849
69	H	1.1392	3.3895	-2.0418
70	H	2.1759	3.1632	-3.4610
71	H	1.4606	1.7621	-2.6476
72	C	-1.4122	-0.1745	-2.0759
73	H	-0.3975	0.2073	-2.1918
74	H	-1.6888	-0.6909	-2.9999
75	H	-2.0794	0.6922	-1.9684
76	C	-0.7126	-1.0562	2.8694
77	H	-1.4548	-0.4068	3.3551
78	H	-0.5489	-1.9165	3.5256
79	H	0.2272	-0.5114	2.7926
80	C	2.5236	-0.9369	-2.2449
81	C	1.5006	-1.2726	-3.1489
82	C	3.6166	-0.2218	-2.7655
83	C	1.5591	-0.9148	-4.5007
84	H	0.6472	-1.8417	-2.7955
85	C	3.6918	0.1357	-4.1166
86	H	4.4206	0.0774	-2.1007
87	C	2.6595	-0.2082	-4.9946
88	H	0.7470	-1.1985	-5.1681
89	H	4.5547	0.6918	-4.4792
90	H	2.7117	0.0699	-6.0450
91	Cl	2.2967	-2.0286	1.8462
92	H	6.4565	3.3857	-1.5641
93	H	8.1646	0.1437	1.7165
94	H	-1.3606	-4.9147	-4.1687
95	H	-3.4315	-3.7356	0.1793

large_basis_D-1_NiIPhen2_bb
Energy (POTENTIAL) = -1546.39870797 Eh

	Atom	X	Y	Z
1	C	1.2292	0.9498	-0.0976
2	C	2.3557	1.6915	-0.1955
3	C	2.9502	-0.4981	-0.6009
4	N	1.5951	-0.3735	-0.3397
5	N	3.3923	0.8119	-0.5053
6	Ni	3.9285	-2.0328	-0.9894
7	C	4.9098	-3.5654	-1.3754
8	N	6.2699	-3.7817	-1.2236
9	N	4.4723	-4.7784	-1.8835
10	C	6.6439	-5.0635	-1.6241
11	C	5.5169	-5.6900	-2.0319
12	H	7.6631	-5.4115	-1.5620
13	H	5.3646	-6.6810	-2.4299
14	H	0.2159	1.2331	0.1409
15	H	2.5118	2.7543	-0.0965
16	C	3.1166	-5.0793	-2.2040
17	C	2.5873	-6.3280	-1.8599
18	C	2.3204	-4.1342	-2.8630
19	C	1.2615	-6.6306	-2.1790
20	C	0.9942	-4.4418	-3.1653
21	C	0.4602	-5.6888	-2.8286
22	H	0.8549	-7.6004	-1.9050
23	H	0.3768	-3.6998	-3.6633
24	C	7.1908	-2.8138	-0.7276
25	C	8.4299	-2.6551	-1.3572
26	C	6.8585	-2.0297	0.3840
27	C	9.3383	-1.7121	-0.8705
28	C	7.7668	-1.0809	0.8529
29	C	9.0086	-0.9198	0.2317
30	H	10.2976	-1.5896	-1.3661
31	H	7.4989	-0.4644	1.7062
32	C	0.6688	-1.4567	-0.3341
33	C	-0.5841	-1.2942	-0.9353
34	C	1.0080	-2.6728	0.2717
35	C	-1.4996	-2.3493	-0.9242
36	C	0.0908	-3.7235	0.2673
37	C	-1.1646	-3.5669	-0.3272
38	H	-2.4695	-2.2193	-1.3966
39	H	0.3638	-4.6693	0.7266
40	C	4.7432	1.2266	-0.6937
41	C	5.2989	2.1783	0.1682
42	C	5.5079	0.6882	-1.7363
43	C	6.6192	2.5944	-0.0180
44	C	6.8294	1.1003	-1.9050
45	C	7.3892	2.0553	-1.0513
46	H	7.0468	3.3308	0.6570
47	H	7.4224	0.6692	-2.7063
48	H	4.7083	2.5754	0.9885
49	H	5.0636	-0.0497	-2.3956
50	H	8.4198	2.3713	-1.1869
51	H	1.9837	-2.7831	0.7327

52	H	-0.8327	-0.3567	-1.4238
53	H	-1.8739	-4.3899	-0.3296
54	H	-0.5743	-5.9216	-3.0656
55	H	3.2023	-7.0495	-1.3301
56	H	2.7444	-3.1699	-3.1228
57	H	9.7113	-0.1779	0.6011
58	H	5.8948	-2.1672	0.8627
59	H	8.6724	-3.2513	-2.2321

large_basis_B-3x-Cl_NiClPhIMes_bb
Energy (POTENTIAL) = -1785.87643322 Eh

	Atom	X	Y	Z
1	Ni	-0.1998	0.3385	0.7299
2	C	0.9180	-0.7514	1.7481
3	N	0.5520	-1.8764	2.4234
4	N	2.2249	-0.5643	2.0782
5	C	1.6111	-2.3769	3.1738
6	C	-0.7601	-2.4638	2.3559
7	C	2.6647	-1.5501	2.9562
8	C	3.0460	0.5034	1.5710
9	H	1.5078	-3.2591	3.7858
10	C	-1.8238	-1.8262	3.0160
11	C	-0.9295	-3.6536	1.6300
12	H	3.6728	-1.5606	3.3396
13	C	3.9993	0.2020	0.5851
14	C	2.8455	1.8052	2.0522
15	C	-3.0927	-2.4037	2.9106
16	C	-1.6136	-0.5615	3.8125
17	C	-2.2194	-4.1911	1.5562
18	C	0.2361	-4.3468	0.9661
19	C	4.7731	1.2536	0.0871
20	C	4.1401	-1.1969	0.0391
21	C	3.6399	2.8250	1.5152
22	C	1.7938	2.1095	3.0902
23	C	-3.3119	-3.5779	2.1799
24	H	-3.9295	-1.9255	3.4147
25	H	-0.6939	-0.6029	4.4061
26	H	-1.5359	0.3157	3.1571
27	H	-2.4546	-0.3866	4.4903
28	H	-2.3722	-5.1094	0.9939
29	H	0.8474	-4.8883	1.6996
30	H	-0.1161	-5.0740	0.2281
31	H	0.8962	-3.6372	0.4580
32	C	4.6090	2.5694	0.5385
33	H	5.5074	1.0427	-0.6870
34	H	4.4941	-1.9006	0.8022
35	H	3.1757	-1.5686	-0.3262
36	H	4.8492	-1.2184	-0.7933
37	H	3.4969	3.8423	1.8721
38	H	1.7888	1.3650	3.8940
39	H	1.9579	3.0962	3.5338
40	H	0.7910	2.1070	2.6428
41	C	-4.7014	-4.1542	2.0537
42	C	5.4753	3.6818	-0.0018
43	H	-4.6750	-5.2282	1.8406
44	H	-5.2829	-3.9993	2.9694
45	H	-5.2512	-3.6706	1.2352
46	H	6.4330	3.7285	0.5347
47	H	5.7052	3.5312	-1.0625
48	H	4.9908	4.6578	0.1088
49	C	0.6204	-0.2475	-0.8209
50	C	1.5243	0.5935	-1.4834
51	C	0.3056	-1.4931	-1.3804

52	C	2.1093	0.1892	-2.6887
53	H	1.7859	1.5565	-1.0556
54	C	0.8888	-1.8936	-2.5894
55	H	-0.3957	-2.1512	-0.8758
56	C	1.7968	-1.0558	-3.2434
57	H	2.8154	0.8483	-3.1893
58	H	0.6354	-2.8627	-3.0141
59	H	2.2567	-1.3699	-4.1772
60	Cl	-1.7211	1.7863	0.1033

large_basis_TS-A-5-6-Br_NiITMe2_ossts_PhBr_t_bb
Energy (POTENTIAL) = -1181.41909459 Eh

	Atom	X	Y	Z
1	C	-3.5750	3.3510	0.1943
2	C	-2.5766	4.1406	-0.3004
3	C	-1.8704	1.9633	-0.4591
4	N	-3.1232	2.0360	0.0827
5	N	-1.5552	3.2739	-0.6923
6	Ni	-0.8002	0.4165	-0.7521
7	C	0.2379	-1.0973	-1.2652
8	N	1.5510	-1.3663	-0.9956
9	N	-0.1711	-2.2056	-1.9560
10	C	1.9486	-2.6076	-1.4921
11	C	0.8519	-3.1428	-2.1048
12	Br	-0.5658	-0.0572	1.8745
13	C	-0.3397	-0.4640	3.9994
14	C	-0.3508	-1.7816	4.4532
15	C	-0.1724	0.5945	4.8906
16	C	-0.1930	-2.0441	5.8203
17	H	-0.4805	-2.6030	3.7509
18	C	-0.0146	0.3297	6.2573
19	H	-0.1633	1.6209	4.5284
20	C	-0.0248	-0.9891	6.7231
21	H	-0.2011	-3.0716	6.1790
22	H	0.1164	1.1530	6.9571
23	H	0.0982	-1.1937	7.7837
24	C	-3.8879	0.8778	0.5172
25	H	-4.8529	0.8419	0.0008
26	H	-3.3085	-0.0144	0.2782
27	H	-4.0590	0.9117	1.5978
28	C	-0.2908	3.7149	-1.2593
29	H	0.3072	2.8259	-1.4709
30	H	-0.4566	4.2719	-2.1874
31	H	0.2477	4.3536	-0.5511
32	C	-2.4755	5.6208	-0.4537
33	H	-3.3836	6.1060	-0.0851
34	H	-1.6253	6.0299	0.1073
35	H	-2.3425	5.9118	-1.5040
36	C	-4.9136	3.6934	0.7557
37	H	-5.7267	3.2478	0.1678
38	H	-5.0242	3.3340	1.7869
39	H	-5.0601	4.7771	0.7610
40	C	-1.5232	-2.4001	-2.4550
41	H	-1.9890	-3.2689	-1.9776
42	H	-2.1004	-1.5045	-2.2157
43	H	-1.5162	-2.5506	-3.5397
44	C	2.4273	-0.4758	-0.2513
45	H	3.3033	-0.2109	-0.8528
46	H	1.8620	0.4238	-0.0067
47	H	2.7591	-0.9506	0.6774
48	C	3.3327	-3.1352	-1.3199
49	H	3.5981	-3.2355	-0.2595
50	H	3.4255	-4.1216	-1.7830
51	H	4.0795	-2.4762	-1.7813

52	C	0.6607	-4.4353	-2.8239
53	H	-0.1326	-5.0410	-2.3673
54	H	0.3869	-4.2790	-3.8756
55	H	1.5836	-5.0220	-2.8032

large_basis_B-4-Cl_transNiClPhIMes2_bb
Energy (POTENTIAL) = -2710.42169637 Eh

	Atom	X	Y	Z
1	C	-0.3846	1.5597	0.6291
2	C	0.7496	2.2954	0.5801
3	C	1.3076	0.1538	0.0061
4	N	-0.0317	0.2601	0.2736
5	N	1.7690	1.4283	0.1886
6	Ni	2.3809	-1.4433	-0.3567
7	C	3.4772	-3.0312	-0.6846
8	N	4.7862	-3.2683	-0.3526
9	N	3.0464	-4.2384	-1.1647
10	C	5.1453	-4.5926	-0.6011
11	C	4.0511	-5.2033	-1.1098
12	H	6.1404	-4.9568	-0.3984
13	H	3.8829	-6.2161	-1.4416
14	H	-1.4010	1.8226	0.8778
15	H	0.9386	3.3390	0.7778
16	C	1.7913	-4.4795	-1.8333
17	C	0.6621	-4.8590	-1.0932
18	C	1.7672	-4.3839	-3.2356
19	C	-0.5304	-5.0805	-1.7918
20	C	0.5514	-4.6132	-3.8871
21	C	-0.6106	-4.9453	-3.1815
22	H	-1.4155	-5.3704	-1.2323
23	H	0.5124	-4.5244	-4.9706
24	C	5.7712	-2.2766	0.0069
25	C	6.4878	-1.6522	-1.0286
26	C	6.0807	-2.0486	1.3592
27	C	7.4481	-0.6936	-0.6817
28	C	7.0488	-1.0835	1.6545
29	C	7.7323	-0.3859	0.6511
30	H	7.9948	-0.1899	-1.4758
31	H	7.2853	-0.8841	2.6976
32	C	-1.0063	-0.7851	0.0952
33	C	-1.5857	-0.9429	-1.1773
34	C	-1.4119	-1.5603	1.1928
35	C	-2.4838	-1.9981	-1.3633
36	C	-2.3153	-2.6036	0.9553
37	C	-2.8429	-2.8526	-0.3152
38	H	-2.9218	-2.1467	-2.3481
39	H	-2.6196	-3.2296	1.7919
40	C	3.0964	1.8985	-0.1133
41	C	4.1328	1.7115	0.8123
42	C	3.2905	2.5801	-1.3268
43	C	5.4005	2.2003	0.4765
44	C	4.5751	3.0493	-1.6160
45	C	5.6436	2.8607	-0.7318
46	H	6.2144	2.0640	1.1824
47	H	4.7457	3.5641	-2.5591
48	C	3.0103	-4.0403	-4.0173
49	H	3.4262	-3.0841	-3.6878
50	H	3.7901	-4.8010	-3.8887
51	H	2.7876	-3.9607	-5.0852

52	C	0.7346	-5.0626	0.3963
53	H	1.4542	-5.8525	0.6501
54	H	1.0666	-4.1529	0.9048
55	H	-0.2420	-5.3506	0.7974
56	C	-1.9257	-5.1301	-3.8992
57	H	-1.7808	-5.5073	-4.9179
58	H	-2.5810	-5.8275	-3.3660
59	H	-2.4623	-4.1749	-3.9805
60	C	5.4603	-2.8727	2.4564
61	H	5.8558	-3.8976	2.4358
62	H	5.6895	-2.4476	3.4390
63	H	4.3753	-2.9324	2.3489
64	C	6.3205	-2.0632	-2.4708
65	H	6.9551	-2.9332	-2.6895
66	H	5.2932	-2.3376	-2.7105
67	H	6.6216	-1.2571	-3.1463
68	C	8.7819	0.6386	1.0099
69	H	9.6844	0.1550	1.4070
70	H	9.0790	1.2321	0.1396
71	H	8.4226	1.3263	1.7844
72	C	3.8967	1.0150	2.1257
73	H	3.0506	1.4578	2.6663
74	H	3.6515	-0.0402	1.9728
75	H	4.7834	1.0769	2.7637
76	C	2.1584	2.7729	-2.3052
77	H	1.3944	3.4560	-1.9140
78	H	2.5280	3.1848	-3.2486
79	H	1.6652	1.8200	-2.5229
80	C	7.0339	3.3275	-1.0907
81	H	7.0098	4.2457	-1.6886
82	H	7.6382	3.5166	-0.1972
83	H	7.5579	2.5669	-1.6852
84	C	-1.3514	0.0560	-2.2851
85	H	-0.3431	0.4709	-2.2730
86	H	-1.5204	-0.3967	-3.2667
87	H	-2.0552	0.8939	-2.1828
88	C	-0.9977	-1.2371	2.6062
89	H	-1.7921	-0.6574	3.0980
90	H	-0.8472	-2.1503	3.1895
91	H	-0.0740	-0.6618	2.6462
92	C	-3.8227	-3.9800	-0.5370
93	H	-4.8453	-3.6695	-0.2816
94	H	-3.8309	-4.3043	-1.5826
95	H	-3.5841	-4.8469	0.0892
96	C	2.5354	-0.9226	-2.1775
97	C	1.5081	-1.2094	-3.0938
98	C	3.6583	-0.2416	-2.6776
99	C	1.5907	-0.8355	-4.4396
100	H	0.6324	-1.7518	-2.7530
101	C	3.7543	0.1365	-4.0220
102	H	4.4732	0.0058	-2.0050
103	C	2.7182	-0.1576	-4.9132
104	H	0.7757	-1.0812	-5.1187
105	H	4.6393	0.6669	-4.3702
106	H	2.7885	0.1353	-5.9586

107	Cl	2.1058	-2.1093	1.8748

large_basis_B-5-Cl_NiIMes2_ClPh_bb
Energy (POTENTIAL) = -2710.33851328 Eh

	Atom	X	Y	Z
1	C	-0.4610	1.0287	0.0803
2	C	0.5697	1.8197	-0.3030
3	C	1.2773	-0.3619	-0.5098
4	N	-0.0223	-0.2886	-0.0471
5	N	1.6145	0.9666	-0.6552
6	Ni	2.3390	-1.8463	-0.8567
7	C	3.4081	-3.3056	-1.2868
8	N	4.6939	-3.6186	-0.8856
9	N	3.0909	-4.3617	-2.1123
10	C	5.1414	-4.8135	-1.4480
11	C	4.1324	-5.2820	-2.2206
12	H	6.1256	-5.2067	-1.2456
13	H	4.0521	-6.1680	-2.8316
14	H	-1.4554	1.2697	0.4231
15	H	0.6626	2.8934	-0.3622
16	C	1.8184	-4.5323	-2.7531
17	C	0.7791	-5.1526	-2.0410
18	C	1.6632	-4.1137	-4.0835
19	C	-0.4253	-5.3851	-2.7114
20	C	0.4343	-4.3535	-4.7086
21	C	-0.6163	-4.9950	-4.0423
22	H	-1.2371	-5.8736	-2.1776
23	H	0.2959	-4.0313	-5.7386
24	C	5.4707	-2.8346	0.0315
25	C	6.0035	-1.6060	-0.3967
26	C	5.7051	-3.3319	1.3244
27	C	6.7579	-0.8631	0.5169
28	C	6.4669	-2.5512	2.2024
29	C	6.9921	-1.3118	1.8219
30	H	7.1721	0.0900	0.1979
31	H	6.6513	-2.9232	3.2082
32	C	-0.8164	-1.4296	0.3045
33	C	-1.3336	-2.2450	-0.7163
34	C	-1.0794	-1.6845	1.6613
35	C	-2.1071	-3.3501	-0.3455
36	C	-1.8603	-2.8009	1.9818
37	C	-2.3743	-3.6500	0.9952
38	H	-2.5095	-3.9904	-1.1264
39	H	-2.0676	-3.0122	3.0290
40	C	2.9098	1.4319	-1.0614
41	C	3.9087	1.5848	-0.0875
42	C	3.1263	1.7644	-2.4082
43	C	5.1398	2.1138	-0.4883
44	C	4.3778	2.2765	-2.7655
45	C	5.3926	2.4660	-1.8188
46	H	5.9222	2.2424	0.2560
47	H	4.5637	2.5333	-3.8063
48	C	2.7802	-3.3914	-4.7933
49	H	3.0173	-2.4551	-4.2719
50	H	3.7023	-3.9848	-4.8146
51	H	2.5029	-3.1522	-5.8248

52	C	0.9492	-5.4999	-0.5853
53	H	1.8495	-6.1014	-0.4112
54	H	1.0599	-4.5802	0.0028
55	H	0.0848	-6.0541	-0.2072
56	C	-1.9495	-5.2112	-4.7180
57	H	-2.4198	-6.1452	-4.3896
58	H	-2.6461	-4.3963	-4.4758
59	H	-1.8514	-5.2417	-5.8086
60	C	5.1634	-4.6698	1.7658
61	H	5.7738	-5.4969	1.3803
62	H	5.1547	-4.7439	2.8575
63	H	4.1429	-4.8242	1.4056
64	C	5.7536	-1.0922	-1.7898
65	H	5.9355	-1.8678	-2.5432
66	H	4.7042	-0.7872	-1.8927
67	H	6.3909	-0.2323	-2.0116
68	C	7.7688	-0.4624	2.8001
69	H	7.1184	0.2866	3.2723
70	H	8.2054	-1.0676	3.6022
71	H	8.5799	0.0828	2.3036
72	C	3.6657	1.1422	1.3316
73	H	2.7768	1.6214	1.7601
74	H	3.4898	0.0597	1.3565
75	H	4.5231	1.3720	1.9710
76	C	2.0457	1.5358	-3.4346
77	H	1.1342	2.0987	-3.1995
78	H	2.3815	1.8315	-4.4335
79	H	1.7666	0.4747	-3.4616
80	C	6.7498	2.9801	-2.2360
81	H	6.6730	3.7242	-3.0371
82	H	7.2835	3.4374	-1.3955
83	H	7.3778	2.1618	-2.6153
84	C	-1.0458	-1.9544	-2.1654
85	H	-1.1744	-0.8904	-2.3959
86	H	-0.0033	-2.2077	-2.3987
87	H	-1.7006	-2.5358	-2.8199
88	C	-0.5436	-0.7863	2.7494
89	H	-1.1537	0.1201	2.8584
90	H	-0.5421	-1.3041	3.7133
91	H	0.4791	-0.4663	2.5328
92	C	-3.1726	-4.8766	1.3678
93	H	-2.5177	-5.7512	1.4838
94	H	-3.7020	-4.7405	2.3175
95	H	-3.9112	-5.1251	0.5973
96	C	2.2664	-3.1573	3.7660
97	C	1.1355	-3.7583	4.3218
98	C	3.4004	-2.8925	4.5362
99	C	1.1468	-4.1003	5.6768
100	H	0.2643	-3.9511	3.7031
101	C	3.3981	-3.2419	5.8891
102	H	4.2670	-2.4236	4.0804
103	C	2.2746	-3.8448	6.4622
104	H	0.2699	-4.5685	6.1166
105	H	4.2783	-3.0396	6.4939
106	H	2.2779	-4.1139	7.5148

107	Cl	2.2648	-2.7175	2.0499

large_basis_B-2x-Cl_NiIMes_e2PhCl_bb
Energy (POTENTIAL) = -1785.80647987 Eh

	Atom	X	Y	Z
1	Ni	0.0148	0.2122	0.0089
2	C	0.8462	-0.5469	1.5063
3	N	0.4609	-1.6260	2.2611
4	N	2.0502	-0.1920	2.0559
5	C	1.4012	-1.9303	3.2434
6	C	-0.7649	-2.3442	2.0490
7	C	2.4036	-1.0251	3.1149
8	C	2.8526	0.8859	1.5490
9	H	1.2655	-2.7519	3.9296
10	C	-1.8350	-2.1344	2.9319
11	C	-0.8585	-3.2289	0.9603
12	H	3.3236	-0.8952	3.6639
13	C	3.8043	0.6098	0.5568
14	C	2.6328	2.1838	2.0329
15	C	-3.0218	-2.8422	2.7052
16	C	-1.7223	-1.1538	4.0734
17	C	-2.0649	-3.9090	0.7728
18	C	0.2921	-3.4147	0.0031
19	C	4.5734	1.6735	0.0724
20	C	3.9434	-0.7817	-0.0061
21	C	3.4239	3.2161	1.5189
22	C	1.5392	2.4520	3.0344
23	C	-3.1551	-3.7325	1.6349
24	H	-3.8622	-2.6857	3.3777
25	H	-0.9706	-1.4670	4.8080
26	H	-1.4206	-0.1629	3.7130
27	H	-2.6789	-1.0514	4.5945
28	H	-2.1563	-4.5944	-0.0674
29	H	1.2344	-3.6010	0.5314
30	H	0.1039	-4.2524	-0.6753
31	H	0.4377	-2.5069	-0.5970
32	C	4.4050	2.9794	0.5475
33	H	5.3141	1.4773	-0.6999
34	H	4.1605	-1.5199	0.7752
35	H	3.0052	-1.0900	-0.4853
36	H	4.7429	-0.8264	-0.7518
37	H	3.2645	4.2298	1.8803
38	H	1.6421	1.8238	3.9272
39	H	1.5416	3.5001	3.3491
40	H	0.5605	2.2251	2.5931
41	C	-4.4380	-4.4957	1.4070
42	C	5.2674	4.1089	0.0357
43	H	-4.3005	-5.5677	1.6014
44	H	-5.2405	-4.1390	2.0609
45	H	-4.7778	-4.3999	0.3687
46	H	6.1160	4.2921	0.7090
47	H	5.6783	3.8845	-0.9546
48	H	4.7018	5.0453	-0.0328
49	C	-1.1227	1.9364	-0.7370
50	H	-2.1282	2.0294	-0.3389
51	C	-0.7947	0.8320	-1.5781

52	C	0.5372	0.7202	-2.0813
53	H	0.8036	-0.1233	-2.7102
54	C	-0.2038	2.9984	-0.6009
55	H	-0.4823	3.8571	0.0042
56	C	1.4255	1.8055	-1.9355
57	H	2.4196	1.7327	-2.3671
58	C	1.0462	2.9533	-1.2299
59	H	1.7390	3.7817	-1.1250
60	Cl	-2.1040	-0.2075	-2.2581

large_basis_NiCOD2_NiCOD2_bb
Energy (POTENTIAL) = -793.668115087 Eh

	Atom	X	Y	Z
1	Ni	1.2955	1.7831	0.0000
2	C	1.6628	1.8252	2.1232
3	H	0.9258	2.5087	2.5397
4	C	2.7329	2.3987	1.4530
5	H	2.7680	3.4870	1.4223
6	C	1.3559	-0.3513	0.2411
7	H	0.6516	-0.7688	-0.4774
8	C	2.5829	0.0608	-0.2533
9	H	2.7338	-0.0403	-1.3257
10	C	-0.7766	1.5888	-0.5253
11	H	-1.1683	0.7487	0.0470
12	C	-0.6180	2.7869	0.1529
13	H	-0.8698	2.7828	1.2115
14	C	1.5389	2.4417	-2.0461
15	H	2.3744	1.8697	-2.4439
16	C	1.8563	3.4806	-1.1854
17	H	2.9147	3.6605	-0.9999
18	C	4.0293	1.7156	1.0644
19	C	1.6234	0.4064	2.6773
20	C	1.0040	-0.6102	1.6923
21	C	3.8510	0.2621	0.5675
22	C	-0.5164	4.1659	-0.4878
23	C	-0.7922	1.3868	-2.0273
24	C	0.2204	2.2701	-2.7902
25	C	0.9413	4.6074	-0.7490
26	H	3.8596	-0.4314	1.4142
27	H	4.7185	-0.0075	-0.0470
28	H	-0.0889	-0.5599	1.7775
29	H	1.2833	-1.6359	1.9860
30	H	2.6324	0.0919	2.9613
31	H	1.0378	0.4011	3.6047
32	H	4.4783	2.3070	0.2567
33	H	4.7524	1.7403	1.8966
34	H	-0.9936	4.9010	0.1715
35	H	-1.0899	4.1854	-1.4197
36	H	1.3529	5.0229	0.1795
37	H	0.9577	5.4307	-1.4824
38	H	-0.2175	3.2497	-3.0057
39	H	0.4199	1.8120	-3.7664
40	H	-0.5449	0.3341	-2.2145
41	H	-1.8057	1.5388	-2.4344

large_basis_A-5-Br_NiITMe2_BrPh_bb
Energy (POTENTIAL) = -1181.44663653 Eh

	Atom	X	Y	Z
1	C	-0.3549	0.3218	-0.0836
2	C	0.1280	0.2431	-1.3579
3	C	-0.2210	2.4694	-0.8959
4	N	-0.5653	1.6772	0.1707
5	N	0.1991	1.5546	-1.8294
6	C	-1.0575	2.1945	1.4361
7	H	-1.1819	3.2732	1.3277
8	H	-2.0197	1.7366	1.6894
9	H	-0.3435	1.9969	2.2424
10	C	0.6691	1.9105	-3.1580
11	H	0.0267	1.4696	-3.9284
12	H	0.6379	2.9993	-3.2393
13	H	1.6966	1.5629	-3.3110
14	C	0.5354	-0.9293	-2.1851
15	H	-0.0517	-0.9983	-3.1102
16	H	1.5928	-0.8734	-2.4756
17	H	0.3912	-1.8595	-1.6282
18	C	-0.6442	-0.7377	0.9256
19	H	-0.3767	-1.7230	0.5335
20	H	-0.0759	-0.5800	1.8516
21	H	-1.7075	-0.7623	1.1980
22	C	-0.2355	6.2173	-1.1696
23	N	0.7982	7.0522	-1.5134
24	N	-1.2629	7.0934	-0.9217
25	C	0.4309	8.3976	-1.4736
26	C	2.1328	6.5889	-1.8541
27	C	-0.8818	8.4243	-1.0994
28	C	-2.5951	6.6820	-0.5102
29	C	1.3806	9.4973	-1.8102
30	H	2.1083	5.4984	-1.8857
31	H	2.4361	6.9788	-2.8317
32	H	2.8597	6.9080	-1.0997
33	C	-1.8281	9.5616	-0.9054
34	H	-3.3469	7.0319	-1.2261
35	H	-2.6076	5.5904	-0.4749
36	H	-2.8355	7.0808	0.4815
37	H	0.8962	10.4709	-1.6940
38	H	2.2654	9.4835	-1.1604
39	H	1.7381	9.4229	-2.8458
40	H	-2.6690	9.5141	-1.6101
41	H	-2.2521	9.5694	0.1070
42	H	-1.3171	10.5161	-1.0602
43	Ni	-0.2199	4.3445	-1.0087
44	Br	1.8522	4.4273	1.1243
45	C	3.2306	4.4974	2.5455
46	C	2.8800	4.9288	3.8270
47	C	4.5425	4.1168	2.2535
48	C	3.8578	4.9789	4.8254
49	H	1.8573	5.2232	4.0457
50	C	5.5127	4.1714	3.2590
51	H	4.8067	3.7819	1.2543

52	C	5.1739	4.6015	4.5449
53	H	3.5861	5.3140	5.8234
54	H	6.5343	3.8760	3.0329
55	H	5.9309	4.6421	5.3235

large_basis_Phrad_Phrad_bb
Energy (POTENTIAL) = -231.634154727 Eh

	Atom	X	Y	Z
1	C	-2.2262	0.0360	0.0001
2	C	-0.8199	0.0232	0.0005
3	C	-0.1934	1.2514	-0.0002
4	C	-0.8199	2.4797	-0.0011
5	C	-2.2260	2.4671	-0.0015
6	C	-2.9185	1.2516	-0.0009
7	H	-2.7717	-0.9050	0.0005
8	H	-0.2699	-0.9145	0.0012
9	H	-0.2697	3.4174	-0.0016
10	H	-2.7716	3.4081	-0.0022
11	H	-4.0052	1.2516	-0.0012

large_basis_NiCODIPhen_NiCODIPhen_bb
Energy (POTENTIAL) = -1170.02023238 Eh

	Atom	X	Y	Z
1	Ni	-0.1561	0.1578	0.1904
2	C	-1.8587	1.4068	-0.0744
3	H	-2.5302	1.1754	0.7548
4	C	-0.7380	2.1675	0.2297
5	H	-0.6233	2.4953	1.2619
6	C	-0.2079	-0.0084	-1.9358
7	H	-0.2262	-1.0771	-2.1577
8	C	0.9966	0.5265	-1.4862
9	H	1.8753	-0.1168	-1.4511
10	C	0.1402	2.8824	-0.7916
11	C	-2.4324	1.1282	-1.4514
12	C	-1.3545	0.8083	-2.5127
13	C	1.2874	2.0140	-1.4021
14	H	0.5979	3.7556	-0.3126
15	H	-0.4910	3.2756	-1.5962
16	H	2.1859	2.1399	-0.7922
17	H	1.5347	2.4151	-2.3989
18	H	-0.9700	1.7353	-2.9510
19	H	-1.8210	0.2577	-3.3399
20	H	-3.0983	0.2607	-1.3578
21	H	-3.0688	1.9614	-1.7958
22	C	0.8841	-0.5494	1.6037
23	N	0.5292	-1.6968	2.3049
24	N	2.1463	-0.2852	2.0858
25	C	1.5542	-2.1219	3.1573
26	C	-0.7423	-2.3035	2.1714
27	C	2.5671	-1.2387	3.0164
28	C	2.9123	0.8575	1.7076
29	H	1.4812	-3.0146	3.7577
30	C	-1.2959	-3.0553	3.2165
31	C	-1.4777	-2.1080	0.9917
32	H	3.5352	-1.1871	3.4908
33	C	4.1570	0.6898	1.0958
34	C	2.4116	2.1373	1.9635
35	C	-2.5740	-3.5981	3.0799
36	C	-2.7610	-2.6433	0.8720
37	C	4.9020	1.8142	0.7323
38	C	3.1594	3.2558	1.5949
39	C	-3.3164	-3.3898	1.9132
40	H	-2.9955	-4.1748	3.8987
41	H	-3.3174	-2.4845	-0.0480
42	C	4.4042	3.0971	0.9775
43	H	5.8673	1.6858	0.2507
44	H	2.7698	4.2508	1.7916
45	H	4.5247	-0.3127	0.8974
46	H	1.4439	2.2425	2.4409
47	H	4.9845	3.9697	0.6905
48	H	-1.0229	-1.6053	0.1288
49	H	-0.7477	-3.1917	4.1434
50	H	-4.3146	-3.8077	1.8170

large_basis_D-2-Cl_NiIPhen2_e2_PhCl_bb
Energy (POTENTIAL) = -2238.36781748 Eh

	Atom	X	Y	Z
1	C	2.0810	1.2427	0.5183
2	C	2.9228	1.5080	-0.5051
3	C	2.0522	-0.5878	-0.8684
4	N	1.5482	-0.0283	0.2866
5	N	2.8878	0.3927	-1.3411
6	Ni	1.8251	-2.3645	-1.5670
7	C	3.5196	-3.3478	-1.2363
8	N	4.2279	-3.5476	-0.0741
9	N	4.2034	-4.1382	-2.1334
10	C	5.2816	-4.4449	-0.2404
11	C	5.2695	-4.8124	-1.5404
12	H	5.9405	-4.7071	0.5727
13	H	5.9272	-5.4537	-2.1058
14	H	1.8317	1.8209	1.3935
15	H	3.5273	2.3733	-0.7290
16	C	3.9290	-4.2459	-3.5305
17	C	3.9144	-5.5074	-4.1340
18	C	3.7362	-3.0904	-4.2868
19	C	3.7132	-5.6056	-5.5113
20	C	3.5217	-3.1998	-5.6601
21	C	3.5159	-4.4532	-6.2774
22	H	3.6997	-6.5846	-5.9822
23	H	3.3628	-2.2985	-6.2442
24	C	3.9701	-2.9346	1.1934
25	C	4.1450	-1.5592	1.3503
26	C	3.5957	-3.7371	2.2745
27	C	3.9156	-0.9785	2.5981
28	C	3.3779	-3.1500	3.5219
29	C	3.5318	-1.7703	3.6835
30	H	4.0371	0.0939	2.7180
31	H	3.0783	-3.7691	4.3626
32	C	0.6060	-0.6345	1.1731
33	C	-0.3630	0.1643	1.7900
34	C	0.6510	-2.0053	1.4334
35	C	-1.2818	-0.4136	2.6669
36	C	-0.2748	-2.5762	2.3048
37	C	-1.2433	-1.7856	2.9276
38	H	-2.0367	0.2117	3.1359
39	H	-0.2300	-3.6442	2.5003
40	C	3.5913	0.3312	-2.5853
41	C	4.9872	0.2865	-2.5887
42	C	2.8724	0.3563	-3.7830
43	C	5.6695	0.2634	-3.8073
44	C	3.5617	0.3376	-4.9963
45	C	4.9590	0.2901	-5.0105
46	H	6.7550	0.2213	-3.8145
47	H	3.0052	0.3554	-5.9289
48	C	0.0919	-2.4020	-2.3475
49	C	0.0033	-1.9561	-3.7208
50	C	0.4183	-3.8021	-2.1294
51	C	0.1809	-2.8278	-4.7656

52	H	-0.2293	-0.9109	-3.9080
53	C	0.5056	-4.6878	-3.2543
54	H	0.1928	-4.2499	-1.1615
55	C	0.4050	-4.2201	-4.5412
56	H	0.1454	-2.4520	-5.7865
57	H	0.6384	-5.7524	-3.0671
58	H	0.5046	-4.8935	-5.3875
59	Cl	-1.4298	-1.6900	-1.3403
60	H	5.5265	0.2634	-1.6462
61	H	5.4925	0.2705	-5.9566
62	H	1.7892	0.3815	-3.7543
63	H	3.3540	-4.5328	-7.3489
64	H	-1.9626	-2.2334	3.6078
65	H	-0.4211	1.2244	1.5640
66	H	1.4036	-2.6163	0.9534
67	H	3.4648	-4.8052	2.1278
68	H	3.3518	-1.3132	4.6525
69	H	4.4489	-0.9586	0.5006
70	H	4.0491	-6.3987	-3.5285
71	H	3.7500	-2.1270	-3.7956

large_basis_NiIMes2_distort_NiIMes2_eta2_PhCl_bb_NiL2frag
Energy (POTENTIAL) = -2018.31962356 Eh

	Atom	X	Y	Z
1	C	1.1354	1.4192	0.0000
2	C	2.1352	1.7031	-0.8560
3	C	1.8781	-0.5999	-0.8586
4	N	0.9715	0.0344	-0.0160
5	N	2.5792	0.4832	-1.3643
6	Ni	2.0746	-2.5050	-1.4154
7	C	3.7583	-3.6476	-1.2841
8	N	4.4943	-3.9520	-0.1529
9	N	4.2055	-4.6234	-2.1668
10	C	5.3284	-5.0567	-0.3283
11	C	5.1508	-5.4735	-1.5981
12	H	5.9678	-5.4167	0.4627
13	H	5.5984	-6.2802	-2.1576
14	H	0.5183	2.0553	0.6149
15	H	2.5765	2.6398	-1.1578
16	C	3.9054	-4.7379	-3.5648
17	C	3.2538	-5.8834	-4.0467
18	C	4.3879	-3.7427	-4.4344
19	C	3.0244	-5.9768	-5.4273
20	C	4.1190	-3.8707	-5.7983
21	C	3.4289	-4.9765	-6.3145
22	H	2.5033	-6.8516	-5.8105
23	H	4.4761	-3.1002	-6.4787
24	C	4.6651	-3.1549	1.0306
25	C	5.6189	-2.1238	0.9903
26	C	4.0368	-3.5390	2.2223
27	C	5.8657	-1.4106	2.1672
28	C	4.3342	-2.8133	3.3819
29	C	5.2259	-1.7356	3.3705
30	H	6.5930	-0.6018	2.1503
31	H	3.8488	-3.0936	4.3140
32	C	-0.1289	-0.5207	0.7274
33	C	-1.4387	-0.1898	0.3360
34	C	0.1210	-1.2538	1.8949
35	C	-2.4992	-0.6536	1.1248
36	C	-0.9670	-1.6909	2.6540
37	C	-2.2858	-1.4091	2.2822
38	H	-3.5173	-0.4173	0.8224
39	H	-0.7778	-2.2682	3.5568
40	C	3.5994	0.4919	-2.3755
41	C	4.9080	0.8479	-2.0107
42	C	3.2223	0.3422	-3.7216
43	C	5.8643	0.9680	-3.0270
44	C	4.2062	0.4941	-4.7020
45	C	5.5341	0.7927	-4.3746
46	H	6.8863	1.2251	-2.7567
47	H	3.9278	0.3747	-5.7469
48	C	5.2262	-2.6067	-3.9105
49	H	4.6401	-1.9376	-3.2772
50	H	6.0544	-2.9852	-3.2993
51	H	5.6455	-2.0230	-4.7326

52	C	2.8092	-7.0096	-3.1425
53	H	3.5600	-7.8106	-3.1165
54	H	2.6509	-6.6820	-2.1118
55	H	1.8761	-7.4506	-3.5088
56	C	3.1242	-5.0689	-7.7904
57	H	2.8379	-6.0853	-8.0807
58	H	2.2948	-4.4017	-8.0609
59	H	3.9873	-4.7706	-8.3975
60	C	3.0666	-4.6919	2.2452
61	H	3.5442	-5.6253	1.9227
62	H	2.6645	-4.8467	3.2512
63	H	2.2285	-4.5104	1.5634
64	C	6.4009	-1.8579	-0.2714
65	H	6.9499	-2.7559	-0.5818
66	H	5.7439	-1.5834	-1.1010
67	H	7.1265	-1.0546	-0.1224
68	C	5.4876	-0.9349	4.6236
69	H	5.3475	-1.5412	5.5254
70	H	6.5060	-0.5306	4.6372
71	H	4.7987	-0.0821	4.6951
72	C	5.2641	1.1678	-0.5793
73	H	4.9010	2.1656	-0.3014
74	H	4.8186	0.4583	0.1231
75	H	6.3483	1.1644	-0.4378
76	C	1.7918	0.0565	-4.0875
77	H	1.1194	0.8319	-3.6982
78	H	1.6654	0.0044	-5.1734
79	H	1.4652	-0.8923	-3.6566
80	C	6.5890	0.8875	-5.4499
81	H	7.4083	1.5527	-5.1557
82	H	7.0282	-0.0994	-5.6528
83	H	6.1701	1.2550	-6.3935
84	C	-1.7231	0.6386	-0.8950
85	H	-1.0382	0.3934	-1.7112
86	H	-2.7461	0.4661	-1.2449
87	H	-1.6216	1.7120	-0.6913
88	C	1.5304	-1.5515	2.3102
89	H	2.0953	-0.6321	2.5110
90	H	1.5552	-2.1711	3.2097
91	H	2.0603	-2.0738	1.5114
92	C	-3.4449	-1.9355	3.0939
93	H	-4.3532	-1.3448	2.9320
94	H	-3.6755	-2.9737	2.8187
95	H	-3.2194	-1.9293	4.1667

large_basis_IPhen_IPhen_bb
Energy (POTENTIAL) = -688.496357545 Eh

	Atom	X	Y	Z
1	C	-0.6466	0.9681	-1.0949
2	C	0.4499	1.7141	-1.3587
3	C	1.1837	-0.2414	-0.3732
4	N	-0.1820	-0.2087	-0.4976
5	N	1.5457	0.9669	-0.9127
6	H	-1.6945	1.1808	-1.2388
7	H	0.5438	2.7045	-1.7763
8	C	-1.0315	-1.2735	-0.0740
9	C	-2.1980	-1.5673	-0.7891
10	C	-0.6968	-2.0198	1.0619
11	C	-3.0312	-2.6020	-0.3596
12	C	-1.5290	-3.0601	1.4744
13	C	-2.7010	-3.3529	0.7708
14	H	-3.9347	-2.8260	-0.9204
15	H	-1.2637	-3.6364	2.3566
16	C	2.8997	1.4059	-1.0115
17	C	3.8175	1.0561	-0.0143
18	C	3.3063	2.1892	-2.0978
19	C	5.1398	1.4888	-0.1109
20	C	4.6292	2.6284	-2.1776
21	C	5.5507	2.2801	-1.1877
22	H	5.8479	1.2141	0.6662
23	H	4.9385	3.2356	-3.0240
24	H	3.4866	0.4507	0.8220
25	H	2.6009	2.4379	-2.8846
26	H	6.5802	2.6208	-1.2546
27	H	0.2100	-1.7800	1.6056
28	H	-3.3497	-4.1599	1.1000
29	H	-2.4434	-1.0067	-1.6858

large_basis_A-6-Br_NiBrITMe2_bb
Energy (POTENTIAL) = -949.818278044 Eh

	Atom	X	Y	Z
1	C	-0.4894	2.1504	1.2060
2	C	-0.0973	2.1475	-0.1025
3	C	-0.0612	4.3188	0.6202
4	N	-0.4605	3.4827	1.6176
5	N	0.1544	3.4800	-0.4330
6	C	-0.8152	3.9248	2.9583
7	H	-0.6376	4.9985	3.0185
8	H	-1.8676	3.7043	3.1667
9	H	-0.1891	3.4230	3.7018
10	C	0.6171	3.9151	-1.7424
11	H	-0.1089	3.6461	-2.5164
12	H	0.7360	5.0003	-1.7166
13	H	1.5805	3.4533	-1.9809
14	C	0.0696	1.0336	-1.0808
15	H	-0.5665	1.1727	-1.9644
16	H	1.1059	0.9566	-1.4343
17	H	-0.1992	0.0784	-0.6218
18	C	-0.8954	1.0405	2.1154
19	H	-0.8426	0.0807	1.5944
20	H	-0.2436	0.9805	2.9963
21	H	-1.9231	1.1703	2.4788
22	C	0.0026	8.1737	0.2801
23	N	0.9428	9.0544	-0.1596
24	N	-1.1144	8.9428	0.4217
25	C	0.4339	10.3472	-0.2843
26	C	2.3193	8.6919	-0.4636
27	C	-0.8785	10.2772	0.0884
28	C	-2.3978	8.4415	0.8896
29	C	1.2690	11.4956	-0.7406
30	H	2.4580	7.6421	-0.2060
31	H	2.5299	8.8505	-1.5267
32	H	3.0108	9.2939	0.1331
33	C	-1.9380	11.3232	0.1736
34	H	-3.1721	8.5996	0.1318
35	H	-2.2930	7.3721	1.0846
36	H	-2.6930	8.9484	1.8137
37	H	0.6710	12.4102	-0.7834
38	H	2.1112	11.6771	-0.0609
39	H	1.6875	11.3203	-1.7401
40	H	-2.7947	11.0874	-0.4709
41	H	-2.3195	11.4295	1.1974
42	H	-1.5423	12.2937	-0.1382
43	Ni	0.2028	6.2627	0.6833
44	Br	2.0449	6.3896	2.5376

large_basis_A-3-Cl_cis-NiClPhITMe2_bb
Energy (POTENTIAL) = -1628.59300135 Eh

	Atom	X	Y	Z
1	C	0.2636	0.4374	-0.8143
2	C	1.2393	-0.0788	-0.0121
3	C	-0.1108	-1.8091	-0.6464
4	N	-0.5471	-0.6400	-1.1843
5	N	0.9827	-1.4506	0.0753
6	Ni	-0.8232	-3.6229	-1.0123
7	C	0.7469	-4.0552	-1.9549
8	N	1.7457	-4.8987	-1.5887
9	N	1.1250	-3.5873	-3.1723
10	C	2.7454	-4.9623	-2.5662
11	C	2.3527	-4.1287	-3.5711
12	C	-1.6891	-5.7121	-2.8953
13	C	-2.1892	-6.9616	-3.2836
14	C	-1.4671	-5.3741	-1.5447
15	C	-2.4605	-7.9375	-2.3208
16	H	-2.3577	-7.1766	-4.3380
17	C	-1.7561	-6.3799	-0.5994
18	C	-2.2360	-7.6401	-0.9721
19	H	-2.8389	-8.9140	-2.6153
20	H	-1.6162	-6.1664	0.4588
21	H	-2.4427	-8.3898	-0.2096
22	C	-1.7357	-0.5072	-2.0149
23	H	-1.4657	-0.1727	-3.0217
24	H	-2.2283	-1.4774	-2.0638
25	H	-2.4255	0.2161	-1.5704
26	C	-0.0058	1.8312	-1.2703
27	H	-0.0031	1.9065	-2.3653
28	H	-0.9829	2.1894	-0.9215
29	H	0.7572	2.5131	-0.8852
30	C	2.3793	0.5717	0.6956
31	H	3.3436	0.1435	0.3933
32	H	2.4029	1.6421	0.4736
33	H	2.2982	0.4581	1.7843
34	C	1.7972	-2.3897	0.8318
35	H	1.2274	-3.3097	0.9522
36	H	2.7338	-2.6061	0.3069
37	H	2.0251	-1.9789	1.8187
38	C	1.7462	-5.7074	-0.3782
39	H	1.7418	-6.7708	-0.6349
40	H	2.6292	-5.4851	0.2282
41	H	0.8450	-5.4790	0.1884
42	C	0.3650	-2.6193	-3.9500
43	H	0.8207	-1.6258	-3.8849
44	H	0.3260	-2.9301	-4.9968
45	H	-0.6481	-2.5784	-3.5524
46	C	3.9504	-5.8260	-2.4135
47	H	4.5270	-5.5632	-1.5172
48	H	3.6795	-6.8861	-2.3280
49	H	4.6082	-5.7177	-3.2800
50	C	2.9968	-3.7787	-4.8695
51	H	2.3766	-4.0784	-5.7241

52	H	3.1744	-2.6992	-4.9561
53	H	3.9607	-4.2861	-4.9628
54	H	-1.4584	-4.9822	-3.6712
55	Cl	-2.7404	-3.1858	0.2028

large_basis_C-1_NiIXy2_bb
Energy (POTENTIAL) = -1861.05447589 Eh

	Atom	X	Y	Z
1	C	-0.0609	0.0050	0.3271
2	C	0.9900	0.7587	-0.0807
3	C	1.5418	-1.4398	-0.4656
4	N	0.2863	-1.3249	0.0888
5	N	1.9546	-0.1284	-0.5547
6	Ni	2.4800	-2.9327	-1.0184
7	C	3.4876	-4.3901	-1.5403
8	N	4.7944	-4.6568	-1.1962
9	N	3.1435	-5.4895	-2.2951
10	C	5.2346	-5.8750	-1.7108
11	C	4.1948	-6.3992	-2.4057
12	H	6.2317	-6.2469	-1.5309
13	H	4.0978	-7.3219	-2.9569
14	H	-1.0129	0.2813	0.7540
15	H	1.1425	1.8272	-0.0847
16	C	1.8500	-5.6664	-2.8906
17	C	0.7809	-6.0892	-2.0820
18	C	1.7028	-5.4191	-4.2664
19	C	-0.4640	-6.2806	-2.6942
20	C	0.4407	-5.6200	-4.8381
21	C	-0.6341	-6.0522	-4.0600
22	H	-1.3041	-6.6085	-2.0884
23	H	0.3036	-5.4307	-5.8999
24	C	5.5918	-3.7741	-0.3921
25	C	6.5096	-2.9241	-1.0305
26	C	5.4259	-3.7930	1.0036
27	C	7.2953	-2.0880	-0.2280
28	C	6.2255	-2.9356	1.7689
29	C	7.1579	-2.0945	1.1602
30	H	8.0080	-1.4179	-0.7011
31	H	6.1113	-2.9296	2.8500
32	C	-0.5522	-2.4501	0.3900
33	C	-1.2434	-3.0840	-0.6570
34	C	-0.6577	-2.8723	1.7268
35	C	-2.0770	-4.1610	-0.3309
36	C	-1.4997	-3.9547	2.0088
37	C	-2.2090	-4.5915	0.9895
38	H	-2.6203	-4.6651	-1.1252
39	H	-1.5927	-4.2997	3.0356
40	C	3.2366	0.2572	-1.0746
41	C	4.2671	0.5613	-0.1699
42	C	3.4154	0.3112	-2.4677
43	C	5.5049	0.9519	-0.6942
44	C	4.6711	0.6985	-2.9510
45	C	5.7065	1.0214	-2.0729
46	H	6.3184	1.1853	-0.0127
47	H	4.8345	0.7417	-4.0250
48	C	2.8645	-4.9192	-5.0879
49	H	3.2670	-3.9901	-4.6654
50	H	3.6897	-5.6410	-5.1114
51	H	2.5576	-4.7222	-6.1197

52	C	0.9619	-6.2796	-0.5989
53	H	1.8200	-6.9244	-0.3742
54	H	1.1599	-5.3089	-0.1248
55	H	0.0679	-6.7153	-0.1436
56	C	4.3766	-4.6655	1.6411
57	H	4.4534	-5.7079	1.3095
58	H	4.4515	-4.6414	2.7329
59	H	3.3781	-4.3121	1.3472
60	C	6.6016	-2.8768	-2.5348
61	H	6.8503	-3.8548	-2.9636
62	H	5.6398	-2.5722	-2.9652
63	H	7.3617	-2.1589	-2.8580
64	C	4.0554	0.4119	1.3156
65	H	3.2511	1.0604	1.6834
66	H	3.7719	-0.6197	1.5569
67	H	4.9686	0.6534	1.8678
68	C	2.3050	-0.0932	-3.4018
69	H	1.3684	0.4297	-3.1745
70	H	2.5718	0.1094	-4.4439
71	H	2.1047	-1.1683	-3.2909
72	C	-1.0488	-2.6509	-2.0862
73	H	-1.1856	-1.5694	-2.2050
74	H	-0.0223	-2.8793	-2.4037
75	H	-1.7451	-3.1667	-2.7535
76	C	0.1416	-2.1987	2.8143
77	H	-0.1339	-1.1438	2.9319
78	H	-0.0104	-2.6979	3.7763
79	H	1.2128	-2.2228	2.5796
80	H	7.7734	-1.4368	1.7689
81	H	-1.6075	-6.2067	-4.5187
82	H	-2.8613	-5.4289	1.2244
83	H	6.6752	1.3219	-2.4641

large_basis_B-2-Cl_NiIMes2_eta2_PhCl_bb
Energy (POTENTIAL) = -2710.32115799 Eh

	Atom	X	Y	Z
1	C	1.1354	1.4192	0.0000
2	C	2.1352	1.7031	-0.8560
3	C	1.8781	-0.5999	-0.8586
4	N	0.9715	0.0344	-0.0160
5	N	2.5792	0.4832	-1.3643
6	Ni	2.0746	-2.5050	-1.4154
7	C	3.7583	-3.6476	-1.2841
8	N	4.4943	-3.9520	-0.1529
9	N	4.2055	-4.6234	-2.1668
10	C	5.3284	-5.0567	-0.3283
11	C	5.1508	-5.4735	-1.5981
12	H	5.9678	-5.4167	0.4627
13	H	5.5984	-6.2802	-2.1576
14	H	0.5183	2.0553	0.6149
15	H	2.5765	2.6398	-1.1578
16	C	3.9054	-4.7379	-3.5648
17	C	3.2538	-5.8834	-4.0467
18	C	4.3879	-3.7427	-4.4344
19	C	3.0244	-5.9768	-5.4273
20	C	4.1190	-3.8707	-5.7983
21	C	3.4289	-4.9765	-6.3145
22	H	2.5033	-6.8516	-5.8105
23	H	4.4761	-3.1002	-6.4787
24	C	4.6651	-3.1549	1.0306
25	C	5.6189	-2.1238	0.9903
26	C	4.0368	-3.5390	2.2223
27	C	5.8657	-1.4106	2.1672
28	C	4.3342	-2.8133	3.3819
29	C	5.2259	-1.7356	3.3705
30	H	6.5930	-0.6018	2.1503
31	H	3.8488	-3.0936	4.3140
32	C	-0.1289	-0.5207	0.7274
33	C	-1.4387	-0.1898	0.3360
34	C	0.1210	-1.2538	1.8949
35	C	-2.4992	-0.6536	1.1248
36	C	-0.9670	-1.6909	2.6540
37	C	-2.2858	-1.4091	2.2822
38	H	-3.5173	-0.4173	0.8224
39	H	-0.7778	-2.2682	3.5568
40	C	3.5994	0.4919	-2.3755
41	C	4.9080	0.8479	-2.0107
42	C	3.2223	0.3422	-3.7216
43	C	5.8643	0.9680	-3.0270
44	C	4.2062	0.4941	-4.7020
45	C	5.5341	0.7927	-4.3746
46	H	6.8863	1.2251	-2.7567
47	H	3.9278	0.3747	-5.7469
48	C	5.2262	-2.6067	-3.9105
49	H	4.6401	-1.9376	-3.2772
50	H	6.0544	-2.9852	-3.2993
51	H	5.6455	-2.0230	-4.7326

52	C	2.8092	-7.0096	-3.1425
53	H	3.5600	-7.8106	-3.1165
54	H	2.6509	-6.6820	-2.1118
55	H	1.8761	-7.4506	-3.5088
56	C	3.1242	-5.0689	-7.7904
57	H	2.8379	-6.0853	-8.0807
58	H	2.2948	-4.4017	-8.0609
59	H	3.9873	-4.7706	-8.3975
60	C	3.0666	-4.6919	2.2452
61	H	3.5442	-5.6253	1.9227
62	H	2.6645	-4.8467	3.2512
63	H	2.2285	-4.5104	1.5634
64	C	6.4009	-1.8579	-0.2714
65	H	6.9499	-2.7559	-0.5818
66	H	5.7439	-1.5834	-1.1010
67	H	7.1265	-1.0546	-0.1224
68	C	5.4876	-0.9349	4.6236
69	H	5.3475	-1.5412	5.5254
70	H	6.5060	-0.5306	4.6372
71	H	4.7987	-0.0821	4.6951
72	C	5.2641	1.1678	-0.5793
73	H	4.9010	2.1656	-0.3014
74	H	4.8186	0.4583	0.1231
75	H	6.3483	1.1644	-0.4378
76	C	1.7918	0.0565	-4.0875
77	H	1.1194	0.8319	-3.6982
78	H	1.6654	0.0044	-5.1734
79	H	1.4652	-0.8923	-3.6566
80	C	6.5890	0.8875	-5.4499
81	H	7.4083	1.5527	-5.1557
82	H	7.0282	-0.0994	-5.6528
83	H	6.1701	1.2550	-6.3935
84	C	-1.7231	0.6386	-0.8950
85	H	-1.0382	0.3934	-1.7112
86	H	-2.7461	0.4661	-1.2449
87	H	-1.6216	1.7120	-0.6913
88	C	1.5304	-1.5515	2.3102
89	H	2.0953	-0.6321	2.5110
90	H	1.5552	-2.1711	3.2097
91	H	2.0603	-2.0738	1.5114
92	C	-3.4449	-1.9355	3.0939
93	H	-4.3532	-1.3448	2.9320
94	H	-3.6755	-2.9737	2.8187
95	H	-3.2194	-1.9293	4.1667
96	C	0.1944	-3.1925	-1.5224
97	C	-0.9413	-2.4416	-1.9783
98	C	1.0252	-3.8947	-2.4764
99	C	-1.0992	-2.1716	-3.3148
100	H	-1.6568	-2.0868	-1.2480
101	C	0.7995	-3.5841	-3.8633
102	H	1.4233	-4.8732	-2.2353
103	C	-0.1982	-2.7293	-4.2699
104	H	-1.9267	-1.5485	-3.6462
105	H	1.4054	-4.0874	-4.6077
106	H	-0.3367	-2.5184	-5.3279

107	Cl	-0.1053	-4.0922	0.0616

large_basis_NiCODIXy_NiCODIXy_bb
Energy (POTENTIAL) = -1327.34590008 Eh

	Atom	X	Y	Z
1	Ni	-1.2346	0.6714	-0.0020
2	C	-3.1362	1.7031	-0.0373
3	H	-3.7201	1.2650	0.7755
4	C	-2.1155	2.5640	0.3293
5	H	-1.9970	2.7700	1.3917
6	C	-1.3866	0.7573	-2.0959
7	H	-1.2858	-0.2706	-2.4547
8	C	-0.2244	1.3752	-1.6240
9	H	0.7297	0.8606	-1.7329
10	C	-1.3574	3.4936	-0.6103
11	C	-3.7195	1.4974	-1.4215
12	C	-2.6512	1.4794	-2.5387
13	C	-0.1077	2.8549	-1.2998
14	H	-1.0136	4.3657	-0.0414
15	H	-2.0418	3.8803	-1.3724
16	H	0.7548	2.9727	-0.6361
17	H	0.1218	3.4408	-2.2057
18	H	-2.4152	2.5011	-2.8539
19	H	-3.0719	0.9841	-3.4240
20	H	-4.2327	0.5267	-1.4158
21	H	-4.4956	2.2493	-1.6470
22	C	-0.2138	-0.0224	1.4286
23	N	-0.6093	-1.1280	2.1522
24	N	0.9973	0.2902	2.0013
25	C	0.3222	-1.4832	3.1277
26	C	-1.8676	-1.7718	1.9128
27	C	1.3356	-0.5886	3.0340
28	C	1.8228	1.3633	1.5318
29	H	0.1739	-2.3276	3.7834
30	C	-2.9677	-1.4167	2.7123
31	C	-1.9695	-2.6927	0.8560
32	H	2.2560	-0.4920	3.5893
33	C	2.7371	1.1047	0.4976
34	C	1.6781	2.6333	2.1119
35	C	-4.1989	-2.0259	2.4421
36	C	-2.8232	-0.3845	3.8024
37	C	-3.2193	-3.2781	0.6169
38	C	-0.7725	-3.0177	-0.0029
39	C	3.5152	2.1712	0.0306
40	C	2.8624	-0.2796	-0.0876
41	C	2.4755	3.6736	1.6186
42	C	0.6858	2.8594	3.2241
43	C	-4.3245	-2.9490	1.4028
44	H	-5.0636	-1.7664	3.0476
45	H	-2.0678	-0.6768	4.5415
46	H	-2.5023	0.5773	3.3842
47	H	-3.7719	-0.2328	4.3260
48	H	-3.3218	-3.9963	-0.1927
49	H	0.0867	-3.3297	0.6026
50	H	-1.0048	-3.8190	-0.7111
51	H	-0.4586	-2.1315	-0.5690

52	C	3.3849	3.4456	0.5849
53	H	4.2243	1.9978	-0.7749
54	H	3.2002	-1.0020	0.6660
55	H	1.8952	-0.6376	-0.4579
56	H	3.5787	-0.2925	-0.9148
57	H	2.3772	4.6672	2.0484
58	H	0.9206	2.2455	4.1025
59	H	0.6759	3.9088	3.5344
60	H	-0.3255	2.5820	2.9069
61	H	-5.2869	-3.4138	1.2048
62	H	3.9941	4.2638	0.2095

large_basis_THFrad_THFrad_bb
Energy (POTENTIAL) = -231.874549871 Eh

	Atom	X	Y	Z
1	C	1.2816	-0.0482	-0.1502
2	O	2.5667	0.4369	0.3069
3	C	2.5281	1.8123	0.3583
4	C	1.2491	2.3388	-0.2178
5	C	0.3136	1.1304	-0.0038
6	H	1.3881	-0.3561	-1.1995
7	H	1.0149	-0.9249	0.4474
8	H	3.5036	2.2850	0.2737
9	H	0.8954	3.2502	0.2780
10	H	1.3394	2.5699	-1.2946
11	H	-0.1066	1.1524	1.0078
12	H	-0.5102	1.0820	-0.7215

large_basis_IMes_IMes_bb
Energy (POTENTIAL) = -924.480889126 Eh

	Atom	X	Y	Z
1	C	-0.5367	1.1347	-0.0962
2	C	0.5622	1.8897	-0.3385
3	C	1.1887	-0.3205	-0.5975
4	N	-0.1352	-0.1932	-0.2601
5	N	1.5884	0.9905	-0.6373
6	H	-1.5465	1.4058	0.1733
7	H	0.7144	2.9586	-0.3264
8	C	-1.0218	-1.3078	-0.0682
9	C	-1.8474	-1.7165	-1.1256
10	C	-1.0501	-1.9444	1.1848
11	C	-2.7178	-2.7918	-0.9038
12	C	-1.9328	-3.0136	1.3594
13	C	-2.7752	-3.4506	0.3281
14	H	-3.3634	-3.1200	-1.7154
15	H	-1.9670	-3.5177	2.3233
16	C	2.9232	1.4092	-0.9644
17	C	3.8544	1.5947	0.0682
18	C	3.2523	1.6379	-2.3106
19	C	5.1417	2.0252	-0.2761
20	C	4.5494	2.0666	-2.6077
21	C	5.5065	2.2688	-1.6045
22	H	5.8746	2.1725	0.5141
23	H	4.8196	2.2457	-3.6465
24	C	3.4795	1.3282	1.5050
25	H	2.6143	1.9271	1.8139
26	H	3.2040	0.2772	1.6520
27	H	4.3120	1.5593	2.1766
28	C	2.2323	1.4109	-3.3986
29	H	1.3292	2.0112	-3.2343
30	H	2.6401	1.6682	-4.3809
31	H	1.9132	0.3623	-3.4216
32	C	6.8904	2.7625	-1.9545
33	H	6.8800	3.8379	-2.1783
34	H	7.5948	2.6038	-1.1310
35	H	7.2835	2.2534	-2.8423
36	C	-1.7896	-1.0271	-2.4667
37	H	-1.9924	0.0470	-2.3798
38	H	-0.7946	-1.1245	-2.9170
39	H	-2.5200	-1.4557	-3.1599
40	C	-0.1425	-1.4874	2.2998
41	H	-0.2720	-0.4190	2.5108
42	H	-0.3388	-2.0451	3.2207
43	H	0.9105	-1.6293	2.0301
44	C	-3.7200	-4.6067	0.5563
45	H	-4.4069	-4.3986	1.3865
46	H	-4.3220	-4.8183	-0.3334
47	H	-3.1723	-5.5214	0.8172

large_basis_TS-B-2x-3x-Cl_NiIMes_PhCl_OATS_bb
Energy (POTENTIAL) = -1785.79704549 Eh

	Atom	X	Y	Z
1	Ni	-0.3376	-0.3197	0.0893
2	C	0.4161	-1.0640	1.6681
3	N	0.0615	-2.1746	2.3867
4	N	1.5984	-0.6811	2.2439
5	C	0.9983	-2.4740	3.3732
6	C	-1.1266	-2.9373	2.1226
7	C	1.9692	-1.5298	3.2827
8	C	2.3552	0.4505	1.7828
9	H	0.8864	-3.3218	4.0311
10	C	-2.2214	-2.8103	2.9945
11	C	-1.1638	-3.7706	0.9941
12	H	2.8779	-1.3840	3.8463
13	C	3.1761	0.3027	0.6520
14	C	2.2177	1.6747	2.4511
15	C	-3.3715	-3.5522	2.7125
16	C	-2.1674	-1.8778	4.1798
17	C	-2.3403	-4.4905	0.7515
18	C	0.0098	-3.8678	0.0506
19	C	3.8738	1.4258	0.2016
20	C	3.2586	-1.0126	-0.0804
21	C	2.9417	2.7709	1.9662
22	C	1.2879	1.8078	3.6314
23	C	-3.4493	-4.3983	1.5984
24	H	-4.2312	-3.4617	3.3732
25	H	-1.4303	-2.2049	4.9233
26	H	-1.8808	-0.8651	3.8719
27	H	-3.1414	-1.8209	4.6750
28	H	-2.3876	-5.1379	-0.1212
29	H	0.9567	-3.9839	0.5900
30	H	-0.1072	-4.7144	-0.6329
31	H	0.1000	-2.9532	-0.5506
32	C	3.7709	2.6663	0.8446
33	H	4.5054	1.3333	-0.6794
34	H	3.4534	-1.8472	0.6033
35	H	2.3063	-1.2238	-0.5829
36	H	4.0485	-0.9921	-0.8372
37	H	2.8443	3.7291	2.4715
38	H	1.5765	1.1429	4.4545
39	H	1.2794	2.8340	4.0111
40	H	0.2624	1.5375	3.3492
41	C	-4.7039	-5.1956	1.3335
42	C	4.5296	3.8592	0.3142
43	H	-4.7082	-5.6157	0.3225
44	H	-4.7993	-6.0304	2.0408
45	H	-5.6006	-4.5751	1.4480
46	H	4.3600	4.7514	0.9256
47	H	5.6097	3.6662	0.2909
48	H	4.2246	4.0929	-0.7141
49	C	-0.4266	1.7154	-1.0314
50	H	-1.1123	2.1934	-0.3384
51	C	-0.6817	0.4101	-1.5294

52	C	0.1045	-0.1575	-2.5609
53	H	-0.1278	-1.1495	-2.9345
54	C	0.6684	2.4255	-1.5613
55	H	0.8841	3.4236	-1.1880
56	C	1.1823	0.5747	-3.0507
57	H	1.8197	0.1376	-3.8157
58	C	1.4644	1.8626	-2.5564
59	H	2.3066	2.4202	-2.9567
60	Cl	-2.5255	-0.3562	-1.2535

large_basis_A-6-I_NiIITMe2_bb
Energy (POTENTIAL) = -948.038890059 Eh

	Atom	X	Y	Z
1	C	-0.4807	2.1421	1.1953
2	C	0.0171	2.1135	-0.0768
3	C	-0.1504	4.3065	0.5448
4	N	-0.5786	3.4882	1.5443
5	N	0.2046	3.4448	-0.4487
6	C	-1.0639	3.9573	2.8344
7	H	-1.0674	5.0474	2.8213
8	H	-2.0784	3.5871	3.0131
9	H	-0.4070	3.6137	3.6386
10	C	0.7459	3.8582	-1.7350
11	H	0.1177	3.4883	-2.5514
12	H	0.7679	4.9495	-1.7579
13	H	1.7630	3.4752	-1.8634
14	C	0.3421	0.9746	-0.9824
15	H	-0.2414	1.0142	-1.9112
16	H	1.4032	0.9729	-1.2628
17	H	0.1242	0.0229	-0.4902
18	C	-0.8755	1.0434	2.1226
19	H	-0.7149	0.0704	1.6503
20	H	-0.2895	1.0687	3.0500
21	H	-1.9345	1.1111	2.4031
22	C	-0.0928	8.1796	0.2344
23	N	0.8621	9.0131	-0.2608
24	N	-1.1413	9.0082	0.4964
25	C	0.4304	10.3381	-0.2978
26	C	2.1902	8.5799	-0.6718
27	C	-0.8480	10.3356	0.1846
28	C	-2.4065	8.5703	1.0674
29	C	1.2927	11.4496	-0.7932
30	H	2.2394	7.4948	-0.5772
31	H	2.3777	8.8677	-1.7111
32	H	2.9541	9.0274	-0.0294
33	C	-1.8285	11.4415	0.3848
34	H	-3.2385	8.8470	0.4125
35	H	-2.3727	7.4843	1.1741
36	H	-2.5586	9.0235	2.0521
37	H	0.7663	12.4045	-0.7128
38	H	2.2213	11.5270	-0.2140
39	H	1.5739	11.3074	-1.8446
40	H	-2.7444	11.2806	-0.1982
41	H	-2.1236	11.5345	1.4377
42	H	-1.3960	12.3958	0.0723
43	Ni	0.0371	6.2556	0.5680
44	I	2.0515	6.3979	2.6989

large_basis_D-3-Cl_cis-NiClPhIPhen2_bb
Energy (POTENTIAL) = -2238.43288662 Eh

	Atom	X	Y	Z
1	C	0.0175	-0.4341	-0.9026
2	C	0.0343	0.6442	-1.7179
3	C	2.1397	-0.2484	-1.7358
4	N	1.3081	-0.9623	-0.9232
5	N	1.3319	0.7509	-2.2159
6	Ni	3.9795	-0.6287	-2.3914
7	C	3.5834	-2.4372	-2.7391
8	N	4.0211	-3.5779	-2.1054
9	N	2.8336	-2.8985	-3.7760
10	C	3.5531	-4.7159	-2.7740
11	C	2.8100	-4.2889	-3.8169
12	H	3.8095	-5.7175	-2.4747
13	H	2.2790	-4.8279	-4.5857
14	H	-0.7646	-0.8644	-0.2969
15	H	-0.7445	1.3336	-2.0033
16	C	2.1951	-2.0728	-4.7607
17	C	0.8796	-1.6542	-4.5572
18	C	2.8990	-1.7236	-5.9149
19	C	0.2572	-0.8717	-5.5313
20	C	2.2663	-0.9434	-6.8849
21	C	0.9478	-0.5197	-6.6946
22	H	-0.7631	-0.5327	-5.3771
23	H	2.8080	-0.6613	-7.7831
24	C	4.8468	-3.6539	-0.9324
25	C	5.6293	-2.5677	-0.5246
26	C	4.8731	-4.8397	-0.1873
27	C	6.4248	-2.6709	0.6160
28	C	5.6848	-4.9380	0.9426
29	C	6.4637	-3.8553	1.3539
30	H	7.0215	-1.8146	0.9174
31	H	5.6900	-5.8646	1.5099
32	C	1.6914	-2.0405	-0.0621
33	C	1.0396	-3.2699	-0.1779
34	C	2.6418	-1.8197	0.9369
35	C	1.3288	-4.2850	0.7358
36	C	2.9220	-2.8392	1.8468
37	C	2.2621	-4.0669	1.7530
38	H	0.8245	-5.2434	0.6512
39	H	3.6627	-2.6752	2.6228
40	C	1.7151	1.8112	-3.1000
41	C	1.3396	3.1205	-2.7857
42	C	2.4220	1.5376	-4.2694
43	C	1.6797	4.1601	-3.6523
44	C	2.7667	2.5832	-5.1256
45	C	2.3953	3.8953	-4.8234
46	H	1.3942	5.1784	-3.4035
47	H	3.3239	2.3630	-6.0318
48	C	5.5085	-0.8406	-3.6190
49	C	5.6936	0.2418	-4.5087
50	C	6.3351	-1.9602	-3.8394
51	C	6.6150	0.2000	-5.5602

52	H	5.1043	1.1428	-4.3724
53	C	7.2737	-2.0102	-4.8784
54	H	6.2557	-2.8306	-3.1929
55	C	7.4124	-0.9321	-5.7553
56	H	6.7144	1.0572	-6.2247
57	H	7.8917	-2.8979	-5.0048
58	H	8.1330	-0.9692	-6.5693
59	Cl	4.7721	1.3647	-1.5010
60	H	0.8069	3.3244	-1.8618
61	H	2.6633	4.7074	-5.4937
62	H	2.7044	0.5204	-4.5006
63	H	0.3638	-1.9269	-3.6416
64	H	0.4616	0.0930	-7.4484
65	H	3.9274	-2.0479	-6.0336
66	H	3.1389	-0.8578	0.9998
67	H	0.3128	-3.4208	-0.9707
68	H	2.4859	-4.8579	2.4629
69	H	7.0896	-3.9328	2.2384
70	H	5.6227	-1.6430	-1.0898
71	H	4.2425	-5.6797	-0.4518

large_basis_A-3-Br_cis-NiBrPhITMe2_bb
Energy (POTENTIAL) = -1181.53805248 Eh

	Atom	X	Y	Z
1	C	0.2820	0.4301	-0.8177
2	C	1.2376	-0.0904	0.0055
3	C	-0.1083	-1.8141	-0.6556
4	N	-0.5258	-0.6436	-1.2053
5	N	0.9721	-1.4611	0.0883
6	Ni	-0.8218	-3.6252	-1.0145
7	C	0.7431	-4.0561	-1.9718
8	N	1.7508	-4.8901	-1.6079
9	N	1.1129	-3.5870	-3.1912
10	C	2.7489	-4.9443	-2.5876
11	C	2.3453	-4.1158	-3.5923
12	C	-1.6869	-5.7310	-2.8807
13	C	-2.1867	-6.9835	-3.2604
14	C	-1.4758	-5.3791	-1.5315
15	C	-2.4672	-7.9494	-2.2903
16	H	-2.3475	-7.2086	-4.3140
17	C	-1.7730	-6.3760	-0.5788
18	C	-2.2520	-7.6389	-0.9428
19	H	-2.8458	-8.9279	-2.5780
20	H	-1.6472	-6.1469	0.4776
21	H	-2.4678	-8.3801	-0.1743
22	C	-1.6989	-0.5042	-2.0557
23	H	-1.4089	-0.1913	-3.0638
24	H	-2.2089	-1.4661	-2.0948
25	H	-2.3829	0.2371	-1.6329
26	C	0.0289	1.8253	-1.2790
27	H	0.0438	1.8990	-2.3740
28	H	-0.9487	2.1926	-0.9411
29	H	0.7933	2.5014	-0.8865
30	C	2.3651	0.5539	0.7387
31	H	3.3314	0.1075	0.4716
32	H	2.4113	1.6206	0.5033
33	H	2.2495	0.4564	1.8260
34	C	1.7620	-2.4021	0.8679
35	H	1.1910	-3.3243	0.9633
36	H	2.7172	-2.6135	0.3756
37	H	1.9532	-1.9966	1.8650
38	C	1.7631	-5.6986	-0.3974
39	H	1.7820	-6.7617	-0.6547
40	H	2.6385	-5.4589	0.2135
41	H	0.8544	-5.4896	0.1649
42	C	0.3403	-2.6291	-3.9689
43	H	0.7778	-1.6280	-3.8979
44	H	0.3120	-2.9369	-5.0169
45	H	-0.6752	-2.6079	-3.5761
46	C	3.9647	-5.7930	-2.4357
47	H	4.5392	-5.5216	-1.5406
48	H	3.7078	-6.8564	-2.3485
49	H	4.6197	-5.6774	-3.3034
50	C	2.9825	-3.7596	-4.8924
51	H	2.3671	-4.0728	-5.7456

52	H	3.1416	-2.6775	-4.9828
53	H	3.9550	-4.2505	-4.9850
54	H	-1.4498	-5.0094	-3.6624
55	Br	-2.8345	-3.1358	0.3394

large_basis_A-2-Br_NiITMe2_eta2_PhBr_bb
Energy (POTENTIAL) = -1181.46957691 Eh

	Atom	X	Y	Z
1	C	-0.0788	-0.2030	0.0575
2	C	0.6201	0.0111	-1.0943
3	C	-0.3188	-2.0721	-1.2399
4	N	-0.6444	-1.4770	-0.0598
5	N	0.4543	-1.1419	-1.8692
6	Ni	-0.7211	-3.8516	-1.8588
7	C	1.0476	-4.6700	-1.6261
8	N	1.7991	-4.8131	-0.4982
9	N	1.8950	-5.0502	-2.6243
10	C	3.0925	-5.2602	-0.7809
11	C	3.1531	-5.4118	-2.1361
12	C	-2.4200	-3.8210	-2.6442
13	C	-2.4460	-3.3176	-3.9972
14	C	-2.1740	-5.2456	-2.4815
15	C	-2.2700	-4.1538	-5.0759
16	H	-2.6011	-2.2522	-4.1475
17	C	-2.1047	-6.0913	-3.6348
18	H	-2.4090	-5.7198	-1.5289
19	C	-2.1259	-5.5643	-4.9062
20	H	-2.2486	-3.7320	-6.0795
21	H	-2.0528	-7.1697	-3.4896
22	H	-2.0495	-6.2084	-5.7786
23	C	-1.4779	-2.0936	0.9599
24	H	-2.3114	-1.4350	1.2189
25	H	-1.8793	-3.0210	0.5522
26	H	-0.8929	-2.3041	1.8621
27	C	-0.2932	0.6570	1.2571
28	H	-1.3534	0.9076	1.3924
29	H	0.0432	0.1611	2.1768
30	H	0.2610	1.5947	1.1599
31	C	1.4184	1.1827	-1.5569
32	H	0.9975	1.6282	-2.4678
33	H	1.4366	1.9582	-0.7861
34	H	2.4571	0.9062	-1.7798
35	C	1.0698	-1.3529	-3.1710
36	H	0.5857	-2.2091	-3.6426
37	H	0.9310	-0.4707	-3.8021
38	H	2.1420	-1.5546	-3.0684
39	C	1.3197	-4.4894	0.8363
40	H	1.5166	-5.3172	1.5238
41	H	1.8080	-3.5848	1.2149
42	H	0.2451	-4.3203	0.7751
43	C	1.5332	-5.0662	-4.0339
44	H	2.1299	-4.3378	-4.5930
45	H	1.6979	-6.0616	-4.4578
46	H	0.4761	-4.8133	-4.1203
47	C	4.1126	-5.4914	0.2822
48	H	4.3050	-4.5808	0.8639
49	H	3.7949	-6.2688	0.9893
50	H	5.0591	-5.8119	-0.1620
51	C	4.2562	-5.8703	-3.0285

52	H	3.9874	-6.7892	-3.5655
53	H	4.5072	-5.1139	-3.7830
54	H	5.1581	-6.0752	-2.4452
55	Br	-4.1153	-3.0233	-1.5383

large_basis_TS-C-5-6-Cl_NiIXy2_ClPh_spt
Energy (POTENTIAL) = -2552.97818662 Eh

	Atom	X	Y	Z
1	C	-0.5015	1.0308	0.0868
2	C	0.5295	1.8151	-0.3102
3	C	1.2511	-0.3593	-0.4163
4	N	-0.0487	-0.2849	0.0187
5	N	1.5844	0.9556	-0.6128
6	Ni	2.3392	-1.8911	-0.6780
7	C	3.4299	-3.3497	-1.2072
8	N	4.7118	-3.6584	-0.8238
9	N	3.1091	-4.3745	-2.0584
10	C	5.1643	-4.8344	-1.4184
11	C	4.1529	-5.2883	-2.1970
12	H	6.1529	-5.2247	-1.2330
13	H	4.0704	-6.1594	-2.8284
14	H	-1.5037	1.2748	0.4036
15	H	0.6182	2.8862	-0.4072
16	C	1.8423	-4.5260	-2.7194
17	C	0.7851	-5.1316	-2.0204
18	C	1.7268	-4.1054	-4.0547
19	C	-0.4078	-5.3596	-2.7171
20	C	0.5114	-4.3392	-4.7097
21	C	-0.5421	-4.9751	-4.0514
22	H	-1.2360	-5.8382	-2.2021
23	H	0.3964	-4.0235	-5.7435
24	C	5.5054	-2.8641	0.0724
25	C	6.0219	-1.6417	-0.3881
26	C	5.7575	-3.3529	1.3657
27	C	6.7962	-0.8844	0.5001
28	C	6.5384	-2.5643	2.2197
29	C	7.0504	-1.3380	1.7940
30	H	7.2013	0.0664	0.1661
31	H	6.7402	-2.9181	3.2276
32	C	-0.8561	-1.4246	0.3538
33	C	-1.3498	-2.2289	-0.6863
34	C	-1.1379	-1.6788	1.7071
35	C	-2.1381	-3.3334	-0.3385
36	C	-1.9311	-2.7924	2.0093
37	C	-2.4243	-3.6164	0.9967
38	H	-2.5273	-3.9712	-1.1269
39	H	-2.1568	-3.0128	3.0496
40	C	2.8774	1.4154	-1.0389
41	C	3.8891	1.5598	-0.0753
42	C	3.0645	1.7442	-2.3915
43	C	5.1148	2.0905	-0.4951
44	C	4.3096	2.2603	-2.7714
45	C	5.3221	2.4448	-1.8287
46	H	5.9107	2.2198	0.2330
47	H	4.4802	2.5214	-3.8127
48	C	2.8695	-3.4014	-4.7431
49	H	3.1257	-2.4727	-4.2177
50	H	3.7773	-4.0162	-4.7601
51	H	2.6095	-3.1497	-5.7759

52	C	0.9252	-5.4743	-0.5605
53	H	1.8038	-6.1035	-0.3723
54	H	1.0574	-4.5585	0.0283
55	H	0.0387	-5.9990	-0.1922
56	C	5.1981	-4.6754	1.8272
57	H	5.7154	-5.5202	1.3546
58	H	5.3034	-4.7835	2.9106
59	H	4.1358	-4.7564	1.5789
60	C	5.7348	-1.1478	-1.7823
61	H	5.8738	-1.9397	-2.5275
62	H	4.6929	-0.8132	-1.8587
63	H	6.3839	-0.3077	-2.0413
64	C	3.6608	1.1223	1.3480
65	H	2.7897	1.6233	1.7888
66	H	3.4616	0.0446	1.3860
67	H	4.5343	1.3364	1.9706
68	C	1.9634	1.5208	-3.3981
69	H	1.0657	2.1023	-3.1556
70	H	2.2893	1.8032	-4.4038
71	H	1.6629	0.4658	-3.4173
72	C	-1.0205	-1.9318	-2.1264
73	H	-1.1379	-0.8664	-2.3561
74	H	0.0240	-2.1942	-2.3376
75	H	-1.6607	-2.5060	-2.8006
76	C	-0.5953	-0.7921	2.7995
77	H	-1.0892	0.1879	2.8075
78	H	-0.7453	-1.2507	3.7812
79	H	0.4769	-0.6218	2.6646
80	C	2.2938	-3.1223	3.7109
81	C	1.1590	-3.7235	4.2404
82	C	3.4208	-2.8734	4.4839
83	C	1.1535	-4.0888	5.5938
84	H	0.2887	-3.9056	3.6123
85	C	3.4117	-3.2419	5.8363
86	H	4.2974	-2.4035	4.0419
87	C	2.2786	-3.8481	6.3905
88	H	0.2726	-4.5607	6.0256
89	H	4.2871	-3.0551	6.4559
90	H	2.2725	-4.1325	7.4398
91	Cl	2.3065	-2.5685	1.7116
92	H	6.2802	2.8551	-2.1372
93	H	-1.4751	-5.1611	-4.5774
94	H	7.6531	-0.7376	2.4708
95	H	-3.0367	-4.4784	1.2492

large_basis_NiCODITMe_NiCODITMe_bb
Energy (POTENTIAL) = -865.091088505 Eh

	Atom	X	Y	Z
1	Ni	0.1638	0.0753	-0.1678
2	C	-1.9572	1.0100	0.2136
3	H	-2.3082	0.4144	1.0573
4	C	-1.0248	1.9727	0.4753
5	H	-0.6846	2.0737	1.5045
6	C	-0.3125	0.3872	-2.1224
7	H	-0.0862	-0.5459	-2.6468
8	C	0.7968	1.1624	-1.7374
9	H	1.7905	0.8435	-2.0584
10	C	-0.5342	3.0289	-0.4960
11	C	-2.6452	0.7420	-1.1076
12	C	-1.7287	0.9110	-2.3469
13	C	0.7301	2.6199	-1.3141
14	H	-0.2956	3.9413	0.0644
15	H	-1.3429	3.2984	-1.1810
16	H	1.6228	2.8285	-0.7103
17	H	0.7993	3.2879	-2.1893
18	H	-1.7034	1.9621	-2.6530
19	H	-2.1875	0.3710	-3.1853
20	H	-3.0071	-0.2939	-1.0815
21	H	-3.5439	1.3709	-1.2199
22	C	1.0829	-0.6584	1.3449
23	N	0.9839	-1.9548	1.7847
24	N	1.8533	-0.0662	2.3118
25	C	1.6599	-2.1601	2.9910
26	C	2.2169	-0.9609	3.3236
27	C	0.2137	-2.9711	1.0886
28	H	-0.7569	-3.1351	1.5710
29	H	0.0481	-2.6260	0.0637
30	H	0.7631	-3.9168	1.0624
31	C	2.2471	1.3313	2.2812
32	H	1.8729	1.7634	1.3524
33	H	1.8226	1.8769	3.1312
34	H	3.3378	1.4277	2.3090
35	C	3.0602	-0.5559	4.4855
36	H	4.0622	-0.2347	4.1714
37	H	2.6116	0.2781	5.0409
38	H	3.1816	-1.3926	5.1794
39	C	1.6936	-3.4845	3.6765
40	H	0.6824	-3.8570	3.8857
41	H	2.2014	-4.2466	3.0707
42	H	2.2263	-3.4088	4.6286

large_basis_B-3-Br_tetNiBrPhIMes2_bb
Energy (POTENTIAL) = -2263.32738065 Eh

	Atom	X	Y	Z
1	C	0.5070	0.4289	-0.0899
2	C	0.7096	1.4758	-0.9167
3	C	2.2392	-0.1442	-1.4812
4	N	1.4295	-0.5540	-0.4559
5	N	1.7549	1.1169	-1.7586
6	Ni	3.9851	-0.6930	-2.4270
7	C	3.9768	-2.5231	-3.0088
8	N	4.8192	-3.4543	-2.4343
9	N	3.6142	-3.1056	-4.1983
10	C	5.0005	-4.5519	-3.2780
11	C	4.2454	-4.3365	-4.3770
12	H	5.6294	-5.3812	-2.9938
13	H	4.0752	-4.9341	-5.2589
14	H	-0.1977	0.2723	0.7112
15	H	0.2213	2.4345	-0.9941
16	C	2.5051	-2.7312	-5.0469
17	C	1.2271	-3.1714	-4.6449
18	C	2.7030	-2.0848	-6.2761
19	C	0.1338	-2.8788	-5.4620
20	C	1.5736	-1.8253	-7.0662
21	C	0.2861	-2.1975	-6.6759
22	H	-0.8563	-3.2052	-5.1511
23	H	1.7146	-1.3181	-8.0181
24	C	5.2469	-3.5445	-1.0483
25	C	6.4379	-2.9500	-0.5949
26	C	4.4887	-4.3872	-0.2103
27	C	6.8046	-3.1517	0.7420
28	C	4.9210	-4.5842	1.1046
29	C	6.0620	-3.9563	1.6094
30	H	7.7152	-2.6793	1.1034
31	H	4.3416	-5.2387	1.7505
32	C	1.3312	-1.8458	0.1729
33	C	0.2077	-2.6354	-0.1365
34	C	2.2287	-2.1960	1.1924
35	C	0.0152	-3.8155	0.5897
36	C	1.9731	-3.3691	1.9100
37	C	0.8801	-4.1923	1.6226
38	H	-0.8413	-4.4432	0.3535
39	H	2.6531	-3.6468	2.7107
40	C	2.1661	1.9785	-2.8356
41	C	2.8265	3.1856	-2.5622
42	C	1.7947	1.6180	-4.1440
43	C	3.2141	3.9757	-3.6545
44	C	2.2008	2.4382	-5.1971
45	C	2.9338	3.6111	-4.9737
46	H	3.7522	4.9012	-3.4607
47	H	1.9363	2.1575	-6.2144
48	C	4.0611	-1.6642	-6.7701
49	H	4.3435	-0.6911	-6.3564
50	H	4.8401	-2.3698	-6.4757
51	H	4.0606	-1.5812	-7.8621

52	C	1.0458	-3.9612	-3.3759
53	H	-0.0032	-4.2312	-3.2302
54	H	1.6355	-4.8853	-3.3958
55	H	1.3761	-3.3926	-2.5041
56	C	-0.9158	-1.8575	-7.5228
57	H	-0.6354	-1.6646	-8.5637
58	H	-1.6577	-2.6642	-7.5101
59	H	-1.4143	-0.9547	-7.1440
60	C	3.2319	-5.0673	-0.6896
61	H	3.3981	-5.6502	-1.6013
62	H	2.8440	-5.7421	0.0773
63	H	2.4543	-4.3319	-0.9091
64	C	7.3437	-2.1514	-1.4889
65	H	8.2384	-1.8381	-0.9419
66	H	7.6670	-2.7405	-2.3540
67	H	6.8397	-1.2571	-1.8580
68	C	6.4648	-4.1266	3.0536
69	H	7.5490	-4.0387	3.1841
70	H	5.9987	-3.3540	3.6805
71	H	6.1483	-5.0991	3.4473
72	C	3.0702	3.6833	-1.1595
73	H	3.1388	2.8680	-0.4394
74	H	4.0042	4.2515	-1.1097
75	H	2.2583	4.3561	-0.8489
76	C	0.9609	0.3914	-4.3954
77	H	0.0711	0.3757	-3.7537
78	H	0.6350	0.3494	-5.4365
79	H	1.5277	-0.5165	-4.1824
80	C	3.4115	4.4463	-6.1365
81	H	2.6099	4.6153	-6.8659
82	H	3.7848	5.4217	-5.8073
83	H	4.2275	3.9397	-6.6689
84	C	-0.8022	-2.2109	-1.1772
85	H	-0.3300	-1.7567	-2.0531
86	H	-1.3934	-3.0684	-1.5121
87	H	-1.5013	-1.4702	-0.7686
88	C	3.4224	-1.3352	1.5035
89	H	3.1289	-0.2992	1.7080
90	H	3.9643	-1.7209	2.3715
91	H	4.1108	-1.2919	0.6541
92	C	0.6717	-5.4837	2.3749
93	H	1.0361	-5.4123	3.4058
94	H	-0.3856	-5.7696	2.4025
95	H	1.2187	-6.3066	1.8935
96	C	5.3443	-0.4248	-3.7901
97	C	5.2814	0.8909	-4.2956
98	C	6.2806	-1.2752	-4.4006
99	C	6.0905	1.3247	-5.3516
100	H	4.6055	1.6060	-3.8446
101	C	7.1194	-0.8457	-5.4359
102	H	6.3679	-2.3072	-4.0821
103	C	7.0254	0.4578	-5.9264
104	H	6.0020	2.3505	-5.7061
105	H	7.8350	-1.5417	-5.8711
106	H	7.6680	0.7936	-6.7372

107	Br	5.2111	0.8919	-0.9075

large_basis_C-6-Cl_NiClIXy2_bb
Energy (POTENTIAL) = -2321.37875378 Eh

	Atom	X	Y	Z
1	C	-0.0216	0.0559	-0.2288
2	C	1.1247	0.7671	-0.3566
3	C	1.6841	-1.4487	-0.4747
4	N	0.3371	-1.2874	-0.3034
5	N	2.1493	-0.1644	-0.5084
6	Ni	2.7093	-3.1067	-0.5872
7	C	3.7348	-4.6145	-1.2817
8	N	5.0839	-4.8259	-1.2342
9	N	3.2617	-5.7446	-1.8843
10	C	5.4377	-6.0535	-1.7900
11	C	4.2849	-6.6355	-2.2007
12	H	6.4637	-6.3841	-1.8378
13	H	4.0899	-7.5818	-2.6815
14	H	-1.0464	0.3662	-0.0951
15	H	1.3152	1.8293	-0.3553
16	C	1.8848	-5.9884	-2.2177
17	C	1.0839	-6.6988	-1.3103
18	C	1.4171	-5.5484	-3.4660
19	C	-0.2236	-7.0065	-1.7054
20	C	0.1046	-5.8788	-3.8225
21	C	-0.7041	-6.6135	-2.9546
22	H	-0.8671	-7.5544	-1.0223
23	H	-0.2811	-5.5559	-4.7860
24	C	6.0520	-3.8785	-0.7506
25	C	6.4262	-2.8214	-1.5963
26	C	6.6216	-4.0769	0.5175
27	C	7.4248	-1.9513	-1.1467
28	C	7.6075	-3.1730	0.9334
29	C	8.0098	-2.1235	0.1078
30	H	7.7329	-1.1276	-1.7830
31	H	8.0606	-3.2997	1.9134
32	C	-0.6229	-2.3569	-0.2517
33	C	-1.0735	-2.9061	-1.4627
34	C	-1.1099	-2.7669	0.9995
35	C	-2.0509	-3.9051	-1.3984
36	C	-2.0791	-3.7777	1.0177
37	C	-2.5482	-4.3395	-0.1697
38	H	-2.4176	-4.3457	-2.3201
39	H	-2.4673	-4.1200	1.9735
40	C	3.5241	0.2197	-0.6821
41	C	4.3379	0.3383	0.4558
42	C	3.9759	0.5190	-1.9771
43	C	5.6431	0.8099	0.2717
44	C	5.2868	0.9911	-2.1161
45	C	6.1086	1.1465	-0.9995
46	H	6.2960	0.9104	1.1344
47	H	5.6599	1.2359	-3.1072
48	C	2.3004	-4.7258	-4.3699
49	H	2.6377	-3.8168	-3.8564
50	H	3.2029	-5.2749	-4.6660
51	H	1.7661	-4.4301	-5.2778

52	C	1.6173	-7.0889	0.0440
53	H	2.5230	-7.7025	-0.0395
54	H	1.8873	-6.1954	0.6219
55	H	0.8705	-7.6549	0.6093
56	C	6.1637	-5.2041	1.4074
57	H	6.2713	-6.1805	0.9201
58	H	6.7404	-5.2238	2.3375
59	H	5.1036	-5.0762	1.6591
60	C	5.7550	-2.6222	-2.9316
61	H	5.7787	-3.5356	-3.5381
62	H	4.7004	-2.3570	-2.7908
63	H	6.2375	-1.8195	-3.4966
64	C	3.8128	-0.0359	1.8173
65	H	2.9085	0.5320	2.0698
66	H	3.5419	-1.0988	1.8489
67	H	4.5633	0.1539	2.5909
68	C	3.0809	0.3179	-3.1744
69	H	2.1538	0.8979	-3.0921
70	H	3.5892	0.6145	-4.0968
71	H	2.7871	-0.7348	-3.2698
72	C	-0.5089	-2.4378	-2.7801
73	H	-0.5852	-1.3486	-2.8865
74	H	0.5548	-2.6928	-2.8550
75	H	-1.0327	-2.9038	-3.6195
76	C	-0.5876	-2.1539	2.2736
77	H	-0.7344	-1.0671	2.2923
78	H	-1.0941	-2.5795	3.1456
79	H	0.4878	-2.3447	2.3703
80	Cl	2.7200	-3.7715	1.7631
81	H	-3.3043	-5.1199	-0.1378
82	H	7.1225	1.5184	-1.1218
83	H	8.7802	-1.4344	0.4444
84	H	-1.7196	-6.8679	-3.2467

large_basis_D-5-Cl_NiIPhen2_ClPh_bb
Energy (POTENTIAL) = -2238.35062724 Eh

	Atom	X	Y	Z
1	C	-0.6139	0.9118	0.0203
2	C	0.1745	1.5950	-0.8385
3	C	1.1717	-0.4576	-0.4921
4	N	-0.0094	-0.3316	0.2222
5	N	1.2541	0.7662	-1.1376
6	Ni	2.3596	-1.8788	-0.7236
7	C	3.5564	-3.2117	-1.2458
8	N	4.7202	-3.6972	-0.6690
9	N	3.5090	-3.9134	-2.4408
10	C	5.3498	-4.6461	-1.4783
11	C	4.5942	-4.7751	-2.5906
12	H	6.2788	-5.1164	-1.1971
13	H	4.7120	-5.4043	-3.4590
14	H	-1.5505	1.1775	0.4851
15	H	0.0841	2.5890	-1.2484
16	C	2.4924	-3.7614	-3.4281
17	C	1.1442	-3.7715	-3.0533
18	C	2.8509	-3.6113	-4.7710
19	C	0.1568	-3.6114	-4.0255
20	C	1.8550	-3.4630	-5.7396
21	C	0.5077	-3.4560	-5.3703
22	H	-0.8890	-3.6185	-3.7302
23	H	2.1373	-3.3409	-6.7818
24	C	5.2685	-3.2663	0.5737
25	C	5.2769	-1.9077	0.9076
26	C	5.8302	-4.2072	1.4439
27	C	5.8408	-1.4957	2.1145
28	C	6.4084	-3.7841	2.6423
29	C	6.4146	-2.4284	2.9835
30	H	5.8399	-0.4394	2.3697
31	H	6.8431	-4.5192	3.3142
32	C	-0.6032	-1.3533	1.0186
33	C	-0.6267	-2.6761	0.5634
34	C	-1.1971	-1.0193	2.2405
35	C	-1.2389	-3.6623	1.3362
36	C	-1.8228	-2.0102	2.9998
37	C	-1.8446	-3.3346	2.5527
38	H	-1.2507	-4.6884	0.9786
39	H	-2.2833	-1.7453	3.9477
40	C	2.2848	1.1252	-2.0547
41	C	3.6281	0.9519	-1.7048
42	C	1.9410	1.6527	-3.3027
43	C	4.6271	1.2954	-2.6159
44	C	2.9480	2.0025	-4.2058
45	C	4.2913	1.8194	-3.8684
46	H	5.6698	1.1602	-2.3411
47	H	2.6779	2.4061	-5.1778
48	C	2.2525	-3.3221	4.4830
49	C	1.0241	-3.4171	5.1385
50	C	3.4546	-3.5602	5.1508
51	C	1.0056	-3.7583	6.4931

52	H	0.1041	-3.2272	4.5961
53	C	3.4189	-3.9008	6.5053
54	H	4.3960	-3.4782	4.6183
55	C	2.1987	-4.0008	7.1792
56	H	0.0525	-3.8341	7.0100
57	H	4.3512	-4.0872	7.0321
58	H	2.1779	-4.2658	8.2327
59	Cl	2.2864	-2.8894	2.7724
60	H	6.8604	-2.1023	3.9192
61	H	5.0724	2.0866	-4.5749
62	H	0.8942	1.7664	-3.5690
63	H	-0.2643	-3.3345	-6.1253
64	H	3.9001	-3.5881	-5.0501
65	H	-2.3280	-4.1043	3.1481
66	H	-0.1679	-2.9130	-0.3889
67	H	-1.1576	0.0048	2.5992
68	H	0.8892	-3.9142	-2.0103
69	H	3.8716	0.5631	-0.7236
70	H	4.8398	-1.1944	0.2191
71	H	5.8012	-5.2631	1.1921

large_basis_A-4-Cl_trans-NiClPhITMe2_bb
Energy (POTENTIAL) = -1628.59992083 Eh

	Atom	X	Y	Z
1	C	-0.6766	2.1781	1.0221
2	C	0.2302	2.1182	0.0049
3	C	-0.0865	4.3203	0.5073
4	N	-0.8519	3.5363	1.3078
5	N	0.5756	3.4419	-0.2873
6	C	-1.7559	4.0454	2.3270
7	H	-1.6366	5.1280	2.3775
8	H	-2.7934	3.8040	2.0754
9	H	-1.5122	3.6137	3.3024
10	C	1.5085	3.8310	-1.3334
11	H	1.0971	3.6019	-2.3215
12	H	1.6793	4.9049	-1.2541
13	H	2.4600	3.3064	-1.2066
14	C	0.8269	0.9601	-0.7200
15	H	0.6320	1.0133	-1.7988
16	H	1.9155	0.9165	-0.5854
17	H	0.4066	0.0214	-0.3489
18	C	-1.3971	1.1075	1.7686
19	H	-1.1272	0.1230	1.3769
20	H	-1.1499	1.1229	2.8381
21	H	-2.4859	1.2168	1.6836
22	C	-0.1198	8.1733	0.2642
23	N	0.6380	8.9612	-0.5394
24	N	-0.9909	9.0330	0.8503
25	C	0.2486	10.3026	-0.4656
26	C	1.7139	8.4686	-1.3852
27	C	-0.7887	10.3483	0.4190
28	C	-2.0255	8.6324	1.7907
29	C	0.9257	11.3740	-1.2509
30	H	1.8634	7.4112	-1.1649
31	H	1.4578	8.5882	-2.4428
32	H	2.6404	9.0113	-1.1755
33	C	-1.6085	11.4872	0.9225
34	H	-3.0194	8.7906	1.3605
35	H	-1.8915	7.5730	2.0103
36	H	-1.9382	9.2049	2.7188
37	H	0.4356	12.3368	-1.0823
38	H	1.9812	11.4800	-0.9686
39	H	0.8950	11.1654	-2.3279
40	H	-2.6763	11.3407	0.7156
41	H	-1.4997	11.6162	2.0072
42	H	-1.2986	12.4198	0.4429
43	Ni	-0.0349	6.2504	0.4454
44	C	-1.3755	6.1492	-0.9023
45	C	-1.0404	6.1646	-2.2714
46	C	-2.7462	6.0499	-0.5908
47	C	-2.0138	6.0801	-3.2735
48	H	0.0042	6.2462	-2.5654
49	C	-3.7280	5.9693	-1.5852
50	H	-3.0583	6.0322	0.4515
51	C	-3.3670	5.9823	-2.9358

52	H	-1.7148	6.0928	-4.3205
53	H	-4.7775	5.8948	-1.3044
54	H	-4.1267	5.9184	-3.7113
55	Cl	1.6545	6.3679	2.0756

large_basis_B-2-Br_NiIMes2_eta2_PhBr_bb
Energy (POTENTIAL) = -2263.26770899 Eh

	Atom	X	Y	Z
1	C	0.4076	0.5604	0.0000
2	C	1.4062	0.8473	-0.8561
3	C	1.1334	-1.4530	-0.8813
4	N	0.2338	-0.8234	-0.0308
5	N	1.8405	-0.3697	-1.3792
6	Ni	1.3266	-3.3446	-1.4900
7	C	3.0322	-4.4894	-1.3712
8	N	3.7701	-4.7919	-0.2420
9	N	3.4684	-5.4701	-2.2513
10	C	4.5957	-5.9025	-0.4151
11	C	4.4102	-6.3240	-1.6825
12	H	5.2368	-6.2626	0.3745
13	H	4.8502	-7.1363	-2.2399
14	H	-0.2039	1.1934	0.6235
15	H	1.8518	1.7846	-1.1496
16	C	3.1621	-5.5927	-3.6481
17	C	2.5087	-6.7425	-4.1173
18	C	3.6449	-4.6070	-4.5279
19	C	2.2851	-6.8543	-5.4973
20	C	3.3821	-4.7537	-5.8914
21	C	2.6958	-5.8669	-6.3962
22	H	1.7641	-7.7333	-5.8708
23	H	3.7410	-3.9916	-6.5801
24	C	3.9496	-3.9870	0.9355
25	C	4.8993	-2.9529	0.8798
26	C	3.3358	-4.3670	2.1358
27	C	5.1519	-2.2294	2.0491
28	C	3.6345	-3.6275	3.2865
29	C	4.5199	-2.5450	3.2591
30	H	5.8761	-1.4182	2.0205
31	H	3.1571	-3.9025	4.2243
32	C	-0.8775	-1.3726	0.7021
33	C	-2.1801	-1.0174	0.3083
34	C	-0.6433	-2.1159	1.8664
35	C	-3.2505	-1.4644	1.0934
36	C	-1.7402	-2.5301	2.6244
37	C	-3.0527	-2.2224	2.2514
38	H	-4.2635	-1.2075	0.7903
39	H	-1.5634	-3.1129	3.5262
40	C	2.8446	-0.3566	-2.4069
41	C	4.1574	0.0039	-2.0648
42	C	2.4458	-0.5069	-3.7477
43	C	5.0976	0.1233	-3.0972
44	C	3.4131	-0.3558	-4.7435
45	C	4.7466	-0.0554	-4.4382
46	H	6.1233	0.3822	-2.8432
47	H	3.1179	-0.4765	-5.7836
48	C	4.4774	-3.4609	-4.0161
49	H	3.8907	-2.7930	-3.3821
50	H	5.3137	-3.8286	-3.4093
51	H	4.8855	-2.8780	-4.8446

52	C	2.0561	-7.8532	-3.1981
53	H	2.8113	-8.6483	-3.1402
54	H	1.8763	-7.5047	-2.1776
55	H	1.1329	-8.3084	-3.5719
56	C	2.3974	-5.9793	-7.8720
57	H	3.2591	-5.6782	-8.4796
58	H	2.1234	-7.0022	-8.1514
59	H	1.5612	-5.3248	-8.1526
60	C	2.3950	-5.5436	2.1808
61	H	2.9268	-6.4844	1.9881
62	H	1.9138	-5.6246	3.1603
63	H	1.6132	-5.4554	1.4193
64	C	5.6716	-2.6954	-0.3894
65	H	6.2113	-3.5980	-0.7026
66	H	5.0092	-2.4178	-1.2135
67	H	6.4042	-1.8969	-0.2493
68	C	4.7837	-1.7292	4.5019
69	H	4.0887	-0.8809	4.5689
70	H	4.6543	-2.3266	5.4111
71	H	5.7990	-1.3171	4.5042
72	C	4.5375	0.3293	-0.6411
73	H	4.1858	1.3313	-0.3634
74	H	4.0985	-0.3731	0.0722
75	H	5.6237	0.3200	-0.5162
76	C	1.0082	-0.7841	-4.0922
77	H	0.3501	0.0072	-3.7098
78	H	0.8689	-0.8534	-5.1753
79	H	0.6737	-1.7204	-3.6412
80	C	5.7791	0.0423	-5.5346
81	H	6.6727	0.5818	-5.2027
82	H	6.1000	-0.9577	-5.8585
83	H	5.3789	0.5526	-6.4185
84	C	-2.4484	-0.1683	-0.9132
85	H	-1.7466	-0.3887	-1.7220
86	H	-3.4632	-0.3428	-1.2854
87	H	-2.3621	0.9019	-0.6856
88	C	0.7589	-2.4597	2.2688
89	H	1.3688	-1.5619	2.4296
90	H	0.7747	-3.0543	3.1858
91	H	1.2457	-3.0303	1.4754
92	C	-4.2223	-2.7243	3.0640
93	H	-5.1217	-2.1229	2.8925
94	H	-4.4666	-3.7622	2.7994
95	H	-4.0008	-2.7099	4.1377
96	C	-0.5192	-3.9730	-1.6886
97	C	-1.6368	-3.1955	-2.1468
98	C	0.2797	-4.7057	-2.6449
99	C	-1.8115	-2.9620	-3.4885
100	H	-2.3261	-2.7926	-1.4168
101	C	0.0376	-4.4365	-4.0353
102	H	0.6879	-5.6738	-2.3860
103	C	-0.9503	-3.5733	-4.4481
104	H	-2.6247	-2.3199	-3.8205
105	H	0.6158	-4.9822	-4.7727
106	H	-1.1125	-3.3938	-5.5084

107	Br	-0.9393	-5.0312	0.0199

large_basis_TS-A-5-6-Br_NiITMe2_ossts_PhBr_t_oss_bb
Energy (POTENTIAL) = -1181.44251873 Eh

	Atom	X	Y	Z
1	C	-3.5750	3.3510	0.1943
2	C	-2.5766	4.1406	-0.3004
3	C	-1.8704	1.9633	-0.4591
4	N	-3.1232	2.0360	0.0827
5	N	-1.5552	3.2739	-0.6923
6	Ni	-0.8002	0.4165	-0.7521
7	C	0.2379	-1.0973	-1.2652
8	N	1.5510	-1.3663	-0.9956
9	N	-0.1711	-2.2056	-1.9560
10	C	1.9486	-2.6076	-1.4921
11	C	0.8519	-3.1428	-2.1048
12	Br	-0.5658	-0.0572	1.8745
13	C	-0.3397	-0.4640	3.9994
14	C	-0.3508	-1.7816	4.4532
15	C	-0.1724	0.5945	4.8906
16	C	-0.1930	-2.0441	5.8203
17	H	-0.4805	-2.6030	3.7509
18	C	-0.0146	0.3297	6.2573
19	H	-0.1633	1.6209	4.5284
20	C	-0.0248	-0.9891	6.7231
21	H	-0.2011	-3.0716	6.1790
22	H	0.1164	1.1530	6.9571
23	H	0.0982	-1.1937	7.7837
24	C	-3.8879	0.8778	0.5172
25	H	-4.8529	0.8419	0.0008
26	H	-3.3085	-0.0144	0.2782
27	H	-4.0590	0.9117	1.5978
28	C	-0.2908	3.7149	-1.2593
29	H	0.3072	2.8259	-1.4709
30	H	-0.4566	4.2719	-2.1874
31	H	0.2477	4.3536	-0.5511
32	C	-2.4755	5.6208	-0.4537
33	H	-3.3836	6.1060	-0.0851
34	H	-1.6253	6.0299	0.1073
35	H	-2.3425	5.9118	-1.5040
36	C	-4.9136	3.6934	0.7557
37	H	-5.7267	3.2478	0.1678
38	H	-5.0242	3.3340	1.7869
39	H	-5.0601	4.7771	0.7610
40	C	-1.5232	-2.4001	-2.4550
41	H	-1.9890	-3.2689	-1.9776
42	H	-2.1004	-1.5045	-2.2157
43	H	-1.5162	-2.5506	-3.5397
44	C	2.4273	-0.4758	-0.2513
45	H	3.3033	-0.2109	-0.8528
46	H	1.8620	0.4238	-0.0067
47	H	2.7591	-0.9506	0.6774
48	C	3.3327	-3.1352	-1.3199
49	H	3.5981	-3.2355	-0.2595
50	H	3.4255	-4.1216	-1.7830
51	H	4.0795	-2.4762	-1.7813

52	C	0.6607	-4.4353	-2.8239
53	H	-0.1326	-5.0410	-2.3673
54	H	0.3869	-4.2790	-3.8756
55	H	1.5836	-5.0220	-2.8032

large_basis_TS-B-2-3-Br_NiIMes2_oa_PhBr_bb
Energy (POTENTIAL) = -2263.26590917 Eh

	Atom	X	Y	Z
1	C	1.2021	1.3375	0.0487
2	C	2.1927	1.6026	-0.8234
3	C	1.9020	-0.6923	-0.8066
4	N	1.0179	-0.0455	0.0433
5	N	2.6118	0.3738	-1.3327
6	Ni	2.1367	-2.5786	-1.3680
7	C	3.8322	-3.7567	-1.2445
8	N	4.5567	-4.0717	-0.1133
9	N	4.2741	-4.7205	-2.1355
10	C	5.3849	-5.1778	-0.2950
11	C	5.2094	-5.5830	-1.5705
12	H	6.0207	-5.5480	0.4941
13	H	5.6543	-6.3877	-2.1350
14	H	0.6023	1.9851	0.6683
15	H	2.6405	2.5316	-1.1386
16	C	3.9874	-4.8048	-3.5407
17	C	3.3062	-5.9226	-4.0451
18	C	4.5176	-3.8162	-4.3884
19	C	3.0963	-5.9928	-5.4295
20	C	4.2658	-3.9194	-5.7582
21	C	3.5471	-4.9950	-6.2976
22	H	2.5542	-6.8459	-5.8318
23	H	4.6598	-3.1537	-6.4232
24	C	4.7222	-3.2699	1.0698
25	C	5.6390	-2.2062	1.0127
26	C	4.1246	-3.6705	2.2720
27	C	5.8720	-1.4757	2.1817
28	C	4.4059	-2.9236	3.4223
29	C	5.2552	-1.8128	3.3935
30	H	6.5704	-0.6423	2.1511
31	H	3.9410	-3.2149	4.3614
32	C	-0.0818	-0.5819	0.8022
33	C	-1.3892	-0.2118	0.4382
34	C	0.1713	-1.3344	1.9570
35	C	-2.4470	-0.6564	1.2419
36	C	-0.9136	-1.7449	2.7335
37	C	-2.2312	-1.4245	2.3896
38	H	-3.4636	-0.3880	0.9620
39	H	-0.7234	-2.3345	3.6280
40	C	3.6130	0.3614	-2.3642
41	C	4.9192	0.7606	-2.0363
42	C	3.2205	0.1434	-3.6984
43	C	5.8548	0.8721	-3.0737
44	C	4.1847	0.2859	-4.6987
45	C	5.5077	0.6413	-4.4073
46	H	6.8740	1.1636	-2.8293
47	H	3.8943	0.1144	-5.7331
48	C	5.3882	-2.7181	-3.8368
49	H	4.8161	-2.0297	-3.2120
50	H	6.1876	-3.1338	-3.2114
51	H	5.8486	-2.1459	-4.6448

52	C	2.8167	-7.0406	-3.1543
53	H	3.5674	-7.8382	-3.0761
54	H	2.6024	-6.7015	-2.1368
55	H	1.9057	-7.4892	-3.5636
56	C	3.2560	-5.0588	-7.7776
57	H	4.1195	-4.7365	-8.3713
58	H	2.9834	-6.0719	-8.0921
59	H	2.4197	-4.3962	-8.0391
60	C	3.2117	-4.8681	2.3224
61	H	3.7488	-5.7908	2.0684
62	H	2.7843	-4.9922	3.3224
63	H	2.3892	-4.7687	1.6061
64	C	6.4000	-1.9199	-0.2568
65	H	6.9470	-2.8108	-0.5896
66	H	5.7303	-1.6341	-1.0716
67	H	7.1248	-1.1161	-0.1068
68	C	5.4936	-0.9884	4.6356
69	H	4.7685	-0.1658	4.7035
70	H	5.3874	-1.5898	5.5453
71	H	6.4935	-0.5402	4.6356
72	C	5.3029	1.1270	-0.6225
73	H	4.9629	2.1405	-0.3743
74	H	4.8591	0.4505	0.1131
75	H	6.3893	1.1101	-0.4995
76	C	1.7994	-0.2132	-4.0394
77	H	1.0915	0.5079	-3.6124
78	H	1.6518	-0.2422	-5.1232
79	H	1.5393	-1.1920	-3.6306
80	C	6.5340	0.7365	-5.5096
81	H	7.4242	1.2874	-5.1877
82	H	6.8618	-0.2636	-5.8257
83	H	6.1248	1.2345	-6.3964
84	C	-1.6811	0.6570	-0.7653
85	H	-0.9715	0.4843	-1.5791
86	H	-2.6890	0.4578	-1.1442
87	H	-1.6329	1.7233	-0.5096
88	C	1.5776	-1.6919	2.3335
89	H	2.2074	-0.8017	2.4547
90	H	1.6048	-2.2627	3.2650
91	H	2.0320	-2.2945	1.5445
92	C	-3.3870	-1.9204	3.2255
93	H	-4.2905	-1.3232	3.0612
94	H	-3.6319	-2.9620	2.9768
95	H	-3.1490	-1.8932	4.2954
96	C	0.3551	-3.1183	-1.7432
97	C	-0.7827	-2.3451	-2.1248
98	C	1.0004	-3.9295	-2.7286
99	C	-1.1052	-2.2090	-3.4585
100	H	-1.3683	-1.8615	-1.3562
101	C	0.6395	-3.7626	-4.0923
102	H	1.5381	-4.8180	-2.4376
103	C	-0.3765	-2.9004	-4.4620
104	H	-1.9361	-1.5652	-3.7413
105	H	1.1372	-4.3733	-4.8394
106	H	-0.6552	-2.7920	-5.5072

107	Br	0.0002	-4.2659	0.0970

large_basis_B-3-Cl_tetNiClPhIMes2_bb
Energy (POTENTIAL) = -2710.38226377 Eh

	Atom	X	Y	Z
1	C	0.4543	0.4003	-0.1511
2	C	0.6598	1.4451	-0.9796
3	C	2.2144	-0.1611	-1.5121
4	N	1.3939	-0.5738	-0.4964
5	N	1.7234	1.0938	-1.8017
6	Ni	3.9775	-0.6974	-2.4381
7	C	3.9604	-2.5217	-3.0185
8	N	4.7960	-3.4550	-2.4367
9	N	3.6006	-3.1054	-4.2077
10	C	4.9764	-4.5553	-3.2776
11	C	4.2270	-4.3396	-4.3804
12	H	5.6015	-5.3860	-2.9895
13	H	4.0592	-4.9381	-5.2622
14	H	-0.2602	0.2410	0.6407
15	H	0.1622	2.3978	-1.0709
16	C	2.4972	-2.7270	-5.0618
17	C	1.2152	-3.1569	-4.6616
18	C	2.7033	-2.0881	-6.2935
19	C	0.1265	-2.8625	-5.4841
20	C	1.5784	-1.8275	-7.0896
21	C	0.2873	-2.1894	-6.7015
22	H	-0.8667	-3.1807	-5.1748
23	H	1.7254	-1.3256	-8.0433
24	C	5.2180	-3.5480	-1.0485
25	C	6.3958	-2.9376	-0.5800
26	C	4.4676	-4.4089	-0.2219
27	C	6.7622	-3.1540	0.7546
28	C	4.9004	-4.6195	1.0906
29	C	6.0325	-3.9855	1.6069
30	H	7.6620	-2.6695	1.1267
31	H	4.3257	-5.2876	1.7267
32	C	1.3298	-1.8499	0.1674
33	C	0.2112	-2.6653	-0.0900
34	C	2.2607	-2.1594	1.1702
35	C	0.0571	-3.8278	0.6728
36	C	2.0430	-3.3163	1.9252
37	C	0.9560	-4.1635	1.6908
38	H	-0.7951	-4.4750	0.4767
39	H	2.7481	-3.5622	2.7143
40	C	2.1574	1.9687	-2.8596
41	C	2.8242	3.1635	-2.5494
42	C	1.8054	1.6369	-4.1794
43	C	3.2346	3.9741	-3.6173
44	C	2.2347	2.4765	-5.2085
45	C	2.9708	3.6394	-4.9485
46	H	3.7787	4.8895	-3.3959
47	H	1.9873	2.2177	-6.2358
48	C	4.0647	-1.6732	-6.7831
49	H	4.3449	-0.6967	-6.3754
50	H	4.8415	-2.3769	-6.4786
51	H	4.0707	-1.5988	-7.8757

52	C	1.0255	-3.9390	-3.3889
53	H	-0.0252	-4.2030	-3.2457
54	H	1.6109	-4.8659	-3.4022
55	H	1.3560	-3.3674	-2.5188
56	C	-0.9096	-1.8460	-7.5541
57	H	-0.6247	-1.6616	-8.5954
58	H	-1.6574	-2.6472	-7.5386
59	H	-1.4025	-0.9373	-7.1823
60	C	3.2121	-5.0882	-0.7063
61	H	3.3808	-5.6769	-1.6138
62	H	2.8173	-5.7572	0.0621
63	H	2.4391	-4.3504	-0.9346
64	C	7.2876	-2.0990	-1.4524
65	H	8.1672	-1.7686	-0.8912
66	H	7.6368	-2.6639	-2.3232
67	H	6.7617	-1.2152	-1.8169
68	C	6.4353	-4.1722	3.0491
69	H	7.5190	-4.0808	3.1812
70	H	5.9653	-3.4095	3.6852
71	H	6.1232	-5.1510	3.4303
72	C	3.0574	3.6084	-1.1278
73	H	3.2784	2.7633	-0.4743
74	H	3.8986	4.3068	-1.0762
75	H	2.1728	4.1278	-0.7342
76	C	0.9680	0.4211	-4.4673
77	H	0.0514	0.4185	-3.8641
78	H	0.6852	0.3828	-5.5210
79	H	1.5125	-0.4946	-4.2298
80	C	3.4691	4.4971	-6.0863
81	H	2.6643	4.7326	-6.7936
82	H	3.8926	5.4403	-5.7258
83	H	4.2512	3.9749	-6.6531
84	C	-0.8353	-2.2870	-1.1123
85	H	-0.3991	-1.8217	-2.0003
86	H	-1.3993	-3.1693	-1.4294
87	H	-1.5546	-1.5713	-0.6942
88	C	3.4449	-1.2689	1.4345
89	H	3.1281	-0.2529	1.7013
90	H	4.0541	-1.6650	2.2516
91	H	4.0758	-1.1707	0.5463
92	C	0.7875	-5.4368	2.4830
93	H	1.2272	-5.3495	3.4827
94	H	-0.2684	-5.7075	2.5943
95	H	1.2862	-6.2771	1.9797
96	C	5.3420	-0.4378	-3.8020
97	C	5.2929	0.8784	-4.3070
98	C	6.2785	-1.2942	-4.4049
99	C	6.1135	1.3074	-5.3562
100	H	4.6150	1.5959	-3.8628
101	C	7.1283	-0.8700	-5.4330
102	H	6.3575	-2.3266	-4.0848
103	C	7.0464	0.4343	-5.9240
104	H	6.0334	2.3332	-5.7128
105	H	7.8441	-1.5699	-5.8616
106	H	7.6976	0.7658	-6.7298

107	Cl	5.0757	0.8497	-1.0615

large_basis_A-5-I_NiITMe2_IPh_bb
Energy (POTENTIAL) = -1179.66794041 Eh

	Atom	X	Y	Z
1	C	-0.3870	0.3171	-0.0350
2	C	0.2182	0.2312	-1.2565
3	C	-0.0962	2.4590	-0.8045
4	N	-0.5714	1.6765	0.2138
5	N	0.3821	1.5428	-1.7026
6	C	-1.1732	2.2014	1.4293
7	H	-1.2354	3.2862	1.3305
8	H	-2.1773	1.7871	1.5676
9	H	-0.5595	1.9558	2.3019
10	C	1.0084	1.8969	-2.9667
11	H	0.4668	1.4467	-3.8051
12	H	0.9806	2.9847	-3.0585
13	H	2.0494	1.5578	-2.9897
14	C	0.6505	-0.9506	-2.0574
15	H	0.1202	-1.0070	-3.0171
16	H	1.7249	-0.9202	-2.2795
17	H	0.4488	-1.8756	-1.5096
18	C	-0.8106	-0.7391	0.9288
19	H	-0.5512	-1.7302	0.5464
20	H	-0.3201	-0.6156	1.9030
21	H	-1.8940	-0.7199	1.1051
22	C	-0.0926	6.2295	-1.0860
23	N	0.8823	7.0814	-1.5316
24	N	-1.1125	7.0778	-0.7451
25	C	0.4889	8.4174	-1.4614
26	C	2.1892	6.6479	-2.0000
27	C	-0.7824	8.4154	-0.9625
28	C	-2.3871	6.6373	-0.2003
29	C	1.3756	9.5389	-1.8856
30	H	2.1936	5.5571	-2.0157
31	H	2.3786	7.0309	-3.0081
32	H	2.9780	7.0010	-1.3278
33	C	-1.7250	9.5323	-0.6662
34	H	-3.2138	6.9662	-0.8386
35	H	-2.3723	5.5461	-0.1594
36	H	-2.5339	7.0367	0.8088
37	H	0.8735	10.4990	-1.7376
38	H	2.3102	9.5567	-1.3104
39	H	1.6478	9.4625	-2.9464
40	H	-2.6566	9.4399	-1.2395
41	H	-1.9986	9.5601	0.3965
42	H	-1.2698	10.4937	-0.9201
43	Ni	-0.0352	4.3474	-0.9000
44	I	1.9460	4.4637	1.1570
45	C	3.5027	4.5496	2.7903
46	C	3.1530	5.0057	4.0646
47	C	4.8144	4.1441	2.5278
48	C	4.1185	5.0561	5.0770
49	H	2.1332	5.3222	4.2733
50	C	5.7775	4.1969	3.5424
51	H	5.0910	3.7875	1.5379

52	C	5.4315	4.6523	4.8180
53	H	3.8424	5.4109	6.0678
54	H	6.7976	3.8812	3.3341
55	H	6.1804	4.6918	5.6049

large_basis_C-5-Cl_NiIXy2_ClPh_bb
Energy (POTENTIAL) = -2553.01330102 Eh

	Atom	X	Y	Z
1	C	-0.4457	1.0354	0.1001
2	C	0.5806	1.8259	-0.2950
3	C	1.2891	-0.3558	-0.5002
4	N	-0.0066	-0.2817	-0.0271
5	N	1.6234	0.9724	-0.6533
6	Ni	2.3447	-1.8440	-0.8504
7	C	3.4060	-3.3084	-1.2827
8	N	4.6912	-3.6216	-0.8801
9	N	3.0893	-4.3661	-2.1064
10	C	5.1387	-4.8183	-1.4384
11	C	4.1307	-5.2874	-2.2114
12	H	6.1220	-5.2123	-1.2330
13	H	4.0509	-6.1745	-2.8208
14	H	-1.4371	1.2768	0.4512
15	H	0.6721	2.8994	-0.3593
16	C	1.8251	-4.5349	-2.7648
17	C	0.7677	-5.1278	-2.0547
18	C	1.7076	-4.1461	-4.1098
19	C	-0.4249	-5.3738	-2.7455
20	C	0.4935	-4.3976	-4.7604
21	C	-0.5598	-5.0199	-4.0886
22	H	-1.2527	-5.8416	-2.2199
23	H	0.3783	-4.1045	-5.8010
24	C	5.4705	-2.8325	0.0307
25	C	6.0008	-1.6075	-0.4121
26	C	5.7019	-3.3268	1.3271
27	C	6.7597	-0.8570	0.4943
28	C	6.4667	-2.5430	2.2009
29	C	6.9882	-1.3156	1.7917
30	H	7.1731	0.0943	0.1721
31	H	6.6515	-2.9042	3.2097
32	C	-0.8030	-1.4225	0.3215
33	C	-1.3233	-2.2256	-0.7091
34	C	-1.0623	-1.6791	1.6795
35	C	-2.1029	-3.3307	-0.3469
36	C	-1.8485	-2.7944	1.9967
37	C	-2.3610	-3.6177	0.9940
38	H	-2.5093	-3.9664	-1.1283
39	H	-2.0555	-3.0139	3.0413
40	C	2.9080	1.4448	-1.0857
41	C	3.9280	1.5884	-0.1303
42	C	3.0811	1.7994	-2.4339
43	C	5.1427	2.1430	-0.5501
44	C	4.3161	2.3375	-2.8161
45	C	5.3345	2.5216	-1.8796
46	H	5.9430	2.2713	0.1737
47	H	4.4742	2.6166	-3.8548
48	C	2.8474	-3.4474	-4.8071
49	H	3.0920	-2.5104	-4.2907
50	H	3.7600	-4.0555	-4.8099
51	H	2.5897	-3.2131	-5.8446

52	C	0.9084	-5.4328	-0.5868
53	H	1.7829	-6.0628	-0.3828
54	H	1.0490	-4.4993	-0.0279
55	H	0.0189	-5.9392	-0.2006
56	C	5.1561	-4.6614	1.7728
57	H	5.7737	-5.4901	1.4025
58	H	5.1346	-4.7255	2.8650
59	H	4.1405	-4.8217	1.4020
60	C	5.7448	-1.1089	-1.8095
61	H	5.9316	-1.8908	-2.5551
62	H	4.6928	-0.8130	-1.9150
63	H	6.3750	-0.2466	-2.0407
64	C	3.7193	1.1152	1.2841
65	H	2.8520	1.5993	1.7504
66	H	3.5243	0.0357	1.2875
67	H	4.6002	1.3126	1.9018
68	C	1.9752	1.5725	-3.4332
69	H	1.0671	2.1284	-3.1698
70	H	2.2838	1.8794	-4.4375
71	H	1.7007	0.5104	-3.4637
72	C	-1.0346	-1.9160	-2.1544
73	H	-1.2091	-0.8571	-2.3797
74	H	0.0208	-2.1194	-2.3795
75	H	-1.6566	-2.5223	-2.8179
76	C	-0.5204	-0.7853	2.7678
77	H	-1.1363	0.1155	2.8890
78	H	-0.5064	-1.3102	3.7279
79	H	0.4979	-0.4564	2.5441
80	C	2.2534	-3.1996	3.8441
81	C	1.1159	-3.8009	4.3859
82	C	3.3835	-2.9473	4.6242
83	C	1.1161	-4.1554	5.7377
84	H	0.2489	-3.9851	3.7589
85	C	3.3697	-3.3092	5.9738
86	H	4.2548	-2.4766	4.1793
87	C	2.2395	-3.9120	6.5332
88	H	0.2342	-4.6237	6.1668
89	H	4.2464	-3.1162	6.5866
90	H	2.2340	-4.1906	7.5833
91	Cl	2.2643	-2.7442	2.1353
92	H	6.2841	2.9506	-2.1892
93	H	-1.4923	-5.2194	-4.6106
94	H	7.5786	-0.7190	2.4825
95	H	-2.9674	-4.4808	1.2573

large_basis_PhH_benzene_bb
Energy (POTENTIAL) = -232.324133299 Eh

	Atom	X	Y	Z
1	C	-2.2263	0.0406	0.0001
2	C	-0.8279	0.0406	0.0006
3	C	-0.1287	1.2514	-0.0001
4	C	-0.8279	2.4624	-0.0010
5	C	-2.2260	2.4625	-0.0014
6	C	-2.9253	1.2515	-0.0010
7	H	-2.7696	-0.9006	0.0004
8	H	-0.2847	-0.9008	0.0014
9	H	0.9582	1.2515	0.0001
10	H	-0.2843	3.4036	-0.0014
11	H	-2.7695	3.4037	-0.0022
12	H	-4.0122	1.2517	-0.0013

large_basis_NiIMes2_distort_NiIMes2_eta2_PhI_fixCI_bb_NiL2frag
Energy (POTENTIAL) = -2018.31627941 Eh

	Atom	X	Y	Z
1	C	0.4072	0.5732	0.0255
2	C	1.4047	0.8576	-0.8331
3	C	1.1193	-1.4392	-0.8658
4	N	0.2285	-0.8096	-0.0095
5	N	1.8313	-0.3596	-1.3623
6	Ni	1.3047	-3.3336	-1.4913
7	C	3.0162	-4.4950	-1.3574
8	N	3.7466	-4.8011	-0.2247
9	N	3.4478	-5.4771	-2.2358
10	C	4.5644	-5.9173	-0.3949
11	C	4.3802	-6.3382	-1.6629
12	H	5.2009	-6.2814	0.3966
13	H	4.8168	-7.1537	-2.2182
14	H	-0.2003	1.2065	0.6526
15	H	1.8540	1.7937	-1.1252
16	C	3.1489	-5.6003	-3.6353
17	C	2.4859	-6.7464	-4.1007
18	C	3.6489	-4.6258	-4.5169
19	C	2.2782	-6.8698	-5.4817
20	C	3.4030	-4.7846	-5.8826
21	C	2.7137	-5.8967	-6.3852
22	H	1.7510	-7.7459	-5.8532
23	H	3.7763	-4.0319	-6.5739
24	C	3.9411	-3.9883	0.9464
25	C	4.8852	-2.9501	0.8673
26	C	3.3557	-4.3662	2.1618
27	C	5.1552	-2.2174	2.0268
28	C	3.6699	-3.6155	3.3013
29	C	4.5468	-2.5273	3.2502
30	H	5.8754	-1.4036	1.9798
31	H	3.2130	-3.8885	4.2499
32	C	-0.8753	-1.3666	0.7274
33	C	-2.1830	-1.0326	0.3316
34	C	-0.6285	-2.1012	1.8954
35	C	-3.2467	-1.5053	1.1105
36	C	-1.7200	-2.5353	2.6511
37	C	-3.0373	-2.2596	2.2691
38	H	-4.2637	-1.2700	0.8037
39	H	-1.5352	-3.1153	3.5528
40	C	2.8366	-0.3501	-2.3897
41	C	4.1500	0.0080	-2.0470
42	C	2.4393	-0.5038	-3.7305
43	C	5.0921	0.1198	-3.0784
44	C	3.4089	-0.3610	-4.7253
45	C	4.7431	-0.0646	-4.4191
46	H	6.1183	0.3760	-2.8238
47	H	3.1148	-0.4852	-5.7653
48	C	4.4775	-3.4769	-4.0053
49	H	3.8835	-2.8016	-3.3860
50	H	5.3050	-3.8398	-3.3836
51	H	4.8978	-2.9024	-4.8337

52	C	2.0060	-7.8363	-3.1704
53	H	2.7710	-8.6135	-3.0419
54	H	1.7635	-7.4569	-2.1735
55	H	1.1131	-8.3219	-3.5772
56	C	2.4326	-6.0214	-7.8634
57	H	3.2972	-5.7140	-8.4636
58	H	2.1731	-7.0490	-8.1392
59	H	1.5918	-5.3785	-8.1569
60	C	2.4330	-5.5550	2.2397
61	H	2.9803	-6.4929	2.0780
62	H	1.9496	-5.6139	3.2197
63	H	1.6532	-5.5042	1.4741
64	C	5.6356	-2.6986	-0.4159
65	H	6.1553	-3.6076	-0.7436
66	H	4.9617	-2.4074	-1.2254
67	H	6.3826	-1.9114	-0.2874
68	C	4.8286	-1.7006	4.4817
69	H	4.1354	-0.8511	4.5507
70	H	4.7117	-2.2896	5.3981
71	H	5.8442	-1.2894	4.4658
72	C	4.5304	0.3359	-0.6239
73	H	4.1850	1.3410	-0.3499
74	H	4.0865	-0.3615	0.0911
75	H	5.6164	0.3201	-0.4979
76	C	1.0011	-0.7748	-4.0767
77	H	0.3461	0.0195	-3.6953
78	H	0.8628	-0.8440	-5.1597
79	H	0.6618	-1.7090	-3.6258
80	C	5.7780	0.0241	-5.5140
81	H	6.6738	0.5598	-5.1821
82	H	6.0938	-0.9786	-5.8342
83	H	5.3820	0.5338	-6.4002
84	C	-2.4625	-0.1674	-0.8760
85	H	-1.7493	-0.3495	-1.6841
86	H	-3.4699	-0.3581	-1.2600
87	H	-2.4051	0.8989	-0.6218
88	C	0.7791	-2.4264	2.2976
89	H	1.3808	-1.5205	2.4425
90	H	0.8031	-3.0075	3.2229
91	H	1.2705	-3.0046	1.5116
92	C	-4.1991	-2.7967	3.0694
93	H	-5.1092	-2.2093	2.9060
94	H	-4.4215	-3.8337	2.7828
95	H	-3.9802	-2.7985	4.1434

large_basis_PhBr_PhBr_bb
Energy (POTENTIAL) = -244.896837913 Eh

	Atom	X	Y	Z
1	C	-2.2270	0.0426	0.0000
2	C	-0.8294	0.0322	0.0006
3	C	-0.1510	1.2514	0.0000
4	C	-0.8293	2.4707	-0.0010
5	C	-2.2269	2.4604	-0.0015
6	C	-2.9269	1.2516	-0.0010
7	H	-2.7640	-0.9018	0.0005
8	H	-0.2848	-0.9060	0.0014
9	H	-0.2846	3.4088	-0.0014
10	H	-2.7639	3.4050	-0.0023
11	H	-4.0131	1.2516	-0.0014
12	Br	1.7869	1.2514	0.0007

large_basis_A-4-Br_trans-NiBrPhITMe2_bb
Energy (POTENTIAL) = -1181.54575592 Eh

	Atom	X	Y	Z
1	C	-0.6690	2.1767	1.0281
2	C	0.2350	2.1176	0.0081
3	C	-0.1017	4.3201	0.4944
4	N	-0.8569	3.5353	1.3033
5	N	0.5653	3.4424	-0.2967
6	C	-1.7556	4.0455	2.3264
7	H	-1.6201	5.1257	2.3883
8	H	-2.7963	3.8198	2.0726
9	H	-1.5179	3.6014	3.2975
10	C	1.5019	3.8335	-1.3382
11	H	1.1003	3.5963	-2.3284
12	H	1.6644	4.9089	-1.2616
13	H	2.4567	3.3172	-1.2020
14	C	0.8414	0.9594	-0.7085
15	H	0.6475	1.0041	-1.7879
16	H	1.9301	0.9243	-0.5723
17	H	0.4275	0.0200	-0.3319
18	C	-1.3754	1.1052	1.7868
19	H	-1.1080	0.1208	1.3932
20	H	-1.1132	1.1233	2.8527
21	H	-2.4655	1.2113	1.7170
22	C	-0.1349	8.1718	0.2537
23	N	0.6297	8.9585	-0.5442
24	N	-1.0000	9.0341	0.8445
25	C	0.2518	10.3026	-0.4609
26	C	1.7049	8.4613	-1.3879
27	C	-0.7856	10.3508	0.4237
28	C	-2.0264	8.6366	1.7946
29	C	0.9378	11.3740	-1.2389
30	H	1.8683	7.4107	-1.1452
31	H	1.4417	8.5569	-2.4463
32	H	2.6265	9.0180	-1.1944
33	C	-1.5953	11.4931	0.9359
34	H	-3.0243	8.8151	1.3822
35	H	-1.9039	7.5728	1.9990
36	H	-1.9164	9.1951	2.7289
37	H	0.4513	12.3384	-1.0688
38	H	1.9924	11.4742	-0.9512
39	H	0.9112	11.1696	-2.3168
40	H	-2.6642	11.3585	0.7264
41	H	-1.4868	11.6113	2.0219
42	H	-1.2760	12.4269	0.4650
43	Ni	-0.0638	6.2479	0.4244
44	C	-1.3978	6.1486	-0.9309
45	C	-1.0601	6.1609	-2.2994
46	C	-2.7694	6.0535	-0.6207
47	C	-2.0326	6.0776	-3.3027
48	H	-0.0149	6.2388	-2.5920
49	C	-3.7499	5.9739	-1.6167
50	H	-3.0827	6.0386	0.4213
51	C	-3.3866	5.9839	-2.9667

52	H	-1.7322	6.0878	-4.3494
53	H	-4.8000	5.9027	-1.3373
54	H	-4.1453	5.9207	-3.7433
55	Br	1.7197	6.3542	2.1975

large_basis_B-6-Br_NiBrIMes2_bb
Energy (POTENTIAL) = -2031.65228445 Eh

	Atom	X	Y	Z
1	C	-0.0785	0.0247	-0.1954
2	C	1.0134	0.7450	-0.5480
3	C	1.6317	-1.4585	-0.5206
4	N	0.3133	-1.3113	-0.1849
5	N	2.0418	-0.1738	-0.7477
6	Ni	2.7077	-3.0906	-0.5932
7	C	3.7882	-4.5853	-1.2455
8	N	5.1070	-4.8633	-1.0117
9	N	3.3783	-5.6383	-2.0147
10	C	5.5003	-6.0559	-1.6135
11	C	4.4073	-6.5485	-2.2450
12	H	6.5097	-6.4286	-1.5338
13	H	4.2577	-7.4439	-2.8281
14	H	-1.0864	0.3251	0.0451
15	H	1.1629	1.8061	-0.6744
16	C	2.0584	-5.7931	-2.5619
17	C	1.0500	-6.3523	-1.7636
18	C	1.8369	-5.4163	-3.8966
19	C	-0.2054	-6.5512	-2.3480
20	C	0.5645	-5.6321	-4.4348
21	C	-0.4669	-6.1994	-3.6764
22	H	-1.0000	-6.9817	-1.7439
23	H	0.3731	-5.3419	-5.4657
24	C	6.0144	-4.0124	-0.2910
25	C	6.4858	-2.8490	-0.9139
26	C	6.4326	-4.3953	0.9950
27	C	7.3937	-2.0503	-0.2074
28	C	7.3322	-3.5606	1.6627
29	C	7.8218	-2.3838	1.0801
30	H	7.7711	-1.1474	-0.6794
31	H	7.6559	-3.8340	2.6648
32	C	-0.5962	-2.3941	0.0746
33	C	-1.0616	-3.1541	-1.0087
34	C	-1.0221	-2.6287	1.3909
35	C	-1.9654	-4.1874	-0.7425
36	C	-1.9226	-3.6774	1.6074
37	C	-2.3955	-4.4734	0.5576
38	H	-2.3374	-4.7832	-1.5718
39	H	-2.2558	-3.8808	2.6228
40	C	3.3606	0.2133	-1.1690
41	C	4.3777	0.3249	-0.2104
42	C	3.5705	0.5184	-2.5248
43	C	5.6275	0.7857	-0.6395
44	C	4.8390	0.9651	-2.9058
45	C	5.8771	1.1103	-1.9763
46	H	6.4258	0.8828	0.0917
47	H	5.0223	1.2012	-3.9519
48	C	2.9328	-4.7726	-4.7104
49	H	3.3104	-3.8709	-4.2122
50	H	3.7898	-5.4435	-4.8451
51	H	2.5669	-4.4872	-5.7013

52	C	1.3072	-6.6931	-0.3196
53	H	2.1687	-7.3638	-0.2100
54	H	1.5373	-5.7878	0.2568
55	H	0.4335	-7.1760	0.1293
56	C	-1.8507	-6.3627	-4.2568
57	H	-1.8173	-6.5717	-5.3319
58	H	-2.4008	-7.1731	-3.7662
59	H	-2.4378	-5.4429	-4.1238
60	C	5.9111	-5.6545	1.6380
61	H	6.2015	-6.5501	1.0749
62	H	6.2973	-5.7585	2.6569
63	H	4.8169	-5.6258	1.6864
64	C	6.0195	-2.4519	-2.2918
65	H	6.0390	-3.3006	-2.9858
66	H	4.9870	-2.0843	-2.2567
67	H	6.6474	-1.6566	-2.7020
68	C	8.8027	-1.5111	1.8271
69	H	9.7826	-1.9988	1.9162
70	H	8.9544	-0.5515	1.3214
71	H	8.4545	-1.3055	2.8466
72	C	4.1390	-0.0700	1.2231
73	H	3.2732	0.4537	1.6473
74	H	3.9248	-1.1437	1.2988
75	H	5.0147	0.1518	1.8407
76	C	2.4652	0.3466	-3.5380
77	H	1.6086	0.9966	-3.3223
78	H	2.8202	0.5792	-4.5466
79	H	2.0883	-0.6836	-3.5375
80	C	7.2510	1.5485	-2.4224
81	H	7.1973	2.3416	-3.1773
82	H	7.8497	1.9154	-1.5818
83	H	7.7993	0.7112	-2.8761
84	C	-0.5954	-2.8783	-2.4159
85	H	-0.6255	-1.8076	-2.6495
86	H	0.4404	-3.2105	-2.5476
87	H	-1.2145	-3.4091	-3.1438
88	C	-0.5169	-1.7839	2.5321
89	H	-0.8655	-0.7460	2.4560
90	H	-0.8598	-2.1828	3.4919
91	H	0.5781	-1.7742	2.5376
92	C	-3.3246	-5.6346	0.8198
93	H	-3.8911	-5.4978	1.7473
94	H	-4.0379	-5.7734	-0.0008
95	H	-2.7591	-6.5716	0.9186
96	Br	2.6642	-3.7086	1.9328

large_basis_PhCl_PhCl_bb
Energy (POTENTIAL) = -691.950431153 Eh

	Atom	X	Y	Z
1	C	-2.2260	0.0425	0.0001
2	C	-0.8288	0.0325	0.0006
3	C	-0.1506	1.2514	-0.0000
4	C	-0.8287	2.4704	-0.0010
5	C	-2.2259	2.4606	-0.0015
6	C	-2.9261	1.2516	-0.0010
7	H	-2.7636	-0.9017	0.0005
8	H	-0.2783	-0.9026	0.0013
9	H	-0.2781	3.4054	-0.0014
10	H	-2.7634	3.4048	-0.0023
11	H	-4.0123	1.2516	-0.0014
12	Cl	1.6179	1.2514	0.0006

large_basis_TS-A-5-6-I_NiITMe2_IPh_ossts_t_ts_bb
Energy (POTENTIAL) = -1179.66802572 Eh

	Atom	X	Y	Z
1	C	-0.9927	1.7727	0.1472
2	C	0.0286	2.5877	-0.2508
3	C	0.7618	0.4238	-0.4532
4	N	-0.5243	0.4664	0.0110
5	N	1.0803	1.7449	-0.6105
6	Ni	1.8537	-1.1003	-0.7579
7	C	2.8962	-2.6008	-1.2834
8	N	4.2191	-2.8604	-1.0528
9	N	2.4692	-3.7211	-1.9434
10	C	4.6039	-4.1091	-1.5394
11	C	3.4900	-4.6567	-2.1095
12	C	2.2763	-2.1725	4.1708
13	C	2.2468	-3.5036	4.5970
14	C	2.4463	-1.1476	5.1064
15	C	2.3851	-3.8091	5.9564
16	H	2.1170	-4.3067	3.8736
17	C	2.5852	-1.4540	6.4658
18	H	2.4720	-0.1086	4.7822
19	C	2.5545	-2.7849	6.8929
20	H	2.3611	-4.8471	6.2825
21	H	2.7170	-0.6524	7.1900
22	H	2.6624	-3.0223	7.9483
23	I	2.0641	-1.6791	1.9503
24	C	-1.3048	-0.7118	0.3569
25	H	-2.2467	-0.7225	-0.2009
26	H	-0.7165	-1.5929	0.0976
27	H	-1.5221	-0.7294	1.4297
28	C	2.3704	2.2174	-1.0884
29	H	2.8410	2.8678	-0.3441
30	H	3.0032	1.3438	-1.2579
31	H	2.2558	2.7714	-2.0260
32	C	0.1259	4.0737	-0.3346
33	H	-0.8125	4.5361	-0.0155
34	H	0.9270	4.4646	0.3060
35	H	0.3348	4.4094	-1.3586
36	C	-2.3657	2.0857	0.6377
37	H	-3.1378	1.6625	-0.0181
38	H	-2.5369	1.6835	1.6444
39	H	-2.5182	3.1677	0.6782
40	C	5.1126	-1.9632	-0.3367
41	H	6.0054	-1.7575	-0.9358
42	H	4.5756	-1.0329	-0.1480
43	H	5.4129	-2.4020	0.6202
44	C	1.0991	-3.9344	-2.3829
45	H	0.5275	-3.0344	-2.1471
46	H	1.0646	-4.1159	-3.4621
47	H	0.6575	-4.7902	-1.8614
48	C	3.2824	-5.9592	-2.8056
49	H	4.2085	-6.5409	-2.8083
50	H	2.5073	-6.5629	-2.3164
51	H	2.9735	-5.8171	-3.8495

52	C	5.9938	-4.6318	-1.4030
53	H	6.7217	-3.9969	-1.9247
54	H	6.3033	-4.6851	-0.3514
55	H	6.0648	-5.6383	-1.8245

large_basis_TS-B-5-6-I_NiIMes2_ossts_PhI_t_ossts_bb
Energy (POTENTIAL) = -2261.50730351 Eh

	Atom	X	Y	Z
1	C	-1.1701	1.7706	-0.0002
2	C	-0.0990	2.5150	-0.3676
3	C	0.5638	0.3183	-0.3855
4	N	-0.7547	0.4412	-0.0141
5	N	0.9447	1.6197	-0.5953
6	Ni	1.6540	-1.1999	-0.5970
7	C	2.7856	-2.6566	-1.0657
8	N	4.0442	-3.0184	-0.6395
9	N	2.5061	-3.6027	-2.0182
10	C	4.5173	-4.1430	-1.3100
11	C	3.5475	-4.5134	-2.1806
12	H	5.4896	-4.5626	-1.1036
13	H	3.4932	-5.3238	-2.8911
14	H	-2.1772	2.0507	0.2667
15	H	0.0252	3.5801	-0.4888
16	C	1.2749	-3.6821	-2.7527
17	C	0.1876	-4.3583	-2.1804
18	C	1.2165	-3.1210	-4.0387
19	C	-0.9658	-4.5120	-2.9575
20	C	0.0382	-3.2884	-4.7720
21	C	-1.0560	-3.9935	-4.2536
22	H	-1.8157	-5.0413	-2.5335
23	H	-0.0281	-2.8582	-5.7692
24	C	4.7824	-2.3350	0.3852
25	C	5.2974	-1.0614	0.1134
26	C	4.9352	-2.9504	1.6405
27	C	5.9320	-0.3741	1.1566
28	C	5.5855	-2.2316	2.6454
29	C	6.0725	-0.9357	2.4288
30	H	6.3174	0.6252	0.9662
31	H	5.6816	-2.6793	3.6319
32	C	-1.6167	-0.6739	0.2545
33	C	-2.0124	-1.4872	-0.8214
34	C	-2.0560	-0.9094	1.5669
35	C	-2.8172	-2.5955	-0.5428
36	C	-2.8589	-2.0333	1.7952
37	C	-3.2351	-2.8953	0.7593
38	H	-3.1262	-3.2373	-1.3641
39	H	-3.1950	-2.2393	2.8092
40	C	2.2405	2.0232	-1.0648
41	C	3.1939	2.4718	-0.1382
42	C	2.4953	1.9926	-2.4452
43	C	4.4144	2.9424	-0.6340
44	C	3.7341	2.4639	-2.8929
45	C	4.6989	2.9535	-2.0046
46	H	5.1638	3.2990	0.0693
47	H	3.9492	2.4478	-3.9593
48	C	2.3847	-2.3366	-4.5828
49	H	2.6639	-1.5317	-3.8915
50	H	3.2731	-2.9675	-4.7111
51	H	2.1412	-1.8906	-5.5519

52	C	0.2518	-4.8500	-0.7575
53	H	1.1126	-5.5094	-0.5917
54	H	0.3660	-3.9988	-0.0739
55	H	-0.6580	-5.3935	-0.4857
56	C	-2.3266	-4.1319	-5.0574
57	H	-2.1147	-4.3646	-6.1075
58	H	-2.9735	-4.9194	-4.6562
59	H	-2.9011	-3.1954	-5.0454
60	C	4.3695	-4.3213	1.9168
61	H	4.9371	-5.1083	1.4042
62	H	4.3871	-4.5370	2.9890
63	H	3.3318	-4.3918	1.5738
64	C	5.1518	-0.4378	-1.2504
65	H	5.3511	-1.1636	-2.0476
66	H	4.1297	-0.0717	-1.3982
67	H	5.8363	0.4057	-1.3693
68	C	6.7192	-0.1723	3.5597
69	H	7.5934	-0.7056	3.9545
70	H	7.0464	0.8228	3.2402
71	H	6.0174	-0.0467	4.3943
72	C	2.9200	2.4049	1.3427
73	H	2.0180	2.9644	1.6185
74	H	2.7590	1.3648	1.6523
75	H	3.7616	2.8069	1.9151
76	C	1.4708	1.4342	-3.4005
77	H	0.5305	1.9983	-3.3616
78	H	1.8400	1.4534	-4.4305
79	H	1.2304	0.3970	-3.1355
80	C	6.0428	3.4243	-2.5062
81	H	5.9826	3.7911	-3.5367
82	H	6.4476	4.2268	-1.8794
83	H	6.7739	2.6038	-2.4947
84	C	-1.5755	-1.1830	-2.2314
85	H	-1.6393	-0.1108	-2.4492
86	H	-0.5314	-1.4811	-2.3802
87	H	-2.1916	-1.7225	-2.9549
88	C	-1.7069	0.0263	2.6983
89	H	-2.3687	0.9030	2.7049
90	H	-1.8151	-0.4755	3.6650
91	H	-0.6792	0.3905	2.6189
92	C	-4.0526	-4.1339	1.0379
93	H	-4.6399	-4.0321	1.9570
94	H	-4.7409	-4.3566	0.2143
95	H	-3.4018	-5.0103	1.1622
96	C	2.2772	-2.1072	4.3017
97	C	2.0877	-3.3871	4.8311
98	C	2.9857	-1.1492	5.0346
99	C	2.6021	-3.7067	6.0941
100	H	1.5500	-4.1410	4.2592
101	C	3.4968	-1.4690	6.2982
102	H	3.1523	-0.1580	4.6175
103	C	3.3084	-2.7494	6.8288
104	H	2.4522	-4.7044	6.5021
105	H	4.0454	-0.7193	6.8652
106	H	3.7099	-2.9997	7.8076

107	I	1.6861	-1.6389	2.1452

large_basis_TS-D-5-6-Cl_NiIPhen2_ossts_PhCl_t_bb
Energy (POTENTIAL) = -2238.31537306 Eh

	Atom	X	Y	Z
1	C	-0.2933	1.1673	0.5594
2	C	0.7123	1.8786	-0.0016
3	C	1.2008	-0.3461	-0.3015
4	N	0.0089	-0.1803	0.3616
5	N	1.6050	0.9499	-0.5312
6	Ni	2.2523	-1.8840	-0.6960
7	C	3.4867	-3.1882	-1.3216
8	N	4.7835	-3.3811	-0.9090
9	N	3.3277	-4.1469	-2.2939
10	C	5.3998	-4.4231	-1.6007
11	C	4.4867	-4.9010	-2.4781
12	H	6.4232	-4.7091	-1.4142
13	H	4.5409	-5.7076	-3.1925
14	H	-1.2030	1.4862	1.0435
15	H	0.8627	2.9423	-0.1022
16	C	2.1100	-4.3674	-3.0050
17	C	0.8984	-4.4070	-2.3055
18	C	2.1383	-4.5468	-4.3906
19	C	-0.2909	-4.6083	-3.0068
20	C	0.9428	-4.7618	-5.0809
21	C	-0.2734	-4.7868	-4.3936
22	H	-1.2320	-4.6362	-2.4643
23	H	0.9648	-4.8984	-6.1586
24	C	5.4239	-2.6271	0.1226
25	C	5.3476	-1.2311	0.1199
26	C	6.1212	-3.2995	1.1297
27	C	5.9590	-0.5095	1.1454
28	C	6.7421	-2.5672	2.1444
29	C	6.6575	-1.1724	2.1587
30	H	5.8926	0.5747	1.1416
31	H	7.2794	-3.0915	2.9299
32	C	-0.8229	-1.2488	0.8104
33	C	-1.0635	-2.3400	-0.0290
34	C	-1.3951	-1.1912	2.0837
35	C	-1.8668	-3.3871	0.4203
36	C	-2.2107	-2.2374	2.5192
37	C	-2.4446	-3.3399	1.6930
38	H	-2.0469	-4.2395	-0.2291
39	H	-2.6492	-2.1950	3.5124
40	C	2.8293	1.2876	-1.1795
41	C	3.6943	2.2132	-0.5905
42	C	3.1660	0.6660	-2.3876
43	C	4.9094	2.5117	-1.2125
44	C	4.3878	0.9612	-2.9943
45	C	5.2621	1.8823	-2.4093
46	H	5.5852	3.2262	-0.7510
47	H	4.6520	0.4722	-3.9278
48	C	2.1202	-3.5693	3.5566
49	C	0.9164	-3.9306	4.1488
50	C	3.3162	-3.5716	4.2639
51	C	0.9126	-4.3144	5.4971

52	H	-0.0077	-3.9116	3.5746
53	C	3.3069	-3.9562	5.6116
54	H	4.2443	-3.2768	3.7773
55	C	2.1063	-4.3274	6.2273
56	H	-0.0213	-4.6018	5.9771
57	H	4.2354	-3.9653	6.1800
58	H	2.1006	-4.6241	7.2733
59	Cl	2.1356	-2.9196	1.5793
60	H	3.4280	2.6720	0.3570
61	H	6.2120	2.1094	-2.8850
62	H	2.4772	-0.0441	-2.8330
63	H	7.1342	-0.6059	2.9540
64	H	-1.1811	-0.3498	2.7357
65	H	-3.0738	-4.1559	2.0377
66	H	-0.6084	-2.3649	-1.0123
67	H	3.0840	-4.5014	-4.9228
68	H	-1.2018	-4.9484	-4.9345
69	H	0.9008	-4.2765	-1.2291
70	H	6.1540	-4.3849	1.1317
71	H	4.8132	-0.7240	-0.6745

large_basis_IXy_IXy_bb
Energy (POTENTIAL) = -845.819164274 Eh

	Atom	X	Y	Z
1	C	-0.5381	1.1362	-0.0969
2	C	0.5597	1.8919	-0.3421
3	C	1.1868	-0.3181	-0.6044
4	N	-0.1359	-0.1914	-0.2626
5	N	1.5848	0.9931	-0.6453
6	H	-1.5471	1.4068	0.1758
7	H	0.7112	2.9608	-0.3298
8	C	-1.0199	-1.3079	-0.0670
9	C	-1.8481	-1.7135	-1.1269
10	C	-1.0360	-1.9424	1.1865
11	C	-2.7139	-2.7923	-0.9058
12	C	-1.9144	-3.0182	1.3660
13	C	-2.7477	-3.4397	0.3294
14	H	-3.3625	-3.1246	-1.7123
15	H	-1.9428	-3.5254	2.3271
16	C	2.9214	1.4088	-0.9692
17	C	3.8451	1.5909	0.0731
18	C	3.2503	1.6343	-2.3158
19	C	5.1366	2.0162	-0.2630
20	C	4.5519	2.0589	-2.6105
21	C	5.4875	2.2495	-1.5931
22	H	5.8686	2.1635	0.5271
23	H	4.8292	2.2396	-3.6461
24	C	3.4519	1.3308	1.5059
25	H	2.6197	1.9740	1.8174
26	H	3.1175	0.2957	1.6414
27	H	4.2933	1.5113	2.1818
28	C	2.2294	1.4119	-3.4036
29	H	1.3273	2.0131	-3.2377
30	H	2.6379	1.6713	-4.3850
31	H	1.9091	0.3638	-3.4297
32	C	-1.7929	-1.0176	-2.4644
33	H	-1.9964	0.0559	-2.3723
34	H	-0.7987	-1.1125	-2.9169
35	H	-2.5243	-1.4440	-3.1578
36	C	-0.1228	-1.4820	2.2954
37	H	-0.2448	-0.4113	2.4989
38	H	-0.3207	-2.0316	3.2207
39	H	0.9286	-1.6335	2.0248
40	H	-3.4252	-4.2754	0.4846
41	H	6.4939	2.5794	-1.8379

large_basis_B-6-Cl_NiClIMes2_bb
Energy (POTENTIAL) = -2478.70682012 Eh

	Atom	X	Y	Z
1	C	-0.0084	0.0587	-0.1487
2	C	1.1352	0.7744	-0.2782
3	C	1.6954	-1.4366	-0.4528
4	N	0.3509	-1.2820	-0.2580
5	N	2.1590	-0.1518	-0.4656
6	Ni	2.7120	-3.0963	-0.5885
7	C	3.7232	-4.6137	-1.2824
8	N	5.0706	-4.8342	-1.2231
9	N	3.2477	-5.7383	-1.8935
10	C	5.4212	-6.0619	-1.7799
11	C	4.2683	-6.6347	-2.2033
12	H	6.4455	-6.3989	-1.8196
13	H	4.0713	-7.5782	-2.6886
14	H	-1.0315	0.3644	0.0067
15	H	1.3240	1.8367	-0.2575
16	C	1.8734	-5.9786	-2.2383
17	C	1.0563	-6.6756	-1.3380
18	C	1.4151	-5.5533	-3.4954
19	C	-0.2435	-6.9916	-1.7510
20	C	0.1090	-5.8884	-3.8616
21	C	-0.7263	-6.6244	-3.0109
22	H	-0.8927	-7.5348	-1.0682
23	H	-0.2643	-5.5701	-4.8329
24	C	6.0367	-3.8928	-0.7261
25	C	6.4225	-2.8296	-1.5569
26	C	6.5989	-4.0944	0.5442
27	C	7.4132	-1.9620	-1.0894
28	C	7.5769	-3.1905	0.9731
29	C	7.9972	-2.1226	0.1721
30	H	7.7312	-1.1396	-1.7235
31	H	8.0210	-3.3266	1.9568
32	C	-0.6017	-2.3581	-0.2319
33	C	-1.0408	-2.8936	-1.4518
34	C	-1.0954	-2.8023	1.0046
35	C	-2.0024	-3.9073	-1.4105
36	C	-2.0449	-3.8290	0.9942
37	C	-2.5089	-4.3930	-0.2002
38	H	-2.3593	-4.3289	-2.3453
39	H	-2.4322	-4.1944	1.9428
40	C	3.5252	0.2373	-0.6846
41	C	4.3725	0.3973	0.4203
42	C	3.9462	0.4966	-1.9985
43	C	5.6658	0.8778	0.1836
44	C	5.2473	0.9717	-2.1855
45	C	6.1135	1.1849	-1.1055
46	H	6.3377	1.0126	1.0280
47	H	5.5912	1.1808	-3.1963
48	C	2.3052	-4.7387	-4.4003
49	H	2.6422	-3.8269	-3.8918
50	H	3.2080	-5.2921	-4.6873
51	H	1.7772	-4.4480	-5.3136

52	C	1.5623	-7.0429	0.0331
53	H	2.4690	-7.6583	-0.0212
54	H	1.8224	-6.1394	0.5999
55	H	0.8040	-7.5979	0.5941
56	C	-2.1182	-7.0080	-3.4533
57	H	-2.0862	-7.8203	-4.1919
58	H	-2.7283	-7.3492	-2.6113
59	H	-2.6347	-6.1657	-3.9289
60	C	6.1426	-5.2296	1.4249
61	H	6.2507	-6.2018	0.9294
62	H	6.7190	-5.2569	2.3551
63	H	5.0825	-5.1040	1.6775
64	C	5.7727	-2.6226	-2.9018
65	H	5.8035	-3.5336	-3.5118
66	H	4.7168	-2.3557	-2.7756
67	H	6.2651	-1.8183	-3.4559
68	C	9.0310	-1.1433	0.6733
69	H	9.7436	-1.6221	1.3542
70	H	9.5943	-0.6938	-0.1517
71	H	8.5531	-0.3242	1.2273
72	C	3.8959	0.0547	1.8082
73	H	3.0253	0.6584	2.0947
74	H	3.5883	-0.9973	1.8628
75	H	4.6866	0.2239	2.5458
76	C	3.0250	0.2438	-3.1658
77	H	2.0971	0.8229	-3.0841
78	H	3.5090	0.5049	-4.1118
79	H	2.7329	-0.8129	-3.2100
80	C	7.4982	1.7425	-1.3342
81	H	7.4600	2.8238	-1.5237
82	H	8.1441	1.5818	-0.4656
83	H	7.9783	1.2827	-2.2060
84	C	-0.4786	-2.4004	-2.7615
85	H	-0.5493	-1.3090	-2.8464
86	H	0.5836	-2.6594	-2.8445
87	H	-1.0064	-2.8480	-3.6087
88	C	-0.5990	-2.2048	2.2965
89	H	-0.7824	-1.1243	2.3419
90	H	-1.0945	-2.6688	3.1552
91	H	0.4817	-2.3619	2.3930
92	C	-3.5034	-5.5286	-0.1785
93	H	-4.2338	-5.4113	0.6304
94	H	-4.0496	-5.6051	-1.1247
95	H	-2.9928	-6.4873	-0.0156
96	Cl	2.7341	-3.7349	1.7725

large_basis_TS-B-5-6-I_NiIMes2_ossts_PhI_t_bb
Energy (POTENTIAL) = -2261.48124081 Eh

	Atom	X	Y	Z
1	C	-1.1701	1.7706	-0.0002
2	C	-0.0990	2.5150	-0.3676
3	C	0.5638	0.3183	-0.3855
4	N	-0.7547	0.4412	-0.0141
5	N	0.9447	1.6197	-0.5953
6	Ni	1.6540	-1.1999	-0.5970
7	C	2.7856	-2.6566	-1.0657
8	N	4.0442	-3.0184	-0.6395
9	N	2.5061	-3.6027	-2.0182
10	C	4.5173	-4.1430	-1.3100
11	C	3.5475	-4.5134	-2.1806
12	H	5.4896	-4.5626	-1.1036
13	H	3.4932	-5.3238	-2.8911
14	H	-2.1772	2.0507	0.2667
15	H	0.0252	3.5801	-0.4888
16	C	1.2749	-3.6821	-2.7527
17	C	0.1876	-4.3583	-2.1804
18	C	1.2165	-3.1210	-4.0387
19	C	-0.9658	-4.5120	-2.9575
20	C	0.0382	-3.2884	-4.7720
21	C	-1.0560	-3.9935	-4.2536
22	H	-1.8157	-5.0413	-2.5335
23	H	-0.0281	-2.8582	-5.7692
24	C	4.7824	-2.3350	0.3852
25	C	5.2974	-1.0614	0.1134
26	C	4.9352	-2.9504	1.6405
27	C	5.9320	-0.3741	1.1566
28	C	5.5855	-2.2316	2.6454
29	C	6.0725	-0.9357	2.4288
30	H	6.3174	0.6252	0.9662
31	H	5.6816	-2.6793	3.6319
32	C	-1.6167	-0.6739	0.2545
33	C	-2.0124	-1.4872	-0.8214
34	C	-2.0560	-0.9094	1.5669
35	C	-2.8172	-2.5955	-0.5428
36	C	-2.8589	-2.0333	1.7952
37	C	-3.2351	-2.8953	0.7593
38	H	-3.1262	-3.2373	-1.3641
39	H	-3.1950	-2.2393	2.8092
40	C	2.2405	2.0232	-1.0648
41	C	3.1939	2.4718	-0.1382
42	C	2.4953	1.9926	-2.4452
43	C	4.4144	2.9424	-0.6340
44	C	3.7341	2.4639	-2.8929
45	C	4.6989	2.9535	-2.0046
46	H	5.1638	3.2990	0.0693
47	H	3.9492	2.4478	-3.9593
48	C	2.3847	-2.3366	-4.5828
49	H	2.6639	-1.5317	-3.8915
50	H	3.2731	-2.9675	-4.7111
51	H	2.1412	-1.8906	-5.5519

52	C	0.2518	-4.8500	-0.7575
53	H	1.1126	-5.5094	-0.5917
54	H	0.3660	-3.9988	-0.0739
55	H	-0.6580	-5.3935	-0.4857
56	C	-2.3266	-4.1319	-5.0574
57	H	-2.1147	-4.3646	-6.1075
58	H	-2.9735	-4.9194	-4.6562
59	H	-2.9011	-3.1954	-5.0454
60	C	4.3695	-4.3213	1.9168
61	H	4.9371	-5.1083	1.4042
62	H	4.3871	-4.5370	2.9890
63	H	3.3318	-4.3918	1.5738
64	C	5.1518	-0.4378	-1.2504
65	H	5.3511	-1.1636	-2.0476
66	H	4.1297	-0.0717	-1.3982
67	H	5.8363	0.4057	-1.3693
68	C	6.7192	-0.1723	3.5597
69	H	7.5934	-0.7056	3.9545
70	H	7.0464	0.8228	3.2402
71	H	6.0174	-0.0467	4.3943
72	C	2.9200	2.4049	1.3427
73	H	2.0180	2.9644	1.6185
74	H	2.7590	1.3648	1.6523
75	H	3.7616	2.8069	1.9151
76	C	1.4708	1.4342	-3.4005
77	H	0.5305	1.9983	-3.3616
78	H	1.8400	1.4534	-4.4305
79	H	1.2304	0.3970	-3.1355
80	C	6.0428	3.4243	-2.5062
81	H	5.9826	3.7911	-3.5367
82	H	6.4476	4.2268	-1.8794
83	H	6.7739	2.6038	-2.4947
84	C	-1.5755	-1.1830	-2.2314
85	H	-1.6393	-0.1108	-2.4492
86	H	-0.5314	-1.4811	-2.3802
87	H	-2.1916	-1.7225	-2.9549
88	C	-1.7069	0.0263	2.6983
89	H	-2.3687	0.9030	2.7049
90	H	-1.8151	-0.4755	3.6650
91	H	-0.6792	0.3905	2.6189
92	C	-4.0526	-4.1339	1.0379
93	H	-4.6399	-4.0321	1.9570
94	H	-4.7409	-4.3566	0.2143
95	H	-3.4018	-5.0103	1.1622
96	C	2.2772	-2.1072	4.3017
97	C	2.0877	-3.3871	4.8311
98	C	2.9857	-1.1492	5.0346
99	C	2.6021	-3.7067	6.0941
100	H	1.5500	-4.1410	4.2592
101	C	3.4968	-1.4690	6.2982
102	H	3.1523	-0.1580	4.6175
103	C	3.3084	-2.7494	6.8288
104	H	2.4522	-4.7044	6.5021
105	H	4.0454	-0.7193	6.8652
106	H	3.7099	-2.9997	7.8076

107	I	1.6861	-1.6389	2.1452

large_basis_TS-B-5-6-Br_NiIMes2_ossts_PhBr_t_oss_bb
Energy (POTENTIAL) = -2263.28344836 Eh

	Atom	X	Y	Z
1	C	-3.7678	3.3353	0.0322
2	C	-2.6772	4.0902	-0.2432
3	C	-2.0410	1.8920	-0.4108
4	N	-3.3676	2.0046	-0.0721
5	N	-1.6385	3.1997	-0.5096
6	Ni	-0.9671	0.3535	-0.6419
7	C	0.1454	-1.1177	-1.1102
8	N	1.4134	-1.4427	-0.6902
9	N	-0.1521	-2.1248	-1.9918
10	C	1.8776	-2.6089	-1.2935
11	C	0.8901	-3.0416	-2.1145
12	H	2.8561	-3.0107	-1.0814
13	H	0.8247	-3.8992	-2.7661
14	H	-4.7796	3.6092	0.2872
15	H	-2.5360	5.1595	-0.2785
16	C	-1.3961	-2.2439	-2.6994
17	C	-2.5008	-2.8071	-2.0443
18	C	-1.4542	-1.8244	-4.0393
19	C	-3.6764	-2.9832	-2.7830
20	C	-2.6548	-2.0063	-4.7310
21	C	-3.7727	-2.5922	-4.1219
22	H	-4.5394	-3.4256	-2.2922
23	H	-2.7208	-1.6817	-5.7676
24	C	2.1735	-0.6790	0.2602
25	C	2.6897	0.5643	-0.1272
26	C	2.3678	-1.1978	1.5521
27	C	3.3775	1.3170	0.8334
28	C	3.0663	-0.4144	2.4731
29	C	3.5633	0.8516	2.1379
30	H	3.7694	2.2908	0.5514
31	H	3.1996	-0.7881	3.4859
32	C	-4.2592	0.8963	0.1213
33	C	-4.6837	0.1627	-0.9998
34	C	-4.7149	0.6056	1.4169
35	C	-5.5752	-0.8933	-0.7911
36	C	-5.6022	-0.4661	1.5747
37	C	-6.0376	-1.2297	0.4869
38	H	-5.9176	-1.4655	-1.6496
39	H	-5.9571	-0.7089	2.5741
40	C	-0.3223	3.6290	-0.8936
41	C	0.6330	3.8851	0.1037
42	C	-0.0507	3.8241	-2.2555
43	C	1.8755	4.3842	-0.2971
44	C	1.2102	4.3190	-2.6095
45	C	2.1790	4.6155	-1.6453
46	H	2.6277	4.5893	0.4615
47	H	1.4384	4.4725	-3.6619
48	C	-0.2596	-1.1742	-4.6919
49	H	0.0825	-0.3132	-4.1044
50	H	0.5894	-1.8646	-4.7668
51	H	-0.5042	-0.8279	-5.7008

52	C	-2.4354	-3.1572	-0.5806
53	H	-1.5886	-3.8175	-0.3564
54	H	-2.2946	-2.2456	0.0149
55	H	-3.3547	-3.6511	-0.2518
56	C	-5.0675	-2.7446	-4.8838
57	H	-4.9011	-3.1690	-5.8812
58	H	-5.7733	-3.3913	-4.3519
59	H	-5.5545	-1.7705	-5.0273
60	C	1.8222	-2.5474	1.9455
61	H	2.4024	-3.3652	1.4982
62	H	1.8450	-2.6726	3.0314
63	H	0.7859	-2.6594	1.6134
64	C	2.4894	1.0945	-1.5236
65	H	2.6703	0.3203	-2.2785
66	H	1.4572	1.4394	-1.6558
67	H	3.1586	1.9350	-1.7226
68	C	4.2754	1.6868	3.1754
69	H	5.1767	1.1823	3.5472
70	H	4.5775	2.6596	2.7728
71	H	3.6290	1.8666	4.0440
72	C	0.3286	3.5951	1.5509
73	H	-0.5414	4.1634	1.9029
74	H	0.0916	2.5332	1.6855
75	H	1.1821	3.8435	2.1892
76	C	-1.0777	3.4658	-3.2998
77	H	-2.0242	3.9960	-3.1395
78	H	-0.7177	3.7039	-4.3054
79	H	-1.3034	2.3925	-3.2576
80	C	3.5353	5.1510	-2.0384
81	H	3.6553	5.1862	-3.1261
82	H	3.6903	6.1662	-1.6505
83	H	4.3418	4.5286	-1.6308
84	C	-4.1852	0.4883	-2.3843
85	H	-4.1807	1.5684	-2.5698
86	H	-3.1540	0.1356	-2.5066
87	H	-4.8039	0.0062	-3.1458
88	C	-4.2759	1.4256	2.6045
89	H	-4.7874	2.3966	2.6343
90	H	-4.5007	0.9035	3.5399
91	H	-3.1995	1.6164	2.5712
92	C	-6.9734	-2.4004	0.6752
93	H	-7.4444	-2.3870	1.6637
94	H	-7.7675	-2.4026	-0.0812
95	H	-6.4358	-3.3535	0.5786
96	Br	-0.9439	-0.1569	1.9382
97	C	-0.3732	-0.4884	4.0078
98	C	-0.5254	-1.7396	4.6027
99	C	0.3212	0.5292	4.6613
100	C	0.0208	-1.9736	5.8721
101	H	-1.0536	-2.5358	4.0812
102	C	0.8643	0.2950	5.9306
103	H	0.4521	1.4959	4.1784
104	C	0.7172	-0.9580	6.5359
105	H	-0.0957	-2.9490	6.3410
106	H	1.4055	1.0880	6.4438

107	H	1.1439	-1.1424	7.5188

large_basis_B-3-I_tetNiIPhIMes2_bb
Energy (POTENTIAL) = -2261.54374849 Eh

	Atom	X	Y	Z
1	C	1.1878	0.1037	0.3014
2	C	1.3745	1.1515	-0.5284
3	C	2.8594	-0.4877	-1.1517
4	N	2.0835	-0.8900	-0.0990
5	N	2.3831	0.7807	-1.4091
6	Ni	4.5715	-1.0526	-2.1463
7	C	4.5961	-2.8876	-2.7077
8	N	5.4491	-3.8112	-2.1416
9	N	4.2201	-3.4735	-3.8917
10	C	5.6231	-4.9117	-2.9820
11	C	4.8535	-4.7025	-4.0729
12	H	6.2559	-5.7389	-2.7005
13	H	4.6725	-5.3049	-4.9494
14	H	0.5071	-0.0487	1.1239
15	H	0.8986	2.1178	-0.5845
16	C	3.0991	-3.1032	-4.7280
17	C	1.8321	-3.5806	-4.3316
18	C	3.2766	-2.4217	-5.9413
19	C	0.7266	-3.2756	-5.1280
20	C	2.1359	-2.1538	-6.7122
21	C	0.8571	-2.5523	-6.3198
22	H	-0.2552	-3.6285	-4.8199
23	H	2.2617	-1.6195	-7.6513
24	C	5.8915	-3.8842	-0.7598
25	C	7.1105	-3.3219	-0.3423
26	C	5.1163	-4.6749	0.1113
27	C	7.4781	-3.4770	1.0002
28	C	5.5457	-4.8242	1.4334
29	C	6.7074	-4.2099	1.9065
30	H	8.4097	-3.0280	1.3363
31	H	4.9502	-5.4335	2.1078
32	C	1.9444	-2.1992	0.4872
33	C	0.8399	-2.9687	0.0741
34	C	2.7586	-2.5820	1.5623
35	C	0.5841	-4.1655	0.7495
36	C	2.4421	-3.7741	2.2244
37	C	1.3686	-4.5792	1.8327
38	H	-0.2584	-4.7770	0.4338
39	H	3.0560	-4.0779	3.0682
40	C	2.7677	1.6292	-2.5055
41	C	3.4258	2.8453	-2.2662
42	C	2.3787	1.2408	-3.8023
43	C	3.8009	3.6107	-3.3809
44	C	2.7736	2.0373	-4.8771
45	C	3.5090	3.2153	-4.6880
46	H	4.3366	4.5424	-3.2132
47	H	2.4961	1.7357	-5.8849
48	C	4.6241	-1.9788	-6.4454
49	H	4.8969	-1.0022	-6.0335
50	H	5.4152	-2.6748	-6.1612
51	H	4.6112	-1.8934	-7.5371

52	C	1.6750	-4.4367	-3.1025
53	H	0.6265	-4.7002	-2.9420
54	H	2.2488	-5.3669	-3.1940
55	H	2.0385	-3.9272	-2.2091
56	C	-0.3572	-2.1998	-7.1434
57	H	-0.0920	-1.9908	-8.1852
58	H	-1.0989	-3.0066	-7.1320
59	H	-0.8500	-1.3028	-6.7439
60	C	3.8539	-5.3600	-0.3443
61	H	4.0037	-5.9301	-1.2667
62	H	3.4923	-6.0477	0.4241
63	H	3.0629	-4.6316	-0.5350
64	C	8.0470	-2.6201	-1.2851
65	H	8.9681	-2.3347	-0.7682
66	H	8.3173	-3.2678	-2.1271
67	H	7.5955	-1.7158	-1.6942
68	C	7.1095	-4.3228	3.3564
69	H	8.1983	-4.3002	3.4766
70	H	6.7020	-3.4839	3.9368
71	H	6.7321	-5.2467	3.8087
72	C	3.6793	3.3916	-0.8818
73	H	3.6633	2.6204	-0.1117
74	H	4.6512	3.8924	-0.8351
75	H	2.9134	4.1381	-0.6287
76	C	1.5304	0.0165	-4.0188
77	H	0.6704	0.0043	-3.3385
78	H	1.1589	-0.0191	-5.0447
79	H	2.0991	-0.8969	-3.8349
80	C	3.9717	4.0256	-5.8740
81	H	3.1615	4.1755	-6.5979
82	H	4.3452	5.0090	-5.5702
83	H	4.7835	3.5098	-6.4039
84	C	-0.0769	-2.4957	-1.0290
85	H	0.4806	-2.1228	-1.8937
86	H	-0.7294	-3.3068	-1.3644
87	H	-0.7177	-1.6744	-0.6841
88	C	3.9360	-1.7491	1.9905
89	H	3.6943	-0.6818	2.0105
90	H	4.2848	-2.0469	2.9839
91	H	4.7683	-1.8706	1.2896
92	C	1.0921	-5.8891	2.5289
93	H	1.4333	-5.8716	3.5697
94	H	0.0240	-6.1330	2.5211
95	H	1.6173	-6.7136	2.0267
96	C	5.9313	-0.7838	-3.4913
97	C	5.8600	0.5414	-3.9675
98	C	6.8702	-1.6196	-4.1161
99	C	6.6721	1.0021	-5.0096
100	H	5.1742	1.2438	-3.5098
101	C	7.7084	-1.1634	-5.1399
102	H	6.9585	-2.6582	-3.8217
103	C	7.6112	0.1508	-5.5997
104	H	6.5804	2.0346	-5.3416
105	H	8.4269	-1.8467	-5.5894
106	H	8.2551	0.5072	-6.4004

107	I	6.0240	0.5453	-0.3672

large_basis_A-5-Cl_NiITMe2_ClPh_bb
Energy (POTENTIAL) = -1628.49916775 Eh

	Atom	X	Y	Z
1	C	-0.5890	0.3177	-0.2354
2	C	-0.1472	0.1934	-1.5209
3	C	-0.4380	2.4400	-1.1137
4	N	-0.7630	1.6838	-0.0130
5	N	-0.0631	1.4890	-2.0320
6	C	-1.2133	2.2464	1.2496
7	H	-1.3226	3.3242	1.1125
8	H	-2.1778	1.8161	1.5400
9	H	-0.4841	2.0556	2.0444
10	C	0.3753	1.7996	-3.3825
11	H	-0.3044	1.3629	-4.1228
12	H	0.3751	2.8868	-3.4879
13	H	1.3862	1.4163	-3.5590
14	C	0.2142	-1.0104	-2.3244
15	H	-0.3908	-1.0864	-3.2373
16	H	1.2674	-0.9909	-2.6342
17	H	0.0545	-1.9218	-1.7412
18	C	-0.8656	-0.7070	0.8127
19	H	-0.6399	-1.7091	0.4372
20	H	-0.2575	-0.5410	1.7117
21	H	-1.9176	-0.6957	1.1270
22	C	-0.4146	6.1745	-1.4184
23	N	0.6712	7.0015	-1.5813
24	N	-1.4600	7.0628	-1.3368
25	C	0.3151	8.3504	-1.5959
26	C	2.0387	6.5250	-1.7092
27	C	-1.0406	8.3894	-1.4413
28	C	-2.8462	6.6638	-1.1593
29	C	1.3176	9.4437	-1.7560
30	H	2.0128	5.4335	-1.6915
31	H	2.4787	6.8652	-2.6531
32	H	2.6554	6.8851	-0.8788
33	C	-1.9890	9.5387	-1.3727
34	H	-3.4599	7.0088	-1.9987
35	H	-2.8725	5.5727	-1.1156
36	H	-3.2529	7.0748	-0.2285
37	H	0.8275	10.4206	-1.7139
38	H	2.0780	9.4159	-0.9646
39	H	1.8463	9.3745	-2.7159
40	H	-2.7435	9.4933	-2.1690
41	H	-2.5284	9.5633	-0.4168
42	H	-1.4507	10.4850	-1.4770
43	Ni	-0.4405	4.3057	-1.2798
44	Cl	1.9336	4.5003	1.6035
45	C	3.1374	4.6094	2.8947
46	C	4.4606	4.2600	2.6220
47	C	2.7441	5.0450	4.1606
48	C	5.4077	4.3516	3.6450
49	H	4.7441	3.9240	1.6297
50	C	3.7033	5.1311	5.1729
51	H	1.7094	5.3121	4.3503

52	C	5.0334	4.7859	4.9193
53	H	6.4400	4.0814	3.4402
54	H	3.4046	5.4693	6.1614
55	H	5.7746	4.8548	5.7106

large_basis_TS-A-2-3-Cl_NiITMe2_OATS_PhCl_bb
Energy (POTENTIAL) = -1628.51976840 Eh

	Atom	X	Y	Z
1	C	-1.3353	1.0580	-0.3955
2	C	-0.0367	0.6441	-0.4385
3	C	-0.0911	2.5957	0.7570
4	N	-1.3404	2.2465	0.3417
5	N	0.6998	1.5964	0.2751
6	C	-2.5342	3.0301	0.6160
7	H	-3.3236	2.3902	1.0202
8	H	-2.2784	3.7887	1.3551
9	H	-2.8984	3.5172	-0.2954
10	C	2.1356	1.5122	0.4915
11	H	2.6770	1.6036	-0.4559
12	H	2.4282	2.3228	1.1581
13	H	2.3943	0.5567	0.9584
14	C	0.5991	-0.5477	-1.0705
15	H	1.3772	-0.2581	-1.7887
16	H	1.0704	-1.2014	-0.3252
17	H	-0.1482	-1.1388	-1.6069
18	C	-2.5808	0.4606	-0.9582
19	H	-2.3473	-0.4440	-1.5266
20	H	-3.2907	0.1849	-0.1676
21	H	-3.0969	1.1570	-1.6315
22	C	0.3285	5.5046	0.2393
23	N	1.1863	5.6435	-0.8096
24	N	-0.6614	6.3994	-0.0371
25	C	0.7404	6.5943	-1.7323
26	C	2.4049	4.8635	-0.9592
27	C	-0.4366	7.0773	-1.2393
28	C	-1.8084	6.6372	0.8249
29	C	1.4999	6.9299	-2.9711
30	H	2.2896	4.1045	-1.7409
31	H	3.2440	5.5166	-1.2155
32	C	-1.3757	8.1107	-1.7626
33	H	-2.7372	6.3372	0.3290
34	H	-1.6781	6.0490	1.7338
35	H	-1.8720	7.6972	1.0896
36	H	0.9585	7.6778	-3.5572
37	H	2.4921	7.3393	-2.7409
38	H	1.6506	6.0475	-3.6061
39	H	-2.3850	7.7044	-1.9073
40	H	-1.4638	8.9640	-1.0776
41	H	-1.0256	8.4902	-2.7266
42	Ni	0.4188	4.1981	1.7052
43	C	0.8453	3.7221	3.4513
44	C	0.7526	5.1698	3.5215
45	C	2.1166	3.1194	3.7481
46	C	1.9029	5.9271	3.9147
47	H	-0.2215	5.6422	3.6424
48	C	3.2167	3.8968	4.0303
49	H	2.1986	2.0362	3.7162
50	C	3.1169	5.3166	4.1323
51	H	1.7934	6.9997	4.0706

52	H	4.1820	3.4175	4.1852
53	H	3.9912	5.8997	4.4109
54	Cl	-0.6493	2.7046	4.5511
55	H	2.6109	4.3740	-0.0073

large_basis_TS-B-2-3-Cl_NiIMes2_oa_PhCl_bb
Energy (POTENTIAL) = -2710.31636386 Eh

	Atom	X	Y	Z
1	C	1.6911	2.2370	0.0220
2	C	2.6748	2.4934	-0.8609
3	C	2.3788	0.2009	-0.8254
4	N	1.5034	0.8543	0.0288
5	N	3.0856	1.2600	-1.3662
6	Ni	2.6609	-1.6796	-1.3298
7	C	4.3230	-2.9112	-1.2134
8	N	5.0517	-3.2248	-0.0862
9	N	4.7740	-3.8609	-2.1129
10	C	5.8951	-4.3171	-0.2783
11	C	5.7213	-4.7156	-1.5567
12	H	6.5376	-4.6849	0.5067
13	H	6.1752	-5.5101	-2.1283
14	H	1.0983	2.8907	0.6419
15	H	3.1221	3.4191	-1.1863
16	C	4.4874	-3.9283	-3.5193
17	C	3.7942	-5.0323	-4.0365
18	C	5.0246	-2.9326	-4.3536
19	C	3.5764	-5.0786	-5.4205
20	C	4.7675	-3.0132	-5.7240
21	C	4.0339	-4.0722	-6.2755
22	H	3.0245	-5.9202	-5.8336
23	H	5.1679	-2.2420	-6.3789
24	C	5.1963	-2.4297	1.1044
25	C	6.1019	-1.3556	1.0627
26	C	4.5820	-2.8377	2.2958
27	C	6.3143	-0.6285	2.2377
28	C	4.8467	-2.0958	3.4534
29	C	5.6884	-0.9788	3.4409
30	H	7.0039	0.2126	2.2182
31	H	4.3721	-2.3950	4.3851
32	C	0.4089	0.3173	0.7936
33	C	-0.9016	0.6849	0.4363
34	C	0.6670	-0.4566	1.9333
35	C	-1.9566	0.2144	1.2287
36	C	-0.4162	-0.8948	2.6977
37	C	-1.7363	-0.5802	2.3574
38	H	-2.9752	0.4780	0.9517
39	H	-0.2225	-1.5030	3.5789
40	C	4.0845	1.2296	-2.3993
41	C	5.3915	1.6350	-2.0779
42	C	3.6945	0.9784	-3.7279
43	C	6.3252	1.7361	-3.1170
44	C	4.6589	1.1095	-4.7307
45	C	5.9780	1.4821	-4.4471
46	H	7.3434	2.0357	-2.8777
47	H	4.3704	0.9135	-5.7612
48	C	5.9053	-1.8502	-3.7870
49	H	5.3350	-1.1556	-3.1669
50	H	6.6906	-2.2800	-3.1535
51	H	6.3839	-1.2822	-4.5871

52	C	3.3015	-6.1582	-3.1578
53	H	4.0527	-6.9558	-3.0840
54	H	3.0835	-5.8277	-2.1381
55	H	2.3921	-6.6035	-3.5739
56	C	3.7346	-4.1108	-7.7549
57	H	3.4541	-5.1171	-8.0839
58	H	2.9009	-3.4392	-8.0011
59	H	4.5968	-3.7842	-8.3481
60	C	3.6513	-4.0221	2.3277
61	H	4.1264	-4.9220	1.9195
62	H	3.3327	-4.2404	3.3517
63	H	2.7571	-3.8313	1.7230
64	C	6.8703	-1.0486	-0.1976
65	H	7.4355	-1.9274	-0.5319
66	H	6.2037	-0.7675	-1.0169
67	H	7.5799	-0.2339	-0.0342
68	C	5.9052	-0.1601	4.6906
69	H	5.7964	-0.7686	5.5952
70	H	6.8999	0.2995	4.7039
71	H	5.1700	0.6537	4.7561
72	C	5.7781	2.0133	-0.6677
73	H	5.4446	3.0309	-0.4277
74	H	5.3316	1.3456	0.0746
75	H	6.8646	1.9906	-0.5457
76	C	2.2806	0.5896	-4.0654
77	H	1.5562	1.2873	-3.6286
78	H	2.1293	0.5670	-5.1488
79	H	2.0486	-0.4004	-3.6653
80	C	7.0071	1.5612	-5.5481
81	H	7.8200	2.2504	-5.2946
82	H	7.4599	0.5763	-5.7296
83	H	6.5598	1.8897	-6.4931
84	C	-1.2006	1.5649	-0.7573
85	H	-0.4964	1.3977	-1.5772
86	H	-2.2111	1.3694	-1.1310
87	H	-1.1492	2.6291	-0.4938
88	C	2.0753	-0.8037	2.3133
89	H	2.6928	0.0930	2.4484
90	H	2.1019	-1.3830	3.2395
91	H	2.5440	-1.3934	1.5228
92	C	-2.8887	-1.1092	3.1770
93	H	-3.8010	-0.5245	3.0168
94	H	-3.1136	-2.1504	2.9089
95	H	-2.6578	-1.0960	4.2487
96	C	0.8962	-2.2317	-1.7591
97	C	-0.2516	-1.4560	-2.0932
98	C	1.4477	-3.0877	-2.7554
99	C	-0.6543	-1.3528	-3.4109
100	H	-0.7800	-0.9388	-1.3065
101	C	1.0212	-2.9542	-4.0952
102	H	2.0525	-3.9315	-2.4654
103	C	-0.0006	-2.0793	-4.4348
104	H	-1.4914	-0.7026	-3.6588
105	H	1.4741	-3.5894	-4.8509
106	H	-0.3358	-1.9938	-5.4652

107	Cl	0.6593	-3.2562	0.0263

large_basis_NiCODIMes_B-1x_NiCODIMes_bb
Energy (POTENTIAL) = -1406.00801396 Eh

	Atom	X	Y	Z
1	Ni	-0.0509	0.1322	0.1509
2	C	-1.9561	1.1564	0.1102
3	H	-2.5430	0.7136	0.9182
4	C	-0.9400	2.0193	0.4857
5	H	-0.8295	2.2227	1.5495
6	C	-0.1933	0.2241	-1.9419
7	H	-0.0872	-0.8017	-2.3054
8	C	0.9651	0.8438	-1.4618
9	H	1.9216	0.3334	-1.5696
10	C	-0.1795	2.9550	-0.4460
11	C	-2.5318	0.9549	-1.2779
12	C	-1.4574	0.9444	-2.3893
13	C	1.0757	2.3226	-1.1315
14	H	0.1589	3.8256	0.1285
15	H	-0.8610	3.3432	-1.2100
16	H	1.9337	2.4401	-0.4621
17	H	1.3087	2.9131	-2.0336
18	H	-1.2227	1.9681	-2.6990
19	H	-1.8720	0.4517	-3.2790
20	H	-3.0421	-0.0174	-1.2788
21	H	-3.3091	1.7053	-1.5044
22	C	0.9707	-0.5587	1.5843
23	N	0.5747	-1.6645	2.3067
24	N	2.1835	-0.2481	2.1541
25	C	1.5082	-2.0224	3.2792
26	C	-0.6833	-2.3089	2.0681
27	C	2.5226	-1.1290	3.1846
28	C	3.0111	0.8225	1.6832
29	H	1.3599	-2.8676	3.9339
30	C	-1.7859	-1.9572	2.8621
31	C	-0.7915	-3.2297	1.0117
32	H	3.4443	-1.0342	3.7382
33	C	3.9235	0.5676	0.6487
34	C	2.8707	2.0967	2.2545
35	C	-3.0156	-2.5678	2.5898
36	C	-1.6489	-0.9237	3.9522
37	C	-2.0400	-3.8132	0.7752
38	C	0.4021	-3.5555	0.1480
39	C	4.6976	1.6346	0.1775
40	C	4.0509	-0.8155	0.0607
41	C	3.6657	3.1327	1.7543
42	C	1.8778	2.3333	3.3642
43	C	-3.1615	-3.4973	1.5539
44	H	-3.8794	-2.3043	3.1962
45	H	-0.8951	-1.2135	4.6940
46	H	-1.3291	0.0388	3.5348
47	H	-2.5996	-0.7742	4.4729
48	H	-2.1401	-4.5297	-0.0376
49	H	1.2612	-3.8747	0.7502
50	H	0.1652	-4.3519	-0.5642
51	H	0.7191	-2.6676	-0.4137

52	C	4.5837	2.9210	0.7171
53	H	5.4019	1.4558	-0.6320
54	H	4.3926	-1.5381	0.8124
55	H	3.0835	-1.1756	-0.3073
56	H	4.7648	-0.8260	-0.7686
57	H	3.5627	4.1282	2.1809
58	H	2.1028	1.7159	4.2427
59	H	1.8779	3.3824	3.6754
60	H	0.8647	2.0671	3.0432
61	C	-4.4880	-4.1704	1.2922
62	C	5.4440	4.0552	0.2119
63	H	-4.4820	-5.2061	1.6584
64	H	-5.3100	-3.6478	1.7927
65	H	-4.7115	-4.2098	0.2197
66	H	6.2928	4.2359	0.8855
67	H	5.8525	3.8389	-0.7809
68	H	4.8762	4.9909	0.1513

large_basis_TS-C-5-6-Cl_NiIXy2_ClPh_spt_sps
Energy (POTENTIAL) = -2553.00094615 Eh

	Atom	X	Y	Z
1	C	-0.5015	1.0308	0.0868
2	C	0.5295	1.8151	-0.3102
3	C	1.2511	-0.3593	-0.4163
4	N	-0.0487	-0.2849	0.0187
5	N	1.5844	0.9556	-0.6128
6	Ni	2.3392	-1.8911	-0.6780
7	C	3.4299	-3.3497	-1.2072
8	N	4.7118	-3.6584	-0.8238
9	N	3.1091	-4.3745	-2.0584
10	C	5.1643	-4.8344	-1.4184
11	C	4.1529	-5.2883	-2.1970
12	H	6.1529	-5.2247	-1.2330
13	H	4.0704	-6.1594	-2.8284
14	H	-1.5037	1.2748	0.4036
15	H	0.6182	2.8862	-0.4072
16	C	1.8423	-4.5260	-2.7194
17	C	0.7851	-5.1316	-2.0204
18	C	1.7268	-4.1054	-4.0547
19	C	-0.4078	-5.3596	-2.7171
20	C	0.5114	-4.3392	-4.7097
21	C	-0.5421	-4.9751	-4.0514
22	H	-1.2360	-5.8382	-2.2021
23	H	0.3964	-4.0235	-5.7435
24	C	5.5054	-2.8641	0.0724
25	C	6.0219	-1.6417	-0.3881
26	C	5.7575	-3.3529	1.3657
27	C	6.7962	-0.8844	0.5001
28	C	6.5384	-2.5643	2.2197
29	C	7.0504	-1.3380	1.7940
30	H	7.2013	0.0664	0.1661
31	H	6.7402	-2.9181	3.2276
32	C	-0.8561	-1.4246	0.3538
33	C	-1.3498	-2.2289	-0.6863
34	C	-1.1379	-1.6788	1.7071
35	C	-2.1381	-3.3334	-0.3385
36	C	-1.9311	-2.7924	2.0093
37	C	-2.4243	-3.6164	0.9967
38	H	-2.5273	-3.9712	-1.1269
39	H	-2.1568	-3.0128	3.0496
40	C	2.8774	1.4154	-1.0389
41	C	3.8891	1.5598	-0.0753
42	C	3.0645	1.7442	-2.3915
43	C	5.1148	2.0905	-0.4951
44	C	4.3096	2.2603	-2.7714
45	C	5.3221	2.4448	-1.8287
46	H	5.9107	2.2198	0.2330
47	H	4.4802	2.5214	-3.8127
48	C	2.8695	-3.4014	-4.7431
49	H	3.1257	-2.4727	-4.2177
50	H	3.7773	-4.0162	-4.7601
51	H	2.6095	-3.1497	-5.7759

52	C	0.9252	-5.4743	-0.5605
53	H	1.8038	-6.1035	-0.3723
54	H	1.0574	-4.5585	0.0283
55	H	0.0387	-5.9990	-0.1922
56	C	5.1981	-4.6754	1.8272
57	H	5.7154	-5.5202	1.3546
58	H	5.3034	-4.7835	2.9106
59	H	4.1358	-4.7564	1.5789
60	C	5.7348	-1.1478	-1.7823
61	H	5.8738	-1.9397	-2.5275
62	H	4.6929	-0.8132	-1.8587
63	H	6.3839	-0.3077	-2.0413
64	C	3.6608	1.1223	1.3480
65	H	2.7897	1.6233	1.7888
66	H	3.4616	0.0446	1.3860
67	H	4.5343	1.3364	1.9706
68	C	1.9634	1.5208	-3.3981
69	H	1.0657	2.1023	-3.1556
70	H	2.2893	1.8032	-4.4038
71	H	1.6629	0.4658	-3.4173
72	C	-1.0205	-1.9318	-2.1264
73	H	-1.1379	-0.8664	-2.3561
74	H	0.0240	-2.1942	-2.3376
75	H	-1.6607	-2.5060	-2.8006
76	C	-0.5953	-0.7921	2.7995
77	H	-1.0892	0.1879	2.8075
78	H	-0.7453	-1.2507	3.7812
79	H	0.4769	-0.6218	2.6646
80	C	2.2938	-3.1223	3.7109
81	C	1.1590	-3.7235	4.2404
82	C	3.4208	-2.8734	4.4839
83	C	1.1535	-4.0888	5.5938
84	H	0.2887	-3.9056	3.6123
85	C	3.4117	-3.2419	5.8363
86	H	4.2974	-2.4035	4.0419
87	C	2.2786	-3.8481	6.3905
88	H	0.2726	-4.5607	6.0256
89	H	4.2871	-3.0551	6.4559
90	H	2.2725	-4.1325	7.4398
91	Cl	2.3065	-2.5685	1.7116
92	H	6.2802	2.8551	-2.1372
93	H	-1.4751	-5.1611	-4.5774
94	H	7.6531	-0.7376	2.4708
95	H	-3.0367	-4.4784	1.2492

large_basis_B-2-I_NiIMes2_eta2_PhI_fixCI_bb
Energy (POTENTIAL) = -2261.48146788 Eh

	Atom	X	Y	Z
1	C	0.4072	0.5732	0.0255
2	C	1.4047	0.8576	-0.8331
3	C	1.1193	-1.4392	-0.8658
4	N	0.2285	-0.8096	-0.0095
5	N	1.8313	-0.3596	-1.3623
6	Ni	1.3047	-3.3336	-1.4913
7	C	3.0162	-4.4950	-1.3574
8	N	3.7466	-4.8011	-0.2247
9	N	3.4478	-5.4771	-2.2358
10	C	4.5644	-5.9173	-0.3949
11	C	4.3802	-6.3382	-1.6629
12	H	5.2009	-6.2814	0.3966
13	H	4.8168	-7.1537	-2.2182
14	H	-0.2003	1.2065	0.6526
15	H	1.8540	1.7937	-1.1252
16	C	3.1489	-5.6003	-3.6353
17	C	2.4859	-6.7464	-4.1007
18	C	3.6489	-4.6258	-4.5169
19	C	2.2782	-6.8698	-5.4817
20	C	3.4030	-4.7846	-5.8826
21	C	2.7137	-5.8967	-6.3852
22	H	1.7510	-7.7459	-5.8532
23	H	3.7763	-4.0319	-6.5739
24	C	3.9411	-3.9883	0.9464
25	C	4.8852	-2.9501	0.8673
26	C	3.3557	-4.3662	2.1618
27	C	5.1552	-2.2174	2.0268
28	C	3.6699	-3.6155	3.3013
29	C	4.5468	-2.5273	3.2502
30	H	5.8754	-1.4036	1.9798
31	H	3.2130	-3.8885	4.2499
32	C	-0.8753	-1.3666	0.7274
33	C	-2.1830	-1.0326	0.3316
34	C	-0.6285	-2.1012	1.8954
35	C	-3.2467	-1.5053	1.1105
36	C	-1.7200	-2.5353	2.6511
37	C	-3.0373	-2.2596	2.2691
38	H	-4.2637	-1.2700	0.8037
39	H	-1.5352	-3.1153	3.5528
40	C	2.8366	-0.3501	-2.3897
41	C	4.1500	0.0080	-2.0470
42	C	2.4393	-0.5038	-3.7305
43	C	5.0921	0.1198	-3.0784
44	C	3.4089	-0.3610	-4.7253
45	C	4.7431	-0.0646	-4.4191
46	H	6.1183	0.3760	-2.8238
47	H	3.1148	-0.4852	-5.7653
48	C	4.4775	-3.4769	-4.0053
49	H	3.8835	-2.8016	-3.3860
50	H	5.3050	-3.8398	-3.3836
51	H	4.8978	-2.9024	-4.8337

52	C	2.0060	-7.8363	-3.1704
53	H	2.7710	-8.6135	-3.0419
54	H	1.7635	-7.4569	-2.1735
55	H	1.1131	-8.3219	-3.5772
56	C	2.4326	-6.0214	-7.8634
57	H	3.2972	-5.7140	-8.4636
58	H	2.1731	-7.0490	-8.1392
59	H	1.5918	-5.3785	-8.1569
60	C	2.4330	-5.5550	2.2397
61	H	2.9803	-6.4929	2.0780
62	H	1.9496	-5.6139	3.2197
63	H	1.6532	-5.5042	1.4741
64	C	5.6356	-2.6986	-0.4159
65	H	6.1553	-3.6076	-0.7436
66	H	4.9617	-2.4074	-1.2254
67	H	6.3826	-1.9114	-0.2874
68	C	4.8286	-1.7006	4.4817
69	H	4.1354	-0.8511	4.5507
70	H	4.7117	-2.2896	5.3981
71	H	5.8442	-1.2894	4.4658
72	C	4.5304	0.3359	-0.6239
73	H	4.1850	1.3410	-0.3499
74	H	4.0865	-0.3615	0.0911
75	H	5.6164	0.3201	-0.4979
76	C	1.0011	-0.7748	-4.0767
77	H	0.3461	0.0195	-3.6953
78	H	0.8628	-0.8440	-5.1597
79	H	0.6618	-1.7090	-3.6258
80	C	5.7780	0.0241	-5.5140
81	H	6.6738	0.5598	-5.1821
82	H	6.0938	-0.9786	-5.8342
83	H	5.3820	0.5338	-6.4002
84	C	-2.4625	-0.1674	-0.8760
85	H	-1.7493	-0.3495	-1.6841
86	H	-3.4699	-0.3581	-1.2600
87	H	-2.4051	0.8989	-0.6218
88	C	0.7791	-2.4264	2.2976
89	H	1.3808	-1.5205	2.4425
90	H	0.8031	-3.0075	3.2229
91	H	1.2705	-3.0046	1.5116
92	C	-4.1991	-2.7967	3.0694
93	H	-5.1092	-2.2093	2.9060
94	H	-4.4215	-3.8337	2.7828
95	H	-3.9802	-2.7985	4.1434
96	C	-0.5191	-3.9255	-1.8039
97	C	-1.6265	-3.1328	-2.2590
98	C	0.2602	-4.6586	-2.7713
99	C	-1.8130	-2.9105	-3.6026
100	H	-2.3009	-2.7070	-1.5282
101	C	0.0171	-4.4007	-4.1586
102	H	0.7043	-5.6085	-2.5126
103	C	-0.9718	-3.5352	-4.5686
104	H	-2.6198	-2.2575	-3.9295
105	H	0.5890	-4.9570	-4.8935
106	H	-1.1475	-3.3632	-5.6279

107	I	-1.0399	-5.1760	0.0195

large_basis_A-2-Cl_NiITMe2_eta2_PhCl_bb
Energy (POTENTIAL) = -1628.52099082 Eh

	Atom	X	Y	Z
1	C	-1.6510	0.8726	0.0118
2	C	-0.3965	0.6479	-0.4731
3	C	-0.3227	2.5917	0.7384
4	N	-1.5771	2.0594	0.7494
5	N	0.3931	1.7077	-0.0145
6	C	-2.7079	2.6666	1.4327
7	H	-2.3257	3.4583	2.0766
8	H	-3.4207	3.0839	0.7127
9	H	-3.2186	1.9255	2.0537
10	C	1.8107	1.8532	-0.3048
11	H	1.9725	2.0534	-1.3699
12	H	2.1924	2.6881	0.2830
13	H	2.3528	0.9442	-0.0267
14	C	0.1538	-0.4507	-1.3184
15	H	0.6051	-0.0636	-2.2411
16	H	0.9304	-1.0209	-0.7917
17	H	-0.6391	-1.1494	-1.5997
18	C	-2.9152	0.0935	-0.1274
19	H	-2.7577	-0.7749	-0.7731
20	H	-3.2760	-0.2712	0.8432
21	H	-3.7184	0.6986	-0.5673
22	C	0.3780	5.5603	0.1839
23	N	1.4894	6.0227	-0.4578
24	N	-0.6409	6.2319	-0.4228
25	C	1.1738	6.9523	-1.4534
26	C	2.8431	5.5922	-0.1405
27	C	-0.1840	7.0862	-1.4305
28	C	-2.0411	6.0588	-0.0708
29	C	2.2135	7.6119	-2.2950
30	H	3.2565	4.9804	-0.9496
31	H	3.4898	6.4606	0.0156
32	C	-1.1072	7.9348	-2.2380
33	H	-2.5792	5.5226	-0.8604
34	H	-2.0861	5.4818	0.8531
35	H	-2.5174	7.0309	0.0875
36	H	1.7451	8.2685	-3.0336
37	H	2.8973	8.2227	-1.6912
38	H	2.8242	6.8781	-2.8365
39	H	-1.8730	7.3321	-2.7428
40	H	-1.6311	8.6716	-1.6150
41	H	-0.5516	8.4818	-3.0048
42	Ni	0.3182	4.2004	1.5961
43	C	0.7998	3.6363	3.3201
44	C	0.8111	5.0925	3.4147
45	C	2.0723	2.9587	3.4256
46	C	2.0472	5.7688	3.6822
47	H	-0.1115	5.6157	3.6652
48	C	3.2418	3.6648	3.5757
49	H	2.0863	1.8735	3.3587
50	C	3.2399	5.0867	3.7292
51	H	2.0225	6.8423	3.8662

52	H	4.1892	3.1286	3.5909
53	H	4.1755	5.6110	3.9074
54	Cl	-0.5794	2.7040	4.4153
55	H	2.8095	5.0071	0.7795

large_basis_D-4-Cl_trans-NiClPhIPhen2_bb
Energy (POTENTIAL) = -2238.44772474 Eh

	Atom	X	Y	Z
1	C	-0.5475	1.4817	-0.1426
2	C	0.5598	2.2536	-0.1924
3	C	1.2528	0.0753	-0.1080
4	N	-0.1112	0.1558	-0.0862
5	N	1.6487	1.3843	-0.1649
6	Ni	2.4233	-1.4595	-0.2974
7	C	3.6113	-2.9096	-0.7915
8	N	4.9698	-3.0202	-0.6914
9	N	3.2558	-4.0038	-1.5331
10	C	5.4433	-4.1472	-1.3680
11	C	4.3649	-4.7652	-1.8965
12	H	6.4898	-4.4080	-1.3717
13	H	4.2718	-5.6802	-2.4598
14	H	-1.5954	1.7345	-0.1063
15	H	0.6835	3.3248	-0.2079
16	C	1.9293	-4.2923	-1.9741
17	C	0.8605	-4.1990	-1.0805
18	C	1.7196	-4.6454	-3.3104
19	C	-0.4308	-4.4608	-1.5394
20	C	0.4247	-4.9125	-3.7551
21	C	-0.6535	-4.8178	-2.8716
22	H	-1.2622	-4.3842	-0.8493
23	H	0.2605	-5.1787	-4.7956
24	C	5.8732	-2.1427	-0.0056
25	C	6.9568	-1.6150	-0.7144
26	C	5.7319	-1.9124	1.3639
27	C	7.9272	-0.8758	-0.0359
28	C	6.7061	-1.1683	2.0322
29	C	7.8112	-0.6626	1.3405
30	H	8.7727	-0.4697	-0.5839
31	H	6.6038	-0.9940	3.0997
32	C	-1.0527	-0.9238	-0.0165
33	C	-2.0430	-1.0109	-0.9999
34	C	-1.0443	-1.7979	1.0716
35	C	-3.0528	-1.9665	-0.8748
36	C	-2.0559	-2.7537	1.1843
37	C	-3.0684	-2.8312	0.2231
38	H	-3.8260	-2.0322	-1.6352
39	H	-2.0559	-3.4314	2.0336
40	C	3.0018	1.8208	-0.2931
41	C	3.9948	1.2702	0.5192
42	C	3.3146	2.7829	-1.2576
43	C	5.3149	1.6911	0.3547
44	C	4.6366	3.2025	-1.4062
45	C	5.6400	2.6550	-0.6028
46	H	6.0881	1.2619	0.9800
47	H	4.8812	3.9443	-2.1614
48	C	2.5231	-0.9669	-2.1409
49	C	1.4427	-1.1863	-3.0157
50	C	3.6786	-0.3727	-2.6820
51	C	1.5118	-0.8350	-4.3685

52	H	0.5326	-1.6437	-2.6348
53	C	3.7528	-0.0117	-4.0320
54	H	4.5338	-0.1844	-2.0369
55	C	2.6690	-0.2437	-4.8847
56	H	0.6601	-1.0252	-5.0197
57	H	4.6593	0.4520	-4.4178
58	H	2.7250	0.0333	-5.9351
59	Cl	2.3032	-2.0790	1.9853
60	H	6.6716	2.9747	-0.7231
61	H	8.5720	-0.0952	1.8693
62	H	-1.6634	-5.0184	-3.2186
63	H	-3.8592	-3.5697	0.3232
64	H	-0.2557	-1.7213	1.8106
65	H	-2.0227	-0.3289	-1.8447
66	H	2.5352	3.1726	-1.9046
67	H	3.7342	0.5167	1.2556
68	H	4.8713	-2.3145	1.8851
69	H	1.0429	-3.9135	-0.0492
70	H	7.0371	-1.7936	-1.7825
71	H	2.5578	-4.6786	-3.9994

large_basis_TS-D-2-3-Cl_NiIPhen_oats_PhCl_bb
Energy (POTENTIAL) = -2238.36769712 Eh

	Atom	X	Y	Z
1	C	-0.8550	-0.7360	0.1365
2	C	-0.0119	-0.4479	-0.8806
3	C	-0.8054	-2.5689	-1.2350
4	N	-1.3410	-2.0260	-0.0908
5	N	0.0028	-1.5702	-1.7072
6	Ni	-1.0024	-4.3190	-1.9565
7	C	0.7155	-5.2482	-1.6297
8	N	1.4577	-5.4146	-0.4861
9	N	1.3987	-6.0167	-2.5425
10	C	2.5392	-6.2720	-0.6783
11	C	2.5056	-6.6464	-1.9766
12	H	3.2280	-6.5079	0.1179
13	H	3.1698	-7.2668	-2.5574
14	H	-1.1319	-0.1613	1.0055
15	H	0.5671	0.4350	-1.1029
16	C	1.0848	-6.1461	-3.9311
17	C	1.0978	-7.4130	-4.5234
18	C	0.8319	-5.0050	-4.6917
19	C	0.8722	-7.5298	-5.8953
20	C	0.5988	-5.1330	-6.0606
21	C	0.6259	-6.3908	-6.6677
22	H	0.8816	-8.5129	-6.3576
23	H	0.3982	-4.2425	-6.6485
24	C	1.1894	-4.8272	0.7929
25	C	1.3131	-3.4490	0.9710
26	C	0.8465	-5.6598	1.8617
27	C	1.0619	-2.8968	2.2278
28	C	0.6064	-5.1008	3.1178
29	C	0.7071	-3.7187	3.3004
30	H	1.1425	-1.8225	2.3642
31	H	0.3301	-5.7435	3.9486
32	C	-2.2664	-2.6678	0.7892
33	C	-3.2621	-1.9061	1.4091
34	C	-2.1736	-4.0376	1.0422
35	C	-4.1610	-2.5205	2.2813
36	C	-3.0818	-4.6457	1.9072
37	C	-4.0772	-3.8921	2.5332
38	H	-4.9377	-1.9244	2.7524
39	H	-3.0000	-5.7125	2.0975
40	C	0.7268	-1.6307	-2.9426
41	C	2.1092	-1.8264	-2.9262
42	C	0.0388	-1.4672	-4.1471
43	C	2.8104	-1.8596	-4.1336
44	C	0.7471	-1.4985	-5.3496
45	C	2.1316	-1.6937	-5.3440
46	H	3.8849	-2.0188	-4.1272
47	H	0.2161	-1.3721	-6.2887
48	C	-2.6588	-4.3704	-2.7901
49	C	-2.7295	-3.9887	-4.1709
50	C	-2.4665	-5.7673	-2.4910
51	C	-2.6467	-4.9352	-5.1679

52	H	-2.8553	-2.9383	-4.4162
53	C	-2.4493	-6.7228	-3.5520
54	H	-2.6522	-6.1341	-1.4821
55	C	-2.5256	-6.3198	-4.8668
56	H	-2.6593	-4.6167	-6.2086
57	H	-2.3975	-7.7818	-3.3038
58	H	-2.4853	-7.0463	-5.6735
59	Cl	-4.3570	-3.4523	-1.8306
60	H	-4.7823	-4.3683	3.2089
61	H	-1.3950	-4.6190	0.5673
62	H	-3.3576	-0.8478	1.1878
63	H	-1.0357	-1.3211	-4.1321
64	H	2.6215	-1.9611	-1.9782
65	H	2.6794	-1.7222	-6.2817
66	H	0.4490	-6.4850	-7.7356
67	H	0.8167	-4.0376	-4.2087
68	H	1.2776	-8.2937	-3.9141
69	H	0.5087	-3.2835	4.2757
70	H	0.7561	-6.7297	1.6982
71	H	1.5927	-2.8210	0.1330

large_basis_ITMe_ITMe_bb
Energy (POTENTIAL) = -383.575486154 Eh

	Atom	X	Y	Z
1	C	-0.1703	8.1023	0.2226
2	N	0.1801	8.9000	-0.8318
3	N	-0.5524	9.0269	1.1554
4	C	0.0238	10.2667	-0.5724
5	C	0.6652	8.3804	-2.0993
6	C	-0.4461	10.3483	0.7058
7	C	-1.0219	8.6730	2.4847
8	C	0.3433	11.3249	-1.5749
9	H	0.7023	7.2924	-2.0290
10	H	-0.0019	8.6641	-2.9212
11	H	1.6695	8.7598	-2.3190
12	C	-0.8148	11.5246	1.5466
13	H	-1.0249	7.5850	2.5655
14	H	-0.3637	9.0884	3.2563
15	H	-2.0371	9.0490	2.6537
16	H	0.1331	12.3174	-1.1656
17	H	1.4011	11.3018	-1.8689
18	H	-0.2491	11.2087	-2.4920
19	H	-1.8737	11.5016	1.8365
20	H	-0.2266	11.5653	2.4729
21	H	-0.6398	12.4564	1.0005

large_basis_NiIMes2_distort_NiIMes2_eta2_PhBr_bb_NiL2frag
Energy (POTENTIAL) = -2018.31733565 Eh

	Atom	X	Y	Z
1	C	0.4076	0.5604	0.0000
2	C	1.4062	0.8473	-0.8561
3	C	1.1334	-1.4530	-0.8813
4	N	0.2338	-0.8234	-0.0308
5	N	1.8405	-0.3697	-1.3792
6	Ni	1.3266	-3.3446	-1.4900
7	C	3.0322	-4.4894	-1.3712
8	N	3.7701	-4.7919	-0.2420
9	N	3.4684	-5.4701	-2.2513
10	C	4.5957	-5.9025	-0.4151
11	C	4.4102	-6.3240	-1.6825
12	H	5.2368	-6.2626	0.3745
13	H	4.8502	-7.1363	-2.2399
14	H	-0.2039	1.1934	0.6235
15	H	1.8518	1.7846	-1.1496
16	C	3.1621	-5.5927	-3.6481
17	C	2.5087	-6.7425	-4.1173
18	C	3.6449	-4.6070	-4.5279
19	C	2.2851	-6.8543	-5.4973
20	C	3.3821	-4.7537	-5.8914
21	C	2.6958	-5.8669	-6.3962
22	H	1.7641	-7.7333	-5.8708
23	H	3.7410	-3.9916	-6.5801
24	C	3.9496	-3.9870	0.9355
25	C	4.8993	-2.9529	0.8798
26	C	3.3358	-4.3670	2.1358
27	C	5.1519	-2.2294	2.0491
28	C	3.6345	-3.6275	3.2865
29	C	4.5199	-2.5450	3.2591
30	H	5.8761	-1.4182	2.0205
31	H	3.1571	-3.9025	4.2243
32	C	-0.8775	-1.3726	0.7021
33	C	-2.1801	-1.0174	0.3083
34	C	-0.6433	-2.1159	1.8664
35	C	-3.2505	-1.4644	1.0934
36	C	-1.7402	-2.5301	2.6244
37	C	-3.0527	-2.2224	2.2514
38	H	-4.2635	-1.2075	0.7903
39	H	-1.5634	-3.1129	3.5262
40	C	2.8446	-0.3566	-2.4069
41	C	4.1574	0.0039	-2.0648
42	C	2.4458	-0.5069	-3.7477
43	C	5.0976	0.1233	-3.0972
44	C	3.4131	-0.3558	-4.7435
45	C	4.7466	-0.0554	-4.4382
46	H	6.1233	0.3822	-2.8432
47	H	3.1179	-0.4765	-5.7836
48	C	4.4774	-3.4609	-4.0161
49	H	3.8907	-2.7930	-3.3821
50	H	5.3137	-3.8286	-3.4093
51	H	4.8855	-2.8780	-4.8446

52	C	2.0561	-7.8532	-3.1981
53	H	2.8113	-8.6483	-3.1402
54	H	1.8763	-7.5047	-2.1776
55	H	1.1329	-8.3084	-3.5719
56	C	2.3974	-5.9793	-7.8720
57	H	3.2591	-5.6782	-8.4796
58	H	2.1234	-7.0022	-8.1514
59	H	1.5612	-5.3248	-8.1526
60	C	2.3950	-5.5436	2.1808
61	H	2.9268	-6.4844	1.9881
62	H	1.9138	-5.6246	3.1603
63	H	1.6132	-5.4554	1.4193
64	C	5.6716	-2.6954	-0.3894
65	H	6.2113	-3.5980	-0.7026
66	H	5.0092	-2.4178	-1.2135
67	H	6.4042	-1.8969	-0.2493
68	C	4.7837	-1.7292	4.5019
69	H	4.0887	-0.8809	4.5689
70	H	4.6543	-2.3266	5.4111
71	H	5.7990	-1.3171	4.5042
72	C	4.5375	0.3293	-0.6411
73	H	4.1858	1.3313	-0.3634
74	H	4.0985	-0.3731	0.0722
75	H	5.6237	0.3200	-0.5162
76	C	1.0082	-0.7841	-4.0922
77	H	0.3501	0.0072	-3.7098
78	H	0.8689	-0.8534	-5.1753
79	H	0.6737	-1.7204	-3.6412
80	C	5.7791	0.0423	-5.5346
81	H	6.6727	0.5818	-5.2027
82	H	6.1000	-0.9577	-5.8585
83	H	5.3789	0.5526	-6.4185
84	C	-2.4484	-0.1683	-0.9132
85	H	-1.7466	-0.3887	-1.7220
86	H	-3.4632	-0.3428	-1.2854
87	H	-2.3621	0.9019	-0.6856
88	C	0.7589	-2.4597	2.2688
89	H	1.3688	-1.5619	2.4296
90	H	0.7747	-3.0543	3.1858
91	H	1.2457	-3.0303	1.4754
92	C	-4.2223	-2.7243	3.0640
93	H	-5.1217	-2.1229	2.8925
94	H	-4.4666	-3.7622	2.7994
95	H	-4.0008	-2.7099	4.1377

large_basis_C-2-Cl_NiIXy2_e2PhCl_bb
Energy (POTENTIAL) = -2552.99589044 Eh

	Atom	X	Y	Z
1	C	1.1287	1.4178	-0.0033
2	C	2.1291	1.7064	-0.8564
3	C	1.8799	-0.5984	-0.8642
4	N	0.9695	0.0323	-0.0222
5	N	2.5781	0.4889	-1.3664
6	Ni	2.0810	-2.5035	-1.4183
7	C	3.7587	-3.6502	-1.2862
8	N	4.4968	-3.9542	-0.1559
9	N	4.2045	-4.6278	-2.1679
10	C	5.3312	-5.0588	-0.3313
11	C	5.1513	-5.4771	-1.6000
12	H	5.9727	-5.4174	0.4587
13	H	5.5984	-6.2844	-2.1591
14	H	0.5090	2.0509	0.6118
15	H	2.5682	2.6452	-1.1549
16	C	3.8988	-4.7528	-3.5642
17	C	3.2472	-5.9088	-4.0272
18	C	4.3729	-3.7592	-4.4395
19	C	3.0160	-6.0214	-5.4060
20	C	4.1047	-3.9021	-5.8048
21	C	3.4261	-5.0229	-6.2871
22	H	2.4983	-6.9004	-5.7819
23	H	4.4525	-3.1372	-6.4945
24	C	4.6699	-3.1579	1.0284
25	C	5.6166	-2.1200	0.9785
26	C	4.0437	-3.5509	2.2195
27	C	5.8651	-1.4034	2.1549
28	C	4.3399	-2.8256	3.3811
29	C	5.2278	-1.7511	3.3474
30	H	6.5834	-0.5878	2.1375
31	H	3.8604	-3.1056	4.3154
32	C	-0.1307	-0.5231	0.7221
33	C	-1.4398	-0.1816	0.3309
34	C	0.1252	-1.2648	1.8832
35	C	-2.5019	-0.6387	1.1224
36	C	-0.9622	-1.6989	2.6487
37	C	-2.2685	-1.3920	2.2724
38	H	-3.5201	-0.3975	0.8273
39	H	-0.7750	-2.2821	3.5469
40	C	3.6045	0.5096	-2.3719
41	C	4.9082	0.8698	-1.9895
42	C	3.2319	0.3637	-3.7204
43	C	5.8728	1.0057	-2.9976
44	C	4.2198	0.5329	-4.6966
45	C	5.5326	0.8416	-4.3394
46	H	6.8916	1.2658	-2.7215
47	H	3.9519	0.4206	-5.7441
48	C	5.1964	-2.6090	-3.9239
49	H	4.6017	-1.9428	-3.2951
50	H	6.0294	-2.9716	-3.3098
51	H	5.6075	-2.0251	-4.7497

52	C	2.8069	-7.0211	-3.1041
53	H	3.5648	-7.8143	-3.0564
54	H	2.6373	-6.6750	-2.0812
55	H	1.8810	-7.4776	-3.4694
56	C	3.0788	-4.7083	2.2378
57	H	3.5633	-5.6400	1.9207
58	H	2.6713	-4.8628	3.2416
59	H	2.2440	-4.5327	1.5503
60	C	6.3853	-1.8500	-0.2901
61	H	6.9343	-2.7456	-0.6068
62	H	5.7194	-1.5764	-1.1129
63	H	7.1095	-1.0445	-0.1467
64	C	5.2491	1.1774	-0.5520
65	H	4.8799	2.1714	-0.2688
66	H	4.8001	0.4604	0.1401
67	H	6.3320	1.1769	-0.4010
68	C	1.8066	0.0613	-4.0918
69	H	1.1220	0.8234	-3.6979
70	H	1.6838	0.0163	-5.1783
71	H	1.4926	-0.8958	-3.6693
72	C	-1.7197	0.6466	-0.9012
73	H	-1.0345	0.3993	-1.7163
74	H	-2.7427	0.4757	-1.2518
75	H	-1.6166	1.7199	-0.6981
76	C	1.5352	-1.5779	2.2832
77	H	2.1148	-0.6660	2.4747
78	H	1.5614	-2.1950	3.1844
79	H	2.0485	-2.1099	1.4800
80	C	0.1967	-3.1906	-1.5272
81	C	-0.9348	-2.4339	-1.9826
82	C	1.0274	-3.8915	-2.4811
83	C	-1.0892	-2.1597	-3.3188
84	H	-1.6510	-2.0795	-1.2529
85	C	0.8049	-3.5781	-3.8675
86	H	1.4235	-4.8707	-2.2402
87	C	-0.1891	-2.7186	-4.2736
88	H	-1.9141	-1.5332	-3.6501
89	H	1.4098	-4.0821	-4.6123
90	H	-0.3258	-2.5053	-5.3313
91	Cl	-0.1038	-4.0903	0.0544
92	H	5.4384	-1.1940	4.2568
93	H	3.2275	-5.1220	-7.3511
94	H	6.2905	0.9615	-5.1094
95	H	-3.1049	-1.7378	2.8746

large_basis_A-3-I_cis-NiIPhITMe2
Energy (POTENTIAL) = -1179.75532412 Eh

	Atom	X	Y	Z
1	C	0.2456	0.4304	-0.8432
2	C	1.2277	-0.0589	-0.0313
3	C	-0.0922	-1.8175	-0.6429
4	N	-0.5445	-0.6652	-1.2032
5	N	0.9939	-1.4334	0.0746
6	Ni	-0.7879	-3.6368	-0.9688
7	C	0.7659	-4.0804	-1.9375
8	N	1.7666	-4.9121	-1.5522
9	N	1.1451	-3.6295	-3.1597
10	C	2.7706	-4.9858	-2.5243
11	C	2.3776	-4.1708	-3.5443
12	C	-1.8618	-5.5659	-2.8691
13	C	-2.4003	-6.7773	-3.3204
14	C	-1.4751	-5.3654	-1.5276
15	C	-2.5473	-7.8507	-2.4375
16	H	-2.6966	-6.8856	-4.3627
17	C	-1.6370	-6.4681	-0.6635
18	C	-2.1577	-7.6900	-1.1036
19	H	-2.9568	-8.7974	-2.7826
20	H	-1.3657	-6.3662	0.3857
21	H	-2.2678	-8.5161	-0.4028
22	C	-1.7486	-0.5609	-2.0151
23	H	-1.5082	-0.1670	-3.0074
24	H	-2.1887	-1.5535	-2.1090
25	H	-2.4735	0.0997	-1.5304
26	C	-0.0489	1.8133	-1.3160
27	H	-0.0371	1.8773	-2.4117
28	H	-1.0372	2.1526	-0.9801
29	H	0.6954	2.5153	-0.9306
30	C	2.3538	0.6209	0.6705
31	H	3.3266	0.2072	0.3756
32	H	2.3576	1.6887	0.4355
33	H	2.2714	0.5195	1.7602
34	C	1.8163	-2.3526	0.8472
35	H	1.2399	-3.2612	1.0151
36	H	2.7384	-2.5983	0.3097
37	H	2.0698	-1.9069	1.8121
38	C	1.7744	-5.6918	-0.3226
39	H	1.7547	-6.7608	-0.5535
40	H	2.6693	-5.4647	0.2642
41	H	0.8866	-5.4377	0.2541
42	C	0.3903	-2.6719	-3.9546
43	H	0.8669	-1.6866	-3.9280
44	H	0.3274	-3.0144	-4.9904
45	H	-0.6142	-2.5982	-3.5418
46	C	3.9814	-5.8372	-2.3497
47	H	4.5619	-5.5402	-1.4667
48	H	3.7167	-6.8948	-2.2254
49	H	4.6331	-5.7559	-3.2237
50	C	3.0258	-3.8366	-4.8446
51	H	2.4084	-4.1466	-5.6974
52	H	3.2044	-2.7583	-4.9437
53	H	3.9900	-4.3452	-4.9280
54	H	-1.7355	-4.7554	-3.5862
55	I	-2.8426	-3.1804	0.7004

large_basis_A-4-I_trans-NiIPhITMe2
Energy (POTENTIAL) = -1179.76388985 Eh

	Atom	X	Y	Z
1	C	-0.6806	2.1774	1.0101
2	C	0.2331	2.1254	-0.0023
3	C	-0.0988	4.3220	0.5053
4	N	-0.8646	3.5330	1.2993
5	N	0.5727	3.4512	-0.2890
6	C	-1.7755	4.0375	2.3152
7	H	-1.6190	5.1128	2.4085
8	H	-2.8144	3.8411	2.0317
9	H	-1.5695	3.5629	3.2788
10	C	1.5217	3.8512	-1.3166
11	H	1.1272	3.6290	-2.3130
12	H	1.6897	4.9247	-1.2239
13	H	2.4717	3.3274	-1.1776
14	C	0.8411	0.9723	-0.7258
15	H	0.6555	1.0290	-1.8060
16	H	1.9284	0.9329	-0.5811
17	H	0.4212	0.0307	-0.3617
18	C	-1.3992	1.1009	1.7498
19	H	-1.1332	0.1198	1.3471
20	H	-1.1463	1.1057	2.8179
21	H	-2.4880	1.2140	1.6710
22	C	-0.1357	8.1723	0.2576
23	N	0.6203	8.9527	-0.5543
24	N	-0.9976	9.0368	0.8493
25	C	0.2400	10.2959	-0.4788
26	C	1.6886	8.4510	-1.4052
27	C	-0.7901	10.3495	0.4148
28	C	-2.0101	8.6449	1.8174
29	C	0.9169	11.3618	-1.2717
30	H	1.8472	7.3979	-1.1698
31	H	1.4194	8.5529	-2.4613
32	H	2.6143	9.0014	-1.2141
33	C	-1.5980	11.4943	0.9239
34	H	-3.0133	8.8260	1.4196
35	H	-1.8882	7.5812	2.0236
36	H	-1.8824	9.2059	2.7478
37	H	0.4319	12.3272	-1.1033
38	H	1.9743	11.4638	-0.9955
39	H	0.8789	11.1494	-2.3477
40	H	-2.6683	11.3541	0.7260
41	H	-1.4786	11.6230	2.0074
42	H	-1.2860	12.4242	0.4408
43	Ni	-0.0646	6.2503	0.4388
44	I	1.8516	6.3834	2.3922
45	C	-1.3913	6.1462	-0.9176
46	C	-1.0489	6.1474	-2.2837
47	C	-2.7613	6.0600	-0.6026
48	C	-2.0225	6.0613	-3.2858
49	H	-0.0032	6.2182	-2.5749
50	C	-3.7410	5.9774	-1.5989
51	H	-3.0731	6.0547	0.4397
52	C	-3.3766	5.9760	-2.9487
53	H	-1.7220	6.0627	-4.3323
54	H	-4.7914	5.9129	-1.3195
55	H	-4.1354	5.9106	-3.7249

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