Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Unusual Mechanism of Paramagnetic Nickel-Catalyzed α-Alkylation of Amides

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Contents

SI1: 3D structure

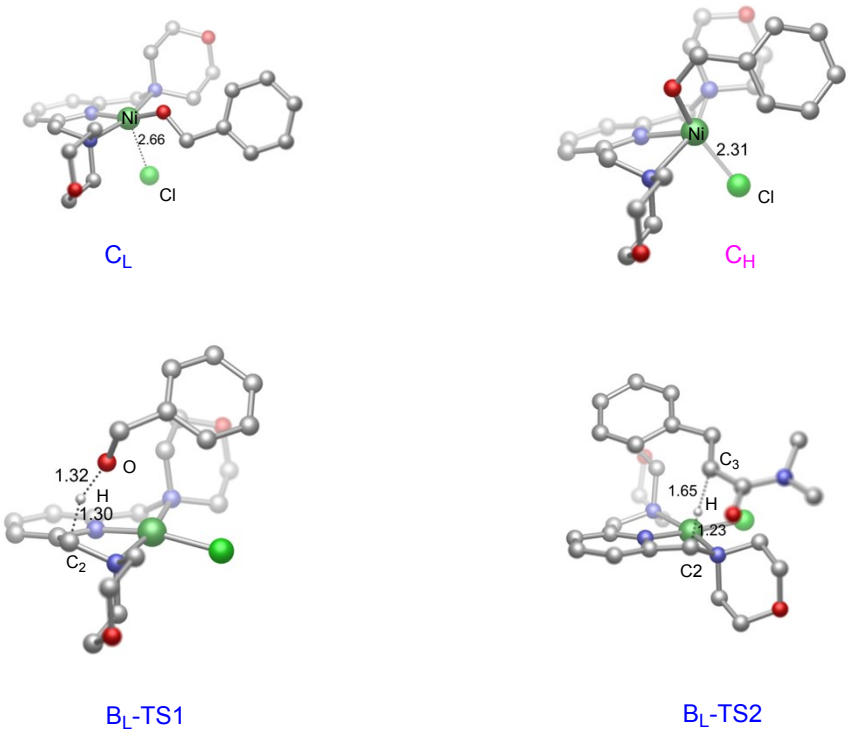

Figure S1. 3D structures of **C_L,C_H B_L-TS1** and **B_{L2}-TS2**. Bond lengths are given in Å. All C–H hydrogen atoms except the reaction site have been omitted for clarity.

SI2: Other mechanisms

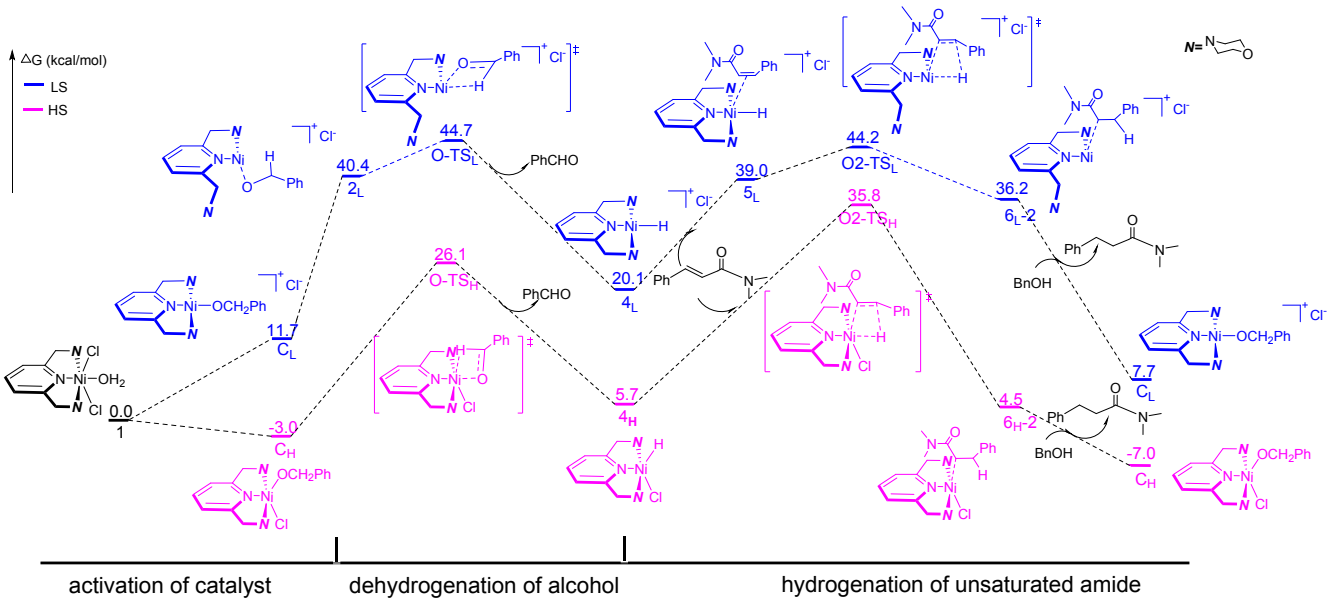

Figure S2. outer sphere mechanism via the second mode . The relevant free energies are given in kcal·mol^{-1}.

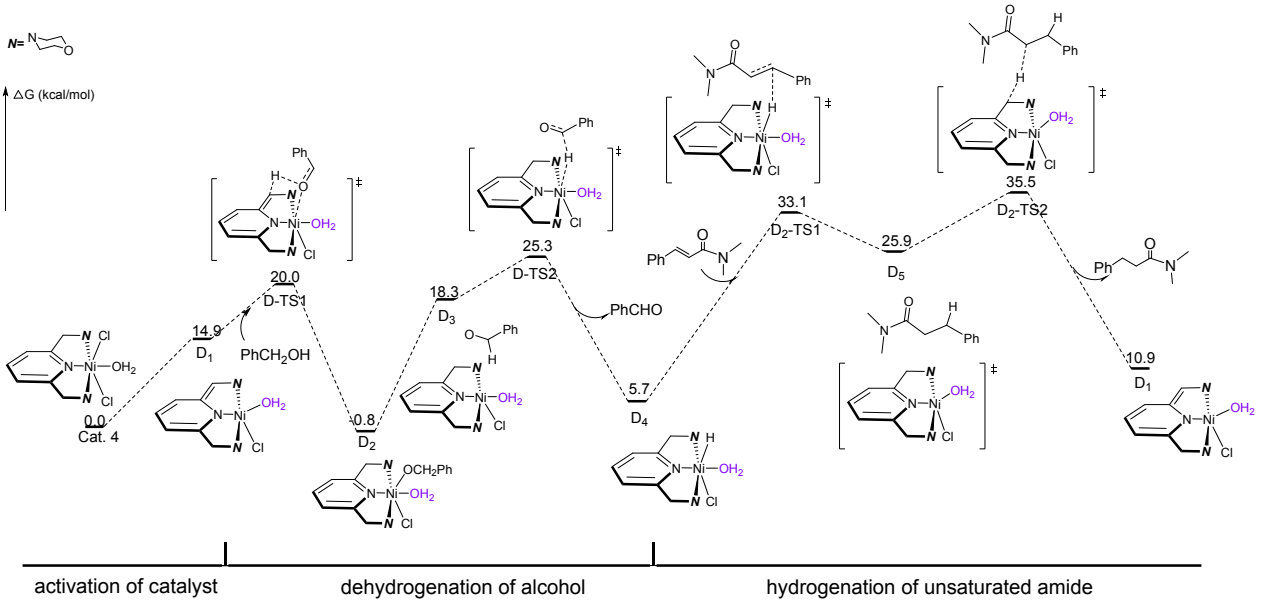

Figure S3. Possible general mechanism paths via H_2O coordinating with Ni. The relevant free energies are given in kcal·mol^{-1}.

SI3: IRC profiles

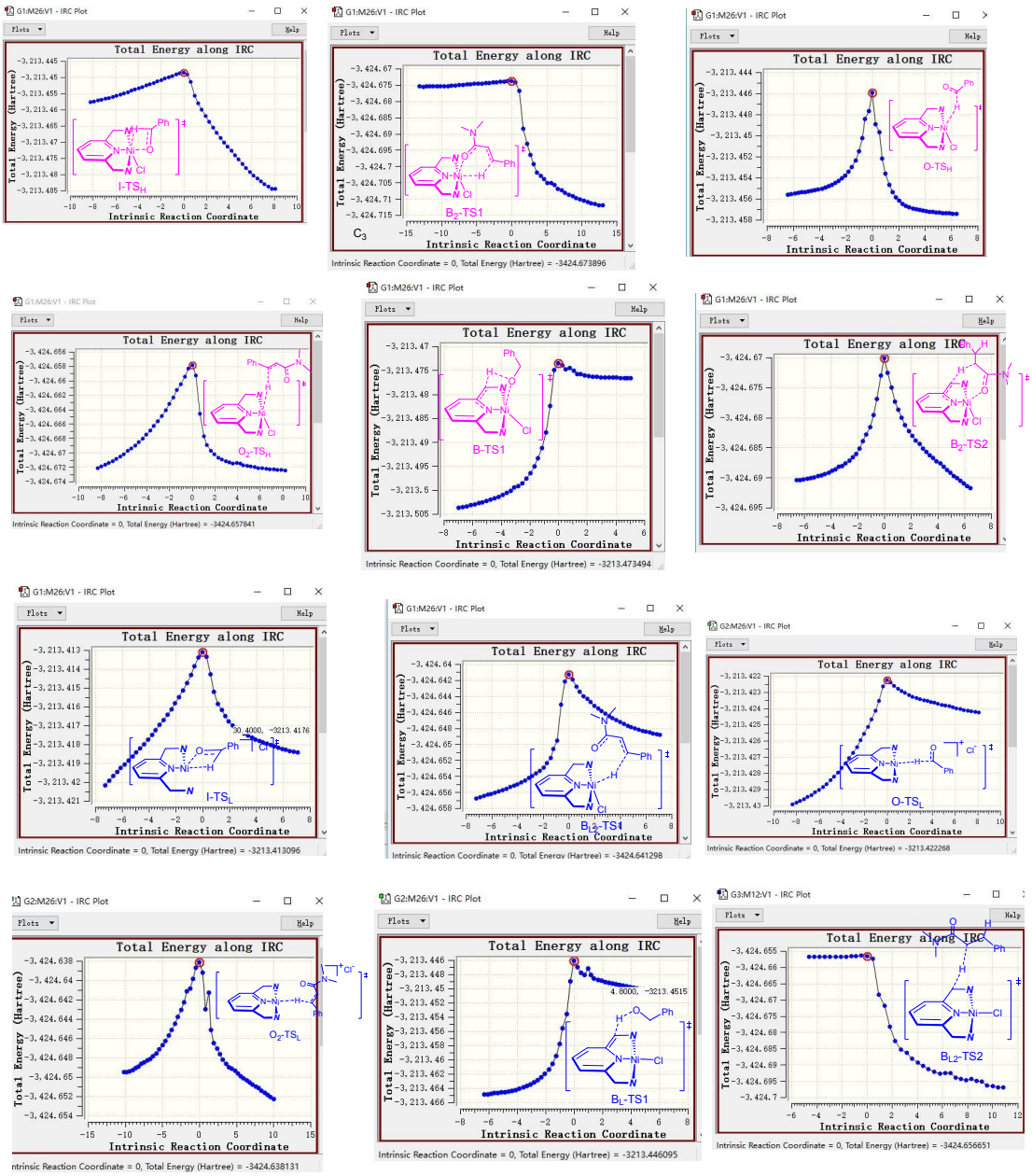

Figure S4: IRC profiles of crucial transition states

SI4: Further exchange of the chloride

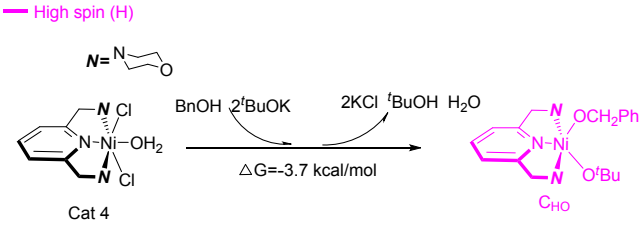

Figure S5. Further exchange of the chloride (C_{HO}). The relevant free energies are given in kcal·mol^{-1}.

SI5: Comparison of activation process

Table S1. Comparison of activation process. The relevant free energies are given in kcal·mol^{-1}.

$\Delta G^{\neq}$(kcal·mol^{-1})	Optimizing structures ： M06-L/def2svp Single-point： M06-L/def2tzvp solvent= n-octane	Optimizing structures: M06-L/def2tzvp solvent= n-octane
ΔG_H	-3.0	-4.9
ΔG_L	9.7	11.7

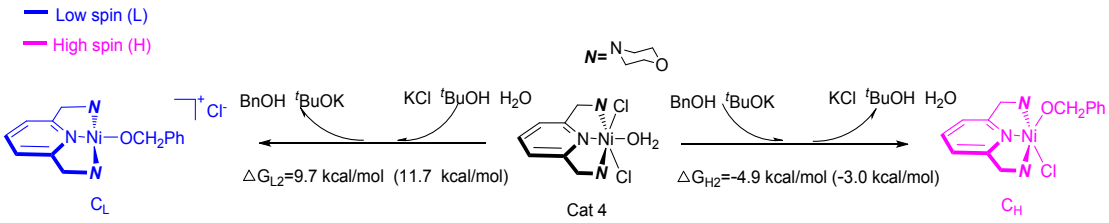

Figure S6. The activated process of Cat.4. ΔG_{L2} and ΔG_{H2} were got at M06-L/def2tzvp levels and adding solvation effect of *n*-octane (ε=1.9406). Raw data is in the bracket.

SI6: Comparison of two calculation methods

Table S2. Comparison of two calculation methods. The relevant free energies are given in kcal·mol^{-1}.

$\Delta G^{\neq}$(kcal·mol^{-1})	Optimizing structures ： M06-L/def2svp Single-point： M06-L/def2tzvp solvent= *n*-octane	Optimizing structures: M06-L/def2tzvp solvent= *n*-octane
C_H	0.0	0.0
C_L	14.7	14.6
O-TS_H	23.7	23.1
B_2-TS1	24.0	25.1
B_2-TS2	27.4	31.2
O_2-TS_L	45.6	44.0

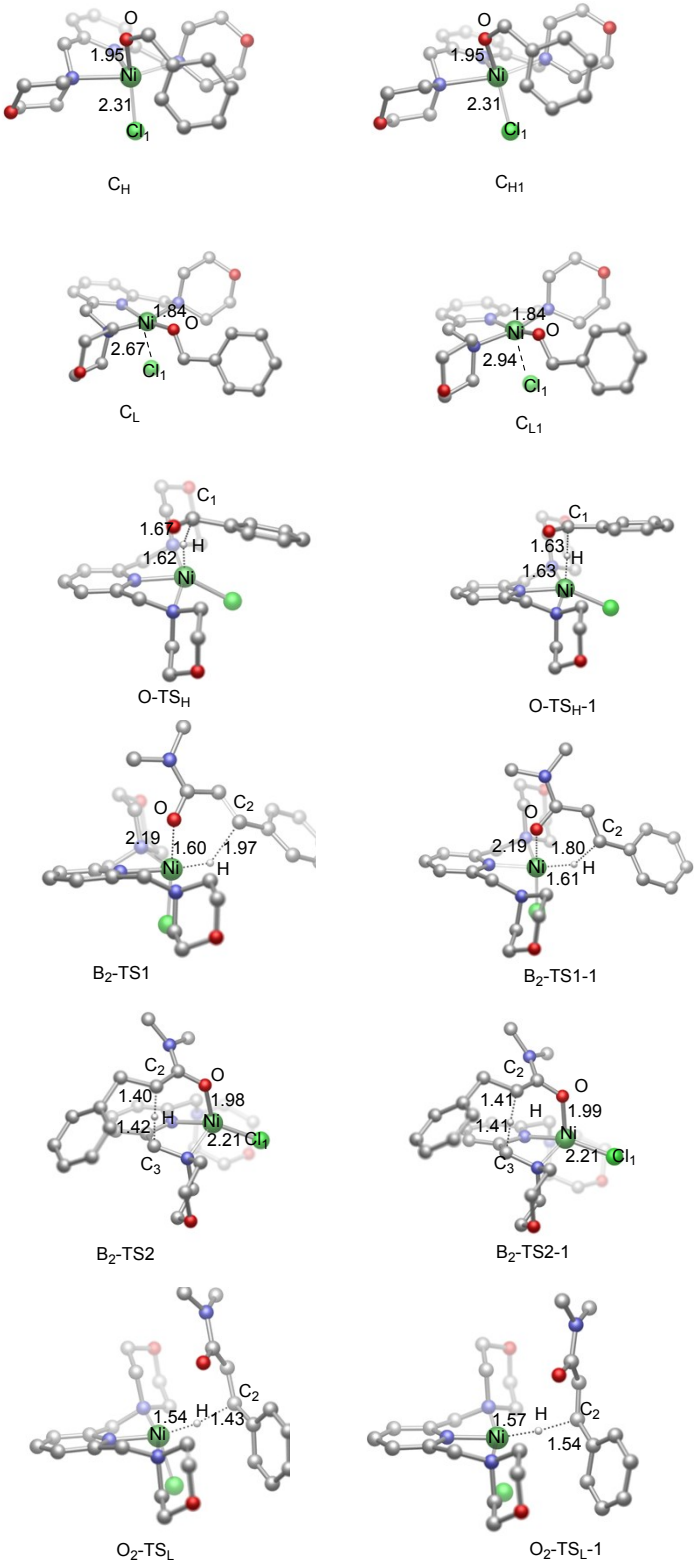

Figure S7. Comparison of crucial intermediates and transition states. Raw data is on the left and structures on the right were got at M06-L/def2tzvp levels and adding solvation effect of *n*-octane (ε=1.9406).

SI7: Discussion about position of chloride

The chloride position of initial structure (Cat.4) was originated from experimental article (CCDC No: 1814945). As for the C_L, We ensure the position of chloride via optimizing and taking the lowest energy. For probing into position influence, with the assistance of the Multiwfn and VMD software (Figure S8), we selected the three largest local maxima to optimize. The result (Figure S9) shows the optimal structure of C_L-1 is same as the C_L, and both of their free energy barriers are 14.7 kcal/mol.

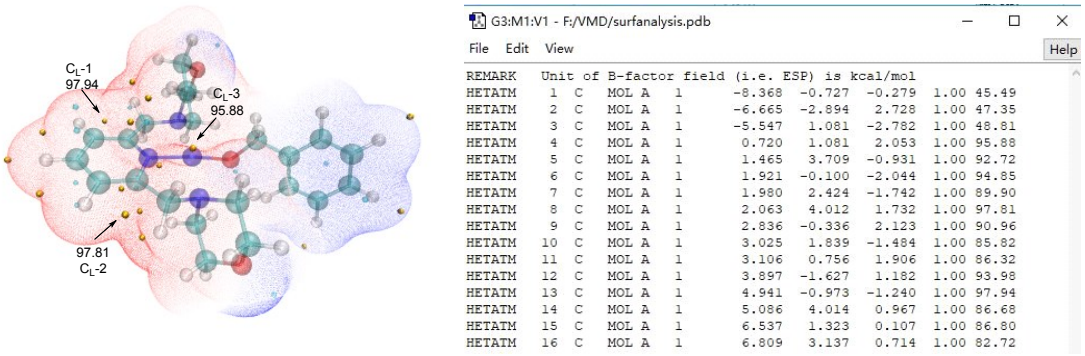

Figure S8. Electrostatic potential analysis via Multiwfn and VMD. Local maxima are indicated by yellow dots and Local minima are indicated by blue dots.

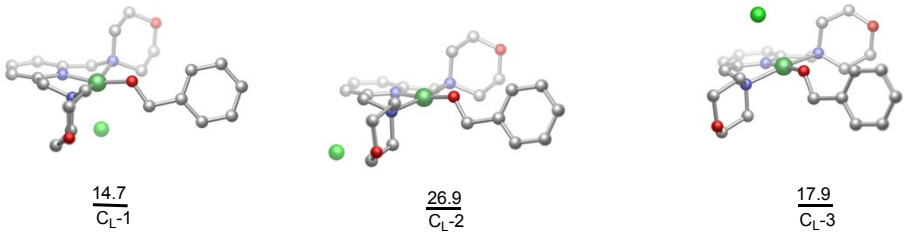

Figure S9. 3D structures of C_L C_L-1 and C_L-2. The relevant free energies are given in kcal·mol^{-1}.

SI9: Cartesian coordinates.

Cat.4

Ni	-0.16737	-0.43624	-0.042
Cl	-0.1781	-0.71951	2.34393
Cl	0.2347	-0.7187	-2.36928
O	4.25049	-1.75584	-0.60742
O	-4.24316	-1.65867	0.48622
O	-0.30399	-2.56291	-0.01247
H	0.3033	-2.84582	-0.71764

H	0.09505	-2.80544	0.8425
N	0.08219	1.58285	-0.02004
N	2.34407	0.07485	0.44505
N	-2.21928	0.14981	-0.44808
C	3.07777	-0.87317	1.28882
H	2.44065	-1.13369	2.14387
H	4.00718	-0.40447	1.67976
C	3.45679	-2.09604	0.4981
H	4.02973	-2.80095	1.11603
H	2.53214	-2.61125	0.16234
C	3.51959	-0.91929	-1.4782
H	2.6353	-1.4532	-1.87393
H	4.17359	-0.67676	-2.33153
C	3.07429	0.3532	-0.79284
H	3.96965	0.98466	-0.56938
H	2.42015	0.92061	-1.475
C	2.12511	1.30441	1.19955
H	3.07462	1.86101	1.35576
H	1.7449	1.01196	2.18847
C	1.09482	2.20172	0.59133
C	1.11307	3.60064	0.71761
H	1.95528	4.0956	1.20801
C	0.03472	4.33266	0.22793
H	0.0149	5.4245	0.32107
C	-1.03683	3.66696	-0.37668
H	-1.89901	4.2104	-0.7558
C	-0.97092	2.27285	-0.49278
C	-2.00229	1.42422	-1.15956
H	-2.95089	1.96925	-1.28604
H	-1.62016	1.16441	-2.16313
C	-2.98034	0.37269	0.79632
H	-3.86107	1.01134	0.56917
H	-2.34035	0.91336	1.51452
C	-3.45102	-0.93332	1.39939
H	-2.57175	-1.52097	1.72272
H	-4.06327	-0.7289	2.28854
C	-3.46308	-1.98745	-0.64371
H	-4.1073	-2.56857	-1.32549
H	-2.61476	-2.62644	-0.35204
C	-2.97348	-0.75131	-1.34842
H	-2.32068	-1.00418	-2.19695
H	-3.85321	-0.19385	-1.73556

C_H

Ni	0.38044	-0.25239	0.14736
C	2.14963	1.77189	-0.71717
C	0.24485	2.67787	0.31128
C	2.69937	3.03603	-0.90517
C	0.73281	3.97695	0.14292
C	1.96993	4.14452	-0.46989
H	3.67273	3.14807	-1.38015
H	0.15027	4.83438	0.48728
H	2.37798	5.14731	-0.61115
C	2.75208	0.4589	-1.14135
H	3.82904	0.5707	-1.34627
C	-1.02866	2.27352	0.99342
H	-0.76893	1.94573	2.01532
H	-1.71082	3.13823	1.08483
N	0.95401	1.64081	-0.12291
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C	2.60292	-1.95207	-0.63749
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H	3.19123	0.62118	1.44491
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H	2.12988	-2.61208	0.11315
H	2.0265	-2.03253	-1.56683
H	5.2329	-0.82278	1.84206
H	5.22126	-0.18588	0.18808
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C	-2.11809	1.43181	-1.02055
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H	-1.30958	1.8829	-1.61495
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H	-2.96948	-0.44274	0.65941
H	-2.35506	0.32719	2.12933
H	-3.75904	2.4604	-1.9876
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H	-4.79862	0.89709	1.5912
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N	-1.62366	1.10481	0.32508
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O	4.75549	-2.19039	0.42634
Cl	0.2591	-0.53983	2.43784

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H	-0.53905	-2.28503	-2.9124
H	-1.51134	-0.81751	-2.94897
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C	-3.21225	-2.0943	-1.43103
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H	-5.13781	-2.64529	-0.63534
H	-1.73877	-3.39578	1.90492
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C_L

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C	-4.44122	-1.16605	-0.14458
C	-3.11336	-3.1311	0.30364
C	-4.35875	-2.51463	0.20521
H	-5.40474	-0.6607	-0.23006
H	-3.02491	-4.18171	0.5847
H	-5.26842	-3.08372	0.40561
C	-3.14152	0.91568	-0.92012
H	-3.97138	1.55346	-0.57502
C	-0.57025	-2.81863	0.31797
H	-0.44008	-2.80822	1.41553
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N	-2.07228	-1.07919	-0.26336
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H	-0.73141	2.23848	1.04376
H	-2.09159	1.23285	1.51204
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H	-0.412	2.84581	-1.31626
H	-1.50006	2.19314	-2.54805
H	-2.45454	3.72106	1.94176
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H	1.33721	-4.32148	-1.27457
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2_L

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H	0.86551	2.9539	0.59002
H	1.94793	1.66699	1.21525
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C	-3.03349	-0.1237	-0.88774
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H	-2.67593	0.14336	-1.89672
H	-2.86524	0.76406	-0.25214
C	-3.98838	-2.73453	-1.31339
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H	-5.07924	0.34082	-1.4239
H	-4.92596	-0.65701	0.03437
H	-4.18814	-3.56516	-2.00563
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C	2.75857	2.48853	-1.671
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H	3.06257	0.73222	-0.40664
C	0.54792	3.03411	-2.12618
H	-0.00741	0.96654	-2.40829
H	-0.92945	1.8642	-1.12127
H	3.75617	2.43385	-2.12942
H	2.82804	3.209	-0.82908
H	-0.10531	3.36881	-2.94155
H	0.47583	3.80599	-1.33596
N	-2.22003	-1.25552	-0.42057
N	0.98884	1.13404	-0.57934
O	1.86343	2.9402	-2.64711
O	-4.7019	-1.61844	-1.7923
C	1.3895	-2.41621	-0.54677
H	1.16277	-1.48574	-1.32872
H	1.41734	-3.17579	-1.36269
O	0.3663	-2.51505	0.29711
C	2.75905	-2.12863	0.02153
C	3.89097	-2.13122	-0.79807
C	2.88421	-1.75815	1.3651
C	5.1314	-1.74663	-0.28987

H	3.79861	-2.42572	-1.8492
C	4.12331	-1.37554	1.87306
H	1.99268	-1.78072	1.99828
C	5.24855	-1.36071	1.04523
H	6.01066	-1.74875	-0.93842
H	4.21538	-1.0896	2.92384
H	6.21903	-1.05642	1.4441
Cl	-1.8669	3.46202	0.30839

I-TS$_L$

Ni	0.27563	-0.70551	-0.24831
C	-1.69076	-0.36835	1.81051
C	-0.08938	1.32647	1.60433
C	-2.23356	0.24386	2.92665
C	-0.59673	1.99684	2.71999
C	-1.63884	1.41121	3.42128
H	-3.13626	-0.166	3.38417
H	-0.20525	2.97797	2.98522
H	-2.062	1.91366	4.29274
C	-2.28933	-1.5186	1.06335
H	-1.75584	-2.45372	1.29525
H	-3.33713	-1.65996	1.39204
C	1.00504	1.817	0.71834
H	0.90041	2.90692	0.59848
H	1.98942	1.60681	1.17288
N	-0.57154	0.13468	1.24755
C	-2.93973	-0.14093	-0.86484
C	-2.42654	-2.46321	-1.18646
C	-4.41001	-0.4864	-0.96346
H	-2.5693	0.10721	-1.87321
H	-2.77324	0.7536	-0.23711
C	-3.91457	-2.74556	-1.28058
H	-2.03482	-2.27502	-2.20092
H	-1.87187	-3.31853	-0.77259
H	-4.9716	0.33874	-1.42105
H	-4.84578	-0.64961	0.04458
H	-4.112	-3.57934	-1.96945
H	-4.31434	-3.04734	-0.28857
C	2.3356	1.11323	-1.21113
C	0.03377	1.73201	-1.58789
C	2.73569	2.49906	-1.68052
H	2.3116	0.43349	-2.07579
H	3.05474	0.70661	-0.4839
C	0.52312	3.07568	-2.07074

H	-0.03911	1.02383	-2.42823
H	-0.94227	1.87325	-1.09461
H	3.72343	2.45266	-2.16108
H	2.83072	3.1889	-0.81587
H	-0.14541	3.44522	-2.8583
H	0.46946	3.81618	-1.24936
N	-2.13643	-1.27811	-0.3771
N	0.97835	1.11032	-0.60606
O	1.82692	2.99858	-2.62084
O	-4.61574	-1.62827	-1.77214
C	1.34603	-2.43717	-0.45463
H	0.86919	-1.27261	-1.49959
H	1.38488	-3.06749	-1.37143
O	0.34559	-2.57283	0.33997
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C	3.8006	-2.03586	-0.78202
C	2.81966	-1.58432	1.38265
C	5.03745	-1.59419	-0.31505
H	3.69536	-2.3864	-1.81402
C	4.0543	-1.14419	1.84678
H	1.94126	-1.60097	2.03444
C	5.16582	-1.14081	0.99751
H	5.90632	-1.60586	-0.97728
H	4.15768	-0.80626	2.88091
H	6.1344	-0.79416	1.36482
Cl	-1.89216	3.3849	0.39803

4_L

Ni	0.23589	-0.71128	-0.24562
C	-1.70859	-0.32447	1.81451
C	-0.078	1.34098	1.59682
C	-2.24206	0.30433	2.9258
C	-0.5721	2.02563	2.70993
C	-1.62573	1.46396	3.41323
H	-3.15174	-0.08653	3.38593
H	-0.16143	2.99996	2.97164
H	-2.03934	1.97884	4.28199
C	-2.31813	-1.47366	1.07547
H	-1.80519	-2.41466	1.32906
H	-3.37369	-1.59106	1.38703
C	1.02667	1.80541	0.70995
H	0.93702	2.89496	0.57671
H	2.0056	1.58902	1.17343
N	-0.5808	0.15555	1.24892

C	-2.9113	-0.11323	-0.88596
C	-2.44208	-2.45143	-1.16105
C	-4.38684	-0.4307	-0.99804
H	-2.52197	0.10769	-1.89345
H	-2.73506	0.78935	-0.27229
C	-3.93437	-2.70426	-1.26902
H	-2.03371	-2.28817	-2.17292
H	-1.91065	-3.31059	-0.72564
H	-4.92438	0.39808	-1.47726
H	-4.83875	-0.56646	0.00685
H	-4.13966	-3.54624	-1.94545
H	-4.35264	-2.9802	-0.27725
C	2.36407	1.04651	-1.1924
C	0.08632	1.72163	-1.60963
C	2.80792	2.41767	-1.66525
H	2.33429	0.36	-2.05143
H	3.06206	0.62848	-0.45157
C	0.61693	3.04854	-2.09522
H	0.01034	1.00879	-2.44558
H	-0.89417	1.89129	-1.13379
H	3.80088	2.34131	-2.13097
H	2.9094	3.11068	-0.80379
H	-0.029	3.42683	-2.89741
H	0.56752	3.79793	-1.28158
N	-2.13714	-1.25831	-0.36716
N	0.99891	1.08444	-0.6069
O	1.92731	2.93592	-2.62225
O	-4.6065	-1.5822	-1.78908
H	0.81008	-1.30055	-1.49841
Cl	-1.85287	3.38741	0.35128

5_L

Ni	-0.0959	0.16888	-0.79771
C	1.66645	0.27361	1.48263
C	-0.21108	-1.07527	1.75517
C	2.08625	0.02074	2.7763
C	0.14932	-1.36945	3.07351
C	1.27051	-0.75474	3.60717
H	3.05609	0.38636	3.11961
H	-0.41533	-2.11036	3.63926
H	1.57962	-0.97256	4.63072
C	2.48622	0.90179	0.40131
H	2.21554	1.95759	0.2295
H	3.55105	0.90574	0.69593

C	-1.32018	-1.73243	1.00369
H	-1.37427	-2.78572	1.32407
H	-2.28791	-1.25769	1.24155
N	0.47297	-0.17836	1.04783
C	2.81353	-1.19713	-0.83375
C	2.77785	0.87713	-2.03106
C	4.32413	-1.17891	-0.92323
H	2.41239	-1.72715	-1.71126
H	2.47487	-1.7511	0.0638
C	4.29465	0.84244	-2.07835
H	2.3778	0.38075	-2.92883
H	2.40823	1.91469	-2.03391
H	4.70355	-2.20572	-1.00143
H	4.77506	-0.7443	-0.00754
H	4.65715	1.31355	-3.00325
H	4.72384	1.42504	-1.23493
C	-2.43821	-1.71841	-1.16483
C	-0.25069	-2.69282	-1.03502
C	-3.01706	-3.11789	-1.0788
H	-2.27651	-1.44928	-2.22008
H	-3.13399	-0.98633	-0.73226
C	-0.89813	-4.05489	-0.98829
H	-0.04152	-2.40509	-2.07753
H	0.67459	-2.74298	-0.43991
H	-3.96489	-3.15785	-1.63479
H	-3.25526	-3.36973	-0.02344
H	-0.25378	-4.78051	-1.50105
H	-0.9754	-4.40456	0.05988
N	2.23262	0.17051	-0.86133
N	-1.12582	-1.61713	-0.47761
O	-2.15751	-4.07218	-1.6372
O	4.77614	-0.47577	-2.06558
C	-1.47737	1.63414	-1.21602
H	-0.24361	0.08125	-2.24078
H	-1.60817	1.61199	-2.30572
C	-2.78456	1.55623	-0.5527
C	-3.91765	1.62087	-1.39004
C	-2.99376	1.34034	0.82241
C	-5.20555	1.49302	-0.88217
H	-3.77315	1.77068	-2.46429
C	-4.28457	1.20517	1.32549
H	-2.13311	1.28272	1.48913
C	-5.39492	1.279	0.48293
H	-6.0642	1.55175	-1.55513

H	-4.42543	1.03635	2.39616
H	-6.403	1.16781	0.88906
Cl	1.47397	-3.62351	1.52977
C	-0.23178	2.21572	-0.83593
H	0.37172	2.54117	-1.68885
C	0.01701	2.92039	0.44775
O	-0.40595	2.52922	1.52998
N	0.8158	4.04839	0.3765
C	1.26873	4.65509	1.60636
H	2.36442	4.77324	1.60125
H	0.8229	5.65145	1.75816
H	0.97688	4.01576	2.44505
C	1.22832	4.69007	-0.84844
H	1.42251	5.75283	-0.65119
H	2.1573	4.26641	-1.27493
H	0.44694	4.64788	-1.61676

I_2-TS_L

Ni	0.37703	-0.17248	-0.6477
C	-1.7177	-0.1929	1.43594
C	0.16375	1.13539	1.78741
C	-2.14177	0.01625	2.73689
C	-0.20432	1.3806	3.11243
C	-1.33549	0.7569	3.60806
H	-3.11239	-0.36783	3.05767
H	0.3704	2.08509	3.71362
H	-1.65261	0.92937	4.63791
C	-2.5528	-0.84303	0.37357
H	-2.24913	-1.89217	0.20873
H	-3.59883	-0.89674	0.7387
C	1.32541	1.78605	1.11103
H	1.34306	2.84592	1.41652
H	2.27443	1.31913	1.42841
N	-0.52197	0.27925	1.02607
C	-2.93732	1.23517	-0.86416
C	-2.96378	-0.85357	-2.03045
C	-4.44936	1.24823	-0.92687
H	-2.54392	1.76002	-1.75045
H	-2.5696	1.78699	0.02202
C	-4.48076	-0.78536	-2.06757
H	-2.56599	-0.39351	-2.95178
H	-2.62078	-1.902	-2.01214
H	-4.82542	2.2769	-1.0015
H	-4.88735	0.81263	-0.00421

H	-4.87362	-1.25548	-2.98107
H	-4.91271	-1.34258	-1.20774
C	2.57984	1.78229	-0.99078
C	0.32466	2.62996	-1.01221
C	3.07263	3.21491	-0.9409
H	2.49046	1.46902	-2.04202
H	3.28362	1.09677	-0.49623
C	0.89993	4.02512	-0.99565
H	0.1732	2.28509	-2.04772
H	-0.62677	2.64693	-0.45815
H	4.04435	3.28799	-1.45023
H	3.23714	3.53221	0.11082
H	0.24464	4.69784	-1.56312
H	0.91229	4.41214	0.04106
N	-2.39469	-0.13609	-0.89436
N	1.23834	1.63505	-0.37108
O	2.18548	4.08137	-1.5914
O	-4.92595	0.5471	-2.06232
C	1.46368	-1.69064	-1.32358
H	0.93544	-0.29459	-1.96153
H	1.57313	-1.87329	-2.40132
C	2.79007	-1.60357	-0.67689
C	3.9252	-1.68465	-1.50326
C	2.98419	-1.34806	0.69388
C	5.20839	-1.52978	-0.98605
H	3.79227	-1.86697	-2.57412
C	4.26872	-1.19825	1.20761
H	2.11756	-1.28701	1.35394
C	5.38576	-1.28447	0.37486
H	6.07319	-1.59738	-1.65014
H	4.39845	-1.00875	2.27618
H	6.39046	-1.15992	0.78536
Cl	-1.41018	3.68065	1.51923
C	0.19574	-2.15148	-0.79793
H	-0.505	-2.41682	-1.59673
C	-0.01379	-2.87369	0.48479
O	0.42857	-2.49762	1.56507
N	-0.81546	-3.99695	0.41057
C	-1.2758	-4.60492	1.6368
H	-2.37239	-4.71304	1.62766
H	-0.8388	-5.60558	1.78541
H	-0.98136	-3.97113	2.47876
C	-1.24994	-4.61818	-0.81734
H	-1.43897	-5.68455	-0.63434

H	-2.18656	-4.187	-1.21876
H	-0.48239	-4.56097	-1.59842

6_L

Ni	-0.84373	0.1306	-0.85721
C	-2.57685	-1.6652	0.33766
C	-3.4487	0.48544	-0.0074
C	-3.71226	-2.04246	1.04531
C	-4.59112	0.18567	0.71529
C	-4.72965	-1.10459	1.23375
H	-3.79026	-3.048	1.46446
H	-5.35981	0.94438	0.87323
H	-5.62201	-1.37146	1.8017
C	-1.33042	-2.47016	0.14315
H	-0.74168	-2.45552	1.07564
H	-1.56566	-3.52558	-0.07999
C	-3.09587	1.76708	-0.6721
H	-3.31643	1.6892	-1.75088
H	-3.69668	2.60366	-0.27812
N	-2.49793	-0.43737	-0.19707
C	-0.9338	-2.28626	-2.26989
C	0.94685	-2.159	-0.76802
C	-0.56704	-3.73244	-2.5521
H	-0.42926	-1.63899	-2.99023
H	-2.01763	-2.11698	-2.35636
C	1.22602	-3.61423	-1.07022
H	1.48186	-1.52428	-1.48809
H	1.28108	-1.87553	0.24281
H	-0.80568	-3.97034	-3.598
H	-1.15803	-4.43283	-1.92511
H	2.30729	-3.79901	-1.01705
H	0.74526	-4.2819	-0.3261
C	-1.24102	2.44606	0.82459
C	-1.18645	3.04563	-1.51746
C	-1.64753	3.87261	1.12233
H	-0.15496	2.30528	0.91008
H	-1.68644	1.76156	1.56175
C	-1.65893	4.42941	-1.13165
H	-0.08999	3.02219	-1.52569
H	-1.50638	2.73685	-2.52638
H	-1.21967	4.18145	2.0885
H	-2.75228	3.95114	1.22883
H	-1.25698	5.1683	-1.83797
H	-2.7667	4.51544	-1.17326

N	-0.49613	-1.844	-0.92255
N	-1.62996	2.01219	-0.55439
O	-1.18877	4.77644	0.1499
O	0.8088	-3.95949	-2.37501
H	1.63649	0.77848	-0.04185
Cl	0.61956	0.64835	-2.51404
C	1.98261	0.03344	1.95937
H	2.78792	-0.2418	2.64231
C	2.2931	0.96684	0.82437
H	2.06024	2.01813	1.08446
C	3.74022	0.89748	0.36743
C	4.09606	0.61826	-0.95638
C	4.77871	1.12715	1.28951
C	5.44243	0.56523	-1.34345
H	3.29212	0.46649	-1.68252
C	6.12138	1.07468	0.91046
H	4.52157	1.35551	2.32858
C	6.45985	0.78935	-0.41213
H	5.6957	0.34925	-2.38446
H	6.90585	1.26041	1.65081
H	7.50985	0.75105	-0.71577
O	-0.32015	-0.02058	1.47182
C	0.67947	-0.41536	2.16945
N	0.41533	-1.41062	3.14649
C	-0.89253	-1.49726	3.74924
H	-0.9243	-1.12028	4.79504
H	-1.59006	-0.88872	3.15733
H	-1.28533	-2.53553	3.77236
C	1.53257	-1.97001	3.88043
H	1.1959	-2.82289	4.48205
H	2.31887	-2.33199	3.19662
H	2.02733	-1.25224	4.57171

6_L-2

Ni	-0.41948	0.18241	-0.53903
C	1.77338	0.19751	1.39287
C	-0.07518	-1.17621	1.77801
C	2.22206	-0.01063	2.68632
C	0.32521	-1.41824	3.09343
C	1.45187	-0.77359	3.57056
H	3.1879	0.39855	2.99017
H	-0.22787	-2.13415	3.70126
H	1.79177	-0.94078	4.59394
C	2.58462	0.88712	0.33626

H	2.21183	1.91293	0.16183
H	3.61653	1.01237	0.72771
C	-1.25579	-1.83367	1.13913
H	-1.24983	-2.89817	1.42961
H	-2.19568	-1.38106	1.50245
N	0.58093	-0.30403	1.00208
C	3.05225	-1.1912	-0.88389
C	3.07545	0.89803	-2.04962
C	4.56548	-1.19063	-0.92565
H	2.67746	-1.72557	-1.77334
H	2.67673	-1.74534	-0.00322
C	4.59354	0.84516	-2.06415
H	2.69962	0.43839	-2.98114
H	2.72036	1.94284	-2.03305
H	4.95607	-2.21443	-0.99468
H	4.98481	-0.747	0.00221
H	4.99874	1.32105	-2.96941
H	5.00672	1.40129	-1.19438
C	-2.57753	-1.80117	-0.92661
C	-0.30017	-2.58248	-1.04143
C	-3.03133	-3.24771	-0.93026
H	-2.52288	-1.44724	-1.96918
H	-3.28552	-1.15212	-0.38869
C	-0.83798	-3.99252	-1.07358
H	-0.182	-2.18749	-2.06463
H	0.66522	-2.59142	-0.51223
H	-4.01445	-3.32874	-1.41594
H	-3.154	-3.61426	0.11097
H	-0.18166	-4.62614	-1.68316
H	-0.81727	-4.41793	-0.05229
N	2.49826	0.17085	-0.92745
N	-1.22621	-1.64618	-0.33711
O	-2.13633	-4.05498	-1.64253
O	5.04876	-0.48467	-2.05572
C	-1.51506	1.67032	-1.41074
H	-1.33262	0.5515	-1.81924
H	-1.59912	2.0701	-2.43786
C	-2.86612	1.68602	-0.75087
C	-3.99813	1.90359	-1.54626
C	-3.04944	1.34051	0.59739
C	-5.28199	1.78026	-1.01693
H	-3.87182	2.16005	-2.60276
C	-4.3323	1.23198	1.1279
H	-2.17476	1.18177	1.23168

C	-5.4528	1.44286	0.32402
H	-6.15097	1.94838	-1.65708
H	-4.45662	0.97471	2.18278
H	-6.45728	1.34581	0.74254
Cl	1.46081	-3.71112	1.44782
C	-0.22196	2.08483	-0.77936
H	0.52414	2.3206	-1.54886
C	-0.08516	2.8899	0.46301
O	-0.56262	2.55757	1.5438
N	0.721	4.00992	0.37439
C	1.15833	4.65222	1.5908
H	2.25083	4.79602	1.57817
H	0.68944	5.64094	1.72525
H	0.88417	4.0234	2.44354
C	1.16406	4.61437	-0.8572
H	1.22685	5.70481	-0.72689
H	2.16517	4.26823	-1.17832
H	0.45713	4.43315	-1.67493

I-TS$_H$

Ni	0.44272	0.13967	-0.25131
C	2.81349	-1.38143	0.42036
C	1.08558	-2.68491	-0.46321
C	3.63957	-2.49828	0.54263
C	1.84672	-3.84644	-0.34558
C	3.14031	-3.74416	0.16563
H	4.6534	-2.3922	0.93477
H	1.43591	-4.8093	-0.65699
H	3.76278	-4.63618	0.26459
C	3.17785	0.00957	0.84783
H	2.81053	0.13695	1.88117
H	4.27735	0.12672	0.86613
C	-0.26678	-2.59692	-1.10227
H	-0.10803	-2.22471	-2.13164
H	-0.7206	-3.60265	-1.18256
N	1.57634	-1.5064	-0.06907
C	3.08381	1.19335	-1.30192
C	2.41898	2.33018	0.70153
C	4.39875	1.94606	-1.25037
H	2.34857	1.74882	-1.90456
H	3.19702	0.20712	-1.77909
C	3.75786	3.03316	0.71122
H	1.697	2.93691	0.1362
H	1.99917	2.18128	1.70657

H	4.76381	2.15172	-2.26669
H	5.18173	1.33777	-0.74803
H	3.66352	4.04147	1.13753
H	4.49322	2.48546	1.33883
C	-1.62845	-2.07459	0.86184
C	-2.24683	-1.19029	-1.2802
C	-2.72473	-3.10804	0.7104
H	-2.01702	-1.19652	1.39772
H	-0.78674	-2.44112	1.46834
C	-3.32269	-2.2526	-1.37405
H	-2.6864	-0.29347	-0.81878
H	-1.85573	-0.89303	-2.26583
H	-3.1556	-3.3571	1.69032
H	-2.3309	-4.0561	0.28449
H	-4.19286	-1.87374	-1.92873
H	-2.9544	-3.14663	-1.92168
N	2.48974	1.01947	0.03353
N	-1.11885	-1.60713	-0.43744
O	-3.77986	-2.62135	-0.0916
O	4.26055	3.18837	-0.60046
C	-1.39852	2.5207	-0.89579
H	-1.52417	1.81029	-1.71288
H	-1.33492	3.59385	-1.19778
O	-0.33913	1.98315	-0.58475
C	-2.6942	2.24183	-0.29176
C	-3.86487	2.73333	-0.8937
C	-2.78186	1.46381	0.87811
C	-5.10966	2.42415	-0.35739
H	-3.78714	3.34689	-1.79671
C	-4.02951	1.16481	1.41082
H	-1.8561	1.1109	1.35221
C	-5.19214	1.63515	0.79283
H	-6.02023	2.79603	-0.83282
H	-4.09965	0.55887	2.31767
H	-6.17041	1.39169	1.21469
Cl	0.19953	0.29076	2.15556

4_H

Ni	-0.29357	-1.11925	-0.69607
C	-0.08883	-0.99196	2.16557
C	-2.30219	-1.07657	1.41476
C	-0.49632	-0.97339	3.49717
C	-2.78358	-1.03089	2.7232
C	-1.86519	-0.99293	3.77222

H	0.24199	-0.93926	4.3015
H	-3.85887	-1.03774	2.91458
H	-2.2155	-0.97542	4.80673
C	1.32325	-0.85246	1.6817
H	2.04098	-1.0679	2.49435
C	-3.14877	-1.20516	0.18105
H	-3.21842	-2.28099	-0.05816
H	-4.17375	-0.83949	0.38141
N	-0.98747	-1.05454	1.17864
C	1.73946	-3.06377	0.70678
C	2.71555	-1.11839	-0.30174
C	3.08827	-3.36817	1.32885
H	1.64689	-3.57564	-0.2622
H	0.9046	-3.42947	1.32357
C	4.02867	-1.46302	0.36524
H	2.67275	-1.57364	-1.30323
H	2.58546	-0.03503	-0.43077
H	3.23706	-4.45443	1.40202
H	3.1508	-2.96729	2.36349
H	4.87776	-1.1422	-0.25543
H	4.13018	-0.93352	1.33682
C	-2.58044	0.91208	-0.90631
C	-3.02373	-1.01701	-2.25943
C	-3.96158	1.42955	-1.24811
H	-1.84046	1.30432	-1.62163
H	-2.24653	1.25042	0.08753
C	-4.39594	-0.45194	-2.56044
H	-2.31843	-0.66183	-3.03105
H	-2.99881	-2.11666	-2.27515
H	-3.95661	2.52743	-1.30038
H	-4.69825	1.1517	-0.46364
H	-4.7237	-0.7337	-3.57094
H	-5.14737	-0.86104	-1.85168
N	1.55879	-1.62298	0.45494
N	-2.50487	-0.55682	-0.96683
O	-4.39048	0.95791	-2.50715
O	4.14672	-2.85781	0.54976
Cl	-1.08131	-3.48426	-1.02072
H	0.19151	0.42448	-0.82339
H	1.46156	0.20748	1.40087

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Ni	0.03669	-0.15253	-0.64052
C	-0.0365	-2.54116	1.12698

C	-2.03314	-2.13156	-0.00147
C	-0.59753	-3.62216	1.80587
C	-2.66799	-3.1777	0.66538
C	-1.93555	-3.92968	1.58095
H	0.0058	-4.20118	2.50798
H	-3.71665	-3.40243	0.45949
H	-2.40717	-4.75822	2.11397
C	1.37282	-2.07593	1.34807
H	1.98131	-2.91544	1.73296
C	-2.67597	-1.32316	-1.08723
H	-2.31403	-1.73019	-2.04704
H	-3.77338	-1.44408	-1.05406
N	-0.7546	-1.83094	0.25496
C	2.28378	-2.46948	-0.87501
C	3.14671	-0.6574	0.41296
C	3.51085	-3.27381	-0.50376
H	2.45881	-1.93756	-1.81987
H	1.40796	-3.10787	-1.05748
C	4.3592	-1.5078	0.73933
H	3.35157	-0.06178	-0.49228
H	2.95626	0.0537	1.22985
H	3.77735	-3.95102	-1.32651
H	3.33045	-3.91202	0.38749
H	5.25032	-0.87283	0.84294
H	4.21978	-2.02736	1.71244
C	-3.00012	0.82063	-0.00463
C	-2.38414	0.79014	-2.31937
C	-4.42748	1.12463	-0.42425
H	-2.48218	1.7771	0.16317
H	-2.97234	0.24992	0.93684
C	-3.82469	1.08238	-2.6681
H	-1.83405	1.74124	-2.22074
H	-1.86739	0.19924	-3.08864
H	-4.91554	1.7603	0.32854
H	-5.02962	0.19393	-0.49222
H	-3.88524	1.68598	-3.58397
H	-4.38135	0.14156	-2.86371
N	1.93809	-1.45338	0.14458
N	-2.24749	0.08309	-1.0317
O	-4.46467	1.82025	-1.64538
O	4.62631	-2.4391	-0.27836
Cl	0.02087	-1.43077	-2.78321
H	0.49324	0.90929	-1.7207
H	1.34279	-1.32892	2.15917

C	-0.81953	0.90405	2.18493
O	-1.04059	-0.15353	2.78051
C	0.25284	0.98395	1.17996
H	1.1648	0.54145	1.58647
C	0.43213	1.81366	0.04995
H	-0.44118	2.38624	-0.2968
C	1.72768	2.50459	-0.20856
C	2.12148	2.9077	-1.49284
C	2.56067	2.83859	0.86991
C	3.30283	3.61074	-1.69361
H	1.49447	2.62787	-2.34495
C	3.75477	3.53236	0.67076
H	2.25802	2.55399	1.88267
C	4.13174	3.92051	-0.61181
H	3.59007	3.90847	-2.70496
H	4.38994	3.77426	1.52665
H	5.06805	4.46019	-0.77232
N	-1.53932	2.0464	2.50308
C	-1.22598	3.38235	2.06685
H	-1.82238	3.71091	1.1934
H	-1.43811	4.09074	2.88204
H	-0.16425	3.48622	1.81475
C	-2.69687	1.92432	3.35232
H	-2.57792	2.50066	4.28467
H	-3.60337	2.29993	2.84471
H	-2.83414	0.87	3.61309

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Ni	-0.04081	-0.36036	-0.58967
C	-0.24116	-2.56408	1.23487
C	-2.19634	-2.11698	0.01908
C	-0.88624	-3.55639	1.96994
C	-2.90827	-3.07124	0.74105
C	-2.23657	-3.79582	1.72668
H	-0.34259	-4.11718	2.73274
H	-3.96407	-3.25146	0.52812
H	-2.76925	-4.5549	2.30382
C	1.17613	-2.11791	1.45124
H	1.75714	-2.91826	1.94701
C	-2.72694	-1.32052	-1.14138
H	-2.30154	-1.7585	-2.06215
H	-3.82699	-1.41305	-1.20098
N	-0.90773	-1.88626	0.29594
C	2.08506	-2.71694	-0.74612

C	3.00737	-0.84162	0.40916
C	3.30027	-3.5217	-0.33725
H	2.25933	-2.25208	-1.72571
H	1.19266	-3.34929	-0.86771
C	4.2059	-1.69635	0.767
H	3.20664	-0.30396	-0.53377
H	2.84283	-0.08305	1.1873
H	3.53733	-4.26769	-1.10828
H	3.12032	-4.08182	0.60604
H	5.11275	-1.07789	0.81779
H	4.06885	-2.15505	1.77034
C	-2.92069	0.8568	-0.04702
C	-2.3944	0.7779	-2.38175
C	-4.33855	1.24659	-0.41622
H	-2.33449	1.77635	0.09263
H	-2.87914	0.29529	0.89985
C	-3.82315	1.17496	-2.67591
H	-1.77838	1.68953	-2.31671
H	-1.95757	0.15782	-3.17504
H	-4.76436	1.90311	0.35586
H	-4.99631	0.35291	-0.47531
H	-3.87267	1.77992	-3.5916
H	-4.45405	0.27704	-2.8482
N	1.77899	-1.62809	0.20532
N	-2.25136	0.07033	-1.0951
O	-4.36899	1.95457	-1.63296
O	4.43446	-2.69492	-0.19609
Cl	0.25455	-1.02482	-2.77995
H	0.16391	1.84296	-1.16141
H	1.11433	-1.27086	2.15855
C	-0.67853	1.04436	2.04396
O	-0.82867	-0.01778	2.66536
C	0.23515	1.1054	0.90032
H	1.19709	0.70778	1.23969
C	0.41038	2.20366	-0.13209
H	-0.32322	3.01462	-0.01478
C	1.80038	2.77742	-0.23448
C	2.31191	3.16497	-1.48068
C	2.63113	2.90545	0.88653
C	3.60322	3.67093	-1.60456
H	1.68708	3.04882	-2.37155
C	3.92653	3.40708	0.7668
H	2.25729	2.59374	1.86682
C	4.41882	3.79131	-0.47972

H	3.98195	3.95904	-2.58843
H	4.55685	3.4974	1.65538
H	5.43645	4.17658	-0.57438
N	-1.43663	2.14803	2.43406
C	-1.06654	3.52318	2.22308
H	-1.65856	4.03455	1.43245
H	-1.22182	4.09631	3.15919
H	0.00082	3.61217	1.9755
C	-2.55574	1.94279	3.31738
H	-2.3683	2.3449	4.32843
H	-3.45959	2.44359	2.92765
H	-2.74192	0.86898	3.41633

O-TS$_L$

C	1.45215	-1.76569	-0.90671
H	0.91014	-2.64333	-0.44522
C	2.87491	-1.74128	-0.38897
C	3.13872	-1.75626	0.9871
C	3.93471	-1.70289	-1.29827
C	4.45412	-1.75048	1.44381
H	2.29944	-1.72281	1.6938
C	5.25036	-1.70283	-0.83858
H	3.69571	-1.67451	-2.36503
C	5.51199	-1.72978	0.53219
H	4.65782	-1.75252	2.51786
H	6.07891	-1.67961	-1.55129
H	6.54405	-1.72747	0.89247
H	0.96297	-0.91246	-0.0478
O	1.21174	-1.5025	-2.12512
Ni	-0.46736	0.14076	0.24359
C	-1.80325	2.47071	-0.43366
C	-3.15448	0.66329	0.26159
C	-2.91515	3.29635	-0.55272
C	-4.30269	1.43204	0.13442
C	-4.17779	2.76824	-0.26495
H	-2.80032	4.33163	-0.88004
H	-5.28082	0.99847	0.3511
H	-5.06554	3.39547	-0.36175
C	-0.39707	2.78458	-0.83617
H	-0.14401	3.82904	-0.59498
C	-3.01816	-0.73953	0.75851
H	-2.75959	-0.69835	1.83404
H	-3.95044	-1.31681	0.63725
N	-1.95019	1.20131	-0.02019

C	1.16711	2.3758	1.01911
C	1.70962	1.56425	-1.15797
C	2.07845	3.55991	0.76022
H	1.7043	1.54887	1.50332
H	0.34948	2.62973	1.70966
C	2.52093	2.81181	-1.41086
H	2.37143	0.8721	-0.62523
H	1.3635	1.02458	-2.05414
H	2.59746	3.82509	1.69163
H	1.49846	4.46016	0.46341
H	3.36209	2.58318	-2.07895
H	1.92259	3.60746	-1.90516
C	-2.05626	-1.66612	-1.332
C	-1.47462	-2.63086	0.81488
C	-2.96817	-2.85835	-1.55781
H	-1.06701	-1.82819	-1.7927
H	-2.47641	-0.76478	-1.80379
C	-2.43367	-3.75961	0.51083
H	-0.4702	-2.91581	0.47012
H	-1.39174	-2.39815	1.88448
H	-2.99314	-3.10492	-2.62798
H	-4.01182	-2.61911	-1.25874
H	-2.07976	-4.68684	0.98085
H	-3.44291	-3.55376	0.92653
N	0.57979	1.83007	-0.23747
N	-1.84075	-1.38406	0.10744
O	-2.51944	-4.00068	-0.87465
O	3.06935	3.28633	-0.20028
Cl	-0.31321	-0.15906	2.68148
H	-0.31556	2.70631	-1.93459

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C	-0.58513	-2.24659	-1.11896
H	-0.22958	-2.13216	-2.15225
C	-2.04943	-2.08648	-1.04151
C	-2.66541	-1.19641	-1.94087
C	-2.85043	-2.79385	-0.13488
C	-4.0408	-0.99136	-1.90476
H	-2.03336	-0.61788	-2.6248
C	-4.2283	-2.59105	-0.10704
H	-2.38586	-3.49796	0.5569
C	-4.828	-1.68494	-0.98337
H	-4.50172	-0.27818	-2.59272
H	-4.84149	-3.14684	0.60724

H	-5.90813	-1.52225	-0.95085
H	-0.32473	-0.7658	-0.78187
Ni	0.23862	0.72694	-0.38725
C	0.46072	2.88618	1.38514
C	2.3402	2.50593	0.02156
C	1.0632	3.9926	1.9691
C	3.00969	3.58334	0.58687
C	2.35415	4.34605	1.56011
H	0.54445	4.55819	2.74583
H	4.02428	3.83051	0.26765
H	2.85468	5.20479	2.01112
C	-0.81928	2.22553	1.77907
H	-1.53562	2.94573	2.20808
C	2.80059	1.57939	-1.05431
H	2.37407	1.92161	-2.01669
H	3.90016	1.54931	-1.14028
N	1.09169	2.19483	0.42171
C	-2.10536	2.34273	-0.31184
C	-2.351	0.43729	1.13275
C	-3.39462	2.89113	0.26453
H	-2.30471	1.73995	-1.20917
H	-1.42184	3.13952	-0.64089
C	-3.61369	1.0592	1.68525
H	-2.61951	-0.17169	0.26469
H	-1.8453	-0.23294	1.84067
H	-3.93695	3.4432	-0.51549
H	-3.19736	3.61777	1.0823
H	-4.32372	0.26596	1.95665
H	-3.41663	1.64522	2.60936
C	2.72604	-0.44849	0.37074
C	2.37005	-0.63845	-2.00154
C	4.13011	-0.9803	0.16031
H	2.04298	-1.28728	0.57935
H	2.68506	0.23763	1.23009
C	3.78957	-1.14373	-2.13086
H	1.70779	-1.49869	-1.84808
H	2.00176	-0.09544	-2.88349
H	4.44618	-1.56751	1.03465
H	4.85603	-0.14602	0.05526
H	3.86174	-1.85885	-2.96128
H	4.49911	-0.31988	-2.35289
N	-1.3906	1.45587	0.64568
N	2.19241	0.23983	-0.82618
O	4.19625	-1.82695	-0.96046

O	-4.24777	1.86973	0.72064
Cl	-0.08822	1.4501	-2.76215
H	-0.59557	1.49479	2.57631
C	0.25393	-2.98107	-0.29332
H	1.20063	-3.30434	-0.73649
C	0.19234	-2.93385	1.16107
O	-0.55814	-2.16815	1.77724
N	1.12014	-3.71256	1.84215
C	1.33469	-3.47961	3.24501
H	0.54358	-2.81835	3.61283
H	1.30773	-4.4211	3.81606
H	2.31248	-3.00032	3.44034
C	2.03618	-4.60022	1.17166
H	2.43268	-5.32703	1.89332
H	1.53145	-5.16911	0.38001
H	2.89841	-4.07746	0.71407

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C	0.57346	2.07694	-1.17207
H	0.27529	2.13128	-2.23236
C	2.07929	2.06519	-1.11155
C	2.78097	1.21924	-1.98497
C	2.79732	2.816	-0.17789
C	4.16685	1.1067	-1.90264
H	2.21682	0.61073	-2.69997
C	4.18559	2.7068	-0.0995
H	2.25289	3.4825	0.49612
C	4.87529	1.84684	-0.95428
H	4.6988	0.43283	-2.57918
H	4.73459	3.29724	0.63931
H	5.96233	1.75777	-0.88654
H	0.29741	0.98916	-0.88637
Ni	-0.27135	-0.68378	-0.34899
C	-0.49303	-2.76208	1.50629
C	-2.3708	-2.41779	0.12535
C	-1.04261	-3.9268	2.02403
C	-2.98719	-3.55775	0.62538
C	-2.3106	-4.32229	1.58188
H	-0.49861	-4.51069	2.76923
H	-3.97344	-3.85511	0.26309
H	-2.77	-5.22825	1.98123
C	0.7861	-2.08437	1.86844
H	1.49168	-2.76958	2.36504
C	-2.8339	-1.51391	-0.97216

H	-2.42976	-1.89146	-1.93076
H	-3.93378	-1.47625	-1.05051
N	-1.16	-2.04796	0.58369
C	2.05196	-2.41444	-0.21667
C	2.36624	-0.40267	1.06003
C	3.33318	-2.94791	0.39458
H	2.25924	-1.89519	-1.16265
H	1.34551	-3.22206	-0.46155
C	3.61377	-1.01436	1.65485
H	2.65088	0.11484	0.13806
H	1.88157	0.33951	1.70843
H	3.85018	-3.58039	-0.34005
H	3.12169	-3.59623	1.27268
H	4.34684	-0.22232	1.8579
H	3.40812	-1.51979	2.62302
C	-2.72467	0.54581	0.4034
C	-2.41117	0.69538	-1.96538
C	-4.13611	1.06276	0.21212
H	-2.04524	1.39756	0.54824
H	-2.65128	-0.1021	1.28841
C	-3.83716	1.19026	-2.08334
H	-1.76249	1.57018	-1.80969
H	-2.0522	0.158	-2.85327
H	-4.43191	1.66536	1.08265
H	-4.86101	0.2231	0.14305
H	-3.91899	1.8917	-2.92452
H	-4.54154	0.35731	-2.28906
N	1.37258	-1.43091	0.66739
N	-2.21699	-0.17706	-0.78744
O	-4.23555	1.88608	-0.92223
O	4.21709	-1.91671	0.75365
Cl	0.14129	-1.27116	-2.64534
H	0.5624	-1.275	2.58546
C	-0.20477	2.99573	-0.34381
H	-0.86683	3.70795	-0.83886
C	-0.28924	2.76099	1.05484
O	0.24508	1.75379	1.59653
N	-1.06889	3.63075	1.82931
C	-1.38061	3.26485	3.18277
H	-0.6457	2.52808	3.52472
H	-1.34472	4.14359	3.84769
H	-2.38903	2.81245	3.28963
C	-1.89192	4.63663	1.21227
H	-2.32635	5.28051	1.98871

H	-1.30266	5.28289	0.54483
H	-2.72646	4.21417	0.61623

O-TS$_H$

Ni	-0.28432	-0.1973	-0.63044
C	-0.3029	-2.51442	1.05609
C	-2.44891	-1.73954	0.5085
C	-0.84394	-3.52748	1.85036
C	-3.05059	-2.70926	1.30384
C	-2.22747	-3.61357	1.97851
H	-0.18441	-4.22453	2.37047
H	-4.13778	-2.75953	1.38902
H	-2.66993	-4.38816	2.60865
C	1.15417	-2.22445	0.9053
H	1.75207	-3.14518	1.0282
C	-3.17605	-0.7467	-0.35439
H	-3.2614	-1.16738	-1.37207
H	-4.21305	-0.61363	0.00419
N	-1.11565	-1.66354	0.41314
C	1.43844	-2.38555	-1.53601
C	2.68505	-0.72934	-0.30255
C	2.70033	-3.22068	-1.61612
H	1.36804	-1.72968	-2.4179
H	0.53783	-3.02138	-1.52033
C	3.90153	-1.61906	-0.43312
H	2.64565	-0.00869	-1.13509
H	2.70598	-0.16979	0.64446
H	2.71719	-3.79594	-2.55264
H	2.74035	-3.95878	-0.78573
H	4.81401	-1.01143	-0.497
H	4.00632	-2.27057	0.46055
C	-2.5142	1.32343	0.76244
C	-2.83979	1.33317	-1.61554
C	-3.87099	1.98115	0.91657
H	-1.73947	2.10339	0.69743
H	-2.2658	0.69547	1.63224
C	-4.19045	1.97728	-1.39054
H	-2.06814	2.10454	-1.75658
H	-2.81741	0.71561	-2.52448
H	-3.86809	2.65662	1.78268
H	-4.66232	1.22411	1.10519
H	-4.43821	2.65147	-2.22151
H	-4.99416	1.21093	-1.34674
N	1.42791	-1.50615	-0.34847

N	-2.4207	0.50883	-0.46713
O	-4.19519	2.75337	-0.21352
O	3.84721	-2.41001	-1.60199
Cl	0.27441	0.7382	-2.58434
C	0.75778	1.03074	1.88047
H	-0.17051	1.51082	2.30963
H	0.28467	0.62954	0.9842
O	1.30374	0.11436	2.608
C	1.65149	2.12599	1.32242
C	2.86039	2.39553	1.9696
C	1.30174	2.87723	0.19656
C	3.69731	3.41072	1.50984
H	3.1226	1.78191	2.83612
C	2.139	3.88738	-0.27065
H	0.38522	2.63407	-0.35424
C	3.33835	4.16078	0.38936
H	4.63903	3.61785	2.0259
H	1.86317	4.45184	-1.16505
H	3.99808	4.95096	0.02182
H	1.41636	-1.52555	1.73765

O_2-TS_H

Ni	-0.01886	-0.96038	-0.74142
C	-0.01669	-1.40338	2.08287
C	-2.11825	-1.72323	1.10302
C	-0.53943	-1.61546	3.35586
C	-2.71302	-1.90376	2.34872
C	-1.90854	-1.85084	3.48715
H	0.11485	-1.58324	4.22961
H	-3.7857	-2.09421	2.42301
H	-2.34787	-1.99781	4.47603
C	1.41361	-1.05092	1.78577
H	2.07656	-1.45092	2.57621
C	-2.81829	-1.86215	-0.22077
H	-2.6647	-2.89256	-0.58865
H	-3.91029	-1.74716	-0.08838
N	-0.80723	-1.45902	1.00063
C	1.95059	-2.92345	0.28744
C	2.98997	-0.79332	-0.07708
C	3.2505	-3.40899	0.89949
H	1.93825	-3.13267	-0.79465
H	1.08404	-3.43707	0.73487
C	4.25237	-1.33627	0.55405
H	3.00566	-0.96061	-1.16578

H	2.8873	0.2864	0.09894
H	3.39269	-4.4798	0.69675
H	3.22825	-3.29272	2.00519
H	5.13858	-0.87688	0.09581
H	4.28999	-1.09662	1.63807
C	-2.62915	0.44611	-0.95269
C	-2.56954	-1.29765	-2.60343
C	-4.05622	0.74083	-1.36363
H	-1.9366	1.08776	-1.52068
H	-2.47221	0.66243	0.11382
C	-4.00509	-0.96412	-2.95015
H	-1.88072	-0.72889	-3.24562
H	-2.33978	-2.35979	-2.7734
H	-4.26396	1.81458	-1.25921
H	-4.7767	0.21088	-0.70357
H	-4.19557	-1.14905	-4.01633
H	-4.71152	-1.60645	-2.38067
N	1.78122	-1.46494	0.4312
N	-2.23923	-0.9516	-1.21184
O	-4.28586	0.39703	-2.70981
O	4.35753	-2.73138	0.36144
Cl	0.82198	-1.36461	-2.78142
H	0.16863	0.73305	-0.28027
H	1.52329	0.0498	1.82352
C	2.9634	2.80525	0.17856
O	3.81808	3.29131	0.92198
C	1.66183	2.4468	0.73855
H	1.68444	2.47896	1.83319
C	0.42116	2.26015	0.11362
H	0.33838	2.58329	-0.93075
C	-0.81998	2.50082	0.88618
C	-1.83109	3.31367	0.35373
C	-1.0407	1.91164	2.14009
C	-3.02687	3.51719	1.03883
H	-1.67463	3.78547	-0.6214
C	-2.23954	2.10236	2.82219
H	-0.25982	1.2848	2.5803
C	-3.2432	2.90187	2.27209
H	-3.7985	4.15843	0.60438
H	-2.39206	1.62207	3.79276
H	-4.18379	3.0532	2.80691
N	3.23247	2.62808	-1.17512
C	2.4484	1.87251	-2.12002
H	1.86161	2.51353	-2.80457

H	3.11362	1.26207	-2.7519
H	1.7626	1.16867	-1.63843
C	4.44653	3.19258	-1.70679
H	5.13958	2.40661	-2.05516
H	4.23253	3.8478	-2.56804
H	4.94287	3.7727	-0.92306

7_H

Ni	-0.04122	-1.05982	-0.75404
C	0.02994	-1.42309	2.0699
C	-2.09578	-1.6978	1.12657
C	-0.47271	-1.64597	3.34785
C	-2.66676	-1.88468	2.37999
C	-1.84286	-1.85935	3.50699
H	0.20089	-1.63584	4.20763
H	-3.74063	-2.06237	2.46995
H	-2.2653	-2.01282	4.50193
C	1.46288	-1.09012	1.76519
H	2.125	-1.53336	2.53318
C	-2.83091	-1.83325	-0.17822
H	-2.73494	-2.87853	-0.52281
H	-3.91366	-1.66526	-0.02581
N	-0.77876	-1.44704	0.99256
C	1.927	-2.92098	0.1937
C	3.03761	-0.81923	-0.09803
C	3.21041	-3.47576	0.78056
H	1.90471	-3.08877	-0.89582
H	1.04468	-3.42119	0.62454
C	4.28362	-1.42917	0.50609
H	3.04225	-0.94907	-1.19195
H	2.98007	0.2581	0.11648
H	3.31295	-4.54215	0.53504
H	3.19623	-3.40244	1.8899
H	5.18372	-0.98578	0.05934
H	4.33405	-1.22902	1.59754
C	-2.55247	0.44184	-0.9949
C	-2.59173	-1.35852	-2.58193
C	-3.96816	0.78924	-1.40379
H	-1.83512	1.02839	-1.59367
H	-2.38164	0.6867	0.06304
C	-4.01411	-0.97299	-2.92746
H	-1.88186	-0.84588	-3.24833
H	-2.41606	-2.4364	-2.71349
H	-4.12622	1.87426	-1.33666

H	-4.70173	0.31653	-0.71562
H	-4.22498	-1.18557	-3.98458
H	-4.74258	-1.56114	-2.3281
N	1.80692	-1.4627	0.39266
N	-2.23208	-0.98099	-1.20696
O	-4.23055	0.40754	-2.73337
O	4.34013	-2.81838	0.26413
Cl	0.79427	-1.12473	-2.82144
H	0.22677	0.96328	-0.1308
H	1.60559	0.00597	1.84348
C	2.89132	2.85015	0.23273
O	3.70072	3.40679	0.98091
C	1.63816	2.36095	0.78398
H	1.63707	2.41809	1.87797
C	0.35046	2.08538	0.12226
H	0.28829	2.56163	-0.86872
C	-0.85007	2.47526	0.93943
C	-1.77792	3.40594	0.45789
C	-1.10256	1.86923	2.17743
C	-2.93624	3.70213	1.1755
H	-1.59313	3.89435	-0.50411
C	-2.26242	2.15496	2.89446
H	-0.37922	1.15365	2.58271
C	-3.19011	3.0683	2.39132
H	-3.64779	4.43117	0.77968
H	-2.44315	1.66005	3.85278
H	-4.1006	3.29418	2.95131
N	3.1672	2.71288	-1.12507
C	2.45204	1.88188	-2.05953
H	1.83279	2.45992	-2.77088
H	3.163	1.29485	-2.66415
H	1.80474	1.15035	-1.56878
C	4.32913	3.37482	-1.65856
H	5.07168	2.64818	-2.03211
H	4.0588	4.03136	-2.50277
H	4.79276	3.97332	-0.86822

B_L

Ni	-0.10775	-0.08591	0.4891
Cl	-1.05594	-1.73475	1.60661
O	-4.04591	-0.48663	-0.7941
O	1.71722	-3.36774	-1.31044
N	0.85971	1.46871	0.22528
N	-1.70812	1.08655	-0.07423

N	1.76947	-0.92909	0.23248
C	-1.99008	0.55022	-1.45353
H	-1.02666	0.42525	-1.96219
H	-2.56429	1.31454	-1.99557
C	-2.79755	-0.72678	-1.41528
H	-3.0074	-1.06239	-2.43553
H	-2.24798	-1.525	-0.88808
C	-3.83185	-0.13276	0.56496
H	-3.37173	-0.96649	1.10609
H	-4.81872	0.06284	0.99368
C	-2.98618	1.12062	0.69577
H	-3.55907	1.9815	0.31872
H	-2.73376	1.31505	1.74154
C	-1.19653	2.44408	-0.18366
H	-1.91708	3.22534	-0.39839
C	0.15931	2.60841	-0.13239
C	0.93603	3.78861	-0.38451
H	0.42727	4.69081	-0.7096
C	2.29621	3.75528	-0.24449
H	2.8739	4.65465	-0.44191
C	2.97338	2.56537	0.13631
H	4.04569	2.54207	0.29321
C	2.20013	1.44856	0.3517
C	2.66353	0.1068	0.82098
H	3.71345	-0.09855	0.5632
H	2.56198	0.02864	1.91125
C	2.0243	-0.99333	-1.23606
H	3.10425	-1.14387	-1.3952
H	1.74145	-0.03422	-1.67948
C	1.27444	-2.14692	-1.85772
H	0.18606	-2.01826	-1.69666
H	1.46275	-2.18488	-2.93401
C	1.40953	-3.39074	0.07576
H	1.77594	-4.34427	0.46376
H	0.32313	-3.34443	0.22248
C	2.07741	-2.25441	0.82775
H	1.73743	-2.24105	1.86754
H	3.17104	-2.38737	0.80616

B_L-TS1

Ni	-0.44784	0.21613	-0.71429
C	-2.01143	1.46519	1.17549
C	-0.26305	2.79709	0.28309
C	-2.39991	2.52803	2.0091

C	-0.58661	3.86763	1.10464
C	-1.68366	3.71675	1.96766
H	-3.24422	2.40359	2.68891
H	-0.00391	4.78928	1.07695
H	-1.97337	4.54381	2.61982
C	-2.44202	0.08551	1.16902
H	-3.43606	-0.10974	1.59496
C	0.81683	2.72105	-0.74456
H	0.41987	3.04478	-1.72198
H	1.65637	3.39502	-0.50994
N	-0.96895	1.6608	0.33095
C	-3.19386	-0.03012	-1.2175
C	-2.3244	-1.98615	-0.1237
C	-4.59112	-0.56241	-0.97475
H	-2.81521	-0.38475	-2.18951
H	-3.18512	1.07003	-1.22835
C	-3.75027	-2.44817	0.09407
H	-1.95133	-2.37948	-1.07876
H	-1.65354	-2.32851	0.67412
H	-5.25561	-0.26142	-1.79645
H	-5.0118	-0.13099	-0.04202
H	-3.79326	-3.54495	0.05718
H	-4.12747	-2.14443	1.0919
C	2.03787	0.82461	0.27415
C	2.08273	1.12011	-2.10759
C	3.40102	1.47467	0.34937
H	2.1607	-0.25651	0.125
H	1.44219	0.93668	1.19245
C	3.44058	1.776	-1.95762
H	2.19952	0.03781	-2.24603
H	1.53408	1.49673	-2.98262
H	3.9747	1.01329	1.16405
H	3.32742	2.55874	0.58078
H	4.05324	1.55686	-2.84291
H	3.35065	2.88223	-1.9004
N	-2.23652	-0.50712	-0.18666
N	1.24724	1.30531	-0.89813
O	4.13352	1.28062	-0.83944
O	-4.6056	-1.96662	-0.91916
Cl	-0.05214	-1.2391	-2.32707
H	-1.47764	-0.41562	1.74876
C	0.24383	-1.8513	2.42605
H	-0.46875	-2.70812	2.30771
H	0.42357	-1.78305	3.52491

O	-0.23258	-0.67833	1.88732
C	1.53791	-2.21442	1.74049
C	1.50893	-2.72286	0.43595
C	2.77902	-1.88301	2.29539
C	2.67909	-2.86877	-0.30553
H	0.54803	-2.96775	-0.02597
C	3.95718	-2.03745	1.56255
H	2.81578	-1.48083	3.31357
C	3.9098	-2.51992	0.2544
H	2.62344	-3.23954	-1.33235
H	4.91863	-1.76912	2.01018
H	4.82916	-2.6215	-0.32759

B_{L2}-TS2

Ni	-0.00885	-1.11884	-0.64932
C	0.06646	-1.24092	2.19478
C	-2.06775	-1.55144	1.28481
C	-0.43001	-1.36789	3.48778
C	-2.63325	-1.63786	2.55229
C	-1.80219	-1.54869	3.6697
H	0.24993	-1.30797	4.3405
H	-3.70948	-1.78981	2.66022
H	-2.21987	-1.62713	4.67541
C	1.49927	-0.93476	1.8627
H	2.16268	-1.31762	2.66156
C	-2.82415	-1.79367	0.00718
H	-2.81887	-2.88083	-0.18801
H	-3.8887	-1.52191	0.13799
N	-0.74886	-1.33298	1.12527
C	1.96656	-2.87941	0.43826
C	3.06987	-0.80041	-0.02031
C	3.25409	-3.38246	1.06048
H	1.94105	-3.13512	-0.63391
H	1.08716	-3.34448	0.9124
C	4.32082	-1.3628	0.61944
H	3.06928	-1.00779	-1.10236
H	3.01021	0.29027	0.11555
H	3.35773	-4.4651	0.90221
H	3.24708	-3.2184	2.16017
H	5.21716	-0.95446	0.13361
H	4.37957	-1.08147	1.69255
C	-2.5107	0.29526	-1.20902
C	-2.48944	-1.77411	-2.42848
C	-3.90699	0.54851	-1.73945

H	-1.76441	0.76026	-1.87574
H	-2.38595	0.73766	-0.20982
C	-3.89932	-1.47377	-2.8898
H	-1.76112	-1.38401	-3.15485
H	-2.30312	-2.8554	-2.34891
H	-4.06562	1.62596	-1.88607
H	-4.67113	0.21095	-1.00624
H	-4.07745	-1.89313	-3.88942
H	-4.64888	-1.93086	-2.20726
N	1.84308	-1.40989	0.52194
N	-2.18331	-1.14083	-1.13547
O	-4.11296	-0.08266	-2.98048
O	4.37739	-2.76651	0.4832
Cl	0.85195	-1.34918	-2.69949
H	0.17672	0.94241	-0.20634
H	1.63966	0.16435	1.8573
C	2.77999	2.94433	-0.01271
O	3.56996	3.60133	0.67173
C	1.56251	2.43269	0.59633
H	1.57328	2.56108	1.68423
C	0.27596	2.08275	-0.03123
H	0.19764	2.48883	-1.05239
C	-0.92713	2.50159	0.76783
C	-1.87962	3.37923	0.2352
C	-1.15244	1.98177	2.04918
C	-3.03393	3.7043	0.94687
H	-1.7169	3.80209	-0.76127
C	-2.30698	2.29747	2.76178
H	-0.40755	1.31744	2.49669
C	-3.25828	3.15549	2.20934
H	-3.76403	4.39149	0.51164
H	-2.4634	1.87082	3.75639
H	-4.16464	3.40522	2.76589
N	3.03122	2.72184	-1.36353
C	2.37208	1.74834	-2.19463
H	1.71225	2.20161	-2.95759
H	3.1174	1.14604	-2.74012
H	1.77614	1.03555	-1.61858
C	4.13837	3.40604	-1.97818
H	4.93892	2.70363	-2.27027
H	3.8168	3.93517	-2.89079
H	4.55229	4.12643	-1.266

B_2

Ni	-0.13362	-0.17582	0.49883
Cl	-0.5976	-1.46464	2.24382
O	-3.7784	-1.23546	-0.87151
O	1.96399	-3.21345	-1.29645
N	0.61201	1.53502	0.09531
N	-1.94916	0.86471	-0.17685
N	1.99037	-0.71481	0.07682
C	-2.10381	0.34564	-1.56543
H	-1.13993	0.46492	-2.07764
H	-2.85424	0.94593	-2.10265
C	-2.54022	-1.1038	-1.52839
H	-2.66332	-1.50062	-2.54043
H	-1.76613	-1.7108	-1.01174
C	-3.64643	-0.80339	0.4782
H	-2.92209	-1.4395	1.00805
H	-4.62794	-0.92857	0.94205
C	-3.20973	0.6444	0.56399
H	-3.99161	1.30066	0.14545
H	-3.03987	0.9319	1.60584
C	-1.58963	2.26024	-0.21035
H	-2.37874	2.98535	-0.39491
C	-0.25793	2.59094	-0.13351
C	0.30692	3.9029	-0.2682
H	-0.357	4.74646	-0.43301
C	1.66107	4.06983	-0.19352
H	2.08864	5.06189	-0.31094
C	2.52192	2.96314	0.04465
H	3.59733	3.08676	0.11641
C	1.94225	1.72797	0.21237
C	2.6769	0.4756	0.60896
H	3.73278	0.50762	0.2936
H	2.66533	0.3831	1.70379
C	2.1953	-0.81387	-1.38088
H	3.27438	-0.88322	-1.60151
H	1.80867	0.09996	-1.84711
C	1.4876	-2.04017	-1.91318
H	0.3966	-1.9327	-1.74093
H	1.65334	-2.14964	-2.98826
C	1.74286	-3.14123	0.10462
H	2.11275	-4.07649	0.53037
H	0.66282	-3.06461	0.31612
C	2.45255	-1.95482	0.72366
H	2.20932	-1.89107	1.78938
H	3.54454	-2.05918	0.60462

B-TS1

Ni	0.53269	0.09074	-0.50502
C	1.15386	2.52596	0.76994
C	3.02674	1.53256	-0.29328
C	2.00556	3.48772	1.36416
C	3.91012	2.44405	0.26925
C	3.36324	3.44207	1.09706
H	1.58857	4.24645	2.02941
H	4.98417	2.37465	0.08961
H	4.02462	4.18463	1.55112
C	-0.23677	2.27739	1.04629
H	-0.77684	3.09576	1.54581
C	3.36906	0.32245	-1.1145
H	3.0197	0.4707	-2.15094
H	4.46096	0.16191	-1.14691
N	1.71455	1.6247	-0.07207
C	-1.03453	2.52295	-1.30024
C	-2.28226	1.17635	0.22151
C	-2.03697	3.63411	-1.09284
H	-1.34281	1.88326	-2.14099
H	-0.03562	2.91139	-1.5464
C	-3.27455	2.31399	0.36774
H	-2.60086	0.51917	-0.60283
H	-2.25843	0.56765	1.13678
H	-2.14454	4.23283	-2.00805
H	-1.6976	4.32281	-0.29015
H	-4.28707	1.91273	0.51748
H	-3.03167	2.93072	1.25978
C	3.04578	-1.24099	0.76207
C	2.70819	-2.0139	-1.48306
C	4.39727	-1.92471	0.75816
H	2.28526	-1.93736	1.15081
H	3.03652	-0.36073	1.4214
C	4.06697	-2.67942	-1.42118
H	1.94227	-2.73449	-1.15061
H	2.43275	-1.70607	-2.50124
H	4.64523	-2.28865	1.765
H	5.199	-1.21221	0.46887
H	4.06963	-3.60168	-2.01813
H	4.85064	-2.01865	-1.84804
N	-0.92817	1.6551	-0.1016
N	2.61723	-0.84257	-0.59342
O	4.40321	-3.04197	-0.09954

O	-3.31415	3.11813	-0.78584
Cl	0.21687	-0.23828	-2.73099
H	0.01053	0.92632	1.6974
H	-2.14882	-3.5012	1.34556
C	-0.54037	-1.13703	1.77141
O	0.35301	-0.12731	1.65363
C	-0.59734	-2.07439	0.77502
H	0.21331	-2.02619	0.03512
C	-1.71454	-3.02857	0.45281
H	-1.31194	-3.85706	-0.15047
C	-2.8124	-2.33803	-0.32121
C	-2.62224	-2.01127	-1.66949
C	-3.99842	-1.93302	0.30224
C	-3.58263	-1.28749	-2.37139
H	-1.68833	-2.28798	-2.16626
C	-4.96756	-1.21535	-0.40004
H	-4.16451	-2.18309	1.3559
C	-4.7605	-0.88515	-1.73906
H	-3.39757	-1.02429	-3.41584
H	-5.8891	-0.90977	0.10317
H	-5.51279	-0.31323	-2.28757
N	-1.29187	-1.14983	2.92802
C	-1.70242	-2.39133	3.53233
H	-1.07245	-3.2158	3.17484
H	-1.5779	-2.32567	4.6244
H	-2.75855	-2.65356	3.34049
C	-1.45735	0.02592	3.74679
H	-0.78914	0.02272	4.62744
H	-1.25971	0.94283	3.17956
H	-2.49324	0.08935	4.11631

B_4

Ni	-0.93794	1.65262	0.15098
C	-1.64054	3.50517	2.18312
C	0.70809	3.08512	1.96004
C	-1.3607	4.30586	3.34243
C	1.00584	3.83263	3.077
C	-0.07025	4.4621	3.76875
H	-2.19199	4.78111	3.86757
H	2.03853	3.93856	3.41559
H	0.14051	5.07226	4.65032
C	-2.89072	3.25561	1.6535
H	-3.80576	3.63419	2.11459

C	1.73715	2.41703	1.08897
H	2.03934	3.11942	0.29478
H	2.65458	2.20923	1.66984
N	-0.56016	2.93757	1.51006
C	-2.74607	3.50771	-0.74431
C	-4.12604	1.73697	0.17164
C	-4.01016	4.2817	-1.04337
H	-2.42081	2.9011	-1.60768
H	-1.94237	4.17833	-0.41532
C	-5.33868	2.58073	-0.16466
H	-3.8935	1.05678	-0.66322
H	-4.29811	1.11805	1.06295
H	-3.89038	4.90723	-1.93572
H	-4.23704	4.95832	-0.19017
H	-6.19506	1.94225	-0.42228
H	-5.64243	3.19664	0.70865
C	1.15374	0.03961	1.30178
C	1.87891	0.87223	-0.82511
C	2.53198	-0.56477	1.49221
H	0.48321	-0.69181	0.82103
H	0.70442	0.32194	2.26741
C	3.24398	0.27829	-0.55946
H	1.24095	0.14355	-1.34969
H	1.94637	1.76943	-1.45829
H	2.46044	-1.50565	2.05566
H	3.18058	0.11441	2.08567
H	3.71936	-0.04083	-1.49775
H	3.91601	1.03187	-0.09386
N	-2.93728	2.57142	0.39985
N	1.18367	1.22687	0.42332
O	3.14308	-0.8644	0.25995
O	-5.09275	3.41047	-1.27939
Cl	-1.43397	0.04582	-1.27877
C	-2.45961	-1.02467	2.5764
H	-1.70181	-0.5512	3.22321
H	-2.11508	-0.83825	1.53428
O	-3.65632	-0.3743	2.84386
C	-2.4962	-2.50564	2.82968
C	-3.54856	-3.08574	3.54562
C	-1.47678	-3.33224	2.34087
C	-3.59371	-4.46526	3.74705
H	-4.34034	-2.44468	3.94111
C	-1.51515	-4.70887	2.55099
H	-0.64982	-2.8887	1.77591

C	−2.58075	−5.28232	3.24822
H	−4.42826	−4.90455	4.29989
H	−0.7142	−5.34136	2.15927
H	−2.61557	−6.36257	3.40631
H	−3.14485	2.25561	2.00495

B_2-TS1

Ni	0.39208	0.20633	-0.57046
C	3.16429	0.08755	0.4441
C	2.51804	-1.80014	-0.768
C	4.45316	-0.41736	0.61891
C	3.77771	-2.37914	-0.61012
C	4.754	-1.67085	0.08793
H	5.20324	0.1605	1.16347
H	3.9895	-3.36229	-1.03616
H	5.75272	-2.09485	0.21575
C	2.6754	1.38712	1.02001
H	3.53708	2.04642	1.23686
C	1.40146	-2.40055	-1.57119
H	1.46753	-1.96277	-2.58283
H	1.54203	-3.49363	-1.66241
N	2.24736	-0.605	-0.2353
C	2.26447	2.68911	-1.00386
C	0.81076	2.96434	0.87672
C	2.95355	3.98118	-0.61953
H	1.4536	2.89101	-1.71782
H	2.9372	1.98882	-1.52136
C	1.54472	4.2459	1.21657
H	-0.03569	3.19964	0.20978
H	0.40491	2.4714	1.772
H	3.29645	4.5116	-1.51843
H	3.85477	3.79352	0.00318
H	0.86379	4.97406	1.6798
H	2.35294	4.04683	1.95397
C	-0.26453	-2.77181	0.17192
C	-1.00469	-2.13103	-2.00786
C	-0.65562	-4.20418	-0.13784
H	-1.13611	-2.27029	0.61965
H	0.56436	-2.71838	0.89572
C	-1.38169	-3.57341	-2.26323
H	-1.86372	-1.58434	-1.58441
H	-0.70907	-1.59468	-2.92052
H	-1.00108	-4.71278	0.77467
H	0.21299	-4.78456	-0.51586

H	-2.26337	-3.63549	-2.91576
H	-0.55842	-4.11025	-2.78129
N	1.66233	2.00738	0.15902
N	0.09264	-2.01257	-1.03275
O	-1.71405	-4.2468	-1.06277
O	2.07522	4.85197	0.06172
Cl	0.89458	0.49459	-2.88901
H	-1.08815	0.70592	-0.72617
H	2.194	1.16482	1.98676
C	-2.1914	-0.14376	1.77829
H	-2.98697	-0.87102	1.95824
C	-2.39563	0.92777	0.94429
H	-1.6311	1.70176	0.93546
C	-3.62938	1.25527	0.24696
C	-3.74358	2.49806	-0.40431
C	-4.72789	0.37741	0.18514
C	-4.9047	2.85421	-1.07883
H	-2.88818	3.17964	-0.38744
C	-5.88972	0.73276	-0.49061
H	-4.66469	-0.604	0.66213
C	-5.98627	1.97298	-1.12437
H	-4.96593	3.82286	-1.58069
H	-6.72883	0.03363	-0.52911
H	-6.89817	2.24747	-1.6598
O	0.15359	0.04126	1.63563
C	-0.85164	-0.44722	2.21254
N	-0.66857	-1.35653	3.2307
C	0.64161	-1.8713	3.52969
H	0.9392	-1.64407	4.56688
H	0.67891	-2.96839	3.40916
H	1.37196	-1.41689	2.85119
C	-1.77099	-1.91403	3.97051
H	-2.57696	-1.17886	4.08628
H	-2.19609	-2.81876	3.49635
H	-1.43392	-2.1967	4.97744

B_{L2}-TS1

Ni	0.59198	0.17854	0.16389
C	3.21082	-0.69757	-0.07838
C	2.95127	1.6441	0.00302
C	4.59299	-0.58448	-0.15487
C	4.32906	1.82428	-0.10252
C	5.15027	0.69842	-0.17869
H	5.22293	-1.47478	-0.1991

H	4.75317	2.83005	-0.10072
H	6.23332	0.81876	-0.24534
C	2.3837	-1.94392	-0.11135
H	2.09185	-2.15051	-1.15526
H	2.94977	-2.82177	0.24356
C	1.91191	2.66916	0.27136
H	1.82381	2.70579	1.38403
H	2.17983	3.66212	-0.12295
N	2.44386	0.40067	-0.00736
C	1.35665	-1.72313	2.12075
C	0.10779	-2.75472	0.34414
C	1.64761	-3.10354	2.66155
H	0.45354	-1.30339	2.58403
H	2.14381	-0.99493	2.35907
C	0.446	-4.10131	0.95395
H	-0.84958	-2.38419	0.74272
H	0.00269	-2.84713	-0.7439
H	1.71318	-3.05759	3.75627
H	2.62419	-3.49069	2.29908
H	-0.37506	-4.80774	0.76644
H	1.3516	-4.53041	0.47113
C	0.40571	2.45377	-1.65738
C	-0.52372	2.87335	0.52785
C	0.22449	3.92745	-1.97005
H	-0.48138	1.8956	-1.98503
H	1.26023	2.02263	-2.20057
C	-0.64899	4.32785	0.14478
H	-1.45092	2.34799	0.26133
H	-0.34456	2.71046	1.60301
H	-0.00224	4.05126	-3.03838
H	1.15767	4.49793	-1.7767
H	-1.52034	4.77351	0.64369
H	0.23867	4.90765	0.47264
N	1.1233	-1.72412	0.64876
N	0.57748	2.19865	-0.20896
O	-0.84449	4.48342	-1.24782
O	0.62337	-4.0198	2.34151
H	-1.26419	-0.05268	0.56498
Cl	1.06581	1.32183	2.97213
C	-2.23548	-1.14292	-1.51041
H	-2.89375	-2.01447	-1.50969
C	-2.51817	-0.06203	-0.6779
H	-2.0721	0.8949	-0.96858
C	-3.74122	0.04552	0.12026

C	-4.32025	1.30382	0.35732
C	-4.36342	-1.08559	0.67683
C	-5.48674	1.4267	1.10592
H	-3.84884	2.19448	-0.07011
C	-5.52594	-0.96292	1.42881
H	-3.91026	-2.07053	0.53043
C	-6.09539	0.2938	1.64537
H	-5.92393	2.41438	1.27106
H	-5.99009	-1.85362	1.85963
H	-7.00709	0.38849	2.23962
O	-0.04015	-0.38588	-1.81536
C	-0.95333	-1.19126	-2.1402
N	-0.68451	-2.19379	-3.06364
C	0.65184	-2.3788	-3.55636
H	0.65016	-2.54933	-4.64395
H	1.23791	-1.47711	-3.3464
H	1.16565	-3.24549	-3.093
C	-1.67441	-3.17496	-3.41984
H	-1.79167	-3.97819	-2.6664
H	-2.65792	-2.70802	-3.56632
H	-1.39296	-3.65217	-4.36762

B_6

Ni	0.46424	0.1431	-0.40555
C	3.2295	-0.10267	0.37896
C	2.43195	-1.89735	-0.90513
C	4.47943	-0.70813	0.51326
C	3.64855	-2.56811	-0.79121
C	4.67949	-1.95491	-0.07813
H	5.27558	-0.21585	1.07531
H	3.78613	-3.54753	-1.25384
H	5.64561	-2.45526	0.01916
C	2.81762	1.19124	1.02299
H	3.71148	1.80285	1.24508
C	1.22542	-2.367	-1.66769
H	1.20383	-1.82498	-2.62969
H	1.30666	-3.44539	-1.89128
N	2.26999	-0.70562	-0.32415
C	2.40356	2.57331	-0.95107
C	1.02716	2.86585	0.98946
C	3.15795	3.82715	-0.55891
H	1.58002	2.82694	-1.6325
H	3.04054	1.86261	-1.49994
C	1.82559	4.10679	1.3287

H	0.17274	3.1592	0.35702
H	0.62364	2.3634	1.88037
H	3.49758	4.36161	-1.45672
H	4.06807	3.58649	0.0326
H	1.18991	4.84987	1.82968
H	2.65197	3.86361	2.03109
C	-0.22258	-2.82582	0.25233
C	-1.21805	-2.09028	-1.79589
C	-0.64845	-4.24111	-0.08278
H	-1.02815	-2.34388	0.82765
H	0.68839	-2.80538	0.86954
C	-1.62034	-3.52264	-2.07312
H	-2.02784	-1.59073	-1.23867
H	-1.05089	-1.51096	-2.71401
H	-0.88328	-4.79029	0.84044
H	0.16665	-4.80318	-0.58847
H	-2.57169	-3.55185	-2.62166
H	-0.86526	-4.02885	-2.71171
N	1.8098	1.89026	0.21528
N	-0.00992	-2.0008	-0.9526
O	-1.80996	-4.24909	-0.87779
O	2.33629	4.71507	0.16454
Cl	0.33858	0.71929	-2.63037
H	-1.59161	0.61208	-0.40182
H	2.34248	0.94126	1.98605
C	-2.07611	-0.01562	1.64136
H	-3.0069	-0.28115	2.13528
C	-2.13005	0.97353	0.52491
H	-1.59305	1.90861	0.77186
C	-3.49532	1.35012	0.02646
C	-3.73336	2.64273	-0.46012
C	-4.55431	0.43337	0.00293
C	-4.98356	3.0122	-0.95141
H	-2.917	3.37184	-0.45047
C	-5.8075	0.79867	-0.48811
H	-4.3912	-0.58101	0.37809
C	-6.02879	2.08935	-0.96728
H	-5.14465	4.02874	-1.32149
H	-6.62125	0.06804	-0.49403
H	-7.01526	2.37625	-1.34576
O	0.27046	-0.08134	1.56119
C	-0.8529	-0.39782	2.14221
N	-0.71856	-1.15917	3.30998
C	0.4762	-1.92385	3.53814

H	0.75097	-1.91238	4.60751
H	0.37488	-2.99319	3.24523
H	1.30259	-1.49	2.96153
C	-1.89619	-1.62019	3.98508
H	-2.59942	-0.78928	4.16009
H	-2.44622	-2.40973	3.4252
H	-1.62262	-2.03503	4.96927

B_2-TS2

Ni	0.86009	0.45385	-1.22975
C	-0.4337	-0.23096	1.17133
C	1.68922	-1.26535	1.13603
C	-0.76195	-0.92669	2.35357
C	1.41231	-1.97203	2.30165
C	0.15797	-1.80275	2.90255
H	-1.73244	-0.74873	2.82223
H	2.18409	-2.61015	2.73445
H	-0.08577	-2.34452	3.82029
C	-1.33469	0.62889	0.45212
H	-2.17791	1.0188	1.04313
C	3.03018	-1.33643	0.46353
H	3.19346	-2.35352	0.06231
H	2.99735	-0.66125	-0.4248
N	0.78137	-0.44456	0.5802
C	0.04068	2.68617	0.40093
C	-1.45132	2.2378	-1.4239
C	-0.96854	3.6782	0.93594
H	0.75221	3.18837	-0.27439
H	0.62477	2.22267	1.21074
C	-2.41438	3.25192	-0.84309
H	-0.76	2.73865	-2.12138
H	-1.97426	1.4519	-1.98415
H	-0.45958	4.50683	1.44721
H	-1.63233	3.19093	1.68023
H	-2.95853	3.76755	-1.64675
H	-3.17088	2.74672	-0.20695
C	4.024	0.22573	2.07527
C	5.42661	-1.18701	0.76291
C	4.39543	1.38979	1.17784
H	4.72149	0.1919	2.93004
H	3.01427	0.35407	2.49711
C	5.7674	0.01317	-0.10675
H	6.17917	-1.2681	1.56623
H	5.46653	-2.12317	0.18306

H	4.41365	2.33416	1.74115
H	3.6568	1.50724	0.35815
H	6.79426	-0.05806	-0.49347
H	5.09028	0.07373	-0.98376
N	-0.62661	1.60913	-0.37587
N	4.11318	-1.06448	1.38925
O	5.69198	1.20458	0.64534
O	-1.73142	4.24149	-0.10719
Cl	2.44363	1.72913	-2.1072
H	-2.96687	-2.73093	-0.02421
H	-1.92076	-0.26786	-0.48954
C	-1.091	-1.67471	-1.82723
O	-0.23681	-0.83226	-2.25866
C	-2.38571	-1.19632	-1.42638
H	-2.78478	-0.48151	-2.15697
C	-3.44072	-1.97474	-0.66896
H	-4.11905	-2.53774	-1.33986
C	-4.2713	-1.06622	0.2052
C	-4.93043	0.04646	-0.33605
C	-4.36723	-1.28042	1.58446
C	-5.64855	0.92121	0.47595
H	-4.87508	0.23375	-1.41331
C	-5.08302	-0.40656	2.4032
H	-3.86123	-2.14555	2.02514
C	-5.72247	0.70209	1.85214
H	-6.15392	1.78299	0.0319
H	-5.13985	-0.59262	3.47887
H	-6.28238	1.38994	2.48985
N	-0.66169	-2.96217	-1.62366
C	-1.52604	-4.11711	-1.6778
H	-2.52392	-3.84457	-2.03274
H	-1.11877	-4.85033	-2.39225
H	-1.62335	-4.62551	-0.70361
C	0.75107	-3.25217	-1.69207
H	1.06333	-3.58125	-2.69805
H	1.32793	-2.35565	-1.44379
H	1.00128	-4.04973	-0.97637

B_3-TS1

Ni	-0.28432	-0.1973	-0.63044
C	-0.3029	-2.51442	1.05609
C	-2.44891	-1.73954	0.5085
C	-0.84394	-3.52748	1.85036
C	-3.05059	-2.70926	1.30384

C	-2.22747	-3.61357	1.97851
H	-0.18441	-4.22453	2.37047
H	-4.13778	-2.75953	1.38902
H	-2.66993	-4.38816	2.60865
C	1.15417	-2.22445	0.9053
H	1.75207	-3.14518	1.0282
C	-3.17605	-0.7467	-0.35439
H	-3.2614	-1.16738	-1.37207
H	-4.21305	-0.61363	0.00419
N	-1.11565	-1.66354	0.41314
C	1.43844	-2.38555	-1.53601
C	2.68505	-0.72934	-0.30255
C	2.70033	-3.22068	-1.61612
H	1.36804	-1.72968	-2.4179
H	0.53783	-3.02138	-1.52033
C	3.90153	-1.61906	-0.43312
H	2.64565	-0.00869	-1.13509
H	2.70598	-0.16979	0.64446
H	2.71719	-3.79594	-2.55264
H	2.74035	-3.95878	-0.78573
H	4.81401	-1.01143	-0.497
H	4.00632	-2.27057	0.46055
C	-2.5142	1.32343	0.76244
C	-2.83979	1.33317	-1.61554
C	-3.87099	1.98115	0.91657
H	-1.73947	2.10339	0.69743
H	-2.2658	0.69547	1.63224
C	-4.19045	1.97728	-1.39054
H	-2.06814	2.10454	-1.75658
H	-2.81741	0.71561	-2.52448
H	-3.86809	2.65662	1.78268
H	-4.66232	1.22411	1.10519
H	-4.43821	2.65147	-2.22151
H	-4.99416	1.21093	-1.34674
N	1.42791	-1.50615	-0.34847
N	-2.4207	0.50883	-0.46713
O	-4.19519	2.75337	-0.21352
O	3.84721	-2.41001	-1.60199
Cl	0.27441	0.7382	-2.58434
C	0.75778	1.03074	1.88047
H	-0.17051	1.51082	2.30963
H	0.22604	0.57981	0.87312
O	1.30374	0.11436	2.608
C	1.65149	2.12599	1.32242

C	2.86039	2.39553	1.9696
C	1.30174	2.87723	0.19656
C	3.69731	3.41072	1.50984
H	3.1226	1.78191	2.83612
C	2.139	3.88738	-0.27065
H	0.38522	2.63407	-0.35424
C	3.33835	4.16078	0.38936
H	4.63903	3.61785	2.0259
H	1.86317	4.45184	-1.16505
H	3.99808	4.95096	0.02182
H	1.36732	-0.81141	2.11666

B_4-TS2

Ni	-0.40504	-1.23339	-0.56748
C	0.37257	-0.74465	2.0964
C	-1.95785	-1.0519	1.83019
C	0.18626	-0.43148	3.45775
C	-2.19786	-0.73266	3.15494
C	-1.09482	-0.42529	3.97885
H	1.05178	-0.18961	4.07855
H	-3.2163	-0.73129	3.54846
H	-1.25462	-0.18335	5.03212
C	1.61949	-0.65282	1.37118
H	2.52148	-0.71284	2.00214
C	-3.00595	-1.49548	0.84398
H	-3.09368	-2.59468	0.90366
H	-3.99659	-1.09863	1.13251
N	-0.70972	-1.05431	1.32717
C	1.69836	-2.93911	0.49625
C	2.67454	-1.18981	-0.79914
C	3.08963	-3.32116	0.96391
H	1.45349	-3.49687	-0.42375
H	0.93745	-3.1858	1.25304
C	4.04023	-1.60139	-0.29714
H	2.42761	-1.72972	-1.72579
H	2.63498	-0.12368	-1.03669
H	3.15624	-4.40649	1.125
H	3.30843	-2.83492	1.9376
H	4.80002	-1.43343	-1.073
H	4.34022	-0.99626	0.58313
C	-2.87374	0.26099	-0.85509
C	-3.24704	-2.00308	-1.55806
C	-4.34264	0.53894	-1.09166
H	-2.29524	0.49077	-1.76506

H	-2.47856	0.88499	-0.03988
C	-4.71049	-1.66465	-1.75415
H	-2.68894	-1.8289	-2.49213
H	-3.11193	-3.06127	-1.28594
H	-4.47817	1.57345	-1.43592
H	-4.92282	0.43883	-0.14897
H	-5.13607	-2.25273	-2.57922
H	-5.29602	-1.91511	-0.84223
N	1.61269	-1.49578	0.17296
N	-2.61651	-1.15891	-0.53146
O	-4.87822	-0.30682	-2.08419
O	4.0658	-2.9826	0.01091
Cl	-0.07827	-0.94339	-2.75391
H	0.56404	1.41435	-1.18087
H	1.72773	0.56174	0.91715
C	3.37324	1.95843	0.18724
O	4.1185	1.88079	1.16797
C	1.92012	1.95382	0.42501
H	1.77894	2.36376	1.43257
C	0.80485	2.28379	-0.52761
H	1.09784	3.07019	-1.24567
C	-0.49924	2.71021	0.09677
C	-1.43595	3.38797	-0.69965
C	-0.8587	2.41741	1.41804
C	-2.68385	3.75051	-0.20306
H	-1.17501	3.62848	-1.73502
C	-2.1127	2.77348	1.91987
H	-0.15565	1.90014	2.07463
C	-3.033	3.43857	1.11317
H	-3.39047	4.2822	-0.84599
H	-2.36475	2.52938	2.95557
H	-4.01145	3.72356	1.50773
N	3.92258	1.96745	-1.09322
C	3.20523	2.00378	-2.34516
H	2.98056	3.02834	-2.69364
H	3.82599	1.532	-3.12106
H	2.26985	1.43342	-2.31997
C	5.35773	2.05938	-1.21304
H	5.65872	2.98723	-1.72879
H	5.7964	2.04976	-0.21092
H	5.76393	1.21264	-1.79196

B_5-TS2

Ni	0.53269	0.09074	-0.50502

C	1.15386	2.52596	0.76994
C	3.02674	1.53256	-0.29328
C	2.00556	3.48772	1.36416
C	3.91012	2.44405	0.26925
C	3.36324	3.44207	1.09706
H	1.58857	4.24645	2.02941
H	4.98417	2.37465	0.08961
H	4.02462	4.18463	1.55112
C	-0.23677	2.27739	1.04629
H	-0.77684	3.09576	1.54581
C	3.36906	0.32245	-1.1145
H	3.0197	0.4707	-2.15094
H	4.46096	0.16191	-1.14691
N	1.71455	1.6247	-0.07207
C	-1.03453	2.52295	-1.30024
C	-2.28226	1.17635	0.22151
C	-2.03697	3.63411	-1.09284
H	-1.34281	1.88326	-2.14099
H	-0.03562	2.91139	-1.5464
C	-3.27455	2.31399	0.36774
H	-2.60086	0.51917	-0.60283
H	-2.25843	0.56765	1.13678
H	-2.14454	4.23283	-2.00805
H	-1.6976	4.32281	-0.29015
H	-4.28707	1.91273	0.51748
H	-3.03167	2.93072	1.25978
C	3.04578	-1.24099	0.76207
C	2.70819	-2.0139	-1.48306
C	4.39727	-1.92471	0.75816
H	2.28526	-1.93736	1.15081
H	3.03652	-0.36073	1.4214
C	4.06697	-2.67942	-1.42118
H	1.94227	-2.73449	-1.15061
H	2.43275	-1.70607	-2.50124
H	4.64523	-2.28865	1.765
H	5.199	-1.21221	0.46887
H	4.06963	-3.60168	-2.01813
H	4.85064	-2.01865	-1.84804
N	-0.92817	1.6551	-0.1016
N	2.61723	-0.84257	-0.59342
O	4.40321	-3.04197	-0.09954
O	-3.31415	3.11813	-0.78584
Cl	0.21687	-0.23828	-2.73099
H	0.01053	0.92632	1.6974

H	-2.14882	-3.5012	1.34556
C	-0.54037	-1.13703	1.77141
O	0.35301	-0.12731	1.65363
C	-0.59734	-2.07439	0.77502
H	0.21331	-2.02619	0.03512
C	-1.71454	-3.02857	0.45281
H	-1.31194	-3.85706	-0.15047
C	-2.8124	-2.33803	-0.32121
C	-2.62224	-2.01127	-1.66949
C	-3.99842	-1.93302	0.30224
C	-3.58263	-1.28749	-2.37139
H	-1.68833	-2.28798	-2.16626
C	-4.96756	-1.21535	-0.40004
H	-4.16451	-2.18309	1.3559
C	-4.7605	-0.88515	-1.73906
H	-3.39757	-1.02429	-3.41584
H	-5.8891	-0.90977	0.10317
H	-5.51279	-0.31323	-2.28757
N	-1.29187	-1.14983	2.92802
C	-1.70242	-2.39133	3.53233
H	-1.07245	-3.2158	3.17484
H	-1.5779	-2.32567	4.6244
H	-2.75855	-2.65356	3.34049
C	-1.45735	0.02592	3.74679
H	-0.78914	0.02272	4.62744
H	-1.25971	0.94283	3.17956
H	-2.49324	0.08935	4.11631

F_2

Ni	0.28415	-0.19691	0.63016
C	0.30266	-2.51428	-1.05596
C	2.44871	-1.73986	-0.50787
C	0.84367	-3.52748	-1.8501
C	3.05037	-2.70978	-1.30298
C	2.22721	-3.61391	-1.97785
H	0.18411	-4.22439	-2.37036
H	4.13757	-2.76033	-1.38784
H	2.66966	-4.38864	-2.60782
C	-1.15437	-2.22417	-0.90524
H	-1.75239	-3.14483	-1.02811
C	3.17582	-0.74693	0.35494
H	3.26081	-1.16725	1.37279
H	4.21292	-0.61415	-0.00344
N	1.11544	-1.66354	-0.41287

C	-1.43857	-2.38516	1.53609
C	-2.68526	-0.72912	0.30264
C	-2.7004	-3.22041	1.61621
H	-1.36823	-1.72926	2.41796
H	-0.53793	-3.02094	1.52046
C	-3.90164	-1.61898	0.43295
H	-2.64602	-0.00868	1.13537
H	-2.70614	-0.16921	-0.64413
H	-2.71727	-3.79554	2.5528
H	-2.74027	-3.95863	0.78592
H	-4.81422	-1.01147	0.49665
H	-4.00618	-2.27053	-0.46072
C	2.51474	1.32294	-0.76279
C	2.83964	1.33347	1.61526
C	3.87176	1.98024	-0.91678
H	1.74017	2.10309	-0.69827
H	2.26643	0.69473	-1.63245
C	4.19058	1.97704	1.39045
H	2.06824	2.1052	1.75566
H	2.81663	0.71632	2.52446
H	3.86926	2.65545	-1.7831
H	4.66289	1.2229	-1.10501
H	4.4383	2.65146	2.22125
H	4.99406	1.21041	1.34719
N	-1.42806	-1.50578	0.34854
N	2.42068	0.50879	0.46703
O	4.19594	2.75271	0.21315
O	-3.8474	-2.40989	1.60187
Cl	-0.27434	0.73883	2.58404
H	-1.41644	-1.52521	-1.73761

H-TS

Ni	-0.00067	-0.83031	-0.31932
C	1.04346	1.85423	-0.33133
C	-1.08746	1.669	0.62576
C	1.07811	3.22411	-0.08308
C	-1.12634	3.03641	0.88953
C	-0.0257	3.81683	0.53238
H	1.95092	3.81508	-0.36842
H	-1.99972	3.48018	1.37203
H	-0.02753	4.88988	0.73534
C	2.09968	1.04641	-1.0267
H	3.05202	1.60757	-1.07691
C	-2.14556	0.66595	0.98625

H	-1.82726	0.16167	1.91717
H	-3.10724	1.17325	1.19132
N	-0.02163	1.12648	0.02524
C	2.83815	-0.22705	0.92976
C	2.89933	-1.26821	-1.22932
C	4.33666	-0.02516	0.83784
H	2.60803	-1.17854	1.43047
H	2.35261	0.55748	1.53088
C	4.39641	-1.0405	-1.26114
H	2.6868	-2.25494	-0.78583
H	2.45057	-1.26191	-2.23394
H	4.7963	-0.09121	1.8338
H	4.58254	0.98218	0.43717
H	4.90289	-1.84803	-1.80788
H	4.63506	-0.09289	-1.79142
C	-2.75185	0.10117	-1.32277
C	-2.97955	-1.56213	0.38666
C	-4.25098	0.31655	-1.27131
H	-2.50157	-0.65933	-2.07794
H	-2.21599	1.01706	-1.61727
C	-4.47063	-1.30289	0.39396
H	-2.74999	-2.36434	-0.33356
H	-2.59713	-1.89439	1.36202
H	-4.63877	0.58342	-2.26454
H	-4.5038	1.1594	-0.59174
H	-5.0252	-2.22356	0.62251
H	-4.73636	-0.56418	1.18033
N	2.20769	-0.27419	-0.40021
N	-2.21925	-0.37867	-0.03863
O	-4.92235	-0.8535	-0.86563
O	4.93761	-1.02048	0.03995
Cl	0.07113	-1.87418	1.73063
H	-0.05152	-0.91176	-1.91591
H	1.76178	0.87578	-2.06571

^{t}BuOK

C	-1.05587	-0.00008	-0.00003
C	-1.6006	1.09544	0.93538
H	-1.22825	0.93339	1.95948
H	-1.24242	2.08458	0.60611
H	-2.7023	1.1326	0.97724
C	-1.59796	-1.35869	0.48085
H	-1.2307	-2.1619	-0.1766
H	-1.23044	-1.57071	1.49723

H	-2.70026	-1.41189	0.50031
C	-1.59762	0.26201	-1.41697
H	-1.23614	1.23622	-1.78352
H	-1.22422	-0.50977	-2.10888
H	-2.69951	0.26682	-1.47502
O	0.30842	0.00011	0.00013
K	2.53364	0.00041	0.00038

BnOH

C	-3.04805	1.9697	0.
C	-1.65289	1.9697	0.
C	-0.95535	3.17745	0.
C	-1.65301	4.38596	-0.0012
C	-3.04783	4.38588	-0.00168
C	-3.74543	3.17767	-0.00068
H	-3.59781	1.01738	0.00045
H	-1.10338	1.01718	0.00132
H	-1.10281	5.3381	-0.00126
H	-3.59796	5.33816	-0.00263
H	-4.84504	3.17786	-0.00086
C	0.58465	3.17756	0.00089
H	0.94182	3.56865	-0.92883
H	0.9408	3.78739	0.80473
O	1.06131	1.83998	0.16995
H	2.02125	1.84084	0.18075

KCl

Cl	-3.40018	3.41792	1.92948
K	-4.86228	5.61857	3.2426

H_2O

O	0.	0.	0.11849
H	0.	0.75464	-0.47394
H	0.	-0.75464	-0.47394

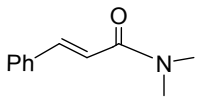
^{t}BuOH

C	-4.99474	-1.00611	-3.85075
O	-3.60578	-0.65048	-3.82766
C	-5.66778	0.0204	-4.74325
C	-5.14096	-2.40793	-4.42521
C	-5.55267	-0.94292	-2.43445
H	-5.24638	-0.00983	-5.75767
H	-6.74769	-0.16599	-4.8172
H	-5.5292	1.03562	-4.34435

H	-5.41747	0.06007	-2.00487
H	-6.62624	-1.17974	-2.41194
H	-5.04306	-1.66429	-1.77818
H	-4.63212	-3.14669	-3.78758
H	-6.19688	-2.70526	-4.49783
H	-4.69617	-2.46706	-5.42842
H	-3.10602	-1.35453	-3.35281

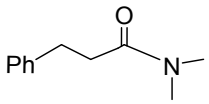
PhCHO

C	-3.04805	1.9697	0.
C	-1.65289	1.9697	0.
C	-0.95535	3.17745	0.
C	-1.65301	4.38596	-0.0012
C	-3.04783	4.38588	-0.00168
C	-3.74543	3.17767	-0.00068
H	-3.59781	1.01738	0.00045
H	-1.10338	1.01718	0.00132
H	-1.10281	5.3381	-0.00126
H	-3.59796	5.33816	-0.00263
H	-4.84504	3.17786	-0.00086
C	0.58465	3.17756	0.00089
H	1.11788	2.24989	0.0015
O	1.21808	4.26491	0.00089



C	3.6558	2.38244	-0.1943
O	4.65877	2.49818	0.50236
C	2.32938	2.49938	0.45505
H	2.37379	2.1989	1.50726
C	1.2051	3.05291	-0.03669
H	1.21341	3.44571	-1.0593
C	-0.06988	3.19536	0.65788
C	-1.08429	3.97925	0.08154
C	-0.35159	2.54847	1.87577
C	-2.32404	4.12527	0.69879
H	-0.8863	4.48424	-0.86855
C	-1.59257	2.68282	2.48695
H	0.41176	1.92598	2.34931
C	-2.58642	3.47334	1.90297
H	-3.09166	4.74971	0.23474
H	-1.78829	2.16631	3.4302
H	-3.55927	3.58157	2.38855

N	3.73438	2.14506	-1.55048
C	2.64456	1.76127	-2.41983
H	2.32405	2.58774	-3.07917
H	2.97802	0.93793	-3.07271
H	1.77283	1.39086	-1.86004
C	5.03966	2.14846	-2.16636
H	5.31963	1.13854	-2.51189
H	5.05423	2.81613	-3.04239
H	5.7825	2.48788	-1.43855



C	2.25296	0.77618	-0.10991
O	2.77945	1.77337	-0.58511
C	0.79636	0.80701	0.16963
H	0.43379	1.71383	-0.26756
C	-0.08706	-0.14837	-0.17838
H	0.13153	-0.37935	-1.20002
C	-1.54237	-0.07694	-0.09966
C	-2.30549	-1.17782	-0.52723
C	-2.22777	1.04819	0.39588
C	-3.69568	-1.16053	-0.4628
H	-1.78924	-2.05939	-0.91845
C	-3.61482	1.06533	0.4612
H	-1.66373	1.92089	0.73289
C	-4.35683	-0.03837	0.03272
H	-4.26674	-2.02794	-0.80195
H	-4.12671	1.94897	0.84967
H	-5.44774	-0.02026	0.08416
N	2.95767	-0.38494	0.12445
C	2.50544	-1.4948	0.92573
H	2.29735	-2.39607	0.32262
H	3.28372	-1.76596	1.65707
H	1.60042	-1.23959	1.48598
C	4.3308	-0.45528	-0.31361
H	5.02807	-0.45405	0.54101
H	4.50626	-1.37738	-0.88954
H	4.55051	0.41286	-0.94207
H	0.1867	-1.01063	0.39299
H	0.70432	0.91825	1.22984

C_{HO}

Ni	-0.12266	0.27542	-0.56032

C	0.00325	1.99702	1.71996
C	-1.37819	0.12298	1.94082
C	-0.428	2.50867	2.94205
C	-1.85833	0.58847	3.16479
C	-1.3815	1.79777	3.66651
H	-0.02153	3.45145	3.31384
H	-2.59633	0.00025	3.71484
H	-1.74568	2.18076	4.62233
C	0.98976	2.68248	0.81932
H	1.58805	3.41627	1.39005
C	-1.79774	-1.18174	1.3265
H	-0.90199	-1.81464	1.22965
H	-2.4782	-1.70446	2.02912
N	-0.4783	0.83668	1.24457
C	2.7478	0.97177	0.96631
C	2.52473	2.24858	-1.05093
C	3.94033	1.83121	1.33822
H	3.09515	0.09169	0.40504
H	2.22521	0.60505	1.86408
C	3.71362	3.07536	-0.61728
H	2.87545	1.39271	-1.65012
H	1.80651	2.80425	-1.66758
H	4.6748	1.2341	1.89656
H	3.634	2.66923	2.00205
H	4.29022	3.40824	-1.49106
H	3.3827	3.99109	-0.08192
C	-3.73452	-0.52932	0.01158
C	-2.24356	-2.18025	-0.864
C	-4.71277	-1.64213	0.35112
H	-3.9716	-0.129	-0.98869
H	-3.83568	0.30748	0.72288
C	-3.24139	-3.25023	-0.47953
H	-2.46022	-1.85709	-1.89643
H	-1.20026	-2.52802	-0.85442
H	-5.75051	-1.29285	0.25137
H	-4.58431	-1.96456	1.40727
H	-3.20804	-4.09602	-1.18057
H	-3.01459	-3.65531	0.53038
N	1.79348	1.68684	0.10002
N	-2.34548	-0.99445	-0.00841
O	-4.5617	-2.74381	-0.51128
O	4.59253	2.32929	0.19569
H	0.42359	3.22507	0.04043
C	-1.10149	3.06345	-2.53405

H	-0.65942	3.90896	-1.94356
H	-2.18003	3.36153	-2.63282
O	-0.91853	1.87248	-1.90312
C	-0.493	3.14149	-3.92033
C	-0.79699	4.1957	-4.79049
C	0.38413	2.14459	-4.35548
C	-0.23974	4.25191	-6.066
H	-1.4866	4.98161	-4.4618
C	0.94438	2.19832	-5.63205
H	0.60871	1.32593	-3.66708
C	0.63429	3.2502	-6.49257
H	-0.48991	5.07981	-6.73492
H	1.62901	1.41082	-5.95918
H	1.06921	3.29043	-7.4943
C	1.10865	-2.60015	1.07189
C	1.21727	-3.50819	-0.15251
H	1.59835	-4.51014	0.09953
H	0.2313	-3.62778	-0.62676
H	1.8918	-3.06183	-0.89738
C	0.14011	-3.21186	2.08786
H	0.4886	-4.17385	2.49764
H	0.00857	-2.50771	2.92313
H	-0.84805	-3.37838	1.62983
C	2.48543	-2.42592	1.71441
H	3.19198	-1.99317	0.9911
H	2.4067	-1.72454	2.55987
H	2.91322	-3.36937	2.09106
O	0.62035	-1.36541	0.65113

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Ni	-0.0335	-0.0055	-1.32
Cl	1.5285	-1.8615	-1.373
Cl	-1.5355	1.8445	-1.591
O	2.6365	3.5475	-1.895
O	-2.3655	-3.3455	-3.332
O	0.2765	0.1455	-3.317
H	0.1425	0.8955	-3.745
H	0.6055	-0.4945	-3.809
N	-0.3485	-0.1975	0.64
N	1.7205	1.2515	-0.384
N	-1.9645	-1.3775	-1.23
C	3.0265	1.2895	-1.098
H	3.2645	0.3765	-1.399
H	3.7325	1.6015	-0.478
C	2.9655	2.2105	-2.292

H	3.8415	2.2105	-2.753
H	2.2835	1.8795	-2.929
C	1.3605	3.5535	-1.234
H	0.6615	3.2565	-1.869
H	1.1435	4.4775	-0.952
C	1.3535	2.6445	-0.02
H	1.9945	2.9885	0.651
H	0.4515	2.6505	0.389
C	1.9385	0.4955	0.872
H	2.4485	1.0575	1.508
H	2.4775	-0.3125	0.679
C	0.6375	0.0865	1.503
C	0.4625	-0.0555	2.876
H	1.1665	0.1485	3.48
C	-0.7615	-0.4995	3.341
H	-0.9055	-0.6015	4.275
C	-1.7815	-0.7985	2.446
H	-2.6255	-1.1065	2.755
C	-1.5365	-0.6335	1.087
C	-2.5705	-0.8535	0.018
H	-3.2495	-1.4945	0.347
H	-3.0285	0.0035	-0.175
C	-1.6945	-2.8285	-1.048
H	-2.4965	-3.2625	-0.664
H	-0.9495	-2.9425	-0.406
C	-1.3355	-3.5115	-2.351
H	-0.4895	-3.1325	-2.697
H	-1.1935	-4.4775	-2.186
C	-2.5455	-1.9495	-3.572
H	-3.2305	-1.8215	-4.275
H	-1.6955	-1.5585	-3.897
C	-2.9795	-1.2335	-2.306
H	-3.1155	-0.2725	-2.502
H	-3.8415	-1.6075	-1.996

C_{L1}

Ni	-0.54905	-0.03217	-0.09812
C	-3.29596	-0.09068	-0.42471
C	-2.3144	-2.10758	0.29891
C	-4.57	-0.6373	-0.33665
C	-3.56038	-2.71958	0.37056
C	-4.69822	-1.97035	0.0627
H	-5.44593	-0.03802	-0.59161
H	-3.64039	-3.76331	0.67966

H	-5.68722	-2.42738	0.1294
C	-2.9215	1.24823	-0.97735
H	-3.71089	1.99837	-0.80241
C	-0.99528	-2.6793	0.69425
H	-0.86133	-2.45149	1.76875
H	-0.95302	-3.77186	0.54844
N	-2.21861	-0.82367	-0.09521
C	-1.72826	2.38731	0.84515
C	-0.90126	2.57605	-1.41343
C	-2.33084	3.76683	0.6897
H	-0.71866	2.44831	1.27435
H	-2.29087	1.74789	1.54023
C	-1.56356	3.93385	-1.49739
H	0.13309	2.66946	-1.06052
H	-0.85099	2.07866	-2.39248
H	-2.30022	4.29142	1.6539
H	-3.4005	3.7118	0.39417
H	-0.98712	4.59338	-2.1605
H	-2.58389	3.85372	-1.93247
C	0.27593	-2.37371	-1.41122
C	1.39656	-2.09392	0.69737
C	0.91914	-3.74417	-1.52777
H	0.92301	-1.6123	-1.8749
H	-0.69973	-2.34928	-1.92221
C	1.97194	-3.48027	0.52788
H	2.07122	-1.35709	0.23938
H	1.23866	-1.80136	1.74585
H	1.12607	-3.97111	-2.58313
H	0.2264	-4.53311	-1.16204
H	2.96549	-3.53302	0.99261
H	1.34088	-4.24677	1.02565
N	-1.59927	1.68236	-0.46119
N	0.09777	-1.95357	-0.00397
O	2.1384	-3.80444	-0.83817
O	-1.61768	4.55324	-0.23642
Cl	-0.55825	-0.09156	2.56476
C	1.853	1.29106	0.41625
H	1.63404	0.91361	1.44172
H	1.61554	2.38573	0.47685
O	1.10615	0.6436	-0.54284
H	-2.8328	1.15232	-2.07362
C	3.33804	1.17189	0.17551
C	3.84423	0.41921	-0.88796
C	4.24404	1.81113	1.03292

C	5.22125	0.30283	-1.08698
H	3.13495	-0.06911	-1.56087
C	5.61671	1.69781	0.83567
H	3.86002	2.40461	1.86912
C	6.11314	0.94013	-0.22757
H	5.5993	-0.29087	-1.9239
H	6.30731	2.20212	1.51695
H	7.19111	0.85019	-0.38303

C_{H1}

Ni	0.20268	-0.18432	0.16462
C	2.17543	1.74784	-0.6965
C	0.28193	2.69141	0.3118
C	2.73513	3.00818	-0.90504
C	0.77411	3.98185	0.12135
C	2.01868	4.13142	-0.49105
H	3.71017	3.10606	-1.38633
H	0.19583	4.84856	0.44726
H	2.43232	5.13002	-0.64807
C	2.76552	0.43588	-1.12404
H	3.84346	0.55027	-1.3423
C	-1.00753	2.32311	0.98359
H	-0.77378	2.01409	2.01858
H	-1.68173	3.19676	1.03819
N	0.98771	1.63457	-0.09698
C	3.25141	-0.46595	1.10094
C	2.63077	-1.9643	-0.66269
C	4.6951	-0.88186	0.90022
H	2.77405	-1.09743	1.86398
H	3.16989	0.56822	1.47052
C	4.09012	-2.33513	-0.82159
H	2.17019	-2.65051	0.0682
H	2.05925	-2.03959	-1.59905
H	5.23518	-0.8662	1.85704
H	5.22534	-0.17789	0.22284
H	4.19437	-3.38383	-1.13272
H	4.56834	-1.71565	-1.61063
C	-2.11438	1.442	-1.0221
C	-2.69172	0.55171	1.12947
C	-3.38286	2.26947	-0.98612
H	-2.33673	0.47645	-1.497
H	-1.3192	1.91275	-1.62014
C	-3.94903	1.39419	1.09886
H	-2.90923	-0.43391	0.69181

H	-2.31827	0.37574	2.14812
H	-3.78374	2.39859	-2.00124
H	-3.18716	3.28903	-0.58857
H	-4.76857	0.87455	1.61416
H	-3.79721	2.35957	1.62768
N	2.46094	-0.60387	-0.13439
N	-1.60505	1.14738	0.33022
O	-4.38091	1.63178	-0.22457
O	4.78666	-2.19583	0.39691
Cl	0.22104	-0.50146	2.44932
C	-0.85654	-1.43692	-2.27087
H	-0.423	-2.26509	-2.88754
H	-1.5109	-0.88775	-2.99541
O	0.12789	-0.65545	-1.73239
H	2.25457	0.13368	-2.05428
C	-1.76858	-2.07744	-1.24458
C	-3.15347	-2.17224	-1.43118
C	-1.23485	-2.55172	-0.03904
C	-3.97525	-2.7257	-0.44946
H	-3.59304	-1.79039	-2.35887
C	-2.0503	-3.08821	0.95654
H	-0.15065	-2.51148	0.12352
C	-3.4264	-3.18101	0.7513
H	-5.05442	-2.78344	-0.6136
H	-1.60443	-3.41697	1.89791
H	-4.07178	-3.5983	1.52795

O-TS_H

Ni	0.28009	-0.16053	0.59385
C	0.43499	-2.52893	-1.02522
C	2.52998	-1.70701	-0.41468
C	1.01514	-3.55388	-1.75503
C	3.17054	-2.69294	-1.145
C	2.39728	-3.62559	-1.8197
H	0.39168	-4.2736	-2.26889
H	4.25137	-2.73187	-1.17784
H	2.87325	-4.40972	-2.3943
C	-1.03768	-2.27934	-0.92365
H	-1.59131	-3.21219	-1.07265
C	3.22479	-0.67855	0.42878
H	3.28778	-1.05344	1.45526
H	4.25686	-0.54563	0.08772
N	1.19691	-1.6402	-0.38229
C	-1.37814	-2.50795	1.505

C	-2.66295	-0.88771	0.27076
C	-2.59877	-3.4024	1.52847
H	-1.36445	-1.87518	2.39485
H	-0.45951	-3.09945	1.49988
C	-3.83713	-1.83644	0.33126
H	-2.69075	-0.19591	1.11603
H	-2.67551	-0.30417	-0.64994
H	-2.62047	-3.98707	2.44865
H	-2.58427	-4.11659	0.69033
H	-4.77378	-1.28052	0.37331
H	-3.87326	-2.47554	-0.56421
C	2.57341	1.34156	-0.78389
C	2.85204	1.446	1.59447
C	3.93112	1.99045	-0.93987
H	1.80112	2.11163	-0.75907
H	2.34618	0.68412	-1.62522
C	4.20602	2.08082	1.37364
H	2.08722	2.21929	1.68101
H	2.82516	0.86822	2.5183
H	3.94524	2.62638	-1.82495
H	4.72201	1.23653	-1.07178
H	4.43341	2.78338	2.17522
H	5.00344	1.32211	1.36722
N	-1.36946	-1.59756	0.33948
N	2.45223	0.57273	0.47495
O	4.23442	2.81948	0.16493
O	-3.79012	-2.64528	1.49512
Cl	-0.35873	0.80083	2.52373
C	-0.94309	1.237	-2.07342
H	0.04994	1.67061	-2.31827
H	-0.23512	0.64114	-0.73391
O	-1.39498	0.30248	-2.75625
C	-1.83712	2.21371	-1.38013
C	-3.21333	2.14743	-1.57334
C	-1.31531	3.22063	-0.57315
C	-4.05336	3.06371	-0.96046
H	-3.60379	1.36903	-2.2191
C	-2.15016	4.1356	0.04083
H	-0.24287	3.26323	-0.40729
C	-3.5244	4.05765	-0.15007
H	-5.12374	3.00659	-1.11765
H	-1.7348	4.90539	0.67929
H	-4.18007	4.77129	0.33322
H	-1.32062	-1.59856	-1.73539

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Ni	0.35164	0.15654	-0.51361
C	3.18372	0.02188	0.32794
C	2.46397	-1.82861	-0.88305
C	4.46426	-0.5013	0.43464
C	3.71477	-2.41972	-0.79419
C	4.72348	-1.73916	-0.13147
H	5.23778	0.0499	0.95337
H	3.89304	-3.38826	-1.2429
H	5.71247	-2.17343	-0.05739
C	2.74433	1.31089	0.95891
H	3.61653	1.94641	1.14626
C	1.30301	-2.4149	-1.62842
H	1.29204	-1.97416	-2.62922
H	1.43404	-3.49552	-1.7422
N	2.23058	-0.64146	-0.32293
C	2.26835	2.67979	-1.00766
C	0.9306	2.94929	0.95552
C	3.0268	3.9298	-0.62225
H	1.43659	2.93653	-1.66289
H	2.89826	1.98691	-1.56676
C	1.72778	4.18974	1.29394
H	0.06866	3.23681	0.34788
H	0.56178	2.45145	1.85308
H	3.34127	4.4688	-1.51605
H	3.93696	3.69272	-0.05006
H	1.10088	4.92037	1.80613
H	2.56418	3.94801	1.96818
C	-0.23584	-2.83181	0.22436
C	-1.12834	-2.19647	-1.90328
C	-0.60911	-4.26831	-0.07659
H	-1.07359	-2.3567	0.73699
H	0.63468	-2.77263	0.88003
C	-1.4744	-3.64527	-2.15154
H	-1.97189	-1.69113	-1.42682
H	-0.9057	-1.65888	-2.82473
H	-0.88617	-4.78532	0.84382
H	0.23486	-4.82155	-0.51542
H	-2.38183	-3.72603	-2.74959
H	-0.671	-4.15534	-2.70392
N	1.69963	1.97593	0.16286
N	0.02471	-2.04256	-0.99399

O	-1.73011	-4.33401	-0.9347
O	2.21584	4.82034	0.12494
Cl	0.60326	0.56656	-2.8537
H	-1.19468	0.62887	-0.51696
H	2.3033	1.0749	1.93082
C	-2.15772	-0.03391	1.79268
H	-2.99352	-0.6956	1.97429
C	-2.26842	1.00264	0.88218
H	-1.55249	1.80716	0.97034
C	-3.49745	1.35737	0.17738
C	-3.58973	2.5972	-0.46327
C	-4.59637	0.49636	0.09881
C	-4.73316	2.96702	-1.1468
H	-2.73622	3.26523	-0.43087
C	-5.7412	0.86523	-0.58477
H	-4.54764	-0.47909	0.56744
C	-5.81722	2.10246	-1.20934
H	-4.77823	3.93068	-1.63877
H	-6.57966	0.18151	-0.6349
H	-6.71181	2.38698	-1.74866
O	0.18768	-0.02639	1.66037
C	-0.86356	-0.41484	2.24733
N	-0.74551	-1.28366	3.30243
C	0.514	-1.90552	3.6167
H	0.81671	-1.68435	4.64366
H	0.45174	-2.99459	3.51842
H	1.27674	-1.52993	2.94049
C	-1.88795	-1.72743	4.05946
H	-2.63016	-0.93565	4.13498
H	-2.36752	-2.61099	3.62019
H	-1.57249	-1.99053	5.06896

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Ni	0.87455	0.46034	-1.22948
C	-0.448	-0.22334	1.16015
C	1.66462	-1.2785	1.13706
C	-0.7902	-0.91561	2.34057
C	1.37355	-1.98375	2.30032
C	0.11779	-1.80093	2.8948
H	-1.76037	-0.72668	2.80516
H	2.1367	-2.62869	2.73803
H	-0.13574	-2.33859	3.81207
C	-1.33689	0.64397	0.43523
H	-2.18365	1.03637	1.01941

C	3.00912	-1.35673	0.47238
H	3.16697	-2.37193	0.06428
H	2.98541	-0.67426	-0.41038
N	0.76755	-0.44966	0.57609
C	0.04857	2.69561	0.39519
C	-1.43651	2.25363	-1.4372
C	-0.96084	3.69117	0.92579
H	0.76499	3.19585	-0.27664
H	0.62856	2.23144	1.2076
C	-2.39982	3.26836	-0.85623
H	-0.74254	2.75544	-2.13147
H	-1.9576	1.46926	-2.0009
H	-0.45224	4.5178	1.4405
H	-1.62988	3.20483	1.66648
H	-2.94464	3.78386	-1.65935
H	-3.15555	2.76245	-0.21936
C	4.00233	0.1759	2.11652
C	5.40221	-1.20134	0.76367
C	4.3653	1.36171	1.24388
H	4.70469	0.12535	2.9663
H	2.99438	0.29109	2.54589
C	5.72809	0.01951	-0.08272
H	6.16211	-1.29605	1.55844
H	5.44149	-2.12428	0.16308
H	4.38413	2.29303	1.82856
H	3.6212	1.49421	0.43115
H	6.74927	-0.03883	-0.4861
H	5.03631	0.10054	-0.94645
N	-0.61768	1.6215	-0.38664
N	4.0926	-1.09886	1.40242
O	5.6586	1.19237	0.69923
O	-1.71658	4.25674	-0.1203
Cl	2.48647	1.7148	-2.0879
H	-2.93368	-2.71914	-0.04183
H	-1.91775	-0.24832	-0.50897
C	-1.08685	-1.64656	-1.85448
O	-0.23954	-0.79475	-2.28145
C	-2.38248	-1.17948	-1.44571
H	-2.78942	-0.46495	-2.17172
C	-3.42343	-1.96569	-0.67814
H	-4.10625	-2.53309	-1.34102
C	-4.25358	-1.06949	0.20982
C	-4.90092	0.06045	-0.30966
C	-4.3677	-1.31881	1.58204

C	-5.62446	0.91789	0.51636
H	-4.83278	0.2767	-1.38055
C	-5.08976	-0.46313	2.41482
H	-3.87103	-2.19739	2.00605
C	-5.71685	0.66323	1.88544
H	-6.11978	1.79373	0.08922
H	-5.16088	-0.67765	3.48424
H	-6.28056	1.33721	2.53437
N	-0.65073	-2.93423	-1.66927
C	-1.51134	-4.09133	-1.73378
H	-2.51398	-3.81546	-2.072
H	-1.11013	-4.81074	-2.46554
H	-1.59598	-4.61634	-0.76736
C	0.76295	-3.21688	-1.74735
H	1.07224	-3.5327	-2.75838
H	1.3361	-2.31993	-1.49204
H	1.02114	-4.02071	-1.04153

O_2-TS_L-1

C	-1.28067	1.76904	1.14277
H	-0.82651	1.7676	2.13226
C	-2.59689	1.09343	1.17632
C	-2.74667	-0.012	2.01966
C	-3.70274	1.53742	0.45446
C	-3.95955	-0.67096	2.11581
H	-1.88048	-0.36809	2.57197
C	-4.91612	0.87374	0.54986
H	-3.61027	2.40659	-0.18178
C	-5.04839	-0.23555	1.37283
H	-4.05276	-1.533	2.76518
H	-5.76579	1.229	-0.02043
H	-5.99709	-0.75339	1.44074
H	-0.4677	0.52182	0.69095
Ni	0.56918	-0.58184	0.25537
C	1.52981	-2.60054	-1.42389
C	3.16043	-1.51623	-0.14321
C	2.47122	-3.46083	-1.95824
C	4.15313	-2.32674	-0.66122
C	3.79638	-3.31717	-1.56743
H	2.17835	-4.2179	-2.67357
H	5.18242	-2.19414	-0.35515
H	4.55345	-3.97333	-1.97602
C	0.09322	-2.49112	-1.80699
H	-0.31401	-3.4557	-2.11532

C	3.30314	-0.44568	0.88313
H	3.13459	-0.88897	1.86997
H	4.29868	0.00393	0.86807
N	1.88906	-1.67854	-0.52762
C	-1.16384	-2.8875	0.26959
C	-1.92276	-1.21008	-1.28252
C	-2.20528	-3.82451	-0.30078
H	-1.57086	-2.33921	1.11771
H	-0.29206	-3.42511	0.6421
C	-2.91537	-2.21216	-1.82315
H	-2.38503	-0.64942	-0.47547
H	-1.61602	-0.48501	-2.03385
H	-2.57952	-4.46975	0.49432
H	-1.78098	-4.48443	-1.07276
H	-3.81399	-1.69176	-2.15449
H	-2.51299	-2.75553	-2.69227
C	2.44503	1.45759	-0.45097
C	2.09164	1.4052	1.92618
C	3.57388	2.44154	-0.21811
H	1.5105	2.00112	-0.61372
H	2.63716	0.84736	-1.33463
C	3.25416	2.35523	2.08217
H	1.18302	1.99162	1.80545
H	1.95719	0.73989	2.779
H	3.62888	3.14231	-1.05202
H	4.5438	1.92462	-0.16492
H	3.0949	3.00053	2.94538
H	4.20015	1.81933	2.24449
N	-0.71045	-1.86215	-0.71728
N	2.21323	0.5613	0.71286
O	3.37031	3.20578	0.95102
O	-3.31978	-3.1305	-0.82452
Cl	0.72127	-1.60374	2.72162
H	0.02137	-1.83113	-2.67609
C	-0.89913	2.83739	0.34672
H	-0.11615	3.47425	0.74106
C	-1.15735	2.91603	-1.07709
O	-1.61824	1.96871	-1.72552
N	-0.78643	4.08576	-1.71359
C	-0.77122	4.13897	-3.15176
H	-1.20976	3.22485	-3.53976
H	-1.34622	4.99331	-3.51704
H	0.24955	4.23513	-3.53834
C	-0.23094	5.2226	-1.02282

H	-0.37454	6.11478	-1.63157
H	-0.7323	5.39081	-0.07191
H	0.84543	5.12291	-0.83184

CL-1

Ni	-0.26311	0.20018	0.22212
C	-2.98387	0.44952	0.52784
C	-1.90371	2.35958	-0.34324
C	-4.21915	1.10333	0.51064
C	-3.08756	3.07195	-0.33999
C	-4.25647	2.43134	0.10317
H	-5.11597	0.56007	0.80322
H	-3.10949	4.10631	-0.68857
H	-5.20515	2.97044	0.09423
C	-2.69581	-0.90097	1.08999
H	-3.52361	-1.58358	0.839
C	-0.57188	2.79194	-0.86697
H	-0.50876	2.562	-1.94434
H	-0.42415	3.88125	-0.77754
N	-1.88111	1.08624	0.11695
C	-1.51336	-2.03988	-0.76231
C	-0.76342	-2.35644	1.52748
C	-2.17858	-3.39501	-0.66877
H	-0.49534	-2.14542	-1.16651
H	-2.12666	-1.38878	-1.40625
C	-1.49337	-3.68414	1.52425
H	0.28107	-2.49316	1.22135
H	-0.74458	-1.89993	2.52796
H	-2.15557	-3.87921	-1.65325
H	-3.24676	-3.27294	-0.40553
H	-0.98094	-4.38962	2.19364
H	-2.52822	-3.56318	1.90892
C	0.8282	2.53685	1.15712
C	1.75916	1.98634	-0.99078
C	1.59028	3.84514	1.10429
H	1.44052	1.7614	1.64359
H	-0.10781	2.64133	1.72681
C	2.46618	3.32445	-0.98526
H	2.40197	1.22853	-0.52163
H	1.52367	1.65177	-2.01158
H	1.89467	4.13898	2.11794
H	0.94734	4.66296	0.71573
H	3.4218	3.24479	-1.52029
H	1.86704	4.10231	-1.50467

N	-1.37644	-1.39253	0.58197
N	0.5087	2.01611	-0.19841
O	2.75856	3.7309	0.33195
O	-1.505	-4.24578	0.24065
Cl	-2.29805	3.59179	-2.99524
C	1.96333	-1.34984	-0.43268
H	1.72621	-1.02651	-1.4792
H	1.5924	-2.40602	-0.39313
O	1.39311	-0.54398	0.52131
H	-2.60972	-0.82408	2.18797
C	3.47027	-1.40233	-0.32379
C	4.15634	-0.61457	0.60346
C	4.20634	-2.24593	-1.16588
C	5.54931	-0.66469	0.6845
H	3.57706	0.02968	1.26936
C	5.59438	-2.298	-1.0859
H	3.6782	-2.87284	-1.89198
C	6.27314	-1.5047	-0.1585
H	6.07226	-0.04465	1.41747
H	6.15302	-2.96304	-1.74946
H	7.36297	-1.5458	-0.0933

CL-2

Ni	-0.54136	-0.02609	-0.19795
C	-3.29023	0.03859	-0.43182
C	-2.38981	-2.0067	0.28045
C	-4.57738	-0.45292	-0.326
C	-3.65297	-2.5603	0.37725
C	-4.75255	-1.76878	0.08029
H	-5.42401	0.17599	-0.56529
H	-3.77231	-3.58766	0.69379
H	-5.75041	-2.17841	0.16416
C	-2.88302	1.37502	-0.95732
H	-3.6136	2.14647	-0.70611
C	-1.09867	-2.64656	0.64814
H	-0.94262	-2.46195	1.71684
H	-1.10749	-3.72385	0.46958
N	-2.24562	-0.73585	-0.11803
C	-1.55989	2.42515	0.8354
C	-0.8193	2.61398	-1.4586
C	-2.10149	3.8315	0.72342
H	-0.54027	2.44112	1.21852
H	-2.13167	1.81137	1.53071
C	-1.41951	4.00076	-1.48912

H	0.22497	2.65342	-1.1554
H	-0.85296	2.13973	-2.43962
H	-2.01039	4.33162	1.68724
H	-3.1692	3.83595	0.45823
H	-0.84771	4.63837	-2.16329
H	-2.4562	3.97955	-1.86084
C	0.19653	-2.42837	-1.45232
C	1.31248	-2.15891	0.6636
C	0.76581	-3.83104	-1.52856
H	0.87918	-1.72183	-1.92784
H	-0.76644	-2.37125	-1.9634
C	1.81303	-3.57623	0.53107
H	2.02451	-1.47508	0.20315
H	1.1606	-1.85708	1.70039
H	0.96749	-4.09074	-2.5681
H	0.04552	-4.56952	-1.14443
H	2.78897	-3.66949	1.00602
H	1.13891	-4.29245	1.02307
N	-1.51183	1.72916	-0.48749
N	0.02569	-1.95926	-0.05176
O	1.98557	-3.93664	-0.8314
O	-1.37456	4.60337	-0.21334
Cl	-0.18495	-1.16561	-3.31995
C	1.88317	1.16119	0.43846
H	1.65631	0.6958	1.41479
H	1.64004	2.23423	0.58431
O	1.1468	0.59348	-0.58451
H	-2.84971	1.32528	-2.04901
C	3.36918	1.06676	0.19787
C	3.88781	0.34023	-0.86762
C	4.25674	1.70361	1.06449
C	5.26035	0.24733	-1.061
H	3.19633	-0.14538	-1.54543
C	5.62428	1.61224	0.87397
H	3.86359	2.27492	1.89921
C	6.13373	0.88099	-0.19224
H	5.64768	-0.32318	-1.89714
H	6.29856	2.1124	1.55897
H	7.20383	0.8097	-0.34245

CL-3

Ni	-0.54136	-0.02609	-0.19795
C	-3.29023	0.03859	-0.43182
C	-2.38981	-2.0067	0.28045

C	-4.57738	-0.45292	-0.326
C	-3.65297	-2.5603	0.37725
C	-4.75255	-1.76878	0.08029
H	-5.42401	0.17599	-0.56529
H	-3.77231	-3.58766	0.69379
H	-5.75041	-2.17841	0.16416
C	-2.88302	1.37502	-0.95732
H	-3.6136	2.14647	-0.70611
C	-1.09867	-2.64656	0.64814
H	-0.94262	-2.46195	1.71684
H	-1.10749	-3.72385	0.46958
N	-2.24562	-0.73585	-0.11803
C	-1.55989	2.42515	0.8354
C	-0.8193	2.61398	-1.4586
C	-2.10149	3.8315	0.72342
H	-0.54027	2.44112	1.21852
H	-2.13167	1.81137	1.53071
C	-1.41951	4.00076	-1.48912
H	0.22497	2.65342	-1.1554
H	-0.85296	2.13973	-2.43962
H	-2.01039	4.33162	1.68724
H	-3.1692	3.83595	0.45823
H	-0.84771	4.63837	-2.16329
H	-2.4562	3.97955	-1.86084
C	0.19653	-2.42837	-1.45232
C	1.31248	-2.15891	0.6636
C	0.76581	-3.83104	-1.52856
H	0.87918	-1.72183	-1.92784
H	-0.76644	-2.37125	-1.9634
C	1.81303	-3.57623	0.53107
H	2.02451	-1.47508	0.20315
H	1.1606	-1.85708	1.70039
H	0.96749	-4.09074	-2.5681
H	0.04552	-4.56952	-1.14443
H	2.78897	-3.66949	1.00602
H	1.13891	-4.29245	1.02307
N	-1.51183	1.72916	-0.48749
N	0.02569	-1.95926	-0.05176
O	1.98557	-3.93664	-0.8314
O	-1.37456	4.60337	-0.21334
Cl	-5.69291	2.84068	-1.8183
C	1.88317	1.16119	0.43846
H	1.65631	0.6958	1.41479
H	1.64004	2.23423	0.58431

O	1.1468	0.59348	-0.58451
H	-2.84971	1.32528	-2.04901
C	3.36918	1.06676	0.19787
C	3.88781	0.34023	-0.86762
C	4.25674	1.70361	1.06449
C	5.26035	0.24733	-1.061
H	3.19633	-0.14538	-1.54543
C	5.62428	1.61224	0.87397
H	3.86359	2.27492	1.89921
C	6.13373	0.88099	-0.19224
H	5.64768	-0.32318	-1.89714
H	6.29856	2.1124	1.55897
H	7.20383	0.8097	-0.34245