SUPPORTING INFORMATION

FOR

Solvent Influence on the Mechanism of a Mechanochemical Metal-Halide Metathesis Reaction

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Experimental Details

General Considerations

Unless noted otherwise, syntheses were conducted under the exclusion of air and moisture using Schlenk line and glovebox techniques. Proton (^{1}H) and carbon (^{13}C) NMR spectra were obtained at ambient temperature on a Bruker AV-400 MHz spectrometer at 400 and 100 MHz, respectively, and were referenced to the residual resonances of C_6D_6.

Materials

HCl in dioxane (4 M) was purchased from Sigma Aldrich. [NiA´$_2$] was prepared according to the literature procedure.[1] Inhibitor-free tetrahydrofuran (THF) and hexanes were degassed and dried by passage through activated alumina columns on an MBRAUN SPS and then stored over 4A molecular sieves before use. Deuterated benzene was purchased from Cambridge Isotopes, degassed and stored over 4A molecular sieves before use.

Mechanochemical protocol

Planetary milling was performed with a Retsch PM100 mill, a 50 mL zirconia grinding jar, and a safety clamp for air-sensitive grinding. Mechanochemical reactions were run by adding the solid reagents into a grinding jar with approximately 25 g of 5 mm zirconia ball bearings (0.340 g each).

Synthesis of [{A´NiCl}$_2$]: In a typical reaction, [NiA'$_2$] (0.057 g, 0.13 mmol) is dissolved in ca. 2.5 mL of THF in an oven-dried 20 mL glass scintillation vial and sealed under an N_2 atmosphere. The solution is cooled to 0 ºC, and 0.03 mL of 4 M HCl in dioxane is added dropwise under nitrogen flow. After 2 h, the reaction is evaporated to dryness under vacuum to yield a dark red solid (0.026 g, 72%). The solid is recrystallized by dissolving in ca. 1 mL of hexanes, followed by slow evaporation to deposit red needles. Satisfactory elemental analysis could not be obtained, although the measured C/H ratio of 2.2 is not far from the 2.3 ratio calculated from the formula $C_9H_{21}ClNiSi_2$. The NMR (^{1}H and ^{13}C) spectra were broad with poor S/N ratios, which made assigning peaks problematic. This difficulty might be from a trace paramagnetic impurity, but it persisted across multiple preparations and concentrations (see Figures S1 and S2).

General Procedures for X-ray Crystallography

Crystals used for crystallographic analysis were grown by slow evaporation from THF solution in glass vials. A suitable crystal of each sample was selected for analysis and mounted in a polyimide loop. All

measurements were made on a Rigaku Oxford Diffraction Supernova Eos CCD with Cu-Kα or Mo-Kα radiation at a temperature of 100 K. Using Olex2,[2] the structures were solved with the ShelXT[3] structure solution program using Direct Methods and refined with the ShelXL refinement package[4] using least squares minimization.

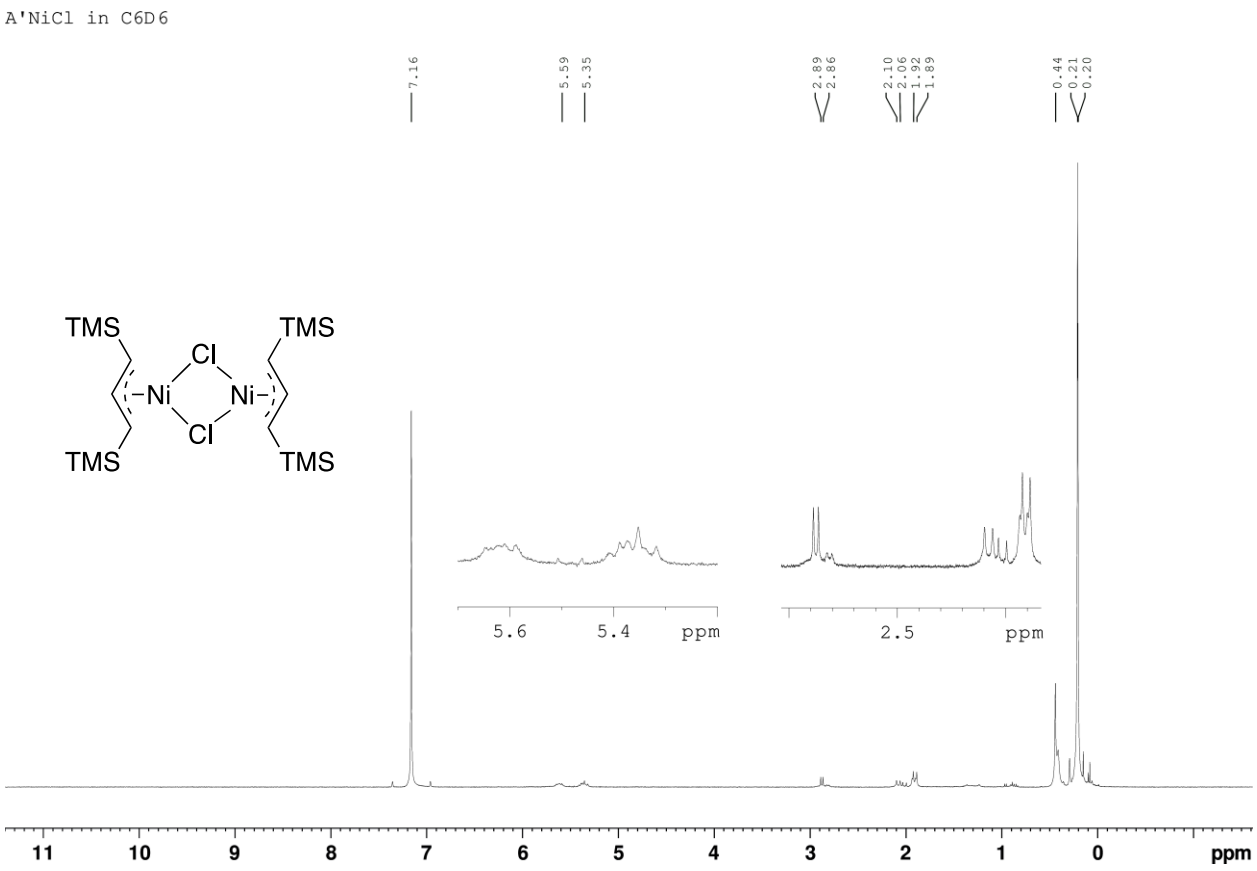

Figure S1. ^{1}H NMR (400 MHz) of [{A´NiCl}$_2$] at 298 K in C_6D_6.

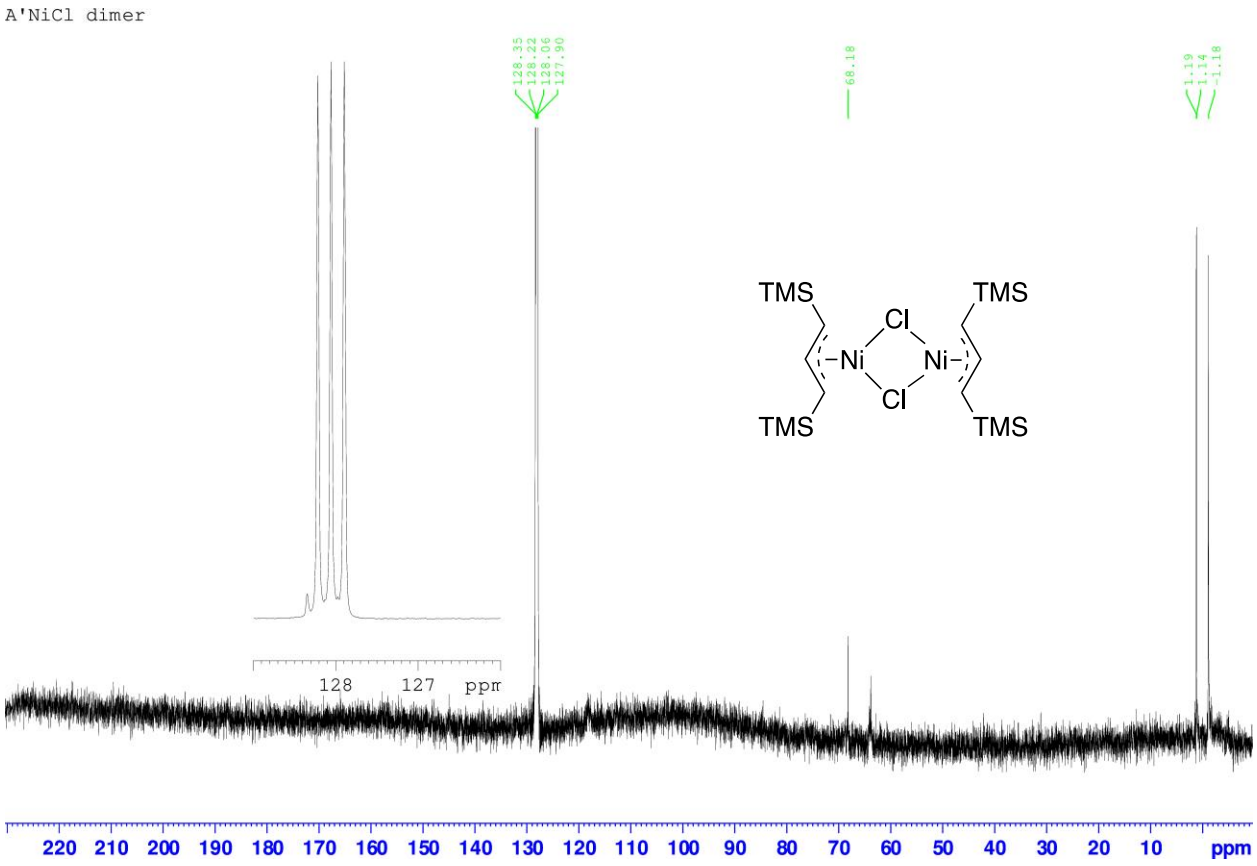

Figure S2. $^{13}C\{^{1}H\}$ NMR (151 MHz) of $[\{A'NiCl\}_2]$ in C_6D_6.

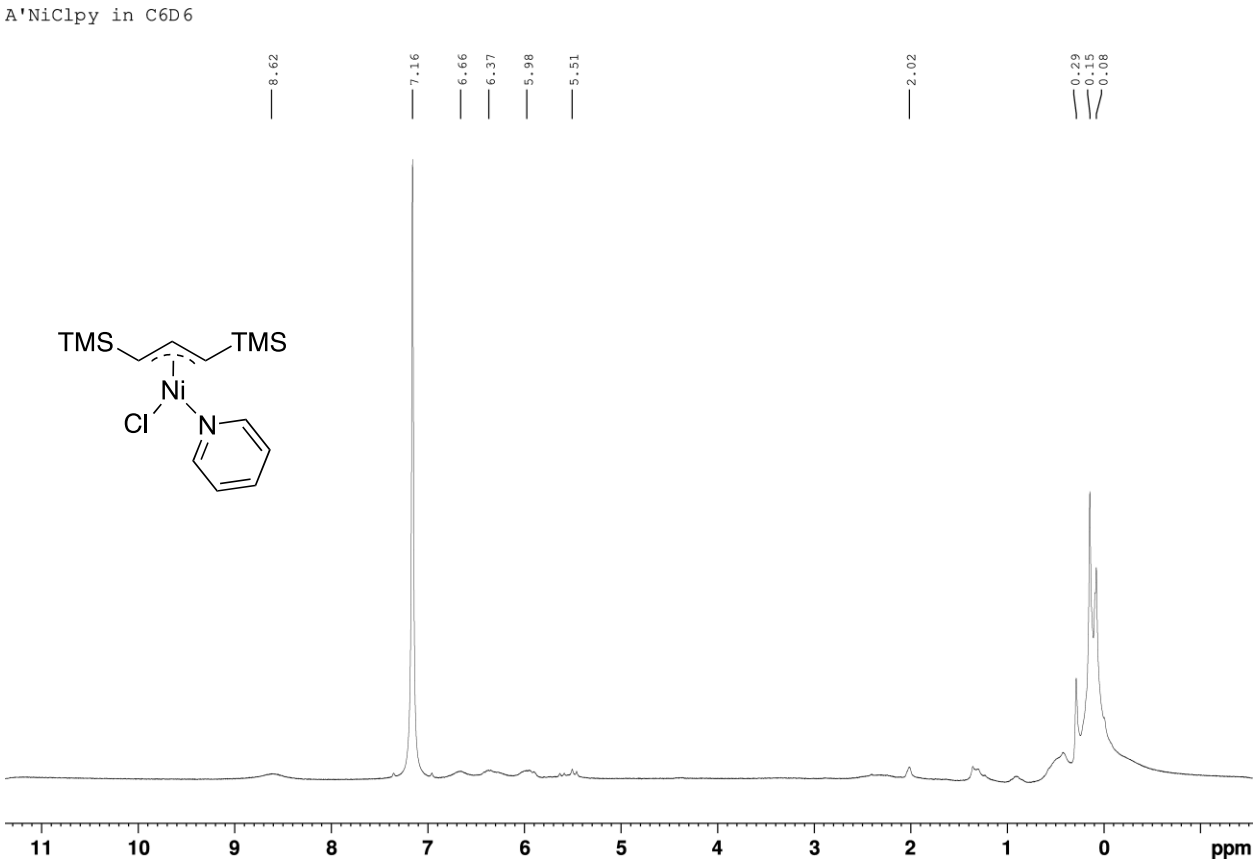

Figure S3. ^{1}H NMR (400 MHz) of [A´Ni(py)Cl] at 298 K in C_6D_6.

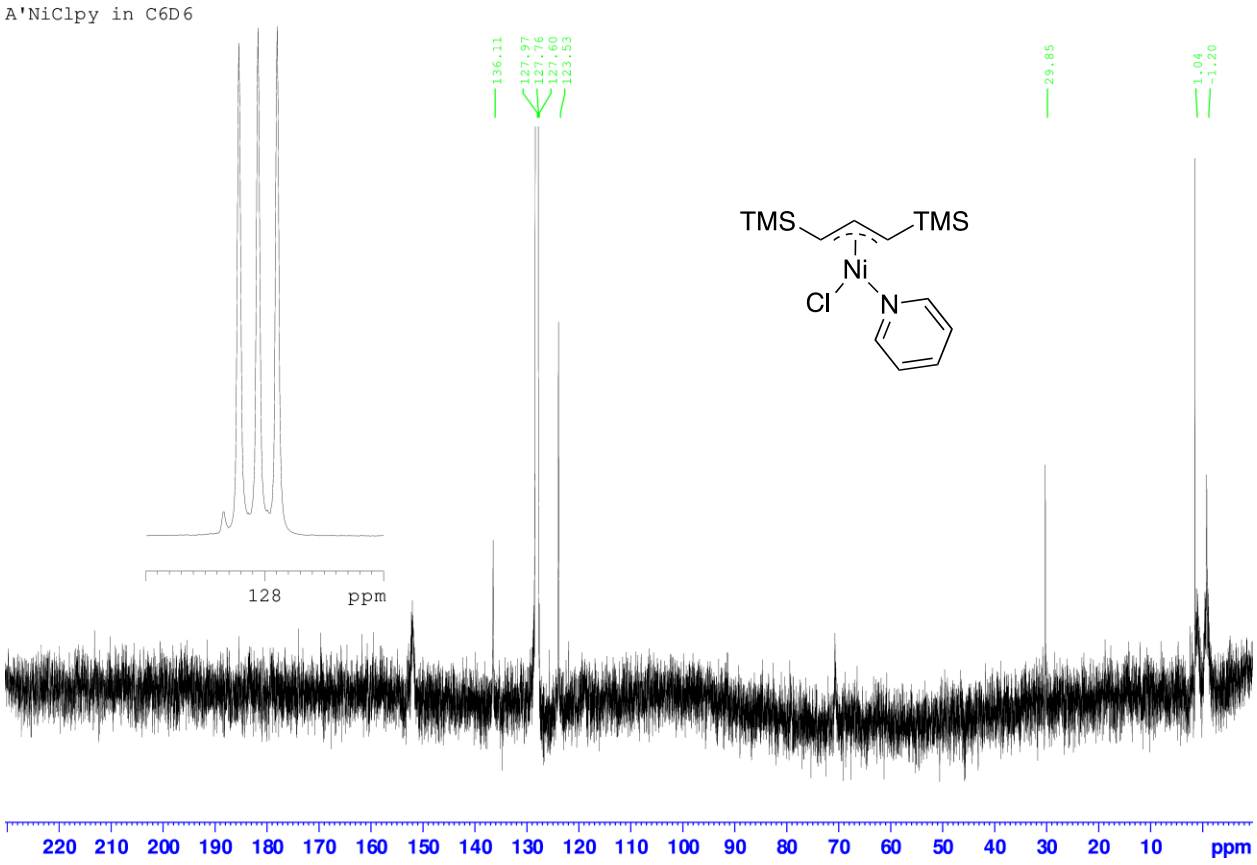

Figure S4. $^{13}C\{^{1}H\}$ NMR (151 MHz) of [A´Ni(py)Cl] at 298 K in C_6D_6.

Formation and structure of [{A´NiCl}$_2$]

[{A´NiCl}$_2$], is generated through the reaction of [NiA´$_2$] with HCl in dioxane. Although lighter and redder in color than [{A´NiBr}$_2$] or [{A´NiI}$_2$],[5] [{A´NiCl}$_2$] is otherwise similar. Slow evaporation of a hexane solution of the compound yielded red needles, allowing its crystal structure to be determined.

The allyl complex crystallizes from hexanes as a chloride-bridged dimer, joining a family of bridged π-allyl nickel species.[5-12] The molecule lies on a crystallographic 2-fold axis, thus only one-half of the molecule is unique (Figure 1). Disorder was found in one of the bridging chlorides and an allyl ligand, which was successfully modeled. The Ni–C bond lengths range from 1.975(7) to 2.041(8) Å, which are similar to those in-[{A´NiBr}$_2$].[5] The Ni(1)···Ni(1)´ separation is 3.18 Å, too long to represent any significant interaction (cf. the 2.49 Å distance in nickel metal[13]).

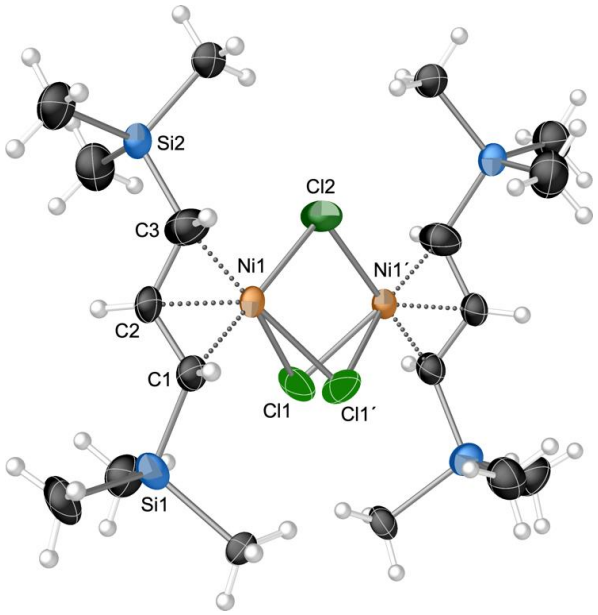

Figure S5. Thermal ellipsoid plot (50% level) of [{A´Ni(μ-Cl)}2]. Disorder in one of the allyl groups is not depicted, but the simpler disorder in one of the bridging chlorides is. Hydrogens have been assigned an arbitrary radius. Selected bond distances (Å) and angles (°): Ni1–Cl(1), 2.285(5); Ni1–Cl(1)´, 2.228(4); Ni1–Cl(1), 2.086(3); Ni1–Cl(2), 2.2182(7); Ni(1)–C(1), 2.041(8); Ni(1)–C(2), 1.975(7); Ni(1)–C(3), 2.019(3); C(1)–C(2), 1.439(6); C(2)–C(3), 1.473(5); C(1) –Si(1), 1.866(9). C(3) –Si(2), 1.849(3), C(1)–C(2)–C(3), 115.3(4).

Table S1: Crystal Data and Summary of X–ray Data Collection

	[A´Ni(μ-Cl)$_2$]	**[A´Ni(py)Cl]**
Empirical formula	$C_9H_{21}ClNiSi_2$	$C_{14}H_{26}ClNNiSi_2$
Formula weight	279.60	358.70
Temperature	100.00(10) K	100.00(10) K
Wavelength	1.54184 Å	1.54184 Å
Crystal system	Monoclinic	Monoclinic
Space group	*I*2/*a*	$P2_1/c$
Unit cell dimensions	*a* = 11.2117(3) Å	*a* = 15.0322(6) Å
	b = 23.0985(4) Å	*b* = 6.3624(2) Å
	c = 11.3080(2) Å	*c* = 20.0761(7) Å
	α = 90°	α = 90°
	β = 100.568(2)°	β = 104.424(4)°
	γ = 90°	γ = 90°
Volume	2878.80(11) Å^3	1859.57(12) Å^3
Z	8	4
Density (calculated)	1.290 g/cm^3	1.281 g/cm^3
Absorption coefficient	4.936 mm^{-1}	3.955 mm^{-1}
F(000)	1184	760
Crystal size (mm^3)	0.199 x 0.17 x 0.083	0.1 x 0.05 x 0.01
Crystal color, habit	red, block	orange, plate
Theta range for data collection	3.7940 to 71.5970°	3.035 to 66.590°
Index ranges	$-13 \le h \le 9$, $-28 \le k \le 28$, $-13 \le l \le 13$	$-17 \le h \le 14$, $-7 \le k \le 7$, $-23 \le l \le 23$
Reflections collected	13 670	10 107
Independent reflections	2794 [*R*(int) = 0.0269]	3277 [*R*(int) = 0.0700]
Absorption correction	Gaussian	Gaussian
Max. and min. transmission	0.685 and 0.440	0.995 and 0.793
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	2794 / 0 / 193	3277 / 0 / 190
Goodness-of-fit on F^2	1.094	1.040
Final R indices [*I*>2sigma(I)]	R_1 = 0.0353, wR_2 = 0.0919	R_1 = 0.0643, wR_2 = 0.1336
R indices (all data)	R_1 = 0.0399, wR_2 = 0.0960	R_1 = 0.0944, wR_2 = 0.1463
Largest diff. peak and hole	0.424 and -0.370 e Å^{-3}	1.648 and -0.526 e Å^{-3}

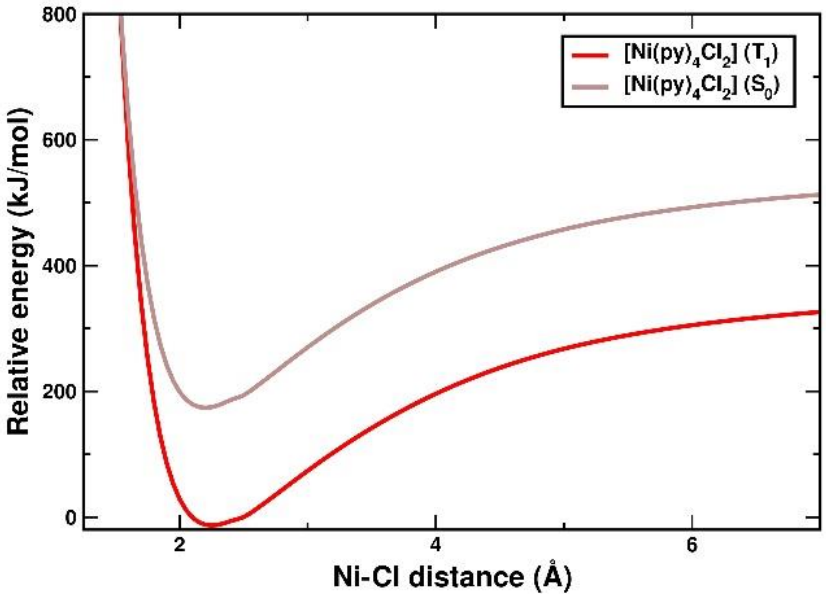

Figure S6. Bond energy scan for the $[Ni(py)_4Cl_2]$ molecule at singlet (S_0) and triplet state (T_1).

The comparison between the optimized singlet (S_0) and triplet (T_1) state energies indicates that the $[Ni(py)_4Cl_2]$ molecule has a global minimum in the T_1 state. Furthermore, the potential energy surface (PES) of the Ni-Cl bond reveals that the energy in the S_0 state remains higher than in the T_1 state. The final energies reported in the manuscript correspond to the triplet state.

Optimized Coordinates for {A´$_2$} Formation

A´ radical (Pyridine)
32

C	0.000000	-0.232422	0.000350
C	-1.234320	-0.865225	0.001132
C	2.636496	1.846628	-0.002880
C	3.846630	-0.526935	1.528545
C	3.847024	-0.531731	-1.526600
C	-3.847034	-0.531748	-1.526585
C	-2.636497	1.846627	-0.002897
C	-3.846619	-0.526921	1.528561
H	1.211165	-1.955723	0.002477
H	-1.211164	-1.955724	0.002477

H	2.085760	2.172661	-0.887658
H	3.602644	2.356370	-0.003083
H	2.084768	2.175285	0.880309
H	3.973775	-1.611294	1.560145
H	3.327638	-0.220674	2.439089
H	4.839491	-0.070616	1.532756
H	3.327968	-0.228907	-2.438255
H	3.974752	-1.616126	-1.554417
H	4.839646	-0.074905	-1.532293
H	-3.327984	-0.228937	-2.438246
H	-4.839655	-0.074920	-1.532277
H	-3.974765	-1.616143	-1.554387
H	-2.084772	2.175294	0.880291
H	-3.602645	2.356369	-0.003110
H	-2.085756	2.172650	-0.887677
H	-3.973760	-1.611280	1.560175
H	-4.839482	-0.070605	1.532771
H	-3.327623	-0.220645	2.439097
Si	2.886851	-0.010230	0.000031
Si	-2.886851	-0.010231	0.000034
H	-0.000000	0.856288	-0.001015
C	1.234320	-0.865224	0.001131

A´ radical (THF)

32

C	0.000000	-0.232715	0.000351
C	-1.234263	-0.865480	0.001135
C	2.636104	1.846469	-0.002879
C	3.846622	-0.526772	1.528536
C	3.847011	-0.531567	-1.526595
C	-3.847021	-0.531584	-1.526579
C	-2.636104	1.846468	-0.002896
C	-3.846611	-0.526758	1.528551
H	1.211032	-1.955954	0.002485
H	-1.211031	-1.955955	0.002485
H	2.085347	2.172559	-0.887616
H	3.602053	2.356575	-0.003089
H	2.084367	2.175183	0.880277
H	3.974256	-1.611064	1.560315
H	3.327470	-0.220905	2.439102
H	4.839367	-0.070213	1.533095
H	3.327793	-0.229138	-2.438269
H	3.975229	-1.615894	-1.554591
H	4.839516	-0.074502	-1.532640
H	-3.327808	-0.229167	-2.438260
H	-4.839525	-0.074517	-1.532624
H	-3.975242	-1.615912	-1.554561

H	-2.084371	2.175192	0.880258
H	-3.602053	2.356574	-0.003116
H	-2.085344	2.172548	-0.887635
H	-3.974241	-1.611049	1.560345
H	-4.839357	-0.070202	1.533110
H	-3.327455	-0.220876	2.439110
Si	2.886611	-0.010425	0.000031
Si	-2.886610	-0.010426	0.000034
H	-0.000000	0.855988	-0.001019
C	1.234264	-0.865479	0.001135

A´ radical (solvent-free)

32

C	-0.002072	1.915551	0.106390
C	1.209332	1.609619	-0.540862
C	-2.767637	1.882589	2.100162
C	-3.465300	3.588165	-0.328165
C	-4.140951	0.623012	-0.347337
C	4.141428	0.634287	-0.341622
C	2.757394	1.882072	2.105326
C	3.456705	3.597163	-0.316103
H	-1.181214	1.613727	-1.630946
H	1.180064	1.617480	-1.629886
H	-2.442611	0.917075	2.488937
H	-3.744425	2.101592	2.537720
H	-2.070206	2.642528	2.458683
H	-3.547885	3.633247	-1.416237
H	-2.761948	4.363228	-0.016910
H	-4.444366	3.828577	0.093334
H	-4.016043	-0.336646	0.153775
H	-4.055596	0.453645	-1.422398
H	-5.153846	0.976999	-0.141993
H	4.018851	-0.326804	0.157310
H	5.152473	0.991641	-0.132962
H	4.059614	0.466752	-1.417237
H	2.058888	2.640619	2.464672
H	3.732946	2.099524	2.546386
H	2.431283	0.915094	2.489570
H	3.542374	3.645602	-1.403798
H	4.433808	3.839282	0.108960
H	2.750143	4.369266	-0.004760
Si	-2.883355	1.889588	0.224428
Si	2.878129	1.895309	0.229955
H	-0.002873	2.161251	1.165869
C	-1.212024	1.606876	-0.541948

A´-A´ diradical *meso* TS (Pyridine)

64

C	-1.712969	-0.264149	-0.674181
C	-0.551869	-1.232310	0.884335
C	-1.313972	2.214897	-0.964910
C	1.794970	-1.676970	0.198955
C	-1.079681	0.810564	-1.278021
C	0.824660	-0.873995	0.689287
C	-1.409621	1.242043	2.509624
C	-0.467079	-2.263199	-2.650956
C	-3.227074	-1.240517	2.393975
C	-2.758791	-3.211624	-0.817159
C	-0.891457	4.679071	0.785066
C	4.103106	0.083429	1.191311
C	0.369426	4.484784	-1.989366
C	3.719699	-0.419579	-1.808637
H	-2.286045	2.606195	-1.277042
H	1.497402	-2.691359	-0.069546
H	-3.718045	-0.961275	3.329252
H	-3.143937	-3.942888	-1.532241
H	-2.946592	-0.408559	-3.636309
H	0.448781	-1.004860	3.950816
H	-0.222355	5.512343	1.013005
H	5.135000	0.392757	1.008586
H	1.060721	5.293545	-1.738440
H	4.751265	-0.123957	-2.015461
H	2.229113	3.545523	0.397826
H	5.692248	-2.444664	-0.190366
H	-0.386388	1.602333	2.627905
H	-0.087091	-1.451735	-3.274668
H	-1.826104	1.706712	1.614514
H	0.318366	-2.540858	-1.948618
H	-3.814422	-0.826798	1.573083
H	-2.035590	-3.721045	-0.179991
H	-4.237068	-0.899862	-2.535181
H	-0.596132	-2.427522	3.889279
H	-1.817350	5.092491	0.379029
H	3.478380	0.977414	1.170560
H	-1.128731	4.166859	1.718595
H	4.049214	-0.343350	2.195028
H	-0.515757	4.924711	-2.453175
H	3.086501	0.464828	-1.906058
H	1.293426	2.311949	1.242595
H	4.593404	-3.149560	1.001386
Si	-0.088883	3.513397	-0.444065
Si	3.558911	-1.170537	-0.092492
H	-2.535963	0.019367	-0.021896

H	-0.758409	-2.268928	0.627039
C	-3.320700	-1.234231	-3.027489
C	-0.591447	-1.335517	3.912312
C	1.471038	2.769753	0.269483
C	4.647875	-2.694898	0.009713
H	-1.983025	1.584530	3.374091
H	-0.666228	-3.117993	-3.301560
H	-3.255966	-2.328991	2.312781
H	-3.592301	-2.888370	-0.190843
H	-0.344411	0.605435	-2.057381
H	1.094738	0.143406	0.963111
H	-1.085308	-1.013501	4.832581
H	-3.578636	-2.062072	-3.692706
H	0.853074	3.839662	-2.725770
H	3.411372	-1.135467	-2.573832
H	1.878294	2.008691	-0.397431
H	4.336235	-3.444535	-0.721507
Si	-1.455105	-0.626288	2.399979
Si	-2.035092	-1.761279	-1.762071

A´-A´ diradical *meso* TS (THF)

64

C	-1.712537	-0.266251	-0.674604
C	-0.551309	-1.232636	0.884882
C	-1.315824	2.213144	-0.966042
C	1.795860	-1.675239	0.199811
C	-1.079906	0.808881	-1.278364
C	0.824865	-0.873033	0.689740
C	-1.410685	1.241576	2.509088
C	-0.462926	-2.260539	-2.653005
C	-3.227094	-1.241605	2.393595
C	-2.750038	-3.217036	-0.817625
C	-0.897006	4.678382	0.783367
C	4.102172	0.086939	1.192893
C	0.365924	4.484427	-1.990152
C	3.719113	-0.415333	-1.807277
H	-2.288046	2.603236	-1.279237
H	1.499370	-2.690151	-0.067863
H	-3.718797	-0.962231	3.328438
H	-3.137048	-3.947553	-1.532447
H	-2.950178	-0.412161	-3.634149
H	0.448541	-1.005173	3.950989
H	-0.229014	5.512395	1.011822
H	5.134136	0.396668	1.011296
H	1.056061	5.294200	-1.739323
H	4.750304	-0.118820	-2.014644

H	2.225273	3.547657	0.398365
H	5.693963	-2.439381	-0.189143
H	-0.387662	1.602304	2.627854
H	-0.089319	-1.449749	-3.281400
H	-1.826747	1.705738	1.613516
H	0.325952	-2.529905	-1.951278
H	-3.814311	-0.828453	1.572318
H	-2.023729	-3.726845	-0.184306
H	-4.237793	-0.909948	-2.532849
H	-0.596626	-2.427344	3.890536
H	-1.822946	5.091045	0.376676
H	3.477345	0.980837	1.171768
H	-1.134699	4.166284	1.716837
H	4.047446	-0.339905	2.196515
H	-0.519294	4.923175	-2.454992
H	3.085259	0.468658	-1.904091
H	1.290098	2.313842	1.243194
H	4.595191	-3.145816	1.001625
Si	-0.092453	3.513084	-0.444819
Si	3.559324	-1.167093	-0.091378
H	-2.536275	0.016632	-0.022972
H	-0.756716	-2.269609	0.628174
C	-3.320451	-1.240140	-3.026150
C	-0.591829	-1.335343	3.912854
C	1.467811	2.771307	0.269953
C	4.649680	-2.690460	0.010292
H	-1.984665	1.584459	3.373005
H	-0.658070	-3.119542	-3.299246
H	-3.255855	-2.330126	2.312957
H	-3.581566	-2.896389	-0.187352
H	-0.343639	0.604003	-2.056824
H	1.093859	0.144772	0.963075
H	-1.085294	-1.012800	4.833139
H	-3.575926	-2.067873	-3.692439
H	0.850879	3.839767	-2.726087
H	3.410859	-1.130947	-2.572734
H	1.876216	2.010152	-0.396142
H	4.339203	-3.440069	-0.721439
Si	-1.455203	-0.626881	2.400152
Si	-2.031716	-1.763916	-1.762575

A´-A´ diradical *meso* TS (solvent-free)

64

C	-0.724797	-0.461036	1.227840
C	0.726276	0.536570	1.201287
C	-2.923823	-0.067906	0.010211

C	2.925038	0.075762	0.005884
C	-1.547574	-0.439090	0.052688
C	1.549392	0.450229	0.028873
C	-0.573667	3.074414	-0.126045
C	0.574725	-3.066345	0.039099
C	-1.227116	2.460692	2.832779
C	1.237357	-2.290157	2.956293
C	-3.054531	-0.564235	-3.032848
C	3.038809	0.358334	-3.065437
C	-4.614996	1.797938	-1.798191
C	4.617594	-1.903181	-1.673291
H	-3.379792	0.158663	0.978641
H	3.383657	-0.091802	0.985004
H	-1.380588	3.509901	3.116941
H	1.391883	-3.321196	3.299998
H	-2.439310	-3.141684	1.529233
H	2.441666	3.233912	1.343592
H	-3.696764	-0.535429	-3.921591
H	3.675924	0.266445	-3.953596
H	-5.278783	1.844902	-2.671490
H	5.278089	-2.009632	-2.543821
H	-6.243060	-0.973132	-2.086070
H	6.229718	0.845179	-2.168785
H	0.211019	3.197231	-0.880276
H	-0.213699	-3.243715	-0.700239
H	-1.355133	2.430419	-0.544547
H	1.344987	-2.438707	-0.422855
H	-2.192564	2.065284	2.498984
H	2.201166	-1.915911	2.594486
H	-1.971557	-2.771963	3.196858
H	1.988194	2.937167	3.029613
H	-2.187976	0.076393	-3.234906
H	2.172387	-0.296569	-3.215509
H	-2.691255	-1.592851	-2.922554
H	2.674104	1.391675	-3.027932
H	-3.777814	2.482739	-1.976624
H	3.783425	-2.603393	-1.798335
H	-5.273776	-2.129559	-1.154647
H	5.259625	2.063784	-1.321165
Si	-4.009291	0.019728	-1.502358
Si	4.004091	-0.111299	-1.502483
H	-1.295475	-0.139551	2.108778
H	1.295680	0.261563	2.098383
C	-1.614767	-3.191962	2.248414
C	1.623367	3.315739	2.066986
C	-5.543729	-1.071165	-1.245964
C	5.534253	1.002742	-1.334566
H	-1.019045	4.059212	0.062490

H	1.034193	-4.032533	0.282237
H	-0.932616	1.916562	3.738452
H	0.948051	-1.694005	3.830405
H	-1.067334	-0.713350	-0.886992
H	1.068573	0.670925	-0.924616
H	1.386574	4.378917	2.198940
H	-1.376634	-4.248436	2.424618
H	-5.175497	2.178742	-0.935713
H	5.183581	-2.218224	-0.788132
H	-6.080612	-0.785873	-0.333090
H	6.076909	0.788702	-0.405801
Si	0.100775	2.353142	1.480386
Si	-0.096360	-2.259061	1.605709

A´-A´ diradical *rac* TS (Pyridine)

64

C	-0.696783	-0.664958	-1.316519
C	0.420031	-1.474303	0.305320
C	-1.837735	1.603204	-0.938522
C	2.736757	-0.951320	-0.454216
C	-0.757247	0.725573	-1.368386
C	1.606519	-0.653427	0.218566
C	-1.594960	-0.127921	2.293087
C	-2.914719	-1.290933	-3.231143
C	-1.355600	-3.198443	2.135376
C	-1.787421	-3.516677	-1.512194
C	-3.080328	3.085931	1.470547
C	3.920681	1.723012	0.421321
C	-1.757207	4.600046	-0.799050
C	4.560625	0.584935	-2.352981
H	-2.718075	1.636197	-1.586292
H	2.759892	-1.912720	-0.970858
H	-1.717846	-3.301390	3.161356
H	-2.664849	-4.128898	-1.733472
H	-3.869179	-0.274982	-0.299205
H	1.477028	-0.623058	3.243439
H	-3.028941	4.005114	2.059510
H	4.803195	2.365888	0.386319
H	-1.663867	5.484292	-0.163135
H	5.455139	1.205624	-2.446317
H	0.105158	3.806544	1.788518
H	6.623429	-0.126757	0.047803
H	-2.401838	-0.427602	2.965523
H	-3.208702	-0.241413	-3.296501
H	-1.062191	0.696807	2.766721
H	-2.157736	-1.476285	-3.996256

H	-2.213746	-3.286186	1.470583
H	-1.039625	-3.714337	-2.283953
H	-3.363527	-1.610887	0.731484
H	1.587530	-2.383951	3.167733
H	-4.038374	3.077426	0.945688
H	3.080269	2.286341	0.011888
H	-3.059896	2.238671	2.155182
H	3.703585	1.507129	1.469438
H	-2.710725	4.662237	-1.327846
H	3.719939	1.133176	-2.783745
H	0.165460	2.048879	1.626043
H	5.581887	-0.984580	1.191840
Si	-1.665817	3.034091	0.240670
Si	4.225727	0.152419	-0.555556
H	0.115579	-1.053666	-1.928098
H	0.545634	-2.443298	-0.176656
C	-3.615063	-1.336323	-0.290575
C	0.896996	-1.547032	3.291395
C	0.005031	2.978998	1.082784
C	5.725144	-0.742577	0.136489
H	-2.039056	0.241797	1.370184
H	-3.789638	-1.902899	-3.464368
H	-0.685152	-4.036865	1.933144
H	-1.379823	-3.845694	-0.557556
H	0.113644	1.244510	-1.775510
H	1.558103	0.306023	0.731741
H	0.452065	-1.616252	4.287394
H	-4.506195	-1.898613	-0.581617
H	-0.955665	4.627363	-1.539903
H	4.714017	-0.317927	-2.948664
H	0.799685	3.074158	0.340444
H	5.903367	-1.676609	-0.401488
Si	-0.440698	-1.568013	1.968440
Si	-2.250518	-1.700641	-1.520576

A´-A´ diradical *rac* TS (THF)

64

C	-0.696797	-0.665028	-1.316687
C	0.420628	-1.473756	0.305312
C	-1.838425	1.602883	-0.939289
C	2.736964	-0.950317	-0.454645
C	-0.757596	0.725422	-1.368713
C	1.606826	-0.652504	0.218135
C	-1.595244	-0.128588	2.293137
C	-2.914900	-1.291742	-3.230906
C	-1.353338	-3.198764	2.135943

C	-1.786459	-3.517086	-1.512051
C	-3.082427	3.084376	1.469815
C	3.920101	1.724500	0.420124
C	-1.758439	4.599795	-0.798389
C	4.561591	0.585107	-2.353268
H	-2.718321	1.635822	-1.587687
H	2.760366	-1.911964	-0.970771
H	-1.715493	-3.302126	3.161907
H	-2.663500	-4.129868	-1.733277
H	-3.868483	-0.276087	-0.297757
H	1.477715	-0.620893	3.243043
H	-3.031495	4.003050	2.059605
H	4.802193	2.367932	0.384955
H	-1.665290	5.483881	-0.162236
H	5.455922	1.206022	-2.446759
H	0.102769	3.804156	1.790655
H	6.623314	-0.125343	0.049724
H	-2.402646	-0.429138	2.964554
H	-3.209114	-0.242311	-3.296407
H	-1.063711	0.696311	2.767867
H	-2.158116	-1.476718	-3.996284
H	-2.211472	-3.287261	1.471232
H	-1.038635	-3.714805	-2.283762
H	-3.362789	-1.612684	0.731789
H	1.589758	-2.381365	3.167487
H	-4.040342	3.076364	0.944716
H	3.079454	2.287326	0.010494
H	-3.062534	2.236635	2.153849
H	3.703107	1.509214	1.468370
H	-2.711735	4.662503	-1.327513
H	3.720989	1.132755	-2.784908
H	0.163690	2.046887	1.625148
H	5.580719	-0.983044	1.192820
Si	-1.667352	3.033292	0.240562
Si	4.225914	0.153413	-0.555786
H	0.115841	-1.053439	-1.928072
H	0.546550	-2.442806	-0.176478
C	-3.614471	-1.337453	-0.290052
C	0.898326	-1.545242	3.291266
C	0.003127	2.977856	1.083411
C	5.724912	-0.741093	0.137611
H	-2.038782	0.241323	1.370050
H	-3.789711	-1.903805	-3.464244
H	-0.682441	-4.036852	1.933847
H	-1.378780	-3.845955	-0.557400
H	0.113292	1.244384	-1.775774
H	1.558216	0.307084	0.731024
H	0.454039	-1.614697	4.287526

H	-4.505910	-1.899263	-0.581057
H	-0.956813	4.627673	-1.539112
H	4.715575	-0.317920	-2.948529
H	0.798333	3.074567	0.341877
H	5.903862	-1.675240	-0.399896
Si	-0.439544	-1.567712	1.968655
Si	-2.250153	-1.701171	-1.520512

A´-A´ diradical *rac* TS (solvent-free)

64

C	-0.693182	-0.671866	-1.317242
C	0.420527	-1.457432	0.323127
C	-1.841780	1.595848	-0.964174
C	2.736110	-0.947440	-0.441362
C	-0.757679	0.716813	-1.382104
C	1.606664	-0.637759	0.224905
C	-1.643064	-0.123089	2.280952
C	-2.901719	-1.324904	-3.232703
C	-1.321590	-3.184090	2.172144
C	-1.762448	-3.531530	-1.493594
C	-3.117616	3.092205	1.415673
C	3.911755	1.747047	0.376775
C	-1.719429	4.593561	-0.818659
C	4.585417	0.534375	-2.357210
H	-2.715522	1.627508	-1.621077
H	2.759919	-1.918593	-0.938891
H	-1.689694	-3.284992	3.196118
H	-2.630821	-4.154837	-1.719128
H	-3.860642	-0.299486	-0.288344
H	1.442070	-0.515713	3.251222
H	-3.066844	4.003561	2.016543
H	4.791610	2.392867	0.334647
H	-1.624646	5.476985	-0.181998
H	5.479380	1.154141	-2.459834
H	0.069973	3.756108	1.819652
H	6.617676	-0.116717	0.098147
H	-2.479319	-0.452106	2.901665
H	-3.201662	-0.277907	-3.307469
H	-1.155868	0.701444	2.801702
H	-2.142592	-1.507035	-3.996121
H	-2.173103	-3.300460	1.502946
H	-1.005873	-3.733556	-2.255510
H	-3.359795	-1.644953	0.729287
H	1.604102	-2.269237	3.202321
H	-4.064489	3.107222	0.871164
H	3.074741	2.298873	-0.054581

H	-3.131323	2.238490	2.092192
H	3.685159	1.561909	1.428544
H	-2.659236	4.676165	-1.368531
H	3.749896	1.067464	-2.815532
H	0.109653	2.001626	1.632709
H	5.553909	-0.947582	1.240362
Si	-1.675983	3.023848	0.218876
Si	4.228306	0.149945	-0.553253
H	0.126819	-1.061270	-1.917922
H	0.548209	-2.433112	-0.144754
C	-3.607395	-1.360911	-0.291128
C	0.886566	-1.453807	3.311405
C	-0.025873	2.941031	1.099178
C	5.715886	-0.727652	0.183239
H	-2.047087	0.258294	1.344553
H	-3.771961	-1.942105	-3.468927
H	-0.633478	-4.011904	1.986834
H	-1.363134	-3.851635	-0.532419
H	0.114726	1.232574	-1.789598
H	1.557994	0.330129	0.721645
H	0.444676	-1.519544	4.308821
H	-4.500685	-1.917009	-0.587014
H	-0.903675	4.611418	-1.543883
H	4.748395	-0.382461	-2.928214
H	0.790807	3.036098	0.381410
H	5.904834	-1.674080	-0.328397
Si	-0.443579	-1.535150	1.984979
Si	-2.238743	-1.718570	-1.518437

A´$_2$ *meso* (Pyridine)

64

C	-0.491248	0.497919	-0.332332
H	1.204400	-4.469808	0.319115
H	-1.228643	-2.622484	2.127031
H	-1.324194	-1.932588	-2.056976
C	1.426833	2.844640	-1.075723
H	1.324001	1.932628	2.057273
H	5.690856	0.218508	-2.242222
C	-4.678150	-0.084308	1.855300
H	-0.449029	0.374620	-1.420650
H	-1.821369	3.239779	-1.430313
C	5.775083	-1.419338	0.585626
C	-2.976116	0.208486	-0.658321
H	5.779661	-1.492948	1.675623
C	-1.891948	0.288551	0.117952
H	-5.779574	1.492944	-1.675771

Si	-0.015177	2.321505	0.005135
H	-4.829539	-2.473673	-0.371344
H	-2.820070	0.273534	-1.736284
C	5.415354	1.613116	0.701616
H	-1.585377	-3.921918	0.984330
C	-1.426827	-2.844405	1.076083
H	2.014901	-0.219358	-1.198735
H	5.410186	1.603776	1.794061
C	-1.480536	3.416437	-0.407496
H	-1.204522	4.469880	-0.318856
H	0.382120	-2.169781	-2.459383
H	1.585326	3.922154	-0.983893
H	1.821385	-3.239666	1.430450
C	-5.775057	1.419240	-0.585780
H	0.630378	3.558405	2.052986
H	6.808171	-1.294522	0.252503
H	4.069407	0.916015	-2.215651
H	-5.401015	2.364562	-0.186770
H	-5.690924	-0.218846	2.241932
Si	-4.704906	-0.015061	-0.017942
H	2.346622	2.337314	-0.788314
H	-2.322521	3.223231	0.258522
C	2.976198	-0.208462	0.658226
C	-0.431012	-2.511038	-1.814912
H	-5.409964	-1.603754	-1.794454
H	2.322410	-3.223242	-0.258424
H	4.276341	-0.838127	-2.280647
H	-4.276455	0.837844	2.280530
C	0.430813	2.511056	1.815176
H	-6.446563	-1.757535	-0.371538
H	4.829716	2.473596	0.370908
H	-2.014931	0.219287	1.198698
Si	4.704960	0.014959	0.017727
C	0.491297	-0.497815	0.332407
H	-0.382354	2.169727	2.459565
H	2.820214	-0.273419	1.736203
C	-5.415194	-1.613189	-0.702010
H	0.449147	-0.374448	1.420720
C	1.891980	-0.288537	-0.117976
C	1.480466	-3.416372	0.407670
C	4.678099	0.084045	-1.855520
H	1.228739	2.622772	-2.126700
H	-2.346614	-2.337053	0.788714
H	-0.630640	-3.558393	-2.052644
H	6.446710	1.757390	0.371072
H	5.400978	-2.364679	0.186719
H	-6.808159	1.294352	-0.252728
H	-4.069444	-0.916284	2.215394

Si	0.015124	-2.321400	-0.004916

A´$_2$ *meso* (THF)

64

C	-0.491219	0.497962	-0.332296
H	1.204995	-4.469686	0.319420
H	-1.229402	-2.622268	2.126577
H	-1.323604	-1.933138	-2.057641
C	1.427014	2.844668	-1.075156
H	1.323384	1.933183	2.057971
H	5.690360	0.218534	-2.242700
C	-4.677798	-0.084336	1.855399
H	-0.449019	0.374511	-1.420619
H	-1.821464	3.239784	-1.430718
C	5.775177	-1.419150	0.585400
C	-2.976125	0.208430	-0.658307
H	5.780302	-1.492739	1.675387
C	-1.891949	0.288512	0.117866
H	-5.780213	1.492726	-1.675550
Si	-0.015330	2.321610	0.005275
H	-4.829398	-2.473912	-0.371288
H	-2.820108	0.273510	-1.736270
C	5.415225	1.613282	0.701318
H	-1.585414	-3.921984	0.984391
C	-1.427005	-2.844406	1.075557
H	2.014978	-0.219288	-1.198660
H	5.410319	1.604186	1.793760
C	-1.480710	3.416222	-0.407850
H	-1.205130	4.469770	-0.319137
H	0.383005	-2.169567	-2.459478
H	1.585362	3.922247	-0.983904
H	1.821484	-3.239655	1.430864
C	-5.775152	1.419035	-0.585570
H	0.628959	3.558386	2.053661
H	6.808205	-1.294573	0.252021
H	4.069103	0.915973	-2.215928
H	-5.401095	2.364540	-0.187075
H	-5.690431	-0.218912	2.242382
Si	-4.704924	-0.015160	-0.017855
H	2.346857	2.337786	-0.787188
H	-2.323038	3.222984	0.257700
C	2.976215	-0.208402	0.658201
C	-0.430180	-2.511005	-1.815166
H	-5.410069	-1.604169	-1.794191
H	2.322913	-3.222994	-0.257598
H	4.276175	-0.838166	-2.280855

H	-4.276300	0.837853	2.280726
C	0.429955	2.511025	1.815457
H	-6.446381	-1.757973	-0.371311
H	4.829603	2.473823	0.370810
H	-2.015011	0.219220	1.198619
Si	4.704985	0.015044	0.017618
C	0.491273	-0.497843	0.332376
H	-0.383270	2.169507	2.459676
H	2.820266	-0.273387	1.736180
C	-5.415042	-1.613369	-0.701751
H	0.449148	-0.374318	1.420694
C	1.891984	-0.288492	-0.117894
C	1.480633	-3.416146	0.408038
C	4.677745	0.084044	-1.855641
H	1.229515	2.622591	-2.126209
H	-2.346848	-2.337497	0.787636
H	-0.629253	-3.558372	-2.053282
H	6.446551	1.757803	0.370801
H	5.401046	-2.364675	0.187018
H	-6.808195	1.294374	-0.252268
H	-4.069138	-0.916269	2.215643
Si	0.015271	-2.321491	-0.005034

A´$_2$ *meso* (solvent-free)

64

C	0.491100	-0.498083	-0.331460
H	-1.216614	4.467544	0.331123
H	1.253382	2.618260	2.117402
H	1.320009	1.947079	-2.059974
C	-1.434534	-2.844809	-1.062995
H	-1.319582	-1.946887	2.060531
H	-5.689634	-0.216304	-2.246631
C	4.677843	0.081384	1.856110
H	0.449709	-0.373128	-1.420653
H	1.819130	-3.233788	-1.445025
C	-5.777130	1.415455	0.589323
C	2.976758	-0.211039	-0.657050
H	-5.787155	1.484056	1.680172
C	1.892149	-0.288101	0.117752
H	5.786962	-1.484405	-1.680341
Si	0.017642	-2.323231	0.005028
H	4.819196	2.475858	-0.367124
H	2.821416	-0.280131	-1.735551
C	-5.409135	-1.617885	0.697062
H	1.589611	3.923996	0.978234
C	1.434278	2.844887	1.063623

H	-2.015543	0.215988	-1.199144
H	-5.406431	-1.613203	1.790106
C	1.483633	-3.411256	-0.420001
H	1.216460	-4.467551	-0.330976
H	-0.390937	2.164689	-2.461792
H	-1.589904	-3.923906	-0.977526
H	-1.819466	3.233713	1.444998
C	5.777030	-1.415646	-0.589502
H	-0.606827	-3.562850	2.059845
H	-6.810385	1.295917	0.252913
H	-4.069102	-0.912808	-2.219403
H	5.401056	-2.364584	-0.199898
H	5.689841	0.216533	2.246221
Si	4.705983	0.015343	-0.017449
H	-2.352329	-2.342865	-0.758071
H	2.331379	-3.214732	0.238407
C	-2.976812	0.210958	0.656933
C	0.419138	2.514044	-1.816700
H	5.406364	1.612851	-1.790698
H	-2.331371	3.214707	-0.238540
H	-4.278385	0.842530	-2.282192
H	4.278550	-0.842234	2.282055
C	-0.418783	-2.513899	1.817100
H	6.440127	1.769035	-0.367087
H	-4.819101	-2.475973	0.366456
H	2.015647	-0.215825	1.199110
Si	-4.705973	-0.015404	0.017151
C	-0.491130	0.498100	0.331586
H	0.391438	-2.164547	2.462009
H	-2.821563	0.279907	1.735456
C	5.409161	1.617693	-0.697654
H	-0.449839	0.373060	1.420773
C	-1.892139	0.288151	-0.117767
C	-1.483766	3.411235	0.420048
C	-4.677673	-0.081169	-1.856416
H	-1.253846	-2.618236	-2.116821
H	2.352155	2.342998	0.758869
H	0.607192	3.563012	-2.059360
H	-6.440066	-1.769224	0.366385
H	-5.401164	2.364467	0.199889
H	6.810319	-1.296103	-0.253197
H	4.069338	0.913103	2.219023
Si	-0.017650	2.323282	-0.004724

A´$_2$ *rac* (Pyridine)

64

C	0.498784	-0.595771	-0.559983
C	-0.498771	0.595816	-0.559987
C	2.975565	-0.395027	-1.019554
C	-2.975547	0.395026	-1.019562
C	1.900569	-0.205835	-0.250481
C	-1.900549	0.205852	-0.250488
C	0.191775	1.776035	2.304954
C	-0.191707	-1.775974	2.304977
C	1.396357	3.047093	-0.232318
C	-1.396468	-3.046929	-0.232258
C	4.679633	0.691194	1.263289
C	-4.679587	-0.691288	1.263257
C	5.398598	1.357563	-1.645296
C	-5.398529	-1.357622	-1.645341
H	2.813895	-0.848746	-1.998630
H	-2.813888	0.848763	-1.998630
H	1.523885	4.004665	0.278795
H	-1.524040	-4.004497	0.278854
H	2.436530	-2.881266	0.852330
H	-2.436583	2.881184	0.852421
H	5.693570	0.938359	1.586148
H	-5.693516	-0.938490	1.586110
H	6.427868	1.607849	-1.377394
H	-6.427793	-1.607942	-1.377446
H	6.819024	-1.254626	-0.319241
H	-6.819032	1.254501	-0.319238
H	-0.662786	1.248982	2.732114
H	0.662901	-1.248976	2.732108
H	1.083720	1.176694	2.488337
H	-1.083609	-1.176581	2.488400
H	2.321673	2.481707	-0.138045
H	-2.321743	-2.481481	-0.137941
H	1.830082	-3.460011	-0.697390
H	-1.830231	3.459978	-0.697318
H	4.072609	1.594141	1.355223
H	-4.072535	-1.594219	1.355173
H	4.280422	-0.055552	1.952871
H	-4.280398	0.055456	1.952855
H	4.803093	2.271741	-1.595973
H	-4.802998	-2.271783	-1.596035
H	5.422030	-2.262284	0.084068
H	-5.422068	2.262192	0.084092
Si	4.704203	0.044540	-0.496948
Si	-4.704174	-0.044600	-0.496967
H	0.487342	-1.024070	-1.571255
H	-0.487338	1.024111	-1.571261
C	1.561434	-3.292546	0.347945
C	-1.561532	3.292520	0.348005

C	5.786733	-1.486145	-0.592210
C	-5.786747	1.486056	-0.592201
H	0.306572	2.718188	2.846966
H	-0.306539	-2.718125	2.846985
H	1.237040	3.251837	-1.293466
H	-1.237208	-3.251675	-1.293413
H	2.043615	0.242767	0.730905
H	-2.043585	-0.242769	0.730891
H	-1.326673	4.259953	0.798311
H	1.326536	-4.259969	0.798253
H	5.395399	1.009784	-2.680926
H	-5.395338	-1.009822	-2.680965
H	5.790376	-1.896997	-1.604493
H	-5.790401	1.896927	-1.604476
Si	-0.083988	2.145576	0.487840
Si	0.083963	-2.145516	0.487849

A´$_2$ *rac* (THF)

64

C	0.498374	-0.596149	-0.559764
C	-0.498369	0.596168	-0.559764
C	2.975286	-0.396075	-1.019202
C	-2.975280	0.396074	-1.019202
C	1.900420	-0.207216	-0.250025
C	-1.900412	0.207223	-0.250026
C	0.193675	1.776114	2.304751
C	-0.193656	-1.776093	2.304754
C	1.398553	3.046302	-0.232995
C	-1.398592	-3.046242	-0.232982
C	4.679328	0.689208	1.263923
C	-4.679309	-0.689243	1.263915
C	5.396795	1.358246	-1.644420
C	-5.396769	-1.358269	-1.644433
H	2.813457	-0.848832	-1.998665
H	-2.813455	0.848839	-1.998663
H	1.527578	4.003653	0.278141
H	-1.527634	-4.003591	0.278153
H	2.434474	-2.882555	0.852789
H	-2.434495	2.882528	0.852823
H	5.693021	0.937020	1.586933
H	-5.692999	-0.937069	1.586923
H	6.425974	1.609446	-1.377108
H	-6.425944	-1.609483	-1.377123
H	6.819487	-1.254667	-0.320720
H	-6.819491	1.254619	-0.320715
H	-0.661065	1.249671	2.732258
H	0.661101	-1.249669	2.732254

H	1.085135	1.176048	2.487998
H	-1.085102	-1.176008	2.488014
H	2.323271	2.479847	-0.139614
H	-2.323296	-2.479764	-0.139587
H	1.828635	-3.461033	-0.696933
H	-1.828686	3.461025	-0.696905
H	4.071724	1.591682	1.356607
H	-4.071695	-1.591711	1.356592
H	4.280975	-0.058209	1.953259
H	-4.280965	0.058174	1.953256
H	4.800430	2.271767	-1.594146
H	-4.800393	-2.271784	-1.594164
H	5.423147	-2.263155	0.082316
H	-5.423162	2.263120	0.082328
Si	4.703899	0.043765	-0.496883
Si	-4.703888	-0.043788	-0.496886
H	0.486892	-1.024068	-1.571192
H	-0.486891	1.024087	-1.571192
C	1.559371	-3.293469	0.348181
C	-1.559405	3.293463	0.348206
C	5.787178	-1.486305	-0.593447
C	-5.787184	1.486271	-0.593441
H	0.309350	2.717939	2.847093
H	-0.309344	-2.717917	2.847094
H	1.239152	3.251516	-1.293993
H	-1.239210	-3.251455	-1.293982
H	2.043640	0.240779	0.731623
H	-2.043627	-0.240780	0.731620
H	-1.324345	4.260918	0.798307
H	1.324296	-4.260921	0.798281
H	5.393326	1.011483	-2.680351
H	-5.393303	-1.011500	-2.680361
H	5.790798	-1.896665	-1.605888
H	-5.790809	1.896637	-1.605879
Si	-0.082290	2.145885	0.487540
Si	0.082280	-2.145862	0.487539

A´$_2$ *rac* (solvent-free)

64

C	-0.494845	0.599086	-0.564167
C	0.494845	-0.599090	-0.564166
C	-2.974256	0.407530	-1.016251
C	2.974255	-0.407532	-1.016248
C	-1.898290	0.218740	-0.249872
C	1.898289	-0.218742	-0.249871
C	-0.225195	-1.775717	2.294166

C	0.225191	1.775715	2.294164
C	-1.413004	-3.041208	-0.254597
C	1.413011	3.041197	-0.254598
C	-4.664958	-0.685581	1.269787
C	4.664954	0.685591	1.269786
C	-5.391656	-1.351272	-1.636048
C	5.391652	1.351274	-1.636050
H	-2.813729	0.854021	-1.998559
H	2.813730	-0.854027	-1.998555
H	-1.576150	-3.983363	0.274503
H	1.576157	3.983354	0.274499
H	-2.412058	2.891947	0.869455
H	2.412060	-2.891942	0.869464
H	-5.673923	-0.944609	1.598244
H	5.673918	0.944622	1.598243
H	-6.417493	-1.612435	-1.365951
H	6.417488	1.612441	-1.365953
H	-6.818247	1.260906	-0.295638
H	6.818249	-1.260896	-0.295632
H	0.617804	-1.235121	2.726952
H	-0.617811	1.235123	2.726950
H	-1.126187	-1.188665	2.473036
H	1.126181	1.188660	2.473038
H	-2.328423	-2.454830	-0.203635
H	2.328428	2.454817	-0.203629
H	-1.825758	3.464639	-0.686218
H	1.825766	-3.464639	-0.686209
H	-4.049866	-1.583349	1.358569
H	4.049859	1.583357	1.358565
H	-4.272798	0.062198	1.962220
H	4.272796	-0.062188	1.962221
H	-4.788774	-2.260614	-1.594022
H	4.788767	2.260615	-1.594027
H	-5.420302	2.271799	0.090715
H	5.420306	-2.271791	0.090724
Si	-4.700479	-0.035601	-0.489905
Si	4.700478	0.035605	-0.489904
H	-0.483695	1.024097	-1.576885
H	0.483696	-1.024102	-1.576883
C	-1.540910	3.298330	0.354772
C	1.540916	-3.298329	0.354780
C	-5.788352	1.491148	-0.578035
C	5.788354	-1.491142	-0.578028
H	-0.329960	-2.715476	2.842041
H	0.329958	2.715475	2.842038
H	-1.231928	-3.277395	-1.305521
H	1.231940	3.277380	-1.305523
H	-2.040333	-0.226464	0.733255

H	2.040331	0.226466	0.733255
H	1.301922	-4.267752	0.798262
H	-1.301915	4.267753	0.798253
H	-5.397548	-1.003879	-2.671610
H	5.397545	1.003877	-2.671612
H	-5.804326	1.901450	-1.590249
H	5.804330	-1.901447	-1.590241
Si	0.065310	-2.147800	0.478653
Si	-0.065309	2.147797	0.478650

Optimized Coordinates for [NiA´$_2$] Formation
[Ni(py)$_4$Cl$_2$]

47
S1

Ni	0.000000	-0.000000	0.000000
Cl	0.000000	-0.000000	2.203512
Cl	0.000000	-0.000000	-2.203512
C	-2.920719	-0.717099	-0.894031
C	-2.920719	0.717099	0.894031
C	-4.306062	-0.750835	-0.927093
H	-2.316923	-1.264461	-1.607378
C	-4.306062	0.750835	0.927093
H	-2.316923	1.264461	1.607378
C	-5.012431	-0.000000	0.000000
H	-4.814419	-1.351733	-1.669828
H	-4.814419	1.351733	1.669828
H	-6.095752	-0.000000	0.000000
C	2.920719	-0.717099	0.894031
C	2.920719	0.717099	-0.894031
C	4.306062	-0.750835	0.927093
H	2.316923	-1.264461	1.607378
C	4.306062	0.750835	-0.927093
H	2.316923	1.264461	-1.607378
C	5.012431	0.000000	0.000000
H	4.814419	-1.351733	1.669828
H	4.814419	1.351733	-1.669828
H	6.095752	0.000000	0.000000
C	-0.717099	2.920719	-0.894031
C	0.717099	2.920719	0.894031
C	-0.750835	4.306062	-0.927093
H	-1.264461	2.316923	-1.607378
C	0.750835	4.306062	0.927093
H	1.264461	2.316923	1.607378
C	0.000000	5.012431	0.000000
H	-1.351733	4.814419	-1.669828
H	1.351733	4.814419	1.669828
H	0.000000	6.095752	0.000000
C	-0.717099	-2.920719	0.894031

C	0.717099	-2.920719	-0.894031
C	-0.750835	-4.306062	0.927093
H	-1.264461	-2.316923	1.607378
C	0.750835	-4.306062	-0.927093
H	1.264461	-2.316923	-1.607378
C	0.000000	-5.012431	0.000000
H	-1.351733	-4.814419	1.669828
H	1.351733	-4.814419	-1.669828
H	0.000000	-6.095752	0.000000
N	-0.000000	2.244728	0.000000
N	2.244728	-0.000000	0.000000
N	0.000000	-2.244728	0.000000
N	-2.244728	-0.000000	0.000000

$[Ni(py)_4Cl_2]$

47

S3

Ni	0.000000	-0.000000	-0.000000
Cl	0.000000	-0.000000	2.443531
Cl	0.000000	-0.000000	-2.443531
C	-2.901628	-0.579481	-0.992941
C	-2.901628	0.579481	0.992941
C	-4.286206	-0.606884	-1.027378
H	-2.293807	-1.005677	-1.781360
C	-4.286206	0.606884	1.027378
H	-2.293807	1.005677	1.781360
C	-4.991812	-0.000000	-0.000000
H	-4.794191	-1.091673	-1.850354
H	-4.794191	1.091673	1.850354
H	-6.075059	-0.000000	-0.000000
C	2.901628	-0.579481	0.992941
C	2.901628	0.579481	-0.992941
C	4.286206	-0.606884	1.027378
H	2.293807	-1.005677	1.781360
C	4.286206	0.606884	-1.027378
H	2.293807	1.005677	-1.781360
C	4.991812	0.000000	-0.000000
H	4.794191	-1.091673	1.850354
H	4.794191	1.091673	-1.850354
H	6.075059	0.000000	-0.000000
C	-0.579481	2.901628	-0.992941
C	0.579481	2.901628	0.992941
C	-0.606884	4.286206	-1.027378
H	-1.005677	2.293807	-1.781360
C	0.606884	4.286206	1.027378
H	1.005677	2.293807	1.781360
C	0.000000	4.991812	-0.000000

H	-1.091673	4.794191	-1.850354
H	1.091673	4.794191	1.850354
H	0.000000	6.075059	-0.000000
C	-0.579481	-2.901628	0.992941
C	0.579481	-2.901628	-0.992941
C	-0.606884	-4.286206	1.027378
H	-1.005677	-2.293807	1.781360
C	0.606884	-4.286206	-1.027378
H	1.005677	-2.293807	-1.781360
C	0.000000	-4.991812	-0.000000
H	-1.091673	-4.794191	1.850354
H	1.091673	-4.794191	-1.850354
H	0.000000	-6.075059	-0.000000
N	-0.000000	2.227783	-0.000000
N	2.227783	-0.000000	-0.000000
N	0.000000	-2.227783	-0.000000
N	-2.227783	-0.000000	-0.000000

IM1

80

Ni	2.230990	-0.104372	0.330018
Cl	-0.240115	-1.067858	-2.461832
Cl	4.244123	0.643914	2.321731
C	4.814501	0.149299	-0.852425
C	3.140102	-0.505143	-2.314293
C	5.755709	0.114001	-1.865867
H	5.048149	0.418223	0.175160
C	4.031796	-0.559700	-3.369535
H	2.086138	-0.737745	-2.448478
C	5.362877	-0.245735	-3.144989
H	6.782448	0.367913	-1.640267
H	3.671941	-0.846070	-4.348194
H	6.082075	-0.280802	-3.953964
C	-0.403162	-0.519029	1.206228
C	1.001176	0.290193	2.863709
C	-1.482244	-0.545913	2.071061
H	-0.504127	-0.816216	0.167729
C	-0.030501	0.277119	3.781064
H	2.013329	0.598537	3.104715
C	-1.289834	-0.147700	3.382342
H	-2.445225	-0.863537	1.688051
H	0.162333	0.603183	4.794136
H	-2.116516	-0.153299	4.081757
C	2.358023	2.733912	0.548814
C	0.982677	1.925072	-1.134029
C	2.060757	4.040787	0.205167
H	3.037663	2.463984	1.352480

C	0.656530	3.206435	-1.532358
H	0.567613	1.047411	-1.623849
C	1.199642	4.284400	-0.852125
H	2.503796	4.849140	0.770187
H	-0.025455	3.344811	-2.358759
H	0.945658	5.297832	-1.135438
C	1.733408	-2.828703	-0.127816
C	3.287308	-2.441710	1.550617
C	1.825124	-4.196238	0.051511
H	1.071657	-2.393035	-0.872602
C	3.425021	-3.799315	1.778177
H	3.831557	-1.679839	2.103402
C	2.683874	-4.691996	1.020252
H	1.223678	-4.850859	-0.563908
H	4.106491	-4.139855	2.545660
H	2.772468	-5.758938	1.182934
N	1.823906	1.704805	-0.116728
N	0.806849	-0.109275	1.598882
N	2.454610	-1.978459	0.612587
N	3.532415	-0.156998	-1.082766
C	-3.800223	-1.071882	-0.305776
C	-3.858804	0.302368	-0.081918
C	-2.860966	1.265608	-0.224712
C	-4.777449	-3.614589	1.116080
C	-6.732328	-1.346473	0.473609
C	-5.596273	-3.107367	-1.743779
C	-1.516417	3.301748	1.582064
C	-4.570176	3.243281	1.343613
C	-2.888161	4.296273	-0.938361
H	-2.819337	-1.488448	-0.556400
H	-1.865675	0.898109	-0.485578
H	-5.576467	-4.357791	1.181091
H	-4.613712	-3.203645	2.114985
H	-3.862090	-4.134402	0.821005
H	-7.042122	-0.575497	-0.235559
H	-6.569843	-0.863042	1.439306
H	-7.562762	-2.047466	0.586016
H	-5.954750	-2.388109	-2.485955
H	-6.368677	-3.871891	-1.624429
H	-4.708835	-3.597016	-2.154923
H	-1.630487	2.715181	2.495484
H	-1.434768	4.355237	1.861292
H	-0.570881	3.002766	1.126079
H	-5.437700	3.088320	0.697936
H	-4.625745	4.262981	1.732249
H	-4.657560	2.555408	2.187152
H	-1.996229	4.187536	-1.558186
H	-2.878768	5.305828	-0.518043

H	-3.757960	4.215124	-1.595539
Si	-5.182427	-2.239673	-0.111672
Si	-2.958563	2.967664	0.410324
H	-4.831099	0.681399	0.237655
K	-2.947820	-0.018336	-2.806740

TS1

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Ni	-0.856653	0.475977	-0.109074
Cl	1.640034	-3.426611	-2.090105
Cl	-4.559361	1.489880	-0.755090
C	-1.886426	0.288063	-2.634903
C	0.308623	-0.440784	-2.620822
C	-2.004890	0.003824	-3.978958
H	-2.725970	0.679934	-2.058770
C	0.253972	-0.762854	-3.965300
H	1.197701	-0.627448	-2.045115
C	-0.919463	-0.533685	-4.658748
H	-2.949364	0.193056	-4.470201
H	1.116695	-1.223489	-4.423807
H	-0.995549	-0.782785	-5.709847
C	-0.396161	1.348397	2.596147
C	-2.595525	1.278428	1.904026
C	-0.758279	1.806011	3.846293
H	0.635556	1.196341	2.326815
C	-3.030902	1.727333	3.139158
H	-3.292334	1.145846	1.073063
C	-2.103981	1.983950	4.133708
H	0.009278	2.013825	4.579050
H	-4.090434	1.880416	3.291272
H	-2.418449	2.331159	5.109866
C	-3.468322	-1.542473	0.243559
C	-1.601445	-2.573216	-0.593697
C	-4.162453	-2.742526	0.281298
H	-3.962805	-0.612977	0.492904
C	-2.220940	-3.810321	-0.591591
H	-0.588671	-2.496314	-0.969448
C	-3.525487	-3.901239	-0.130872
H	-5.190238	-2.750491	0.618589
H	-1.674663	-4.670125	-0.955214
H	-4.040592	-4.853932	-0.109379
C	0.572070	2.856123	-0.730477
C	-1.714066	3.219552	-0.756790
C	0.829798	4.184377	-1.008613
H	1.368429	2.132375	-0.605706
C	-1.525358	4.562295	-1.045076
H	-2.712682	2.781212	-0.670671

C	-0.238420	5.056160	-1.168039
H	1.853087	4.521981	-1.099175
H	-2.392001	5.197087	-1.170790
H	-0.066066	6.102278	-1.389116
N	-2.200774	-1.460587	-0.161641
N	-1.298244	1.063257	1.652030
N	-0.677565	2.391008	-0.600208
N	-0.737286	0.065735	-1.972382
C	2.980907	0.234904	-0.269054
C	2.040296	-0.059007	0.689479
C	0.915831	-0.934628	0.655165
C	4.024263	2.503666	1.471489
C	5.998442	0.524663	0.245327
C	4.566052	2.495256	-1.558928
C	-1.206282	-2.042606	2.858224
C	1.634806	-1.368216	3.609159
C	1.027907	-3.741536	1.828574
H	2.881593	-0.238291	-1.247378
H	0.881355	-1.543024	-0.248360
H	4.831622	3.225040	1.615904
H	3.949271	1.910237	2.385576
H	3.092539	3.062430	1.359127
H	6.225514	-0.136288	-0.595760
H	5.960639	-0.083574	1.153080
H	6.834957	1.220272	0.348231
H	4.780384	1.877011	-2.434102
H	5.388241	3.205628	-1.445840
H	3.658100	3.060010	-1.777891
H	-1.661162	-1.075466	3.062510
H	-1.159330	-2.593799	3.801692
H	-1.869482	-2.591470	2.191372
H	2.692197	-1.345973	3.333288
H	1.526011	-2.059486	4.448443
H	1.371874	-0.374898	3.975980
H	0.860432	-4.016153	0.783644
H	0.438356	-4.421059	2.447667
H	2.074991	-3.944025	2.079890
Si	4.360626	1.421642	-0.029085
Si	0.540514	-1.940702	2.176700
H	2.213974	0.443592	1.642931
K	3.398714	-2.684742	-0.026399

IM2

67

Ni	-0.707209	-0.174609	0.052569
Cl	-1.746151	-0.083133	2.864489
C	0.536704	-2.098949	1.723190

C	1.066151	-2.289802	-0.517195
C	1.249707	-3.247774	2.019620
H	-0.005249	-1.519186	2.467665
C	1.777895	-3.453906	-0.294866
H	1.004472	-1.844879	-1.500269
C	1.872511	-3.945304	0.997272
H	1.304634	-3.582621	3.046444
H	2.253624	-3.955948	-1.125673
H	2.429262	-4.850875	1.202961
C	-1.978798	1.538793	-1.816530
C	-2.752031	1.744001	0.346410
C	-2.927516	2.423377	-2.291040
H	-1.258281	1.082265	-2.480597
C	-3.723841	2.643773	-0.056445
H	-2.636559	1.403764	1.374428
C	-3.818636	2.991610	-1.393613
H	-2.955306	2.663868	-3.344950
H	-4.393939	3.059467	0.683651
H	-4.569317	3.694506	-1.732179
C	-2.224322	-1.962861	-1.631545
C	-3.008312	-1.966655	0.533652
C	-3.164334	-2.893646	-2.030611
H	-1.502183	-1.562085	-2.332464
C	-3.980054	-2.901527	0.210209
H	-2.882508	-1.547067	1.532376
C	-4.062762	-3.374140	-1.088288
H	-3.187093	-3.231736	-3.057789
H	-4.658282	-3.246685	0.979028
H	-4.812695	-4.104581	-1.365532
N	-1.890119	1.205384	-0.525251
N	-2.146727	-1.508082	-0.378283
N	0.443754	-1.637671	0.469699
C	2.562545	0.439415	-1.683695
C	1.391200	0.941702	-1.236142
C	0.867193	1.014086	0.126384
C	5.389359	1.203647	-0.945450
C	3.890256	-0.554148	1.026077
C	4.748472	-1.658080	-1.692290
C	0.018431	2.939999	2.444592
C	-0.116687	3.955724	-0.454617
C	2.541539	3.388101	0.823178
H	2.712563	0.509685	-2.763384
H	1.555194	0.531841	0.823325
H	6.346329	0.870119	-0.536114
H	5.085153	2.101925	-0.405995
H	5.548814	1.479099	-1.990235
H	3.140188	-1.323009	1.205496
H	3.620380	0.324665	1.612294

H	4.844633	-0.926423	1.408326
H	4.068877	-2.506636	-1.609321
H	5.714429	-1.962206	-1.282117
H	4.890772	-1.445641	-2.754476
H	0.581154	2.333001	3.156158
H	-1.009310	2.585707	2.499683
H	0.058409	3.981208	2.775839
H	0.215057	3.803900	-1.483688
H	0.131588	4.984448	-0.181414
H	-1.201736	3.865712	-0.427622
H	3.133589	2.773992	1.505148
H	2.592565	4.420583	1.177257
H	3.011899	3.342603	-0.160933
Si	4.086034	-0.142968	-0.792124
Si	0.756440	2.788165	0.737823
H	0.744287	1.384748	-1.996033

TS2

67

Ni	0.664651	-0.018357	0.311263
Cl	0.309055	0.147544	2.658693
C	-0.630942	2.709827	0.793484
C	-0.664283	2.160953	-1.429753
C	-0.963422	4.027006	0.515692
H	-0.464732	2.346514	1.803211
C	-0.971687	3.459482	-1.800038
H	-0.580154	1.375241	-2.169272
C	-1.123191	4.413699	-0.805569
H	-1.088676	4.732105	1.326783
H	-1.106055	3.707646	-2.844540
H	-1.373724	5.437020	-1.056388
C	1.744431	-1.398484	-2.012961
C	2.769231	-1.814644	0.001191
C	2.657664	-2.187078	-2.689590
H	0.938371	-0.902040	-2.533644
C	3.713888	-2.624855	-0.599668
H	2.767688	-1.629719	1.066995
C	3.660700	-2.817878	-1.971920
H	2.570565	-2.305890	-3.761040
H	4.473295	-3.098472	0.007411
H	4.383822	-3.450514	-2.470338
C	2.669354	1.785842	-0.757674
C	2.856409	1.606726	1.523327
C	3.716293	2.684965	-0.826635
H	2.142319	1.474701	-1.650410
C	3.919972	2.495367	1.539566
H	2.440967	1.161101	2.420903

C	4.358281	3.048361	0.348261
H	4.016929	3.089672	-1.783630
H	4.387203	2.747500	2.482151
H	5.182985	3.749982	0.332536
N	1.793155	-1.212937	-0.690767
N	2.240978	1.257556	0.391194
N	-0.477286	1.794322	-0.162694
C	-2.692549	-0.429431	-1.450805
C	-1.521439	-1.028025	-1.158516
C	-0.897553	-1.188124	0.151748
C	-5.568835	-0.626375	-0.616826
C	-3.610737	0.357073	1.491990
C	-4.275538	2.112444	-0.901325
C	0.329577	-3.317548	2.137230
C	-0.049886	-4.051311	-0.793591
C	-2.465675	-3.599444	0.979511
H	-2.980255	-0.442545	-2.504371
H	-1.521963	-0.747987	0.925946
H	-6.398009	-0.187302	-0.056514
H	-5.450695	-1.661225	-0.288854
H	-5.848000	-0.641326	-1.672880
H	-2.673773	0.856890	1.738230
H	-3.560686	-0.652411	1.901832
H	-4.420471	0.883675	2.005343
H	-3.433306	2.753128	-0.638624
H	-5.168495	2.518781	-0.419785
H	-4.419908	2.174241	-1.982247
H	0.081278	-2.611174	2.929216
H	1.395804	-3.215097	1.933381
H	0.156916	-4.336310	2.494399
H	-0.593881	-3.878916	-1.724471
H	-0.164985	-5.107845	-0.538358
H	1.010085	-3.877332	-0.982001
H	-2.868756	-3.098717	1.862495
H	-2.492420	-4.676111	1.163594
H	-3.128253	-3.379290	0.139680
Si	-3.977301	0.340462	-0.343761
Si	-0.718849	-2.995157	0.619484
H	-0.987415	-1.480368	-1.996913

IM3

56

Ni	-0.118822	0.038188	0.283421
Cl	0.670993	-0.926342	2.639028
Si	-1.765980	2.491674	-0.831895
Si	3.199875	0.975627	0.360416

N	-1.834784	-0.850157	0.460939
C	-0.858986	1.874601	0.678716
H	-1.464339	1.955116	1.582634
C	0.520796	1.813276	0.928416
H	0.854949	1.817340	1.959734
C	1.406439	1.339598	-0.054475
H	1.164011	1.570985	-1.091088
C	-1.223923	1.753312	-2.473869
H	-0.199269	2.031688	-2.725602
H	-1.870443	2.128885	-3.271358
H	-1.292397	0.665334	-2.473232
C	-1.537743	4.351914	-0.944124
H	-1.874204	4.842708	-0.028637
H	-2.099729	4.774353	-1.780583
H	-0.483364	4.599669	-1.084109
C	-3.583049	2.106953	-0.569236
H	-3.767733	1.033197	-0.517872
H	-4.188335	2.513150	-1.382676
H	-3.939721	2.550022	0.363119
C	4.231683	1.952155	-0.874660
H	5.299708	1.813496	-0.691353
H	4.016469	3.021198	-0.812860
H	4.027787	1.629743	-1.899108
C	3.545607	1.546129	2.106071
H	2.936550	0.965709	2.803036
H	3.324905	2.606679	2.243300
H	4.596753	1.385848	2.356965
C	3.655127	-0.834035	0.231733
H	3.069691	-1.397224	0.959904
H	4.714450	-0.959542	0.469421
H	3.485204	-1.248606	-0.762842
C	-2.476263	-1.372684	-0.587566
H	-1.970747	-1.305849	-1.541140
C	-3.717405	-1.970584	-0.478483
H	-4.195258	-2.378785	-1.358561
C	-4.321819	-2.027607	0.768156
H	-5.296310	-2.483816	0.888336
C	-3.649676	-1.495605	1.856382
H	-4.073673	-1.527845	2.850725
C	-2.404999	-0.920106	1.669498
H	-1.802397	-0.537406	2.484303
N	0.647519	-1.446420	-0.732419
C	0.980114	-1.329337	-2.021328
H	0.851968	-0.350344	-2.462194
C	1.474441	-2.387939	-2.759605
H	1.735405	-2.241364	-3.798930
C	1.633826	-3.617864	-2.138150
H	2.025488	-4.465621	-2.686146

C	1.291011	-3.735226	-0.801543
H	1.409411	-4.669591	-0.269885
C	0.801733	-2.629217	-0.128069
H	0.560138	-2.633174	0.931305

TS3

56

Ni	0.206695	0.152893	-0.744472
Cl	-0.615100	-1.576238	-2.102877
Si	1.093067	2.779228	1.318455
Si	-3.335151	0.598134	-0.827222
N	2.023183	-0.412329	-0.988165
C	0.634582	2.065589	-0.392730
H	1.336658	2.466503	-1.131643
C	-0.703243	1.905420	-0.905047
H	-0.943083	2.223355	-1.918698
C	-1.588481	1.052391	-0.213340
H	-1.459322	0.970206	0.869278
C	0.540130	1.757464	2.845962
H	-0.552000	1.727346	2.928900
H	0.932177	2.224745	3.757452
H	0.911285	0.729134	2.798957
C	0.323007	4.533510	1.477745
H	0.658622	5.179482	0.658614
H	0.614079	5.001997	2.425678
H	-0.770917	4.480913	1.440842
C	3.005527	2.960859	1.370848
H	3.507887	1.990751	1.291070
H	3.319908	3.432315	2.309397
H	3.355214	3.589532	0.543445
C	-4.550921	1.844408	0.002726
H	-5.583749	1.627065	-0.295987
H	-4.319038	2.874327	-0.292281
H	-4.494689	1.782157	1.096138
C	-3.463673	0.782412	-2.727693
H	-2.755369	0.104062	-3.212558
H	-3.250406	1.809090	-3.048613
H	-4.476675	0.530431	-3.063433
C	-3.809484	-1.166048	-0.258089
H	-3.140143	-1.893319	-0.725785
H	-4.843479	-1.396118	-0.541581
H	-3.725324	-1.263625	0.830889
C	2.836569	-0.594176	0.083315
H	2.386228	-0.427151	1.051002
C	4.162418	-0.999106	-0.056785
H	4.775054	-1.141617	0.825600

C	4.678025	-1.215608	-1.339561
H	5.708501	-1.524966	-1.476104
C	3.836053	-1.032785	-2.440994
H	4.190289	-1.200587	-3.451046
C	2.514066	-0.641539	-2.233406
H	1.810776	-0.535201	-3.047055
N	-0.015029	-1.751739	1.383913
C	-0.761508	-1.673888	2.511407
H	-0.947158	-0.677381	2.892780
C	-1.274827	-2.796925	3.165623
H	-1.872158	-2.677372	4.062698
C	-1.003328	-4.064238	2.639017
H	-1.387316	-4.957169	3.121261
C	-0.235206	-4.157036	1.473939
H	-0.011344	-5.117978	1.024831
C	0.233023	-2.983872	0.875931
H	0.790444	-3.011500	-0.050624

IM4

45

Ni	2.637178	4.199559	7.252172
Cl	2.452364	5.961596	8.698951
Si	3.397227	3.910029	4.135874
Si	-0.800107	4.709802	7.443533
N	4.411050	3.751485	7.842961
C	2.634172	3.018939	5.650781
H	3.059034	2.015319	5.741859
C	1.314064	3.144839	6.178270
H	0.851734	2.279291	6.654958
C	0.789491	4.438200	6.422681
H	1.014138	5.232944	5.710472
C	3.036054	5.790197	4.012604
H	1.981425	5.987014	3.792170
H	3.631911	6.215568	3.195683
H	3.294708	6.321419	4.934624
C	2.735574	3.051105	2.549635
H	2.965423	1.979681	2.558962
H	3.191881	3.491608	1.655106
H	1.648581	3.165309	2.473035
C	5.296952	3.656684	4.227229
H	5.729151	4.197878	5.075658
H	5.773888	4.024873	3.311443
H	5.549645	2.595347	4.335157
C	-1.083077	6.581397	7.702908
H	-2.002040	6.759516	8.273605
H	-1.175138	7.100765	6.741477

H	-0.237059	7.008787	8.248680
C	-2.275598	3.984045	6.439000
H	-2.144530	2.910291	6.260202
H	-2.367563	4.481474	5.466537
H	-3.216536	4.125886	6.984373
C	-0.686812	3.785493	9.119192
H	-0.499446	2.714054	8.976509
H	-1.624492	3.889680	9.677765
H	0.126708	4.205341	9.718806
C	5.341156	4.720105	8.057911
H	5.013546	5.736050	7.890067
C	6.624486	4.421968	8.512752
H	7.335218	5.225491	8.663980
C	6.966575	3.093330	8.781692
H	7.955909	2.838902	9.145545
C	6.003866	2.098925	8.578155
H	6.220662	1.057235	8.782610
C	4.745320	2.460145	8.103876
H	3.978599	1.719378	7.924458

IM5

78

Ni	-1.777536	-0.407426	0.143129
Cl	-0.694626	-0.158219	2.046719
Si	-4.520442	-1.616961	-0.525041
Si	0.609107	-2.889504	-0.113944
N	-2.663878	1.312287	0.254573
C	-2.922640	-1.070850	-1.350588
H	-3.102233	-0.397312	-2.188809
C	-1.664823	-1.697498	-1.372138
H	-0.973060	-1.447842	-2.173877
C	-1.169496	-2.322998	-0.218358
H	-1.892002	-2.791693	0.446169
C	-4.346939	-2.099316	1.279506
H	-3.838796	-3.057375	1.399658
H	-5.342971	-2.200588	1.718603
H	-3.795401	-1.358906	1.860838
C	-5.197782	-3.080241	-1.482105
H	-5.356642	-2.826109	-2.531981
H	-6.152082	-3.413488	-1.067417
H	-4.501373	-3.920405	-1.444063
C	-5.702440	-0.168908	-0.662475
H	-5.375820	0.678649	-0.058461
H	-6.698566	-0.457266	-0.319770
H	-5.793429	0.171020	-1.696222
C	1.077727	-3.239205	1.666871

H	2.152978	-3.409962	1.762460
H	0.574107	-4.142185	2.019045
H	0.771298	-2.426650	2.326303
C	0.794803	-4.475557	-1.098646
H	0.519552	-4.322851	-2.144247
H	0.160804	-5.268833	-0.697191
H	1.828974	-4.827428	-1.072916
C	1.689535	-1.571046	-0.884467
H	1.596853	-1.589782	-1.972199
H	2.745628	-1.723271	-0.658573
H	1.411925	-0.563396	-0.575023
C	-3.172233	1.732931	1.418324
H	-2.982452	1.098308	2.272016
C	-3.874388	2.917842	1.532391
H	-4.268703	3.211354	2.495415
C	-4.046867	3.709581	0.409014
H	-4.586445	4.645914	0.469561
C	-3.503582	3.282530	-0.791413
H	-3.594353	3.870292	-1.694264
C	-2.824859	2.080341	-0.827910
H	-2.380939	1.717039	-1.741709
C	2.693077	2.430069	0.252992
C	3.586273	1.470959	-0.221097
C	4.675227	0.888687	0.420817
C	1.628941	4.622773	-1.712468
C	0.486730	1.830447	-1.784236
C	-0.027855	3.659324	0.633256
C	7.562779	-0.029261	-0.084200
C	5.353751	-0.741892	-2.075731
C	5.494866	-2.079775	0.660791
H	2.959235	2.906858	1.202679
H	4.972210	1.341192	1.373379
H	0.728931	5.017503	-2.193563
H	2.347075	4.366671	-2.495244
H	2.071136	5.424098	-1.115540
H	-0.034634	1.058037	-1.211103
H	1.247942	1.336554	-2.391742
H	-0.227052	2.294465	-2.469667
H	-0.388496	2.803749	1.207659
H	-0.884849	4.153064	0.170283
H	0.417971	4.367920	1.336439
H	7.813841	0.866865	-0.655538
H	8.196152	-0.848230	-0.435056
H	7.819476	0.165227	0.960493
H	4.308613	-1.008240	-2.242628
H	5.969693	-1.557560	-2.462149
H	5.565893	0.150699	-2.667956
H	5.690659	-1.952027	1.729671

H	6.173071	-2.855713	0.294932
H	4.475341	-2.461485	0.555620
Si	1.263210	3.116001	-0.631506
Si	5.728939	-0.430711	-0.256161
H	3.353499	1.058845	-1.206100
K	2.308105	0.117827	1.922225

TS5

76

Ni	-0.068818	0.218351	-0.141922
Si	-1.234370	-2.680620	-1.686506
Si	3.538444	-0.704391	-0.894706
N	-0.144590	-1.392366	2.018374
C	-0.633137	-0.866609	-1.763994
H	-1.266137	-0.313441	-2.460858
C	0.755224	-0.494153	-1.831214
H	1.083394	0.240136	-2.566374
C	1.647764	-0.894774	-0.809914
H	1.361444	-1.789714	-0.257132
C	-0.050834	-3.916436	-0.813913
H	0.938755	-3.925844	-1.282395
H	-0.474075	-4.925261	-0.897311
H	0.070800	-3.685644	0.248913
C	-1.411094	-3.263548	-3.514846
H	-2.114137	-2.626780	-4.064660
H	-1.779074	-4.295846	-3.560048
H	-0.443336	-3.220393	-4.027599
C	-2.964202	-2.876002	-0.872673
H	-2.914779	-2.721634	0.209809
H	-3.337797	-3.891661	-1.051599
H	-3.691962	-2.170979	-1.287329
C	4.315581	0.414561	0.457102
H	5.409491	0.360215	0.400631
H	4.012116	0.098323	1.461790
H	4.016211	1.457519	0.328782
C	4.261140	-2.469949	-0.635875
H	3.902983	-3.155495	-1.412435
H	3.964612	-2.878947	0.337720
H	5.356762	-2.450422	-0.675175
C	4.103066	-0.088851	-2.624745
H	3.761211	-0.779704	-3.403799
H	5.198137	-0.046100	-2.664614
H	3.719355	0.908143	-2.864208
C	1.046848	-1.578846	2.637020
H	1.913854	-1.212994	2.102201
C	1.165924	-2.193138	3.886226

H	2.143732	-2.317621	4.337678
C	0.008291	-2.638040	4.533830
H	0.067596	-3.119621	5.504072
C	-1.227479	-2.447469	3.906421
H	-2.149803	-2.774667	4.372947
C	-1.259607	-1.823277	2.656611
H	-2.196791	-1.649283	2.143760
C	-1.599518	1.626907	-0.175210
C	-0.897616	1.601750	1.059207
C	0.512589	1.813907	1.088796
C	-4.018856	0.959619	-2.077970
C	-4.259020	0.341637	1.003410
C	-4.213805	3.264157	-0.022232
C	0.045916	4.812613	0.266484
C	1.956928	3.158046	-1.508046
C	2.752993	3.922739	1.426567
H	-1.175299	2.250352	-0.968974
H	0.993735	1.553993	2.033167
H	-5.109251	1.011234	-2.180431
H	-3.701072	-0.063650	-2.298528
H	-3.578700	1.621506	-2.833386
H	-3.932494	0.616261	2.013197
H	-3.994068	-0.703800	0.819915
H	-5.352153	0.422554	0.973741
H	-3.964555	3.624586	0.982306
H	-5.305885	3.255839	-0.124037
H	-3.810207	3.980825	-0.747017
H	-0.823579	4.593690	-0.361544
H	0.526300	5.720579	-0.118205
H	-0.315494	5.018140	1.280465
H	2.715235	2.373855	-1.573730
H	2.404729	4.099850	-1.847638
H	1.142375	2.902210	-2.195163
H	2.360682	4.208595	2.409849
H	3.258987	4.795730	0.997316
H	3.499588	3.136661	1.576702
Si	-3.489091	1.504410	-0.316302
Si	1.308391	3.359401	0.288050
H	-1.402216	1.209188	1.940646

IM6

76

Ni	-0.627972	0.417085	-0.103350
Si	-3.398193	1.836140	-0.314937
Si	-1.523276	-2.921166	-1.280753
N	0.227738	2.116922	0.110399

C	-2.026522	1.180099	-1.399968
H	-1.682304	1.899718	-2.142824
C	-1.705682	-0.151147	-1.676125
H	-1.153345	-0.368337	-2.590245
C	-1.799427	-1.168826	-0.699865
H	-2.569121	-1.034106	0.058799
C	-3.367945	1.206929	1.455783
H	-3.753815	0.189086	1.524088
H	-3.997449	1.841837	2.084651
H	-2.363643	1.192555	1.881642
C	-5.053618	1.368857	-1.064005
H	-5.154149	1.766589	-2.075769
H	-5.883980	1.750222	-0.464761
H	-5.149952	0.282614	-1.122622
C	-3.213942	3.703532	-0.309538
H	-2.254175	4.011991	0.108463
H	-4.003923	4.173648	0.280112
H	-3.274902	4.101355	-1.324996
C	-2.025223	-4.187090	0.006238
H	-1.909634	-5.192664	-0.405539
H	-3.079454	-4.058116	0.263149
H	-1.448652	-4.133493	0.926436
C	-2.669426	-3.175258	-2.753683
H	-2.428417	-2.488095	-3.567709
H	-3.710044	-3.000340	-2.471716
H	-2.592902	-4.193727	-3.142275
C	0.226190	-3.188414	-1.899526
H	0.503730	-2.399384	-2.602124
H	0.301957	-4.141643	-2.427630
H	0.965562	-3.188764	-1.100662
C	0.037624	2.927195	1.156590
H	-0.675749	2.592997	1.896759
C	0.714138	4.122285	1.302094
H	0.522301	4.742552	2.166875
C	1.634119	4.495532	0.332324
H	2.182781	5.424483	0.419842
C	1.839908	3.650908	-0.744575
H	2.554375	3.885969	-1.520883
C	1.122237	2.470129	-0.818135
H	1.260669	1.777249	-1.634670
C	2.882757	0.202891	0.313024
C	1.780171	-0.569712	0.438888
C	0.612916	-0.321057	1.276822
C	5.896692	-0.292023	0.133004
C	3.975604	-1.752190	-1.760498
C	4.492186	1.246558	-2.073511
C	0.957466	-1.253110	4.106995
C	0.924527	-3.333160	1.931534

C	-1.674215	-1.878458	2.798241
H	2.934995	1.091052	0.944796
H	0.815733	0.546926	1.916823
H	6.747932	-0.459489	-0.531333
H	5.852504	-1.119790	0.843755
H	6.090995	0.620913	0.701057
H	3.066687	-1.695820	-2.362101
H	3.868576	-2.596062	-1.076047
H	4.807899	-1.972015	-2.432931
H	3.609811	1.340616	-2.710750
H	5.355298	1.079469	-2.722377
H	4.642266	2.200011	-1.561544
H	2.033582	-1.107736	3.987501
H	0.802884	-2.036162	4.853479
H	0.539499	-0.325732	4.506920
H	0.647944	-3.642158	0.925910
H	0.635010	-4.132712	2.617517
H	2.012954	-3.244909	1.961684
H	-2.078216	-0.940803	3.185004
H	-1.843847	-2.648354	3.555073
H	-2.245047	-2.146503	1.911824
Si	4.286428	-0.154477	-0.827342
Si	0.162936	-1.696190	2.455129
H	1.732095	-1.468878	-0.171644

IM7

76

Ni	-0.686035	0.441033	-0.123311
Si	-3.407333	1.898324	0.028923
Si	-1.747665	-2.820844	-1.335834
N	0.278603	2.109281	-0.058080
C	-2.190091	1.271935	-1.245045
H	-1.919328	2.010354	-1.999359
C	-1.930489	-0.054426	-1.590667
H	-1.480360	-0.252935	-2.563043
C	-1.948279	-1.101639	-0.637322
H	-2.654270	-0.992502	0.184425
C	-3.135529	1.257604	1.775895
H	-3.464635	0.222831	1.877075
H	-3.718222	1.860241	2.477900
H	-2.090662	1.286513	2.087409
C	-5.141827	1.411150	-0.494160
H	-5.384414	1.817703	-1.477893
H	-5.888803	1.771678	0.217127
H	-5.228134	0.324126	-0.553391
C	-3.248051	3.768655	0.030375

H	-2.240536	4.086294	0.305088
H	-3.947105	4.222436	0.736132
H	-3.462807	4.176086	-0.960091
C	-2.040940	-4.180281	-0.080175
H	-1.986002	-5.150244	-0.580730
H	-3.044940	-4.086569	0.340699
H	-1.332474	-4.186548	0.743802
C	-3.094209	-3.019656	-2.639203
H	-2.993681	-2.274713	-3.431490
H	-4.085157	-2.897931	-2.195974
H	-3.053265	-4.008791	-3.102090
C	-0.103337	-3.002064	-2.221324
H	-0.001766	-2.233994	-2.991715
H	-0.038055	-3.974044	-2.715668
H	0.747656	-2.905517	-1.549412
C	0.219688	2.983878	0.948206
H	-0.470775	2.749309	1.746255
C	1.004259	4.121666	0.989690
H	0.920914	4.797639	1.829672
C	1.889499	4.364611	-0.048989
H	2.523129	5.242076	-0.041682
C	1.950027	3.456219	-1.093933
H	2.630464	3.594199	-1.922756
C	1.131964	2.342815	-1.061446
H	1.162880	1.595941	-1.842024
C	2.543123	-0.662408	-0.176363
C	1.905074	-0.022609	0.820182
C	0.530137	-0.249831	1.297953
C	4.201281	0.228379	-2.571217
C	4.936237	1.182412	0.243148
C	5.382038	-1.741584	-0.577245
C	1.330357	-1.642901	3.850606
C	1.101969	-3.335274	1.399450
C	-1.435524	-2.124436	2.763239
H	1.989053	-1.443944	-0.693777
H	0.305017	0.505477	2.069267
H	5.204824	0.409460	-2.963542
H	3.614155	1.136504	-2.724070
H	3.747276	-0.563901	-3.170997
H	5.021843	0.928730	1.301658
H	4.296823	2.063718	0.160733
H	5.931327	1.454962	-0.115828
H	5.470254	-2.040045	0.469415
H	6.384818	-1.530456	-0.956357
H	4.987728	-2.595995	-1.132275
H	2.381276	-1.439507	3.631352
H	1.286000	-2.545194	4.465900
H	0.947667	-0.812506	4.449144

H	0.700200	-3.530476	0.409011
H	0.951810	-4.231193	2.007087
H	2.176969	-3.176232	1.295734
H	-1.789213	-1.264916	3.337600
H	-1.522402	-3.006981	3.401383
H	-2.102017	-2.255014	1.913739
Si	4.247127	-0.254618	-0.750593
Si	0.349073	-1.841757	2.249089
H	2.454606	0.781222	1.313705

TS5

76

Ni	-0.068818	0.218351	-0.141922
Si	-1.234370	-2.680620	-1.686506
Si	3.538444	-0.704391	-0.894706
N	-0.144590	-1.392366	2.018374
C	-0.633137	-0.866609	-1.763994
H	-1.266137	-0.313441	-2.460858
C	0.755224	-0.494153	-1.831214
H	1.083394	0.240136	-2.566374
C	1.647764	-0.894774	-0.809914
H	1.361444	-1.789714	-0.257132
C	-0.050834	-3.916436	-0.813913
H	0.938755	-3.925844	-1.282395
H	-0.474075	-4.925261	-0.897311
H	0.070800	-3.685644	0.248913
C	-1.411094	-3.263548	-3.514846
H	-2.114137	-2.626780	-4.064660
H	-1.779074	-4.295846	-3.560048
H	-0.443336	-3.220393	-4.027599
C	-2.964202	-2.876002	-0.872673
H	-2.914779	-2.721634	0.209809
H	-3.337797	-3.891661	-1.051599
H	-3.691962	-2.170979	-1.287329
C	4.315581	0.414561	0.457102
H	5.409491	0.360215	0.400631
H	4.012116	0.098323	1.461790
H	4.016211	1.457519	0.328782
C	4.261140	-2.469949	-0.635875
H	3.902983	-3.155495	-1.412435
H	3.964612	-2.878947	0.337720
H	5.356762	-2.450422	-0.675175
C	4.103066	-0.088851	-2.624745
H	3.761211	-0.779704	-3.403799
H	5.198137	-0.046100	-2.664614
H	3.719355	0.908143	-2.864208

C	1.046848	-1.578846	2.637020
H	1.913854	-1.212994	2.102201
C	1.165924	-2.193138	3.886226
H	2.143732	-2.317621	4.337678
C	0.008291	-2.638040	4.533830
H	0.067596	-3.119621	5.504072
C	-1.227479	-2.447469	3.906421
H	-2.149803	-2.774667	4.372947
C	-1.259607	-1.823277	2.656611
H	-2.196791	-1.649283	2.143760
C	-1.599518	1.626907	-0.175210
C	-0.897616	1.601750	1.059207
C	0.512589	1.813907	1.088796
C	-4.018856	0.959619	-2.077970
C	-4.259020	0.341637	1.003410
C	-4.213805	3.264157	-0.022232
C	0.045916	4.812613	0.266484
C	1.956928	3.158046	-1.508046
C	2.752993	3.922739	1.426567
H	-1.175299	2.250352	-0.968974
H	0.993735	1.553993	2.033167
H	-5.109251	1.011234	-2.180431
H	-3.701072	-0.063650	-2.298528
H	-3.578700	1.621506	-2.833386
H	-3.932494	0.616261	2.013197
H	-3.994068	-0.703800	0.819915
H	-5.352153	0.422554	0.973741
H	-3.964555	3.624586	0.982306
H	-5.305885	3.255839	-0.124037
H	-3.810207	3.980825	-0.747017
H	-0.823579	4.593690	-0.361544
H	0.526300	5.720579	-0.118205
H	-0.315494	5.018140	1.280465
H	2.715235	2.373855	-1.573730
H	2.404729	4.099850	-1.847638
H	1.142375	2.902210	-2.195163
H	2.360682	4.208595	2.409849
H	3.258987	4.795730	0.997316
H	3.499588	3.136661	1.576702
Si	-3.489091	1.504410	-0.316302
Si	1.308391	3.359401	0.288050
H	-1.402216	1.209188	1.940646

[NiA´$_2$]

65

C	-0.565825	-1.611517	1.052402

C	0.818329	-1.359898	1.171342
C	1.627308	-1.252453	0.025404
C	-1.237833	-2.382661	-1.947726
C	-0.165798	-4.434018	0.009464
C	-2.982716	-3.344303	0.378434
C	4.059450	0.349635	-1.035516
C	4.191456	-2.655167	-0.615390
C	4.080099	-0.824752	1.818086
H	-1.147464	-1.464767	1.958668
H	1.272376	-1.786924	-0.858331
H	-1.804945	-3.109613	-2.535255
H	-0.227378	-2.346995	-2.358231
H	-1.690049	-1.403471	-2.098186
H	-0.194857	-4.829290	1.026925
H	0.875277	-4.210015	-0.229715
H	-0.507092	-5.218996	-0.669528
H	-3.006777	-3.660264	1.423741
H	-3.350087	-4.175787	-0.227611
H	-3.682500	-2.517194	0.264229
H	3.614118	0.276827	-2.029687
H	5.145671	0.329783	-1.149065
H	3.782311	1.316125	-0.618430
H	3.872955	-3.509347	-0.014203
H	5.283724	-2.631719	-0.615418
H	3.863154	-2.830076	-1.642679
H	3.625530	0.032686	2.315396
H	5.162670	-0.678977	1.829999
H	3.859502	-1.712453	2.415001
Si	-1.236022	-2.897315	-0.139012
Si	3.475322	-1.052804	0.056902
H	1.223989	-1.023470	2.123121
C	0.505963	1.622887	-1.134274
C	-0.875937	1.332654	-1.172636
C	-1.613312	1.230051	0.021540
C	-0.127381	4.274404	0.317486
C	1.936000	2.419793	1.553270
C	2.513487	3.885983	-1.087270
C	-4.260672	2.634875	0.172844
C	-3.834301	0.093329	1.780209
C	-4.118307	-0.012885	-1.306614
H	1.047167	1.444324	-2.060576
H	-1.215444	1.792257	0.870384
H	0.341374	5.174352	0.723761
H	-0.857235	3.926377	1.048319
H	-0.671730	4.556341	-0.585614
H	2.790694	1.765195	1.390541
H	1.199843	1.863820	2.137711
H	2.270958	3.270180	2.152041

H	3.290591	3.212790	-1.449939
H	2.995645	4.669602	-0.498236
H	2.053736	4.359458	-1.957954
H	-3.889722	3.242394	1.001239
H	-5.344933	2.551085	0.279301
H	-4.053038	3.176174	-0.752584
H	-3.402631	-0.904858	1.833428
H	-4.913272	0.005207	1.925707
H	-3.433999	0.674793	2.614176
H	-3.890187	0.498002	-2.244725
H	-5.205893	-0.084417	-1.231127
H	-3.722654	-1.024873	-1.371307
Si	1.203553	3.003695	-0.071191
Si	-3.442989	0.942102	0.157187
H	-1.321215	0.956180	-2.091388
Ni	0.009416	0.010512	-0.003737

K[A´]
33

C	1.258978	-0.014908	-0.822922
C	-0.001462	0.344236	-0.347419
C	-1.261876	-0.008696	-0.827647
C	3.963057	1.469057	-1.133291
C	2.545709	1.346954	1.576617
C	3.837286	-1.138685	0.380842
C	-3.955743	1.492790	-1.145849
C	-2.550652	1.355361	1.569475
C	-3.852033	-1.119614	0.361915
H	1.284625	-0.498427	-1.806334
H	-1.286213	-0.492119	-1.811138
H	4.925947	1.674328	-0.658212
H	3.486299	2.423502	-1.366332
H	4.160149	0.961650	-2.081109
H	1.946013	0.759741	2.276377
H	2.022310	2.289251	1.402352
H	3.494207	1.578120	2.066994
H	3.327109	-1.740115	1.140614
H	4.832834	-0.905900	0.767985
H	3.969531	-1.763317	-0.507445
H	-3.472120	2.444807	-1.374642
H	-4.919221	1.702914	-0.674087
H	-4.152208	0.988939	-2.095689
H	-1.957550	0.762853	2.270394
H	-3.499856	1.591099	2.056301
H	-2.020847	2.294912	1.399799
H	-3.983577	-1.741496	-0.528398
H	-4.848074	-0.881820	0.744707

H	-3.349110	-1.725724	1.122798
Si	2.843004	0.423605	-0.037132
Si	-2.846623	0.437694	-0.047783
H	-0.001827	0.907439	0.588923
K	-0.009020	-2.391246	0.065305

Pyridine

11

N	-1.472341	0.795959	0.000000
C	-2.616345	0.116990	0.000000
C	-2.686507	-1.269216	0.000000
C	-1.502036	-1.989695	0.000000
C	-0.302475	-1.294629	0.000000
C	-0.343072	0.092757	0.000000
H	-3.524432	0.711890	0.000000
H	-3.646941	-1.768875	0.000000
H	-1.513581	-3.072732	0.000000
H	0.647089	-1.814648	0.000000
H	0.577491	0.668164	0.000000

KCl

2

K	-3.332844	1.217558	0.000000
Cl	-0.654238	0.951415	-0.000000

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