Supporting Information

Fluxional Interconversion of Divalent Palladium Complexes Having NSNSN Ligands between Flexible SNS and Rigid NNN-Coordinated Structures

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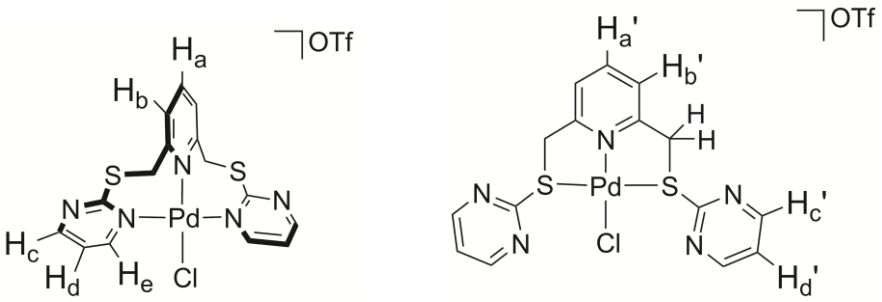
COSY spectrum for 1-NNN and 1-SNS (300 MHz, CD_3OD)



1-NNN **1**-SNS

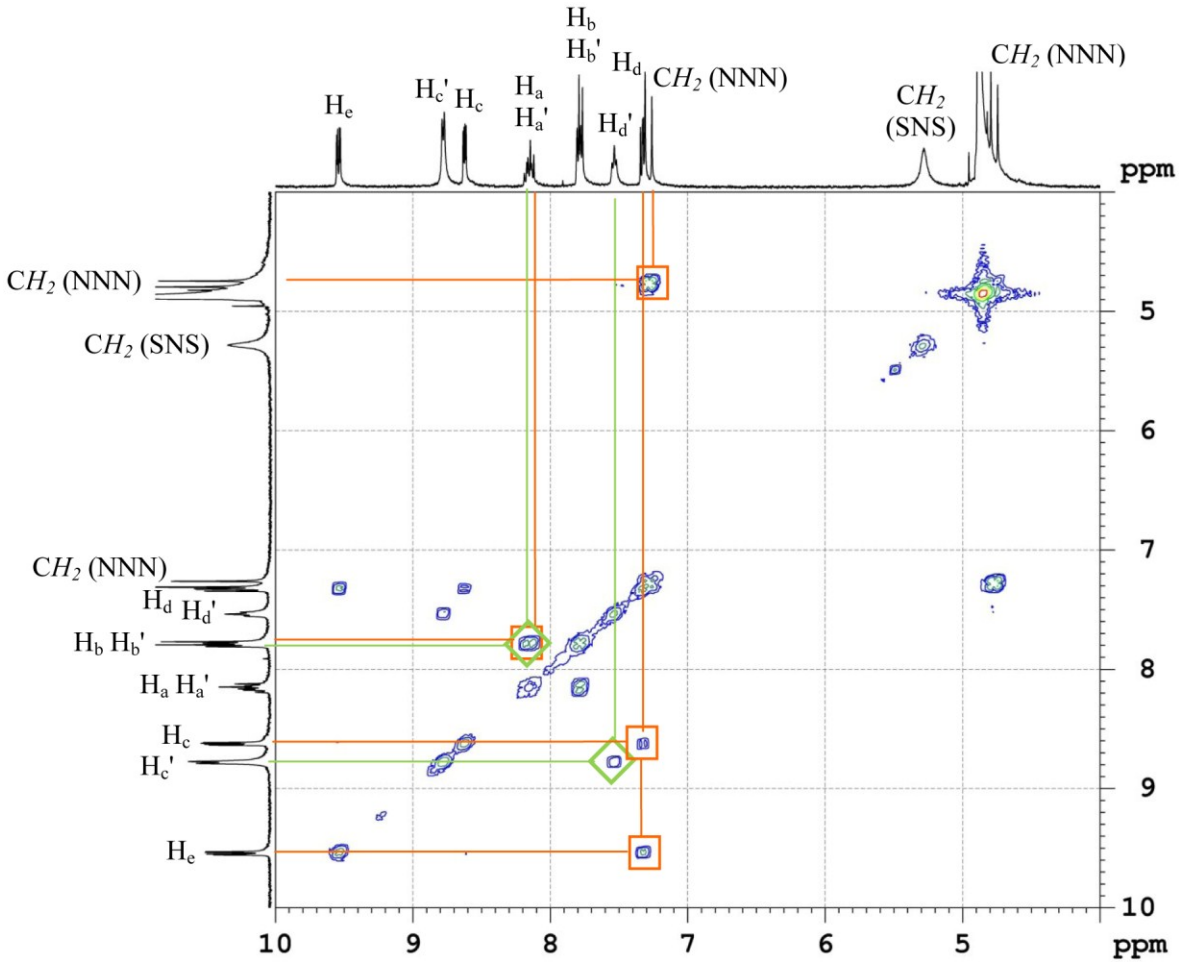


Fig. S1 COSY spectrum for **1**-NNN and **1**-SNS.

van't Hoff plot for the equilibrium between 1-NNN and 1-SNS

Table S1 Equilibrium constants (*K*), 1/T, and -ln*K*

T (K)	243	253	263	273	283	293	303	313	323
K	0.30	0.41	0.58	0.82	0.86	1.07	1.33	1.63	2.02
1/T	0.00412	0.00395	0.00380	0.00366	0.00353	0.00341	0.00330	0.00319	0.00310
-ln*K*	1.20	0.89	0.54	0.20	0.15	-0.07	-0.29	-0.49	-0.70

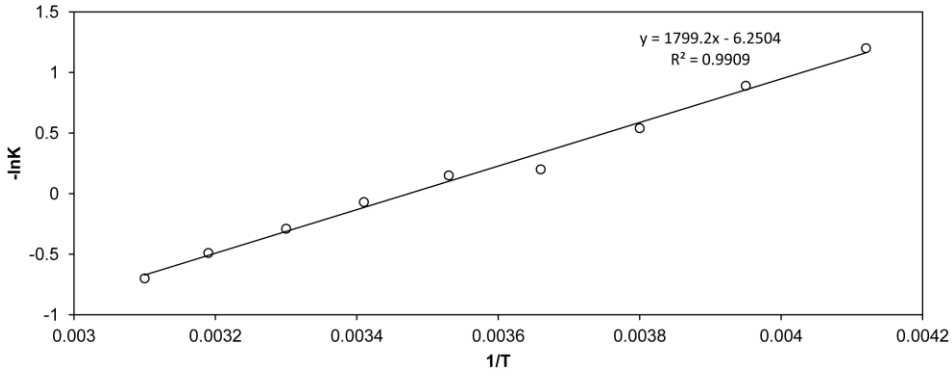


Fig. S2 van't Hoff plot for the equilibrium between **1**-NNN and **1**-SNS.

Eyring plots for 2 (in CD_3CN, 17 mM)

Table S2 Rate constants (k) obtained by line-shape analysis, 1/T, and ln(k/T)

T (K)	233	238	243	248	253	258
k (s^{-1})	1.33	1.37	1.91	2.70	3.13	4.01
1/T	0.00429	0.00420	0.00412	0.00403	0.00395	0.00388
ln(k/T)	-5.17	-5.16	-4.84	-4.52	-4.39	-4.16

Table S3 Rate constants (k_{-1}) obtained by line-shape analysis, 1/T, and ln(k_{-1}/T)

T (K)	233	238	243	248	253	258
k_{-1} (s^{-1})	6.91	7.40	11.1	13.4	19.0	27.6
1/T	0.00429	0.00420	0.00412	0.00403	0.00395	0.00388
ln(k_{-1}/T)	-3.52	-3.47	-3.09	-2.92	-2.59	-2.24

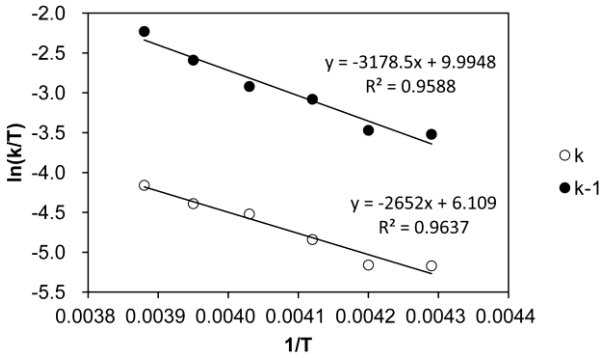


Fig. S3 Eyring plot for **2** (in CD_3CN).

Eyring plots for 4 (in CD_2Cl_2, 11 mM)

Table S4 Rate constants (k) obtained by line-shape analysis, 1/T, and ln(k/T)

T (K)	240	249	254	259	263	268	273	277
k (s^{-1})	0.22	0.92	1.21	1.57	3.32	2.94	4.63	6.03
1/T	0.00417	0.00402	0.00394	0.00386	0.00380	0.00373	0.00366	0.00361
ln(k/T)	-6.99	-5.60	-5.35	-5.11	-4.37	-4.51	-4.08	-3.83

Table S5 Rate constants (k_{-1}) obtained by line-shape analysis, 1/T, and ln(k_{-1}/T)

T (K)	240	249	254	259	263	268	273	277
k_{-1} (s^{-1})	0.92	2.85	3.90	5.11	8.41	9.39	13.7	18.3
1/T	0.00417	0.00402	0.00394	0.00386	0.00380	0.00373	0.00366	0.00361
ln(k_{-1}/T)	-5.56	-4.47	-4.18	-3.93	-3.44	-3.35	-2.99	-2.72

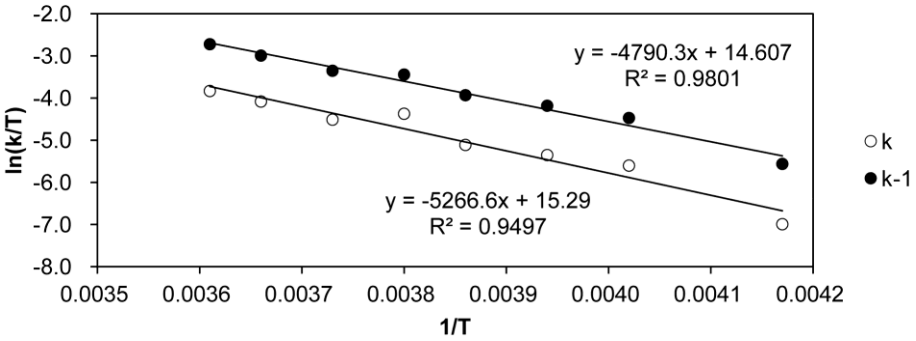


Fig. S4 Eyring plot for **4** (in CD_2Cl_2).

Eyring plots for 4 (in CD_3OD, 9.4 mM)

Table S6 Rate constants (k) obtained by line-shape analysis, 1/T, and ln(k/T)

T (K)	253	258	263	268	273	278
k (s^{-1})	5.24	8.14	11.1	14.0	18.7	24.7
1/T	0.00395	0.00388	0.00380	0.00373	0.00366	0.00360
ln(k/T)	-3.88	-3.46	-3.17	-2.95	-2.68	-2.42

Table S7 Rate constants (k_{-1}) obtained by line-shape analysis, 1/T, and ln(k_{-1}/T)

T (K)	253	258	263	268	273	278
k_{-1} (s^{-1})	9.33	14.3	16.4	21.9	31.9	54.1
1/T	0.00395	0.00388	0.00380	0.00373	0.00366	0.00360
ln(k_{-1}/T)	-3.30	-2.89	-2.78	-2.50	-2.15	-1.64

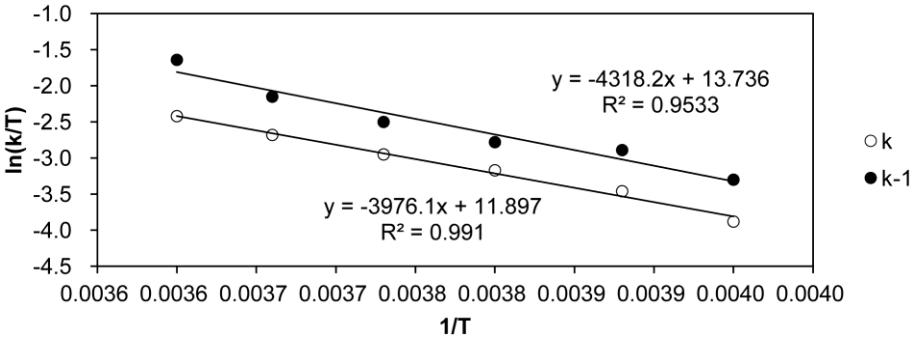


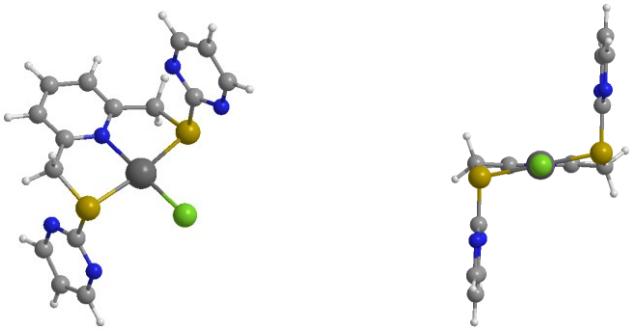
Fig. S5 Eyring plot for **4** (in CD_3OD).

Table S8 Summary of Crystal Data, Collection Data, and Refinement of Complexes **2** and **4**

	2	**4**
formula	$C_{18}H_{15}ClF_3N_3O_3PdS_3$	$C_{35}H_{28}F_6N_5O_6PPdS_4$
fw	616.36	994.23
cryst size, mm	0.05 × 0.05 × 0.05	0.30 × 0.20 × 0.20
cryst syst	triclinic	monoclinic
space group	*P*-1	$P2_1/a$
a, Å	8.755(3)	17.7910(13)
b, Å	10.203(3)	12.9731(6)
c, Å	13.952(4)	18.4171(11)
α, deg	65.946(17)	90
β, deg	74.499(18)	110.727(2)
γ, deg	78.61(2)	90
V, Å^3	1091.2(6)	3975.6(4)
Z	2	4
D (calcd), g cm^{-3}	1.876	1.661
data collection temp, K	153(2)	173(2)
μ (Mo Kα), mm^{-1}	1.313	0.797
$2\theta_{max}$, deg	52.0	55.0
no. of measd reflns	7610	30328
no. of unique reflns	4148	8934
no. of obsd reflns ($I > 2\sigma(I)$)	3333	7329
no. of variables	282	540
$R_1{}^a$ ($I > 2\sigma(I)$)	0.065	0.054
$wR_2{}^a$ ($I > 2\sigma(I)$)	0.157	0.138
$R_1{}^a$ (all data)	0.079	0.066
$wR_2{}^a$ (all data)	0.172	0.149
GOF	1.082	1.107

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2]^{1/2}$.

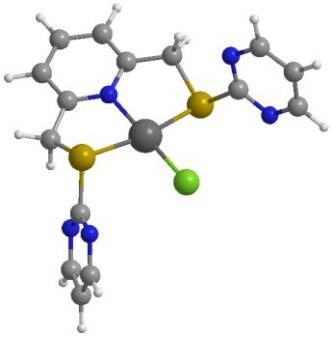
Table S9 Optimized geometries and energies for **1**-*rac*(*ax*,*ax*)-SNS at B3LYP/LANL2DZ+6-31G(d) level

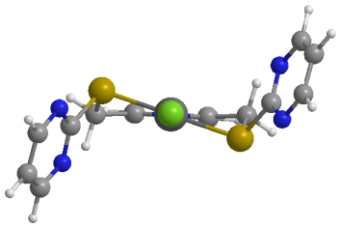


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000003	-0.720736	-0.000010
2	17	0	0.000052	-3.026718	-0.000058
3	16	0	1.796605	-0.549691	1.538108
4	16	0	-1.796624	-0.549710	-1.538117
5	7	0	3.777983	-1.586074	0.149147
6	7	0	-3.777930	-1.586112	-0.149066
7	7	0	-0.000013	1.349993	-0.000010
8	6	0	-3.247065	-0.408726	-0.443358
9	6	0	3.247054	-0.408698	0.443361
10	6	0	0.743473	2.016526	0.913280
11	6	0	4.737133	0.830621	-0.699834
12	1	0	5.086761	1.813668	-1.005212
13	6	0	0.770181	3.409670	0.925155
14	1	0	1.379292	3.931933	1.655107
15	6	0	1.478790	1.217257	1.961069
16	1	0	0.878520	1.161872	2.877681
17	1	0	2.435377	1.682392	2.207602
18	6	0	-0.743514	2.016519	-0.913295
19	6	0	-0.770243	3.409662	-0.925164
20	1	0	-1.379365	3.931918	-1.655112
21	6	0	-0.000036	4.111446	-0.000004
22	1	0	-0.000045	5.197022	-0.000001
23	6	0	5.389417	-0.333805	-1.097458
24	1	0	-0.878552	1.161856	-2.877692
25	1	0	-2.435414	1.682368	-2.207620
26	1	0	6.269422	-0.302853	-1.729869
27	6	0	-1.478824	1.217241	-1.961082
28	6	0	-4.859740	-1.542521	0.639808
29	1	0	-5.306611	-2.499168	0.897900
30	6	0	4.859822	-1.542473	-0.639688
31	1	0	5.306742	-2.499113	-0.897722
32	6	0	-5.389371	-0.333854	1.097542
33	1	0	-6.269355	-0.302911	1.729982
34	6	0	-4.737147	0.830581	0.699845
35	1	0	-5.086804	1.813627	1.005194
36	7	0	-3.641320	0.803166	-0.079476
37	7	0	3.641278	0.803195	0.079448

Zero-point correction =	0.267019 (Hartree/Particle)
Thermal correction to Energy =	0.288923
Thermal correction to Enthalpy =	0.289867
Thermal correction to Gibbs Free Energy =	0.212094
Sum of electronic and zero-point Energies =	-2236.069668
Sum of electronic and thermal Energies =	-2236.047764
Sum of electronic and thermal Enthalpies =	-2236.046820
Sum of electronic and thermal Free Energies =	-2236.124593

Table S10 Optimized geometries and energies for **1**-*rac*(*eq*,*eq*)-SNS at B3LYP/LANL2DZ+6-31G(d) level

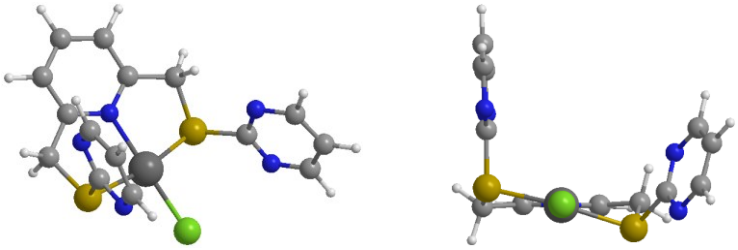




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000022	-0.039882	0.000019
2	17	0	0.000021	-2.354740	0.000066
3	16	0	-2.008185	0.192704	1.250668
4	16	0	2.008141	0.192765	-1.250630
5	7	0	-3.777236	-0.347764	-0.741142
6	7	0	3.776823	-0.347832	0.741483
7	7	0	-0.000069	2.024658	-0.000005
8	6	0	3.247234	-0.822224	-0.374084
9	6	0	-3.247230	-0.822358	0.374141
10	6	0	-1.136426	2.688523	0.317574
11	6	0	-4.330517	-2.790384	0.356883
12	1	0	-4.519719	-3.748890	0.832928
13	6	0	-1.154863	4.082322	0.344682
14	1	0	-2.064892	4.605986	0.616799
15	6	0	-2.379639	1.877942	0.571350
16	1	0	-2.921131	1.692886	-0.365410
17	1	0	-3.049314	2.389344	1.267609
18	6	0	1.136256	2.688569	-0.317605
19	6	0	1.154625	4.082368	-0.344752
20	1	0	2.064628	4.606069	-0.616887
21	6	0	-0.000135	4.782969	-0.000044
22	1	0	-0.000162	5.868469	-0.000059
23	6	0	-4.958127	-2.424018	-0.834410
24	1	0	2.921032	1.693047	0.365385
25	1	0	3.049147	2.389461	-1.267653
26	1	0	-5.656965	-3.084926	-1.334453
27	6	0	2.379510	1.878045	-0.571369
28	6	0	4.652235	-1.165422	1.348903
29	1	0	5.105620	-0.794352	2.264347
30	6	0	-4.652507	-1.165445	-1.348642
31	1	0	-5.106242	-0.794209	-2.263845
32	6	0	4.958422	-2.423703	0.834295
33	1	0	5.657369	-3.084545	1.334271
34	6	0	4.331235	-2.789860	-0.357285
35	1	0	4.520888	-3.748128	-0.833628
36	7	0	3.469178	-1.975490	-0.983546
37	7	0	-3.468603	-1.975931	0.983232

Zero-point correction =	0.267247 (Hartree/Particle)
Thermal correction to Energy =	0.289056
Thermal correction to Enthalpy =	0.290000
Thermal correction to Gibbs Free Energy =	0.213198
Sum of electronic and zero-point Energies =	-2236.071543
Sum of electronic and thermal Energies =	-2236.049733
Sum of electronic and thermal Enthalpies =	-2236.048789
Sum of electronic and thermal Free Energies =	-2236.125592

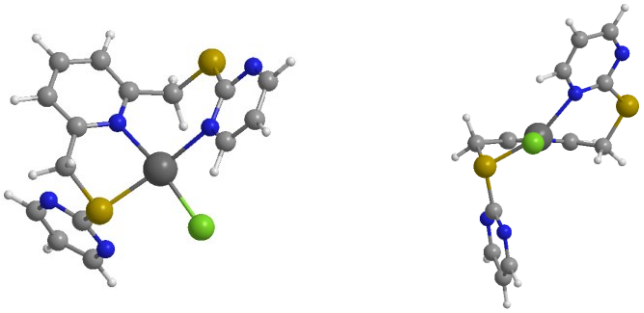
Table S11 Optimized geometries and energies for **1**-*asymm*(*ax*,*eq*)-SNS at B3LYP/LANL2DZ+6-31G(d) level



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.118741	0.088761	-0.964360
2	17	0	1.231669	-1.692677	-1.923734
3	16	0	-2.048820	-0.759161	-1.445566
4	16	0	2.067157	1.353332	-0.471916
5	7	0	-2.138623	-2.901626	0.081966
6	7	0	2.976646	-0.047690	1.672557
7	7	0	-0.876427	1.668063	-0.071539
8	6	0	3.208831	0.228709	0.399498
9	6	0	-2.518588	-1.631874	0.082219
10	6	0	-2.203828	1.822910	-0.276693
11	6	0	-3.551421	-1.682533	2.081852
12	1	0	-4.118057	-1.157746	2.847017
13	6	0	-2.891034	2.883315	0.311859
14	1	0	-3.957891	2.992135	0.149287
15	6	0	-2.894419	0.864156	-1.215036
16	1	0	-2.925361	1.287612	-2.226714
17	1	0	-3.919558	0.670239	-0.893454
18	6	0	-0.179730	2.536857	0.699552
19	6	0	-0.816144	3.631044	1.282468
20	1	0	-0.246632	4.331565	1.883596
21	6	0	-2.187215	3.798944	1.091350
22	1	0	-2.702697	4.639025	1.546257
23	6	0	-3.210790	-3.026049	2.216336
24	1	0	1.400082	1.576302	1.811138
25	1	0	1.838675	3.162296	1.135358
26	1	0	-3.497772	-3.599026	3.090797
27	6	0	1.276165	2.243801	0.949214
28	6	0	3.846799	-0.901818	2.236056
29	1	0	3.682637	-1.137576	3.284378
30	6	0	-2.486648	-3.601317	1.169698
31	1	0	-2.181043	-4.644364	1.189534
32	6	0	4.900913	-1.458774	1.514737
33	1	0	5.594095	-2.155373	1.972462
34	6	0	5.028019	-1.072250	0.179774
35	1	0	5.825909	-1.450911	-0.453549
36	7	0	4.178652	-0.204705	-0.389384
37	7	0	-3.199059	-0.962492	1.002161

Zero-point correction =	0.267108 (Hartree/Particle)
Thermal correction to Energy =	0.288969
Thermal correction to Enthalpy =	0.289913
Thermal correction to Gibbs Free Energy =	0.212616
Sum of electronic and zero-point Energies =	-2236.069972
Sum of electronic and thermal Energies =	-2236.048111
Sum of electronic and thermal Enthalpies =	-2236.047167
Sum of electronic and thermal Free Energies =	-2236.124464

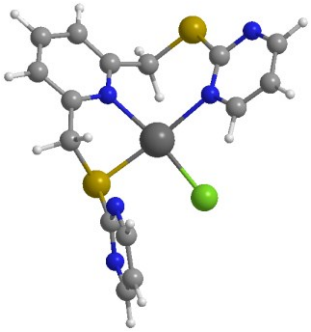
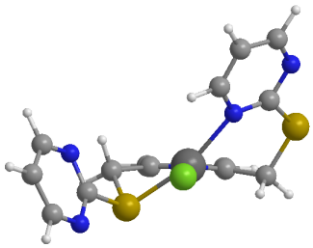
Table S12 Optimized geometries and energies for **1**-*ax*-SNN at B3LYP/LANL2DZ+6-31G(d) level



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.334095	-0.800900	0.143166
2	6	0	-3.078154	-0.753624	-0.003580
3	6	0	-1.621542	0.264229	2.225509
4	6	0	-1.085324	1.455445	1.473697
5	6	0	-0.992417	3.803059	0.981345
6	6	0	-0.212912	3.510358	-0.134407
7	6	0	0.131623	2.183302	-0.398976
8	6	0	0.872773	1.773624	-1.641100
9	6	0	-1.462606	2.759648	1.779086
10	16	0	2.694511	1.891534	-1.530255
11	6	0	3.250372	0.511242	-0.573133
12	16	0	-1.745008	-1.230159	1.144753
13	7	0	-0.249967	1.197995	0.439395
14	7	0	2.495920	-0.476926	-0.040706
15	6	0	3.176035	-1.434904	0.648793
16	6	0	4.550048	-1.411737	0.800459
17	6	0	5.228330	-0.349777	0.201455
18	6	0	-4.779264	0.602606	-0.577869
19	6	0	-5.083370	-0.242206	-1.642266
20	6	0	-4.276015	-1.370704	-1.804710
21	7	0	-3.258989	-1.637032	-0.974248
22	17	0	0.615214	-3.070273	-0.268249
23	1	0	-2.607807	0.472054	2.644586
24	1	0	-0.952679	-0.049260	3.035645
25	1	0	-1.268699	4.829115	1.203502
26	1	0	0.116191	4.294209	-0.808386
27	1	0	0.635425	2.464681	-2.455776
28	1	0	0.575669	0.771733	-1.965974
29	1	0	-2.130533	2.948554	2.612388
30	1	0	2.580324	-2.237914	1.059699
31	1	0	5.060042	-2.190960	1.354170
32	1	0	6.309579	-0.248215	0.259179
33	1	0	-5.356947	1.501745	-0.378847
34	1	0	-5.909506	-0.034312	-2.312835
35	1	0	-4.441004	-2.083184	-2.608890
36	7	0	4.580090	0.594178	-0.471553
37	7	0	-3.757711	0.352132	0.261161

Zero-point correction =	0.267666 (Hartree/Particle)
Thermal correction to Energy =	0.289255
Thermal correction to Enthalpy =	0.290199
Thermal correction to Gibbs Free Energy =	0.214422
Sum of electronic and zero-point Energies =	-2236.064862
Sum of electronic and thermal Energies =	-2236.043273
Sum of electronic and thermal Enthalpies =	-2236.042329
Sum of electronic and thermal Free Energies =	-2236.118106

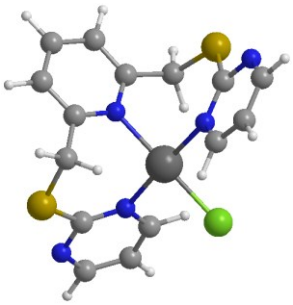
Table S13 Optimized geometries and energies for **1**-*eq*-SNN at B3LYP/LANL2DZ+6-31G(d) level

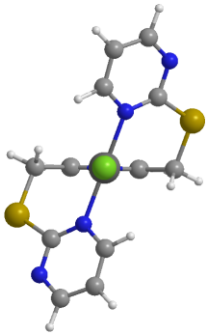



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.003443	-0.164477	-0.505155
2	6	0	-3.289115	0.375960	0.002924
3	6	0	-1.271117	2.143587	0.963421
4	6	0	0.172893	2.518115	0.764733
5	6	0	2.039250	4.022142	0.891957
6	6	0	2.766045	3.146534	0.090819
7	6	0	2.171316	1.957619	-0.339752
8	6	0	2.840533	1.020232	-1.305031
9	6	0	0.711956	3.722541	1.205676
10	16	0	3.942316	-0.221373	-0.537002
11	6	0	2.914202	-1.472261	0.176535
12	16	0	-1.846165	1.313534	-0.598825
13	7	0	0.923724	1.638544	0.057555
14	7	0	1.563179	-1.538346	0.160844
15	6	0	1.015563	-2.618352	0.783592
16	6	0	1.779620	-3.595412	1.394036
17	6	0	3.164245	-3.431107	1.341055
18	6	0	-5.226337	-0.600393	-0.580879
19	6	0	-5.403420	-1.013172	0.740135
20	6	0	-4.418953	-0.644855	1.655864
21	7	0	-3.334952	0.056840	1.286599
22	17	0	-1.246546	-1.943956	-1.348057
23	1	0	-1.893606	3.023510	1.143791
24	1	0	-1.428088	1.425408	1.774461
25	1	0	2.484718	4.951629	1.232455
26	1	0	3.777588	3.383385	-0.221559
27	1	0	3.521742	1.581639	-1.951788
28	1	0	2.105900	0.529755	-1.951068
29	1	0	0.099026	4.418146	1.768546
30	1	0	-0.062982	-2.684227	0.756807
31	1	0	1.312011	-4.444088	1.878711
32	1	0	3.849088	-4.149751	1.785275
33	1	0	-5.949513	-0.835526	-1.357308
34	1	0	-6.270694	-1.588880	1.043089
35	1	0	-4.486579	-0.912441	2.707205
36	7	0	3.714265	-2.381513	0.741792
37	7	0	-4.158710	0.117756	-0.959905

Zero-point correction =	0.267699 (Hartree/Particle)
Thermal correction to Energy =	0.289277
Thermal correction to Enthalpy =	0.290222
Thermal correction to Gibbs Free Energy =	0.214904
Sum of electronic and zero-point Energies =	-2236.066232
Sum of electronic and thermal Energies =	-2236.044653
Sum of electronic and thermal Enthalpies =	-2236.043709
Sum of electronic and thermal Free Energies =	-2236.119027

Table S14 Optimized geometries and energies for **1**-NNN at B3LYP/LANL2DZ+6-31G(d) level

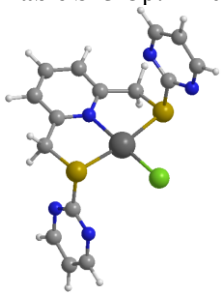


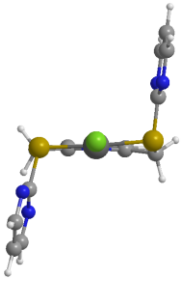


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.000038	-0.679407	-0.000156
2	6	0	3.076478	-0.173983	-0.301929
3	6	0	1.219982	1.247300	-2.092868
4	6	0	0.577047	2.083504	-1.024030
5	6	0	-0.000340	4.181697	0.000021
6	6	0	-0.590228	3.478252	1.048302
7	6	0	-0.577225	2.083346	1.024039
8	6	0	-1.219751	1.246992	2.093000
9	6	0	0.589747	3.478412	-1.048255
10	16	0	-2.982360	0.840169	1.754636
11	6	0	-3.076420	-0.174476	0.302449
12	16	0	2.982591	0.840874	-1.753994
13	7	0	-0.000048	1.419712	-0.000027
14	7	0	-2.058121	-0.727143	-0.396794
15	6	0	-2.395295	-1.477694	-1.480053
16	6	0	-3.708812	-1.675655	-1.859170
17	6	0	-4.685884	-1.082476	-1.055705
18	6	0	4.685831	-1.082690	1.055890
19	6	0	3.708691	-1.676268	1.858972
20	6	0	2.395211	-1.478230	1.479770
21	7	0	2.058130	-0.727168	0.396826
22	17	0	0.000055	-3.012837	-0.000514
23	1	0	1.292891	1.809421	-3.028898
24	1	0	0.648715	0.336675	-2.292900
25	1	0	-0.000449	5.267248	0.000042
26	1	0	-1.061437	3.997656	1.875875
27	1	0	-1.292548	1.809089	3.029055
28	1	0	-0.648236	0.336489	2.292880
29	1	0	1.060909	3.997940	-1.875777
30	1	0	-1.574370	-1.934698	-2.016460
31	1	0	-3.954586	-2.278215	-2.725300
32	1	0	-5.747417	-1.201316	-1.259641
33	1	0	5.747345	-1.201521	1.259937
34	1	0	3.954390	-2.279239	2.724838
35	1	0	1.574253	-1.935586	2.015819
36	7	0	-4.366249	-0.341260	-0.000817
37	7	0	4.366285	-0.340975	0.001326

Zero-point correction =	0.268573 (Hartree/Particle)
Thermal correction to Energy =	0.289677
Thermal correction to Enthalpy =	0.290621
Thermal correction to Gibbs Free Energy =	0.217570
Sum of electronic and zero-point Energies =	-2236.076861
Sum of electronic and thermal Energies =	-2236.055757
Sum of electronic and thermal Enthalpies =	-2236.054813
Sum of electronic and thermal Free Energies =	-2236.127864

Table S15 Optimized geometries and energies for **1**-TS_{ri1} at B3LYP/LANL2DZ+6-31G(d) level

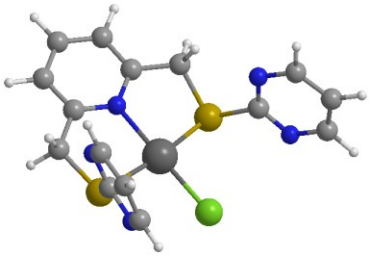


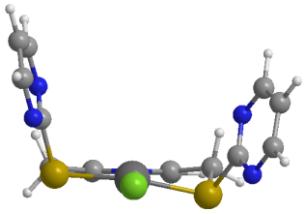


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.071937	-0.515472	0.093721
2	17	0	-0.340504	-2.807963	0.065928
3	16	0	1.798280	-0.612512	1.546769
4	16	0	-1.803979	-0.137520	-1.470915
5	7	0	3.510245	-2.014266	0.119600
6	7	0	-3.812188	-1.551331	-0.530397
7	7	0	0.180960	1.540082	0.113877
8	6	0	-3.334768	-0.317679	-0.487066
9	6	0	3.180302	-0.755596	0.366284
10	6	0	1.141908	2.079967	0.903632
11	6	0	4.751958	0.177476	-0.945997
12	1	0	5.220621	1.077356	-1.336379
13	6	0	1.439248	3.438229	0.835087
14	1	0	2.217626	3.852982	1.466338
15	6	0	1.818179	1.192840	1.919184
16	1	0	1.293889	1.267079	2.880215
17	1	0	2.856148	1.493730	2.073415
18	6	0	-0.533087	2.314742	-0.734772
19	6	0	-0.276133	3.682831	-0.833206
20	1	0	-0.855214	4.291367	-1.519959
21	6	0	0.723874	4.246922	-0.046465
22	1	0	0.941929	5.308077	-0.115963
23	6	0	5.194161	-1.092966	-1.306670
24	1	0	-1.484481	1.932969	-2.627533
25	1	0	-2.599930	2.105542	-1.253266
26	1	0	6.020727	-1.231354	-1.994369
27	6	0	-1.632546	1.700029	-1.568366
28	6	0	-4.930012	-1.754037	0.180432
29	1	0	-5.333811	-2.763009	0.164988
30	6	0	4.526944	-2.179528	-0.737008
31	1	0	4.808512	-3.205820	-0.958138
32	6	0	-5.547975	-0.723484	0.891674
33	1	0	-6.455649	-0.890676	1.460343
34	6	0	-4.948982	0.532419	0.829808
35	1	0	-5.369824	1.393394	1.342796
36	7	0	-3.817421	0.745599	0.135921
37	7	0	3.722671	0.360338	-0.100054

Zero-point correction = 0.266866 (Hartree/Particle)
Thermal correction to Energy = 0.287919
Thermal correction to Enthalpy = 0.288863
Thermal correction to Gibbs Free Energy = 0.213986
Sum of electronic and zero-point Energies = -2236.068917
Sum of electronic and thermal Energies = -2236.047864
Sum of electronic and thermal Enthalpies = -2236.046920
Sum of electronic and thermal Free Energies = -2236.121797
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -25.2539

Table S16 Optimized geometries and energies for **1**-TS_{ri2} at B3LYP/LANL2DZ+6-31G(d) level

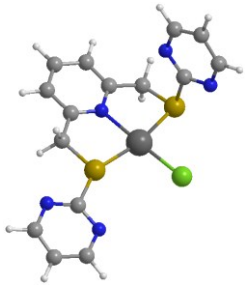
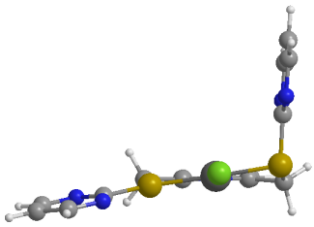




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.029447	0.149364	-0.829857
2	17	0	-0.631673	-1.870210	-1.779988
3	16	0	-2.255967	0.954794	-0.691763
4	16	0	2.292749	-0.181142	-1.167777
5	7	0	-3.969544	-1.032821	-0.552955
6	7	0	3.228093	-0.968458	1.267464
7	7	0	0.496375	1.944243	0.056218
8	6	0	2.812283	-1.402988	0.088637
9	6	0	-3.210578	-0.291974	0.238441
10	6	0	-0.486896	2.754841	0.525186
11	6	0	-3.780702	-1.306983	2.163642
12	1	0	-3.683677	-1.367788	3.244580
13	6	0	-0.197184	4.046324	0.956557
14	1	0	-0.994783	4.688880	1.313195
15	6	0	-1.876800	2.187526	0.636907
16	1	0	-2.631379	2.977051	0.598147
17	1	0	-1.991385	1.635908	1.578850
18	6	0	1.784729	2.353829	0.043037
19	6	0	2.125093	3.636512	0.477294
20	1	0	3.162301	3.954184	0.456240
21	6	0	1.124297	4.491673	0.928189
22	1	0	1.370166	5.496048	1.258474
23	6	0	-4.601909	-2.177630	1.449797
24	1	0	3.475762	1.108220	0.453843
25	1	0	3.516215	1.882382	-1.147990
26	1	0	-5.171278	-2.954495	1.947390
27	6	0	2.867082	1.403262	-0.408908
28	6	0	3.610715	-1.928563	2.126785
29	1	0	3.965186	-1.593468	3.098210
30	6	0	-4.664470	-1.997377	0.067393
31	1	0	-5.286400	-2.625232	-0.565237
32	6	0	3.554186	-3.279129	1.791823
33	1	0	3.858666	-4.049508	2.491160
34	6	0	3.097211	-3.593151	0.510240
35	1	0	3.029877	-4.620349	0.161190
36	7	0	2.729224	-2.645218	-0.362125
37	7	0	-3.063740	-0.349817	1.552500

Zero-point correction = 0.266964 (Hartree/Particle)
Thermal correction to Energy = 0.287998
Thermal correction to Enthalpy = 0.288942
Thermal correction to Gibbs Free Energy = 0.214271
Sum of electronic and zero-point Energies = -2236.068528
Sum of electronic and thermal Energies = -2236.047494
Sum of electronic and thermal Enthalpies = -2236.046550
Sum of electronic and thermal Free Energies = -2236.121221
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -23.8553

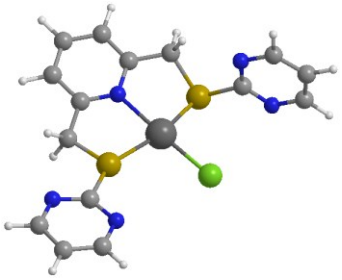
Table S17 Optimized geometries and energies for **1**-TS_{Si1} at B3LYP/LANL2DZ+6-31G(d) level

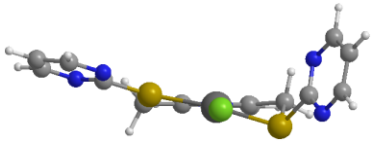



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.136680	-0.490625	-0.689524
2	17	0	0.178105	-2.744749	-1.032814
3	16	0	-2.373621	-0.662009	-1.307864
4	16	0	2.025033	0.152329	0.095594
5	7	0	-3.351273	-2.174664	0.615475
6	7	0	4.479323	0.776556	0.903310
7	7	0	-0.490212	1.565555	-0.395079
8	6	0	3.769177	-0.203644	0.368874
9	6	0	-3.223071	-0.897547	0.291662
10	6	0	-1.692134	2.049351	-0.802023
11	6	0	-4.293913	-0.070805	2.088255
12	1	0	-4.659079	0.795380	2.634192
13	6	0	-2.047089	3.375506	-0.575618
14	1	0	-3.016494	3.737281	-0.900661
15	6	0	-2.605563	1.143834	-1.589232
16	1	0	-2.414313	1.263709	-2.663036
17	1	0	-3.654179	1.381055	-1.399466
18	6	0	0.402265	2.379830	0.218927
19	6	0	0.095078	3.722440	0.451793
20	1	0	0.824753	4.359482	0.940566
21	6	0	-1.141206	4.222922	0.059156
22	1	0	-1.395736	5.262445	0.240650
23	6	0	-4.486603	-1.367520	2.558996
24	1	0	1.803611	1.876914	1.772472
25	1	0	2.553293	2.491633	0.300885
26	1	0	-5.005330	-1.560318	3.491258
27	6	0	1.747263	1.856924	0.678922
28	6	0	5.778698	0.486745	1.095500
29	1	0	6.386952	1.274464	1.532785
30	6	0	-3.986288	-2.407402	1.772176
31	1	0	-4.096771	-3.449624	2.060117
32	6	0	6.315274	-0.752060	0.754976
33	1	0	7.363085	-0.979398	0.914098
34	6	0	5.439801	-1.687973	0.199208
35	1	0	5.773925	-2.679336	-0.096025
36	7	0	4.142835	-1.417478	-0.001077
37	7	0	-3.645955	0.179614	0.936652

Zero-point correction = 0.266203 (Hartree/Particle)
Thermal correction to Energy = 0.287742
Thermal correction to Enthalpy = 0.288686
Thermal correction to Gibbs Free Energy = 0.211119
Sum of electronic and zero-point Energies = -2236.045339
Sum of electronic and thermal Energies = -2236.023800
Sum of electronic and thermal Enthalpies = -2236.022855
Sum of electronic and thermal Free Energies = -2236.100423
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -176.7425

Table S18 Optimized geometries and energies for **1**-TS_{Si2} at B3LYP/LANL2DZ+6-31G(d) level

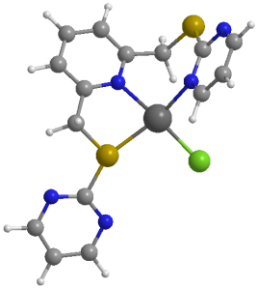
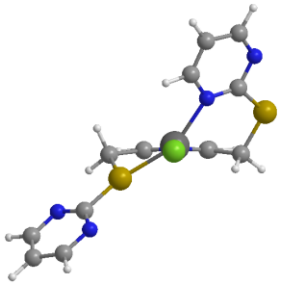




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.252964	-0.103110	-0.451603
2	17	0	0.621031	-2.336227	-0.890456
3	16	0	2.462073	0.478696	-0.929686
4	16	0	-2.123621	-0.081331	-0.118224
5	7	0	3.596170	-0.490964	1.340161
6	7	0	-4.749919	-0.136749	0.304621
7	7	0	-0.011402	1.939294	-0.024620
8	6	0	-3.690282	-0.918875	0.177137
9	6	0	3.525190	-0.658119	0.030496
10	6	0	1.116423	2.680847	0.137070
11	6	0	4.872919	-2.450572	-0.079680
12	1	0	5.362390	-3.206912	-0.687402
13	6	0	1.048360	4.057474	0.327935
14	1	0	1.960559	4.633524	0.438350
15	6	0	2.436701	1.960160	0.181306
16	1	0	2.635462	1.568353	1.186723
17	1	0	3.259237	2.618675	-0.109464
18	6	0	-1.231330	2.523675	0.033964
19	6	0	-1.347726	3.899403	0.250848
20	1	0	-2.333443	4.349881	0.300429
21	6	0	-0.201259	4.673283	0.389083
22	1	0	-0.277711	5.744675	0.545617
23	6	0	5.027873	-2.404969	1.306216
24	1	0	-2.955361	1.955524	-1.117572
25	1	0	-3.219005	1.928996	0.625557
26	1	0	5.639833	-3.128636	1.832623
27	6	0	-2.490013	1.705586	-0.157662
28	6	0	-5.906167	-0.788720	0.520758
29	1	0	-6.793430	-0.170098	0.629322
30	6	0	4.367671	-1.381279	1.984522
31	1	0	4.446716	-1.262977	3.061967
32	6	0	-5.965158	-2.177559	0.599562
33	1	0	-6.901049	-2.696868	0.770757
34	6	0	-4.761461	-2.869555	0.447185
35	1	0	-4.715369	-3.954533	0.496200
36	7	0	-3.599522	-2.237859	0.232676
37	7	0	4.117761	-1.557031	-0.736765

Zero-point correction = 0.266282 (Hartree/Particle)
Thermal correction to Energy = 0.287781
Thermal correction to Enthalpy = 0.288725
Thermal correction to Gibbs Free Energy = 0.211839
Sum of electronic and zero-point Energies = -2236.046133
Sum of electronic and thermal Energies = -2236.024634
Sum of electronic and thermal Enthalpies = -2236.023690
Sum of electronic and thermal Free Energies = -2236.100576
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -174.2029

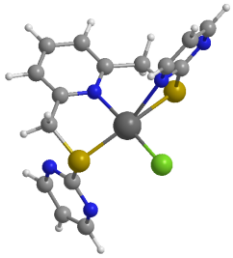
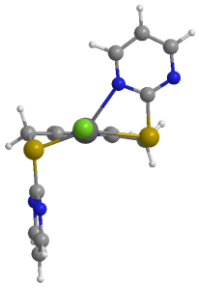
Table S19 Optimized geometries and energies for **1**-TS_{Si3} at B3LYP/LANL2DZ+6-31G(d) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.307151	-0.584346	-0.248290
2	6	0	-3.776173	-0.282389	0.045178
3	6	0	-1.660342	1.312334	1.369451
4	6	0	-0.524676	2.139573	0.814597
5	6	0	0.568887	4.247806	0.434621
6	6	0	1.432189	3.610127	-0.451579
7	6	0	1.305559	2.235733	-0.658658
8	6	0	2.119524	1.504340	-1.691140
9	6	0	-0.440624	3.509920	1.051777
10	16	0	3.763421	0.925926	-1.131551
11	6	0	3.498355	-0.420500	-0.020503
12	16	0	-1.990758	-0.044277	0.182802
13	7	0	0.383978	1.519958	0.021358
14	7	0	2.319804	-0.992449	0.317122
15	6	0	2.374952	-2.014291	1.217086
16	6	0	3.566307	-2.460278	1.755652
17	6	0	4.728321	-1.821206	1.317955
18	6	0	-5.449563	-1.430589	-0.903777
19	6	0	-6.369413	-0.664133	-0.185006
20	6	0	-5.850445	0.315783	0.657644
21	7	0	-4.526433	0.517139	0.782218
22	17	0	0.034137	-2.823020	-0.756599
23	1	0	-2.574121	1.900914	1.480162
24	1	0	-1.410810	0.874912	2.342176
25	1	0	0.651598	5.315984	0.609467
26	1	0	2.186405	4.167292	-0.997094
27	1	0	2.377710	2.188784	-2.505278
28	1	0	1.553025	0.678143	-2.131869
29	1	0	-1.170122	3.989645	1.695408
30	1	0	1.432315	-2.475570	1.475126
31	1	0	3.582195	-3.275477	2.469010
32	1	0	5.714927	-2.115984	1.667791
33	1	0	-5.766845	-2.214852	-1.586253
34	1	0	-7.437392	-0.823889	-0.278418
35	1	0	-6.492686	0.959982	1.252627
36	7	0	4.684326	-0.816546	0.451487
37	7	0	-4.126708	-1.242155	-0.793486

Zero-point correction = 0.266793 (Hartree/Particle)
Thermal correction to Energy = 0.287962
Thermal correction to Enthalpy = 0.288906
Thermal correction to Gibbs Free Energy = 0.214138
Sum of electronic and zero-point Energies = -2236.037920
Sum of electronic and thermal Energies = -2236.016751
Sum of electronic and thermal Enthalpies = -2236.015806
Sum of electronic and thermal Free Energies = -2236.090575
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -181.7958

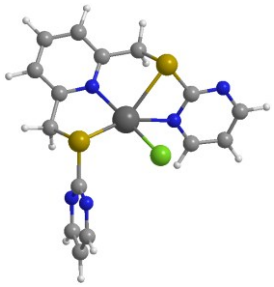
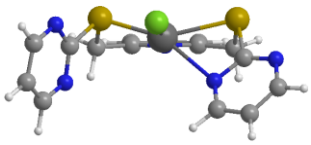
Table S20 Optimized geometries and energies for **1**-$TS_{SNS\text{-}SNN1}$ at B3LYP/LANL2DZ+6-31G(d) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.252338	-0.718683	-0.223084
2	17	0	-0.564484	-3.003759	-0.225077
3	16	0	-1.709347	0.012725	1.986246
4	16	0	1.766977	-0.908359	-1.388393
5	7	0	-2.662014	-0.497712	-0.420907
6	7	0	3.414021	-1.782861	0.468197
7	7	0	0.116628	1.350106	-0.246789
8	6	0	3.090343	-0.662363	-0.162262
9	6	0	-3.058962	-0.091468	0.793411
10	6	0	-0.462410	2.234041	0.599702
11	6	0	-5.250939	-0.020407	0.250561
12	1	0	-6.270584	0.196889	0.558579
13	6	0	-0.268385	3.608191	0.433053
14	1	0	-0.757297	4.300586	1.110919
15	6	0	-1.263303	1.785076	1.810339
16	1	0	-0.668142	1.995712	2.707371
17	1	0	-2.178541	2.378185	1.901656
18	6	0	0.962034	1.791559	-1.214476
19	6	0	1.207860	3.148984	-1.399000
20	1	0	1.892042	3.471431	-2.176386
21	6	0	0.566201	4.072346	-0.577580
22	1	0	0.730125	5.137127	-0.711192
23	6	0	-4.959932	-0.483859	-1.032058
24	1	0	1.014477	0.613077	-3.021288
25	1	0	2.609289	1.111176	-2.421676
26	1	0	-5.740683	-0.660295	-1.763241
27	6	0	1.615641	0.775004	-2.118238
28	6	0	4.410422	-1.671348	1.355671
29	1	0	4.687643	-2.578989	1.885776
30	6	0	-3.618450	-0.706495	-1.336766
31	1	0	-3.291521	-1.058981	-2.310278
32	6	0	5.063386	-0.457242	1.582206
33	1	0	5.874340	-0.373393	2.296803
34	6	0	4.626641	0.639475	0.843879
35	1	0	5.083226	1.619985	0.954127
36	7	0	3.619772	0.547278	-0.043269
37	7	0	-4.297487	0.173474	1.177157

Zero-point correction = 0.266533 (Hartree/Particle)
Thermal correction to Energy = 0.287776
Thermal correction to Enthalpy = 0.288720
Thermal correction to Gibbs Free Energy = 0.213245
Sum of electronic and zero-point Energies = -2236.050804
Sum of electronic and thermal Energies = -2236.029561
Sum of electronic and thermal Enthalpies = -2236.028617
Sum of electronic and thermal Free Energies = -2236.104093
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -118.7350

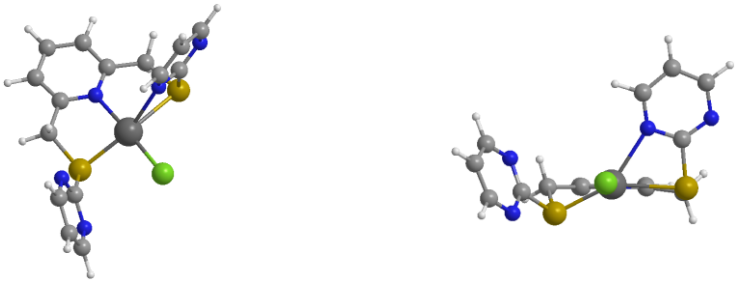
Table S21 Optimized geometries and energies for **1**-$TS_{SNS\text{-}SNN2}$ at B3LYP/LANL2DZ+6-31G(d) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.112229	-0.035877	0.374152
2	6	0	-3.250678	-0.199215	0.054895
3	6	0	-1.837166	2.211996	-0.403452
4	6	0	-0.444550	2.777356	-0.405885
5	6	0	1.089635	4.613630	-0.621493
6	6	0	2.139289	3.710190	-0.480057
7	6	0	1.864505	2.352538	-0.306339
8	6	0	2.994410	1.356960	-0.244540
9	6	0	-0.219870	4.141054	-0.585475
10	16	0	2.795162	0.003435	1.017049
11	6	0	2.824077	-1.415857	-0.100658
12	16	0	-1.996599	0.862086	0.852614
13	7	0	0.586173	1.906421	-0.262608
14	7	0	1.769306	-1.476392	-0.927158
15	6	0	1.718144	-2.528048	-1.754477
16	6	0	2.704568	-3.513924	-1.732512
17	6	0	3.738520	-3.351961	-0.813675
18	6	0	-4.294045	-0.974941	-1.781060
19	6	0	-5.070540	-1.806960	-0.975776
20	6	0	-4.850689	-1.739957	0.400521
21	7	0	-3.935514	-0.915784	0.931693
22	17	0	-0.514518	-2.089831	1.244060
23	1	0	-2.082174	1.748244	-1.366374
24	1	0	-2.581003	2.981043	-0.181075
25	1	0	1.288981	5.672877	-0.749901
26	1	0	3.169828	4.047976	-0.500331
27	1	0	3.934192	1.871783	-0.034018
28	1	0	3.092004	0.866069	-1.217699
29	1	0	-1.061421	4.817467	-0.687253
30	1	0	0.860815	-2.582121	-2.418853
31	1	0	2.656461	-4.375031	-2.389272
32	1	0	4.537727	-4.082815	-0.720177
33	1	0	-4.410232	-0.953142	-2.861648
34	1	0	-5.815951	-2.470060	-1.400096
35	1	0	-5.417805	-2.346051	1.102145
36	7	0	3.811671	-2.286814	0.004446
37	7	0	-3.360652	-0.160300	-1.263950

Zero-point correction = 0.266635 (Hartree/Particle)
Thermal correction to Energy = 0.287929
Thermal correction to Enthalpy = 0.288874
Thermal correction to Gibbs Free Energy = 0.213118
Sum of electronic and zero-point Energies = -2236.050085
Sum of electronic and thermal Energies = -2236.028790
Sum of electronic and thermal Enthalpies = -2236.027846
Sum of electronic and thermal Free Energies = -2236.103602
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -133.3557

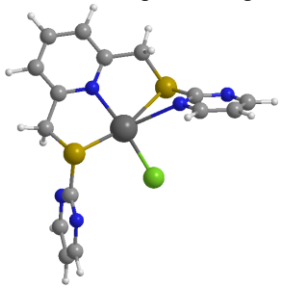
Table S22 Optimized geometries and energies for **1**-$TS_{SNS\text{-}SNN3}$ at B3LYP/LANL2DZ+6-31G(d) level

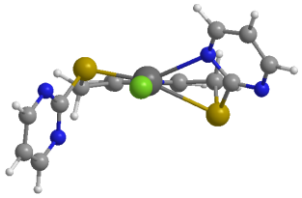


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.002172	-0.173550	0.562751
2	7	0	-1.004334	1.555462	-0.085775
3	16	0	1.854936	1.271941	0.632163
4	7	0	4.144749	0.009610	0.861230
5	16	0	-2.515619	-0.731027	1.510234
6	6	0	-2.328036	1.779293	0.079767
7	6	0	-0.231933	2.472249	-0.728673
8	6	0	3.275632	0.371167	-0.069347
9	6	0	4.380798	-0.520870	-1.812613
10	6	0	-2.602992	-1.671858	-0.026386
11	6	0	-3.193174	0.877142	0.942041
12	6	0	-2.929770	2.912305	-0.477817
13	6	0	-0.781526	3.632623	-1.265373
14	6	0	1.241030	2.185239	-0.857537
15	17	0	1.184454	-2.022148	1.274756
16	7	0	3.312224	0.165492	-1.376568
17	6	0	5.360760	-0.989316	-0.939265
18	7	0	-1.447428	-1.685105	-0.706112
19	7	0	-3.722644	-2.300505	-0.349631
20	6	0	-2.155014	3.844093	-1.158509
21	6	0	5.195516	-0.693118	0.414254
22	6	0	-1.396560	-2.453015	-1.803853
23	6	0	-3.671621	-3.053002	-1.461045
24	6	0	-2.509636	-3.179612	-2.221722
25	1	0	4.439977	-0.694111	-2.884139
26	1	0	-3.418155	1.410747	1.873879
27	1	0	-4.153807	0.691295	0.451697
28	1	0	-3.996813	3.064554	-0.351088
29	1	0	-0.141489	4.353403	-1.762491
30	1	0	1.463495	1.541015	-1.715624
31	1	0	1.812420	3.111491	-0.961132
32	1	0	6.215304	-1.552432	-1.296965
33	1	0	-2.610009	4.733336	-1.583465
34	1	0	5.915929	-1.011740	1.163066
35	1	0	-0.450825	-2.477024	-2.336664
36	1	0	-4.588644	-3.569194	-1.733926
37	1	0	-2.473442	-3.809994	-3.103032

Zero-point correction = 0.266513 (Hartree/Particle)
Thermal correction to Energy = 0.287774
Thermal correction to Enthalpy = 0.288718
Thermal correction to Gibbs Free Energy = 0.213429
Sum of electronic and zero-point Energies = -2236.051028
Sum of electronic and thermal Energies = -2236.029767
Sum of electronic and thermal Enthalpies = -2236.028823
Sum of electronic and thermal Free Energies = -2236.104112
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -120.9510

Table S23 Optimized geometries and energies for **1**-$TS_{SNS\text{-}SNN4}$ at B3LYP/LANL2DZ+6-31G(d) level

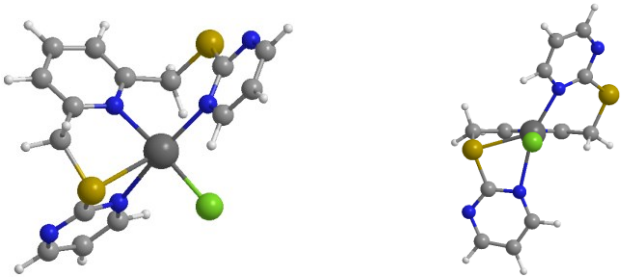




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.179247	-0.000341	0.048120
2	17	0	-0.031556	-2.304339	0.273805
3	16	0	1.879136	0.065747	-1.042174
4	16	0	-2.270366	0.885524	1.907773
5	7	0	3.549514	-0.464250	1.033305
6	7	0	-2.624554	-0.651150	-0.216973
7	7	0	-0.049658	2.105415	0.009270
8	6	0	-3.155771	-0.383618	0.983697
9	6	0	3.073529	-0.949870	-0.100705
10	6	0	1.150254	2.657800	-0.294279
11	6	0	4.171483	-2.907539	-0.026138
12	1	0	4.392706	-3.865252	-0.489730
13	6	0	1.316468	4.042357	-0.354436
14	1	0	2.282491	4.456558	-0.622336
15	6	0	2.340453	1.756207	-0.469281
16	1	0	2.845928	1.604319	0.493108
17	1	0	3.057592	2.174306	-1.181089
18	6	0	-1.098410	2.903886	0.328359
19	6	0	-0.970275	4.292123	0.322701
20	1	0	-1.820592	4.907198	0.596441
21	6	0	0.243724	4.870134	-0.040952
22	1	0	0.354772	5.949588	-0.066798
23	6	0	4.737430	-2.531805	1.192553
24	1	0	-3.115397	3.001294	1.040358
25	1	0	-2.838976	1.811287	-0.246439
26	1	0	5.415720	-3.185873	1.728671
27	6	0	-2.413883	2.257480	0.657359
28	6	0	-3.230525	-1.597043	-0.946353
29	1	0	-2.790722	-1.822226	-1.913152
30	6	0	4.399916	-1.272443	1.686132
31	1	0	4.807988	-0.893648	2.619470
32	6	0	-4.345364	-2.278154	-0.458843
33	1	0	-4.831548	-3.052852	-1.040579
34	6	0	-4.781538	-1.939839	0.819891
35	1	0	-5.625128	-2.443385	1.285227
36	7	0	-4.194979	-0.973119	1.548373
37	7	0	3.331334	-2.103254	-0.694810

Zero-point correction = 0.266893 (Hartree/Particle)
Thermal correction to Energy = 0.288069
Thermal correction to Enthalpy = 0.289014
Thermal correction to Gibbs Free Energy = 0.214155
Sum of electronic and zero-point Energies = -2236.048072
Sum of electronic and thermal Energies = -2236.026896
Sum of electronic and thermal Enthalpies = -2236.025951
Sum of electronic and thermal Free Energies = -2236.100810
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -133.7389

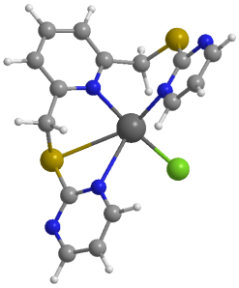
Table S24 Optimized geometries and energies for **1**-$TS_{SNN\text{-}NNN1}$ at B3LYP/LANL2DZ+6-31G(d) level

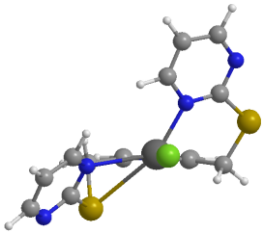


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.137299	-0.725763	-0.026773
2	6	0	-2.932002	-0.700767	0.242357
3	6	0	-1.587733	0.653019	2.357376
4	6	0	-1.023152	1.685853	1.409464
5	6	0	-0.809687	3.993188	0.745523
6	6	0	-0.031593	3.579714	-0.330449
7	6	0	0.231487	2.219729	-0.503019
8	6	0	1.011959	1.720692	-1.688664
9	6	0	-1.328297	3.032535	1.610810
10	16	0	2.826857	1.670641	-1.435121
11	6	0	3.180197	0.282691	-0.393296
12	16	0	-1.865780	-1.030956	1.661957
13	7	0	-0.229700	1.303010	0.378633
14	7	0	2.296430	-0.606824	0.106697
15	6	0	2.812251	-1.602671	0.876473
16	6	0	4.165169	-1.705568	1.142858
17	6	0	4.991253	-0.736138	0.571070
18	6	0	-4.971621	-0.466393	-0.700742
19	6	0	-4.395081	-0.479740	-1.970387
20	6	0	-3.005957	-0.575547	-2.034671
21	7	0	-2.264211	-0.673910	-0.921700
22	17	0	0.312027	-2.962936	-0.590558
23	1	0	-2.521087	1.015621	2.795528
24	1	0	-0.889875	0.467470	3.183645
25	1	0	-1.030893	5.045341	0.895434
26	1	0	0.362355	4.295189	-1.044415
27	1	0	0.909501	2.424807	-2.520046
28	1	0	0.651021	0.748051	-2.034595
29	1	0	-1.969263	3.317555	2.438375
30	1	0	2.104180	-2.326263	1.256281
31	1	0	4.550924	-2.509010	1.758940
32	1	0	6.068998	-0.739093	0.716407
33	1	0	-6.045493	-0.367267	-0.564011
34	1	0	-4.997774	-0.411342	-2.869016
35	1	0	-2.468713	-0.576822	-2.978725
36	7	0	4.498789	0.241132	-0.182454
37	7	0	-4.239091	-0.587375	0.418778

Zero-point correction = 0.267052 (Hartree/Particle)
Thermal correction to Energy = 0.288023
Thermal correction to Enthalpy = 0.288967
Thermal correction to Gibbs Free Energy = 0.215326
Sum of electronic and zero-point Energies = -2236.048797
Sum of electronic and thermal Energies = -2236.027826
Sum of electronic and thermal Enthalpies = -2236.026881
Sum of electronic and thermal Free Energies = -2236.100522
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -130.9426

Table S25 Optimized geometries and energies for **1**-$TS_{SNN\text{-}NNN2}$ at B3LYP/LANL2DZ+6-31G(d) level

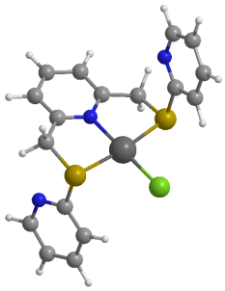


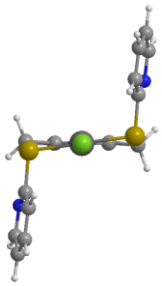


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.070637	-0.323083	-0.442380
2	6	0	-3.371316	0.481813	-0.000597
3	6	0	-1.402770	2.036219	1.265246
4	6	0	0.004472	2.420240	0.915138
5	6	0	1.833045	3.983229	0.838823
6	6	0	2.462534	3.156456	-0.084957
7	6	0	1.846720	1.960381	-0.465011
8	6	0	2.433169	1.075344	-1.532101
9	6	0	0.574599	3.623176	1.323365
10	16	0	3.717812	-0.096065	-0.954341
11	6	0	2.921156	-1.221469	0.143214
12	16	0	-2.376584	1.942430	-0.321179
13	7	0	0.668321	1.587685	0.077294
14	7	0	1.598851	-1.298756	0.412547
15	6	0	1.205901	-2.230473	1.322407
16	6	0	2.104176	-3.073586	1.945403
17	6	0	3.445014	-2.940845	1.570499
18	6	0	-5.388259	-0.539323	-0.019444
19	6	0	-4.793613	-1.740554	0.359915
20	6	0	-3.409017	-1.733104	0.519619
21	7	0	-2.687672	-0.619546	0.329986
22	17	0	-0.656509	-2.372904	-1.352593
23	1	0	-1.449411	1.051118	1.737340
24	1	0	-1.860918	2.774783	1.925982
25	1	0	2.294646	4.915946	1.147509
26	1	0	3.415123	3.430795	-0.525704
27	1	0	2.985050	1.686899	-2.253126
28	1	0	1.655073	0.543567	-2.088470
29	1	0	0.025008	4.275913	1.992951
30	1	0	0.144816	-2.282323	1.524540
31	1	0	1.771897	-3.807546	2.669640
32	1	0	4.221854	-3.581224	1.981767
33	1	0	-6.459109	-0.462351	-0.191056
34	1	0	-5.373428	-2.645623	0.500351
35	1	0	-2.854463	-2.633998	0.762722
36	7	0	3.837418	-2.024258	0.695609
37	7	0	-4.679287	0.588347	-0.190434

Zero-point correction = 0.266992 (Hartree/Particle)
Thermal correction to Energy = 0.288072
Thermal correction to Enthalpy = 0.289016
Thermal correction to Gibbs Free Energy = 0.214917
Sum of electronic and zero-point Energies = -2236.030784
Sum of electronic and thermal Energies = -2236.009704
Sum of electronic and thermal Enthalpies = -2236.008760
Sum of electronic and thermal Free Energies = -2236.082859
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -114.1877

Table S26 Optimized geometries and energies for **2**-*rac*(*ax*,*ax*)-SNS at B3LYP/LANL2DZ+6-31G(d) level

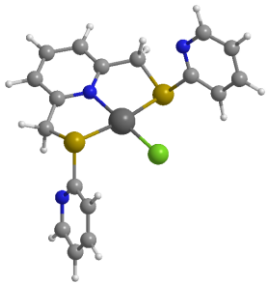


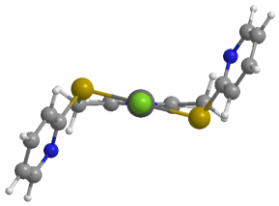


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000046	-0.641140	0.000105
2	17	0	-0.000166	-2.967321	0.000075
3	16	0	1.776558	-0.486588	1.542689
4	16	0	-1.776509	-0.486327	-1.542589
5	6	0	3.655071	-1.692334	-0.088452
6	6	0	-3.655382	-1.692096	0.088126
7	7	0	0.000114	1.421505	0.000111
8	6	0	-3.243019	-0.470750	-0.449623
9	6	0	3.242906	-0.471019	0.449519
10	6	0	0.777484	2.089717	0.886329
11	6	0	4.964599	0.691406	-0.477890
12	1	0	5.452287	1.654258	-0.605207
13	6	0	0.804464	3.483071	0.894874
14	1	0	1.441154	4.004638	1.601509
15	6	0	1.565977	1.305752	1.908008
16	1	0	1.054918	1.328097	2.877539
17	1	0	2.567202	1.726732	2.026930
18	6	0	-0.777072	2.089844	-0.886169
19	6	0	-0.803662	3.483209	-0.894844
20	1	0	-1.440206	4.004887	-1.601530
21	6	0	0.000498	4.185523	-0.000020
22	1	0	0.000650	5.271052	-0.000074
23	6	0	5.478338	-0.461488	-1.069206
24	1	0	-1.054987	1.328458	-2.877404
25	1	0	-2.567060	1.727090	-2.026412
26	1	0	6.380380	-0.410559	-1.669744
27	6	0	-1.565830	1.306032	-1.907763
28	6	0	-4.808813	-1.671275	0.870929
29	1	0	-5.178076	-2.589578	1.317236
30	6	0	4.808393	-1.671530	-0.871418
31	1	0	5.177501	-2.589812	-1.317895
32	6	0	-5.478667	-0.461193	1.068776
33	1	0	-6.380785	-0.410250	1.669199
34	6	0	-4.964739	0.691725	0.477669
35	1	0	-5.452345	1.654610	0.605040
36	7	0	-3.852609	0.689827	-0.275857
37	7	0	3.852583	0.689526	0.275804
38	1	0	-3.093873	-2.604723	-0.083966
39	1	0	3.093492	-2.604925	0.083600

Zero-point correction =	0.290915 (Hartree/Particle)
Thermal correction to Energy =	0.313086
Thermal correction to Enthalpy =	0.314030
Thermal correction to Gibbs Free Energy =	0.235087
Sum of electronic and zero-point Energies =	-2203.980456
Sum of electronic and thermal Energies =	-2203.958285
Sum of electronic and thermal Enthalpies =	-2203.957341
Sum of electronic and thermal Free Energies =	-2204.036284

Table S27 Optimized geometries and energies for **2**-*rac*(*eq*,*eq*)-SNS at B3LYP/LANL2DZ+6-31G(d) level

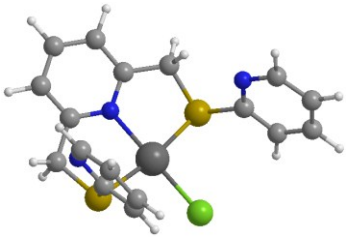
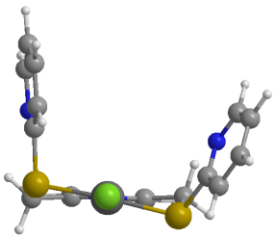




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000008	-0.097967	-0.000072
2	17	0	-0.000105	-2.425137	-0.000106
3	16	0	1.958338	0.098238	-1.313865
4	16	0	-1.958285	0.098352	1.313803
5	7	0	3.925134	-0.143843	0.534291
6	7	0	-3.925044	-0.143731	-0.534394
7	7	0	0.000077	1.962863	-0.000029
8	6	0	-3.274851	-0.795677	0.413226
9	6	0	3.274796	-0.795851	-0.413184
10	6	0	1.097544	2.629441	-0.433486
11	6	0	3.509702	-2.119427	-0.786229
12	1	0	2.935414	-2.597533	-1.571628
13	6	0	4.507054	-2.799383	-0.087205
14	1	0	4.730623	-3.833688	-0.329607
15	6	0	1.111734	4.023497	-0.462322
16	1	0	1.989251	4.546543	-0.826854
17	6	0	2.321539	1.840976	-0.815550
18	1	0	3.003445	1.738084	0.041564
19	1	0	2.861696	2.325268	-1.633249
20	6	0	-1.097328	2.629506	0.433497
21	6	0	-1.111382	4.023557	0.462476
22	1	0	-1.988846	4.546653	0.827065
23	6	0	0.000211	4.724739	0.000113
24	1	0	0.000265	5.810249	0.000171
25	6	0	5.210122	-2.133962	0.918449
26	1	0	-3.003247	1.738244	-0.041688
27	1	0	-2.861588	2.325423	1.633129
28	1	0	5.994072	-2.631340	1.479587
29	6	0	-2.321393	1.841107	0.815470
30	6	0	-4.888563	-0.804508	-1.192950
31	1	0	-5.412024	-0.244707	-1.963197
32	6	0	4.888579	-0.804657	1.192918
33	1	0	5.412163	-0.244804	1.963044
34	6	0	-5.210329	-2.133715	-0.918264
35	1	0	-5.994331	-2.631066	-1.479354
36	6	0	-3.509986	-2.119151	0.786490
37	1	0	-2.935812	-2.597210	1.572001
38	6	0	-4.507414	-2.799072	0.087538
39	1	0	-4.731156	-3.833300	0.330108

Zero-point correction =	0.291197 (Hartree/Particle)
Thermal correction to Energy =	0.313187
Thermal correction to Enthalpy =	0.314132
Thermal correction to Gibbs Free Energy =	0.237042
Sum of electronic and zero-point Energies =	-2203.980996
Sum of electronic and thermal Energies =	-2203.959005
Sum of electronic and thermal Enthalpies =	-2203.958061
Sum of electronic and thermal Free Energies =	-2204.035151

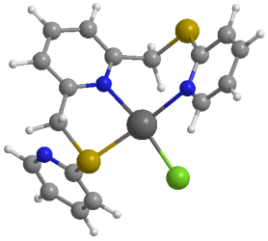
Table S28 Optimized geometries and energies for **2**-*asymm*(*ax*,*eq*)-SNS at B3LYP/LANL2DZ+6-31G(d) level

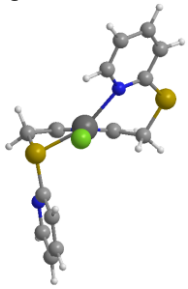



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.057228	0.168153	-1.020467
2	17	0	1.100554	-1.615199	-2.085175
3	16	0	-2.111564	-0.678105	-1.409611
4	16	0	2.052192	1.358273	-0.578088
5	6	0	-1.860543	-2.982957	0.089457
6	7	0	2.984219	0.138226	1.653905
7	7	0	-0.880184	1.718907	-0.034337
8	6	0	3.149793	0.227109	0.345587
9	6	0	-2.415623	-1.701101	0.071890
10	6	0	-2.226961	1.841590	-0.108596
11	6	0	-3.447655	-1.957777	2.083271
12	1	0	-4.081243	-1.515335	2.847515
13	6	0	-2.880388	2.879129	0.553864
14	1	0	-3.960652	2.958990	0.497015
15	6	0	-2.999067	0.876332	-0.975241
16	1	0	-3.225543	1.336782	-1.944191
17	1	0	-3.936608	0.590824	-0.493210
18	6	0	-0.136005	2.602415	0.674806
19	6	0	-0.743368	3.676279	1.324459
20	1	0	-0.136544	4.386957	1.875155
21	6	0	-2.129199	3.809243	1.269117
22	1	0	-2.619929	4.631809	1.779946
23	6	0	-2.953157	-3.253934	2.218342
24	1	0	1.571206	1.776839	1.705751
25	1	0	1.893733	3.307272	0.855951
26	1	0	-3.197644	-3.842036	3.096599
27	6	0	1.344991	2.363415	0.803415
28	6	0	3.792896	-0.694558	2.325524
29	1	0	3.642420	-0.743945	3.400604
30	6	0	-2.144298	-3.771386	1.203358
31	1	0	-1.741523	-4.777267	1.273276
32	6	0	4.774351	-1.460338	1.695805
33	1	0	5.404333	-2.124064	2.278467
34	6	0	4.926114	-1.348875	0.312734
35	1	0	5.680273	-1.927634	-0.211495
36	6	0	4.098373	-0.477872	-0.395810
37	7	0	-3.180467	-1.182975	1.019009
38	1	0	-1.230667	-3.337407	-0.720135
39	1	0	4.179919	-0.360508	-1.470536

Zero-point correction =	0.291001 (Hartree/Particle)
Thermal correction to Energy =	0.313098
Thermal correction to Enthalpy =	0.314043
Thermal correction to Gibbs Free Energy =	0.235889
Sum of electronic and zero-point Energies =	-2203.980236
Sum of electronic and thermal Energies =	-2203.958139
Sum of electronic and thermal Enthalpies =	-2203.957194
Sum of electronic and thermal Free Energies =	-2204.035348

Table S29 Optimized geometries and energies for **2**-*ax*-SNN at B3LYP/LANL2DZ+6-31G(d) level

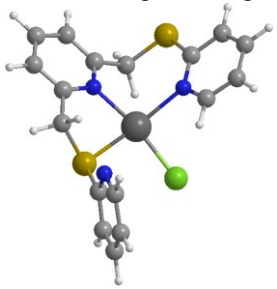


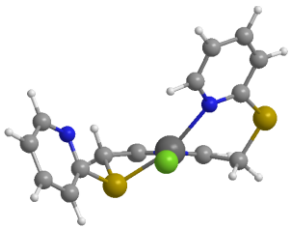


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.327580	-0.764788	0.166032
2	6	0	-3.053458	-0.772673	0.051707
3	6	0	-1.622920	0.383266	2.237242
4	6	0	-1.065863	1.542347	1.453193
5	6	0	-0.949727	3.874027	0.893271
6	6	0	-0.163129	3.541294	-0.206584
7	6	0	0.172562	2.204829	-0.427419
8	6	0	0.902462	1.751780	-1.661935
9	6	0	-1.436234	2.858516	1.715467
10	16	0	2.722826	1.837321	-1.571024
11	6	0	3.273330	0.460839	-0.588503
12	16	0	-1.715175	-1.158388	1.225550
13	7	0	-0.219191	1.247492	0.438852
14	7	0	2.499681	-0.509788	-0.062395
15	6	0	3.120217	-1.498823	0.642819
16	6	0	4.486690	-1.553688	0.844026
17	6	0	5.284879	-0.547287	0.295153
18	6	0	-4.737844	0.613588	-0.590726
19	6	0	-5.120062	-0.257209	-1.610389
20	6	0	-4.404737	-1.445108	-1.781784
21	6	0	-3.338005	-1.725908	-0.929173
22	17	0	0.461761	-3.042875	-0.327533
23	1	0	-2.623538	0.606843	2.611895
24	1	0	-0.979816	0.105989	3.080569
25	1	0	-1.220867	4.908193	1.081475
26	1	0	0.175160	4.301238	-0.903025
27	1	0	0.671100	2.425352	-2.492533
28	1	0	0.587603	0.746905	-1.959226
29	1	0	-2.113727	3.076501	2.533823
30	1	0	2.476679	-2.274154	1.032608
31	1	0	4.908094	-2.373380	1.414805
32	1	0	6.362741	-0.551464	0.424597
33	1	0	-5.268324	1.546985	-0.421355
34	1	0	-5.958840	-0.009823	-2.252455
35	1	0	-4.674183	-2.147578	-2.564576
36	6	0	4.671362	0.462810	-0.423975
37	7	0	-3.709684	0.362209	0.236397
38	1	0	-2.749815	-2.633497	-1.023296
39	1	0	5.253942	1.263110	-0.869435

Zero-point correction =	0.291603 (Hartree/Particle)
Thermal correction to Energy =	0.313487
Thermal correction to Enthalpy =	0.314431
Thermal correction to Gibbs Free Energy =	0.238005
Sum of electronic and zero-point Energies =	-2203.971367
Sum of electronic and thermal Energies =	-2203.949482
Sum of electronic and thermal Enthalpies =	-2203.948538
Sum of electronic and thermal Free Energies =	-2204.024964

Table S30 Optimized geometries and energies for **2**-*eq*-SNN at B3LYP/LANL2DZ+6-31G(d) level

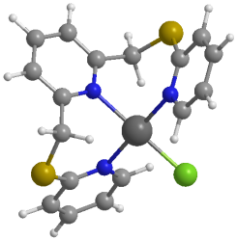
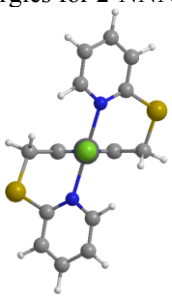




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.016284	-0.136745	-0.560936
2	6	0	-3.255431	0.402490	0.005935
3	6	0	-1.265440	2.196347	0.904776
4	6	0	0.191845	2.533191	0.751723
5	6	0	2.088181	3.991257	0.961793
6	6	0	2.822790	3.105139	0.178650
7	6	0	2.214940	1.936019	-0.284046
8	6	0	2.887406	1.000834	-1.250756
9	6	0	0.743830	3.721705	1.222441
10	16	0	3.941557	-0.282949	-0.495140
11	6	0	2.873596	-1.518120	0.211546
12	16	0	-1.828347	1.330178	-0.639885
13	7	0	0.947437	1.641164	0.067588
14	7	0	1.527660	-1.554641	0.144584
15	6	0	0.892756	-2.602154	0.743531
16	6	0	1.553526	-3.620451	1.404598
17	6	0	2.948633	-3.584295	1.464729
18	6	0	-5.335263	-0.672083	-0.400346
19	6	0	-5.364557	-0.994112	0.956359
20	6	0	-4.307261	-0.577499	1.768548
21	7	0	-3.258218	0.109784	1.297155
22	17	0	-1.202851	-1.847639	-1.574564
23	1	0	-1.873044	3.093734	1.045594
24	1	0	-1.470600	1.497352	1.723555
25	1	0	2.542803	4.906766	1.327208
26	1	0	3.849893	3.320783	-0.096102
27	1	0	3.597019	1.558820	-1.869181
28	1	0	2.156862	0.541276	-1.923592
29	1	0	0.127028	4.427763	1.767830
30	1	0	-0.183891	-2.611044	0.655665
31	1	0	0.980594	-4.423533	1.854060
32	1	0	3.509984	-4.365108	1.968495
33	1	0	-6.140269	-0.976848	-1.061806
34	1	0	-6.189480	-1.555178	1.382628
35	1	0	-4.294352	-0.800432	2.832141
36	6	0	3.607643	-2.525693	0.865855
37	6	0	-4.254493	0.054723	-0.902312
38	1	0	4.690729	-2.457896	0.890284
39	1	0	-4.189608	0.330084	-1.949181

Zero-point correction =	0.291645 (Hartree/Particle)
Thermal correction to Energy =	0.313515
Thermal correction to Enthalpy =	0.314459
Thermal correction to Gibbs Free Energy =	0.238247
Sum of electronic and zero-point Energies =	-2203.972019
Sum of electronic and thermal Energies =	-2203.950150
Sum of electronic and thermal Enthalpies =	-2203.949206
Sum of electronic and thermal Free Energies =	-2204.025418

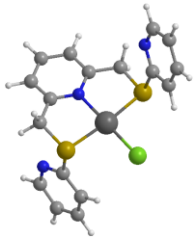
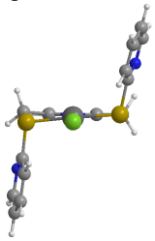
Table S31 Optimized geometries and energies for **2**-NNN at B3LYP/LANL2DZ+6-31G(d) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.000030	-0.719865	0.000016
2	6	0	-3.031062	-0.135623	0.379399
3	6	0	-1.077995	1.204992	2.161727
4	6	0	-0.520501	2.050008	1.053162
5	6	0	-0.000182	4.148211	0.000407
6	6	0	0.537475	3.445109	-1.076238
7	6	0	0.520318	2.050224	-1.052692
8	6	0	1.077804	1.205443	-2.161441
9	6	0	-0.537787	3.444888	1.076932
10	16	0	2.836619	0.712615	-1.936634
11	6	0	3.031077	-0.135400	-0.379533
12	16	0	-2.836760	0.712060	1.936705
13	7	0	-0.000047	1.386550	0.000190
14	7	0	2.063482	-0.736775	0.345060
15	6	0	2.415154	-1.424003	1.464654
16	6	0	3.722008	-1.535481	1.902243
17	6	0	4.727968	-0.910777	1.160749
18	6	0	4.377972	-0.203442	0.022048
19	6	0	-4.377921	-0.203642	-0.022308
20	6	0	-4.727790	-0.910764	-1.161181
21	6	0	-3.721742	-1.535282	-1.902713
22	6	0	-2.414929	-1.423841	-1.464989
23	7	0	-2.063384	-0.736819	-0.345230
24	17	0	0.000092	-3.049276	-0.000204
25	1	0	-1.123369	1.772552	3.096051
26	1	0	-0.459615	0.320347	2.333200
27	1	0	-0.000237	5.233799	0.000491
28	1	0	0.966898	3.964562	-1.926242
29	1	0	1.123067	1.773168	-3.095670
30	1	0	0.459482	0.320778	-2.333026
31	1	0	-0.967285	3.964165	1.927007
32	1	0	1.604849	-1.913385	1.988091
33	1	0	3.939591	-2.104909	2.798620
34	1	0	5.767363	-0.969558	1.468565
35	1	0	5.131456	0.304133	-0.571077
36	1	0	-5.131475	0.303785	0.570854
37	1	0	-5.767156	-0.969525	-1.469098
38	1	0	-3.939228	-2.104544	-2.799219
39	1	0	-1.604561	-1.913090	-1.988452

Zero-point correction =	0.292668 (Hartree/Particle)
Thermal correction to Energy =	0.314092
Thermal correction to Enthalpy =	0.315037
Thermal correction to Gibbs Free Energy =	0.241087
Sum of electronic and zero-point Energies =	-2203.982465
Sum of electronic and thermal Energies =	-2203.961041
Sum of electronic and thermal Enthalpies =	-2203.960097
Sum of electronic and thermal Free Energies =	-2204.034046

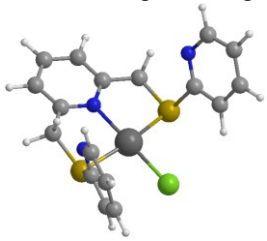
Table S32 Optimized geometries and energies for **2**-TS_{ri1} at B3LYP/LANL2DZ+6-31G(d) level

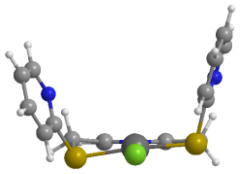



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.043960	-0.546450	0.078822
2	17	0	0.197664	-2.869463	0.027853
3	16	0	-1.800324	-0.567875	1.550379
4	16	0	1.789883	-0.238840	-1.471119
5	7	0	-3.889455	0.435426	0.163410
6	7	0	4.002448	0.729062	-0.245520
7	7	0	-0.125432	1.509378	0.100940
8	6	0	3.324647	-0.381035	-0.473664
9	6	0	-3.207574	-0.675582	0.387773
10	6	0	-1.042837	2.091020	0.914456
11	6	0	-3.500954	-1.930168	-0.151284
12	1	0	-2.884396	-2.796699	0.064125
13	6	0	-4.608438	-2.003230	-0.994800
14	1	0	-4.885284	-2.951391	-1.445551
15	6	0	-1.263875	3.464823	0.866882
16	1	0	-2.009076	3.913039	1.515098
17	6	0	-1.767499	1.234405	1.923885
18	1	0	-2.803531	1.560667	2.035765
19	1	0	-1.268509	1.298456	2.898180
20	6	0	0.612331	2.253955	-0.756948
21	6	0	0.434974	3.636179	-0.827132
22	1	0	1.035573	4.220253	-1.516580
23	6	0	-0.515970	4.244853	-0.013403
24	1	0	-0.672495	5.317923	-0.062504
25	6	0	-5.352222	-0.847878	-1.247734
26	1	0	1.401333	1.770874	-2.701384
27	1	0	2.636612	1.980019	-1.434003
28	1	0	-6.221361	-0.870275	-1.896588
29	6	0	1.634121	1.588048	-1.647681
30	6	0	5.160212	0.621233	0.426580
31	1	0	5.700079	1.548315	0.599327
32	6	0	-4.956107	0.346566	-0.648259
33	1	0	-5.504787	1.269461	-0.816753
34	6	0	5.654023	-0.600001	0.881162
35	1	0	6.594452	-0.641095	1.420365
36	6	0	3.712419	-1.661359	-0.073665
37	1	0	3.097434	-2.530462	-0.282117
38	6	0	4.914283	-1.757565	0.626635
39	1	0	5.266471	-2.726725	0.966539

Zero-point correction = 0.290882 (Hartree/Particle)
Thermal correction to Energy = 0.312111
Thermal correction to Enthalpy = 0.313055
Thermal correction to Gibbs Free Energy = 0.237720
Sum of electronic and zero-point Energies = -2203.980392
Sum of electronic and thermal Energies = -2203.959163
Sum of electronic and thermal Enthalpies = -2203.958219
Sum of electronic and thermal Free Energies = -2204.033554
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -9.5572

Table S33 Optimized geometries and energies for **2**-TS_{ri2} at B3LYP/LANL2DZ+6-31G(d) level

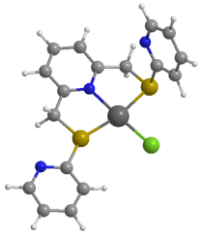
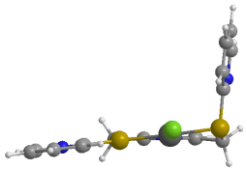




Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.387939	-0.863201	-0.225396
2	17	0	1.480826	-2.207838	-0.573388
3	16	0	-0.405631	-1.202946	2.112467
4	16	0	-0.781781	-0.546082	-2.528915
5	6	0	2.209579	-1.534486	2.917316
6	7	0	-0.031240	1.953367	-3.261996
7	7	0	-2.042022	0.327049	0.086550
8	6	0	0.425265	0.731612	-3.054611
9	6	0	1.194358	-0.591985	2.750733
10	6	0	-2.429315	0.597219	1.360095
11	6	0	2.475027	1.139497	3.489502
12	1	0	2.533712	2.202139	3.709012
13	6	0	-3.627992	1.261102	1.610700
14	1	0	-3.932538	1.457006	2.633068
15	6	0	-1.505500	0.232038	2.490897
16	1	0	-2.066491	0.002119	3.400114
17	1	0	-0.809250	1.055616	2.707456
18	6	0	-2.792414	0.727907	-0.966797
19	6	0	-3.992052	1.411125	-0.762346
20	1	0	-4.582540	1.726509	-1.616132
21	6	0	-4.416189	1.672243	0.537073
22	1	0	-5.352182	2.193001	0.713301
23	6	0	3.568458	0.296786	3.690786
24	1	0	-2.101652	1.392582	-2.891184
25	1	0	-3.094906	-0.087027	-2.937614
26	1	0	4.502083	0.697682	4.070980
27	6	0	-2.324822	0.449194	-2.374972
28	6	0	0.839900	2.875192	-3.702961
29	1	0	0.438177	3.871207	-3.868548
30	6	0	3.430636	-1.061060	3.397796
31	1	0	4.258985	-1.747404	3.543902
32	6	0	2.182449	2.586905	-3.940561
33	1	0	2.851701	3.362502	-4.297550
34	6	0	2.637869	1.286075	-3.711745
35	1	0	3.676876	1.023693	-3.886443
36	6	0	1.743241	0.317662	-3.258464
37	7	0	1.299603	0.698009	3.018355
38	1	0	2.057773	-2.580168	2.674774
39	1	0	2.054043	-0.701411	-3.054695

Zero-point correction = 0.290884 (Hartree/Particle)
Thermal correction to Energy = 0.312087
Thermal correction to Enthalpy = 0.313031
Thermal correction to Gibbs Free Energy = 0.238040
Sum of electronic and zero-point Energies = -2203.980065
Sum of electronic and thermal Energies = -2203.958862
Sum of electronic and thermal Enthalpies = -2203.957918
Sum of electronic and thermal Free Energies = -2204.032909
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -16.8178

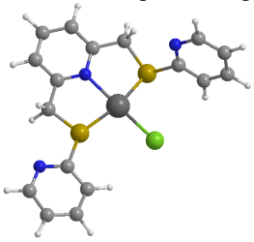
Table S34 Optimized geometries and energies for **2**-TS_{Si1} at B3LYP/LANL2DZ+6-31G(d) level

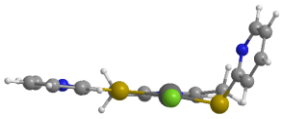



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.128253	-0.404453	-0.732378
2	17	0	-0.234694	-2.667088	-1.097444
3	16	0	2.359568	-0.601950	-1.345204
4	16	0	-2.008123	0.219687	0.050246
5	6	0	3.146430	-2.313715	0.676630
6	7	0	-4.468148	0.755490	0.864096
7	7	0	0.513482	1.623331	-0.371779
8	6	0	-3.736839	-0.213219	0.351998
9	6	0	3.180493	-0.987238	0.241530
10	6	0	1.747988	2.089728	-0.697905
11	6	0	4.444404	-0.281647	1.995123
12	1	0	4.947498	0.548700	2.483501
13	6	0	2.130434	3.388700	-0.378433
14	1	0	3.124930	3.735880	-0.636628
15	6	0	2.673250	1.205242	-1.495489
16	1	0	2.552172	1.404785	-2.567146
17	1	0	3.714693	1.380176	-1.219176
18	6	0	-0.384693	2.431542	0.245004
19	6	0	-0.046804	3.747820	0.568352
20	1	0	-0.779062	4.380218	1.059328
21	6	0	1.221697	4.227874	0.263331
22	1	0	1.499702	5.245551	0.518931
23	6	0	4.482711	-1.566717	2.535404
24	1	0	-1.935725	1.999534	1.678146
25	1	0	-2.532748	2.569075	0.120782
26	1	0	5.019580	-1.753105	3.459502
27	6	0	-1.774860	1.940173	0.597207
28	6	0	-5.763309	0.480312	1.102341
29	1	0	-6.351578	1.290316	1.524906
30	6	0	3.820280	-2.597104	1.864016
31	1	0	3.828545	-3.609900	2.255005
32	6	0	-6.329917	-0.761761	0.829409
33	1	0	-7.379496	-0.940119	1.037204
34	6	0	-5.519493	-1.764526	0.286556
35	1	0	-5.928237	-2.745094	0.061940
36	6	0	-4.175355	-1.499794	0.033214
37	7	0	3.795443	0.010070	0.856273
38	1	0	2.608143	-3.076994	0.124338
39	1	0	-3.505309	-2.243754	-0.385246

Zero-point correction = 0.290106 (Hartree/Particle)
Thermal correction to Energy = 0.311888
Thermal correction to Enthalpy = 0.312833
Thermal correction to Gibbs Free Energy = 0.234758
Sum of electronic and zero-point Energies = -2203.954612
Sum of electronic and thermal Energies = -2203.932829
Sum of electronic and thermal Enthalpies = -2203.931885
Sum of electronic and thermal Free Energies = -2204.009959
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -199.1258

Table S35 Optimized geometries and energies for **2**-TS_{Si2} at B3LYP/LANL2DZ+6-31G(d) level

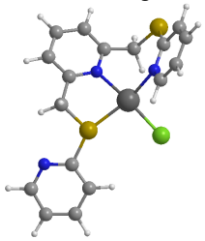


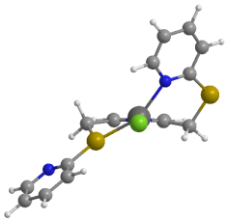


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.214457	-0.115380	-0.462859
2	17	0	0.353452	-2.380831	-0.951160
3	16	0	-2.092392	0.024001	0.020713
4	16	0	2.430466	0.258608	-1.070537
5	6	0	-3.764691	-2.179257	0.006405
6	7	0	3.754515	-0.327514	1.218202
7	7	0	0.114510	1.932536	-0.040359
8	6	0	3.468827	-0.786739	0.012534
9	6	0	-3.686300	-0.801966	0.222479
10	6	0	-1.062510	2.569127	0.183102
11	6	0	-5.887865	-0.580603	0.728345
12	1	0	-6.696365	0.087949	1.011433
13	6	0	-1.099979	3.958168	0.326957
14	1	0	-2.050645	4.449059	0.506858
15	6	0	-2.364461	1.801908	0.299430
16	1	0	-2.799535	1.945960	1.293263
17	1	0	-3.091212	2.171512	-0.430138
18	6	0	1.276179	2.637163	-0.105624
19	6	0	1.279072	4.024709	0.009686
20	1	0	2.214233	4.569377	-0.061653
21	6	0	0.076064	4.692766	0.229494
22	1	0	0.058085	5.773780	0.325886
23	6	0	-6.104158	-1.943924	0.547101
24	1	0	2.965472	1.636163	0.781606
25	1	0	3.329921	2.480580	-0.744523
26	1	0	-7.094754	-2.362753	0.688250
27	6	0	2.577527	1.889773	-0.215962
28	6	0	4.515505	-1.096600	2.009362
29	1	0	4.741720	-0.695561	2.993500
30	6	0	-5.022649	-2.751918	0.180450
31	1	0	-5.155750	-3.818820	0.028509
32	6	0	4.994738	-2.344687	1.607290
33	1	0	5.602894	-2.936905	2.282776
34	6	0	4.678079	-2.804998	0.328671
35	1	0	5.035390	-3.769394	-0.018752
36	6	0	3.895277	-2.008412	-0.508171
37	7	0	-4.680500	-0.009327	0.568189
38	1	0	-2.895756	-2.761681	-0.282241
39	1	0	3.621792	-2.326313	-1.507837

Zero-point correction = 0.290130 (Hartree/Particle)
Thermal correction to Energy = 0.311873
Thermal correction to Enthalpy = 0.312818
Thermal correction to Gibbs Free Energy = 0.235157
Sum of electronic and zero-point Energies = -2203.954760
Sum of electronic and thermal Energies = -2203.933017
Sum of electronic and thermal Enthalpies = -2203.932073
Sum of electronic and thermal Free Energies = -2204.009734
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -200.6079

Table S36 Optimized geometries and energies for **2**-TS_{Si3} at B3LYP/LANL2DZ+6-31G(d) level



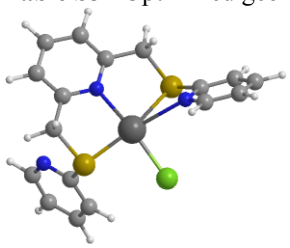
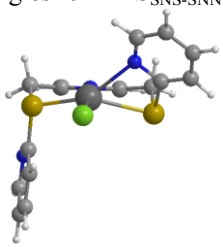


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.297640	-0.560206	-0.261607
2	6	0	-3.749269	-0.263730	0.056862
3	6	0	-1.645996	1.394635	1.344703
4	6	0	-0.467493	2.178575	0.815898
5	6	0	0.712251	4.248255	0.479285
6	6	0	1.555052	3.592356	-0.414240
7	6	0	1.374627	2.228589	-0.644988
8	6	0	2.139405	1.484475	-1.706534
9	6	0	-0.331278	3.541432	1.075034
10	16	0	3.768006	0.821819	-1.212320
11	6	0	3.489964	-0.475128	-0.032102
12	16	0	-1.960187	0.010403	0.189644
13	7	0	0.426097	1.536945	0.023331
14	7	0	2.305064	-1.031552	0.291324
15	6	0	2.292718	-2.041010	1.208993
16	6	0	3.435080	-2.526186	1.815421
17	6	0	4.666109	-1.959545	1.473624
18	6	0	-5.585511	-1.563692	-0.668777
19	6	0	-6.417605	-0.581215	-0.122838
20	6	0	-5.832756	0.519851	0.497834
21	7	0	-4.500212	0.681277	0.579820
22	17	0	-0.085330	-2.777951	-0.828161
23	1	0	-2.550759	2.007018	1.386579
24	1	0	-1.452406	0.987045	2.342853
25	1	0	0.835110	5.309401	0.672399
26	1	0	2.331642	4.128978	-0.948930
27	1	0	2.408567	2.173327	-2.513352
28	1	0	1.526086	0.693083	-2.147938
29	1	0	-1.049365	4.040221	1.717067
30	1	0	1.325181	-2.468815	1.427847
31	1	0	3.354308	-3.334402	2.533267
32	1	0	5.589302	-2.312707	1.922455
33	1	0	-6.007009	-2.439343	-1.153147
34	1	0	-7.497548	-0.669007	-0.173403
35	1	0	-6.436182	1.305790	0.943608
36	6	0	4.688657	-0.928616	0.551656
37	6	0	-4.201952	-1.420694	-0.578769
38	1	0	5.622800	-0.454610	0.267607
39	1	0	-3.514351	-2.163725	-0.969168

Zero-point correction =	0.290629 (Hartree/Particle)
Thermal correction to Energy =	0.312135
Thermal correction to Enthalpy =	0.313079
Thermal correction to Gibbs Free Energy =	0.237208
Sum of electronic and zero-point Energies =	-2203.943048
Sum of electronic and thermal Energies =	-2203.921541
Sum of electronic and thermal Enthalpies =	-2203.920597
Sum of electronic and thermal Free Energies =	-2203.996469

****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -203.9621

Table S37 Optimized geometries and energies for **2**-$TS_{SNS-SNN1}$ at B3LYP/LANL2DZ+6-31G(d) level

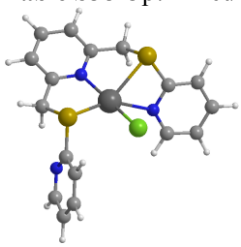



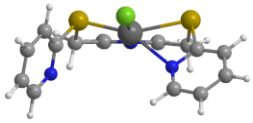
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.160947	-0.474751	0.307877
2	6	0	-3.104259	-0.855749	0.015790
3	6	0	-2.044369	0.601514	2.204941
4	6	0	-1.422188	1.760552	1.473305
5	6	0	-1.331256	4.101745	0.942156
6	6	0	-0.183277	3.852621	0.193960
7	6	0	0.320071	2.554117	0.112290
8	6	0	1.617046	2.295290	-0.610071
9	6	0	-1.955757	3.042718	1.593181
10	16	0	1.645464	0.748413	-1.649596
11	6	0	3.005184	-0.105396	-0.840489
12	16	0	-1.856262	-1.009695	1.338384
13	7	0	-0.305233	1.526973	0.740000
14	7	0	2.701479	-0.552071	0.386077
15	6	0	3.631769	-1.230055	1.067077
16	6	0	4.897067	-1.496237	0.536638
17	6	0	5.197957	-1.038605	-0.743916
18	6	0	-4.800138	0.334175	-0.925000
19	6	0	-5.031054	-0.664183	-1.870256
20	6	0	-4.233091	-1.810522	-1.842661
21	6	0	-3.237466	-1.924755	-0.873796
22	17	0	0.384606	-2.704381	-0.312091
23	1	0	-3.108080	0.769146	2.379579
24	1	0	-1.544413	0.442123	3.167987
25	1	0	-1.735964	5.106659	1.010686
26	1	0	0.326519	4.656557	-0.325956
27	1	0	2.421502	2.183033	0.123365
28	1	0	1.861429	3.143139	-1.253465
29	1	0	-2.854752	3.196686	2.179536
30	1	0	3.341940	-1.587214	2.050543
31	1	0	5.618270	-2.063227	1.115533
32	1	0	6.168759	-1.236352	-1.188131
33	1	0	-5.397997	1.241764	-0.909352
34	1	0	-5.816975	-0.544520	-2.608510
35	1	0	-4.383024	-2.608632	-2.563340
36	6	0	4.234040	-0.317230	-1.457657
37	7	0	-3.842451	0.243539	0.012080
38	1	0	-2.583178	-2.788438	-0.819417
39	1	0	4.431484	0.061978	-2.453853

Zero-point correction =	0.290862 (Hartree/Particle)
Thermal correction to Energy =	0.312253
Thermal correction to Enthalpy =	0.313197
Thermal correction to Gibbs Free Energy =	0.237759
Sum of electronic and zero-point Energies =	-2203.962670
Sum of electronic and thermal Energies =	-2203.941279
Sum of electronic and thermal Enthalpies =	-2203.940335
Sum of electronic and thermal Free Energies =	-2204.015773

****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -125.9955

Table S38 Optimized geometries and energies for **2**-$TS_{SNS\text{-}SNN2}$ at B3LYP/LANL2DZ+6-31G(d) level

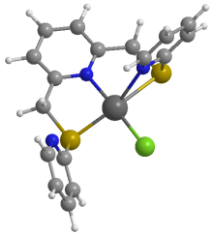


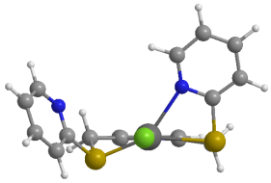


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.149535	0.017718	-0.511303
2	6	0	-3.191409	-0.198617	-0.084447
3	6	0	-1.851583	2.257578	0.267401
4	6	0	-0.454133	2.803328	0.343357
5	6	0	1.069909	4.631951	0.679653
6	6	0	2.124198	3.728279	0.576630
7	6	0	1.856139	2.376049	0.360945
8	6	0	2.983825	1.377276	0.339327
9	6	0	-0.235301	4.163204	0.563573
10	16	0	2.853815	0.084374	-0.996274
11	6	0	2.856603	-1.384611	0.039534
12	16	0	-1.980159	0.866484	-0.939576
13	7	0	1.733701	-1.538050	0.754607
14	7	0	0.580733	1.931889	0.238023
15	6	0	1.617293	-2.617966	1.534686
16	6	0	2.616628	-3.591613	1.614588
17	6	0	3.773876	-3.429142	0.856626
18	6	0	-4.253737	-0.802028	1.837082
19	6	0	-4.990177	-1.782014	1.169187
20	6	0	-4.793530	-1.949664	-0.202116
21	6	0	-3.872638	-1.135671	-0.862487
22	17	0	-0.440734	-1.958208	-1.584103
23	1	0	-2.567745	3.031212	-0.019994
24	1	0	-2.166628	1.824067	1.226502
25	1	0	1.263410	5.687811	0.840830
26	1	0	3.152782	4.062128	0.660048
27	1	0	3.939121	1.893960	0.226388
28	1	0	2.999823	0.833465	1.288777
29	1	0	-1.080126	4.839468	0.634918
30	1	0	0.688025	-2.711442	2.088283
31	1	0	2.476271	-4.461248	2.247670
32	1	0	4.565668	-4.171370	0.889200
33	1	0	-4.378841	-0.632311	2.903203
34	1	0	-5.701138	-2.394293	1.713870
35	1	0	-5.350062	-2.699865	-0.755330
36	6	0	3.909358	-2.294398	0.048941
37	7	0	-3.358483	-0.021686	1.216015
38	1	0	-3.685750	-1.230744	-1.926042
39	1	0	4.796969	-2.126771	-0.550418

Zero-point correction = 0.290774 (Hartree/Particle)
Thermal correction to Energy = 0.312202
Thermal correction to Enthalpy = 0.313147
Thermal correction to Gibbs Free Energy = 0.237698
Sum of electronic and zero-point Energies = -2203.962136
Sum of electronic and thermal Energies = -2203.940708
Sum of electronic and thermal Enthalpies = -2203.939764
Sum of electronic and thermal Free Energies = -2204.015212
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -127.0253

Table S39 Optimized geometries and energies for **2**-$TS_{SNS\text{-}SNN3}$ at B3LYP/LANL2DZ+6-31G(d) level





Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.057133	-0.077752	-0.677630
2	17	0	-0.972391	-1.975620	-1.511761
3	16	0	2.629573	-0.549543	-1.479850
4	16	0	-1.910320	1.198306	-0.774902
5	6	0	3.742178	-2.340477	0.378549
6	7	0	-3.259092	0.145735	1.323300
7	7	0	0.918417	1.694449	0.018657
8	6	0	-3.243291	0.228366	0.002711
9	6	0	2.659944	-1.540454	0.017697
10	6	0	2.240954	1.965117	-0.064165
11	6	0	1.392761	-2.253448	1.807842
12	1	0	0.440780	-2.197902	2.326655
13	6	0	2.763085	3.128794	0.508850
14	1	0	3.829779	3.319499	0.449201
15	6	0	3.195461	1.085971	-0.853871
16	1	0	3.472471	1.628059	-1.766767
17	1	0	4.120768	0.940807	-0.288341
18	6	0	0.071979	2.591066	0.591639
19	6	0	0.543224	3.781329	1.139502
20	1	0	-0.154248	4.484972	1.580786
21	6	0	1.911349	4.042744	1.118614
22	1	0	2.304411	4.955643	1.555063
23	6	0	2.424239	-3.083116	2.253488
24	1	0	-1.644992	1.664494	1.541925
25	1	0	-2.003662	3.161952	0.654158
26	1	0	2.285992	-3.688906	3.142760
27	6	0	-1.393556	2.254745	0.651208
28	6	0	-4.241611	-0.572492	1.884657
29	1	0	-4.240031	-0.618880	2.970509
30	6	0	3.613586	-3.125999	1.528304
31	1	0	4.429808	-3.769304	1.842758
32	6	0	-5.218174	-1.231015	1.135522
33	1	0	-5.990883	-1.806432	1.634290
34	6	0	-5.176899	-1.129364	-0.255367
35	1	0	-5.919745	-1.626737	-0.871252
36	6	0	-4.166721	-0.374240	-0.851742
37	7	0	1.512682	-1.497938	0.710179
38	1	0	4.644768	-2.360007	-0.221986
39	1	0	-4.095828	-0.266236	-1.928382

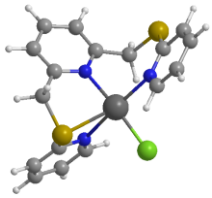
Zero-point correction = 0.290462 (Hartree/Particle)
Thermal correction to Energy = 0.311979
Thermal correction to Enthalpy = 0.312923
Thermal correction to Gibbs Free Energy = 0.236829
Sum of electronic and zero-point Energies = -2203.961992
Sum of electronic and thermal Energies = -2203.940475
Sum of electronic and thermal Enthalpies = -2203.939531
Sum of electronic and thermal Free Energies = -2204.015625
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -119.7989

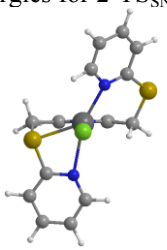
Table S40 Optimized geometries and energies for **2**-$TS_{SNS-SNN4}$ at B3LYP/LANL2DZ+6-31G(d) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.216373	-0.105709	-0.055560
2	17	0	-0.132354	-2.432079	-0.016829
3	16	0	1.830459	-0.084272	-1.159691
4	16	0	-2.103037	0.601796	1.960445
5	7	0	3.705303	-0.238839	0.791839
6	7	0	-0.033772	1.990269	0.011556
7	7	0	-2.694707	-0.656463	-0.274720
8	6	0	-3.156864	-0.459650	0.966956
9	6	0	3.075283	-0.945159	-0.130436
10	6	0	1.125286	2.545580	-0.418668
11	6	0	4.248642	-2.943804	0.389237
12	1	0	4.458789	-3.996958	0.230485
13	6	0	1.312623	3.930013	-0.411298
14	1	0	2.243395	4.345909	-0.782261
15	6	0	2.276696	1.668319	-0.826817
16	1	0	3.005515	1.608899	-0.005183
17	1	0	2.778554	2.061079	-1.715705
18	6	0	-1.011207	2.784644	0.520504
19	6	0	-0.850175	4.167054	0.590582
20	1	0	-1.640824	4.774841	1.016910
21	6	0	0.316075	4.750980	0.101499
22	1	0	0.449533	5.827777	0.132162
23	6	0	4.924803	-2.221641	1.373428
24	1	0	-2.888828	1.875137	0.076661
25	1	0	-2.889591	2.875810	1.540058
26	1	0	5.672721	-2.692807	2.002325
27	6	0	-2.306622	2.158597	0.958598
28	6	0	-3.393056	-1.442676	-1.101380
29	1	0	-2.974381	-1.589350	-2.092084
30	6	0	4.625223	-0.868287	1.536227
31	1	0	5.131683	-0.264121	2.283959
32	6	0	-4.575946	-2.072404	-0.706256
33	1	0	-5.106285	-2.713698	-1.402021
34	6	0	-5.039412	-1.875005	0.592419
35	1	0	-5.950819	-2.356655	0.933471
36	6	0	-4.321494	-1.041419	1.457474
37	6	0	3.295493	-2.296826	-0.397819
38	1	0	2.743540	-2.818550	-1.170524
39	1	0	-4.656744	-0.849538	2.470363

Zero-point correction = 0.290825 (Hartree/Particle)
Thermal correction to Energy = 0.312232
Thermal correction to Enthalpy = 0.313177
Thermal correction to Gibbs Free Energy = 0.237499
Sum of electronic and zero-point Energies = -2203.959512
Sum of electronic and thermal Energies = -2203.938105
Sum of electronic and thermal Enthalpies = -2203.937161
Sum of electronic and thermal Free Energies = -2204.012838
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -128.7937

Table S41 Optimized geometries and energies for **2**-$TS_{SNN\text{-}NNN1}$ at B3LYP/LANL2DZ+6-31G(d) level



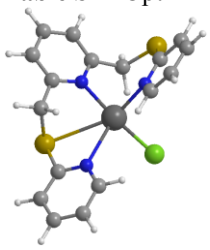


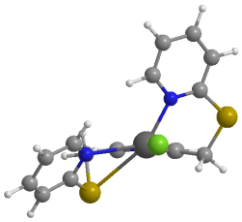
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.154055	-0.727968	-0.030447
2	6	0	-2.953284	-0.692694	0.254186
3	6	0	-1.491247	0.559862	2.403205
4	6	0	-0.961291	1.634265	1.485280
5	6	0	-0.772950	3.958296	0.878026
6	6	0	-0.024263	3.577175	-0.230732
7	6	0	0.236031	2.222890	-0.446412
8	6	0	0.959486	1.743712	-1.675724
9	6	0	-1.266784	2.973294	1.731182
10	16	0	2.779507	1.657626	-1.514845
11	6	0	3.178726	0.292680	-0.442385
12	16	0	-1.853095	-1.079244	1.622089
13	7	0	-0.192842	1.285227	0.426389
14	7	0	2.316431	-0.610066	0.061200
15	6	0	2.813786	-1.610359	0.840638
16	6	0	4.157105	-1.740862	1.140151
17	6	0	5.053253	-0.805130	0.616451
18	6	0	-3.044593	-0.338255	-2.017642
19	6	0	-4.441679	-0.324093	-1.997788
20	6	0	-5.097850	-0.502804	-0.781668
21	6	0	-4.341702	-0.699323	0.377795
22	17	0	0.286611	-2.947765	-0.665631
23	1	0	-2.379359	0.918650	2.929369
24	1	0	-0.744293	0.301626	3.164547
25	1	0	-0.993181	5.005293	1.061758
26	1	0	0.345333	4.312700	-0.937332
27	1	0	0.833557	2.468658	-2.485617
28	1	0	0.565400	0.785487	-2.025521
29	1	0	-1.887605	3.234607	2.581574
30	1	0	2.091198	-2.327525	1.202990
31	1	0	4.486757	-2.563282	1.764842
32	1	0	6.116920	-0.871266	0.823321
33	1	0	-2.492162	-0.218067	-2.945068
34	1	0	-4.995168	-0.187790	-2.920867
35	1	0	-6.182484	-0.506301	-0.732722
36	6	0	4.558862	0.216057	-0.175923
37	7	0	-2.312449	-0.516815	-0.911935
38	1	0	-4.815480	-0.868674	1.338391
39	1	0	5.221427	0.963598	-0.600736

Zero-point correction =	0.291102 (Hartree/Particle)
Thermal correction to Energy =	0.312331
Thermal correction to Enthalpy =	0.313275
Thermal correction to Gibbs Free Energy =	0.239047
Sum of electronic and zero-point Energies =	-2203.956623
Sum of electronic and thermal Energies =	-2203.935395
Sum of electronic and thermal Enthalpies =	-2203.934450
Sum of electronic and thermal Free Energies =	-2204.008678

****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -123.5331

Table S42 Optimized geometries and energies for **2**-$TS_{SNN\text{-}NNN2}$ at B3LYP/LANL2DZ+6-31G(d) level





Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.028215	-0.235130	-0.680174
2	6	0	-3.313625	0.411943	0.014324
3	6	0	-1.356741	2.048722	1.161677
4	6	0	0.023130	2.482706	0.763797
5	6	0	1.818062	4.083037	0.672130
6	6	0	2.428654	3.297692	-0.299896
7	6	0	1.818688	2.104778	-0.697408
8	6	0	2.365571	1.272075	-1.826289
9	6	0	0.584401	3.684610	1.188681
10	16	0	3.680608	0.081997	-1.372088
11	6	0	2.993961	-1.021495	-0.166365
12	16	0	-2.368013	1.875505	-0.396766
13	7	0	0.668887	1.690824	-0.124361
14	7	0	1.688205	-1.161317	0.130014
15	6	0	1.317960	-2.071471	1.072321
16	6	0	2.224410	-2.871718	1.739251
17	6	0	3.582425	-2.743252	1.428055
18	6	0	3.965269	-1.810556	0.481178
19	6	0	-4.705043	0.441921	0.099566
20	6	0	-5.365723	-0.763356	0.355721
21	6	0	-4.616102	-1.925456	0.522988
22	6	0	-3.225015	-1.847864	0.419245
23	7	0	-2.585775	-0.699900	0.165836
24	17	0	-0.534021	-2.266712	-1.672118
25	1	0	-1.824466	2.775237	1.829070
26	1	0	-1.345482	1.067611	1.645040
27	1	0	2.273903	5.014095	0.994201
28	1	0	3.359527	3.603766	-0.765506
29	1	0	2.882846	1.917216	-2.543630
30	1	0	1.563719	0.760947	-2.367248
31	1	0	0.048100	4.305312	1.898335
32	1	0	0.256541	-2.145084	1.265196
33	1	0	1.870268	-3.581504	2.478035
34	1	0	4.328519	-3.356138	1.924142
35	1	0	5.010668	-1.668908	0.226543
36	1	0	-5.248489	1.371239	-0.028257
37	1	0	-6.449192	-0.787615	0.423182
38	1	0	-5.092501	-2.881109	0.714360
39	1	0	-2.601626	-2.732645	0.500972

Zero-point correction = 0.291095 (Hartree/Particle)
Thermal correction to Energy = 0.312399
Thermal correction to Enthalpy = 0.313344
Thermal correction to Gibbs Free Energy = 0.238988
Sum of electronic and zero-point Energies = -2203.940215
Sum of electronic and thermal Energies = -2203.918911
Sum of electronic and thermal Enthalpies = -2203.917967
Sum of electronic and thermal Free Energies = -2203.992323
****** 1 imaginary frequencies (negative Signs) ******
Frequencies -- -106.5224