Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

The On-and-Off Dynamics of Thiophene on a Nickel Cluster Enables Efficient Hydrodesulfurization and Excellent Stability at High Temperatures

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Supporting Figures and Tables:

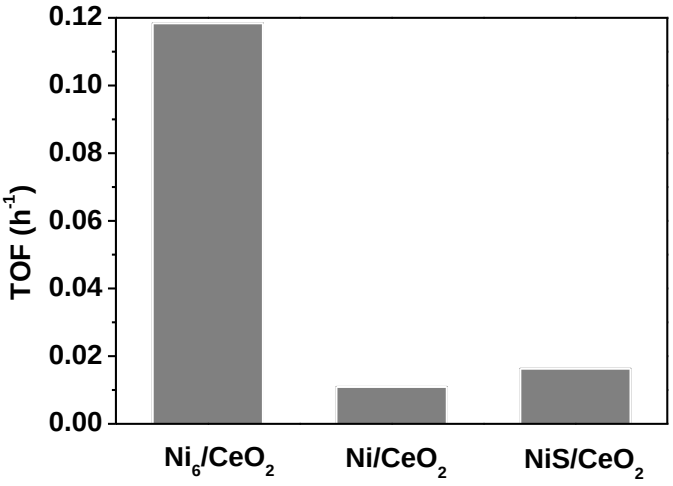

Figure S1. Comparison of catalytic hydrodesulfurization of thiophene over different catalysts. Reaction conditions: 100 mg catalyst, 0.15 % thiophene in hexane with 0.002 cm^3/min flow, 14 bar H_2, space velocity = 12000 cm^3/g/h, room temperature = 400 ^oC.

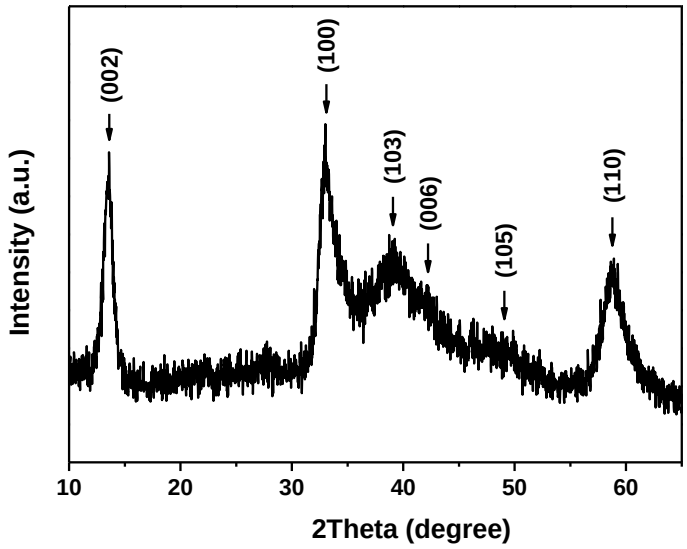

Figure S2. XRD pattern of MoS_2.

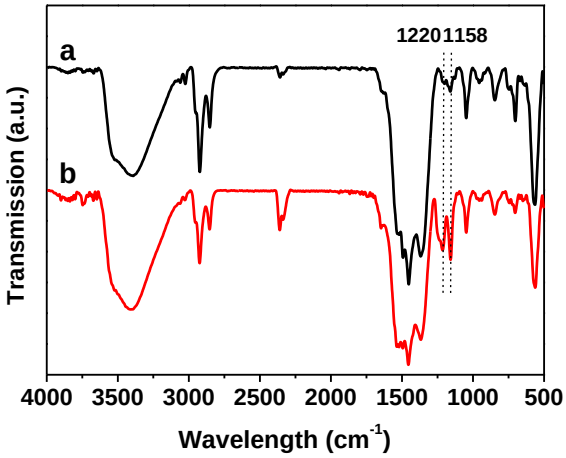

Figure S3. IR spectra of the pretreated $Ni_6(SR)_{12}/CeO_2$ (a) before and (b) after the adsorption of thiophene.

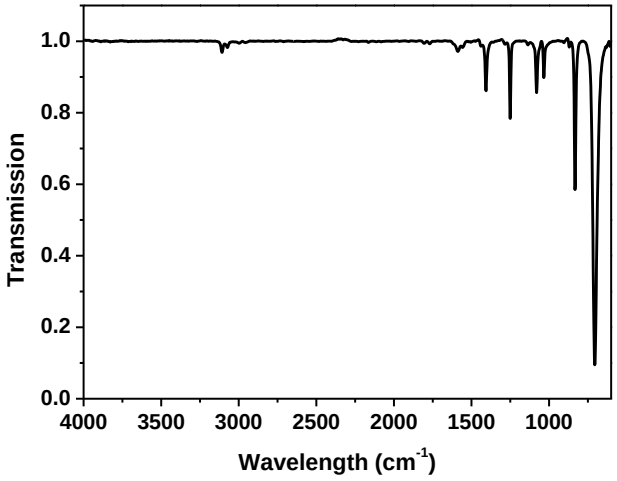

Figure S4. FT-IR spectrum of thiophene.

Table S1. The bond lengths of the $Ni_6(SC_2H_4Ph)_{12}$ cluster.

No.	Atom1	Atom2	Distance(Å)
1	Ni1	S6	2.1822(19)
2	Ni1	S1	2.1969(19)
3	Ni1	S7	2.2001(19)
4	Ni1	S9	2.2281(19)
5	Ni1	Ni2	2.8345(14)
6	Ni1	Ni3	2.9450(14)
7	Ni2	S5	2.192(2)
8	Ni2	S7	2.1931(19)
9	Ni2	S8	2.1961(19)
10	Ni2	S1	2.205(2)
11	Ni3	S8	2.1949(19)
12	Ni3	S5	2.198(2)
13	Ni3	S6	2.2046(19)
14	Ni3	S9	2.212(2)
15	S1	C23	1.822(6)
16	S5	C13	1.841(7)
17	S5	Ni3	2.198(2)
18	S6	C5	1.829(7)
19	S7	C1	1.817(7)
20	S8	C2	1.829(7)
21	S8	Ni3	2.1948(19)
22	S9	C16	1.836(6)
23	C1	C26	1.525(9)
24	C1	H1A	0.97
25	C1	H1B	0.97
26	C2	C9	1.512(9)
27	C2	H2A	0.97
28	C2	H2B	0.97
29	C3	C11	1.373(10)
30	C3	C27	1.383(10)
31	C3	C4	1.515(10)
32	C4	C5	1.535(9)
33	C4	H4A	0.97
34	C4	H4B	0.97
35	C5	H5A	0.97
36	C5	H5B	0.97
37	C6	C15	1.500(10)
38	C6	C16	1.520(9)
39	C6	H6A	0.97
40	C6	H6B	0.97

41	C7	C30	1.371(8)
42	C7	C20	1.379(8)
43	C7	C9	1.510(9)
44	C8	C10	1.374(9)
45	C8	C22	1.392(10)
46	C8	H8A	0.93
47	C9	H9A	0.97
48	C9	H9B	0.97
49	C10	C29	1.385(9)
50	C10	C26	1.495(9)
51	C11	C21	1.387(10)
52	C11	H11A	0.93
53	C12	C13	1.513(9)
54	C12	C25	1.521(9)
55	C12	H12A	0.97
56	C12	H12B	0.97
57	C13	H13A	0.97
58	C13	H13B	0.97
59	C14	C24	1.344(11)
60	C14	C22	1.379(11)
61	C14	H14A	0.93
62	C15	C32	1.352(11)
63	C15	C33	1.388(10)
64	C16	H16A	0.97
65	C16	H16B	0.97
66	C17	C31	1.365(9)
67	C17	C44	1.376(9)
68	C17	C18	1.511(10)
69	C18	C23	1.508(9)
70	C18	H18A	0.97
71	C18	H18B	0.97
72	C19	C35	1.362(8)
73	C19	C20	1.366(8)
74	C19	H19A	0.93
75	C20	H20A	0.93
76	C21	C34	1.364(12)
77	C21	H21A	0.93
78	C22	H22A	0.93
79	C23	H23A	0.97
80	C23	H23B	0.97
81	C24	C29	1.368(10)
82	C24	H24A	0.93
83	C25	C38	1.370(10)

84	C25	C42	1.373(9)
85	C26	H26A	0.97
86	C26	H26B	0.97
87	C27	C47	1.381(12)
88	C27	H27A	0.93
89	C29	H29A	0.93
90	C30	C43	1.369(8)
91	C30	H30A	0.93
92	C31	C49	1.378(9)
93	C31	H31A	0.93
94	C32	C36	1.387(12)
95	C32	H32A	0.93
96	C33	C46	1.387(13)
97	C33	H33A	0.93
98	C34	C47	1.370(13)
99	C34	H34A	0.93
100	C35	C43	1.368(9)
101	C35	H35A	0.93
102	C36	C37	1.350(14)
103	C36	H36A	0.93
104	C37	C46	1.353(15)
105	C37	H37A	0.93
106	C38	C39	1.382(12)
107	C38	H38A	0.93
108	C39	C40	1.360(12)
109	C39	H39A	0.93
110	C40	C41	1.362(11)
111	C40	H40A	0.93
112	C41	C42	1.382(10)
113	C41	H41A	0.93
114	C42	H42A	0.93
115	C43	H43A	0.93
116	C44	C45	1.367(10)
117	C44	H44A	0.93
118	C45	C48	1.359(11)
119	C45	H45A	0.93
120	C46	H46A	0.93
121	C47	H47A	0.93
122	C48	C49	1.365(11)
123	C48	H48A	0.93
124	C49	H49A	0.93

Table S2. Cartesian coordinates in Angstroms for the stationary states in Figure 5.
Figure 5A.
$Ni_6(SCH_2CH_2Ph)_{12}$, E_0 = -9520.372618, G_{298} = -9520.549698

Ni	2.178369	-1.803948	0.892011
Ni	2.498248	1.081191	0.737589
Ni	-0.358999	-2.919051	0.155309
S	2.394301	-0.282202	2.486366
S	2.231128	2.255957	-1.118313
S	0.849413	-3.187909	1.99049
S	3.698704	-0.565772	-0.130207
S	1.614161	2.884796	1.663761
S	1.61402	-3.077905	-0.837814
C	3.597159	-0.669469	-1.965628
H	2.54336	-0.772722	-2.261448
H	3.972558	0.28878	-2.355734
C	0.678264	2.519022	3.2053
H	-0.074628	3.313951	3.308207
H	0.166988	1.553162	3.085473
C	-1.745762	-2.831377	5.212795
C	-0.909138	-3.459772	4.116298
H	-1.577163	-3.853013	3.330451
H	-0.340247	-4.313752	4.516105
C	0.063611	-2.453995	3.482553
H	0.879063	-2.204334	4.176127
H	-0.456076	-1.530702	3.191388
C	1.245105	-5.858306	-0.897513
H	1.68994	-6.843383	-0.656379
H	0.330555	-5.765341	-0.28788
C	0.952479	2.016361	5.675719
C	5.417986	-1.882884	-4.844402
H	6.400062	-1.6576	-4.415962
C	1.628806	2.505539	4.410375
H	2.030009	3.519568	4.563817
H	2.483663	1.847411	4.175623
C	4.302969	-2.006809	-3.991762
C	-2.611744	-1.756979	4.917206
H	-2.660009	-1.379337	3.89178
C	4.886907	3.109274	-1.159647
H	4.985464	2.680342	-2.170909
H	5.068603	2.297689	-0.434454
C	3.45463	3.631178	-0.959631
H	3.200335	4.381897	-1.726321

H	3.340499	4.094977	0.032375
C	4.021817	-2.330477	-6.791168
H	3.909237	-2.445761	-7.87302
C	0.86582	-5.833142	-2.365376
C	2.230832	-4.779408	-0.442449
H	3.210324	-4.870425	-0.940438
H	2.391973	-4.849003	0.643368
C	3.573413	-2.467582	4.614196
C	4.449065	-1.903433	3.512227
H	5.506207	-1.934122	3.840689
H	4.372774	-2.554438	2.624409
C	-0.226584	0.254256	6.901029
H	-0.678204	-0.740375	6.912036
C	0.37919	0.728828	5.728826
H	0.420142	0.084961	4.846276
C	-3.403828	-1.16949	5.913186
H	-4.049751	-0.323471	5.667221
C	5.281859	-2.04823	-6.235236
H	6.15835	-1.949753	-6.882798
C	4.143354	-0.469786	3.072727
H	4.816693	-0.175774	2.254615
H	4.268802	0.255405	3.893709
C	2.9024	-2.451622	-5.949389
H	1.915563	-2.654787	-6.372391
C	5.888331	4.225923	-0.967896
C	4.440354	-1.840139	-2.491293
H	5.498019	-1.682467	-2.223518
H	4.112216	-2.763092	-1.983233
C	-1.696601	-3.306875	6.537377
H	-1.027754	-4.137623	6.782047
C	3.04568	-2.29447	-4.56351
H	2.170864	-2.404986	-3.916933
C	0.906204	2.818635	6.833128
H	1.348749	3.818963	6.807092
C	3.098471	-1.672326	5.677023
H	3.308993	-0.599469	5.701118
C	1.800569	-5.5189	-3.373084
H	2.821016	-5.229237	-3.106634
C	-0.448762	-6.164027	-2.752076
H	-1.195286	-6.376651	-1.980493
C	-3.349666	-1.655311	7.231622
H	-3.960615	-1.191536	8.011346
C	-0.263281	1.061636	8.051125

H	-0.740809	0.694238	8.964116
C	1.436901	-5.549108	-4.729195
H	2.17246	-5.277448	-5.491091
C	0.12982	-5.904385	-5.102778
H	-0.149962	-5.931336	-6.159363
C	6.416035	4.927668	-2.07007
H	6.126191	4.631396	-3.083752
C	7.309884	5.996156	-1.881252
H	7.714289	6.528263	-2.747397
C	7.687673	6.379109	-0.582362
H	8.385197	7.208206	-0.433869
C	7.165922	5.685532	0.525002
H	7.458962	5.975091	1.538576
C	6.272784	4.619306	0.331666
H	5.868913	4.080336	1.195896
C	0.30789	2.346092	8.015189
H	0.284295	2.982269	8.905334
C	3.241379	-3.837748	4.604461
H	3.574509	-4.461308	3.768999
C	2.477052	-4.406099	5.636538
H	2.229261	-5.471296	5.606025
C	-0.815262	-6.208069	-4.107421
H	-1.841479	-6.468097	-4.383733
C	-2.495162	-2.727553	7.541129
H	-2.444365	-3.11035	8.565103
C	2.01999	-3.603872	6.696854
H	1.419841	-4.038138	7.501116
C	2.326707	-2.232963	6.70805
H	1.948666	-1.591069	7.50809
Ni	-2.178369	1.803948	-0.892011
Ni	-2.498248	-1.081191	-0.737589
Ni	0.358999	2.919051	-0.155309
S	-2.394301	0.282202	-2.486366
S	-2.231128	-2.255957	1.118313
S	-0.849413	3.187909	-1.99049
S	-3.698704	0.565772	0.130207
S	-1.614161	-2.884796	-1.663761
S	-1.61402	3.077905	0.837814
C	-3.597159	0.669469	1.965628
H	-2.54336	0.772722	2.261448
H	-3.972558	-0.28878	2.355734
C	-0.678264	-2.519022	-3.2053
H	0.074628	-3.313951	-3.308207

H	-0.166988	-1.553162	-3.085473
C	1.745762	2.831377	-5.212795
C	0.909138	3.459772	-4.116298
H	1.577163	3.853013	-3.330451
H	0.340247	4.313752	-4.516105
C	-0.063611	2.453995	-3.482553
H	-0.879063	2.204334	-4.176127
H	0.456076	1.530702	-3.191388
C	-1.245105	5.858306	0.897513
H	-1.68994	6.843383	0.656379
H	-0.330555	5.765341	0.28788
C	-0.952479	-2.016361	-5.675719
C	-5.417986	1.882884	4.844402
H	-6.400062	1.6576	4.415962
C	-1.628806	-2.505539	-4.410375
H	-2.030009	-3.519568	-4.563817
H	-2.483663	-1.847411	-4.175623
C	-4.302969	2.006809	3.991762
C	2.611744	1.756979	-4.917206
H	2.660009	1.379337	-3.89178
C	-4.886907	-3.109274	1.159647
H	-4.985464	-2.680342	2.170909
H	-5.068603	-2.297689	0.434454
C	-3.45463	-3.631178	0.959631
H	-3.200335	-4.381897	1.726321
H	-3.340499	-4.094977	-0.032375
C	-4.021817	2.330477	6.791168
H	-3.909237	2.445761	7.87302
C	-0.86582	5.833142	2.365376
C	-2.230832	4.779408	0.442449
H	-3.210324	4.870425	0.940438
H	-2.391973	4.849003	-0.643368
C	-3.573413	2.467582	-4.614196
C	-4.449065	1.903433	-3.512227
H	-5.506207	1.934122	-3.840689
H	-4.372774	2.554438	-2.624409
C	0.226584	-0.254256	-6.901029
H	0.678204	0.740375	-6.912036
C	-0.37919	-0.728828	-5.728826
H	-0.420142	-0.084961	-4.846276
C	3.403828	1.16949	-5.913186
H	4.049751	0.323471	-5.667221
C	-5.281859	2.04823	6.235236

H	-6.15835	1.949753	6.882798
C	-4.143354	0.469786	-3.072727
H	-4.816693	0.175774	-2.254615
H	-4.268802	-0.255405	-3.893709
C	-2.9024	2.451622	5.949389
H	-1.915563	2.654787	6.372391
C	-5.888331	-4.225923	0.967896
C	-4.440354	1.840139	2.491293
H	-5.498019	1.682467	2.223518
H	-4.112216	2.763092	1.983233
C	1.696601	3.306875	-6.537377
H	1.027754	4.137623	-6.782047
C	-3.04568	2.29447	4.56351
H	-2.170864	2.404986	3.916933
C	-0.906204	-2.818635	-6.833128
H	-1.348749	-3.818963	-6.807092
C	-3.098471	1.672326	-5.677023
H	-3.308993	0.599469	-5.701118
C	-1.800569	5.5189	3.373084
H	-2.821016	5.229237	3.106634
C	0.448762	6.164027	2.752076
H	1.195286	6.376651	1.980493
C	3.349666	1.655311	-7.231622
H	3.960615	1.191536	-8.011346
C	0.263281	-1.061636	-8.051125
H	0.740809	-0.694238	-8.964116
C	-1.436901	5.549108	4.729195
H	-2.17246	5.277448	5.491091
C	-0.12982	5.904385	5.102778
H	0.149962	5.931336	6.159363
C	-6.416035	-4.927668	2.07007
H	-6.126191	-4.631396	3.083752
C	-7.309884	-5.996156	1.881252
H	-7.714289	-6.528263	2.747397
C	-7.687673	-6.379109	0.582362
H	-8.385197	-7.208206	0.433869
C	-7.165922	-5.685532	-0.525002
H	-7.458962	-5.975091	-1.538576
C	-6.272784	-4.619306	-0.331666
H	-5.868913	-4.080336	-1.195896
C	-0.30789	-2.346092	-8.015189
H	-0.284295	-2.982269	-8.905334
C	-3.241379	3.837748	-4.604461

H	-3.574509	4.461308	-3.768999
C	-2.477052	4.406099	-5.636538
H	-2.229261	5.471296	-5.606025
C	0.815262	6.208069	4.107421
H	1.841479	6.468097	4.383733
C	2.495162	2.727553	-7.541129
H	2.444365	3.11035	-8.565103
C	-2.01999	3.603872	-6.696854
H	-1.419841	4.038138	-7.501116
C	-2.326707	2.232963	-6.70805
H	-1.948666	1.591069	-7.50809

Figure 5B for Ni-S bond cleavage

$Ni_6(SCH_2CH_2Ph)_{11}(H)$, E_0 = -8813.081139, G_{298} = -8813.244839

Ni	0.333608	1.951849	2.086355
Ni	0.463854	-0.924292	2.132062
Ni	-0.206163	3.166847	-0.423467
S	2.044343	0.591309	2.477443
S	-1.160557	-2.149962	1.256236
S	1.478062	3.455412	0.937394
S	-0.791474	0.480259	3.301141
S	1.718906	-2.547483	1.309239
S	-1.395778	3.16517	1.420259
C	-2.569449	0.392653	2.831881
H	-2.662836	0.605183	1.757588
H	-2.885164	-0.647276	3.004125
C	3.428099	-2.020904	0.884835
H	3.785304	-2.716077	0.11088
H	3.397025	-1.002823	0.471144
C	5.128954	3.769153	-0.952276
C	3.647252	3.914403	-0.670072
H	3.064272	3.865916	-1.608303
H	3.46858	4.919247	-0.251588
C	3.09809	2.867462	0.308107
H	3.753192	2.765657	1.185551
H	2.958838	1.880501	-0.153702
C	-1.833956	5.919217	1.357895
H	-1.767809	6.870028	1.920714
H	-1.216329	6.039326	0.452591
C	5.722209	-1.588741	1.862249
C	-5.865904	0.860464	4.207796
H	-5.565639	0.602701	5.228639

C	4.316922	-2.084688	2.134775
H	4.349267	-3.123294	2.500769
H	3.852821	-1.472559	2.927268
C	-4.886964	1.265838	3.278839
C	5.717847	2.513634	-1.198277
H	5.112178	1.604336	-1.172953
C	-1.900488	-3.386408	3.642389
H	-2.928333	-3.027694	3.465447
H	-1.344353	-2.580332	4.150884
C	-1.221701	-3.677591	2.293798
H	-1.791224	-4.433358	1.728159
H	-0.19652	-4.051877	2.440041
C	-7.614381	1.1173	2.528511
H	-8.666309	1.053942	2.235553
C	-3.272804	5.674875	0.942235
C	-1.205702	4.81887	2.222231
H	-1.68704	4.735096	3.21062
H	-0.133947	5.015747	2.376388
C	3.662181	2.93379	4.015286
C	2.525048	2.217783	4.719026
H	2.700208	2.231821	5.812177
H	1.588287	2.771827	4.537374
C	7.252649	0.22124	1.25611
H	7.404221	1.261366	0.956459
C	5.952076	-0.244234	1.501915
H	5.107238	0.447695	1.423457
C	7.088768	2.400588	-1.478631
H	7.512575	1.414341	-1.681647
C	-7.221965	0.790035	3.838632
H	-7.9696	0.476448	4.573456
C	2.299343	0.758593	4.305459
H	1.417015	0.351523	4.821083
H	3.16444	0.120329	4.54995
C	-6.644367	1.513652	1.591891
H	-6.933493	1.757167	0.567115
C	-1.930725	-4.632627	4.498216
C	-3.423957	1.356441	3.665252
H	-3.300859	1.129902	4.737121
H	-3.057279	2.384497	3.501714
C	5.956308	4.911086	-0.974292
H	5.516301	5.893285	-0.771812
C	-5.29595	1.587071	1.96786
H	-4.55268	1.910439	1.234824

C	6.829647	-2.452882	1.970762
H	6.663737	-3.496436	2.253287
C	4.907858	2.312434	3.791189
H	5.071802	1.277419	4.106272
C	-4.229043	5.167587	1.846173
H	-3.935522	4.917025	2.870314
C	-3.685079	5.969001	-0.372876
H	-2.949921	6.339504	-1.093664
C	7.902099	3.545752	-1.502553
H	8.97053	3.459459	-1.720476
C	8.350126	-0.649786	1.365493
H	9.362766	-0.287103	1.167642
C	-5.557984	4.953516	1.447915
H	-6.276069	4.531402	2.155342
C	-5.957167	5.249931	0.133009
H	-6.988388	5.066633	-0.181031
C	-3.054082	-5.484126	4.495523
H	-3.930828	-5.214442	3.896992
C	-3.060825	-6.6663	5.255635
H	-3.942154	-7.314492	5.24765
C	-1.939839	-7.014468	6.029741
H	-1.945563	-7.932007	6.624848
C	-0.813263	-6.172064	6.038175
H	0.060689	-6.434331	6.641877
C	-0.810288	-4.992315	5.276134
H	0.068121	-4.337617	5.28555
C	8.135115	-1.991169	1.727113
H	8.982243	-2.677618	1.819251
C	3.492366	4.2632	3.579387
H	2.524753	4.752554	3.7251
C	4.529514	4.951021	2.927026
H	4.366062	5.974281	2.576287
C	-5.016028	5.764044	-0.775163
H	-5.313071	5.995253	-1.802664
C	7.330711	4.805259	-1.245427
H	7.954697	5.704187	-1.256296
C	5.764002	4.318018	2.701954
H	6.563803	4.837431	2.167513
C	5.948764	2.996662	3.142462
H	6.899917	2.487598	2.967311
Ni	0.064908	-0.927022	-2.805664
Ni	-0.291293	1.90052	-2.558196
Ni	0.294394	-2.455535	-0.375906

S	-1.641319	0.360018	-3.357535
S	-1.121793	-2.638242	-2.065032
S	1.263377	0.763521	-3.62051
S	-1.788724	3.290327	-1.868447
S	1.756026	-2.144583	-2.00758
C	2.992676	0.73073	-2.985733
H	2.990152	0.313593	-1.968316
H	3.353451	1.769539	-2.950267
C	-3.351641	2.467962	-1.328566
H	-3.716598	3.051254	-0.469684
H	-3.12574	1.44155	-1.006355
C	-4.806238	-3.178069	-0.243621
C	-3.492097	-3.464683	-0.941873
H	-2.783323	-3.889773	-0.2097
H	-3.641915	-4.228851	-1.720713
C	-2.845974	-2.224558	-1.577442
H	-3.37429	-1.924817	-2.493721
H	-2.818282	-1.378672	-0.876567
C	1.934417	-4.947314	-2.194907
H	1.903359	-5.815532	-2.88169
H	1.066726	-5.043061	-1.521303
C	-5.660122	1.787562	-2.145102
C	6.360787	-0.04836	-4.25419
H	6.203109	0.486202	-5.196327
C	-4.363825	2.495038	-2.482032
H	-4.568662	3.542309	-2.755501
H	-3.901726	2.010151	-3.360236
C	5.248136	-0.407595	-3.468614
C	-4.868366	-2.25433	0.821709
H	-3.963567	-1.711717	1.111327
C	7.877921	-1.047212	-2.630018
H	8.892834	-1.289488	-2.301582
C	3.208639	-5.013683	-1.376972
C	1.741244	-3.685126	-3.038752
H	2.543032	-3.551912	-3.783607
H	0.781927	-3.736097	-3.57351
C	-3.045675	-1.757909	-5.288971
C	-1.808941	-1.028542	-5.781525
H	-1.850291	-0.938013	-6.884098
H	-0.919811	-1.63761	-5.545584
C	-6.855914	-0.266621	-1.560313
H	-6.828519	-1.329852	-1.311784
C	-5.660377	0.412651	-1.834771

H	-4.716154	-0.137058	-1.823605
C	-6.067157	-2.023899	1.511016
H	-6.096717	-1.291119	2.32102
C	7.666633	-0.371373	-3.844611
H	8.518688	-0.085981	-4.468903
C	-1.593039	0.375493	-5.206192
H	-0.618609	0.773912	-5.526101
H	-2.376521	1.083355	-5.523164
C	6.775289	-1.397403	-1.830641
H	6.926633	-1.908189	-0.876378
C	3.836779	-0.126723	-3.944165
H	3.865142	0.362513	-4.931553
H	3.309143	-1.087068	-4.083838
C	-5.983278	-3.861071	-0.607077
H	-5.952332	-4.575946	-1.435598
C	5.474339	-1.085727	-2.252168
H	4.621203	-1.38763	-1.638772
C	-6.892193	2.471038	-2.170934
H	-6.906651	3.538628	-2.411271
C	-4.265356	-1.088666	-5.057623
H	-4.33578	-0.007799	-5.210883
C	4.451769	-4.604038	-1.90149
H	4.509373	-4.165201	-2.901966
C	3.173426	-5.540528	-0.070266
H	2.211599	-5.829265	0.364386
C	-7.233095	-2.721318	1.147891
H	-8.169907	-2.538111	1.681867
C	-8.080506	0.422084	-1.597073
H	-9.013841	-0.105528	-1.380331
C	5.630598	-4.740843	-1.151172
H	6.58148	-4.405196	-1.573752
C	5.586531	-5.295322	0.13941
H	6.506973	-5.411834	0.717804
C	-8.096083	1.794787	-1.903165
H	-9.044717	2.339516	-1.932003
C	-2.99304	-3.14754	-5.05973
H	-2.047233	-3.677645	-5.208161
C	-4.125322	-3.852962	-4.618808
H	-4.058577	-4.93064	-4.442313
C	4.350604	-5.687067	0.682374
H	4.299975	-6.09979	1.694339
C	-7.188623	-3.639877	0.084649
H	-8.092469	-4.182109	-0.209709

C	-5.33266	-3.172096	-4.38434
H	-6.212124	-3.711201	-4.021406
C	-5.39758	-1.785287	-4.604588
H	-6.322699	-1.240513	-4.399449
H	0.774237	2.677525	-1.61759

Figure 5B for C-S bond cleavage

$Ni_6(SCH_2CH_2Ph)_{11}(SH)$, E_0 = -9211.151877, G_{298} = -9211.313998

Ni	-0.358704	-1.770989	2.213218
Ni	-0.482295	1.124791	2.130492
Ni	0.059643	-3.317745	-0.255903
S	-2.053609	-0.382942	2.558256
S	1.15001	2.383789	1.328624
S	-1.509571	-3.421469	1.307534
S	0.77056	-0.241937	3.345313
S	-1.755879	2.668922	1.190845
S	1.360489	-2.976379	1.495539
C	2.555669	-0.198777	2.906336
H	2.664286	-0.424322	1.835962
H	2.900053	0.831985	3.079861
C	-3.399838	2.021162	0.674989
H	-3.737301	2.6507	-0.160885
H	-3.272319	0.988981	0.319566
C	-5.236678	-3.750348	-0.525051
C	-3.893939	-4.125448	0.069847
H	-3.241858	-4.53708	-0.720155
H	-4.031671	-4.922083	0.817463
C	-3.192098	-2.936491	0.744246
H	-3.738507	-2.623662	1.646068
H	-3.111502	-2.064149	0.076294
C	1.728852	-5.758588	1.614201
H	1.670703	-6.657932	2.2577
H	0.993783	-5.900281	0.804197
C	-5.703611	1.394237	1.510283
C	5.816825	-0.842101	4.303125
H	5.532892	-0.510564	5.307258
C	-4.396672	2.087705	1.841173
H	-4.582663	3.142004	2.098597
H	-3.940714	1.608913	2.725021
C	4.813832	-1.223777	3.389969
C	-5.33305	-2.789016	-1.55253
H	-4.435049	-2.275845	-1.908442

C	1.491842	3.697296	3.764985
H	2.519848	3.297509	3.774635
H	0.833921	2.929106	4.205845
C	1.050665	3.943274	2.313158
H	1.712349	4.676425	1.82266
H	0.018267	4.323669	2.273987
C	7.546239	-1.309387	2.65009
H	8.600512	-1.334756	2.359885
C	3.11751	-5.67112	1.01031
C	1.28483	-4.559373	2.456015
H	1.924211	-4.408667	3.341575
H	0.251147	-4.704791	2.80312
C	-3.641922	-2.554047	4.41784
C	-2.471911	-1.764175	4.971178
H	-2.592007	-1.664596	6.067523
H	-1.541703	-2.333185	4.803838
C	-6.919836	-0.64077	0.895983
H	-6.90399	-1.702364	0.638799
C	-5.719514	0.01995	1.193314
H	-4.781266	-0.54144	1.192883
C	-6.566965	-2.464507	-2.133447
H	-6.61397	-1.70593	-2.917721
C	7.175369	-0.888064	3.939175
H	7.941696	-0.589939	4.661086
C	-2.27373	-0.359025	4.399117
H	-1.383908	0.105851	4.847957
H	-3.136521	0.299398	4.593362
C	6.552711	-1.687418	1.730482
H	6.826026	-2.003343	0.721113
C	1.428085	4.980183	4.563074
C	3.348065	-1.188779	3.771714
H	3.239448	-0.916847	4.834587
H	2.906386	-2.192338	3.647272
C	-6.420822	-4.375521	-0.087135
H	-6.364208	-5.120445	0.711869
C	5.201349	-1.646222	2.101221
H	4.437605	-1.952917	1.381311
C	-6.927573	2.091994	1.528298
H	-6.931012	3.157745	1.776287
C	-4.870869	-1.943607	4.094832
H	-4.987456	-0.859661	4.181212
C	4.201617	-5.100915	1.708202
H	4.048212	-4.658373	2.696765

C	3.352393	-6.198849	-0.275628
H	2.514348	-6.611362	-0.84547
C	-7.73966	-3.101552	-1.692206
H	-8.704459	-2.847035	-2.140081
C	-8.13486	0.065147	0.915247
H	-9.070411	-0.447626	0.673882
C	5.487612	-5.071303	1.144496
H	6.307392	-4.601528	1.694201
C	5.713371	-5.620518	-0.128874
H	6.715475	-5.598163	-0.565762
C	2.577799	5.772754	4.752876
H	3.537121	5.431616	4.349548
C	2.505722	6.988382	5.45491
H	3.408334	7.589806	5.597889
C	1.277129	7.429944	5.976649
H	1.219837	8.373535	6.526489
C	0.122978	6.647126	5.79141
H	-0.835639	6.98243	6.198413
C	0.199612	5.433446	5.088681
H	-0.70074	4.825284	4.947721
C	-8.136488	1.434161	1.236564
H	-9.077796	1.991973	1.25589
C	-3.524081	-3.949003	4.251981
H	-2.565883	-4.432848	4.465551
C	-4.609653	-4.719531	3.803868
H	-4.495296	-5.800852	3.682697
C	4.638521	-6.181615	-0.840451
H	4.797279	-6.596119	-1.840456
C	-7.663187	-4.05755	-0.664395
H	-8.570761	-4.556547	-0.311161
C	-5.834944	-4.100001	3.501318
H	-6.684002	-4.693494	3.151694
C	-5.957541	-2.707098	3.638206
H	-6.893394	-2.207962	3.373547
Ni	0.165233	1.039182	-2.825657
Ni	0.346364	-1.904425	-2.737354
Ni	-0.218935	2.575372	-0.397796
S	1.871231	-0.34421	-3.126408
S	1.309165	2.73647	-1.992398
S	-0.93217	-0.532265	-3.923673
S	1.671877	-3.403788	-1.776984
S	-1.570105	2.239885	-2.117108
C	-2.722006	-0.5742	-3.497999

H	-2.837372	-0.341595	-2.428254
H	-3.075903	-1.599968	-3.687833
C	3.262365	-2.675474	-1.202196
H	3.592486	-3.281305	-0.34581
H	3.079418	-1.645548	-0.865286
C	4.950976	3.184284	-0.054583
C	3.65487	3.52951	-0.75933
H	2.948907	3.969135	-0.033659
H	3.838845	4.289109	-1.53505
C	2.994558	2.30107	-1.40245
H	3.5605	1.965692	-2.282952
H	2.912119	1.46997	-0.688106
C	-1.842701	5.035698	-2.243749
H	-1.791721	5.925621	-2.900957
H	-1.044878	5.151484	-1.490817
C	5.574064	-1.980121	-1.985605
C	-6.007166	0.257663	-4.807236
H	-5.781864	-0.105858	-5.815109
C	4.298115	-2.72093	-2.334459
H	4.526043	-3.771266	-2.573652
H	3.853012	-2.271273	-3.239191
C	-4.948829	0.565265	-3.929416
C	4.956332	2.266617	1.017232
H	4.014608	1.800721	1.320817
C	-7.641354	0.879673	-3.108963
H	-8.680403	0.99151	-2.786076
C	-3.187138	5.017257	-1.542952
C	-1.511897	3.810661	-3.099645
H	-2.223264	3.675857	-3.931364
H	-0.503733	3.913872	-3.526833
C	3.487637	1.799115	-5.019403
C	2.321993	0.995596	-5.562351
H	2.449228	0.872146	-6.655467
H	1.390463	1.568187	-5.414567
C	6.713032	0.094166	-1.357351
H	6.657727	1.150319	-1.084908
C	5.536493	-0.611802	-1.646529
H	4.576951	-0.088272	-1.626291
C	6.143312	1.946282	1.690474
H	6.129057	1.216181	2.503212
C	-7.345861	0.419855	-4.404364
H	-8.155676	0.179226	-5.099724
C	2.120238	-0.398035	-4.964044

H	1.238903	-0.875618	-5.416085
H	2.986596	-1.058428	-5.133072
C	-6.592417	1.180963	-2.22276
H	-6.809095	1.522764	-1.207893
C	-3.502964	0.427034	-4.364215
H	-3.452721	0.112885	-5.419355
H	-3.000732	1.407232	-4.294836
C	6.170414	3.775915	-0.43662
H	6.181826	4.484018	-1.270773
C	-5.260754	1.03011	-2.634523
H	-4.450868	1.289281	-1.947472
C	6.825764	-2.62605	-2.029175
H	6.869643	-3.687221	-2.292971
C	4.709572	1.19678	-4.657693
H	4.825628	0.1107	-4.710169
C	-4.345865	4.50824	-2.164422
H	-4.283902	4.056184	-3.158383
C	-3.304462	5.554003	-0.244688
H	-2.407927	5.919105	0.265626
C	7.354324	2.548122	1.304602
H	8.282488	2.292898	1.823968
C	7.956488	-0.558236	-1.409371
H	8.873538	-0.009067	-1.177015
C	-5.590481	4.552521	-1.51545
H	-6.47168	4.134087	-2.009111
C	-5.698687	5.113376	-0.231522
H	-6.669675	5.151964	0.269752
C	8.010839	-1.92198	-1.748668
H	8.974267	-2.439244	-1.790882
C	3.371472	3.199204	-4.900747
H	2.418978	3.678491	-5.147484
C	4.450085	3.980575	-4.455082
H	4.336356	5.065368	-4.369378
C	-4.548226	5.609634	0.40581
H	-4.615519	6.030703	1.413358
C	7.364816	3.46514	0.23932
H	8.303415	3.934814	-0.07057
C	5.666855	3.3677	-4.107269
H	6.509083	3.969376	-3.754826
C	5.789183	1.971433	-4.202622
H	6.717811	1.478105	-3.90428
S	-1.187663	-3.37549	-2.097169
H	-2.204878	-2.546182	-1.734927

Figure 5C.
$Ni_6(SCH_2CH_3)_{12}$, E_0 = -6751.525897, G_{298} = -6751.636562

Ni	0	2.910532	0.002502
Ni	-2.520595	1.455266	-0.002502
Ni	2.520595	1.455266	-0.002502
S	-1.63052	2.820564	1.506264
S	-3.25794	-0.00179	-1.506264
S	1.695009	2.932169	1.431073
S	-1.691828	2.934006	-1.431073
S	-3.386838	0.001837	1.431073
S	1.62742	2.822353	-1.506264
C	-1.234645	2.169008	-3.046923
H	-0.399873	1.472065	-2.879227
H	-2.112	1.583972	-3.361491
C	-2.495738	0.01527	3.046923
H	-2.42776	-1.03706	3.361491
H	-1.474783	0.389732	2.879227
C	2.373945	2.373943	4.07011
H	3.304808	1.881534	3.749215
H	2.578815	3.447126	4.211845
C	1.261093	2.153738	3.046923
H	0.31576	2.621032	3.361491
H	1.074909	1.082333	2.879227
C	4.033298	4.197447	-1.812624
H	4.588857	5.148365	-1.748092
H	4.547221	3.446093	-1.192496
C	-3.242868	0.868925	4.07011
H	-4.274707	0.509756	4.211845
H	-3.28186	1.92128	3.749215
C	-5.651744	1.394215	-1.812624
H	-5.367523	1.59254	-2.858765
H	-5.258014	2.214963	-1.192496
C	-5.100312	0.05299	-1.328585
H	-5.482843	-0.787884	-1.930206
H	-5.354623	-0.13083	-0.27372
C	2.596046	4.390505	-1.328585
H	2.059094	5.142224	-1.930206
H	2.564009	4.702654	-0.27372
C	-1.618446	5.591662	1.812624
H	-2.164186	6.548249	1.748092
H	-0.710793	5.661055	1.192496

C	-2.504265	4.443494	1.328585
H	-2.790613	4.571824	0.27372
H	-3.423749	4.35434	1.930206
C	-0.868923	3.242868	-4.07011
H	-1.695891	3.956883	-4.211845
H	0.022948	3.802814	-3.749215
Ni	0	-2.910532	-0.002502
Ni	2.520595	-1.455266	0.002502
Ni	-2.520595	-1.455266	0.002502
S	1.63052	-2.820564	-1.506264
S	3.25794	0.00179	1.506264
S	-1.695009	-2.932169	-1.431073
S	1.691828	-2.934006	1.431073
S	3.386838	-0.001837	-1.431073
S	-1.62742	-2.822353	1.506264
C	1.234645	-2.169008	3.046923
H	0.399873	-1.472065	2.879227
H	2.112	-1.583972	3.361491
C	2.495738	-0.01527	-3.046923
H	2.42776	1.03706	-3.361491
H	1.474783	-0.389732	-2.879227
C	-2.373945	-2.373943	-4.07011
H	-3.304808	-1.881534	-3.749215
H	-2.578815	-3.447126	-4.211845
C	-1.261093	-2.153738	-3.046923
H	-0.31576	-2.621032	-3.361491
H	-1.074909	-1.082333	-2.879227
C	-4.033298	-4.197447	1.812624
H	-4.588857	-5.148365	1.748092
H	-4.547221	-3.446093	1.192496
C	3.242868	-0.868925	-4.07011
H	4.274707	-0.509756	-4.211845
H	3.28186	-1.92128	-3.749215
C	5.651744	-1.394215	1.812624
H	5.367523	-1.59254	2.858765
H	5.258014	-2.214963	1.192496
C	5.100312	-0.05299	1.328585
H	5.482843	0.787884	1.930206
H	5.354623	0.13083	0.27372
C	-2.596046	-4.390505	1.328585
H	-2.059094	-5.142224	1.930206
H	-2.564009	-4.702654	0.27372
C	1.618446	-5.591662	-1.812624

H	2.164186	-6.548249	-1.748092
H	0.710793	-5.661055	-1.192496
C	2.504265	-4.443494	-1.328585
H	2.790613	-4.571824	-0.27372
H	3.423749	-4.35434	-1.930206
C	0.868923	-3.242868	4.07011
H	1.695891	-3.956883	4.211845
H	-0.022948	-3.802814	3.749215
H	-2.079598	-1.947553	-5.044435
H	0.646832	-2.774761	5.044435
H	-2.72643	0.827208	5.044435
H	-4.062942	-3.852141	2.858765
H	-6.753043	1.399884	-1.748092
H	1.304581	-5.444682	-2.858765
H	-0.646832	2.774761	-5.044435
H	-1.304581	5.444682	2.858765
H	2.72643	-0.827208	-5.044435
H	6.753043	-1.399884	1.748092
H	2.079598	1.947553	5.044435
H	4.062942	3.852141	-2.858765

Figure 5D. TS1

$Ni_6(SCH_2CH_3)_{12} + H_2 \rightarrow Ni_6(SCH_2CH_3)_{11}(SH) + C_2H_6$, $E_0 = -6752.58524$, $G_{298} = -6752.70046$

Ni	-3.114014	-0.58027	-0.242286
Ni	-0.989906	-2.317351	-0.016767
Ni	-1.988552	1.970471	-0.318779
S	-2.588875	-1.88356	1.468695
S	0.694256	-2.557269	-1.454801
S	-3.63799	1.206664	0.962074
S	-2.70049	-2.385447	-1.470911
S	0.566871	-2.408676	1.470015
S	-3.102623	0.890173	-1.910011
C	-2.157322	-1.982459	-3.184852
H	-1.580129	-1.047057	-3.159815
H	-1.472975	-2.79228	-3.480066
C	-0.615974	-1.569041	4.541352
H	0.31537	-1.803861	5.065181
H	-0.541409	-0.876157	3.702054
C	-3.557998	2.326894	3.499991
H	-3.007783	3.203393	3.124815
H	-4.636871	2.529718	3.406856

C	-3.161417	1.065008	2.73533
H	-3.682922	0.17503	3.118352
H	-2.079467	0.881459	2.794281
C	-4.557225	3.179847	-2.537712
H	-5.539014	3.669143	-2.654983
H	-3.949824	3.770218	-1.833448
C	-1.934747	-1.800047	5.189713
H	-1.937869	-2.677948	5.854877
H	-2.732359	-1.905456	4.434369
C	-0.083523	-5.12464	-2.285085
H	-0.036398	-4.807982	-3.339654
H	-1.100678	-4.931464	-1.908433
C	0.955776	-4.39305	-1.436765
H	1.978164	-4.556125	-1.815537
H	0.923237	-4.711294	-0.384138
C	-4.735547	1.754191	-2.015095
H	-5.352559	1.143158	-2.694468
H	-5.202529	1.746388	-1.018652
C	-5.110483	-2.94757	1.986476
H	-5.772507	-3.829564	2.015383
H	-5.569316	-2.188616	1.333406
C	-3.728393	-3.339389	1.462005
H	-3.783972	-3.745378	0.440706
H	-3.242823	-4.089212	2.108426
C	-3.352526	-1.88484	-4.131109
H	-3.939036	-2.817454	-4.133457
H	-4.017296	-1.059278	-3.833265
Ni	3.234208	0.459061	0.201439
Ni	1.016068	2.399877	-0.005175
Ni	2.138057	-1.912941	0.093973
S	2.749328	1.981267	-1.331404
S	-0.73426	2.811379	1.299941
S	3.804245	-1.158163	-1.224222
S	2.489979	2.008707	1.606209
S	-0.439007	2.88055	-1.609884
S	3.437209	-1.146034	1.7443
C	1.658268	1.227227	3.057088
H	1.34636	0.212132	2.764721
H	0.7526	1.827318	3.233771
C	-0.095892	1.884735	-3.128051
H	-1.078197	1.561682	-3.505182
H	0.469599	0.990435	-2.828198
C	3.551957	-2.042418	-3.834222

H	3.021293	-2.947489	-3.499418
H	4.633004	-2.255254	-3.82741
C	3.212005	-0.8498	-2.940106
H	3.701944	0.073749	-3.283433
H	2.12583	-0.677562	-2.915165
C	4.952646	-3.487906	1.779685
H	5.948856	-3.962308	1.762948
H	4.338949	-3.928745	0.978292
C	0.663894	2.714171	-4.162018
H	0.0984	3.617762	-4.440442
H	1.646062	3.021953	-3.771694
C	0.233639	5.359372	1.8939
H	0.257733	5.073873	2.95801
H	1.206753	5.095252	1.450873
C	-0.901027	4.651189	1.15346
H	-1.88636	4.901116	1.580587
H	-0.912407	4.913383	0.084281
C	5.081431	-1.978138	1.572708
H	5.720682	-1.515468	2.342636
H	5.503139	-1.744803	0.584126
C	5.34935	2.984662	-1.397551
H	6.035319	3.833918	-1.238901
H	5.696779	2.134938	-0.788695
C	3.924274	3.374448	-1.003203
H	3.861122	3.644284	0.062177
H	3.552486	4.22493	-1.598153
C	2.573877	1.213051	4.278844
H	2.892858	2.23182	4.551724
H	3.470758	0.603498	4.091046
H	3.247549	-1.834421	-4.874109
H	2.037292	0.776235	5.139064
H	-2.215742	-0.919353	5.809303
H	4.472449	-3.723479	2.742974
H	0.098228	-6.211955	-2.24981
H	5.406823	2.690067	-2.457832
H	-3.006248	-1.69186	-5.160913
H	-5.053507	-2.532176	3.006288
H	0.830225	2.116108	-5.074506
H	0.103396	6.453066	1.833663
H	-3.320063	2.209283	4.571055
H	-4.04816	3.189762	-3.515066
H	-0.374203	-3.862426	3.272838
H	-0.513237	-3.242814	3.749786

Figure 5D. IM1

$Ni_6(SCH_2CH_3)_{11}(SH)$, E_0 = -6673.04190, G_{298} = -6673.14839

Ni	-1.608362	2.285992	-0.219843
Ni	-2.834406	-0.369767	0.10596
Ni	1.261578	2.50887	-0.260798
S	-2.830975	1.420414	1.41403
S	-2.644889	-2.157003	-1.19424
S	-0.242885	3.478718	1.050851
S	-3.008456	1.140812	-1.50467
S	-2.757715	-1.886193	1.721311
S	-0.238788	2.946585	-1.83844
C	-2.200687	0.595279	-3.071211
H	-1.115084	0.544554	-2.898451
H	-2.568181	-0.424116	-3.263371
C	-2.00506	-1.214801	3.267117
H	-1.393624	-2.02945	3.684488
H	-1.342201	-0.378284	2.998604
C	0.69332	3.788627	3.64588
H	1.733154	3.801618	3.284979
H	0.305984	4.819844	3.628815
C	-0.165345	2.862028	2.78687
H	-1.20683	2.822956	3.140071
H	0.230192	1.835098	2.777807
C	0.997413	5.357543	-2.484525
H	0.93421	6.455659	-2.569102
H	1.845605	5.102642	-1.82946
C	-3.090486	-0.770506	4.246997
H	-3.774603	-1.600209	4.48593
H	-3.680426	0.058994	3.827831
C	-5.401804	-2.289059	-1.555468
H	-5.237668	-2.110394	-2.630473
H	-5.51642	-1.310845	-1.062131
C	-4.23903	-3.063196	-0.934334
H	-4.103089	-4.050239	-1.405957
H	-4.383915	-3.212161	0.146338
C	-0.303185	4.795359	-1.909809
H	-1.170544	5.039947	-2.544772
H	-0.494596	5.179417	-0.89637
C	-4.43263	3.691787	1.59839
H	-5.43166	4.150732	1.507892
H	-3.735047	4.234805	0.941181

C	-4.491003	2.215042	1.207025
H	-4.812298	2.0869	0.161997
H	-5.178815	1.646214	1.854237
C	-2.542846	1.549126	-4.214567
H	-3.632276	1.617286	-4.363614
H	-2.15619	2.559727	-4.011391
Ni	1.550585	-2.603888	0.350049
Ni	2.807618	0.077032	0.043501
Ni	-1.263416	-2.842139	0.389276
S	2.771183	-1.712694	-1.260301
S	2.64978	1.867435	1.34749
S	0.21965	-3.811136	-0.948124
S	2.919899	-1.440568	1.65154
S	2.78887	1.591412	-1.576446
S	0.218794	-3.404197	1.968135
C	2.080784	-0.891792	3.201944
H	0.996792	-0.866776	3.017113
H	2.42012	0.140148	3.3791
C	2.0794	0.923406	-3.143211
H	1.489651	1.742842	-3.58073
H	1.392292	0.100446	-2.894275
C	-0.73478	-4.056071	-3.544622
H	-1.774484	-4.057616	-3.183047
H	-0.36514	-5.093862	-3.545554
C	0.140027	-3.158077	-2.671436
H	1.180359	-3.126563	-3.029178
H	-0.24081	-2.126097	-2.640381
C	3.190546	0.458291	-4.083465
H	3.897179	1.275231	-4.300498
H	3.753196	-0.379754	-3.643935
C	5.411974	1.972718	1.691105
H	5.251063	1.783046	2.764682
H	5.518859	0.999319	1.186735
C	4.250586	2.759364	1.083399
H	4.126408	3.743963	1.563584
H	4.390696	2.915197	0.003018
C	4.367075	-3.986817	-1.483129
H	5.362704	-4.451963	-1.38779
H	3.657856	-4.541716	-0.848829
C	4.426365	-2.519591	-1.058137
H	4.739099	-2.414534	-0.007952
H	5.120333	-1.937526	-1.686923
C	2.436659	-1.815374	4.366219

H	3.525295	-1.840673	4.533009
H	2.090976	-2.842715	4.175676
H	-0.733937	-3.688072	-4.584835
H	1.955089	-1.45644	5.292013
H	-2.629233	-0.421982	5.186873
H	-6.341285	-2.855415	-1.440217
H	4.040114	-4.089506	-2.530578
H	-2.08776	1.190867	-5.153831
H	-4.089973	3.819225	2.638083
H	2.756752	0.114764	-5.038138
H	6.354439	2.534712	1.577812
H	0.697386	3.438454	4.692227
H	1.20548	4.946979	-3.48584
H	0.328898	-4.722571	1.635035

Figure 5D. IM2

$Ni_6(SCH_2CH_3)_{10}(SH)_2$, E_0 = -6594.55549, G_{298} = -6594.65973

Ni	0.941489	-2.811724	-0.640483
Ni	-1.952031	-2.336164	-0.762047
Ni	2.81915	-0.657962	-0.030296
S	-0.499643	-2.971562	-2.327639
S	-3.260952	-1.562622	0.852796
S	2.72265	-2.073017	-1.728965
S	-0.756437	-3.725382	0.469475
S	-3.246424	-1.083643	-2.07386
S	2.23476	-2.462072	1.119159
C	-0.749468	-3.252826	2.253281
H	-0.227562	-2.289811	2.356231
H	-1.804223	-3.105922	2.529735
C	3.636053	-0.889967	-4.070493
H	4.208738	-0.14833	-3.493522
H	4.271327	-1.775874	-4.227919
C	2.344735	-1.263459	-3.341559
H	1.767627	-2.000055	-3.922768
H	1.715443	-0.378105	-3.158415
C	4.866462	-3.048181	1.803598
H	5.724412	-3.738998	1.7468
H	5.179891	-2.06483	1.418275
C	-4.977238	-3.755354	0.702439
H	-4.700754	-4.009231	1.738566
H	-4.273116	-4.265655	0.026719
C	-4.940303	-2.244612	0.470011

H	-5.636794	-1.710877	1.137575
H	-5.199165	-1.990602	-0.568979
C	3.69563	-3.591559	0.984294
H	3.353226	-4.571395	1.355806
H	3.959065	-3.69672	-0.079077
C	-0.08663	-4.342238	3.09489
H	-0.586317	-5.314039	2.95529
H	0.974933	-4.456694	2.826398
Ni	-1.074734	2.461104	0.193591
Ni	1.799668	2.020387	0.379048
Ni	-2.98738	0.281604	-0.348112
S	0.315867	2.618401	1.914583
S	3.108809	1.196677	-1.2133
S	-2.837622	1.723215	1.31301
S	0.619286	3.384907	-0.901509
S	3.037251	0.72361	1.684638
S	-2.340085	2.015843	-1.572346
C	0.660338	2.904398	-2.681707
H	0.178883	1.920702	-2.7864
H	1.724376	2.796388	-2.940275
C	2.128666	0.16422	3.188313
H	2.46109	-0.867541	3.377145
H	1.052508	0.141864	2.959815
C	-3.657692	0.59326	3.713676
H	-4.292556	-0.128384	3.176537
H	-4.250305	1.502346	3.903359
C	-2.397614	0.91216	2.910376
H	-1.740776	1.620443	3.437456
H	-1.817248	0.003034	2.692533
C	-4.946133	2.651727	-2.332783
H	-5.781097	3.372329	-2.318279
H	-5.30181	1.69299	-1.923687
C	2.432554	1.085178	4.369068
H	3.51423	1.126852	4.57392
H	2.077859	2.108103	4.169136
C	4.887078	3.337731	-1.050476
H	4.639288	3.594635	-2.093159
H	4.183311	3.870529	-0.391686
C	4.801169	1.830404	-0.809407
H	5.493903	1.271742	-1.460363
H	5.027679	1.575797	0.237093
C	-3.77638	3.183476	-1.505228
H	-3.400623	4.143693	-1.895845

H	-4.056874	3.325353	-0.450341
C	-0.787515	5.034215	2.755871
H	-0.655807	6.111241	2.954526
H	-1.617499	4.907172	2.042913
C	0.501245	4.441144	2.185399
H	0.772581	4.910588	1.227568
H	1.347226	4.557348	2.882666
C	-0.031929	3.959875	-3.542623
H	0.430744	4.950683	-3.408795
H	-1.099973	4.038666	-3.287158
H	-3.383608	0.150103	4.686236
H	0.043383	3.685359	-4.60859
H	-4.653117	2.485148	-3.38177
H	-5.991713	-4.144484	0.512663
H	-1.071878	4.543911	3.701075
H	-0.141339	-4.076174	4.164313
H	1.92302	0.717445	5.275997
H	5.90806	3.699256	-0.841337
H	3.401496	-0.45269	-5.055743
H	4.593701	-2.927399	2.864596
H	-0.307232	-1.779025	-2.959811
H	-2.406738	-0.541001	-3.002966

Figure 5D. CAT
$Ni_6(SCH_2CH_3)_{10}(S)(H_2S)$, E_0 = -6594.49358, G_{298} = -6594.59806

Ni	1.927455	-2.206814	-0.554586
Ni	-1.322933	-2.361632	-0.827702
Ni	3.218686	0.065425	0.054439
S	0.389616	-1.978925	-2.125169
S	-2.984557	-2.34396	0.610115
S	3.735932	-1.3742	-1.569754
S	0.257022	-3.331793	0.456396
S	-2.731343	-1.460522	-2.216539
S	3.062786	-1.768877	1.292313
C	0.046612	-2.849815	2.225329
H	0.428536	-1.82418	2.340419
H	-1.042207	-2.83859	2.391499
C	4.607783	-0.034321	-3.839341
H	4.857077	0.851052	-3.234159
H	5.483909	-0.701476	-3.854269
C	3.381015	-0.741425	-3.26341
H	3.102704	-1.619497	-3.869217

H	2.526755	-0.048518	-3.218853
C	5.747229	-1.820235	2.014587
H	6.711436	-2.35583	2.016052
H	5.89594	-0.830635	1.55474
C	-3.735077	-4.953302	-0.030076
H	-3.444326	-5.253568	0.989715
H	-2.853403	-5.062507	-0.681628
C	-4.244151	-3.513314	-0.07035
H	-5.139967	-3.377852	0.55873
H	-4.465237	-3.180656	-1.094968
C	4.704615	-2.618348	1.230676
H	4.537431	-3.616602	1.667047
H	5.00049	-2.743322	0.178286
C	0.750178	-3.824356	3.167484
H	0.379404	-4.851545	3.024495
H	1.838281	-3.821708	2.999844
Ni	-1.951734	1.886697	0.1892
Ni	1.183422	2.048941	0.272755
Ni	-3.293108	-0.39259	-0.393191
S	-0.432953	2.167581	1.781497
S	2.783508	1.797891	-1.257778
S	-3.509424	0.895813	1.422569
S	-0.389283	2.815845	-1.078845
S	2.832537	1.526561	1.669394
S	-3.390746	1.536308	-1.487285
C	-0.354494	1.96854	-2.72656
H	-0.958029	1.049339	-2.640999
H	0.702411	1.713131	-2.909845
C	2.229098	0.766542	3.236931
H	2.956137	-0.01601	3.500481
H	1.257374	0.288302	3.044668
C	-3.826487	-0.658152	3.703648
H	-4.251881	-1.478508	3.105388
H	-4.647446	0.010425	4.008546
C	-2.763797	0.09895	2.907807
H	-2.314066	0.909897	3.501173
H	-1.952112	-0.56595	2.577376
C	-6.175908	1.475351	-1.585178
H	-7.136897	1.977192	-1.379201
H	-6.187683	0.481727	-1.109787
C	2.115779	1.826303	4.332398
H	3.073722	2.348353	4.485991
H	1.34884	2.573654	4.078363

C	3.34861	4.523149	-1.257416
H	3.040291	4.557113	-2.314787
H	2.456377	4.710279	-0.639654
C	3.970328	3.173086	-0.900314
H	4.867982	2.962388	-1.504568
H	4.246404	3.122676	0.164069
C	-5.014609	2.305672	-1.036704
H	-4.990994	3.315984	-1.477523
H	-5.074727	2.404222	0.057313
C	-1.807712	4.301039	2.934168
H	-1.872044	5.384033	3.132941
H	-2.717028	3.98839	2.397013
C	-0.561605	3.989458	2.104706
H	-0.583151	4.510121	1.134914
H	0.363907	4.277323	2.629954
C	-0.901133	2.882715	-3.822194
H	-0.315767	3.813296	-3.894305
H	-1.951495	3.141641	-3.620084
H	-3.380021	-1.092989	4.614428
H	-0.859161	2.368023	-4.797457
H	-6.086473	1.328837	-2.673534
H	-4.520423	-5.643719	-0.382043
H	-1.784813	3.776024	3.902898
H	0.564448	-3.533698	4.215819
H	1.824726	1.351723	5.284808
H	4.076392	5.333711	-1.083998
H	4.406744	0.298288	-4.871572
H	5.438569	-1.669369	3.061628
H	0.436443	-2.607903	-3.349113
H	0.309373	-0.72604	-2.670429

Figure 5D. IM3

$Ni_6(SCH_2CH_3)_{10}(S)(SC_4H_4)$, E_0 = -6747.917757, G_{298} = -6748.025619

Ni	-1.832997	-1.80324	0.289619
Ni	-2.998777	0.433637	0.089816
Ni	1.003037	-2.558588	0.039357
S	-4.073764	-1.159131	-1.038858
S	-2.675886	2.334862	1.164757
S	-0.639426	-2.46185	-1.454679
S	-2.950811	-0.871237	1.925171
S	-2.620274	1.636361	-1.683614
S	-0.585331	-3.207465	1.435667

C	-1.688249	-0.182466	3.083481
H	-0.736172	-0.122987	2.534785
H	-2.016576	0.843139	3.313758
C	0.099667	-1.431971	-3.93934
H	1.018081	-2.039171	-3.945794
H	-0.711874	-2.020164	-4.398257
C	-0.271504	-0.997661	-2.524446
H	-1.171179	-0.366057	-2.500938
H	0.527344	-0.41973	-2.034862
C	0.156406	-5.843471	0.8848
H	-0.134708	-6.847516	0.532069
H	1.006452	-5.489148	0.280073
C	-5.401378	2.948768	1.153057
H	-5.405582	2.758071	2.238347
H	-5.641018	2.004354	0.638863
C	-4.048396	3.475756	0.67945
H	-3.794882	4.439137	1.154563
H	-4.005217	3.585038	-0.413047
C	-1.021086	-4.876647	0.755963
H	-1.894974	-5.215949	1.336369
H	-1.326585	-4.747801	-0.293476
C	-3.748971	-2.953632	-2.850364
C	-3.743179	-1.585006	-2.696191
H	-3.588779	-0.790961	-3.423801
C	-1.576414	-1.035459	4.345552
H	-2.537029	-1.074569	4.883183
H	-1.273837	-2.06497	4.101557
Ni	1.795107	2.114666	-0.185316
Ni	2.917825	-0.516607	0.130829
Ni	-1.114687	2.54344	-0.378737
S	2.708689	1.141594	1.594717
S	2.62131	-2.074377	-1.422846
S	0.454715	3.520416	0.857765
S	3.476328	1.124789	-1.238186
S	2.606368	-2.215021	1.525835
S	0.484006	2.553682	-1.931849
C	3.1842	0.78052	-3.023173
H	2.118105	0.565336	-3.176394
H	3.756526	-0.129139	-3.261333
C	1.905981	-1.70992	3.151959
H	1.253958	-2.536056	3.473573
H	1.287369	-0.814299	2.999852
C	-0.536746	4.32444	3.325617

H	-1.564986	4.356036	2.933535
H	-0.069665	5.306508	3.148961
C	0.265825	3.204099	2.664307
H	1.285268	3.140808	3.073373
H	-0.213242	2.225	2.802128
C	-0.662695	4.857181	-3.012262
H	-0.560117	5.923228	-3.277284
H	-1.529666	4.738646	-2.34288
C	3.023131	-1.441706	4.158628
H	3.674406	-2.322017	4.279019
H	3.644614	-0.592842	3.833791
C	5.312505	-2.752089	-1.613934
H	5.294246	-2.438149	-2.670292
H	5.570644	-1.874109	-1.000863
C	3.963203	-3.32502	-1.178068
H	3.673941	-4.196445	-1.788001
H	3.978934	-3.630793	-0.121089
C	0.608788	4.360901	-2.324212
H	1.492407	4.473369	-2.974246
H	0.796652	4.902508	-1.384493
C	4.257028	3.340586	2.337363
H	5.257513	3.789911	2.454637
H	3.673284	3.963521	1.641048
C	4.379284	1.914	1.801677
H	4.8888	1.892409	0.826088
H	4.933358	1.262598	2.497536
C	3.633032	1.974383	-3.86493
H	4.698556	2.203296	-3.703766
H	3.048217	2.871881	-3.610965
H	-0.591445	4.159762	4.415442
H	3.483196	1.759728	-4.936586
H	-0.870207	4.288871	-3.93303
H	-6.194669	3.681512	0.927279
H	3.758312	3.360661	3.320119
H	-0.819914	-0.603603	5.023225
H	-3.601808	-3.438792	-3.817132
H	2.592689	-1.19291	5.143551
H	6.105501	-3.509884	-1.495758
H	0.269564	-0.538799	-4.565005
H	0.494186	-5.929743	1.930004
C	-4.052128	-2.843761	-0.519732
H	-4.329103	-3.092845	0.503611
C	-3.948081	-3.673249	-1.621106

H	-3.981222	-4.761918	-1.553647

Figure 5D. TS2
$Ni_6(SCH_2CH_3)_{10}(S)(c\text{-}SC_4H_4) + H_2 \rightarrow Ni_6(SCH_2CH_3)_{10}(SH)(c\text{-}SC_4H_5)$, E_0 = -6749.03112, G_{298} = -6749.13877

Ni	-1.1509	-1.97955	0.407682
Ni	-3.008673	-0.277276	0.276565
Ni	1.655345	-2.362126	-0.011398
S	-3.649856	-2.287862	-0.714173
S	-2.995925	1.685369	1.308178
S	-0.051485	-2.429332	-1.450027
S	-2.463532	-1.48746	2.068098
S	-3.069053	1.004117	-1.454077
S	0.258012	-3.337609	1.399415
C	-1.473775	-0.48185	3.262283
H	-0.599608	-0.086976	2.722242
H	-2.107081	0.368305	3.559897
C	0.364338	-1.235475	-3.942197
H	1.310519	-1.785752	-4.064532
H	-0.448788	-1.847628	-4.365169
C	0.09915	-0.904803	-2.477562
H	-0.842993	-0.358413	-2.349252
H	0.889991	-0.285034	-2.031998
C	1.333318	-5.796614	0.632125
H	1.170892	-6.806042	0.217533
H	2.09966	-5.285478	0.02741
C	-5.8014	1.644629	1.305786
H	-5.751658	1.275716	2.342794
H	-5.819049	0.775065	0.62864
C	-4.61006	2.538731	0.970858
H	-4.585668	3.439515	1.607612
H	-4.617857	2.844782	-0.084004
C	0.027869	-5.000519	0.610648
H	-0.766308	-5.495559	1.192622
H	-0.335627	-4.850139	-0.416974
C	-4.903561	-2.42249	-3.012503
C	-3.570553	-2.374372	-2.516681
H	-2.95353	-1.060105	-2.926678
C	-1.065993	-1.333179	4.464302
H	-1.951188	-1.711099	4.999924
H	-0.462355	-2.197644	4.148902
Ni	1.323845	2.344609	-0.227875

Ni	3.050135	0.017017	0.062444
Ni	-1.597319	2.20041	-0.34071
S	2.452716	1.574099	1.529139
S	3.131612	-1.569915	-1.49476
S	-0.231334	3.502156	0.827169
S	3.163868	1.761371	-1.306594
S	3.178277	-1.710826	1.450035
S	-0.081683	2.508839	-1.94698
C	2.970043	1.400318	-3.10302
H	2.180503	2.071038	-3.474783
H	2.626524	0.363287	-3.219897
C	2.402784	-1.400213	3.090494
H	2.021306	-2.375298	3.430217
H	1.548868	-0.722421	2.953114
C	-1.296848	4.179811	3.300744
H	-2.319055	3.989221	2.939068
H	-1.044008	5.229237	3.08056
C	-0.302071	3.221339	2.647401
H	0.720671	3.386223	3.01778
H	-0.564877	2.172109	2.837782
C	-1.553984	4.566637	-3.114614
H	-1.624958	5.630907	-3.396036
H	-2.417406	4.31103	-2.480049
C	3.421957	-0.819002	4.069001
H	4.296308	-1.480446	4.176908
H	3.773459	0.166739	3.726707
C	5.899214	-1.718516	-1.760935
H	5.780377	-1.430705	-2.818054
H	6.01573	-0.799029	-1.165957
C	4.698164	-2.524944	-1.266121
H	4.565287	-3.454249	-1.843643
H	4.799906	-2.789436	-0.202797
C	-0.247388	4.304728	-2.364888
H	0.633178	4.551277	-2.981385
H	-0.191428	4.887776	-1.432971
C	3.539515	4.03109	2.311439
H	4.43265	4.670222	2.413308
H	2.822123	4.540658	1.648541
C	3.930347	2.672122	1.731115
H	4.408574	2.778635	0.745408
H	4.622906	2.128436	2.394822
C	4.301371	1.617414	-3.82274
H	5.072449	0.930599	-3.439398

H	4.668197	2.647843	-3.691196
H	-1.290603	4.045336	4.395878
H	4.181465	1.429346	-4.903347
H	-1.618667	3.961266	-4.032824
H	-6.743457	2.205258	1.181282
H	3.080983	3.929315	3.308519
H	-0.467659	-0.729574	5.168265
H	-5.1232	-2.544203	-4.074155
H	2.960503	-0.691436	5.062969
H	6.822759	-2.315008	-1.669676
H	0.424256	-0.301367	-4.526224
H	1.722601	-5.903142	1.657391
C	-5.379242	-2.03638	-0.732582
H	-5.904887	-1.866176	0.20437
C	-5.880254	-2.152956	-2.028202
H	-6.947626	-2.072621	-2.249088
H	-2.732516	-2.972223	-2.888733
H	-2.732233	-0.178474	-2.70114

Figure 5D. IM4
$Ni_6(SCH_2CH_3)_{10}(SH)(c\text{-}SC_4H_5)$, E_0 = -6749.080378, G_{298} = -6749.18808

Ni	0.718892	2.565467	-0.065816
Ni	3.010127	0.722056	-0.160745
Ni	-2.08678	1.909497	0.322829
S	1.895747	1.777681	-1.732906
S	3.332127	-0.696684	1.536718
S	-1.100523	3.331775	-1.069483
S	2.733549	2.626032	0.932737
S	3.789852	-0.934417	-1.444383
S	-0.581926	2.676579	1.764138
C	2.679313	2.393053	2.760532
H	1.803048	1.773862	3.001079
H	3.584951	1.827229	3.025838
C	-2.525733	3.508705	-3.446341
H	-3.432048	3.126192	-2.952709
H	-2.511363	4.60541	-3.343198
C	-1.272057	2.87544	-2.84344
H	-0.362563	3.234983	-3.349171
H	-1.290668	1.779445	-2.930877
C	-2.406341	4.534092	2.770412
H	-2.685066	5.590649	2.922438
H	-3.215608	4.033066	2.215818

C	5.989122	0.049686	1.950277
H	5.718108	0.413349	2.954773
H	5.857369	0.878065	1.236468
C	5.129159	-1.146099	1.538923
H	5.230252	-1.982454	2.250366
H	5.405603	-1.509712	0.538323
C	-1.092075	4.441349	1.994746
H	-0.266939	4.932432	2.536133
H	-1.177372	4.907025	1.000685
C	2.477142	2.650092	-4.21221
C	2.685768	3.104715	-2.794828
H	2.159317	4.035128	-2.527468
C	2.625393	3.742252	3.474935
H	3.495232	4.367642	3.218148
H	1.715297	4.297223	3.200545
Ni	-0.664229	-2.617873	-0.080182
Ni	-2.873869	-0.846572	0.163217
Ni	2.305181	-1.865657	-0.049861
S	-2.202376	-2.471569	1.515321
S	-3.326657	0.855151	-1.186189
S	1.037906	-3.108818	1.248331
S	-2.423701	-2.338328	-1.408593
S	-3.239334	0.663987	1.742976
S	0.919966	-2.57749	-1.631904
C	-2.003473	-1.566705	-3.028494
H	-1.135841	-0.906313	-2.889485
H	-2.865649	-0.937246	-3.296091
C	-2.325738	0.292483	3.3012
H	-2.010223	1.267516	3.702028
H	-1.418421	-0.276708	3.052567
C	1.898338	-2.971332	3.890354
H	2.913018	-2.698613	3.561328
H	1.832607	-4.069893	3.941366
C	0.847106	-2.397983	2.942049
H	-0.174995	-2.65263	3.261305
H	0.927478	-1.303045	2.863418
C	2.640079	-4.5282	-2.651218
H	2.858394	-5.598012	-2.807757
H	3.478639	-4.076142	-2.099053
C	-3.219484	-0.465204	4.28126
H	-4.138403	0.100436	4.503525
H	-3.504547	-1.445426	3.869708
C	-6.011919	0.150664	-1.401872

H	-5.85855	0.010387	-2.484159
H	-5.803314	-0.808171	-0.901137
C	-5.103117	1.247817	-0.846692
H	-5.2935	2.220611	-1.329524
H	-5.234341	1.369057	0.239354
C	1.334454	-4.367271	-1.87333
H	0.478178	-4.806029	-2.412135
H	1.392348	-4.838206	-0.879773
C	-2.524267	-5.238766	1.537065
H	-3.193068	-6.109793	1.4318
H	-1.684909	-5.350234	0.832619
C	-3.289292	-3.946834	1.248302
H	-3.665339	-3.923779	0.214364
H	-4.142673	-3.815084	1.933518
C	-1.733547	-2.637394	-4.084618
H	-2.592525	-3.319259	-4.189066
H	-0.846261	-3.234131	-3.823456
H	1.748628	-2.568095	4.906498
H	-1.548602	-2.163437	-5.063674
H	2.581187	-4.041225	-3.637827
H	7.05508	-0.233845	1.966779
H	-2.11135	-5.243238	2.558879
H	2.618517	3.592934	4.568001
H	2.925565	3.185707	-5.049357
H	-2.680697	-0.634492	5.229214
H	-7.070915	0.411275	-1.235862
H	-2.591075	3.263835	-4.520137
H	-2.325036	4.056187	3.760258
C	1.321314	0.894942	-3.090751
H	0.78852	-0.039794	-2.932418
C	1.740516	1.494368	-4.315838
H	1.496489	1.02715	-5.273981
H	3.738596	3.194157	-2.483029
H	3.050366	-0.735265	-2.58091

Figure 5D. TS3
$Ni_6(SCH_2CH_3)_{10}(SH)(c\text{-}SC_4H_5)$ -> $Ni_6(SCH_2CH_3)_{10}(SH)(a\text{-}SC_4H_5)$, E_0 = -6749.077170, G_{298} = -6749.184668

Ni	1.1798	-2.587654	-0.24599
Ni	-1.890503	-2.201299	-0.472554
Ni	2.939317	-0.515434	0.280241
S	-0.231247	-2.177306	-1.908091
S	-3.199549	-1.563767	1.20011

S	3.125445	-2.152577	-1.213041
S	-0.599637	-3.62821	0.599398
S	-3.481866	-1.284751	-1.784841
S	2.330418	-2.163762	1.648048
C	-0.709967	-3.496135	2.436162
H	-0.317736	-2.512476	2.733836
H	-1.780145	-3.532841	2.688346
C	4.394915	-1.205647	-3.497364
H	4.792266	-0.343757	-2.939371
H	5.117422	-2.032908	-3.411681
C	3.018736	-1.603534	-2.964661
H	2.601479	-2.457874	-3.522015
H	2.303601	-0.772558	-3.032678
C	4.952765	-2.574812	2.51827
H	5.821167	-3.250853	2.597997
H	5.267434	-1.659182	1.99306
C	-4.645903	-3.946061	1.32352
H	-4.329026	-4.075219	2.371232
H	-3.895872	-4.425458	0.674991
C	-4.79913	-2.46756	0.963619
H	-5.527116	-1.962508	1.61956
H	-5.129788	-2.341011	-0.078037
C	3.817559	-3.258629	1.755449
H	3.480512	-4.175614	2.267176
H	4.125176	-3.526447	0.733114
C	-0.505013	-1.667699	-4.628797
C	-0.83948	-2.80021	-3.773191
H	-0.43621	-3.787703	-4.044694
C	0.070453	-4.631095	3.097651
H	-0.308979	-5.615733	2.781281
H	1.138502	-4.57391	2.837335
Ni	-1.247487	2.404536	0.185995
Ni	1.676377	2.099075	0.385759
Ni	-3.151084	0.191429	-0.142185
S	0.156388	2.689057	1.879628
S	3.025141	1.195651	-1.131457
S	-2.984494	1.754837	1.396754
S	0.413039	3.330864	-0.957732
S	3.047385	1.081851	1.801131
S	-2.570518	1.852577	-1.510042
C	0.498536	2.891931	-2.748271
H	-0.509308	2.562965	-3.044177
H	1.198027	2.04938	-2.852585

C	2.246186	0.636338	3.400176
H	2.709462	-0.31253	3.709817
H	1.178141	0.449275	3.215874
C	-3.753831	0.740234	3.862717
H	-4.335316	-0.054299	3.369867
H	-4.405184	1.619872	3.987877
C	-2.508695	1.08581	3.047813
H	-1.907278	1.870932	3.530379
H	-1.863615	0.207721	2.896018
C	-5.19822	2.47642	-2.190809
H	-6.024463	3.20721	-2.18721
H	-5.544162	1.551746	-1.702602
C	2.458397	1.738483	4.436706
H	3.530159	1.946153	4.585134
H	1.964913	2.672273	4.126188
C	4.549904	3.512246	-1.415884
H	4.303599	3.529443	-2.489973
H	3.772104	4.076195	-0.876742
C	4.633073	2.080207	-0.887326
H	5.390686	1.489466	-1.428182
H	4.87849	2.058303	0.185614
C	-3.9856	3.045948	-1.454189
H	-3.616349	3.971791	-1.924913
H	-4.216939	3.262187	-0.399882
C	-1.024185	5.079177	2.688451
H	-0.941859	6.170198	2.828073
H	-1.881627	4.873608	2.02826
C	0.264158	4.526727	2.078069
H	0.467638	4.970836	1.091651
H	1.135693	4.709508	2.728303
C	0.969111	4.097414	-3.562116
H	1.973706	4.42198	-3.247484
H	0.284273	4.952614	-3.447685
H	-3.462032	0.380317	4.86395
H	1.014582	3.835354	-4.633313
H	-4.955288	2.235518	-3.238131
H	-5.607804	-4.469591	1.192438
H	-1.231908	4.624043	3.670522
H	-0.018656	-4.56193	4.195066
H	-0.180754	-1.807064	-5.663402
H	2.029038	1.432136	5.405841
H	5.516339	4.025847	-1.277981
H	4.32135	-0.919413	-4.560309

H	4.642298	-2.29474	3.538054
C	-0.097346	-0.565442	-2.544968
H	0.200047	0.224581	-1.855725
C	-0.257059	-0.476542	-3.937429
H	-0.050165	0.467838	-4.449968
H	-1.886853	-2.88195	-3.449638
H	-2.757711	-0.696823	-2.783329

Figure 5D. IM5

$Ni_6(SCH_2CH_3)_{10}(SH)(a\text{-}SC_4H_5)$, E_0 = -6749.12487, G_{298} = -6749.233615

Ni	-0.727867	-2.659853	0.122786
Ni	2.273289	-2.002698	0.269436
Ni	-2.902785	-0.834528	-0.209615
S	0.727672	-2.546968	1.806711
S	3.555493	-1.129351	-1.317686
S	-2.638272	-2.485957	1.232136
S	1.057606	-3.314299	-1.011892
S	3.687093	-0.922462	1.633081
S	-2.059147	-2.323785	-1.617883
C	1.023044	-2.769197	-2.775812
H	0.437065	-1.839983	-2.839001
H	2.06622	-2.542515	-3.042287
C	-3.946001	-2.020978	3.623725
H	-4.61189	-1.289015	3.139771
H	-4.403819	-3.018417	3.527639
C	-2.551843	-1.980535	2.998859
H	-1.86452	-2.689483	3.487316
H	-2.114766	-0.976462	3.068302
C	-4.535571	-3.259546	-2.477879
H	-5.259877	-4.08913	-2.538328
H	-5.020715	-2.406594	-1.977053
C	5.289632	-3.306633	-1.307806
H	4.944548	-3.540371	-2.328032
H	4.634088	-3.834025	-0.597362
C	5.258259	-1.801791	-1.039673
H	5.911048	-1.248067	-1.734307
H	5.571311	-1.569422	-0.011096
C	-3.294924	-3.697981	-1.699656
H	-2.779276	-4.539804	-2.190782
H	-3.545752	-3.997175	-0.670579
C	1.059967	-1.570468	4.843862
C	1.250022	-1.222011	6.142104

H	1.565915	-1.956879	6.886961
C	0.435328	-3.862465	-3.666488
H	1.000125	-4.803164	-3.568903
H	-0.615363	-4.06106	-3.405647
Ni	0.866026	2.427742	-0.182671
Ni	-2.069376	1.857293	-0.309752
Ni	3.156957	0.559476	0.064247
S	-0.623803	2.570932	-1.82346
S	-3.26384	0.803528	1.243079
S	2.649068	2.074781	-1.450045
S	-0.849485	3.126733	1.031446
S	-3.385603	0.732753	-1.695745
S	2.311028	2.063374	1.468204
C	-0.822614	2.56196	2.785587
H	0.230983	2.605206	3.102691
H	-1.159154	1.516176	2.815505
C	-2.643391	0.4368	-3.356228
H	-3.042897	-0.532272	-3.691936
H	-1.553228	0.33882	-3.251609
C	3.472827	1.295014	-3.985913
H	4.257396	0.657679	-3.549522
H	3.888444	2.304735	-4.132465
C	2.238335	1.329939	-3.086793
H	1.438701	1.956445	-3.510359
H	1.830667	0.321707	-2.92031
C	4.797161	3.162214	2.086542
H	5.467565	4.038183	2.077137
H	5.298588	2.330635	1.566787
C	-3.014916	1.564053	-4.318833
H	-4.107432	1.685695	-4.391801
H	-2.582164	2.520608	-3.98785
C	-5.209613	2.794231	1.50605
H	-4.952603	2.904138	2.571886
H	-4.573032	3.480605	0.925409
C	-5.018333	1.354831	1.029737
H	-5.627121	0.64743	1.616581
H	-5.285258	1.243291	-0.032252
C	3.475813	3.501513	1.396473
H	2.953223	4.334067	1.895426
H	3.629319	3.772612	0.340699
C	0.299398	5.055024	-2.690449
H	0.118206	6.13609	-2.812721
H	1.212392	4.918246	-2.089599

C	-0.897433	4.394472	-2.005877
H	-1.078905	4.818864	-1.006433
H	-1.819809	4.502964	-2.600176
C	-1.720076	3.448168	3.647223
H	-2.766322	3.394037	3.309253
H	-1.400965	4.501764	3.607186
H	3.20789	0.883479	-4.974783
H	-1.682658	3.115767	4.698883
H	4.638521	2.86069	3.134256
H	6.316664	-3.692813	-1.194843
H	0.47958	4.624135	-3.688783
H	0.469745	-3.546163	-4.722983
H	1.228148	-2.607928	4.531547
H	-2.624311	1.343723	-5.326845
H	-6.261933	3.098814	1.37675
H	-3.884068	-1.770957	4.696374
H	-4.279918	-2.954226	-3.505644
C	0.439383	-0.933817	2.498339
H	0.124925	-0.165706	1.783456
C	0.639181	-0.635493	3.814321
H	0.472937	0.403365	4.123698
H	1.096666	-0.192879	6.483085
H	2.885258	-0.535829	2.667983