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ELECTRONIC SUPPLEMENTARY INFORMATION

Role of Solvent on phophatase activity of a dinuclear Nickel(II) complex of a Schiff-base ligand: mechanistic interpretation by DFT studies

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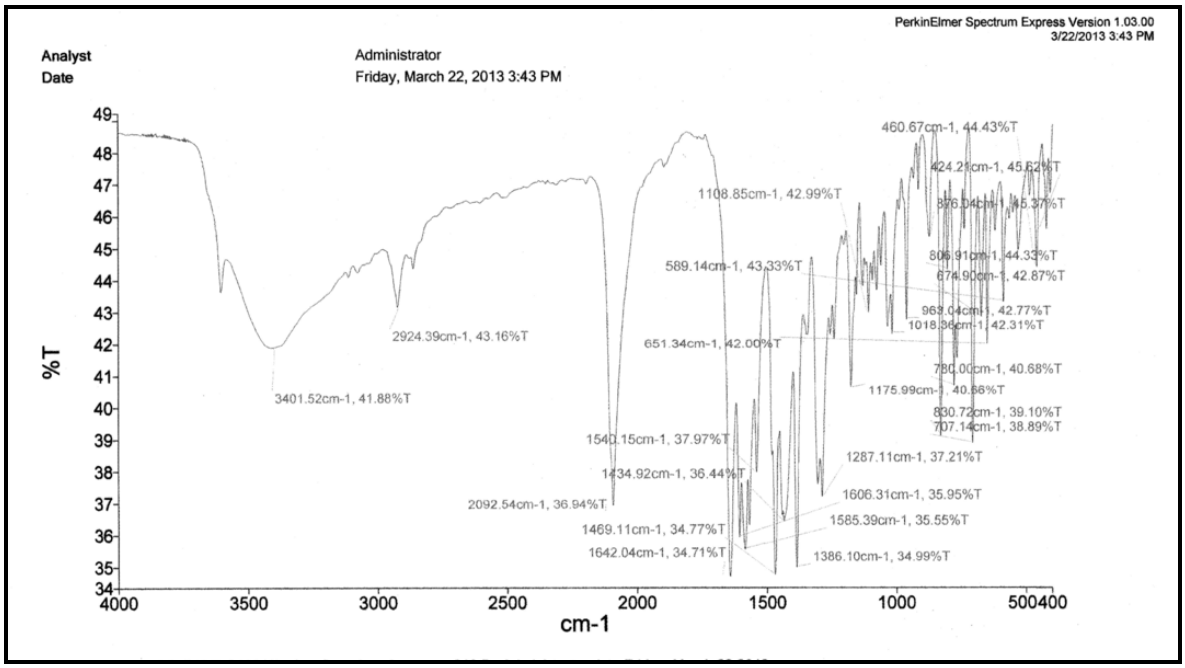

Fig. S1 FT-IR spectrum of complex at 298 K.

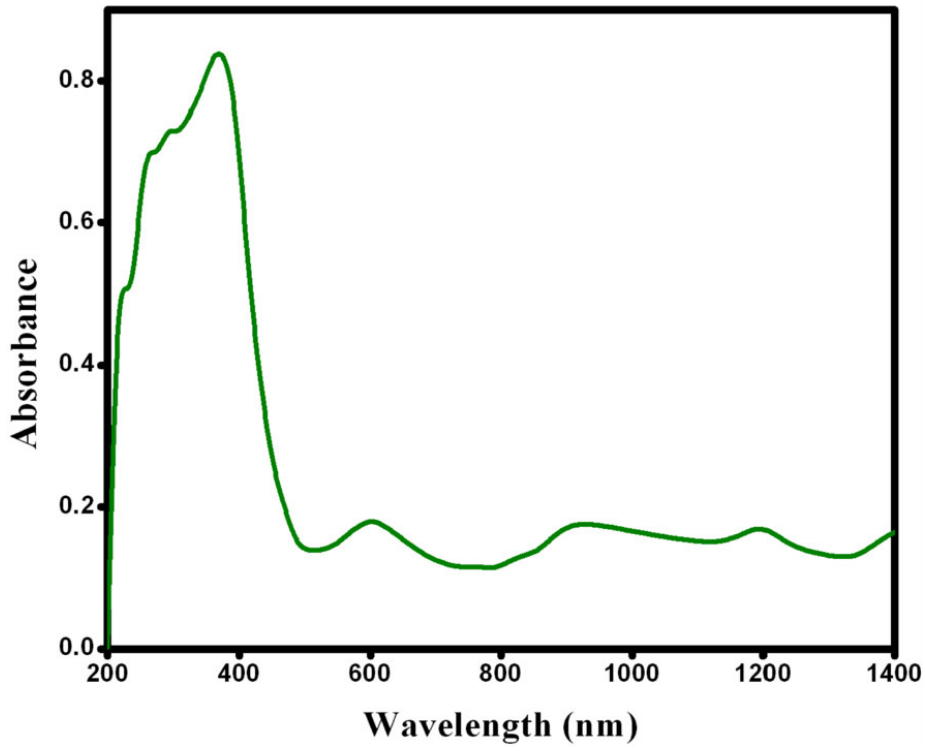

Fig. S2 Absorption spectra of complex in the solid phase at 298K.

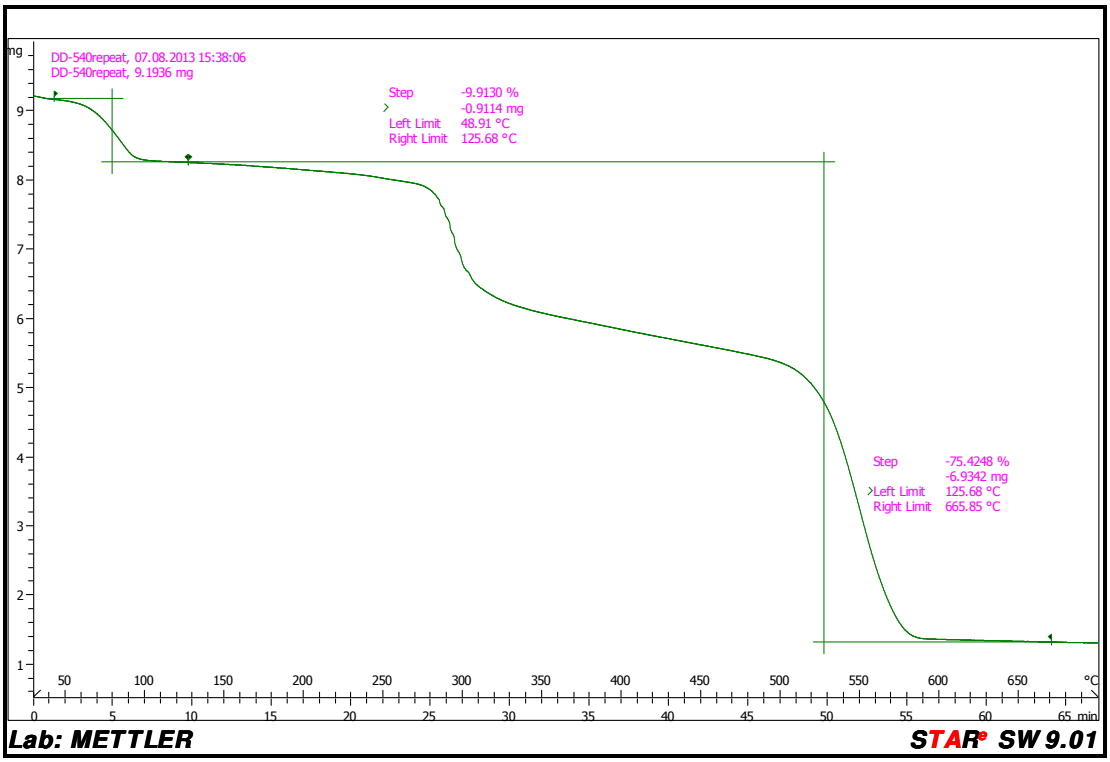

Fig. S3 TGA curve of complex from 30°C – 700°C.

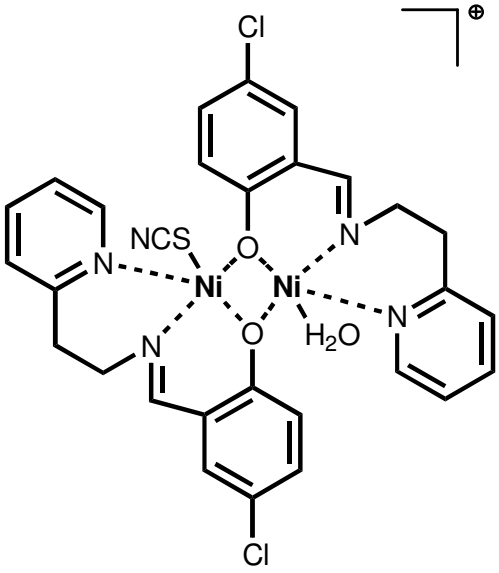

Fig. S4 Solution-state structure of the complex in acetonitrile and DMF.

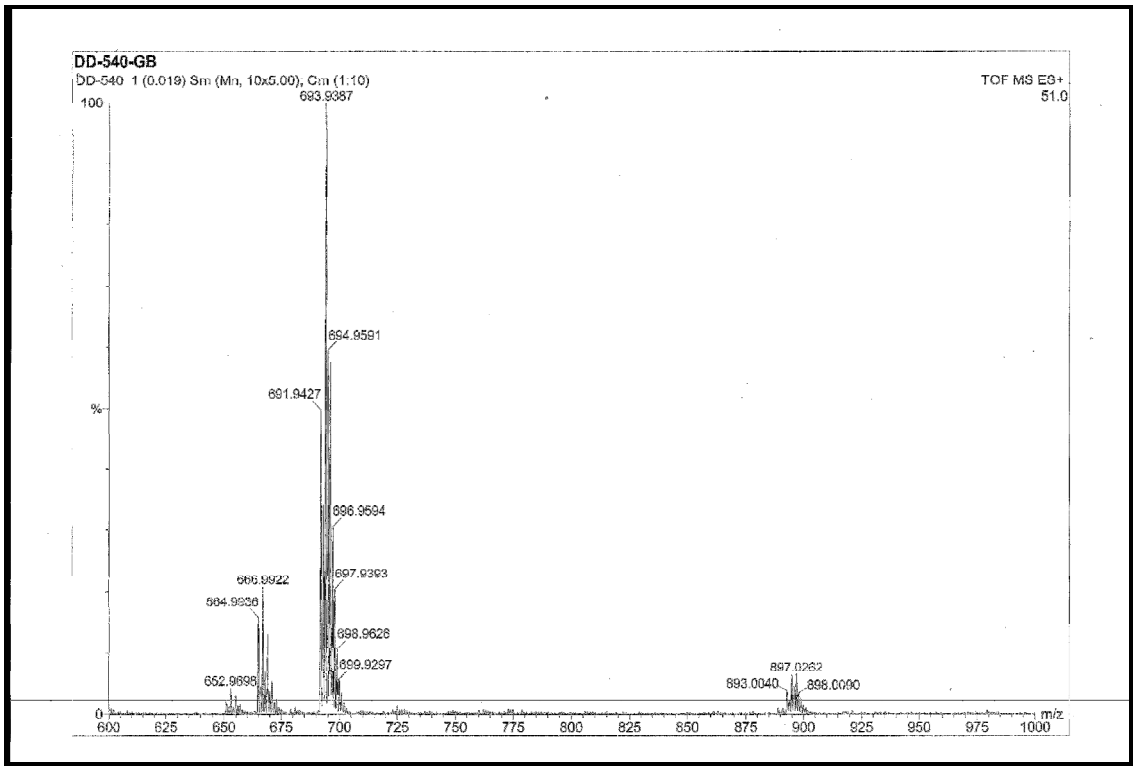

Fig. S5 ESI-MS of complex in acetonitrile.

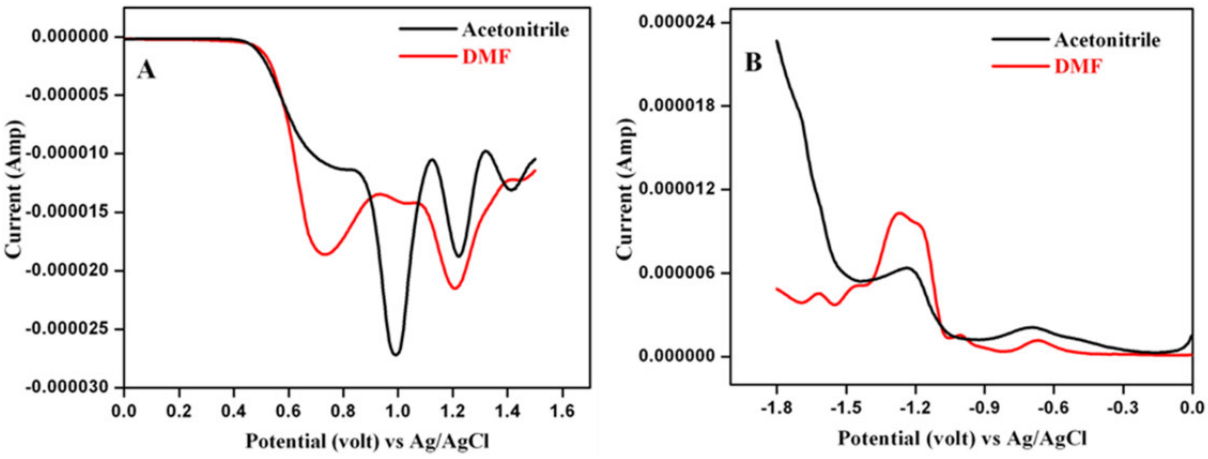

Fig. S6 Differential Pulse Voltammogram of complex in acetonitrile and DMF.

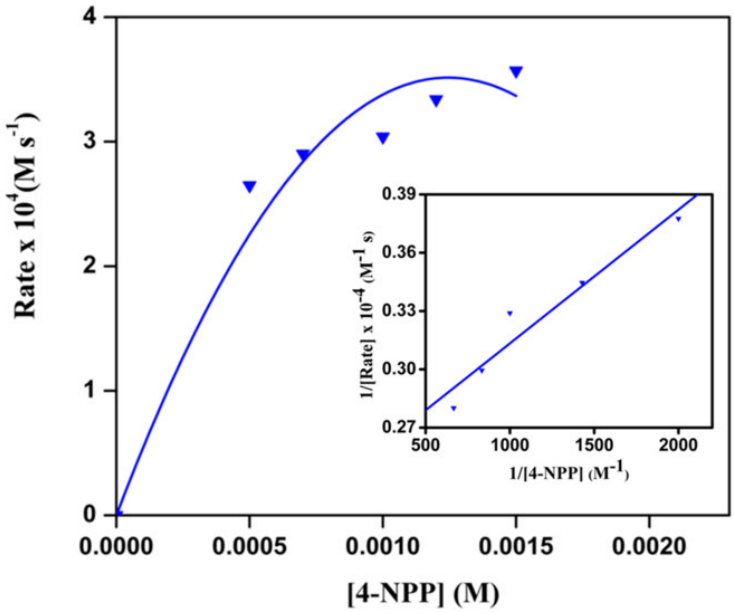

Fig. S7 Kinetic plot of V vs S for phosphatase activity where V = initial rate and [S] = [4-NPP].

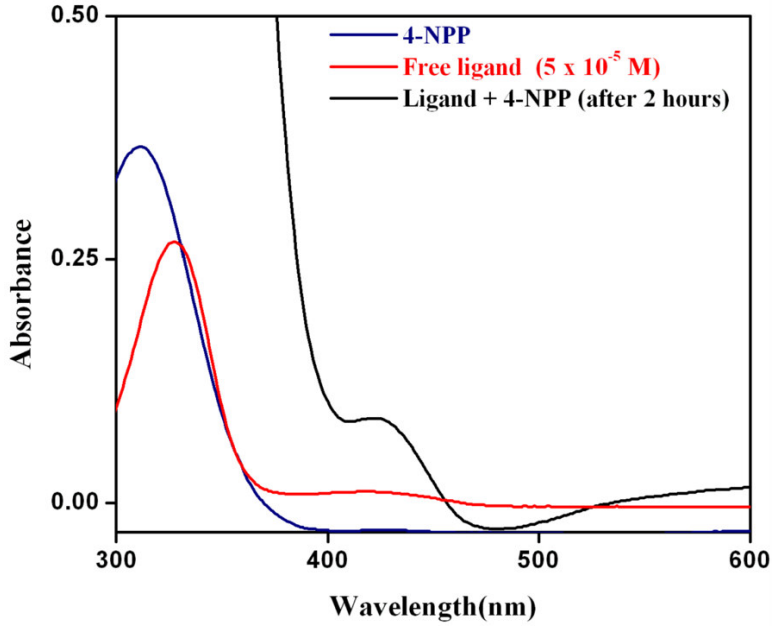

Fig. S8 Control experiment of phosphatase activity with free ligand HL. Conditions: [4-NPP]=1 × 10^{-3} (M), [HL]=5 × 10^{-5} (M), Temperature=298 K.

Table S1 Selected Coordination Bond Lengths (Å) and Angles (deg) with Esds in Parentheses.

Ni(1)-O(1)	2.076(5)	Ni(2)-O(2)	2.063(5)
Ni(1)-N(1)	2.067(6)	Ni(2)-N(3)	2.081(6)

Ni(1)-N(2)	2.132(6)	Ni(2)-N(4)	2.137(7)
Ni(1)-O(2)	2.106(4)	Ni(2)-O(1)	2.198(5)
Ni(1)-O(5)	2.059(5)	Ni(2)-O(4)	2.076(5)
Ni(1)-O(3)	2.166(6)	Ni(2)-N(5)	2.054(6)
O(5)-Ni(1)-N(1)	177.3(2)	N(5)-Ni(2)-O(2)	92.5(2)
O(5)-Ni(1)-O(1)	87.94(19)	N(5)-Ni(2)-O(4)	88.3(2)
N(1)-Ni(1)-O(1)	90.0(2)	O(2)-Ni(2)-O(4)	88.0(2)
O(5)-Ni(1)-O(2)	88.24(19)	N(5)-Ni(2)-N(3)	90.9(2)
N(1)-Ni(1)-O(2)	93.4(2)	O(2)-Ni(2)-N(3)	90.8(2)
O(1)-Ni(1)-O(2)	84.97(18)	O(4)-Ni(2)-N(3)	178.5(2)
O(5)-Ni(1)-N(2)	89.0(2)	N(5)-Ni(2)-N(4)	93.3(2)
N(1)-Ni(1)-N(2)	92.9(2)	O(2)-Ni(2)-N(4)	173.6(2)
O(1)-Ni(1)-N(2)	176.1(2)	O(4)-Ni(2)-N(4)	89.6(3)
O(2)-Ni(1)-N(2)	97.48(19)	N(3)-Ni(2)-N(4)	91.7(3)
O(5)-Ni(1)-O(3)	84.0(2)	N(5)-Ni(2)-O(1)	174.1(2)
N(1)-Ni(1)-O(3)	94.1(2)	O(2)-Ni(2)-O(1)	82.95(17)
O(1)-Ni(1)-O(3)	88.0(2)	O(4)-Ni(2)-O(1)	87.71(18)
O(2)-Ni(1)-O(3)	169.7(2)	N(3)-Ni(2)-O(1)	93.01(19)
N(2)-Ni(1)-O(3)	89.2(2)	N(4)-Ni(2)-O(1)	91.1(2)

Cartesian coordinates of optimized structures.

RC1-1

Ni	2.81258	-1.0596	0.79713
Ni	-1.95099	1.38318	-0.90715
Cl	8.04312	1.79244	-3.35513
Cl	-0.69624	7.11362	3.35418
O	3.13242	0.20748	-0.51815
O	-0.77572	2.07116	0.32643
N	4.60585	-1.73053	0.76033
N	2.2601	-2.22179	2.29505
N	-3.23211	2.78654	-0.65099
N	-2.99194	0.51216	-2.35306
C	4.23851	0.52318	-1.11378
C	4.23005	1.59456	-2.0551
H	3.28741	2.10424	-2.22599
C	5.37687	1.97091	-2.7203
H	5.35355	2.79094	-3.43148
C	6.59258	1.29164	-2.48522
C	6.64637	0.24855	-1.59106
H	7.58128	-0.27604	-1.41499
C	5.4789	-0.1483	-0.89022
C	5.55647	-1.24994	0.00996
H	6.52788	-1.75088	0.06126
C	4.94188	-2.91707	1.55954
H	5.15251	-2.6023	2.591
H	5.85294	-3.376	1.15855
C	3.80839	-3.94891	1.54776
H	3.45401	-4.09979	0.51717
H	4.19265	-4.90631	1.91531
C	2.68232	-3.49885	2.43342
C	2.1271	-4.33395	3.40736
H	2.47185	-5.36028	3.47991

C	1.15201	-3.84178	4.26941
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C	0.75853	-2.51044	4.14558
H	0.01149	-2.07293	4.79867
C	1.32426	-1.73745	3.1394
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C	0.3107	3.53376	1.7931
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C	0.33304	4.71441	2.50207
H	1.18719	4.96347	3.12428
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C	-1.84753	5.32687	1.64592
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C	-3.03867	3.82427	0.11888
H	-3.85618	4.5484	0.1863
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H	-5.25643	3.34593	-0.78102
C	-5.07501	1.26849	-1.34031
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C	-5.01953	-0.29997	-3.3313
H	-6.1033	-0.34598	-3.30261
C	-4.29871	-0.97428	-4.31379
H	-4.81459	-1.56329	-5.06647
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H	-2.30061	-1.36747	-5.06107
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RC1-2

Ni	-2.29629	-1.46175	-0.07226
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O	2.85469	1.01895	-0.05085
N	-3.84827	-2.50107	-0.45317

N	-1.75045	-1.76533	-1.89348
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H	-2.12946	-5.08322	-1.88226
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C	-1.04922	-2.20266	-4.52892
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C	-0.96337	4.74043	2.82278
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C	-2.20294	4.10236	2.77528
H	-3.05757	4.52653	3.29482
C	-2.32717	2.92862	2.03721
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O	1.45642	-1.7408	0.6097
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O	6.50305	-3.66714	3.82306
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H	-1.76248	-1.54952	2.31771

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Ni	-1.52948	0.1049	-2.15056
Ni	0.9211	-0.56863	1.66511
Cl	-7.733	-2.49018	1.02843
Cl	1.1172	6.48606	3.13392
O	-2.41399	-0.12866	0.02869
O	1.78412	0.98364	1.14321
N	-3.30604	0.06552	-2.83668
N	-1.70717	2.03401	-2.13993
N	0.52731	0.10665	3.40651
N	-0.01366	-2.25832	1.99695
C	-3.56045	-0.64528	0.19637
C	-3.97674	-1.10301	1.50352
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H	-5.48034	-1.99246	2.74244
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C	2.10015	3.29192	0.87513
H	2.58588	3.08797	-0.07321
C	1.94363	4.58213	1.33635
H	2.31222	5.4201	0.75254
C	1.30505	4.8256	2.57232
C	0.84213	3.77866	3.33577
H	0.3677	3.96679	4.29478
C	0.97927	2.44576	2.87224
C	0.56562	1.37153	3.71483

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C	0.17286	-0.82651	4.48769
H	-0.91903	-0.93895	4.52557
H	0.50257	-0.41065	5.44675
C	0.81756	-2.20303	4.28081
H	0.72499	-2.78473	5.20354
H	1.88945	-2.07669	4.07883
C	0.13743	-2.93696	3.15514
C	-0.38793	-4.21966	3.31069
H	-0.24128	-4.7458	4.24856
C	-1.10125	-4.80104	2.263
H	-1.51472	-5.79998	2.36876
C	-1.29057	-4.07085	1.09326
H	-1.8616	-4.46224	0.25897
C	-0.72833	-2.80194	0.99137
H	-0.86111	-2.20324	0.10174
O	1.0965	-1.94507	-2.42281
P	1.3277	-0.77644	-1.40674
O	0.30503	0.35009	-1.58985
O	1.47346	-1.34308	0.0206
O	2.76343	-0.07993	-1.83111
C	3.99788	-0.63961	-1.6779
C	4.21335	-2.01918	-1.52997
C	5.08341	0.24956	-1.71022
C	5.51128	-2.49839	-1.40145
H	3.37372	-2.7035	-1.52516
C	6.37958	-0.22764	-1.58612
H	4.8857	1.30913	-1.83123
C	6.58341	-1.60244	-1.42819
H	5.70278	-3.55825	-1.28657
H	7.2298	0.44289	-1.60521
N	7.94465	-2.11109	-1.28958
O	8.87657	-1.29961	-1.32823
O	8.10027	-3.32801	-1.13849
O	-1.30844	-1.78556	-2.38352
H	-1.86837	-2.11838	-3.09902
H	-0.04541	-1.99996	-2.53518

RC2

Ni	-1.47725	0.34329	-2.20559
Ni	0.81917	-0.7932	1.37768
Cl	-7.27543	-2.81436	1.24874
Cl	0.55122	5.91566	4.01042
O	-2.18984	-0.06238	0.04291
O	1.59027	0.87468	1.14768
N	-3.29865	0.22367	-2.75121
N	-1.79444	2.25539	-2.0306
N	0.33663	-0.44057	3.19056
N	0.02524	-2.58311	1.39627
C	-3.28869	-0.65943	0.25343
C	-3.58666	-1.2149	1.55581
H	-2.81966	-1.0921	2.31524
C	-4.76342	-1.8607	1.8459
H	-4.94382	-2.26593	2.83791
C	-5.76179	-1.99097	0.85221
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H	-6.34147	-1.55917	-1.15151
C	-4.3411	-0.81896	-0.7476
C	-4.29438	-0.27593	-2.06882
H	-5.26279	-0.27246	-2.58519
C	-3.58768	0.86673	-4.03701
H	-4.63357	1.20016	-4.05865

H	-3.44829	0.1479	-4.85592
C	-2.6482	2.07176	-4.29121
H	-1.68294	1.69563	-4.65291
H	-3.07439	2.69349	-5.08584
C	-2.3848	2.90222	-3.05838
C	-2.69316	4.25931	-2.95668
H	-3.16623	4.76725	-3.79122
C	-2.37759	4.94613	-1.78329
H	-2.60884	6.00355	-1.69037
C	-1.7621	4.26027	-0.73749
H	-1.49629	4.75614	0.18992
C	-1.48749	2.90436	-0.89858
H	-1.02476	2.3022	-0.12685
C	1.33625	1.96089	1.80904
C	1.77467	3.20965	1.28049
H	2.2952	3.19713	0.32868
C	1.53127	4.39291	1.94696
H	1.86505	5.33634	1.52568
C	0.84975	4.38794	3.18337
C	0.43049	3.20259	3.74301
H	-0.07853	3.19911	4.70269
C	0.65783	1.97769	3.06714
C	0.28756	0.75536	3.70315
H	-0.04532	0.83865	4.74229
C	0.0108	-1.55748	4.09092
H	-1.07008	-1.74869	4.05435
H	0.26971	-1.28078	5.11939
C	0.76426	-2.83462	3.70053
H	0.68296	-3.56213	4.51446
H	1.83008	-2.60389	3.5719
C	0.1819	-3.42335	2.44262
C	-0.25227	-4.74693	2.37443
H	-0.10404	-5.40121	3.22759
C	-0.87869	-5.20505	1.21613
H	-1.2218	-6.23351	1.14791
C	-1.07087	-4.3164	0.16273
H	-1.57326	-4.61323	-0.75118
C	-0.60275	-3.01066	0.28186
H	-0.73497	-2.29858	-0.5239
O	1.38197	-1.41448	-2.89205
P	1.43613	-0.41623	-1.65093
O	0.38988	0.68509	-1.77033
O	1.47716	-1.24428	-0.35737
O	2.87382	0.35286	-1.84691
C	4.11138	-0.17941	-1.61351
C	4.37992	-1.55621	-1.64171
C	5.1405	0.74337	-1.37624
C	5.67661	-2.00334	-1.41722
H	3.58418	-2.2629	-1.84279
C	6.43618	0.29897	-1.1565
H	4.9014	1.80119	-1.36695
C	6.69268	-1.07557	-1.1747
H	5.91016	-3.06082	-1.43376
H	7.24471	0.99441	-0.96828
N	8.05332	-1.55127	-0.93565
O	8.93662	-0.71059	-0.73506
O	8.25391	-2.77056	-0.94363
O	-1.1333	-1.4713	-2.60632
H	-1.8568	-1.82991	-3.13902
H	0.37872	-1.61607	-3.01079

TS1

Ni	1.44409	2.20669	-0.36991
Ni	-0.86975	-1.54378	1.29212
Cl	8.13411	-0.57546	-0.08825
Cl	3.54595	-5.50125	-2.84973
O	2.35811	0.55377	-0.45499
O	-0.40572	-1.85131	-0.46673
N	2.91683	3.11335	0.42288
N	0.56146	3.92416	-0.84744
N	-0.07178	-3.15931	1.90431
N	-1.53212	-1.03143	3.0766
C	3.63583	0.35688	-0.38046
C	4.16677	-0.91873	-0.74066
H	3.4702	-1.67063	-1.09494
C	5.51623	-1.18876	-0.65707
H	5.89707	-2.1642	-0.94482
C	6.41266	-0.20084	-0.1965
C	5.94918	1.04082	0.17149
H	6.63945	1.7977	0.53385
C	4.56769	1.34449	0.07764
C	4.11779	2.62534	0.51956
H	4.87005	3.25034	1.01237
C	2.68827	4.42718	1.05538
H	3.08979	5.21399	0.4004
H	3.24139	4.46399	2.0007
C	1.20325	4.68798	1.34446
H	0.78105	3.79292	1.83993
H	1.11226	5.56442	1.99455
C	0.44939	4.90696	0.06972
C	-0.31717	6.04766	-0.1981
H	-0.40451	6.81901	0.5604
C	-0.95903	6.17393	-1.42655
H	-1.55963	7.05228	-1.6457
C	-0.81393	5.15681	-2.37462
H	-1.28527	5.21656	-3.34994
C	-0.04517	4.04603	-2.04419
H	0.07532	3.20874	-2.72186
C	0.48385	-2.66071	-0.94544
C	0.84464	-2.55305	-2.32025
H	0.38125	-1.76175	-2.89929
C	1.76685	-3.4097	-2.88123
H	2.04012	-3.31046	-3.92719
C	2.37194	-4.42147	-2.1001
C	2.04625	-4.56681	-0.77255
H	2.50542	-5.35034	-0.17649
C	1.10488	-3.68961	-0.17325
C	0.72709	-3.89792	1.18238
H	1.1381	-4.79187	1.66052
C	-0.39077	-3.65216	3.25026
H	0.25501	-3.15092	3.98342
H	-0.18634	-4.72783	3.30146
C	-1.86021	-3.39228	3.60259
H	-2.13606	-3.99688	4.47267
H	-2.49533	-3.7153	2.76675
C	-2.07845	-1.9363	3.92166
C	-2.74594	-1.53109	5.07661
H	-3.18431	-2.28023	5.72833
C	-2.82831	-0.17281	5.38262
H	-3.34747	0.15651	6.27867
C	-2.21572	0.74142	4.53205
H	-2.22313	1.80638	4.73878
C	-1.58124	0.28652	3.37694
H	-1.07491	0.97324	2.68287

O	-2.10629	2.46555	0.2005
P	-1.37945	1.10557	-0.33316
O	-0.09273	1.30371	-1.13002
O	-1.76748	0.00481	0.64839
O	-2.36929	0.8023	-1.68276
C	-3.64852	0.35191	-1.67641
C	-4.50755	0.40125	-0.56232
C	-4.12145	-0.15646	-2.90081
C	-5.81409	-0.05628	-0.67907
H	-4.14947	0.78787	0.38237
C	-5.42513	-0.61147	-3.01929
H	-3.44004	-0.18605	-3.74455
C	-6.26664	-0.55903	-1.90224
H	-6.48989	-0.02501	0.167
H	-5.7992	-1.00786	-3.95527
N	-7.63855	-1.03696	-2.01609
O	-8.01855	-1.46612	-3.11204
O	-8.35905	-0.99147	-1.01134
O	0.19234	1.82648	1.55493
H	0.81901	1.11642	1.77571
H	-2.19173	3.10945	-0.5222

IM

Ni	-2.66102	-1.75243	-0.31869
Ni	1.77703	1.18553	0.78588
Cl	-7.31457	3.28094	2.11098
Cl	-1.35223	6.23787	-3.35768
O	-2.76301	0.00703	0.30822
O	0.47355	1.44551	-0.48162
N	-4.50122	-2.128	0.11648
N	-2.35704	-3.51225	-1.17061
N	2.58753	2.89345	0.45222
N	3.07705	0.70391	2.20585
C	-3.79547	0.68931	0.69015
C	-3.62855	2.06893	1.01231
H	-2.63512	2.49228	0.90252
C	-4.68997	2.8399	1.43293
H	-4.54486	3.89077	1.66643
C	-5.97676	2.27164	1.56323
C	-6.18456	0.94516	1.2697
H	-7.17374	0.50794	1.37523
C	-5.10701	0.13574	0.82452
C	-5.3489	-1.24433	0.56491
H	-6.36242	-1.59445	0.78377
C	-5.00509	-3.50149	-0.00732
H	-5.32393	-3.67925	-1.04385
H	-5.88252	-3.62942	0.6373
C	-3.93548	-4.5298	0.37921
H	-3.46632	-4.22581	1.3236
H	-4.41136	-5.50242	0.5425
C	-2.90163	-4.65774	-0.70647
C	-2.55697	-5.89518	-1.2542
H	-3.00258	-6.79856	-0.84951
C	-1.6522	-5.95344	-2.31243
H	-1.37278	-6.90836	-2.74533
C	-1.11869	-4.76433	-2.80142
H	-0.41097	-4.75213	-3.62352
C	-1.48462	-3.56541	-2.19918
H	-1.05023	-2.61799	-2.49164
C	0.11529	2.52185	-1.09873
C	-1.04878	2.4792	-1.92306
H	-1.57897	1.53483	-1.98061

C	-1.4801	3.60198	-2.59473
H	-2.37276	3.56133	-3.21153
C	-0.7669	4.81887	-2.48824
C	0.37181	4.89817	-1.72329
H	0.9252	5.83076	-1.6546
C	0.8307	3.75557	-1.01591
C	2.0489	3.8274	-0.28612
H	2.6043	4.76573	-0.37867
C	3.90736	3.20025	1.02007
H	3.78369	3.58376	2.04214
H	4.38593	3.98617	0.42566
C	4.81217	1.96372	1.04388
H	5.84806	2.27464	1.21537
H	4.77811	1.46379	0.06764
C	4.38928	1.02173	2.13723
C	5.29839	0.53895	3.08203
H	6.34787	0.79456	2.98483
C	4.84781	-0.26209	4.12763
H	5.54583	-0.6451	4.86649
C	3.48736	-0.55336	4.20912
H	3.08157	-1.16159	5.00995
C	2.63748	-0.0614	3.22547
H	1.5826	-0.30088	3.20324
O	0.84603	-3.14215	0.49563
P	0.25094	-1.60112	0.32507
O	-0.86759	-1.37006	-0.74769
O	0.91687	-0.46145	1.17863
O	1.45095	-1.43772	-1.05922
C	2.76941	-1.42292	-1.01384
C	3.5604	-1.95591	0.03975
C	3.44242	-0.83361	-2.12037
C	4.94232	-1.87548	-0.00564
H	3.06878	-2.44185	0.87124
C	4.82189	-0.75493	-2.16654
H	2.8334	-0.43786	-2.92678
C	5.57699	-1.26506	-1.09721
H	5.54693	-2.28381	0.79577
H	5.32956	-0.29733	-3.00757
N	7.01519	-1.14275	-1.11071
O	7.55776	-0.63016	-2.10264
O	7.65359	-1.53998	-0.12094
O	-0.86767	-2.02215	1.63286
H	-1.16408	-1.19722	2.0484
H	0.38984	-3.52523	1.26489

TS2

Ni	-2.80547	-1.48056	-0.44811
Ni	1.84236	0.71881	0.98083
Cl	-6.85258	4.12221	1.74596
Cl	-0.14662	6.4565	-2.95954
O	-2.70857	0.3393	-0.05169
O	0.87117	1.21758	-0.49045
N	-4.53726	-1.6927	0.34901
N	-2.79583	-3.28106	-1.2235
N	2.71502	2.41498	1.12373
N	2.74844	-0.02714	2.59629
C	-3.65847	1.13351	0.33151
C	-3.40958	2.53816	0.36496
H	-2.43548	2.88262	0.03297
C	-4.37588	3.42798	0.78177
H	-4.17011	4.49411	0.78878
C	-5.64049	2.96141	1.20392

C	-5.92361	1.61591	1.19618
H	-6.89582	1.25895	1.52452
C	-4.9503	0.68392	0.75195
C	-5.26502	-0.70627	0.79153
H	-6.21936	-0.96298	1.26294
C	-5.0601	-3.04865	0.58268
H	-5.69771	-3.33929	-0.2637
H	-5.68387	-3.04362	1.4844
C	-3.93863	-4.08277	0.75615
H	-3.19987	-3.7133	1.47857
H	-4.36667	-5.01061	1.14961
C	-3.25555	-4.35683	-0.55399
C	-3.12884	-5.64155	-1.0873
H	-3.4926	-6.49148	-0.51914
C	-2.53776	-5.81193	-2.33655
H	-2.4342	-6.80528	-2.76408
C	-2.08323	-4.68808	-3.02627
H	-1.61766	-4.77064	-4.00236
C	-2.21601	-3.4391	-2.42982
H	-1.82373	-2.5383	-2.88565
C	0.68118	2.38929	-1.00213
C	-0.26508	2.52538	-2.06122
H	-0.79081	1.63002	-2.37482
C	-0.50568	3.75291	-2.6391
H	-1.2337	3.84756	-3.4392
C	0.19057	4.90271	-2.19836
C	1.12192	4.81272	-1.19226
H	1.66273	5.6952	-0.86289
C	1.37975	3.55965	-0.5765
C	2.3826	3.46837	0.42595
H	2.9494	4.38428	0.61667
C	3.84202	2.58763	2.051
H	3.45486	2.82283	3.05221
H	4.45377	3.43561	1.72331
C	4.71612	1.33248	2.1225
H	5.66868	1.58261	2.59987
H	4.94244	0.98001	1.10787
C	4.03013	0.25762	2.91826
C	4.66533	-0.37909	3.98748
H	5.69914	-0.13436	4.20759
C	3.96785	-1.30843	4.75435
H	4.45037	-1.80899	5.58874
C	2.63908	-1.57459	4.43237
H	2.04571	-2.28437	4.99856
C	2.07002	-0.92194	3.34542
H	1.06278	-1.13266	3.01672
O	0.41663	-3.45544	-0.07108
P	0.04003	-1.8567	0.01314
O	-0.99659	-1.33474	-1.02939
O	0.93858	-0.95215	0.90375
O	1.35144	-1.72328	-1.53742
C	2.6436	-1.51436	-1.48104
C	3.47647	-1.95816	-0.40985
C	3.27371	-0.84353	-2.56882
C	4.84378	-1.74491	-0.43536
H	3.02461	-2.47879	0.42653
C	4.6369	-0.62713	-2.59305
H	2.63951	-0.50496	-3.38184
C	5.42917	-1.0719	-1.51967
H	5.47724	-2.10108	0.36902
H	5.10793	-0.11324	-3.42274
N	6.84839	-0.83009	-1.52584

O	7.35402	-0.27312	-2.51381
O	7.51424	-1.17837	-0.5331
O	-1.06123	-2.25098	1.28285
H	-1.1393	-1.45711	1.83392
H	0.97026	-3.56252	-0.86398

PC

Ni	1.92517	-0.74792	-1.34687
Ni	-2.93088	-1.22636	1.32959
Cl	8.62536	-3.42686	-0.4538
Cl	-7.95447	-0.21066	-3.81076
O	2.93201	-1.91533	-0.27393
O	-3.30087	-1.56886	-0.46371
N	3.4973	0.02933	-2.14688
N	0.66963	0.36385	-2.39426
N	-4.42084	-0.03279	1.53813
N	-2.47296	-1.19727	3.23646
C	4.19823	-2.22793	-0.34856
C	4.69906	-3.28977	0.4516
H	4.00294	-3.82191	1.09243
C	6.03189	-3.64725	0.41257
H	6.39567	-4.46498	1.02676
C	6.92994	-2.95385	-0.42393
C	6.48635	-1.91271	-1.20751
H	7.18019	-1.37277	-1.84534
C	5.11953	-1.53876	-1.18802
C	4.70564	-0.42657	-1.98205
H	5.51081	0.10497	-2.49834
C	3.37044	1.23042	-2.98516
H	3.11003	0.92569	-4.00774
H	4.33474	1.74976	-3.02554
C	2.30042	2.18188	-2.44469
H	2.44727	2.32814	-1.36676
H	2.41459	3.16002	-2.92203
C	0.92197	1.65068	-2.72646
C	-0.0458	2.43583	-3.35578
H	0.18614	3.46861	-3.59437
C	-1.28778	1.88816	-3.66529
H	-2.05003	2.49092	-4.15073
C	-1.52868	0.55523	-3.34304
H	-2.47885	0.0776	-3.55592
C	-0.53305	-0.17126	-2.6994
H	-0.68983	-1.18837	-2.36681
C	-4.35421	-1.2619	-1.15046
C	-4.49605	-1.79337	-2.46808
H	-3.72624	-2.4731	-2.82004
C	-5.58282	-1.47915	-3.2574
H	-5.67781	-1.90255	-4.25276
C	-6.58401	-0.60846	-2.77558
C	-6.49162	-0.07522	-1.5106
H	-7.26447	0.59277	-1.14055
C	-5.39027	-0.39685	-0.67794
C	-5.3154	0.19283	0.61858
H	-6.09631	0.9233	0.85219
C	-4.54648	0.75191	2.7756
H	-5.11262	0.16755	3.51389
H	-5.11349	1.66679	2.56773
C	-3.17789	1.12478	3.35842
H	-3.31332	1.90215	4.11738
H	-2.54035	1.54126	2.56779
C	-2.52382	-0.07551	3.98405
C	-2.03636	-0.06328	5.29232

H	-2.0764	0.85749	5.86518
C	-1.5052	-1.22786	5.84105
H	-1.11585	-1.2293	6.85511
C	-1.485	-2.38691	5.06779
H	-1.08401	-3.31973	5.44844
C	-1.96796	-2.33018	3.76566
H	-1.92041	-3.18108	3.09898
O	-0.10453	-0.06245	1.43551
P	-0.04076	-1.48946	0.88299
O	0.404	-1.57042	-0.62101
O	-1.3748	-2.27539	1.07881
O	-0.71756	2.2902	0.64748
C	0.31461	3.12091	0.82342
C	1.53758	2.7024	1.39874
C	0.16743	4.46233	0.40842
C	2.58308	3.60347	1.53948
H	1.6344	1.67251	1.72806
C	1.21118	5.36113	0.54993
H	-0.78048	4.77047	-0.02132
C	2.42101	4.92752	1.11
H	3.5245	3.29896	1.98142
H	1.11063	6.39271	0.23447
N	3.52203	5.86442	1.2435
O	3.34932	7.03095	0.86334
O	4.58638	5.455	1.72621
O	1.06591	-2.35322	1.70973
H	1.87567	-2.38331	1.15137
H	-0.48161	1.33193	0.91915

[Ni]-H_2O

Ni	-1.24310000	0.98733100	-0.59807800
Cl	5.88377200	-1.16308200	0.14772700
O	0.58188700	1.33428100	0.95490200
N	-0.38491900	-0.67147900	-1.06775300
N	-2.53670700	-0.02312000	0.40715000
C	1.72866800	0.77826400	0.73703200
C	2.90945400	1.26636300	1.38848800
H	2.79749700	2.12273100	2.04820900
C	4.15196700	0.69490900	1.20936000
H	5.02007500	1.09933400	1.72166600
C	4.28588200	-0.42179300	0.36264200
C	3.19093600	-0.94375300	-0.28924300
H	3.30030800	-1.81207600	-0.93292700
C	1.90623300	-0.35889500	-0.14044600
C	0.84772000	-1.02599600	-0.85991200
H	1.14444900	-1.98699900	-1.29082100
C	-1.23648600	-1.63954400	-1.79451700
H	-1.03063200	-2.64922200	-1.42439500
H	-0.98507000	-1.61002700	-2.86072800
C	-2.73246400	-1.32440200	-1.63413700
H	-2.98119700	-0.42990400	-2.21946900
H	-3.30870000	-2.15868900	-2.04297400
C	-3.12013000	-1.08357900	-0.20078400
C	-4.01957200	-1.88956800	0.49826300
H	-4.47830000	-2.73277600	-0.00673200
C	-4.31625000	-1.59894900	1.82882800
H	-5.01549200	-2.21899700	2.38127400
C	-3.70243200	-0.50492000	2.43954200
H	-3.89971600	-0.24513100	3.47356700
C	-2.81448200	0.26131000	1.69474300
H	-2.30405900	1.11739900	2.12091600
O	-2.07207100	2.62907100	-0.29250700

H	-2.91162500	2.50224800	0.17680100
O	-0.14185100	2.02106000	-1.94311300
H	-0.34233600	2.94763300	-1.71064800
H	0.81085800	1.91180500	-1.76811300

[Ni]-MeCN

Ni	1.20856400	0.92019700	-0.27598700
Cl	-5.73451200	-1.41074600	0.63439600
O	-0.36824500	-0.41122700	-1.65010900
N	0.49203900	-0.10219100	1.20673200
N	2.71966300	-0.28792100	-0.29300900
C	-1.53372000	-0.58220000	-1.11660000
C	-2.70381900	-0.70352400	-1.93677100
H	-2.57263800	-0.60815000	-3.01143800
C	-3.96030200	-0.94002200	-1.41673500
H	-4.81931800	-1.02333300	-2.07617300
C	-4.11997200	-1.08347500	-0.02613800
C	-3.03688100	-0.97931300	0.81944600
H	-3.16588000	-1.09873100	1.89175500
C	-1.74371200	-0.69638600	0.31121800
C	-0.69709200	-0.61175300	1.30258700
H	-0.96259700	-1.03205300	2.27809600
C	1.36219000	-0.20527800	2.39931700
H	1.33865200	-1.23399400	2.77377300
H	0.97614000	0.45244500	3.18633600
C	2.80988500	0.19704900	2.08420000
H	2.85587800	1.27725200	1.89604600
H	3.42953900	-0.01496600	2.95965800
C	3.34282200	-0.53449900	0.88370500
C	4.39505800	-1.44893100	0.94834900
H	4.88139500	-1.62988300	1.90085000
C	4.80354100	-2.11353600	-0.20637800
H	5.62079500	-2.82717100	-0.16719900
C	4.14560800	-1.85337900	-1.40890300
H	4.42455700	-2.35187400	-2.33052300
C	3.10670900	-0.93104300	-1.41287800
H	2.55820400	-0.69712700	-2.31819800
O	1.91727900	1.98359900	-1.63932300
C	-0.97390200	3.09944800	0.15073200
N	-0.17609500	2.28166400	-0.03061700
C	-1.97323100	4.12327500	0.39554700
H	-2.34053400	4.51590200	-0.55738600
H	-2.80740300	3.69176500	0.95713400
H	-1.52732000	4.93741200	0.97517000
H	2.77683600	1.62123400	-1.90547000

[Ni]-DMF

Ni	1.32092600	0.78064800	0.11131700
Cl	-5.29629300	-2.49211400	0.25505100
O	-0.18254700	-0.22527000	-1.67694800
N	0.79256000	-0.78077000	1.13077900
N	2.97112600	-0.12081300	-0.31575400
C	-1.29479600	-0.68298300	-1.20336500
C	-2.49669500	-0.63647600	-1.98541100
H	-2.43588800	-0.17241800	-2.96637700
C	-3.69537000	-1.16686500	-1.55020900
H	-4.57886700	-1.11306800	-2.17964600
C	-3.76036800	-1.78901100	-0.29040400
C	-2.64389000	-1.86164500	0.51504600
H	-2.70142100	-2.34621100	1.48588900
C	-1.41309600	-1.28895400	0.10660000
C	-0.33152500	-1.42384700	1.05635700

H	-0.50716800	-2.17610800	1.83238500
C	1.72155300	-1.20033900	2.20388900
H	1.84943900	-2.28726100	2.16565200
H	1.28899700	-0.94322700	3.17749600
C	3.08942500	-0.51528000	2.07698900
H	2.98331900	0.55439700	2.29917100
H	3.76477300	-0.94382000	2.82238100
C	3.67454700	-0.67331200	0.70083200
C	4.86167500	-1.36160500	0.44584900
H	5.41200800	-1.79305100	1.27497700
C	5.32088000	-1.48340400	-0.86430100
H	6.24411100	-2.01500100	-1.07355600
C	4.57685500	-0.91820500	-1.90073200
H	4.89148200	-0.99522100	-2.93546400
C	3.40381400	-0.24379600	-1.58641200
H	2.78675000	0.21167000	-2.35237900
O	1.83356900	2.34545600	-0.76614800
H	2.75837100	2.26698200	-1.04797400
C	-0.96003300	2.44852000	0.00268100
O	-0.27382000	1.72710300	0.78255500
N	-2.11842500	3.00059700	0.33769500
H	-0.61590900	2.65222900	-1.01220900
C	-2.71503000	2.83236800	1.66276500
H	-2.64570200	3.76833400	2.22682300
H	-3.76899200	2.56555300	1.54591400
H	-2.19872100	2.04167200	2.20525600
C	-2.83236100	3.87604700	-0.59415400
H	-3.83401100	3.47745400	-0.78001500
H	-2.92257200	4.87875500	-0.16487600
H	-2.28688800	3.93745100	-1.53703700