

Electronic Supplementary Information

Part II: Theoretical Calculations

Stereochemistry and mechanistic insights in the $[2^t + 2^i + 2^i]$ annulations of thioketenes and imines

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1. Details of Calculations

All the DFT calculations were performed using Gaussian 09 program package.^[1] The optimization and frequency calculation of the minima and transition states were performed at B3LYP/6-31g(d) level. Frequency calculations were used to verify if the real minima or transition states were obtained and to produce thermal corrections to Gibbs free energy. IRC calculations were performed at the same level of theory to confirm the calculated transition states connect the correct reactants and products. The single point energies based on the optimized structures were calculated at M06-2x/6-311++g(d,p) level.

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09*, Revision D.01, (Gaussian, Inc., Wallingford CT, 2009).

2. Computed energies of all stationary points

Table SI-1 Calculated Gibbs free energy changes at 298 K (ΔG , in kcal/mol)

Entry	1	TS1-endo	C-endo	TS2-Si	7	4	TS1-exo	C-exo	TS2-Re	8
1	1c	6.9	-17.4	3.4	-27.9	-32.9	9.64	-11.4	18.2	-17.0
2	1g	7.4	-20.3	6.6	-31.7	-35.9	10.5	-13.5	18.1	-22.7
3	1k	7.2	-20.0	5.8	-23.8	-33.5	10.4	-13.5	17.3	-14.3
4	1m	4.4	-20.2	2.8	-33.0	-35.9	8.2	-12.3	15.7	-23.6
5	1n	7.0	-18.6	7.8	-16.5	-29.9	10.3	-12.2	18.8	-10.3

Table SI-2. Sum of electronic and thermal free energies (G , in Hartree, m06-2x/6-311++g(d,p)), thermal corrections to Gibbs free energy (TCGFE, in Hartree, b3lyp/6-31g(d)), total free energies (G' , in Hartree), and Gibbs free energy changes (ΔG , in kcal/mol) at 298 K in the gas phase

Structure	G	TCGFE	G'	ΔG , in kcal/mol
1c	-1109.61305771	0.232007	-1109.38105071	

imine 5	-403.045003056	0.127196	-402.91780706	
1c + imine 5			-1512.29885777	0
TS1-endo-c	-1512.67079475	0.382958	-1512.28783675	6.91579
C-endo-c	-1512.71393503	0.387308	-1512.32662703	-17.42547
TS2-Si-c	-1512.67977689	0.386368	-1512.29340889	3.41922
7c	-1512.73349630	0.390189	-1512.34330730	-27.8925
4c	-1512.74135734	0.390101	-1512.35125634	-32.8806
TS1-exo-c	-1512.66607451	0.382583	-1512.28349151	9.64247
C-exo-c	-1512.70288443	0.385817	-1512.31706743	-11.42673
TS2-Re-c	-1512.65625498	0.386336	-1512.26991898	18.15937
8c	-1512.71607029	0.390176	-1512.32589429	-16.96567
1g	-917.899888260	0.182858	-917.71703026	
1g + imine 5			-1320.63483732	0
TS1-endo-g	-1320.95700391	0.334004	-1320.62299991	7.42809
C-endo-g	-1321.00646446	0.339229	-1320.66723546	-20.33014
TS2-Si-g	-1320.96072859	0.336420	-1320.62430859	6.60688
7g	-1321.02818063	0.342803	-1320.68537763	-31.71452
4g	-1321.03469897	0.342718	-1320.69198097	-35.85818
TS1-exo-g	-1320.95149910	0.333466	-1320.61803310	10.54481
C-exo-g	-1320.99429934	0.338015	-1320.65628434	-13.45821
TS2-Re-g	-1320.94295241	0.337001	-1320.60595141	18.12618
8g	-1321.01428475	0.343327	-1320.67095775	-22.66591
1k	-996.508908539	0.236243	-996.27266554	
1k + imine 5			-1399.1904726	0
TS1-endo-k	-1399.56547256	0.386424	-1399.17904856	7.16869
C-endo-k	-1399.61438286	0.392036	-1399.22234686	-20.0014
TS2-Si-k	-1399.57062649	0.389349	-1399.18127749	5.77002
7k	-1399.62626850	0.397907	-1399.22836150	-23.77564
4k	-1399.64092180	0.397105	-1399.24381680	-33.47399
TS1-exo-k	-1399.56031010	0.386393	-1399.17391710	10.38873
C-exo-k	-1399.60296462	0.391032	-1399.21193262	-13.46637
TS2-Re-k	-1399.55372204	0.390807	-1399.16291504	17.29263
8k	-1399.60927807	0.396065	-1399.21321307	-14.26986
1m	-1145.76216224	0.220389	-1145.54175604	
1m + imine 5			-1548.4595631	0
TS1-endo-m	-1548.82195380	0.371044	-1548.45248385	4.4423
C-endo-m	-1548.86600834	0.376636	-1548.49180865	-20.23439
TS2-Si-m	-1548.82989985	0.375484	-1548.45517483	2.75368
7m	-1548.89192517	0.379871	-1548.51219554	-33.02736
4m	-1548.89533214	0.378501	-1548.51683114	-35.93624
TS1-exo-m	-1548.81846585	0.371947	-1548.44651885	8.18539
C-exo-m	-1548.85354274	0.374454	-1548.47908874	-12.25252

TS2-Re-m	-1548.80950682	0.374970	-1548.43453682	15.70423
8m	-1548.87606380	0.378911	-1548.49715280	-23.58789
1n	-1035.81289694	0.263739	-1035.54915794	
1n + imine 5			-1438.466965	0
TS1-endo-n	-1438.86984265	0.414090	-1438.45575265	7.03586
C-endo-n	-1438.91623988	0.419592	-1438.49664788	-18.62629
TS2-Si-n	-1438.87245119	0.417890	-1438.45456119	7.78351
7n	-1438.91819648	0.424965	-1438.49323148	-16.48247
4n	-1438.93929991	0.424712	-1438.51458791	-29.88383
TS1-exo-n	-1438.86487638	0.414384	-1438.45049238	10.33673
C-exo-n	-1438.90495975	0.418630	-1438.48632975	-12.15156
TS2-Re-n	-1438.85503200	0.417975	-1438.43705700	18.76755
8n	-1438.90753075	0.424082	-1438.48344875	-10.34371

3. Intrinsic reaction coordinate (IRC) analysis

Surprisingly, the IRC analyses of **TS2-Re** converged at **C-endo** rather than **C-exo** (see Figures SI4, SI8, SI12, SI16, and SI20). One of the reviewers thought that during the IRC the molecule was jumping off to a different part of PES, and also suggested that smaller steps for IRC might be helpful. During the revision of the manuscript, we met some difficulties in calculating the IRC analysis of **TS2-Re**. If we set the default stepsize as 5 or 10, the IRC calculation would normally terminate only after several steps. We have tried to use "calcall" in the command line with default stepsize, but the calculation also normally terminated only after several steps. When we set the stepsize as 20, the IRC calculations of the five **TS2-Re** transition states (Figures SI4, SI8, SI12, SI16, and SI20) all converged at **C-endo**. However, the *forward calculations* led to the correct products **8**. The *backward calculations* showed that the energy decreased very slowly and did not converge to **C-exo**. The final structures in the backward calculations seemed to be the structures between **C-exo** and **C-endo**. Further optimization of these final structures led to **C-endo**. We thought there might be transition states between **C-exo** and **C-endo**, but we could not locate it. The backward PES from **TS2-Re** to **C-exo** were more complex.

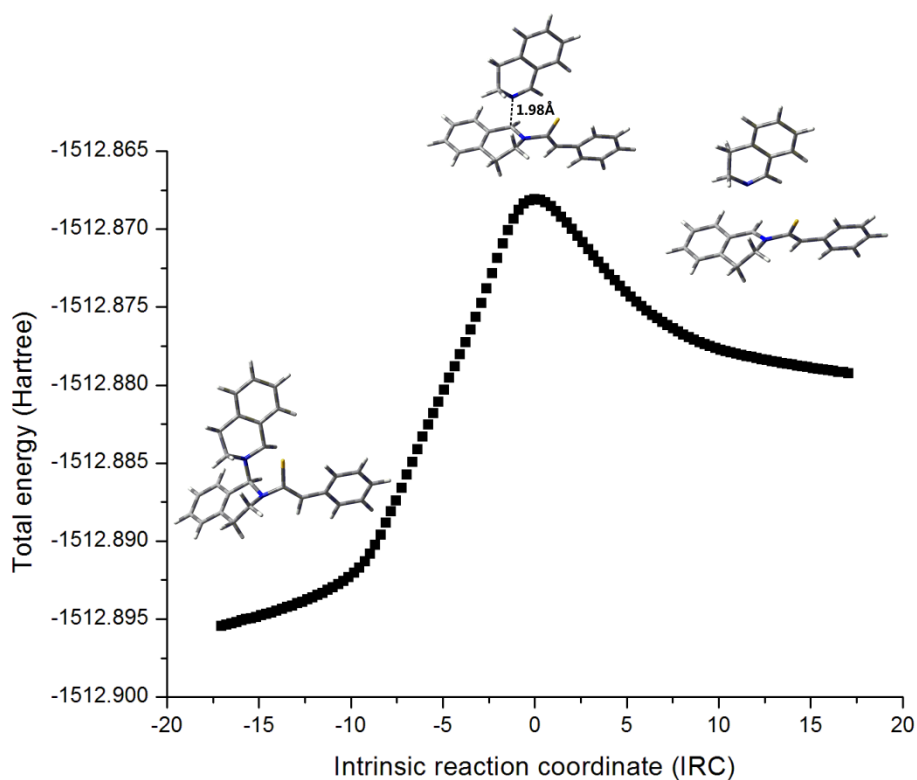


Figure SI-1. The IRC analysis of **TS1-endo-c**.

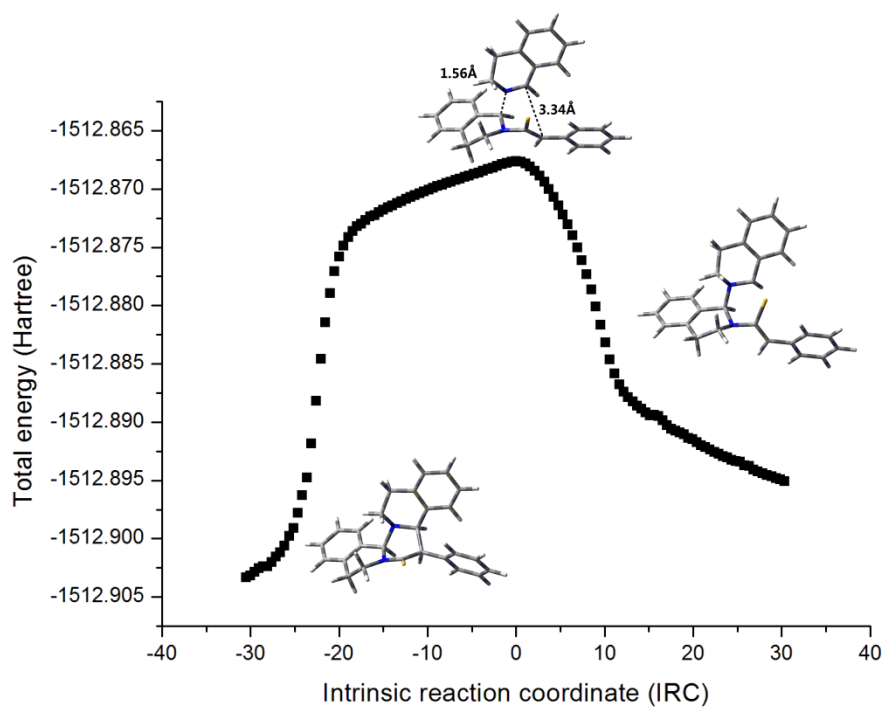


Figure SI-2. The IRC analysis of **TS2-Si-c**.

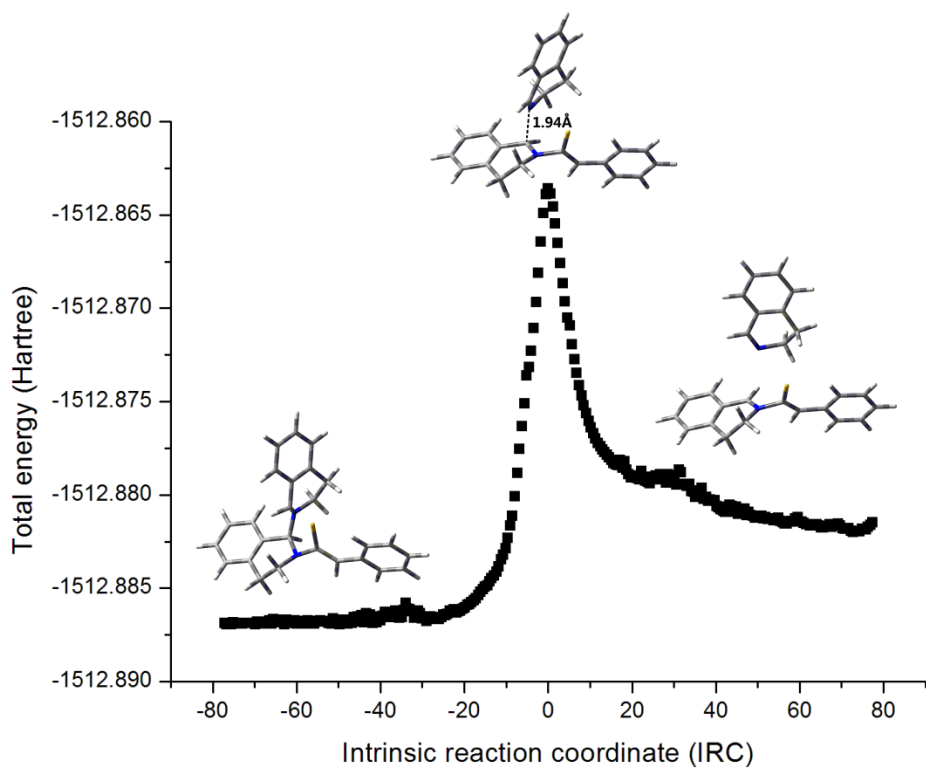


Figure SI-3. The IRC analysis of **TS1-exo-c**.

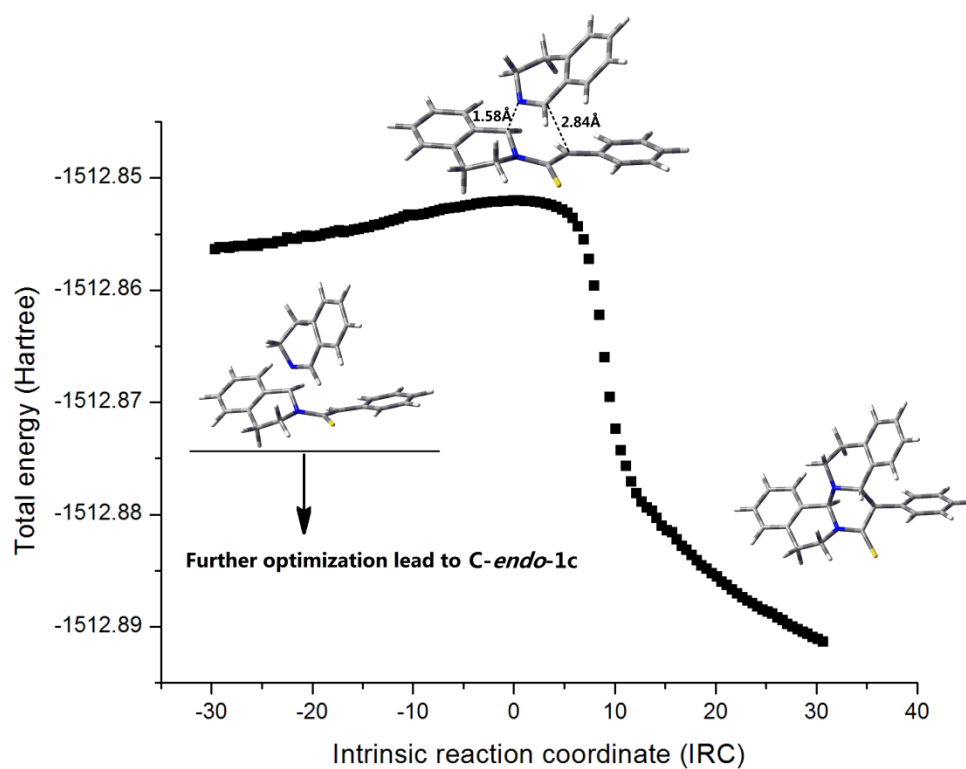


Figure SI-4. The IRC analysis of **TS2-Re-c**.

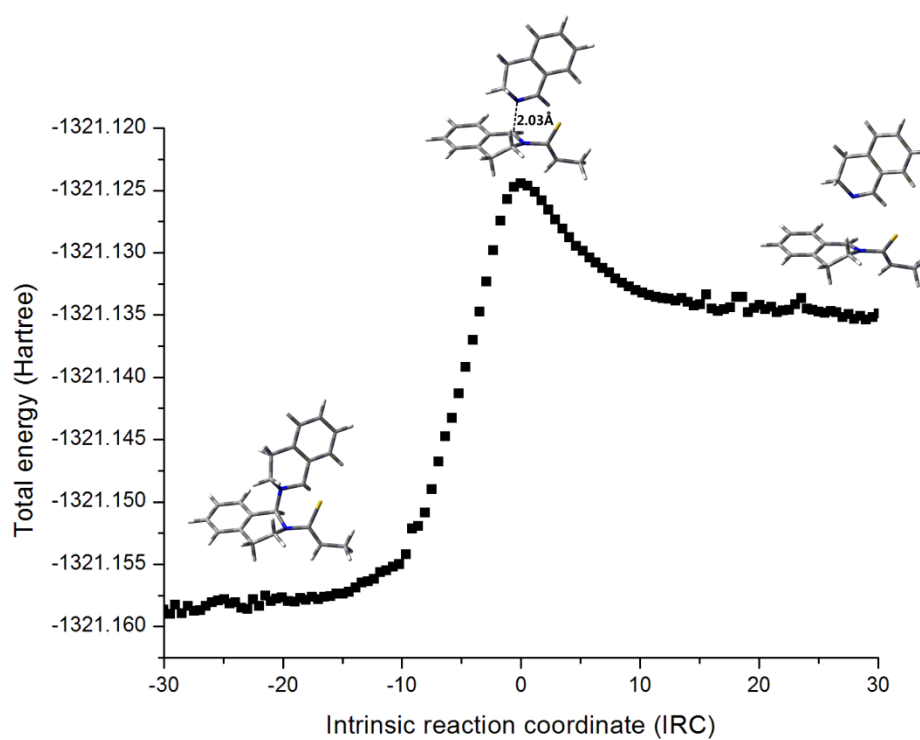


Figure SI-5. The IRC analysis of **TS1-endo-g**.

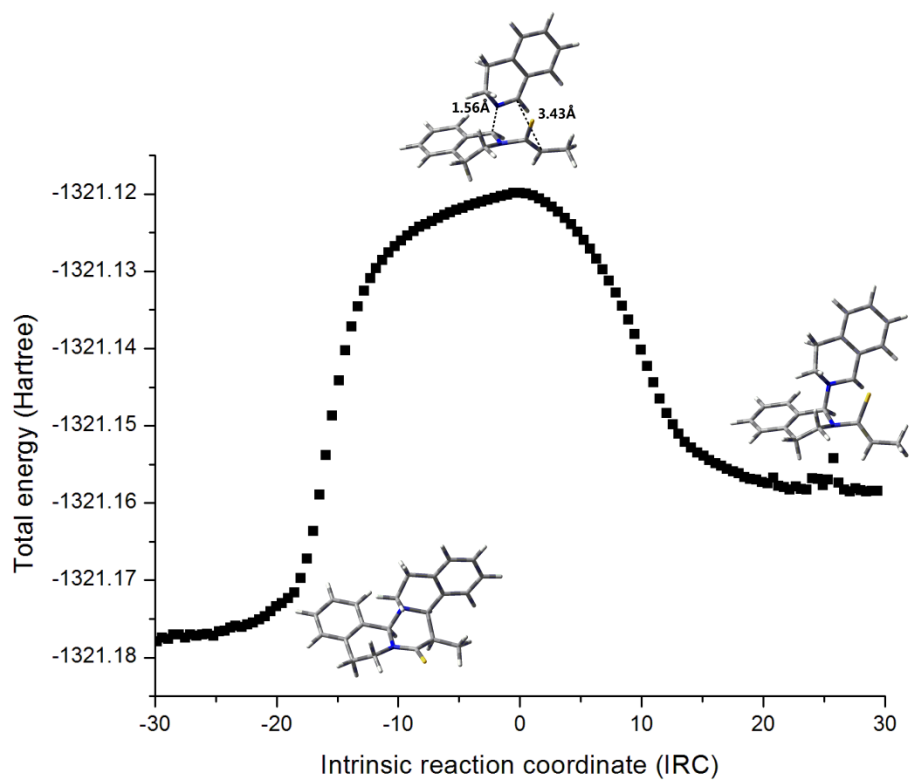


Figure SI-6. The IRC analysis of **TS2-Si-g**.

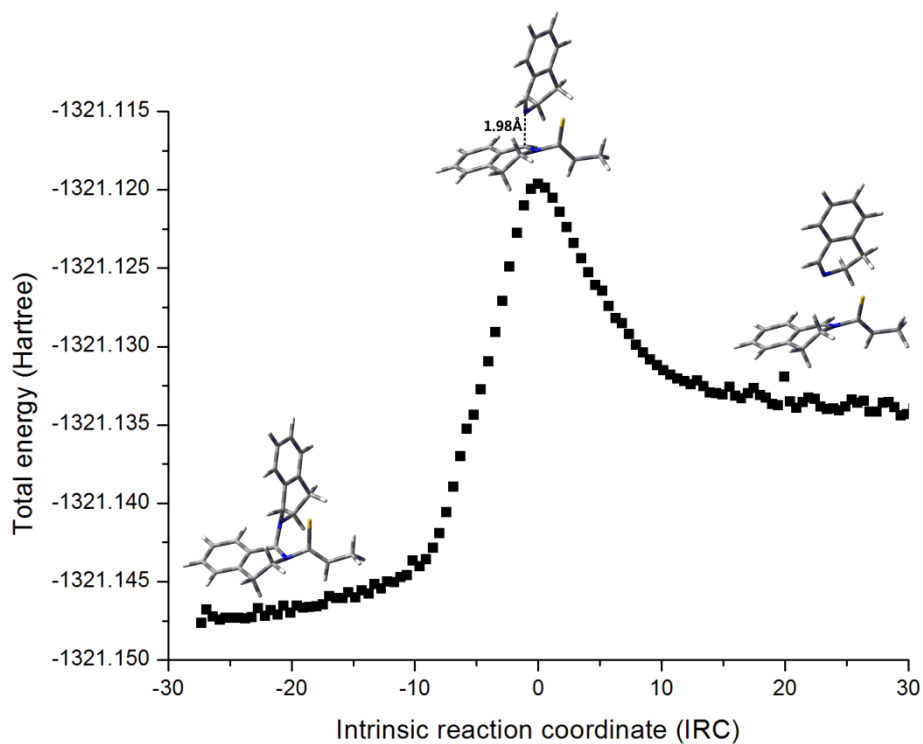


Figure SI-7. The IRC analysis of **TS1-exo-g**.

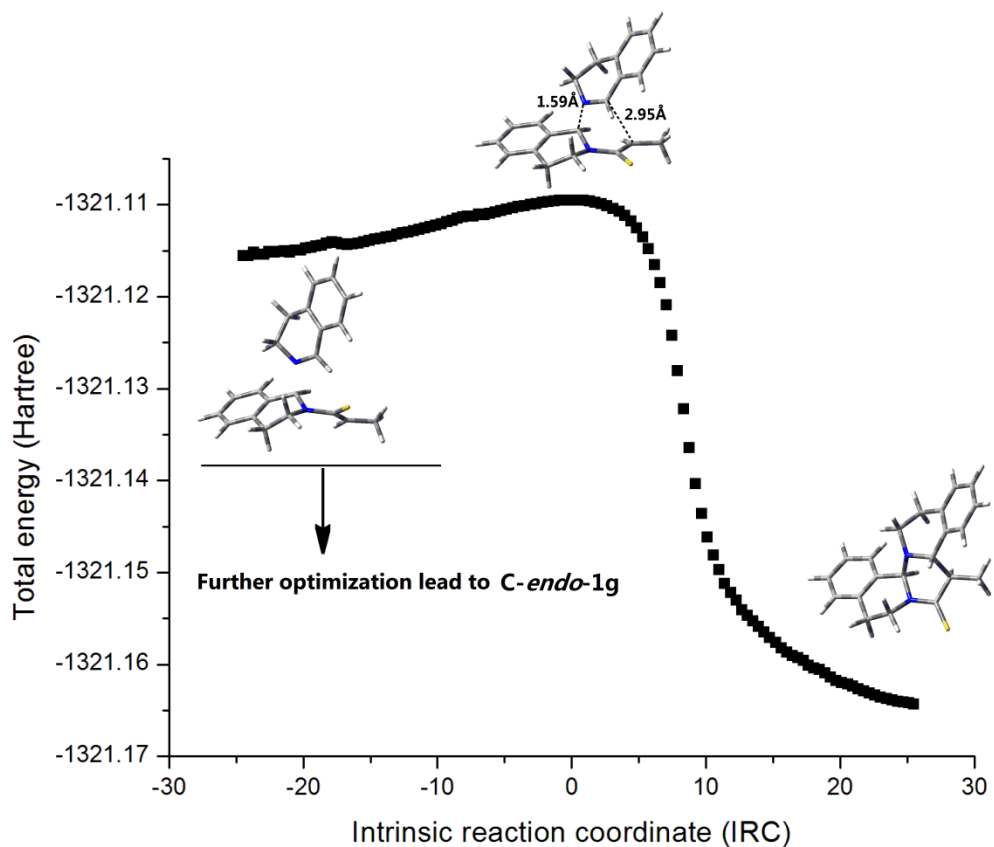


Figure SI-8. The IRC analysis of TS2-Re-g.

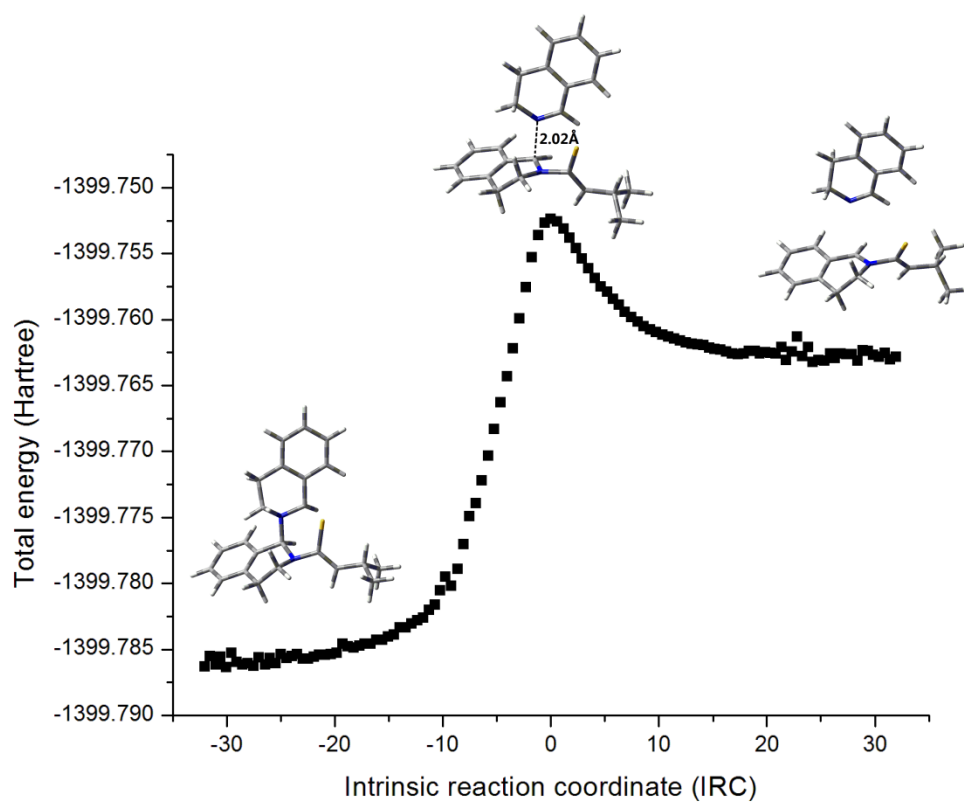


Figure SI-9. The IRC analysis of **TS1-endo-k**.

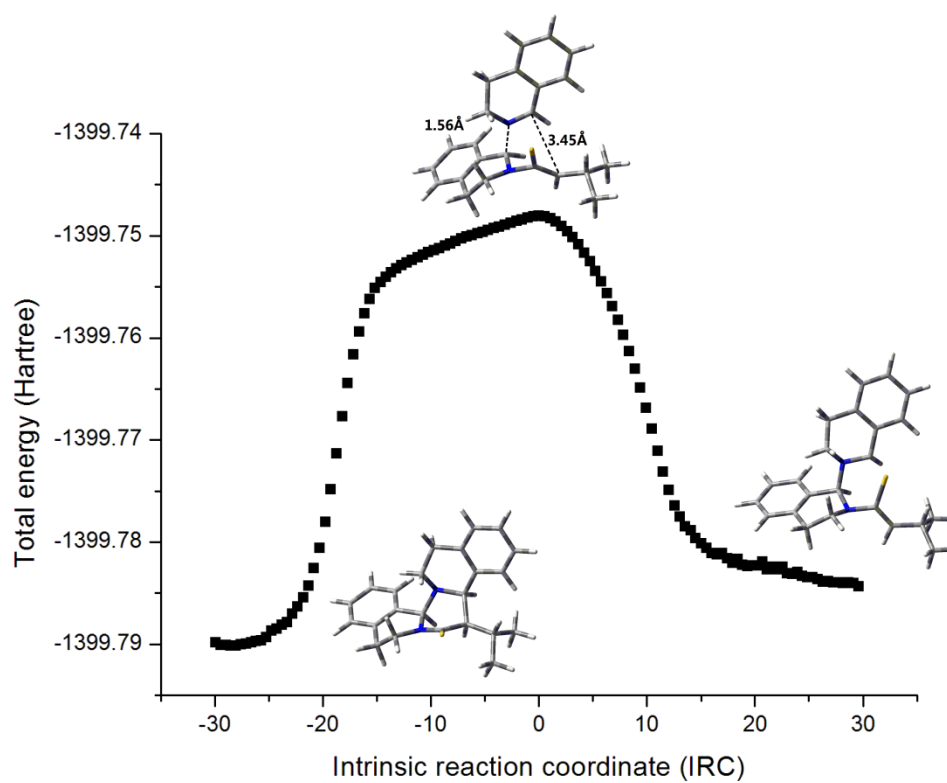


Figure SI-10. The IRC analysis of **TS2-Si-k**.

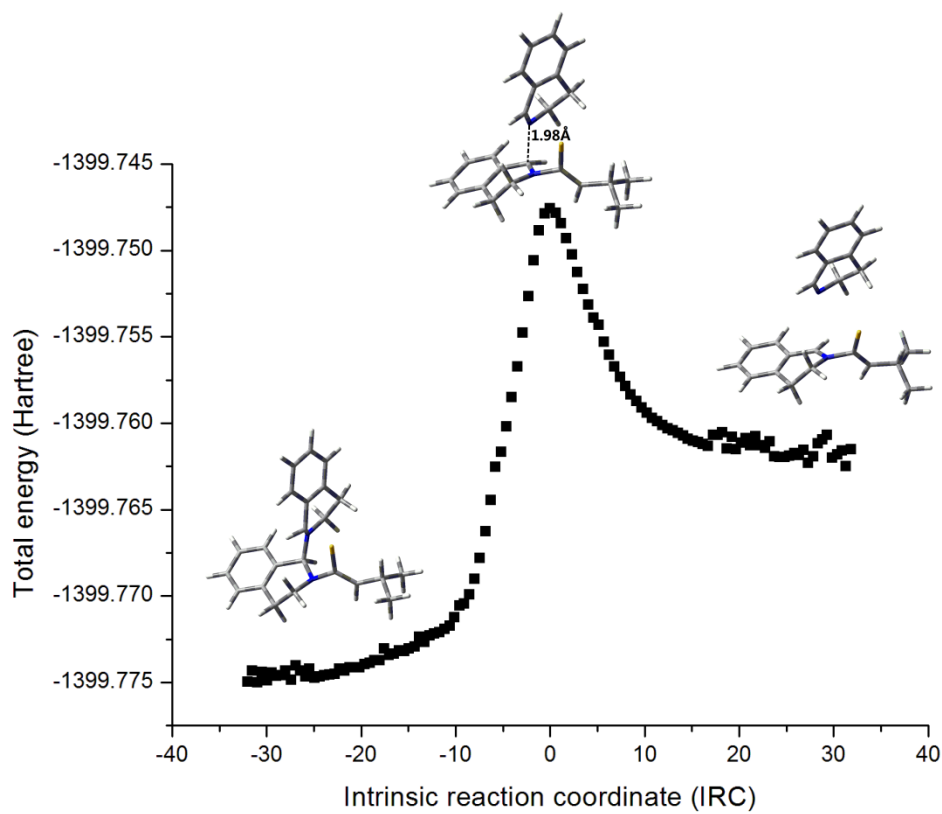


Figure SI-11. The IRC analysis of **TS1-exo-k**.

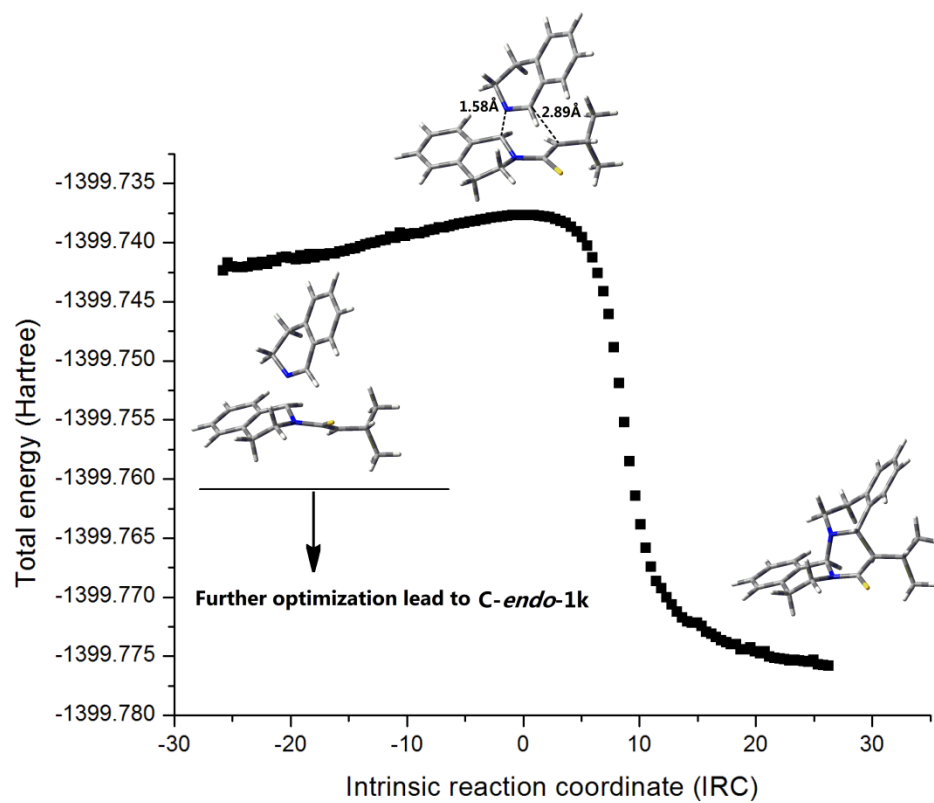


Figure SI-12. The IRC analysis of **TS2-*Re-k***.

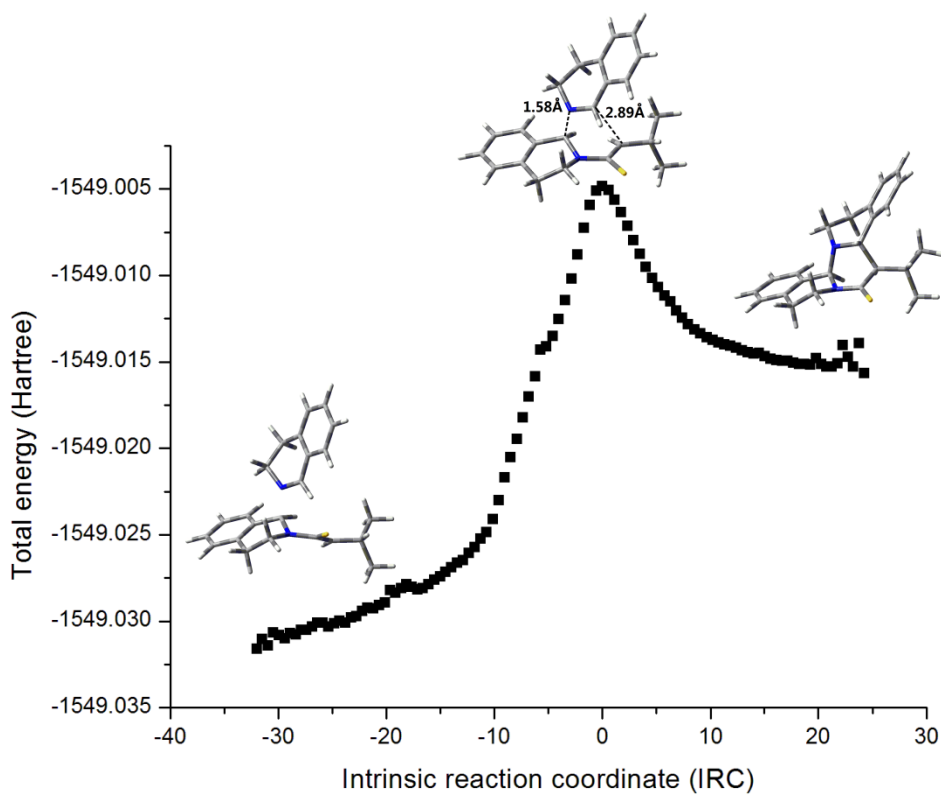


Figure SI-13. The IRC analysis of **TS1-*endo-m***.

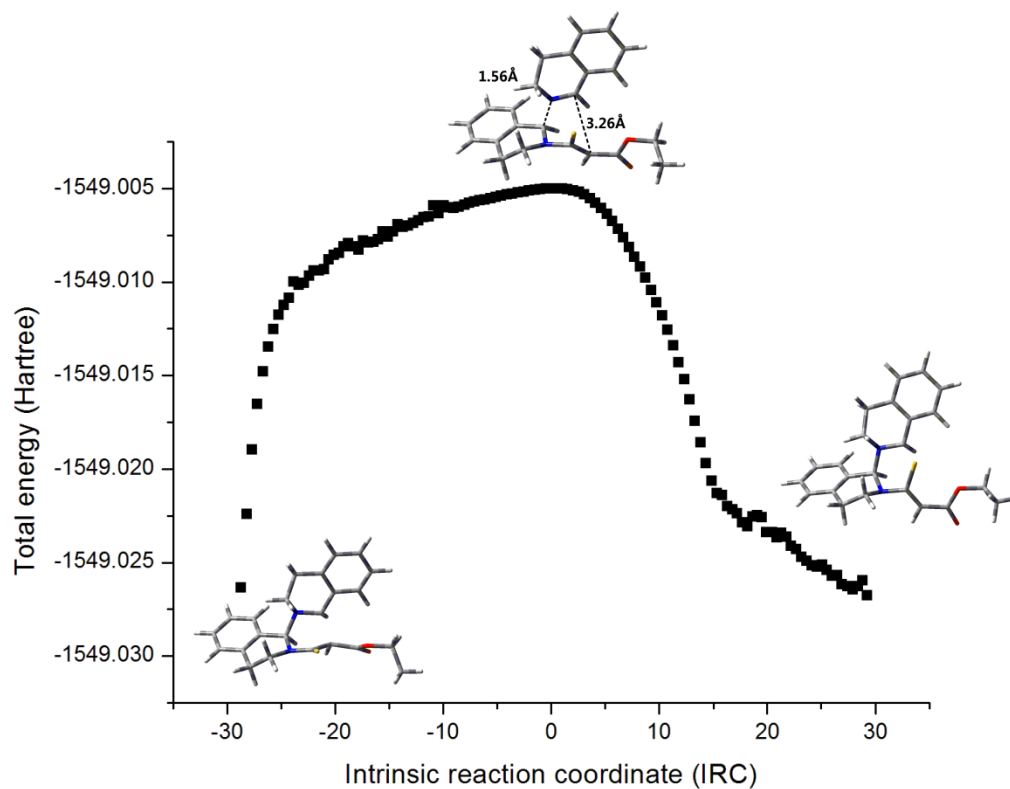


Figure SI-14. The IRC analysis of **TS2-Si-m**.

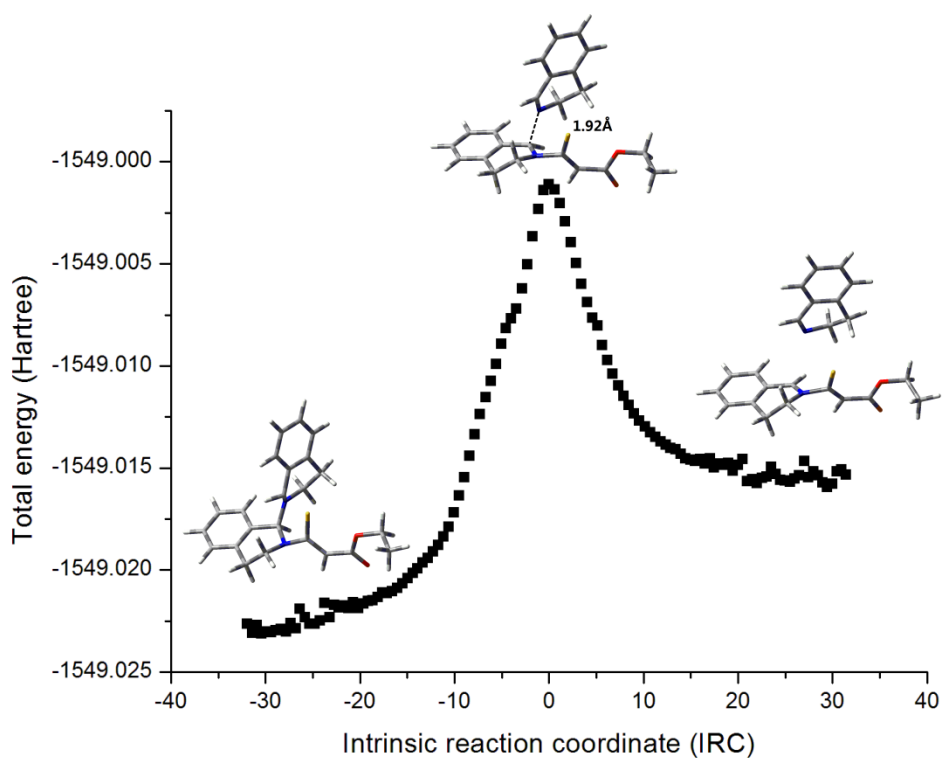


Figure SI-15. The IRC analysis of **TS1-exo-m**.

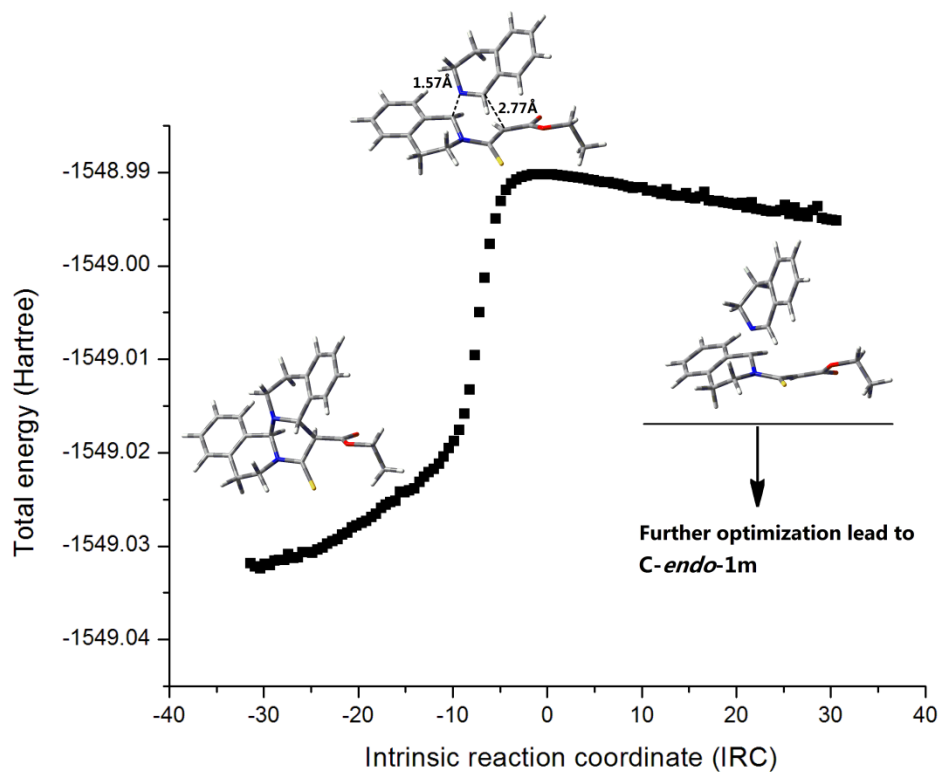


Figure SI-16. The IRC analysis of **TS2-*Re-m***.

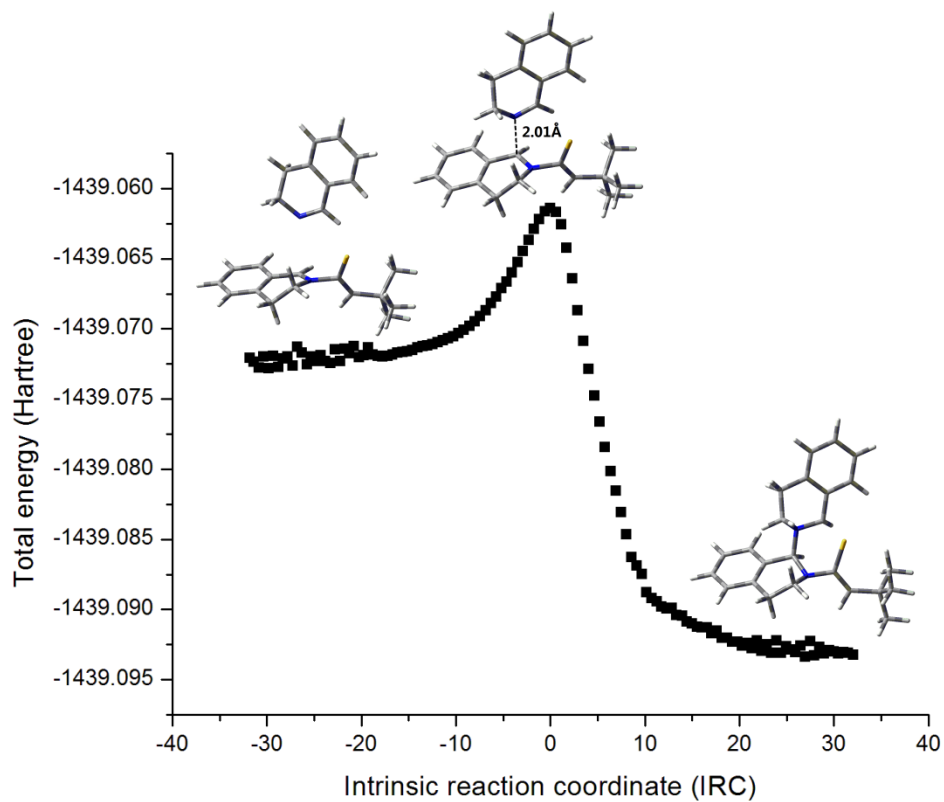


Figure SI-17. The IRC analysis of **TS1-*endo-n***.

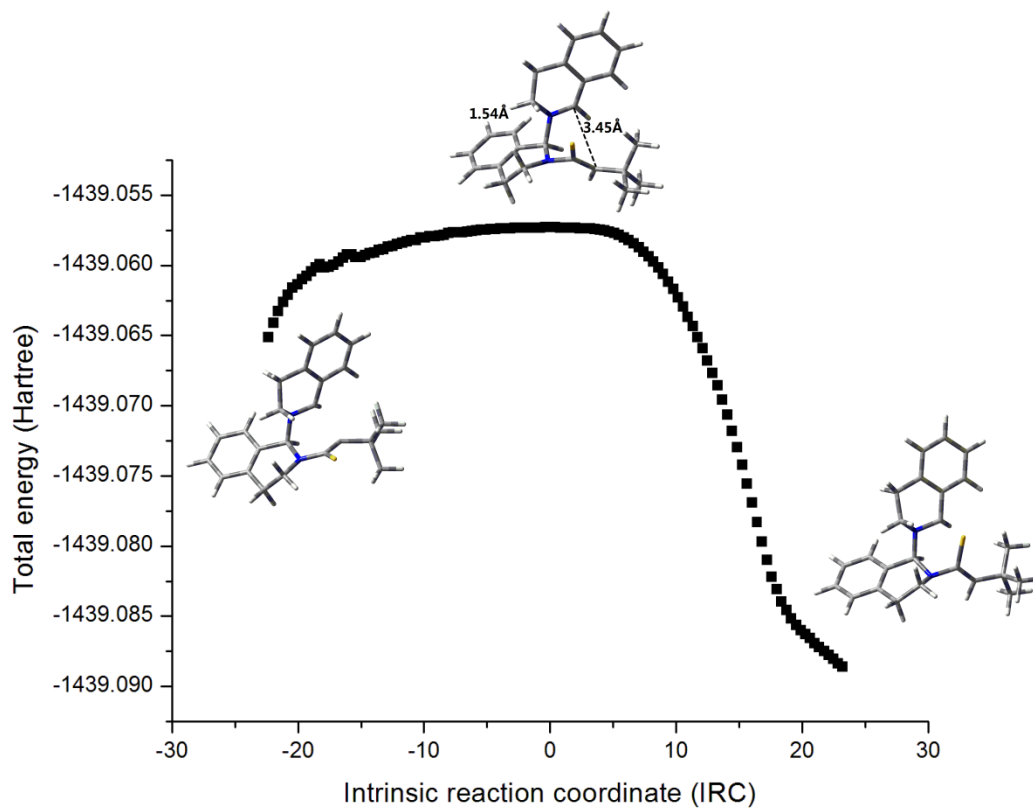


Figure SI-18. The IRC analysis of **TS2-Si-n**.

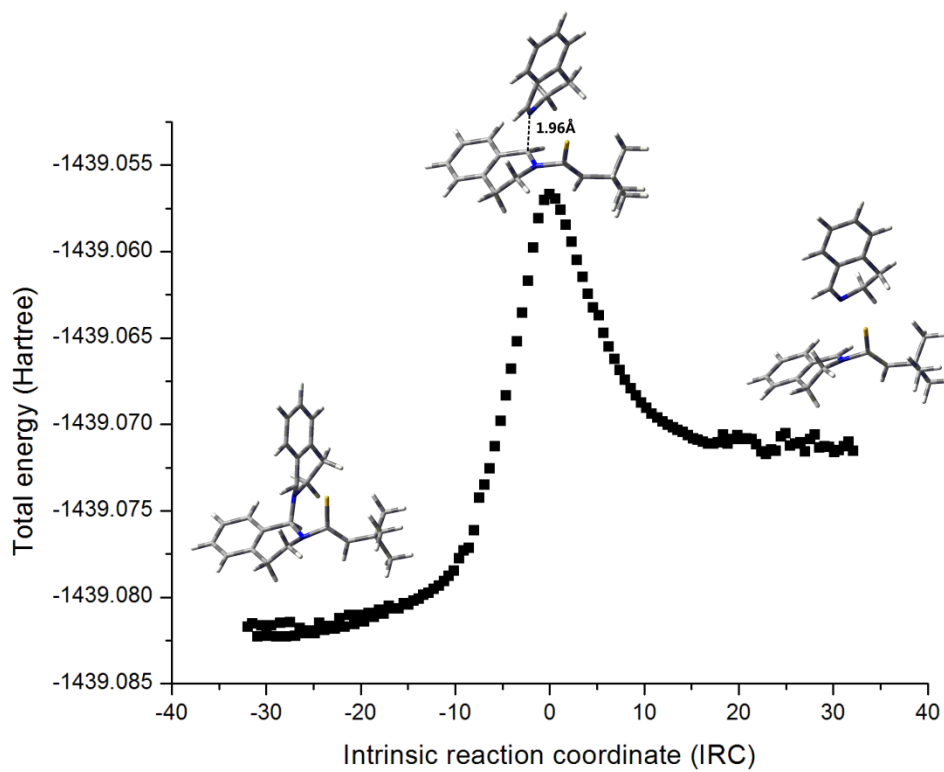


Figure SI-19. The IRC analysis of **TS1-exo-n**.

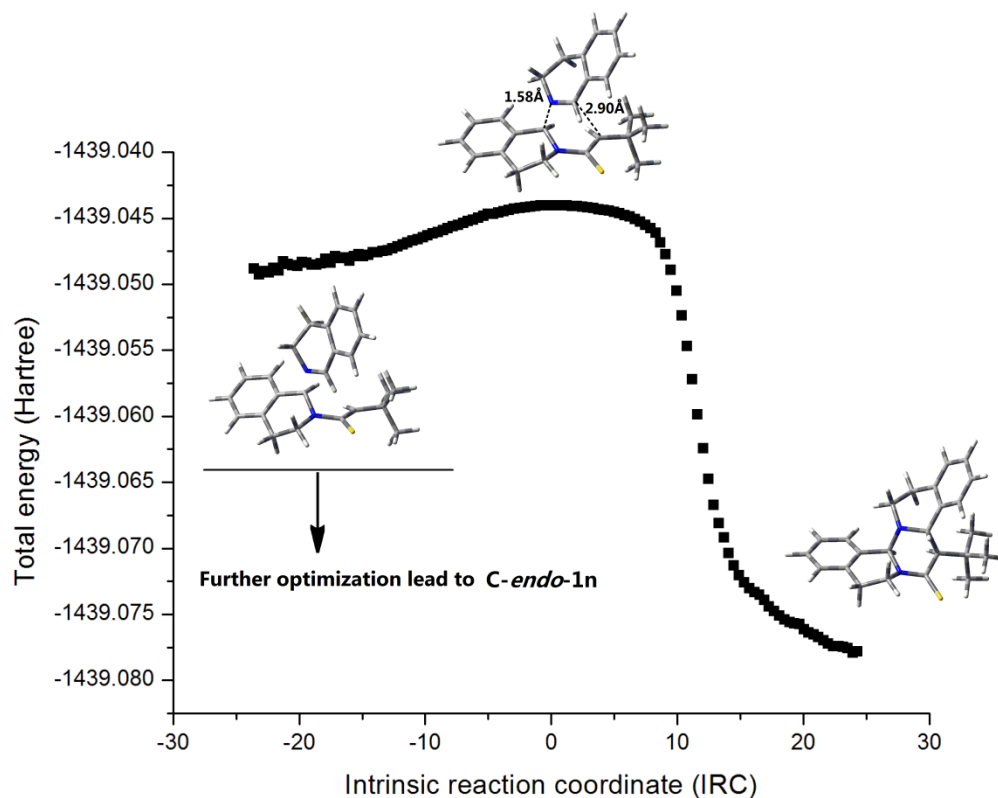
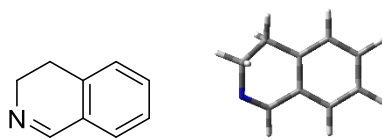


Figure SI-20. The IRC analysis of **TS2-*Re-n***.

4. Coordinates of all stationary points

The structures of all stationary points are optimized at b3lyp/6-31g(d) level in gas phase.

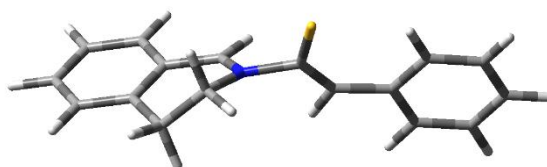
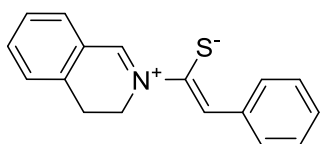
imine **5**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.294275	1.389329	0.003908
2	6	0	-0.079795	0.699831	-0.089044
3	6	0	-0.064351	-0.708373	-0.102980
4	6	0	-1.270009	-1.402292	-0.011081
5	6	0	-2.480391	-0.709960	0.092717
6	6	0	-2.494960	0.686720	0.097911
7	1	0	-1.292489	2.477330	0.010141

8	1	0	-1.265890	-2.490106	-0.021347
9	1	0	-3.413010	-1.262987	0.167748
10	1	0	-3.436693	1.223153	0.174402
11	6	0	1.281506	-1.373904	-0.279675
12	1	0	1.491376	-1.474481	-1.355948
13	1	0	1.278225	-2.389266	0.133866
14	6	0	1.209959	1.409703	-0.162252
15	1	0	1.172636	2.483769	-0.372250
16	7	0	2.363671	0.892633	0.030416
17	6	0	2.394046	-0.537054	0.367499
18	1	0	3.376111	-0.929606	0.083772
19	1	0	2.333655	-0.610234	1.464689

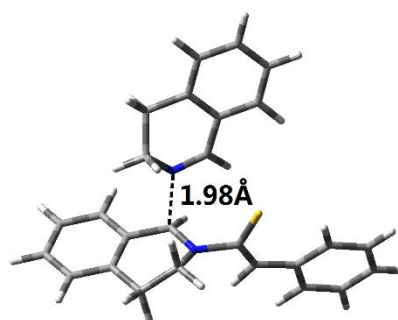
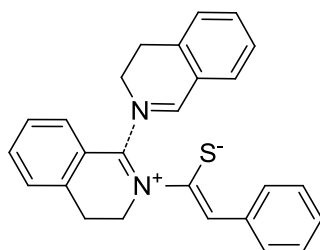
1c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.396335	-1.507593	-1.175368
2	6	0	-2.723032	-0.574132	-0.367004
3	6	0	-3.424838	0.145353	0.627302
4	6	0	-4.791668	-0.069760	0.778224
5	6	0	-5.459188	-0.989793	-0.036757
6	6	0	-4.762019	-1.711181	-1.011362
7	1	0	-2.844567	-2.057251	-1.933675
8	1	0	-5.340969	0.479682	1.538631
9	1	0	-6.526512	-1.145944	0.091773
10	1	0	-5.284592	-2.426095	-1.639608
11	6	0	-2.615986	1.071156	1.505393
12	1	0	-2.222045	0.507289	2.364063
13	1	0	-3.242041	1.871040	1.914814
14	6	0	-1.305279	-0.350261	-0.527006
15	1	0	-0.710789	-1.009221	-1.150633
16	7	0	-0.669787	0.644419	0.038923
17	6	0	-1.459206	1.700327	0.729510
18	1	0	-0.767124	2.245400	1.370716
19	1	0	-1.820382	2.395420	-0.033432
20	6	0	0.770796	0.846262	-0.166314

21	16	0	1.150552	2.393946	-0.784111
22	6	0	1.506015	-0.256399	0.204504
23	1	0	0.948861	-1.074243	0.658807
24	6	0	2.940230	-0.478859	0.149905
25	6	0	3.444293	-1.666305	0.730498
26	6	0	3.868247	0.403888	-0.447267
27	6	0	4.802661	-1.959730	0.722822
28	1	0	2.747693	-2.361854	1.195065
29	6	0	5.228829	0.105374	-0.448104
30	1	0	3.505892	1.317670	-0.902055
31	6	0	5.707047	-1.071546	0.132622
32	1	0	5.158739	-2.880763	1.177904
33	1	0	5.923766	0.800800	-0.912569
34	1	0	6.770339	-1.296815	0.123925

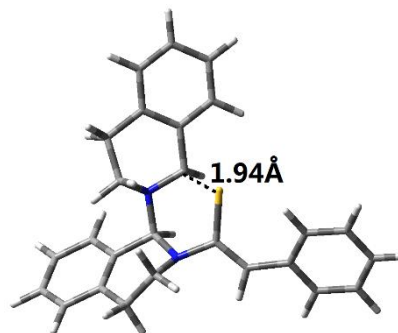
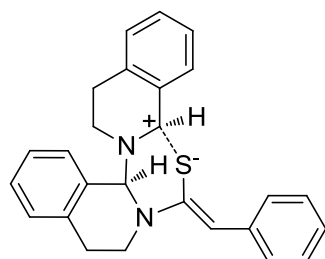
TS1-endo-c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.314135	-0.072173	0.301871
2	6	0	3.625402	-1.209971	-0.172232
3	6	0	4.352491	-2.126110	-0.965265
4	6	0	5.692501	-1.920659	-1.277077
5	6	0	6.356425	-0.786187	-0.802939
6	6	0	5.656804	0.129307	-0.013691
7	1	0	3.783761	0.640914	0.921622
8	1	0	3.845885	-3.013771	-1.340015
9	1	0	6.220625	-2.647043	-1.890525
10	1	0	7.403900	-0.621305	-1.042437
11	1	0	6.163581	1.013363	0.367020
12	6	0	2.221494	-1.511348	0.093008
13	6	0	1.265829	-0.807363	0.765911
14	16	0	1.289089	0.698694	1.623141
15	7	0	-0.069718	-1.430750	0.707634

16	6	0	-0.820692	-1.276885	-0.390094
17	6	0	-0.744172	-1.772727	1.972375
18	6	0	-2.090215	-2.036478	-0.501584
19	6	0	-1.604880	-3.018564	1.764156
20	1	0	0.033246	-1.943266	2.717535
21	1	0	-1.348564	-0.925673	2.318670
22	6	0	-2.863160	-1.941534	-1.667270
23	6	0	-2.489526	-2.887113	0.543953
24	1	0	-0.949977	-3.893430	1.640896
25	1	0	-2.210176	-3.201991	2.659577
26	6	0	-4.033330	-2.682891	-1.798872
27	1	0	-2.543276	-1.272239	-2.461855
28	6	0	-3.669044	-3.625212	0.399498
29	6	0	-4.437783	-3.526099	-0.759255
30	1	0	-4.627842	-2.605672	-2.704638
31	1	0	-3.984158	-4.284987	1.204545
32	1	0	-5.352053	-4.105777	-0.852817
33	1	0	1.890145	-2.463692	-0.321280
34	1	0	-0.248332	-1.140740	-1.302442
35	7	0	-1.444763	0.594845	-0.485427
36	6	0	-0.489472	1.459751	-0.624261
37	6	0	-2.655132	1.033176	0.215492
38	6	0	-0.654157	2.894952	-0.381307
39	1	0	0.438987	1.118189	-1.074582
40	6	0	-3.106415	2.418193	-0.258871
41	1	0	-3.439309	0.289219	0.053125
42	1	0	-2.430254	1.062545	1.293076
43	6	0	0.448896	3.760314	-0.386157
44	6	0	-1.956804	3.399910	-0.200439
45	1	0	-3.479178	2.345393	-1.292001
46	1	0	-3.946511	2.762196	0.355314
47	6	0	0.260834	5.126452	-0.202590
48	1	0	1.446461	3.345579	-0.499419
49	6	0	-2.131613	4.772342	-0.022061
50	6	0	-1.030612	5.631545	-0.020293
51	1	0	1.115436	5.796642	-0.194631
52	1	0	-3.133051	5.172323	0.119698
53	1	0	-1.180219	6.697685	0.127824

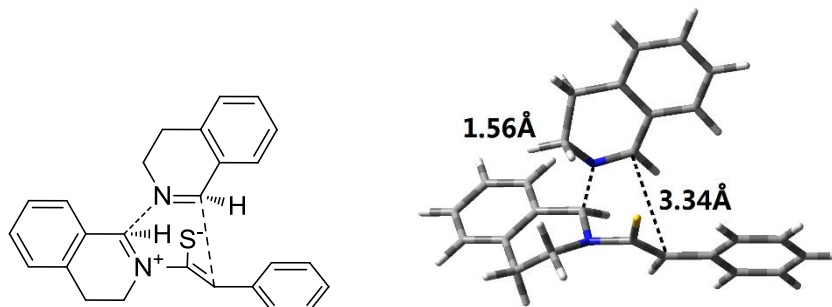
C-endo-c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.330406	-0.085757	0.551561
2	6	0	3.757842	-1.204342	-0.084982
3	6	0	4.620259	-2.061205	-0.800693
4	6	0	5.982085	-1.797540	-0.909406
5	6	0	6.527818	-0.671409	-0.288554
6	6	0	5.695613	0.176058	0.444354
7	1	0	3.712463	0.572681	1.149620
8	1	0	4.203437	-2.941248	-1.285339
9	1	0	6.618940	-2.473026	-1.474793
10	1	0	7.591734	-0.463702	-0.365856
11	1	0	6.111987	1.044964	0.947572
12	6	0	2.338450	-1.568227	-0.040271
13	6	0	1.218087	-0.847560	0.198626
14	16	0	1.193727	0.915511	0.565691
15	7	0	-0.028778	-1.542477	0.225831
16	6	0	-1.111603	-0.949783	-0.561217
17	6	0	-0.419812	-2.128271	1.516197
18	6	0	-2.366247	-1.811440	-0.528878
19	6	0	-1.359281	-3.303295	1.252571
20	1	0	0.490776	-2.474268	2.011287
21	1	0	-0.896020	-1.396476	2.188019
22	6	0	-3.418870	-1.480560	-1.394005
23	6	0	-2.490286	-2.917759	0.324602
24	1	0	-0.779522	-4.119493	0.799136
25	1	0	-1.760185	-3.685546	2.199944
26	6	0	-4.585793	-2.238004	-1.422535
27	1	0	-3.312872	-0.612478	-2.039064
28	6	0	-3.673156	-3.670683	0.290214
29	6	0	-4.713538	-3.341055	-0.573426
30	1	0	-5.391374	-1.971200	-2.101226
31	1	0	-3.772760	-4.525567	0.955876

32	1	0	-5.621598	-3.938181	-0.583459
33	1	0	2.139025	-2.616895	-0.258887
34	1	0	-0.741537	-0.928463	-1.595702
35	7	0	-1.444897	0.464508	-0.276225
36	6	0	-0.342916	1.334212	-0.533372
37	6	0	-2.156672	0.791811	0.964027
38	6	0	-0.657354	2.797830	-0.338884
39	1	0	0.019060	1.154625	-1.550264
40	6	0	-2.822985	2.157913	0.797297
41	1	0	-2.909290	0.022315	1.147174
42	1	0	-1.471216	0.814306	1.826402
43	6	0	0.238049	3.764842	-0.816169
44	6	0	-1.839196	3.197634	0.304922
45	1	0	-3.648952	2.063305	0.078524
46	1	0	-3.265232	2.476231	1.749758
47	6	0	-0.030475	5.121609	-0.659863
48	1	0	1.152795	3.444011	-1.308735
49	6	0	-2.097203	4.566022	0.456368
50	6	0	-1.204939	5.524149	-0.018539
51	1	0	0.671108	5.861070	-1.035976
52	1	0	-3.011600	4.878579	0.956449
53	1	0	-1.422792	6.580923	0.111564

TS2-Si-c

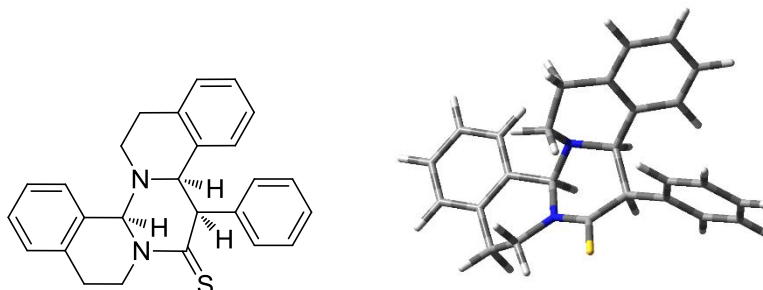


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.594999	-1.522207	0.523829
2	6	0	2.577130	-2.181305	-0.206048
3	6	0	2.986544	-2.987026	-1.296586
4	6	0	4.325248	-3.126274	-1.645312
5	6	0	5.315470	-2.460226	-0.916465
6	6	0	4.935308	-1.663107	0.165678
7	1	0	3.313026	-0.915033	1.375927

8	1	0	2. 226851	-3. 512312	-1. 873315
9	1	0	4. 598672	-3. 757342	-2. 488231
10	1	0	6. 363666	-2. 567704	-1. 184013
11	1	0	5. 694817	-1. 147346	0. 749895
12	6	0	1. 149517	-2. 076017	0. 059841
13	6	0	0. 446917	-1. 342195	0. 987156
14	16	0	0. 992561	-0. 335357	2. 290647
15	7	0	-0. 998033	-1. 364635	0. 753642
16	6	0	-1. 434935	-0. 654317	-0. 395044
17	6	0	-1. 904412	-1. 412800	1. 905483
18	6	0	-2. 930883	-0. 671868	-0. 631653
19	6	0	-3. 224897	-2. 043387	1. 463448
20	1	0	-1. 416896	-2. 018630	2. 669847
21	1	0	-2. 078189	-0. 425932	2. 356207
22	6	0	-3. 447274	-0. 042124	-1. 772749
23	6	0	-3. 791556	-1. 343115	0. 249861
24	1	0	-3. 051759	-3. 101977	1. 224434
25	1	0	-3. 948821	-2. 016465	2. 287197
26	6	0	-4. 812624	-0. 066755	-2. 041830
27	1	0	-2. 770492	0. 470695	-2. 452765
28	6	0	-5. 164350	-1. 360090	-0. 032654
29	6	0	-5. 675255	-0. 729885	-1. 164427
30	1	0	-5. 201763	0. 423449	-2. 929761
31	1	0	-5. 835947	-1. 875407	0. 650175
32	1	0	-6. 743271	-0. 754101	-1. 363369
33	1	0	0. 534298	-2. 682481	-0. 606833
34	1	0	-0. 914896	-1. 031096	-1. 280767
35	7	0	-0. 930712	0. 819759	-0. 347199
36	6	0	0. 288667	1. 050050	-0. 754297
37	6	0	-1. 522479	1. 755995	0. 633264
38	6	0	0. 994612	2. 280816	-0. 490242
39	1	0	0. 772800	0. 267716	-1. 330822
40	6	0	-1. 203898	3. 203396	0. 259566
41	1	0	-2. 598277	1. 579674	0. 659555
42	1	0	-1. 074960	1. 491220	1. 604003
43	6	0	2. 368336	2. 378749	-0. 766382
44	6	0	0. 278819	3. 383934	0. 022704
45	1	0	-1. 762664	3. 490335	-0. 644233
46	1	0	-1. 550644	3. 858471	1. 065625
47	6	0	3. 033736	3. 576360	-0. 527029
48	1	0	2. 906464	1. 507201	-1. 129019
49	6	0	0. 956674	4. 578611	0. 242645
50	6	0	2. 326293	4. 673668	-0. 027689
51	1	0	4. 098763	3. 655058	-0. 721655

52	1	0	0.420579	5.438663	0.635873
53	1	0	2.844634	5.609898	0.160196

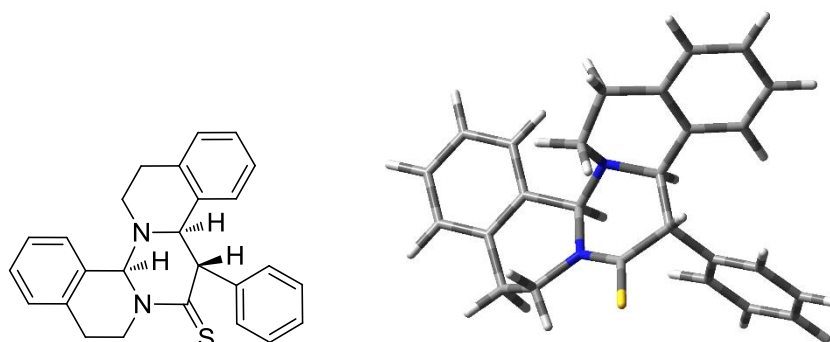
7c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.032836	-0.938559	0.680147
2	6	0	2.330001	-1.260968	-0.489946
3	6	0	3.030140	-1.869066	-1.537994
4	6	0	4.394458	-2.150311	-1.429672
5	6	0	5.079411	-1.825197	-0.260501
6	6	0	4.391661	-1.218969	0.794443
7	1	0	2.512441	-0.467871	1.507475
8	1	0	2.500796	-2.135959	-2.450875
9	1	0	4.915007	-2.626382	-2.256606
10	1	0	6.140250	-2.043093	-0.168177
11	1	0	4.916468	-0.964221	1.711360
12	6	0	0.859188	-0.946537	-0.669589
13	6	0	-0.088812	-1.717541	0.277605
14	16	0	0.441587	-2.893718	1.342884
15	7	0	-1.404933	-1.425178	0.096296
16	6	0	-1.751830	-0.167050	-0.635196
17	6	0	-2.444851	-2.165078	0.821279
18	6	0	-3.216648	0.231659	-0.499935
19	6	0	-3.764174	-2.141418	0.053243
20	1	0	-2.081545	-3.184796	0.954369
21	1	0	-2.575226	-1.738427	1.825886
22	6	0	-3.590546	1.556083	-0.760641
23	6	0	-4.201027	-0.725815	-0.219153
24	1	0	-3.641718	-2.696430	-0.888471
25	1	0	-4.523603	-2.675751	0.635094
26	6	0	-4.932293	1.931059	-0.727195
27	1	0	-2.817063	2.283861	-0.983026

28	6	0	-5.544950	-0.337831	-0.182709
29	6	0	-5.914228	0.981579	-0.436447
30	1	0	-5.209847	2.962551	-0.926304
31	1	0	-6.304583	-1.080687	0.050177
32	1	0	-6.961836	1.268556	-0.403988
33	1	0	0.584080	-1.354236	-1.652352
34	1	0	-1.566855	-0.352729	-1.704512
35	7	0	-0.843874	0.898113	-0.254588
36	6	0	0.481487	0.626552	-0.814683
37	6	0	-0.814870	1.170595	1.191596
38	6	0	1.503501	1.653798	-0.346731
39	1	0	0.386335	0.774720	-1.897509
40	6	0	-0.093146	2.489528	1.433003
41	1	0	-1.847207	1.227598	1.547779
42	1	0	-0.316143	0.364810	1.755107
43	6	0	2.708316	1.789255	-1.054123
44	6	0	1.237537	2.532217	0.715939
45	1	0	-0.724413	3.314580	1.074267
46	1	0	0.046416	2.644373	2.510280
47	6	0	3.651306	2.747239	-0.697490
48	1	0	2.912397	1.125545	-1.889240
49	6	0	2.197753	3.489679	1.072987
50	6	0	3.399088	3.599421	0.380590
51	1	0	4.578968	2.827817	-1.257231
52	1	0	1.986498	4.161088	1.902872
53	1	0	4.130791	4.348102	0.672563

4c

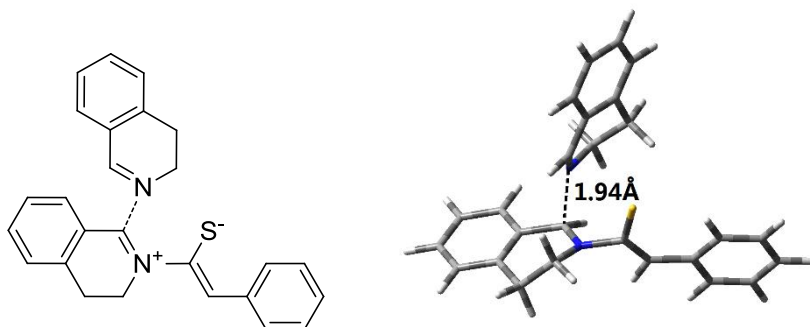


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.232789	0.543015	0.497750
2	6	0	-0.071654	1.277263	1.200198

3	16	0	-0.417719	2.153820	2.587212
4	7	0	1.166038	1.178372	0.664159
5	6	0	1.430575	0.151632	-0.409819
6	6	0	2.283447	1.917536	1.269413
7	6	0	2.911204	-0.169071	-0.577634
8	6	0	3.420792	2.118728	0.270972
9	1	0	1.890037	2.873866	1.617923
10	1	0	2.640590	1.377663	2.157016
11	6	0	3.299079	-1.394570	-1.133176
12	6	0	3.882071	0.801058	-0.292402
13	1	0	3.078571	2.782857	-0.536649
14	1	0	4.244209	2.637803	0.773831
15	6	0	4.644924	-1.666283	-1.374558
16	1	0	2.535350	-2.126114	-1.375639
17	6	0	5.230418	0.517010	-0.532486
18	6	0	5.615431	-0.709917	-1.069959
19	1	0	4.934050	-2.623336	-1.800098
20	1	0	5.980758	1.267801	-0.295175
21	1	0	6.666410	-0.918323	-1.251091
22	1	0	1.093829	0.596073	-1.358119
23	7	0	0.614357	-1.023072	-0.218644
24	6	0	-0.791097	-0.666263	-0.427240
25	6	0	0.827664	-1.758726	1.037889
26	6	0	-1.704796	-1.867831	-0.249792
27	1	0	-0.868807	-0.333332	-1.468981
28	6	0	0.161562	-3.127717	0.914950
29	1	0	1.903072	-1.871710	1.196435
30	1	0	0.425045	-1.218353	1.910441
31	6	0	-3.015207	-1.815498	-0.746726
32	6	0	-1.264760	-3.023497	0.415827
33	1	0	0.744883	-3.744238	0.216568
34	1	0	0.188161	-3.640481	1.884535
35	6	0	-3.887945	-2.887602	-0.578594
36	1	0	-3.351300	-0.924286	-1.269623
37	6	0	-2.153164	-4.094632	0.580588
38	6	0	-3.455600	-4.033873	0.092304
39	1	0	-4.899262	-2.829969	-0.971932
40	1	0	-1.811205	-4.988019	1.099380
41	1	0	-4.129071	-4.875308	0.231846
42	6	0	-2.110024	1.542567	-0.251061
43	6	0	-1.616528	2.285761	-1.333560
44	6	0	-3.444477	1.729269	0.130335
45	6	0	-2.434933	3.182457	-2.019463
46	1	0	-0.578490	2.176914	-1.638548

47	6	0	-4.267645	2.623411	-0.556424
48	1	0	-3.838352	1.172372	0.975945
49	6	0	-3.766456	3.352529	-1.634893
50	1	0	-2.030598	3.751438	-2.852647
51	1	0	-5.300138	2.752691	-0.242641
52	1	0	-4.405228	4.050923	-2.168748
53	1	0	-1.832317	0.144318	1.317350

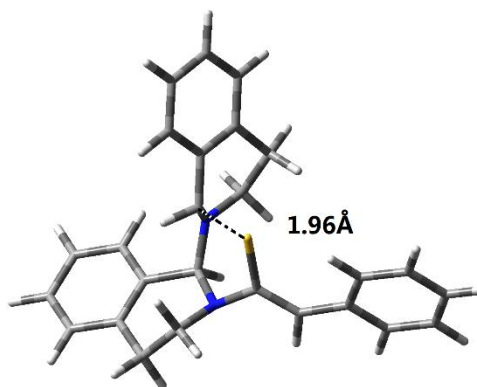
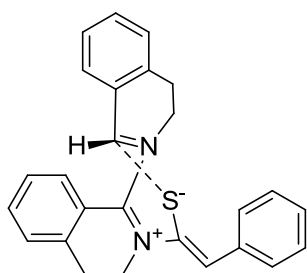
TS1-exo-c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.010172	0.891761	0.486079
2	6	0	-3.131020	1.865978	-0.035692
3	6	0	-3.691244	2.877349	-0.848535
4	6	0	-5.052053	2.915793	-1.134406
5	6	0	-5.905814	1.939392	-0.614097
6	6	0	-5.372730	0.933782	0.195193
7	1	0	-3.610913	0.111177	1.122702
8	1	0	-3.036308	3.643442	-1.260041
9	1	0	-5.448126	3.709484	-1.763795
10	1	0	-6.970312	1.965794	-0.832863
11	1	0	-6.026734	0.171163	0.612257
12	6	0	-1.691077	1.903785	0.197930
13	6	0	-0.870662	1.043757	0.866932
14	16	0	-1.165440	-0.401968	1.778760
15	7	0	0.560479	1.378239	0.761502
16	6	0	1.202464	1.120289	-0.389996
17	6	0	1.332348	1.555790	2.006337
18	6	0	2.645574	1.471477	-0.493623
19	6	0	2.454750	2.561191	1.762395
20	1	0	0.632364	1.909184	2.764044
21	1	0	1.737478	0.601752	2.361091
22	6	0	3.366776	1.154496	-1.653052

23	6	0	3.269156	2.179545	0.548278
24	1	0	2.019190	3.559751	1.612101
25	1	0	3.093669	2.624329	2.650771
26	6	0	4.701203	1.525217	-1.779079
27	1	0	2.877908	0.604678	-2.452619
28	6	0	4.613205	2.544141	0.411266
29	6	0	5.327665	2.220486	-0.740112
30	1	0	5.253032	1.272332	-2.679853
31	1	0	5.099797	3.088284	1.217350
32	1	0	6.371518	2.508866	-0.828931
33	1	0	-1.194411	2.767275	-0.245786
34	1	0	0.599177	1.289968	-1.277436
35	7	0	1.122527	-0.786119	-0.748716
36	6	0	1.104095	-1.581623	0.276216
37	6	0	0.467170	-1.223393	-1.989270
38	6	0	0.599875	-2.953741	0.221952
39	1	0	1.625919	-1.258088	1.170446
40	6	0	-0.706794	-2.178184	-1.742138
41	1	0	0.124495	-0.332590	-2.527313
42	1	0	1.229771	-1.706318	-2.618534
43	6	0	0.993899	-3.913592	1.162619
44	6	0	-0.281245	-3.296556	-0.822623
45	1	0	-1.524668	-1.621142	-1.263725
46	1	0	-1.080676	-2.563540	-2.697226
47	6	0	0.523097	-5.220636	1.060967
48	1	0	1.665444	-3.631584	1.969758
49	6	0	-0.749469	-4.604897	-0.910687
50	6	0	-0.346790	-5.564898	0.023208
51	1	0	0.828156	-5.967114	1.788576
52	1	0	-1.436091	-4.877407	-1.708636
53	1	0	-0.716937	-6.583295	-0.058373

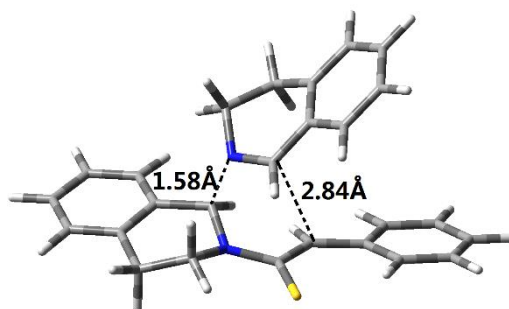
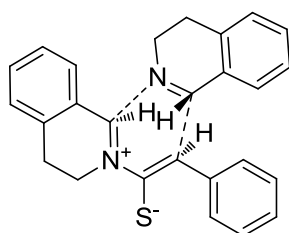
C-*exo-c*



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.112624	-0.391673	-0.724734
2	6	0	-3.515485	-1.406104	0.050220
3	6	0	-4.352112	-2.144987	0.913795
4	6	0	-5.711041	-1.868491	1.024429
5	6	0	-6.280610	-0.845593	0.262303
6	6	0	-5.474645	-0.115254	-0.612309
7	1	0	-3.516550	0.175506	-1.429198
8	1	0	-3.916336	-2.942478	1.511541
9	1	0	-6.327072	-2.452745	1.703217
10	1	0	-7.342342	-0.627756	0.341851
11	1	0	-5.909534	0.672199	-1.222590
12	6	0	-2.095582	-1.766753	0.025625
13	6	0	-0.998406	-1.119721	-0.429994
14	16	0	-0.975939	0.474325	-1.252677
15	7	0	0.277519	-1.747600	-0.274621
16	6	0	1.163996	-1.077031	0.695662
17	6	0	0.868664	-2.233921	-1.528135
18	6	0	2.637127	-1.455870	0.503376
19	6	0	2.007535	-3.194215	-1.201187
20	1	0	0.073572	-2.748737	-2.075042
21	1	0	1.237828	-1.423021	-2.179371
22	6	0	3.602982	-0.776697	1.258564
23	6	0	3.039187	-2.493330	-0.351476
24	1	0	1.594570	-4.063720	-0.670927
25	1	0	2.464772	-3.566221	-2.126074
26	6	0	4.948415	-1.125171	1.182289
27	1	0	3.291457	0.041174	1.901456
28	6	0	4.397169	-2.831265	-0.428382
29	6	0	5.348960	-2.161826	0.335282
30	1	0	5.682606	-0.586969	1.775798
31	1	0	4.704688	-3.625948	-1.104905
32	1	0	6.397704	-2.437737	0.263122
33	1	0	-1.868234	-2.730016	0.479993
34	1	0	0.865315	-1.431435	1.692255
35	7	0	0.984532	0.386078	0.748035
36	6	0	0.756889	1.009724	-0.505128
37	6	0	0.395851	0.966243	1.966341
38	6	0	0.770981	2.509378	-0.437630
39	1	0	1.487845	0.644091	-1.229187
40	6	0	-0.462301	2.214640	1.696390

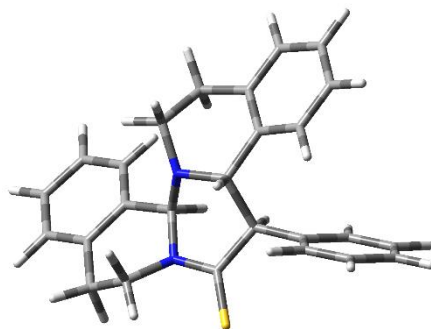
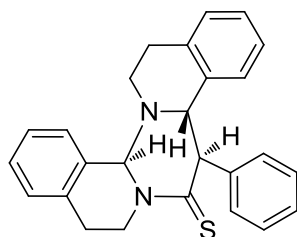
41	1	0	-0.219971	0.213334	2.474871
42	1	0	1.207220	1.236818	2.658930
43	6	0	1.352980	3.286045	-1.441380
44	6	0	0.181225	3.122449	0.679169
45	1	0	-1.443796	1.899075	1.320341
46	1	0	-0.631410	2.740664	2.642671
47	6	0	1.353536	4.678226	-1.338309
48	1	0	1.810545	2.801400	-2.300810
49	6	0	0.198230	4.514090	0.781031
50	6	0	0.778167	5.291518	-0.224565
51	1	0	1.808750	5.279758	-2.120253
52	1	0	-0.248915	4.993137	1.649256
53	1	0	0.783431	6.374622	-0.135498

TS2-Re-c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.825347	-1.439399	0.684956
2	6	0	-0.018714	-1.850177	-0.382859
3	16	0	-0.541594	-2.793699	-1.712921
4	7	0	1.341856	-1.347700	-0.391324
5	6	0	1.673900	-0.178400	0.350266
6	6	0	2.148694	-1.488283	-1.618127
7	6	0	3.171092	0.041967	0.523337
8	6	0	3.626373	-1.638158	-1.292608
9	1	0	1.772929	-2.354473	-2.158282
10	1	0	1.999850	-0.608663	-2.265084
11	6	0	3.641207	0.817509	1.595788
12	6	0	4.103710	-0.611854	-0.296888
13	1	0	3.803532	-2.637810	-0.870768
14	1	0	4.209157	-1.581956	-2.220495
15	6	0	5.002893	1.036423	1.789426
16	1	0	2.938801	1.227213	2.317131

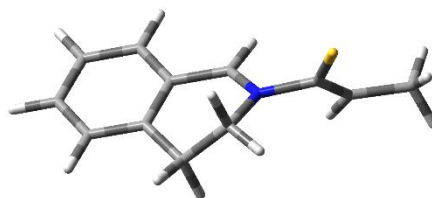
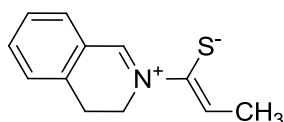
17	6	0	5.471058	-0.384152	-0.098140
18	6	0	5.924248	0.449403	0.920623
19	1	0	5.341046	1.645547	2.622825
20	1	0	6.186118	-0.888664	-0.744126
21	1	0	6.989522	0.614403	1.057162
22	1	0	1.243384	-0.226212	1.350462
23	6	0	-0.207636	0.814310	-0.921945
24	6	0	-1.302223	1.750083	-0.998563
25	7	0	0.917793	1.069638	-0.252308
26	6	0	-2.310813	1.579907	-1.966249
27	6	0	-1.393443	2.800704	-0.056254
28	6	0	1.020567	2.392144	0.398106
29	6	0	-3.385754	2.460808	-2.010535
30	1	0	-2.240029	0.754307	-2.668888
31	6	0	-2.475735	3.671576	-0.112274
32	6	0	-0.310246	2.864658	0.992533
33	1	0	1.799411	2.355760	1.154394
34	1	0	1.354346	3.101490	-0.370398
35	6	0	-3.465878	3.508673	-1.088081
36	1	0	-4.163209	2.331123	-2.757412
37	1	0	-2.553168	4.481501	0.609207
38	1	0	-0.585737	2.225946	1.845265
39	1	0	-0.192285	3.882140	1.382241
40	1	0	-4.303631	4.199489	-1.123762
41	1	0	-0.236568	-0.047578	-1.575548
42	1	0	-0.314042	-1.014890	1.544717
43	6	0	-2.241789	-1.620593	0.968140
44	6	0	-2.690467	-1.201441	2.246118
45	6	0	-3.220444	-2.135064	0.085978
46	6	0	-4.023394	-1.292566	2.627365
47	1	0	-1.963444	-0.800790	2.951148
48	6	0	-4.556336	-2.220375	0.471999
49	1	0	-2.912293	-2.479116	-0.892144
50	6	0	-4.972764	-1.804621	1.738454
51	1	0	-4.322936	-0.965716	3.620466
52	1	0	-5.282383	-2.624785	-0.229742
53	1	0	-6.016976	-1.881126	2.030400



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.953703	-0.752049	0.321530
2	6	0	-0.007272	-1.931594	0.014693
3	16	0	-0.513265	-3.498089	-0.253010
4	7	0	1.296538	-1.544546	-0.064683
5	6	0	1.590734	-0.129631	0.206526
6	6	0	2.217079	-2.229368	-0.985065
7	6	0	3.100122	0.128051	0.310044
8	6	0	3.631479	-2.231391	-0.441106
9	1	0	1.840922	-3.239450	-1.132749
10	1	0	2.178080	-1.692384	-1.944496
11	6	0	3.547579	1.336264	0.871618
12	6	0	4.056998	-0.852955	-0.000992
13	1	0	3.692192	-2.919891	0.413644
14	1	0	4.314984	-2.619837	-1.206062
15	6	0	4.901038	1.606848	1.044983
16	1	0	2.824773	2.077530	1.193347
17	6	0	5.419568	-0.571732	0.175001
18	6	0	5.849478	0.649861	0.679362
19	1	0	5.211207	2.556045	1.472830
20	1	0	6.146870	-1.339404	-0.080180
21	1	0	6.910417	0.847822	0.805162
22	1	0	1.216733	0.067956	1.222503
23	6	0	-0.642310	0.400864	-0.733838
24	6	0	-1.468607	1.679312	-0.490426
25	7	0	0.834491	0.632557	-0.807437
26	6	0	-2.856659	1.669252	-0.711724
27	6	0	-0.869845	2.899410	-0.123674
28	6	0	1.212246	2.008610	-1.104516
29	6	0	-3.640095	2.798228	-0.487581
30	1	0	-3.337961	0.765752	-1.063562
31	6	0	-1.665148	4.031636	0.097252

32	6	0	0.633499	3.013507	-0.099237
33	1	0	2.299688	2.070486	-1.164693
34	1	0	0.826861	2.253521	-2.103251
35	6	0	-3.046223	3.986150	-0.059775
36	1	0	-4.712444	2.748120	-0.656015
37	1	0	-1.179619	4.965434	0.373584
38	1	0	1.026269	2.817203	0.907788
39	1	0	0.937233	4.036834	-0.355216
40	1	0	-3.647781	4.874103	0.115993
41	1	0	-0.958293	0.003870	-1.710137
42	1	0	-0.677632	-0.351772	1.304439
43	6	0	-2.417294	-1.139380	0.424280
44	6	0	-3.095420	-0.928890	1.628416
45	6	0	-3.130062	-1.685911	-0.654167
46	6	0	-4.448774	-1.249052	1.761720
47	1	0	-2.561349	-0.504896	2.475874
48	6	0	-4.481661	-1.999451	-0.529259
49	1	0	-2.625272	-1.871869	-1.596339
50	6	0	-5.147162	-1.783267	0.680943
51	1	0	-4.952692	-1.076513	2.709026
52	1	0	-5.015233	-2.422143	-1.376500
53	1	0	-6.200426	-2.033108	0.777969

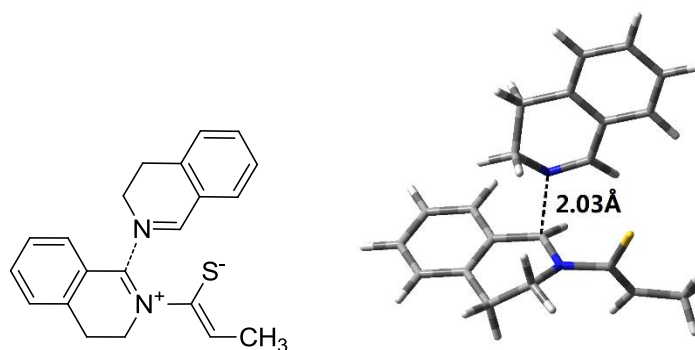
1g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.389062	1.544804	-0.596966
2	6	0	1.500312	0.559538	-0.131331
3	6	0	1.995306	-0.654398	0.398198
4	6	0	3.370912	-0.865675	0.429667
5	6	0	4.250203	0.112062	-0.046615
6	6	0	3.760510	1.318756	-0.556788
7	1	0	1.995602	2.475257	-0.998356
8	1	0	3.761961	-1.796729	0.832385
9	1	0	5.321143	-0.067693	-0.016268

10	1	0	4.447539	2.075690	-0.922888
11	6	0	0.981257	-1.628562	0.950988
12	1	0	0.781166	-1.386528	2.005449
13	1	0	1.368838	-2.652668	0.930727
14	6	0	0.072451	0.778215	-0.167154
15	1	0	-0.331362	1.759688	-0.391370
16	7	0	-0.799998	-0.172835	0.044356
17	6	0	-0.323576	-1.577579	0.156265
18	1	0	-1.127049	-2.148132	0.622007
19	1	0	-0.189220	-1.962780	-0.857989
20	6	0	-2.240992	0.084877	-0.033607
21	16	0	-3.048389	-0.874825	-1.208193
22	6	0	-2.680878	1.019972	0.852187
23	1	0	-1.966837	1.463629	1.544638
24	6	0	-4.111977	1.438612	0.962975
25	1	0	-4.754477	0.736694	0.422929
26	1	0	-4.432374	1.489414	2.011908
27	1	0	-4.276271	2.437476	0.530520

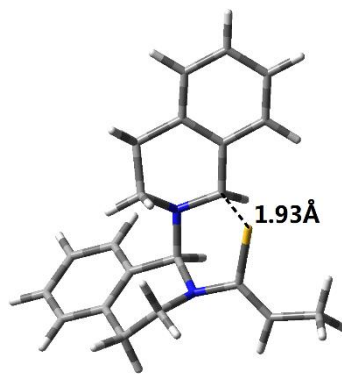
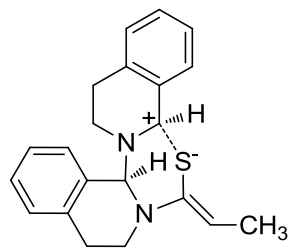
TS1-endo-g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.729153	3.493221	-0.796403
2	6	0	0.330598	2.510596	0.041056
3	16	0	-1.169896	2.289286	0.906023
4	7	0	1.301840	1.423608	0.240380
5	6	0	1.383937	0.432283	-0.647608
6	6	0	1.816441	1.189779	1.602229
7	6	0	2.456002	-0.578236	-0.507900
8	6	0	3.253305	0.674934	1.521659
9	1	0	1.759677	2.138967	2.135689
10	1	0	1.167734	0.478591	2.126791

11	6	0	2.580020	-1.604897	-1.454666
12	6	0	3.376502	-0.478097	0.550327
13	1	0	3.913216	1.492480	1.196196
14	1	0	3.592851	0.374871	2.519819
15	6	0	3.610681	-2.534203	-1.354374
16	1	0	1.851287	-1.674226	-2.257991
17	6	0	4.405985	-1.420470	0.640982
18	6	0	4.525276	-2.441820	-0.300556
19	1	0	3.701624	-3.327786	-2.090490
20	1	0	5.120525	-1.350124	1.457855
21	1	0	5.329996	-3.166735	-0.212982
22	1	0	1.741312	3.439258	-1.198093
23	1	0	1.076289	0.701571	-1.652248
24	7	0	-0.276869	-0.723655	-0.481737
25	6	0	-1.374771	-0.081810	-0.744277
26	6	0	-0.351790	-1.788482	0.519933
27	6	0	-2.705966	-0.560733	-0.351841
28	1	0	-1.318378	0.750986	-1.440095
29	6	0	-1.564858	-2.694887	0.284070
30	1	0	0.577192	-2.364436	0.486732
31	1	0	-0.427106	-1.321215	1.514680
32	6	0	-3.846833	0.232574	-0.538137
33	6	0	-2.825930	-1.869011	0.155748
34	1	0	-1.408590	-3.278221	-0.636342
35	1	0	-1.652442	-3.417665	1.103756
36	6	0	-5.103942	-0.267371	-0.214493
37	1	0	-3.728462	1.249384	-0.901463
38	6	0	-4.093225	-2.359404	0.474483
39	6	0	-5.226743	-1.564923	0.293447
40	1	0	-5.986109	0.352067	-0.348994
41	1	0	-4.194004	-3.368081	0.869086
42	1	0	-6.206864	-1.956385	0.552772
43	6	0	-0.107187	4.671132	-1.194992
44	1	0	-1.114022	4.586754	-0.777690
45	1	0	0.332676	5.613651	-0.837315
46	1	0	-0.184795	4.756984	-2.288660

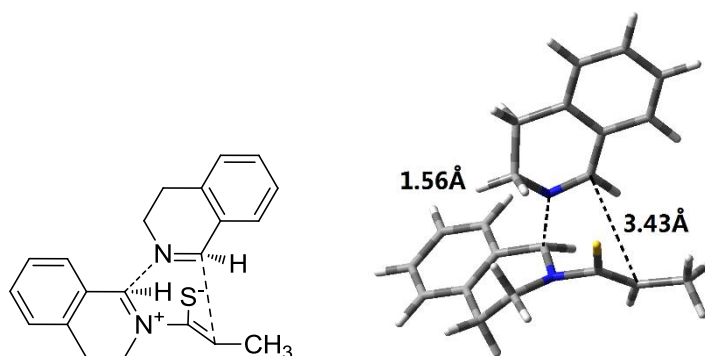
C-endo-g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.511065	3.688228	-0.464490
2	6	0	0.258756	2.430962	-0.064193
3	16	0	-1.393939	1.882916	0.431296
4	7	0	1.325044	1.490974	0.045558
5	6	0	1.093096	0.212611	-0.632032
6	6	0	1.997153	1.407947	1.348881
7	6	0	2.306791	-0.699840	-0.534161
8	6	0	3.406979	0.859788	1.131925
9	1	0	2.042733	2.418850	1.762127
10	1	0	1.448720	0.785975	2.073836
11	6	0	2.324663	-1.866462	-1.311762
12	6	0	3.396388	-0.403320	0.298221
13	1	0	4.005203	1.626461	0.619841
14	1	0	3.891451	0.670958	2.098379
15	6	0	3.411656	-2.734368	-1.274018
16	1	0	1.466929	-2.089642	-1.940646
17	6	0	4.484118	-1.288273	0.331550
18	6	0	4.499210	-2.442724	-0.445638
19	1	0	3.412389	-3.632926	-1.885111
20	1	0	5.327074	-1.062648	0.981521
21	1	0	5.352326	-3.114862	-0.404152
22	1	0	1.553820	3.910456	-0.690820
23	1	0	0.943195	0.469469	-1.689922
24	7	0	-0.140458	-0.522078	-0.267307
25	6	0	-1.324235	0.227047	-0.557009
26	6	0	-0.203973	-1.210451	1.026760
27	6	0	-2.603959	-0.530187	-0.292549
28	1	0	-1.285696	0.552466	-1.601430
29	6	0	-1.283506	-2.290814	0.951315
30	1	0	0.769217	-1.660940	1.231182

31	1	0	-0.435827	-0.509140	1.844266
32	6	0	-3.815580	-0.029087	-0.788008
33	6	0	-2.591597	-1.730926	0.434803
34	1	0	-0.936800	-3.091988	0.283677
35	1	0	-1.429799	-2.742540	1.940726
36	6	0	-5.010265	-0.708778	-0.569378
37	1	0	-3.814842	0.905168	-1.344340
38	6	0	-3.800877	-2.404776	0.649291
39	6	0	-5.002568	-1.903814	0.154991
40	1	0	-5.942035	-0.309748	-0.960739
41	1	0	-3.793788	-3.334158	1.215143
42	1	0	-5.930117	-2.440885	0.335021
43	6	0	-0.467555	4.813986	-0.607608
44	1	0	-1.501063	4.464189	-0.539446
45	1	0	-0.316198	5.573970	0.172047
46	1	0	-0.330543	5.322098	-1.571013

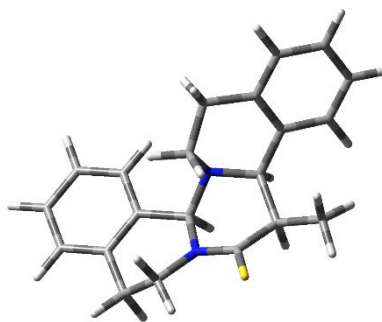
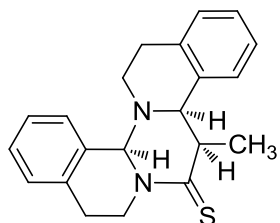
TS2-Si-g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.241579	2.945394	1.155519
2	6	0	0.071656	2.307754	-0.034850
3	16	0	1.134896	2.281112	-1.424376
4	7	0	-1.139536	1.491498	-0.124605
5	6	0	-1.158597	0.309572	0.650071
6	6	0	-1.913961	1.514665	-1.368450
7	6	0	-2.424272	-0.516313	0.535369
8	6	0	-3.374488	1.202780	-1.043904
9	1	0	-1.806050	2.514636	-1.789553
10	1	0	-1.531126	0.817063	-2.125856
11	6	0	-2.535454	-1.699995	1.277739
12	6	0	-3.495476	-0.085060	-0.261947

13	1	0	-3.793685	2.029672	-0.453567
14	1	0	-3.961704	1.139877	-1.968404
15	6	0	-3.699050	-2.462505	1.230988
16	1	0	-1.700518	-2.023835	1.895164
17	6	0	-4.660896	-0.862671	-0.301225
18	6	0	-4.767587	-2.039641	0.435515
19	1	0	-3.774291	-3.377773	1.811420
20	1	0	-5.491394	-0.535078	-0.922406
21	1	0	-5.680116	-2.627932	0.389227
22	1	0	-0.573914	2.894137	1.879237
23	1	0	-0.964516	0.547473	1.701155
24	7	0	0.075863	-0.578924	0.304191
25	6	0	1.185356	-0.349369	0.954223
26	6	0	0.165832	-1.151966	-1.055972
27	6	0	2.473937	-0.834569	0.522947
28	1	0	1.108437	0.236509	1.864914
29	6	0	1.225463	-2.250775	-1.116153
30	1	0	-0.819516	-1.537762	-1.320925
31	1	0	0.432270	-0.303754	-1.710822
32	6	0	3.647424	-0.390977	1.154219
33	6	0	2.534567	-1.777350	-0.526360
34	1	0	0.877999	-3.141478	-0.570474
35	1	0	1.357501	-2.552620	-2.160432
36	6	0	4.883060	-0.872488	0.735418
37	1	0	3.582587	0.345738	1.950237
38	6	0	3.777232	-2.257387	-0.926605
39	6	0	4.945435	-1.805163	-0.303612
40	1	0	5.793985	-0.520348	1.209513
41	1	0	3.839273	-2.982175	-1.734423
42	1	0	5.909371	-2.181012	-0.635231
43	6	0	1.424606	3.792672	1.517228
44	1	0	1.155877	4.858717	1.577096
45	1	0	1.838142	3.524450	2.502155
46	1	0	2.210571	3.690023	0.763944

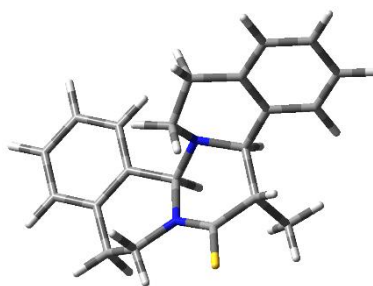
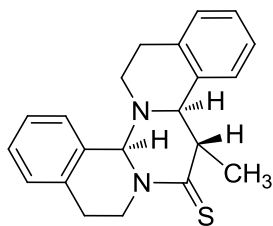
7g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.111332	1.577307	-0.955671
2	6	0	0.018394	2.110037	-0.053466
3	16	0	-0.151058	3.483200	0.894487
4	7	0	1.183809	1.415853	-0.137774
5	6	0	1.127519	0.026763	-0.694167
6	6	0	2.383267	1.875914	0.571231
7	6	0	2.382408	-0.790890	-0.412265
8	6	0	3.646659	1.339887	-0.097732
9	1	0	2.363409	2.966623	0.565520
10	1	0	2.339975	1.561383	1.623589
11	6	0	2.318263	-2.187883	-0.490087
12	6	0	3.613585	-0.164125	-0.175345
13	1	0	3.735125	1.777570	-1.102975
14	1	0	4.520791	1.679200	0.469327
15	6	0	3.466781	-2.958580	-0.319573
16	1	0	1.358294	-2.657219	-0.678732
17	6	0	4.759890	-0.947284	-0.000367
18	6	0	4.692905	-2.337210	-0.073408
19	1	0	3.403717	-4.041822	-0.377065
20	1	0	5.710619	-0.457529	0.198084
21	1	0	5.591320	-2.932597	0.065433
22	1	0	-0.738765	1.798501	-1.967769
23	1	0	1.039810	0.119705	-1.787555
24	7	0	-0.084878	-0.639248	-0.253515
25	6	0	-1.233438	-0.030358	-0.933819
26	6	0	-0.239601	-0.671836	1.211881
27	6	0	-2.544825	-0.623950	-0.433627
28	1	0	-1.150117	-0.332153	-1.985671
29	6	0	-1.375277	-1.616997	1.581058
30	1	0	0.702602	-1.021165	1.643685
31	1	0	-0.443091	0.327293	1.629093
32	6	0	-3.692667	-0.528368	-1.236220

33	6	0	-2.621374	-1.344886	0.769241
34	1	0	-1.055012	-2.653027	1.401907
35	1	0	-1.588998	-1.534750	2.654057
36	6	0	-4.908531	-1.071458	-0.832961
37	1	0	-3.627854	-0.031246	-2.200749
38	6	0	-3.851923	-1.882245	1.172228
39	6	0	-4.993534	-1.741316	0.389907
40	1	0	-5.782532	-0.978645	-1.471792
41	1	0	-3.903111	-2.430591	2.110704
42	1	0	-5.938096	-2.164699	0.720751
43	6	0	-2.427053	2.338937	-0.791220
44	1	0	-2.253204	3.411656	-0.891151
45	1	0	-3.145765	2.032658	-1.555628
46	1	0	-2.875398	2.164674	0.190439

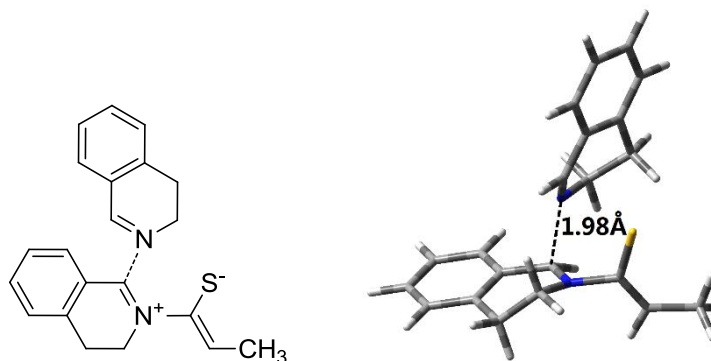
4g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.212394	1.608221	0.623211
2	6	0	0.013110	2.082863	-0.204832
3	16	0	0.173643	3.457534	-1.154033
4	7	0	-1.133885	1.376951	-0.079242
5	6	0	-1.072339	0.037896	0.599616
6	6	0	-2.352529	1.793806	-0.783547
7	6	0	-2.327923	-0.800170	0.390791
8	6	0	-3.598799	1.305903	-0.049284
9	1	0	-2.329751	2.882287	-0.852193
10	1	0	-2.335588	1.404934	-1.811312
11	6	0	-2.264822	-2.187640	0.571109
12	6	0	-3.562832	-0.189699	0.129135
13	1	0	-3.662203	1.810626	0.926006
14	1	0	-4.486883	1.607311	-0.615932
15	6	0	-3.416206	-2.966680	0.472327

16	1	0	-1.304161	-2.643726	0.786754
17	6	0	-4.711965	-0.981364	0.027375
18	6	0	-4.644946	-2.362749	0.198196
19	1	0	-3.353304	-4.042843	0.608596
20	1	0	-5.665450	-0.505227	-0.189947
21	1	0	-5.545703	-2.964930	0.115339
22	1	0	-0.996575	0.236970	1.679105
23	7	0	0.143635	-0.662261	0.243772
24	6	0	1.284423	0.040442	0.844827
25	6	0	0.312174	-0.919143	-1.194786
26	6	0	2.615928	-0.546968	0.399205
27	1	0	1.198187	-0.131400	1.926845
28	6	0	1.452387	-1.915060	-1.381792
29	1	0	-0.623548	-1.332895	-1.580304
30	1	0	0.523854	0.002762	-1.761899
31	6	0	3.787339	-0.164377	1.069654
32	6	0	2.703197	-1.462892	-0.660817
33	1	0	1.136741	-2.894444	-0.995619
34	1	0	1.658314	-2.047426	-2.451148
35	6	0	5.029515	-0.668783	0.695847
36	1	0	3.724076	0.534643	1.900301
37	6	0	3.959091	-1.962889	-1.031388
38	6	0	5.116998	-1.574352	-0.364223
39	1	0	5.923895	-0.359253	1.229657
40	1	0	4.021576	-2.666651	-1.858955
41	1	0	6.081243	-1.972723	-0.668168
42	6	0	1.209052	2.362260	1.970845
43	1	0	1.211461	3.442236	1.800056
44	1	0	0.326367	2.110218	2.571416
45	1	0	2.097656	2.102884	2.557703
46	1	0	2.093766	1.931510	0.067692

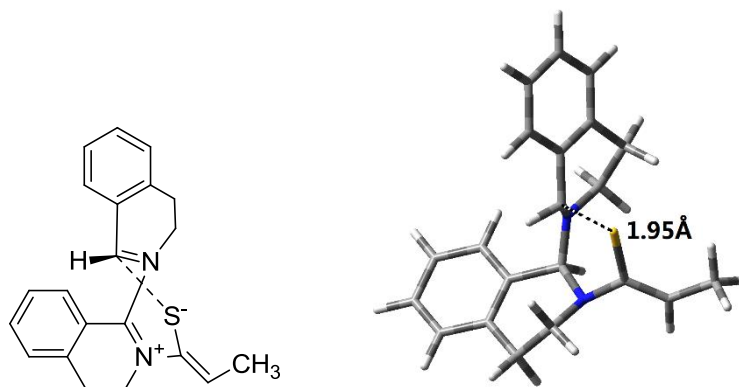
TS1-*exo-g*



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.523533	3.320685	0.835611
2	6	0	-0.244346	2.358266	-0.069725
3	16	0	1.187847	2.089782	-1.036251
4	7	0	-1.290750	1.347523	-0.274645
5	6	0	-1.427725	0.355887	0.613997
6	6	0	-1.857620	1.200611	-1.629062
7	6	0	-2.502944	-0.648294	0.406346
8	6	0	-3.310667	0.744589	-1.522288
9	1	0	-1.775495	2.174444	-2.112870
10	1	0	-1.270963	0.492171	-2.223982
11	6	0	-2.629087	-1.738213	1.278692
12	6	0	-3.433649	-0.470762	-0.632194
13	1	0	-3.917214	1.563643	-1.108747
14	1	0	-3.705590	0.531882	-2.522386
15	6	0	-3.663400	-2.654193	1.120630
16	1	0	-1.901870	-1.870996	2.074720
17	6	0	-4.467770	-1.400994	-0.783665
18	6	0	-4.584911	-2.486105	0.082365
19	1	0	-3.750910	-3.497938	1.799126
20	1	0	-5.186521	-1.268781	-1.589054
21	1	0	-5.392313	-3.200980	-0.051067
22	1	0	-1.516927	3.322005	1.285420
23	1	0	-1.214985	0.645498	1.638525
24	7	0	0.241300	-0.716616	0.649310
25	6	0	0.938170	-0.727685	-0.449029
26	6	0	0.955781	-0.817182	1.928084
27	6	0	2.371213	-1.031332	-0.489492
28	1	0	0.393343	-0.707793	-1.386606
29	6	0	2.386145	-0.265235	1.868367
30	1	0	0.375129	-0.281683	2.688905
31	1	0	0.968186	-1.876941	2.225068
32	6	0	2.984176	-1.516143	-1.651197
33	6	0	3.119633	-0.858198	0.690925
34	1	0	2.339720	0.825048	1.736854
35	1	0	2.906409	-0.468370	2.811352
36	6	0	4.339749	-1.838322	-1.640546
37	1	0	2.397459	-1.636222	-2.558669
38	6	0	4.474218	-1.180486	0.689387
39	6	0	5.083339	-1.672080	-0.469639
40	1	0	4.816245	-2.214520	-2.541382
41	1	0	5.060333	-1.043529	1.595242

42	1	0	6.140748	-1.922454	-0.458053
43	6	0	0.422213	4.406586	1.250900
44	1	0	1.413953	4.238904	0.822073
45	1	0	0.072773	5.394711	0.916809
46	1	0	0.515175	4.460638	2.345281

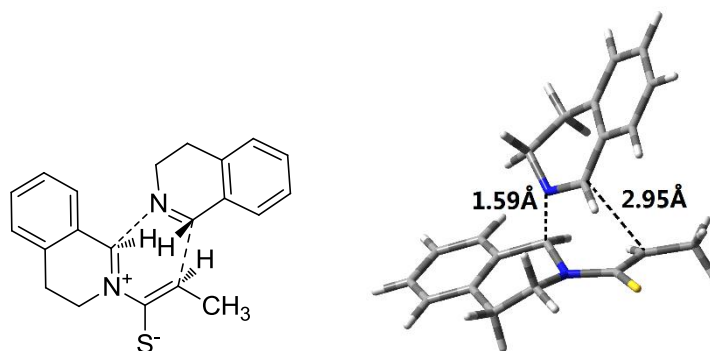
C-*exo-g*



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.179633	3.591604	0.465709
2	6	0	-0.219863	2.375678	-0.101869
3	16	0	1.147535	1.687004	-1.059458
4	7	0	-1.392877	1.568173	-0.011103
5	6	0	-1.211996	0.347822	0.804203
6	6	0	-2.140961	1.450760	-1.269236
7	6	0	-2.246362	-0.736592	0.479246
8	6	0	-3.519589	0.866618	-0.979524
9	1	0	-2.227083	2.460096	-1.682140
10	1	0	-1.625251	0.834205	-2.025358
11	6	0	-2.087795	-2.003705	1.056813
12	6	0	-3.372495	-0.481706	-0.318271
13	1	0	-4.067515	1.561061	-0.327142
14	1	0	-4.093918	0.774365	-1.909275
15	6	0	-3.035101	-3.004807	0.861071
16	1	0	-1.203116	-2.203655	1.653904
17	6	0	-4.316257	-1.498490	-0.516983
18	6	0	-4.159167	-2.750304	0.071228
19	1	0	-2.894640	-3.981211	1.317058
20	1	0	-5.179087	-1.300591	-1.149542
21	1	0	-4.901526	-3.526816	-0.093788
22	1	0	-1.094089	3.911618	0.963407

23	1	0	-1.373677	0.643764	1.850239
24	7	0	0.159977	-0.186530	0.774063
25	6	0	0.800041	-0.149977	-0.494765
26	6	0	0.967657	-0.077896	1.999565
27	6	0	2.103107	-0.896728	-0.520904
28	1	0	0.115276	-0.540556	-1.250862
29	6	0	2.472306	0.091673	1.725402
30	1	0	0.617838	0.769950	2.602878
31	1	0	0.817669	-0.984382	2.605661
32	6	0	2.486210	-1.673183	-1.616105
33	6	0	2.938513	-0.800536	0.603038
34	1	0	2.668655	1.136174	1.451531
35	1	0	3.027316	-0.112216	2.648059
36	6	0	3.702222	-2.358898	-1.598578
37	1	0	1.830801	-1.745512	-2.480979
38	6	0	4.145876	-1.499969	0.618689
39	6	0	4.530665	-2.274157	-0.478779
40	1	0	3.996485	-2.963096	-2.452360
41	1	0	4.791187	-1.435125	1.492055
42	1	0	5.474346	-2.812785	-0.456659
43	6	0	0.972227	4.551110	0.457535
44	1	0	1.902784	4.062525	0.152572
45	1	0	0.792531	5.385513	-0.235144
46	1	0	1.117132	4.993204	1.451594

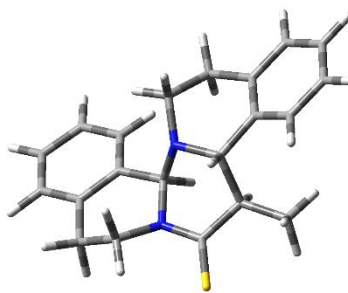
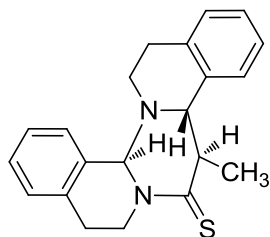
TS2-Re-g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.642947	1.848729	1.765945
2	6	0	-0.001215	2.237821	0.605345
3	16	0	0.534721	3.565391	-0.353364
4	7	0	-1.090801	1.415588	0.122785

5	6	0	-1.127593	0.043307	0.479649
6	6	0	-1.662673	1.671353	-1.208749
7	6	0	-2.480255	-0.611169	0.249709
8	6	0	-3.142120	1.311168	-1.240208
9	1	0	-1.500012	2.722686	-1.438418
10	1	0	-1.122342	1.084381	-1.969354
11	6	0	-2.843354	-1.745666	0.992871
12	6	0	-3.424451	-0.032875	-0.613874
13	1	0	-3.710569	2.072797	-0.687616
14	1	0	-3.503558	1.340704	-2.275803
15	6	0	-4.079534	-2.362170	0.814065
16	1	0	-2.165405	-2.136200	1.748384
17	6	0	-4.662962	-0.662102	-0.791198
18	6	0	-4.987275	-1.827845	-0.101858
19	1	0	-4.337037	-3.242102	1.396693
20	1	0	-5.387589	-0.213801	-1.467358
21	1	0	-5.953768	-2.300329	-0.255044
22	1	0	-0.866457	-0.081816	1.530853
23	6	0	1.165648	-0.015802	-0.460695
24	6	0	2.481037	-0.609533	-0.515533
25	7	0	0.067430	-0.728712	-0.219405
26	6	0	3.551710	0.101176	-1.091244
27	6	0	2.702570	-1.881409	0.062100
28	6	0	0.234177	-2.185909	-0.047204
29	6	0	4.826158	-0.455305	-1.105759
30	1	0	3.367713	1.084329	-1.515992
31	6	0	3.983444	-2.422978	0.041151
32	6	0	1.514352	-2.547085	0.712891
33	1	0	-0.647176	-2.587618	0.445507
34	1	0	0.266254	-2.624942	-1.053063
35	6	0	5.041489	-1.718001	-0.544131
36	1	0	5.651886	0.091300	-1.551524
37	1	0	4.161838	-3.400667	0.482850
38	1	0	1.430794	-2.216913	1.759601
39	1	0	1.630442	-3.636682	0.732413
40	1	0	6.035514	-2.156315	-0.559797
41	1	0	1.061166	1.010572	-0.792270
42	1	0	0.167817	1.134230	2.435098
43	6	0	1.853983	2.535599	2.321567
44	1	0	2.548362	2.825619	1.526735
45	1	0	1.589802	3.463081	2.852759
46	1	0	2.373883	1.885480	3.036462

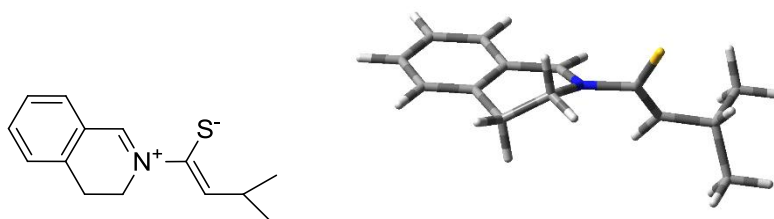
8g



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.113184	1.484518	-0.741444
2	6	0	0.145783	2.266283	-0.355397
3	16	0	0.156933	3.918421	-0.115862
4	7	0	1.212925	1.452478	-0.117626
5	6	0	0.987686	0.009706	-0.294989
6	6	0	2.223874	1.827649	0.882425
7	6	0	2.290308	-0.790656	-0.212915
8	6	0	3.583580	1.253591	0.531868
9	1	0	2.247376	2.914532	0.932958
10	1	0	1.882828	1.439693	1.853629
11	6	0	2.303052	-2.112474	-0.690392
12	6	0	3.505408	-0.214228	0.190878
13	1	0	3.998629	1.799564	-0.327238
14	1	0	4.272583	1.418855	1.369170
15	6	0	3.465059	-2.877340	-0.689696
16	1	0	1.389668	-2.548277	-1.083352
17	6	0	4.671788	-0.992861	0.190376
18	6	0	4.659091	-2.317925	-0.229865
19	1	0	3.439915	-3.899790	-1.056061
20	1	0	5.604487	-0.536184	0.514343
21	1	0	5.574092	-2.903811	-0.219655
22	1	0	0.661198	-0.122081	-1.336948
23	6	0	-1.331987	0.460549	0.447987
24	6	0	-2.601117	-0.379321	0.285708
25	7	0	-0.084637	-0.345120	0.661378
26	6	0	-3.851111	0.211213	0.528779
27	6	0	-2.558186	-1.744030	-0.051469
28	6	0	-0.322244	-1.750255	0.971439
29	6	0	-5.035724	-0.499958	0.353604
30	1	0	-3.896251	1.243313	0.863322
31	6	0	-3.753183	-2.454548	-0.219625

32	6	0	-1.220893	-2.443468	-0.067410
33	1	0	0.637975	-2.253476	1.084479
34	1	0	-0.820104	-1.801597	1.948582
35	6	0	-4.988903	-1.838083	-0.042153
36	1	0	-5.990123	-0.014027	0.537398
37	1	0	-3.704904	-3.512278	-0.470263
38	1	0	-0.753040	-2.400236	-1.061732
39	1	0	-1.348614	-3.506932	0.171864
40	1	0	-5.906388	-2.404577	-0.177107
41	1	0	-1.481962	1.084497	1.342504
42	1	0	-0.906380	0.895947	-1.644474
43	6	0	-2.309377	2.374932	-1.071319
44	1	0	-2.641745	2.953768	-0.205226
45	1	0	-2.023954	3.093074	-1.843847
46	1	0	-3.142556	1.774009	-1.443160

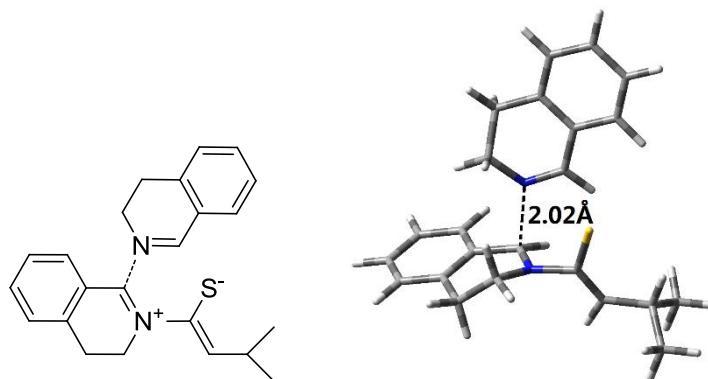
1k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.787883	-1.610337	-0.776072
2	6	0	-2.029882	-0.568252	-0.213171
3	6	0	-2.662888	0.448536	0.538235
4	6	0	-4.045996	0.412664	0.691725
5	6	0	-4.796888	-0.618724	0.118783
6	6	0	-4.168621	-1.632127	-0.612369
7	1	0	-2.288451	-2.388214	-1.347997
8	1	0	-4.542866	1.191174	1.265278
9	1	0	-5.875636	-0.632751	0.246255
10	1	0	-4.756087	-2.431862	-1.053120
11	6	0	-1.771824	1.489108	1.175568
12	1	0	-1.439984	1.130693	2.161441
13	1	0	-2.318639	2.422332	1.347211
14	6	0	-0.594397	-0.530192	-0.374585
15	1	0	-0.060215	-1.383520	-0.778510
16	7	0	0.129993	0.514399	-0.067665

17	6	0	-0.554552	1.783276	0.299367
18	1	0	0.185608	2.410798	0.795642
19	1	0	-0.842719	2.283388	-0.629108
20	6	0	1.582073	0.522978	-0.274991
21	16	0	2.120541	1.783277	-1.312557
22	6	0	2.242128	-0.454395	0.403703
23	1	0	1.675301	-1.125254	1.050218
24	6	0	3.730516	-0.653359	0.346439
25	1	0	4.163562	0.269146	-0.060575
26	6	0	4.096789	-1.802772	-0.616595
27	1	0	5.185172	-1.933114	-0.670389
28	1	0	3.662748	-2.754413	-0.281898
29	1	0	3.727464	-1.593816	-1.625774
30	6	0	4.311483	-0.901812	1.749048
31	1	0	3.891050	-1.812302	2.197871
32	1	0	5.399934	-1.027964	1.704849
33	1	0	4.094805	-0.065092	2.422658

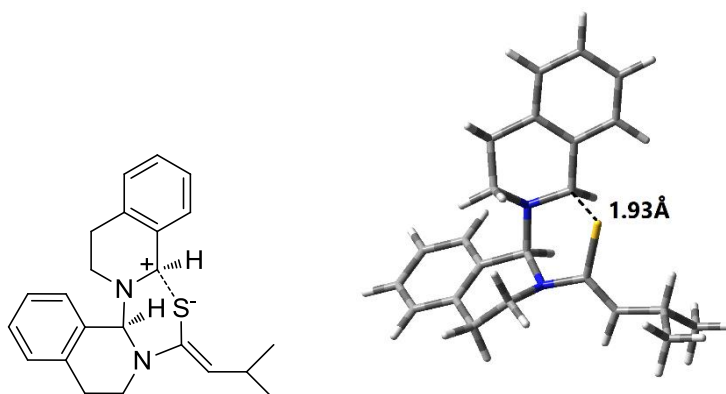
TS1-endo-k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.886919	3.040680	-0.283755
2	6	0	0.442286	1.999988	0.454755
3	16	0	-1.055664	1.775781	1.322767
4	7	0	1.347225	0.840211	0.511844
5	6	0	1.366354	-0.034496	-0.495542
6	6	0	1.838763	0.399802	1.829695
7	6	0	2.375460	-1.117765	-0.493166
8	6	0	3.241757	-0.187167	1.677445
9	1	0	1.837655	1.272339	2.483539
10	1	0	1.144710	-0.332303	2.258920

11	6	0	2.439573	-2.018777	-1.565288
12	6	0	3.298326	-1.209869	0.563807
13	1	0	3.951538	0.623991	1.458237
14	1	0	3.558448	-0.634561	2.626788
15	6	0	3.412560	-3.013086	-1.591980
16	1	0	1.709557	-1.939479	-2.366569
17	6	0	4.269819	-2.215309	0.525538
18	6	0	4.329378	-3.111782	-0.540652
19	1	0	3.457465	-3.708859	-2.424904
20	1	0	4.986063	-2.292831	1.340227
21	1	0	5.089548	-3.888140	-0.552353
22	1	0	1.891338	2.976137	-0.707118
23	1	0	1.082685	0.381941	-1.456180
24	7	0	-0.354990	-1.089092	-0.467330
25	6	0	-1.411574	-0.352510	-0.630089
26	6	0	-0.497921	-2.292011	0.356106
27	6	0	-2.770251	-0.804050	-0.306591
28	1	0	-1.300685	0.571361	-1.191060
29	6	0	-1.762647	-3.075030	-0.011893
30	1	0	0.394264	-2.910729	0.226415
31	1	0	-0.546528	-1.984085	1.412631
32	6	0	-3.859704	0.076714	-0.360547
33	6	0	-2.970835	-2.164816	-0.003821
34	1	0	-1.637877	-3.516515	-1.012558
35	1	0	-1.897253	-3.909765	0.685917
36	6	0	-5.145740	-0.389617	-0.108110
37	1	0	-3.677953	1.128001	-0.564429
38	6	0	-4.266405	-2.620431	0.244756
39	6	0	-5.348656	-1.739944	0.195535
40	1	0	-5.988105	0.295493	-0.139221
41	1	0	-4.429715	-3.669595	0.481059
42	1	0	-6.351409	-2.106297	0.399012
43	6	0	0.125310	4.311318	-0.552678
44	1	0	-0.885304	4.182067	-0.148414
45	6	0	0.018057	4.578938	-2.065909
46	1	0	-0.540946	5.501875	-2.265387
47	1	0	1.012189	4.689273	-2.520219
48	1	0	-0.493052	3.756056	-2.579303
49	6	0	0.778978	5.507120	0.167393
50	1	0	1.809544	5.662823	-0.179210
51	1	0	0.221170	6.433487	-0.021026
52	1	0	0.808781	5.340581	1.249293

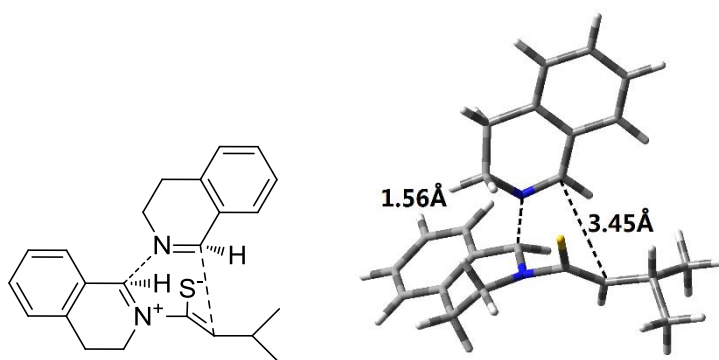
C-endo-k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.098613	3.271056	0.218437
2	6	0	-0.013008	1.969763	-0.103437
3	16	0	1.551107	1.178298	-0.557381
4	7	0	-1.194406	1.173045	-0.165056
5	6	0	-1.132503	-0.084575	0.583184
6	6	0	-1.878507	1.108522	-1.462886
7	6	0	-2.459886	-0.827266	0.537515
8	6	0	-3.348244	0.770226	-1.217278
9	1	0	-1.788834	2.091366	-1.932677
10	1	0	-1.423604	0.378000	-2.150645
11	6	0	-2.631838	-1.933136	1.381996
12	6	0	-3.504780	-0.432314	-0.311229
13	1	0	-3.833684	1.639300	-0.751527
14	1	0	-3.860083	0.593370	-2.171854
15	6	0	-3.828195	-2.643687	1.395057
16	1	0	-1.808260	-2.234748	2.023732
17	6	0	-4.704193	-1.159209	-0.292651
18	6	0	-4.871870	-2.253416	0.550996
19	1	0	-3.947825	-3.496362	2.057976
20	1	0	-5.513227	-0.857173	-0.954580
21	1	0	-5.809799	-2.802562	0.549144
22	1	0	-1.104148	3.642958	0.424243
23	1	0	-0.941253	0.207378	1.625278
24	7	0	-0.012664	-0.998832	0.260401
25	6	0	1.262714	-0.403920	0.512450
26	6	0	-0.052724	-1.762294	-0.991765
27	6	0	2.428552	-1.336154	0.283791
28	1	0	1.275719	-0.024438	1.539139
29	6	0	0.874476	-2.970660	-0.856248

30	1	0	-1.079024	-2.090678	-1.167530
31	1	0	0.261997	-1.146666	-1.849667
32	6	0	3.701441	-0.973095	0.745056
33	6	0	2.250989	-2.561028	-0.378620
34	1	0	0.431873	-3.678292	-0.141223
35	1	0	0.948047	-3.494556	-1.817709
36	6	0	4.794442	-1.813556	0.555272
37	1	0	3.830038	-0.019083	1.250625
38	6	0	3.359216	-3.397456	-0.564840
39	6	0	4.622263	-3.032946	-0.105287
40	1	0	5.775203	-1.519928	0.919256
41	1	0	3.223380	-4.345754	-1.080867
42	1	0	5.469769	-3.694887	-0.262584
43	6	0	1.010897	4.285515	0.301309
44	1	0	1.969871	3.759688	0.225958
45	6	0	0.963579	5.018664	1.654862
46	1	0	1.771581	5.756493	1.726252
47	1	0	0.012511	5.552174	1.781546
48	1	0	1.067905	4.317426	2.490078
49	6	0	0.922888	5.287548	-0.867678
50	1	0	-0.031682	5.829204	-0.852175
51	1	0	1.728491	6.029197	-0.804352
52	1	0	1.004229	4.776836	-1.833209

TS2-Si-k

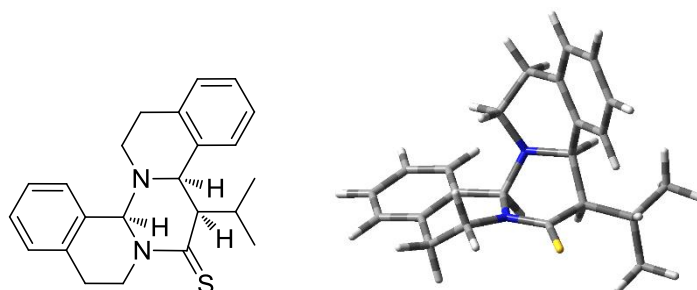


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.662202	2.641005	-0.486022
2	6	0	-0.295487	1.852447	0.560688
3	16	0	-1.244729	1.385379	1.953316
4	7	0	1.049991	1.283301	0.462778
5	6	0	1.233247	0.277103	-0.512215

6	6	0	1.881417	1.235080	1.669307
7	6	0	2.634194	-0.294624	-0.593472
8	6	0	3.352702	1.261544	1.255643
9	1	0	1.623139	2.110036	2.266570
10	1	0	1.672846	0.359239	2.298858
11	6	0	2.913012	-1.280770	-1.549727
12	6	0	3.656100	0.182673	0.241304
13	1	0	3.584571	2.244863	0.822829
14	1	0	3.994446	1.141357	2.137212
15	6	0	4.196947	-1.801957	-1.680453
16	1	0	2.114185	-1.640554	-2.194437
17	6	0	4.944254	-0.351461	0.100285
18	6	0	5.217811	-1.333211	-0.848769
19	1	0	4.402016	-2.565200	-2.425871
20	1	0	5.738396	0.011341	0.748836
21	1	0	6.223700	-1.734167	-0.940217
22	1	0	0.097542	2.890957	-1.230756
23	1	0	0.924113	0.648505	-1.494520
24	7	0	0.212769	-0.882572	-0.288103
25	6	0	-0.956776	-0.779792	-0.858214
26	6	0	0.322939	-1.682785	0.950537
27	6	0	-2.095922	-1.583656	-0.485120
28	1	0	-1.053018	-0.045541	-1.652344
29	6	0	-0.493942	-2.969004	0.844250
30	1	0	1.379647	-1.897666	1.114788
31	1	0	-0.062096	-1.028113	1.751934
32	6	0	-3.369890	-1.290655	-0.998300
33	6	0	-1.904389	-2.681585	0.381637
34	1	0	-0.012209	-3.665807	0.141230
35	1	0	-0.499198	-3.461620	1.822181
36	6	0	-4.458100	-2.079208	-0.640468
37	1	0	-3.500062	-0.433484	-1.653291
38	6	0	-3.000967	-3.467160	0.721364
39	6	0	-4.271117	-3.165968	0.218201
40	1	0	-5.447724	-1.847267	-1.021687
41	1	0	-2.869473	-4.315434	1.388283
42	1	0	-5.119586	-3.782316	0.502163
43	6	0	-2.005937	3.304592	-0.643682
44	1	0	-2.722660	2.746729	-0.028527
45	6	0	-2.480637	3.276435	-2.107727
46	1	0	-3.461176	3.756248	-2.219151
47	1	0	-1.777527	3.807728	-2.763899
48	1	0	-2.566963	2.248022	-2.484387
49	6	0	-1.973253	4.752163	-0.111418

50	1	0	-1.247619	5.361108	-0.667143
51	1	0	-2.956391	5.233375	-0.204900
52	1	0	-1.686568	4.759249	0.944692

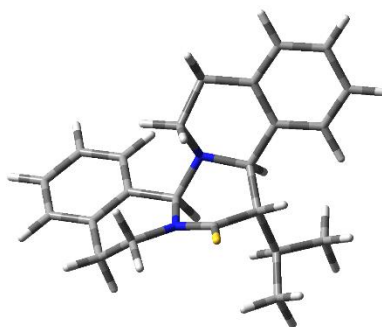
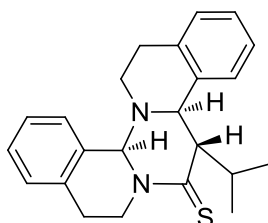
7k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.101624	1.264693	0.854786
2	6	0	0.482897	1.615410	-0.505238
3	16	0	1.269953	2.477254	-1.707673
4	7	0	-0.756508	1.074751	-0.640773
5	6	0	-1.282541	0.320237	0.524681
6	6	0	-1.472986	1.031497	-1.918628
7	6	0	-2.740810	-0.091491	0.383348
8	6	0	-2.959270	1.297223	-1.709839
9	1	0	-1.019661	1.777071	-2.571804
10	1	0	-1.321182	0.044167	-2.377112
11	6	0	-3.316150	-0.864087	1.404033
12	6	0	-3.548738	0.390893	-0.655638
13	1	0	-3.095745	2.348138	-1.416688
14	1	0	-3.485383	1.168295	-2.663105
15	6	0	-4.668081	-1.191221	1.375628
16	1	0	-2.687825	-1.204567	2.222511
17	6	0	-4.908506	0.049336	-0.676870
18	6	0	-5.469287	-0.737886	0.323835
19	1	0	-5.095851	-1.795513	2.170795
20	1	0	-5.529373	0.414624	-1.491922
21	1	0	-6.524906	-0.993099	0.288679
22	1	0	0.392698	1.591789	1.625734
23	1	0	-1.293528	1.036001	1.352820
24	7	0	-0.373425	-0.758470	0.914856
25	6	0	1.066981	-0.302044	0.985395
26	6	0	-0.598041	-2.049420	0.249350

27	6	0	2.004180	-1.107752	0.071946
28	1	0	1.396944	-0.516988	2.010091
29	6	0	0.521418	-3.020115	0.627631
30	1	0	-1.564589	-2.442605	0.571635
31	1	0	-0.628916	-1.966115	-0.851066
32	6	0	3.096815	-0.575084	-0.622527
33	6	0	1.794234	-2.500211	0.017834
34	1	0	0.581647	-3.085016	1.724232
35	1	0	0.291388	-4.024261	0.255218
36	6	0	3.979724	-1.404325	-1.318961
37	1	0	3.260618	0.492313	-0.653995
38	6	0	2.677206	-3.323250	-0.682580
39	6	0	3.781901	-2.782813	-1.340562
40	1	0	4.817519	-0.961959	-1.851075
41	1	0	2.487385	-4.393839	-0.721764
42	1	0	4.467176	-3.430223	-1.881320
43	6	0	2.403603	2.018039	1.244089
44	1	0	3.057190	2.086261	0.371392
45	6	0	3.171701	1.333485	2.385699
46	1	0	4.035837	1.945608	2.668045
47	1	0	2.547885	1.220489	3.282505
48	1	0	3.546940	0.344660	2.103594
49	6	0	2.054636	3.462746	1.645866
50	1	0	1.433853	3.480432	2.552405
51	1	0	2.967442	4.030912	1.858519
52	1	0	1.517666	3.980239	0.846198

4k

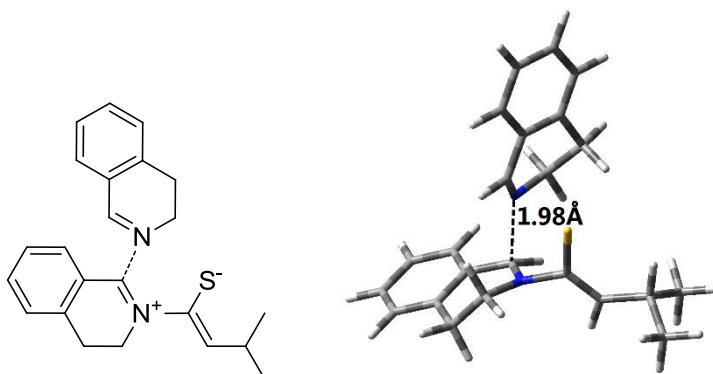


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.184515	1.368753	0.276350
2	6	0	0.131622	1.648709	-0.794096

3	16	0	0.515338	2.527542	-2.168608
4	7	0	-1.102926	1.151192	-0.530220
5	6	0	-1.183765	0.038466	0.476786
6	6	0	-2.221023	1.389550	-1.448273
7	6	0	-2.529506	-0.675649	0.482790
8	6	0	-3.551960	1.274542	-0.710480
9	1	0	-2.084160	2.384772	-1.873734
10	1	0	-2.178516	0.675410	-2.283137
11	6	0	-2.628539	-1.921159	1.117233
12	6	0	-3.680663	-0.068775	-0.038547
13	1	0	-3.622458	2.084228	0.030485
14	1	0	-4.370511	1.429051	-1.422565
15	6	0	-3.858039	-2.567600	1.220967
16	1	0	-1.728367	-2.375314	1.519082
17	6	0	-4.910369	-0.729811	0.066561
18	6	0	-5.005006	-1.970384	0.692824
19	1	0	-3.920348	-3.535385	1.711028
20	1	0	-5.799003	-0.262580	-0.351998
21	1	0	-5.966853	-2.470863	0.765155
22	1	0	-1.067159	0.494186	1.467895
23	7	0	-0.060043	-0.861852	0.314673
24	6	0	1.184907	-0.167594	0.701093
25	6	0	-0.008366	-1.521823	-0.998796
26	6	0	2.433573	-0.924871	0.247884
27	1	0	1.188941	-0.181498	1.799406
28	6	0	1.014045	-2.647815	-0.935257
29	1	0	-1.003692	-1.919566	-1.214163
30	1	0	0.257769	-0.824539	-1.809999
31	6	0	3.699411	-0.450815	0.626895
32	6	0	2.356996	-2.112686	-0.498855
33	1	0	0.660299	-3.411590	-0.228617
34	1	0	1.100553	-3.132869	-1.915206
35	6	0	4.863482	-1.131278	0.281570
36	1	0	3.779533	0.464732	1.203308
37	6	0	3.534879	-2.787305	-0.847326
38	6	0	4.783271	-2.310522	-0.461396
39	1	0	5.829229	-0.739562	0.589335
40	1	0	3.461111	-3.698875	-1.436832
41	1	0	5.685153	-2.847312	-0.743012
42	1	0	2.144516	1.612437	-0.181407
43	6	0	1.004399	2.327828	1.509982
44	1	0	0.109153	2.009989	2.063764
45	6	0	0.798305	3.796350	1.105771
46	1	0	0.719210	4.420020	2.004230

47	1	0	1.639849	4.165401	0.508922
48	1	0	-0.109192	3.941244	0.514203
49	6	0	2.197187	2.237661	2.476402
50	1	0	3.118698	2.581245	1.989607
51	1	0	2.024849	2.883419	3.344949
52	1	0	2.370641	1.225142	2.855367

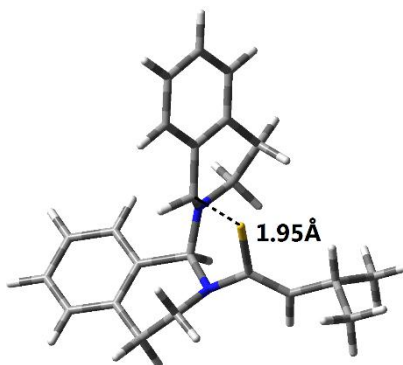
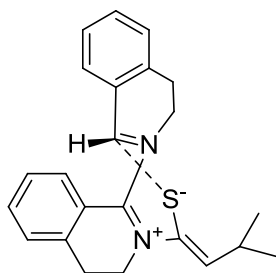
TS1-*exo-k*



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.449609	2.985300	0.209225
2	6	0	-0.204686	1.876597	-0.521728
3	16	0	1.208504	1.413616	-1.441795
4	7	0	-1.280582	0.875918	-0.551360
5	6	0	-1.434435	0.044296	0.486259
6	6	0	-1.875073	0.536565	-1.858267
7	6	0	-2.545256	-0.943291	0.452314
8	6	0	-3.340529	0.157616	-1.662004
9	1	0	-1.767749	1.417554	-2.491890
10	1	0	-1.323834	-0.278539	-2.339635
11	6	0	-2.691305	-1.879566	1.485240
12	6	0	-3.487684	-0.897067	-0.589897
13	1	0	-3.910206	1.053607	-1.375122
14	1	0	-3.761237	-0.195211	-2.610620
15	6	0	-3.757629	-2.772336	1.484540
16	1	0	-1.954738	-1.912245	2.283045
17	6	0	-4.554206	-1.802648	-0.581458
18	6	0	-4.691456	-2.735299	0.444382
19	1	0	-3.860498	-3.496722	2.287420
20	1	0	-5.282417	-1.772381	-1.388626
21	1	0	-5.523959	-3.433553	0.434126

22	1	0	-1.438615	3.094727	0.659289
23	1	0	-1.198817	0.489023	1.448399
24	7	0	0.197023	-1.062592	0.677589
25	6	0	0.879770	-1.271859	-0.409275
26	6	0	0.922077	-0.987840	1.952315
27	6	0	2.300981	-1.628350	-0.410656
28	1	0	0.324812	-1.375973	-1.335276
29	6	0	2.369796	-0.503802	1.798107
30	1	0	0.369278	-0.319113	2.622936
31	1	0	0.900945	-1.987854	2.411446
32	6	0	2.884188	-2.308381	-1.486603
33	6	0	3.068659	-1.298828	0.723371
34	1	0	2.359650	0.553553	1.497911
35	1	0	2.893477	-0.575868	2.758103
36	6	0	4.228459	-2.671254	-1.434573
37	1	0	2.283446	-2.547862	-2.360596
38	6	0	4.411858	-1.663448	0.763224
39	6	0	4.990770	-2.350303	-0.308731
40	1	0	4.681781	-3.199085	-2.268790
41	1	0	5.012890	-1.406649	1.632517
42	1	0	6.039464	-2.631800	-0.265014
43	6	0	0.521702	4.114006	0.431800
44	1	0	1.497105	3.789311	0.050632
45	6	0	0.662071	4.432266	1.931867
46	1	0	1.375684	5.248986	2.097943
47	1	0	-0.300075	4.740524	2.363322
48	1	0	1.013122	3.557161	2.491361
49	6	0	0.099219	5.369193	-0.357140
50	1	0	-0.888688	5.725787	-0.035720
51	1	0	0.814068	6.188477	-0.206469
52	1	0	0.047875	5.153598	-1.429446

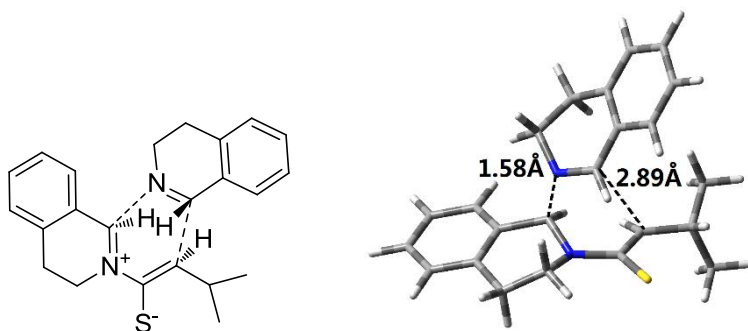
C-*exo*-k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.643090	2.709402	0.233830
2	6	0	0.873146	1.727248	-0.260723
3	16	0	1.529356	0.333829	-1.207143
4	7	0	-0.545199	1.764120	-0.101278
5	6	0	-1.074516	0.694133	0.772576
6	6	0	-1.279296	2.072076	-1.334998
7	6	0	-2.557889	0.402138	0.516528
8	6	0	-2.725367	2.408676	-0.987098
9	1	0	-0.781723	2.932077	-1.792982
10	1	0	-1.252563	1.251540	-2.072695
11	6	0	-3.138487	-0.706933	1.146716
12	6	0	-3.360511	1.243648	-0.268983
13	1	0	-2.736642	3.307361	-0.354433
14	1	0	-3.287339	2.647220	-1.898222
15	6	0	-4.497937	-0.976123	1.014641
16	1	0	-2.508820	-1.368860	1.733647
17	6	0	-4.726288	0.959774	-0.403038
18	6	0	-5.298877	-0.135685	0.237309
19	1	0	-4.930193	-1.841064	1.510698
20	1	0	-5.340273	1.606285	-1.026598
21	1	0	-6.360034	-0.340605	0.122273
22	1	0	1.114150	3.521774	0.734396
23	1	0	-0.993005	1.063914	1.804448
24	7	0	-0.270945	-0.539372	0.752237
25	6	0	0.205708	-0.929555	-0.529749
26	6	0	0.527982	-0.851482	1.948888
27	6	0	0.818410	-2.301056	-0.534710
28	1	0	-0.617620	-0.871988	-1.245234
29	6	0	1.818385	-1.630277	1.635815
30	1	0	0.791531	0.075651	2.474617
31	1	0	-0.088704	-1.446486	2.639176
32	6	0	0.613275	-3.197824	-1.584846
33	6	0	1.604374	-2.672123	0.567504
34	1	0	2.583179	-0.924418	1.287977
35	1	0	2.192930	-2.084292	2.560168
36	6	0	1.188452	-4.469400	-1.543422
37	1	0	-0.001529	-2.903651	-2.432421
38	6	0	2.164076	-3.949734	0.608107
39	6	0	1.961513	-4.845948	-0.444390
40	1	0	1.025535	-5.165127	-2.361956

41	1	0	2.766013	-4.244002	1.465119
42	1	0	2.404140	-5.837671	-0.403305
43	6	0	3.141669	2.834049	0.150399
44	1	0	3.548780	1.883961	-0.217884
45	6	0	3.737757	3.109319	1.543217
46	1	0	4.829750	3.193369	1.490779
47	1	0	3.350649	4.048848	1.958824
48	1	0	3.492125	2.306077	2.246982
49	6	0	3.544461	3.940078	-0.845949
50	1	0	3.146509	4.914397	-0.534639
51	1	0	4.636029	4.029111	-0.907538
52	1	0	3.161653	3.725684	-1.849361

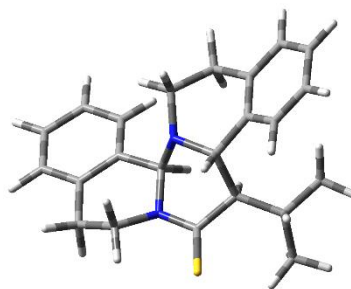
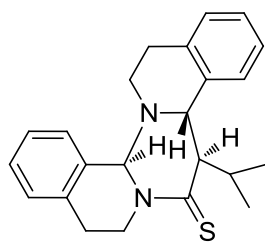
TS2-Re-k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.805120	1.802064	1.012173
2	6	0	0.067856	2.040595	-0.136311
3	16	0	0.607661	3.088526	-1.393308
4	7	0	-1.144932	1.277342	-0.334010
5	6	0	-1.296509	0.034081	0.335195
6	6	0	-1.815644	1.304603	-1.644872
7	6	0	-2.726630	-0.484727	0.347878
8	6	0	-3.320198	1.133936	-1.489583
9	1	0	-1.567942	2.252109	-2.119679
10	1	0	-1.417600	0.502931	-2.287920
11	6	0	-3.137977	-1.374977	1.352757
12	6	0	-3.680988	0.001192	-0.560230
13	1	0	-3.748487	2.061463	-1.083498
14	1	0	-3.774207	0.985927	-2.477477
15	6	0	-4.441850	-1.862719	1.398456
16	1	0	-2.441398	-1.665357	2.135578
17	6	0	-4.988632	-0.497535	-0.510007

18	6	0	-5.368093	-1.437353	0.444805
19	1	0	-4.735366	-2.555130	2.182302
20	1	0	-5.720898	-0.122861	-1.221802
21	1	0	-6.387802	-1.812270	0.465292
22	1	0	-0.966208	0.118914	1.370799
23	6	0	0.874621	-0.503663	-0.730169
24	6	0	2.117492	-1.241838	-0.740802
25	7	0	-0.253841	-1.009878	-0.231822
26	6	0	3.173512	-0.835613	-1.578821
27	6	0	2.287492	-2.341223	0.132235
28	6	0	-0.193114	-2.382366	0.310492
29	6	0	4.381266	-1.524908	-1.556981
30	1	0	3.032523	0.020415	-2.233220
31	6	0	3.502285	-3.018578	0.143863
32	6	0	1.125154	-2.671096	1.035842
33	1	0	-1.047126	-2.544042	0.962517
34	1	0	-0.305413	-3.068497	-0.539224
35	6	0	4.545002	-2.617284	-0.698984
36	1	0	5.195554	-1.213116	-2.204296
37	1	0	3.640685	-3.864445	0.813203
38	1	0	1.184623	-2.064411	1.952172
39	1	0	1.147581	-3.721582	1.347022
40	1	0	5.486621	-3.159080	-0.684367
41	1	0	0.824416	0.405010	-1.317533
42	1	0	0.344153	1.282829	1.852128
43	6	0	2.121651	2.453579	1.348308
44	1	0	2.650987	2.651812	0.409266
45	6	0	1.903356	3.813122	2.047646
46	1	0	2.864509	4.287491	2.286298
47	1	0	1.337283	4.486616	1.397841
48	1	0	1.347839	3.688576	2.986644
49	6	0	2.983117	1.525536	2.222152
50	1	0	3.947063	1.992440	2.457833
51	1	0	2.485094	1.303377	3.176445
52	1	0	3.182617	0.573249	1.717167

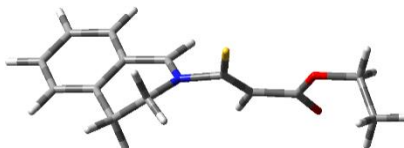
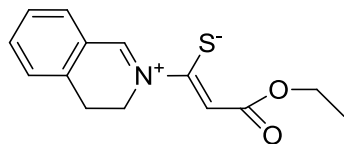
8k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.023990	1.198733	0.548217
2	6	0	-0.080100	2.073965	-0.058529
3	16	0	0.213090	3.536148	-0.817349
4	7	0	-1.274853	1.412831	-0.130567
5	6	0	-1.254195	-0.008403	0.263823
6	6	0	-2.228316	1.750702	-1.201061
7	6	0	-2.646447	-0.635874	0.284255
8	6	0	-3.653803	1.403657	-0.810066
9	1	0	-2.122722	2.812325	-1.413931
10	1	0	-1.925988	1.191743	-2.098730
11	6	0	-2.826452	-1.844036	0.979432
12	6	0	-3.773467	0.011264	-0.242753
13	1	0	-4.011353	2.124434	-0.060821
14	1	0	-4.302156	1.521444	-1.686957
15	6	0	-4.075840	-2.449260	1.072170
16	1	0	-1.976111	-2.310511	1.470431
17	6	0	-5.029002	-0.605742	-0.146499
18	6	0	-5.185228	-1.833020	0.488453
19	1	0	-4.184709	-3.388702	1.606747
20	1	0	-5.895130	-0.098928	-0.566514
21	1	0	-6.166640	-2.295328	0.549636
22	1	0	-0.948854	-0.035515	1.318490
23	6	0	1.078631	0.077118	-0.595481
24	6	0	2.273288	-0.861859	-0.569628
25	7	0	-0.248675	-0.637149	-0.625272
26	6	0	3.478688	-0.440085	-1.148047
27	6	0	2.190699	-2.155361	-0.026303
28	6	0	-0.161320	-2.092517	-0.691605
29	6	0	4.613243	-1.247372	-1.110361
30	1	0	3.528579	0.539504	-1.617620
31	6	0	3.333041	-2.962977	0.002056
32	6	0	0.822810	-2.678551	0.339476

33	1	0	-1.161508	-2.510571	-0.587632
34	1	0	0.188578	-2.371563	-1.694279
35	6	0	4.545620	-2.509240	-0.514808
36	1	0	5.542895	-0.897489	-1.550803
37	1	0	3.260443	-3.967607	0.413465
38	1	0	0.520410	-2.382846	1.355264
39	1	0	0.815075	-3.775399	0.312625
40	1	0	5.423486	-3.149028	-0.484049
41	1	0	1.171390	0.642289	-1.533055
42	1	0	0.649021	0.712799	1.454798
43	6	0	2.319049	1.908285	1.025756
44	1	0	2.872346	2.290102	0.159103
45	6	0	1.986675	3.094921	1.956447
46	1	0	2.916373	3.519895	2.352375
47	1	0	1.437032	3.887471	1.451390
48	1	0	1.394178	2.752341	2.816104
49	6	0	3.224372	0.964800	1.848090
50	1	0	4.107777	1.517812	2.187623
51	1	0	2.694374	0.621990	2.747367
52	1	0	3.572858	0.086325	1.309228

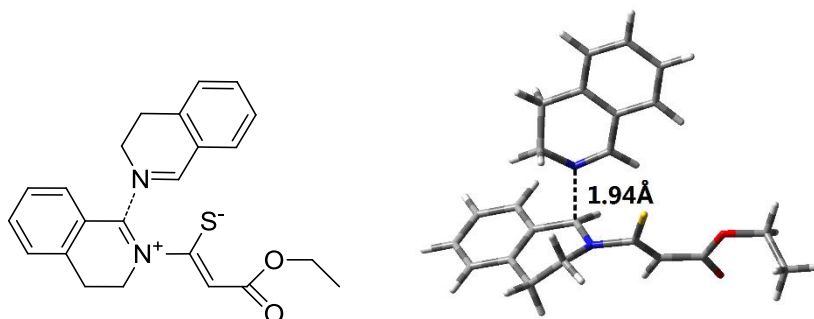
1m



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.555325	-0.586822	0.384493
2	6	0	0.936868	0.459040	-0.254293
3	16	0	1.393754	1.743829	-1.255250
4	7	0	-0.532578	0.457798	0.003266
5	6	0	-1.279056	-0.535744	-0.386477
6	6	0	-1.177239	1.698469	0.513492
7	6	0	-2.718101	-0.546216	-0.245126
8	6	0	-2.409904	1.350276	1.346878
9	1	0	-0.421429	2.235000	1.087099
10	1	0	-1.438293	2.312857	-0.351600
11	6	0	-3.496134	-1.509569	-0.909872
12	6	0	-3.326123	0.408480	0.600797
13	1	0	-2.098308	0.880723	2.291701

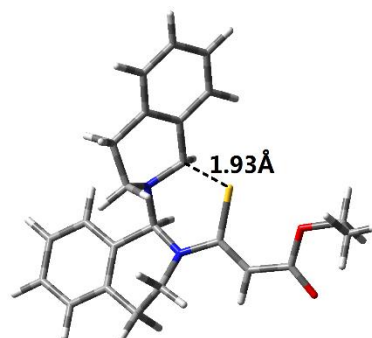
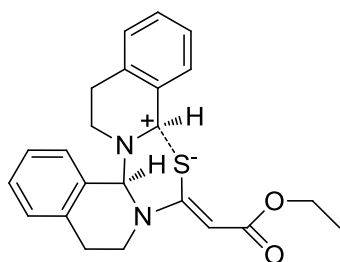
14	1	0	-2.929637	2.276854	1.612073
15	6	0	-4.878250	-1.509452	-0.755318
16	1	0	-3.012592	-2.241481	-1.551576
17	6	0	-4.710261	0.393048	0.747265
18	6	0	-5.482784	-0.556408	0.070553
19	1	0	-5.484208	-2.245795	-1.274100
20	1	0	-5.190897	1.121343	1.395392
21	1	0	-6.562248	-0.554511	0.192466
22	1	0	0.963826	-1.229842	1.028100
23	1	0	-0.762573	-1.372874	-0.846241
24	6	0	2.964525	-0.974055	0.371135
25	8	0	3.383993	-1.930274	1.011860
26	8	0	3.750537	-0.198252	-0.409877
27	6	0	5.150016	-0.537852	-0.449809
28	1	0	5.255178	-1.626091	-0.452251
29	1	0	5.497130	-0.136381	-1.405562
30	6	0	5.908893	0.080691	0.716396
31	1	0	5.564590	-0.344098	1.663439
32	1	0	6.982030	-0.122217	0.616189
33	1	0	5.762527	1.165568	0.739454

TS1-endo-m



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.590529	-2.193860	-0.332537
2	6	0	0.995811	-1.334004	0.554759
3	16	0	1.584564	-0.081622	1.564621
4	7	0	-0.473026	-1.490693	0.585997
5	6	0	-1.189740	-1.028300	-0.452879
6	6	0	-1.151735	-1.634137	1.885578
7	6	0	-2.646479	-1.310935	-0.493942
8	6	0	-2.393843	-2.506885	1.705322
9	1	0	-0.440100	-2.086054	2.576575

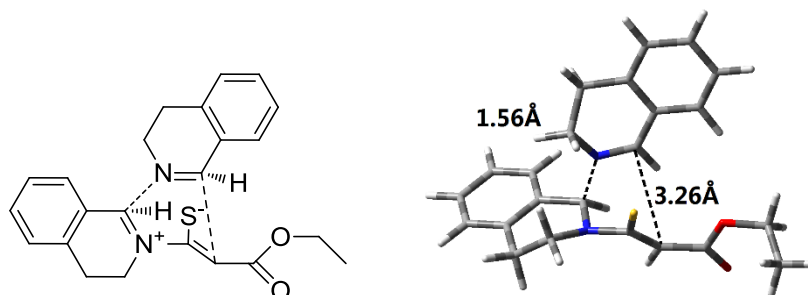
10	1	0	-1.414403	-0.648957	2.289523
11	6	0	-3.406325	-0.906146	-1.600451
12	6	0	-3.249933	-2.026445	0.554823
13	1	0	-2.082056	-3.543679	1.513152
14	1	0	-2.973036	-2.518949	2.635999
15	6	0	-4.764651	-1.200584	-1.667724
16	1	0	-2.924215	-0.351573	-2.401665
17	6	0	-4.616576	-2.314722	0.474910
18	6	0	-5.371175	-1.905595	-0.623504
19	1	0	-5.348225	-0.885438	-2.527871
20	1	0	-5.090507	-2.867521	1.282632
21	1	0	-6.431869	-2.137179	-0.667171
22	1	0	0.968179	-2.957692	-0.789560
23	1	0	-0.662146	-1.064058	-1.401172
24	7	0	-1.121288	0.914134	-0.438370
25	6	0	0.065493	1.404583	-0.606205
26	6	0	-2.090286	1.718355	0.314536
27	6	0	0.416560	2.794237	-0.314457
28	1	0	0.806476	0.775491	-1.093141
29	6	0	-2.043090	3.190702	-0.105909
30	1	0	-3.086188	1.297227	0.157407
31	1	0	-1.845295	1.625333	1.383657
32	6	0	1.752521	3.219429	-0.337169
33	6	0	-0.623217	3.711139	-0.063430
34	1	0	-2.443678	3.291694	-1.126115
35	1	0	-2.696122	3.779454	0.548170
36	6	0	2.057450	4.556612	-0.102902
37	1	0	2.539074	2.489156	-0.504913
38	6	0	-0.303520	5.049416	0.162988
39	6	0	1.028514	5.470326	0.146265
40	1	0	3.091847	4.887257	-0.108079
41	1	0	-1.097609	5.766696	0.356958
42	1	0	1.264503	6.514604	0.332419
43	6	0	2.979125	-2.293469	-0.772406
44	8	0	3.363543	-3.171194	-1.536599
45	8	0	3.803177	-1.327400	-0.289975
46	6	0	5.184793	-1.418054	-0.681608
47	1	0	5.244571	-1.722488	-1.730253
48	1	0	5.563738	-0.397196	-0.577288
49	6	0	5.957735	-2.382597	0.208135
50	1	0	5.580598	-3.400931	0.080369
51	1	0	7.021722	-2.371315	-0.058373
52	1	0	5.860376	-2.097677	1.260844

C-endo-m

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.637539	-2.475160	-0.163175
2	6	0	0.849493	-1.359136	-0.194575
3	16	0	1.560647	0.282501	-0.389805
4	7	0	-0.523945	-1.476348	0.022657
5	6	0	-1.445906	-0.507222	-0.581273
6	6	0	-1.037383	-2.328364	1.103076
7	6	0	-2.912668	-0.890262	-0.398173
8	6	0	-2.262240	-3.100258	0.623272
9	1	0	-0.244291	-3.002387	1.421241
10	1	0	-1.312119	-1.713980	1.974940
11	6	0	-3.887774	0.014237	-0.842827
12	6	0	-3.307453	-2.134309	0.117473
13	1	0	-1.960975	-3.797285	-0.171203
14	1	0	-2.669143	-3.703931	1.443848
15	6	0	-5.240618	-0.306712	-0.778664
16	1	0	-3.568700	0.976337	-1.231858
17	6	0	-4.672578	-2.444552	0.180363
18	6	0	-5.636252	-1.544843	-0.265998
19	1	0	-5.983599	0.405704	-1.126660
20	1	0	-4.975802	-3.404699	0.592101
21	1	0	-6.690128	-1.803688	-0.208804
22	1	0	1.138115	-3.435015	-0.090646
23	1	0	-1.249966	-0.526508	-1.662613
24	7	0	-1.196162	0.883356	-0.189435
25	6	0	0.015056	1.358626	-0.788807
26	6	0	-1.294938	1.179835	1.244570
27	6	0	0.369066	2.775567	-0.406362
28	1	0	-0.086769	1.283243	-1.875212
29	6	0	-1.365284	2.694892	1.433985

30	1	0	-2.204498	0.708586	1.626473
31	1	0	-0.437916	0.767721	1.801073
32	6	0	1.350624	3.460170	-1.135857
33	6	0	-0.272008	3.410429	0.669223
34	1	0	-2.345243	3.050457	1.086078
35	1	0	-1.302106	2.937985	2.501870
36	6	0	1.705505	4.764231	-0.801458
37	1	0	1.839454	2.962208	-1.970140
38	6	0	0.092151	4.723118	0.993117
39	6	0	1.073182	5.398425	0.270547
40	1	0	2.468331	5.283491	-1.374778
41	1	0	-0.402954	5.218070	1.826005
42	1	0	1.343148	6.415635	0.541276
43	6	0	3.086070	-2.624583	-0.237968
44	8	0	3.640664	-3.711597	-0.302507
45	8	0	3.768135	-1.446860	-0.230064
46	6	0	5.204413	-1.530067	-0.339767
47	1	0	5.460100	-2.329769	-1.039342
48	1	0	5.499532	-0.566731	-0.764089
49	6	0	5.854835	-1.761760	1.016793
50	1	0	5.559742	-2.734970	1.418060
51	1	0	6.946659	-1.745271	0.916092
52	1	0	5.562146	-0.980420	1.726114

TS2-Si-m

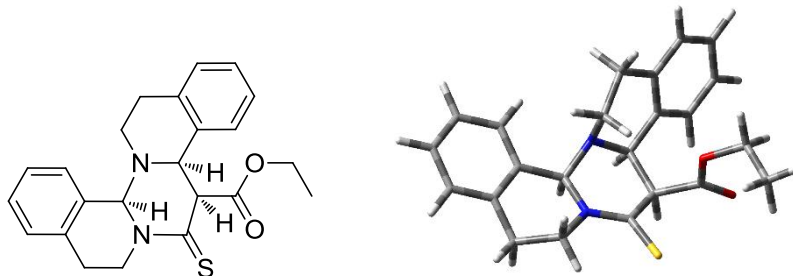


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.970442	-2.137455	-0.506150
2	6	0	0.417749	-1.557995	0.625326
3	16	0	1.139729	-0.922600	2.039894
4	7	0	-1.037419	-1.436357	0.521177
5	6	0	-1.491579	-0.550467	-0.492575
6	6	0	-1.859938	-1.564069	1.728936

7	6	0	-2.994985	-0.400896	-0.592583
8	6	0	-3.261257	-2.018032	1.321849
9	1	0	-1.375931	-2.303398	2.367300
10	1	0	-1.910266	-0.636220	2.314958
11	6	0	-3.531003	0.424478	-1.591124
12	6	0	-3.848347	-1.109642	0.266274
13	1	0	-3.205379	-3.043503	0.930864
14	1	0	-3.915550	-2.047091	2.201684
15	6	0	-4.908419	0.557862	-1.738514
16	1	0	-2.860517	0.964216	-2.256317
17	6	0	-5.233397	-0.965234	0.107847
18	6	0	-5.763415	-0.141661	-0.882052
19	1	0	-5.313361	1.198504	-2.516722
20	1	0	-5.899027	-1.508786	0.774357
21	1	0	-6.840527	-0.043721	-0.986835
22	1	0	0.288686	-2.637572	-1.189840
23	1	0	-1.082560	-0.850577	-1.460812
24	7	0	-0.834377	0.851550	-0.298514
25	6	0	0.346105	1.045411	-0.819825
26	6	0	-1.232510	1.679348	0.861997
27	6	0	1.201719	2.148310	-0.454639
28	1	0	0.683392	0.322048	-1.555561
29	6	0	-0.805049	3.133004	0.660459
30	1	0	-2.313800	1.595606	0.975811
31	1	0	-0.731486	1.234391	1.735333
32	6	0	2.547928	2.157593	-0.854570
33	6	0	0.659339	3.215831	0.292926
34	1	0	-1.414091	3.596546	-0.130357
35	1	0	-1.007140	3.689532	1.581467
36	6	0	3.357930	3.234842	-0.511824
37	1	0	2.951966	1.302602	-1.388618
38	6	0	1.479655	4.292109	0.614718
39	6	0	2.820927	4.300742	0.215969
40	1	0	4.403808	3.243594	-0.802228
41	1	0	1.078633	5.124323	1.187546
42	1	0	3.452632	5.142971	0.484392
43	6	0	2.351244	-2.286287	-0.929814
44	8	0	2.690181	-3.007054	-1.863885
45	8	0	3.250979	-1.508010	-0.253914
46	6	0	4.635239	-1.716804	-0.579728
47	1	0	4.741425	-1.836307	-1.662088
48	1	0	5.131416	-0.793363	-0.264968
49	6	0	5.209793	-2.920271	0.156144
50	1	0	4.722976	-3.838522	-0.183582

51	1	0	6.285833	-3.005866	-0.039895
52	1	0	5.057444	-2.817948	1.235277

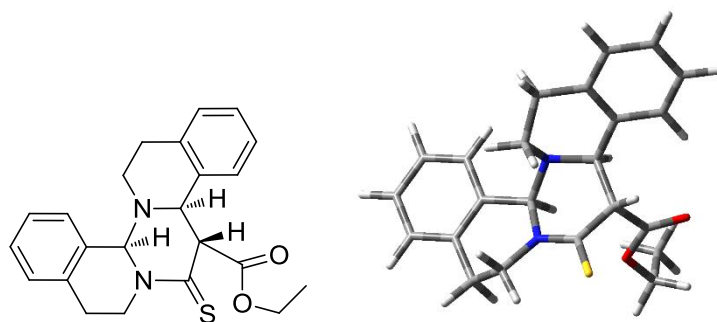
7m



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.912416	0.926357	-1.096855
2	6	0	0.181265	1.849811	-0.524913
3	16	0	-0.226850	3.440134	-0.179140
4	7	0	1.427685	1.347069	-0.387164
5	6	0	1.693978	-0.102191	-0.704192
6	6	0	2.516078	2.202342	0.112055
7	6	0	3.047947	-0.588026	-0.200851
8	6	0	3.873095	1.752236	-0.422773
9	1	0	2.292979	3.225416	-0.193048
10	1	0	2.510957	2.183762	1.210230
11	6	0	3.251844	-1.950691	0.048382
12	6	0	4.125795	0.302991	-0.104831
13	1	0	3.904684	1.917314	-1.510028
14	1	0	4.651195	2.389389	0.011908
15	6	0	4.510222	-2.419517	0.422831
16	1	0	2.417132	-2.635344	-0.059325
17	6	0	5.383090	-0.175434	0.277456
18	6	0	5.579280	-1.529652	0.542588
19	1	0	4.654556	-3.478256	0.619804
20	1	0	6.212468	0.522800	0.364397
21	1	0	6.561026	-1.888847	0.839052
22	1	0	-1.016020	1.226951	-2.143970
23	1	0	1.719710	-0.172312	-1.802774
24	7	0	0.599264	-0.938347	-0.284040
25	6	0	-0.580001	-0.636450	-1.090050
26	6	0	0.312213	-0.962348	1.160503
27	6	0	-1.747749	-1.536009	-0.716658
28	1	0	-0.305503	-0.879750	-2.123981

29	6	0	-0.583881	-2.166479	1.447713
30	1	0	1.258432	-1.057307	1.698720
31	1	0	-0.176088	-0.037513	1.498040
32	6	0	-2.825080	-1.664141	-1.603802
33	6	0	-1.754083	-2.253953	0.489573
34	1	0	0.015429	-3.084480	1.367419
35	1	0	-0.945769	-2.118966	2.482488
36	6	0	-3.905422	-2.489571	-1.303354
37	1	0	-2.821768	-1.102127	-2.534387
38	6	0	-2.846465	-3.081311	0.780892
39	6	0	-3.916232	-3.202731	-0.102683
40	1	0	-4.732616	-2.575697	-2.002265
41	1	0	-2.852104	-3.637114	1.716502
42	1	0	-4.754281	-3.849432	0.143446
43	6	0	-2.282218	1.251378	-0.495356
44	8	0	-3.246002	1.556104	-1.162352
45	8	0	-2.305744	1.056275	0.837163
46	6	0	-3.573152	1.279947	1.503253
47	1	0	-4.372134	0.900399	0.862024
48	1	0	-3.510655	0.665708	2.405085
49	6	0	-3.775262	2.749328	1.838232
50	1	0	-3.848647	3.346249	0.925667
51	1	0	-4.702502	2.871428	2.410762
52	1	0	-2.942626	3.130191	2.437456

4m

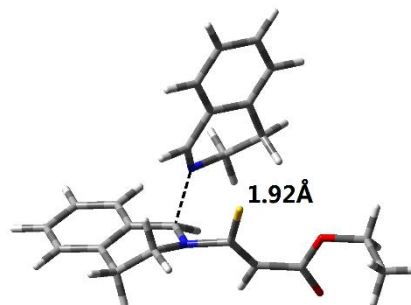
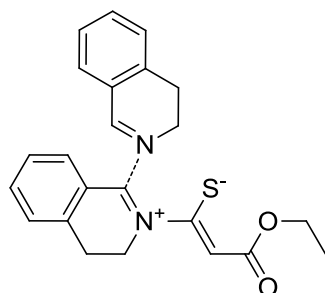


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.204608	-1.035334	0.525825
2	6	0	0.019496	-1.120396	1.492099
3	16	0	0.258754	-1.837067	2.988233
4	7	0	-1.152730	-0.613076	1.058589
5	6	0	-1.158263	0.164274	-0.224911

6	6	0	-2.358627	-0.680750	1.891036
7	6	0	-2.473753	0.885861	-0.485365
8	6	0	-3.612938	-0.750154	1.023309
9	1	0	-2.263682	-1.562137	2.526458
10	1	0	-2.397606	0.195599	2.553071
11	6	0	-2.499317	1.963906	-1.379007
12	6	0	-3.672069	0.417487	0.072577
13	1	0	-3.611955	-1.699951	0.469038
14	1	0	-4.495261	-0.765984	1.672865
15	6	0	-3.704000	2.584668	-1.704071
16	1	0	-1.564895	2.307666	-1.810605
17	6	0	-4.875242	1.051761	-0.255766
18	6	0	-4.897195	2.128420	-1.140141
19	1	0	-3.710189	3.423265	-2.394945
20	1	0	-5.800810	0.694910	0.190414
21	1	0	-5.839379	2.611094	-1.385338
22	1	0	2.102665	-1.011160	1.140505
23	1	0	-1.026179	-0.573698	-1.028193
24	7	0	-0.005745	1.040416	-0.290171
25	6	0	1.204279	0.232217	-0.451555
26	6	0	0.085161	2.029831	0.794910
27	6	0	2.481788	1.050503	-0.320298
28	1	0	1.170526	-0.154258	-1.478576
29	6	0	1.144383	3.062439	0.424049
30	1	0	-0.893405	2.505353	0.902954
31	1	0	0.337141	1.565678	1.762990
32	6	0	3.708384	0.442062	-0.628281
33	6	0	2.457380	2.393972	0.083271
34	1	0	0.786283	3.648124	-0.434281
35	1	0	1.282797	3.766841	1.253475
36	6	0	4.898845	1.158144	-0.542731
37	1	0	3.725109	-0.603807	-0.924076
38	6	0	3.664091	3.102032	0.168288
39	6	0	4.877786	2.497189	-0.144190
40	1	0	5.840114	0.671855	-0.783804
41	1	0	3.643062	4.141266	0.490101
42	1	0	5.802824	3.062782	-0.070275
43	6	0	1.341518	-2.299197	-0.321455
44	8	0	2.405194	-2.716309	-0.728885
45	8	0	0.150467	-2.855534	-0.621693
46	6	0	0.178065	-4.058218	-1.434947
47	1	0	1.038151	-4.659844	-1.133455
48	1	0	-0.743071	-4.580302	-1.166175
49	6	0	0.224581	-3.728004	-2.918572

50	1	0	1.160859	-3.223887	-3.173685
51	1	0	0.163246	-4.652363	-3.504317
52	1	0	-0.616119	-3.086881	-3.204640

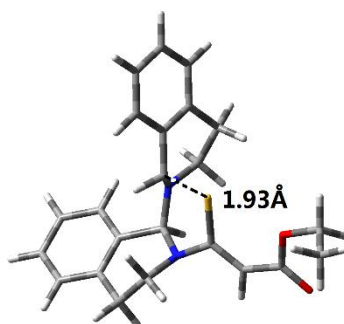
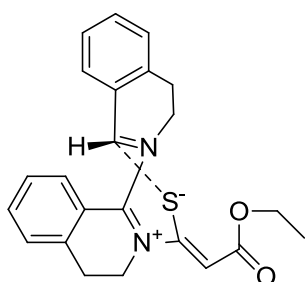
TS1-*exo-m*



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.028793	-2.364937	-0.212518
2	6	0	0.531775	-1.444209	0.674213
3	16	0	1.263426	-0.330700	1.749041
4	7	0	-0.942722	-1.359415	0.648455
5	6	0	-1.514118	-0.843453	-0.459974
6	6	0	-1.678199	-1.324810	1.926960
7	6	0	-2.993722	-0.680309	-0.485866
8	6	0	-3.079351	-1.891074	1.711763
9	1	0	-1.106691	-1.922524	2.637384
10	1	0	-1.727963	-0.308440	2.331765
11	6	0	-3.614986	-0.073096	-1.586284
12	6	0	-3.772640	-1.193580	0.565336
13	1	0	-3.006491	-2.967040	1.497211
14	1	0	-3.662780	-1.789646	2.634035
15	6	0	-5.000022	0.037193	-1.643015
16	1	0	-3.004152	0.323649	-2.392698
17	6	0	-5.165294	-1.074698	0.497665
18	6	0	-5.777803	-0.463811	-0.594289
19	1	0	-5.473167	0.512143	-2.497587
20	1	0	-5.771046	-1.467370	1.310891
21	1	0	-6.860350	-0.377285	-0.629530
22	1	0	0.324397	-3.044232	-0.684635
23	1	0	-1.055235	-1.175519	-1.386471
24	7	0	-0.795892	0.909635	-0.755065
25	6	0	-0.579576	1.660117	0.277947
26	6	0	0.035117	1.112750	-1.953691

27	6	0	0.367276	2.772264	0.284575
28	1	0	-1.219645	1.516177	1.143539
29	6	0	1.450937	1.596579	-1.620206
30	1	0	0.074767	0.168632	-2.505567
31	1	0	-0.481704	1.843606	-2.593163
32	6	0	0.271584	3.803566	1.227735
33	6	0	1.383693	2.785558	-0.692339
34	1	0	2.003066	0.785891	-1.123514
35	1	0	1.982597	1.842559	-2.546138
36	6	0	1.177302	4.860956	1.194734
37	1	0	-0.510667	3.772445	1.982182
38	6	0	2.287812	3.844164	-0.709011
39	6	0	2.183669	4.879446	0.225641
40	1	0	1.104484	5.663584	1.922694
41	1	0	3.081380	3.860663	-1.452056
42	1	0	2.894066	5.701225	0.198494
43	6	0	2.401119	-2.630766	-0.626417
44	8	0	2.705286	-3.579929	-1.339235
45	8	0	3.312455	-1.715364	-0.196296
46	6	0	4.684503	-1.970134	-0.548623
47	1	0	4.729882	-2.353845	-1.571644
48	1	0	5.162276	-0.987092	-0.506915
49	6	0	5.340816	-2.939402	0.425460
50	1	0	4.868392	-3.923266	0.358432
51	1	0	6.405880	-3.050048	0.187521
52	1	0	5.250129	-2.572149	1.452841

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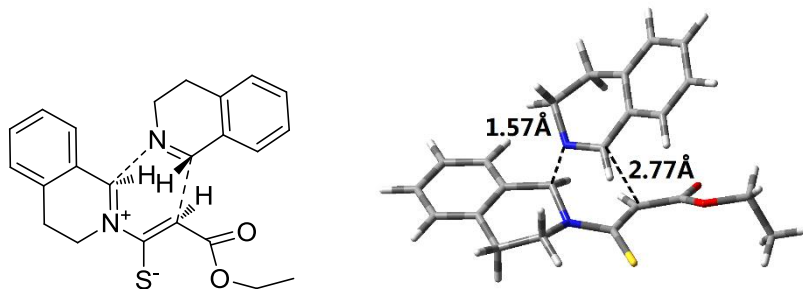


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.127317	-1.998585	0.529460
2	6	0	-1.132307	-1.197684	0.076449

3	16	0	-1.361701	0.437575	-0.613367
4	7	0	0.188525	-1.729624	0.061297
5	6	0	1.226395	-0.987579	0.802774
6	6	0	0.552697	-2.374566	-1.209224
7	6	0	2.644017	-1.382919	0.367648
8	6	0	1.740307	-3.302186	-0.979002
9	1	0	-0.321530	-2.940016	-1.541815
10	1	0	0.795246	-1.647589	-2.004115
11	6	0	3.720289	-0.618605	0.837986
12	6	0	2.899813	-2.512556	-0.424452
13	1	0	1.437477	-4.095602	-0.281608
14	1	0	2.024377	-3.788265	-1.920091
15	6	0	5.033927	-0.972249	0.542373
16	1	0	3.519104	0.269914	1.428307
17	6	0	4.224775	-2.855615	-0.724516
18	6	0	5.289350	-2.100243	-0.241263
19	1	0	5.855147	-0.366555	0.915981
20	1	0	4.415040	-3.722600	-1.353608
21	1	0	6.310915	-2.380811	-0.483652
22	1	0	-1.835584	-2.967006	0.921654
23	1	0	1.122356	-1.275748	1.859050
24	7	0	1.044916	0.472455	0.781802
25	6	0	0.480887	0.974595	-0.427052
26	6	0	0.716513	1.129747	2.058147
27	6	0	0.529937	2.475583	-0.506694
28	1	0	1.008662	0.530758	-1.274385
29	6	0	-0.114359	2.417494	1.894131
30	1	0	0.167632	0.437435	2.712244
31	1	0	1.655881	1.373815	2.574997
32	6	0	0.838684	3.141802	-1.694179
33	6	0	0.272673	3.202252	0.665935
34	1	0	-1.174483	2.146341	1.814797
35	1	0	-0.006626	3.026282	2.798668
36	6	0	0.897685	4.536060	-1.720822
37	1	0	1.039286	2.569191	-2.596798
38	6	0	0.348037	4.595919	0.634244
39	6	0	0.655771	5.262501	-0.553885
40	1	0	1.139997	5.051287	-2.646127
41	1	0	0.159113	5.163251	1.542873
42	1	0	0.709338	6.347846	-0.566697
43	6	0	-3.575566	-1.761992	0.582374
44	8	0	-4.355135	-2.531598	1.118501
45	8	0	-3.959151	-0.609261	-0.021384
46	6	0	-5.368523	-0.292461	0.018057

47	1	0	-5.767849	-0.583948	0.992679
48	1	0	-5.401912	0.795575	-0.079306
49	6	0	-6.124571	-0.976082	-1.111843
50	1	0	-6.095444	-2.062166	-0.989268
51	1	0	-7.173138	-0.655767	-1.105744
52	1	0	-5.690264	-0.715554	-2.082661

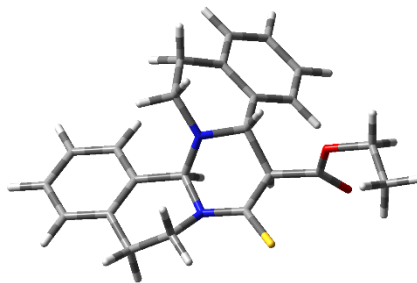
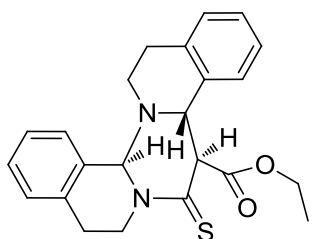
TS2-Re-m



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.812661	-1.319186	1.009889
2	6	0	-0.119089	-1.875860	-0.082813
3	16	0	-0.776505	-2.942483	-1.226583
4	7	0	1.228026	-1.395353	-0.265886
5	6	0	1.636496	-0.184383	0.369602
6	6	0	1.914577	-1.630361	-1.548078
7	6	0	3.145289	0.010297	0.405230
8	6	0	3.417295	-1.770501	-1.356412
9	1	0	1.483094	-2.528862	-1.985281
10	1	0	1.702631	-0.795840	-2.236200
11	6	0	3.716429	0.824580	1.396997
12	6	0	3.991599	-0.704343	-0.456790
13	1	0	3.633870	-2.750515	-0.908013
14	1	0	3.909944	-1.760358	-2.336696
15	6	0	5.093465	1.018989	1.468182
16	1	0	3.081833	1.285910	2.149883
17	6	0	5.375052	-0.498827	-0.381793
18	6	0	5.927042	0.369917	0.555704
19	1	0	5.512188	1.657360	2.240790
20	1	0	6.024846	-1.049547	-1.058232
21	1	0	7.003089	0.515057	0.596661
22	1	0	1.281407	-0.166116	1.399850
23	6	0	-0.351786	0.772774	-0.741429

24	6	0	-1.403050	1.763236	-0.801093
25	7	0	0.852763	1.032516	-0.241930
26	6	0	-2.534152	1.537229	-1.606649
27	6	0	-1.321315	2.919044	0.007035
28	6	0	1.107798	2.412043	0.226353
29	6	0	-3.563641	2.471882	-1.630379
30	1	0	-2.595720	0.625789	-2.194184
31	6	0	-2.361270	3.842088	-0.024013
32	6	0	-0.113947	3.036538	0.904959
33	1	0	1.968961	2.407112	0.888234
34	1	0	1.385540	3.001783	-0.656943
35	6	0	-3.474178	3.624633	-0.843795
36	1	0	-4.436530	2.303211	-2.253654
37	1	0	-2.309174	4.733852	0.595739
38	1	0	-0.316320	2.524270	1.857404
39	1	0	0.103127	4.083225	1.145587
40	1	0	-4.277173	4.356268	-0.862473
41	1	0	-0.499133	-0.146593	-1.291523
42	1	0	-0.254348	-0.972153	1.872875
43	6	0	-2.233313	-1.321019	1.333662
44	8	0	-2.642163	-1.054091	2.459894
45	8	0	-3.072857	-1.532357	0.285873
46	6	0	-4.477751	-1.561280	0.594769
47	1	0	-4.706910	-0.772147	1.316354
48	1	0	-4.968292	-1.335782	-0.356785
49	6	0	-4.907781	-2.923781	1.121868
50	1	0	-4.430868	-3.125880	2.084808
51	1	0	-5.995498	-2.947600	1.262259
52	1	0	-4.628495	-3.713544	0.417402

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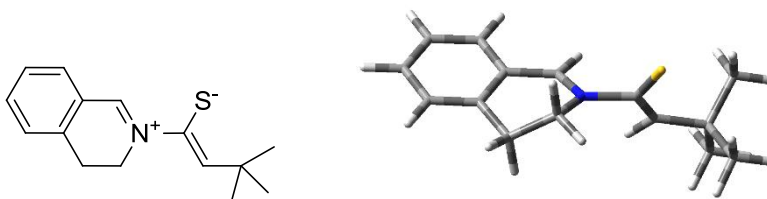


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.340775	-0.438251	0.538711
2	6	0	-0.684278	-1.816074	0.367331
3	16	0	-1.584827	-3.212524	0.226142
4	7	0	0.675983	-1.764717	0.349776
5	6	0	1.265955	-0.403870	0.232640
6	6	0	1.431506	-2.867529	-0.259375
7	6	0	2.786293	-0.404807	0.202913
8	6	0	2.850332	-2.925574	0.281220
9	1	0	0.890176	-3.790163	-0.056461
10	1	0	1.437769	-2.713860	-1.349179
11	6	0	3.449822	0.829085	0.293190
12	6	0	3.541333	-1.586490	0.210825
13	1	0	2.824999	-3.265202	1.326485
14	1	0	3.415654	-3.680545	-0.278160
15	6	0	4.838861	0.900242	0.315995
16	1	0	2.866242	1.741059	0.371085
17	6	0	4.940988	-1.504517	0.228372
18	6	0	5.591783	-0.275933	0.267723
19	1	0	5.331106	1.866478	0.381748
20	1	0	5.520287	-2.425164	0.223175
21	1	0	6.677465	-0.233920	0.279480
22	1	0	1.000160	0.115739	1.166518
23	6	0	-0.792907	0.595931	-0.506906
24	6	0	-0.849421	2.052308	-0.022475
25	7	0	0.565225	0.210932	-0.892175
26	6	0	-1.786293	2.497346	0.923063
27	6	0	0.059128	2.980506	-0.569937
28	6	0	1.136163	1.068511	-1.914918
29	6	0	-1.831453	3.831367	1.324140
30	1	0	-2.490263	1.800828	1.366792
31	6	0	0.006408	4.316880	-0.150498
32	6	0	1.109333	2.582223	-1.593524
33	1	0	2.154848	0.738724	-2.130139
34	1	0	0.548121	0.890234	-2.826327
35	6	0	-0.929997	4.748879	0.784339
36	1	0	-2.564802	4.147718	2.060946
37	1	0	0.716541	5.027156	-0.570312
38	1	0	2.091603	2.913123	-1.233872
39	1	0	0.939750	3.139852	-2.524843
40	1	0	-0.953273	5.790990	1.091823
41	1	0	-1.418034	0.499293	-1.403396
42	1	0	-1.086681	-0.090631	1.546980
43	6	0	-2.870036	-0.531753	0.547921
44	8	0	-3.525081	-0.528553	1.568093

45	8	0	-3.388317	-0.534574	-0.692342
46	6	0	-4.832490	-0.621863	-0.795546
47	1	0	-5.273491	-0.033260	0.012613
48	1	0	-5.058713	-0.149654	-1.754854
49	6	0	-5.306917	-2.065498	-0.754234
50	1	0	-5.063624	-2.523109	0.207720
51	1	0	-6.394089	-2.097004	-0.893657
52	1	0	-4.835835	-2.653505	-1.547466

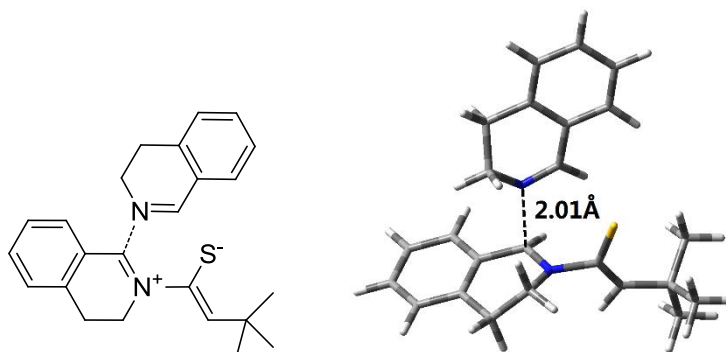
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.069197	1.527943	-0.893102
2	6	0	2.298224	0.538027	-0.259062
3	6	0	2.915305	-0.423237	0.573512
4	6	0	4.297200	-0.385850	0.737847
5	6	0	5.061533	0.592717	0.094424
6	6	0	4.448733	1.551528	-0.718697
7	1	0	2.581214	2.263418	-1.527544
8	1	0	4.782452	-1.121292	1.374638
9	1	0	6.139151	0.608366	0.230999
10	1	0	5.046917	2.310377	-1.213872
11	6	0	2.009797	-1.404897	1.280543
12	1	0	1.676112	-0.970742	2.234880
13	1	0	2.546188	-2.327842	1.525068
14	6	0	0.862544	0.500956	-0.427089
15	1	0	0.338503	1.328262	-0.893876
16	7	0	0.126675	-0.509319	-0.049104
17	6	0	0.795053	-1.752536	0.420641
18	1	0	0.045559	-2.331107	0.960311
19	1	0	1.083041	-2.326503	-0.464083
20	6	0	-1.330797	-0.520773	-0.274519
21	16	0	-1.831093	-1.839457	-1.257688
22	6	0	-1.969864	0.502921	0.356568
23	1	0	-1.357545	1.158296	0.975319
24	6	0	-3.461617	0.805019	0.351404

25	6	0	-3.967588	1.062208	-1.086776
26	1	0	-5.040247	1.295575	-1.074682
27	1	0	-3.442499	1.912461	-1.539542
28	1	0	-3.807480	0.185215	-1.719112
29	6	0	-3.699531	2.073780	1.195766
30	1	0	-3.158291	2.934505	0.781796
31	1	0	-4.765488	2.328731	1.219060
32	1	0	-3.365784	1.931964	2.231714
33	6	0	-4.251192	-0.368917	0.975799
34	1	0	-4.078708	-1.293439	0.417858
35	1	0	-3.947384	-0.532643	2.016935
36	1	0	-5.326940	-0.150403	0.967321

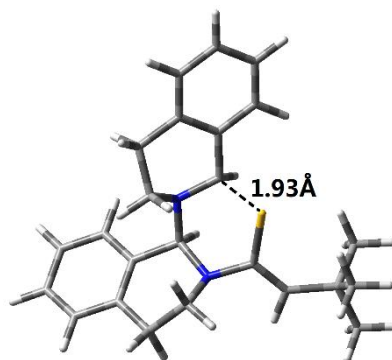
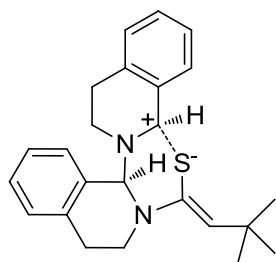
TS1-endo-n



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.700062	-2.952006	-0.230030
2	6	0	-0.294340	-1.865233	0.466493
3	16	0	1.191550	-1.487227	1.300855
4	7	0	-1.287655	-0.775497	0.520357
5	6	0	-1.386527	0.091045	-0.489869
6	6	0	-1.817172	-0.379809	1.837488
7	6	0	-2.495570	1.074209	-0.489905
8	6	0	-3.269129	0.072064	1.684662
9	1	0	-1.733974	-1.247537	2.492395
10	1	0	-1.196051	0.415459	2.266650
11	6	0	-2.646476	1.962022	-1.564300
12	6	0	-3.422320	1.080440	0.567400
13	1	0	-3.899713	-0.803031	1.469542
14	1	0	-3.625860	0.491629	2.632528
15	6	0	-3.710129	2.858687	-1.592610
16	1	0	-1.913712	1.950331	-2.366891

17	6	0	-4.485603	1.988436	0.527493
18	6	0	-4.631432	2.872289	-0.540731
19	1	0	-3.822122	3.544249	-2.427699
20	1	0	-5.205524	1.999500	1.342580
21	1	0	-5.462354	3.572373	-0.553889
22	1	0	-1.722161	-2.920077	-0.609208
23	1	0	-1.072042	-0.305122	-1.449919
24	7	0	0.216690	1.299124	-0.469999
25	6	0	1.338296	0.674586	-0.658233
26	6	0	0.248561	2.490744	0.380826
27	6	0	2.648910	1.249075	-0.334676
28	1	0	1.312653	-0.246589	-1.234241
29	6	0	1.426720	3.402872	0.023089
30	1	0	-0.701678	3.020660	0.272927
31	1	0	0.337828	2.162101	1.428369
32	6	0	3.818658	0.480845	-0.419308
33	6	0	2.718515	2.615660	-0.000736
34	1	0	1.249735	3.854044	-0.965299
35	1	0	1.486012	4.229649	0.740460
36	6	0	5.055494	1.064972	-0.165983
37	1	0	3.740159	-0.577641	-0.650173
38	6	0	3.965769	3.190220	0.247623
39	6	0	5.128399	2.421260	0.168079
40	1	0	5.960525	0.466861	-0.221059
41	1	0	4.028390	4.244546	0.507716
42	1	0	6.092677	2.879468	0.371278
43	6	0	0.071720	-4.233671	-0.527839
44	6	0	0.434667	-4.967210	0.783579
45	1	0	0.982752	-5.893930	0.566450
46	1	0	1.057145	-4.334733	1.422515
47	1	0	-0.470718	-5.232962	1.342756
48	6	0	1.360482	-3.935726	-1.326493
49	1	0	1.899593	-4.866547	-1.547099
50	1	0	1.123435	-3.450607	-2.282181
51	1	0	2.023763	-3.277543	-0.758195
52	6	0	-0.832284	-5.152265	-1.375836
53	1	0	-0.318944	-6.091379	-1.614601
54	1	0	-1.757157	-5.401865	-0.840317
55	1	0	-1.111566	-4.672099	-2.322676

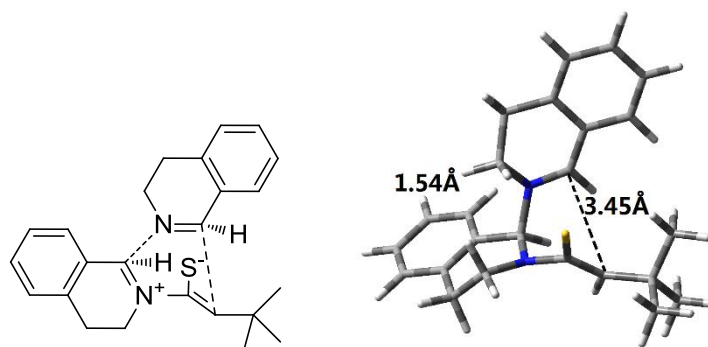
C-endo-n



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.450939	-2.759721	0.173586
2	6	0	-0.872203	-1.589345	-0.148683
3	16	0	-1.774779	-0.092421	-0.615096
4	7	0	0.555421	-1.518912	-0.196794
5	6	0	1.151654	-0.424522	0.571514
6	6	0	1.182006	-1.797999	-1.495375
7	6	0	2.671809	-0.484201	0.539881
8	6	0	2.611613	-2.278458	-1.247816
9	1	0	0.597813	-2.583396	-1.981792
10	1	0	1.178442	-0.927142	-2.170061
11	6	0	3.388068	0.353745	1.406160
12	6	0	3.364707	-1.351122	-0.318143
13	1	0	2.570157	-3.282046	-0.801653
14	1	0	3.147870	-2.376067	-2.200444
15	6	0	4.779227	0.334038	1.432421
16	1	0	2.837614	1.030388	2.054502
17	6	0	4.766902	-1.358400	-0.286371
18	6	0	5.473510	-0.528630	0.579297
19	1	0	5.320062	0.986431	2.112652
20	1	0	5.305154	-2.026588	-0.955539
21	1	0	6.560101	-0.550580	0.587552
22	1	0	-0.733473	-3.553990	0.382594
23	1	0	0.825112	-0.586058	1.608230
24	7	0	0.678231	0.944787	0.260357
25	6	0	-0.723490	1.095734	0.490855
26	6	0	1.127564	1.591102	-0.977476
27	6	0	-1.231960	2.501124	0.274517
28	1	0	-0.950509	0.761735	1.508251
29	6	0	0.962218	3.103435	-0.825498
30	1	0	2.177016	1.339120	-1.141993
31	1	0	0.549993	1.238817	-1.847009

32	6	0	-2.513247	2.847753	0.724752
33	6	0	-0.433227	3.463773	-0.363033
34	1	0	1.697638	3.468405	-0.094847
35	1	0	1.186086	3.601018	-1.777652
36	6	0	-3.005944	4.137394	0.548158
37	1	0	-3.126046	2.093457	1.212451
38	6	0	-0.941162	4.757717	-0.536247
39	6	0	-2.215087	5.097885	-0.088036
40	1	0	-4.000394	4.392545	0.903808
41	1	0	-0.324523	5.504473	-1.032303
42	1	0	-2.591283	6.106865	-0.235022
43	6	0	-2.919815	-3.164565	0.278313
44	6	0	-3.660345	-2.967993	-1.064205
45	1	0	-4.690574	-3.338040	-0.985851
46	1	0	-3.703154	-1.913720	-1.352221
47	1	0	-3.164091	-3.520749	-1.870562
48	6	0	-3.632798	-2.366520	1.394355
49	1	0	-4.677073	-2.691943	1.483031
50	1	0	-3.145405	-2.529503	2.362793
51	1	0	-3.625251	-1.294012	1.182877
52	6	0	-2.965965	-4.664265	0.643155
53	1	0	-4.002157	-5.007324	0.743239
54	1	0	-2.482430	-5.275394	-0.129058
55	1	0	-2.454365	-4.856838	1.594135

TS2-Si-n

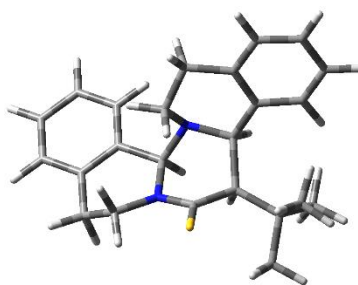
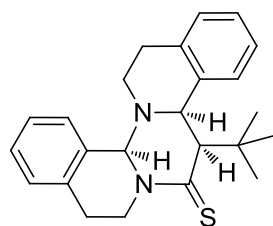


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.820937	2.393542	-0.496889
2	6	0	-0.355464	1.726562	0.602807
3	16	0	-1.162925	1.328083	2.091391
4	7	0	1.031496	1.271451	0.473795

5	6	0	1. 296719	0. 270722	-0. 494599
6	6	0	1. 907727	1. 350843	1. 645658
7	6	0	2. 747802	-0. 163922	-0. 590981
8	6	0	3. 350251	1. 528960	1. 173746
9	1	0	1. 573640	2. 207679	2. 231574
10	1	0	1. 825883	0. 476685	2. 306307
11	6	0	3. 100683	-1. 156928	-1. 515306
12	6	0	3. 738005	0. 448931	0. 191122
13	1	0	3. 450863	2. 513668	0. 696208
14	1	0	4. 031372	1. 519483	2. 033658
15	6	0	4. 427416	-1. 549912	-1. 665551
16	1	0	2. 326586	-1. 624777	-2. 119312
17	6	0	5. 070087	0. 043362	0. 031141
18	6	0	5. 417450	-0. 944741	-0. 886379
19	1	0	4. 688878	-2. 320196	-2. 385664
20	1	0	5. 839538	0. 512096	0. 640357
21	1	0	6. 456252	-1. 245286	-0. 993414
22	1	0	-0. 084530	2. 589655	-1. 278997
23	1	0	0. 953312	0. 602990	-1. 479938
24	7	0	0. 401261	-0. 960982	-0. 244445
25	6	0	-0. 741243	-1. 033608	-0. 880402
26	6	0	0. 565242	-1. 694188	1. 033651
27	6	0	-1. 793530	-1. 947282	-0. 511416
28	1	0	-0. 878144	-0. 363193	-1. 722494
29	6	0	-0. 111017	-3. 062202	0. 967746
30	1	0	1. 636337	-1. 797117	1. 215339
31	1	0	0. 115936	-1. 057661	1. 810721
32	6	0	-3. 064088	-1. 853271	-1. 106413
33	6	0	-1. 522345	-2. 958592	0. 437877
34	1	0	0. 469426	-3. 736654	0. 319700
35	1	0	-0. 103080	-3. 504850	1. 969260
36	6	0	-4. 067404	-2. 744826	-0. 746155
37	1	0	-3. 260556	-1. 065656	-1. 827988
38	6	0	-2. 536127	-3. 847466	0. 782723
39	6	0	-3. 802708	-3. 739807	0. 200294
40	1	0	-5. 053501	-2. 663564	-1. 192923
41	1	0	-2. 339857	-4. 628371	1. 513048
42	1	0	-4. 586473	-4. 434930	0. 488032
43	6	0	-2. 175886	3. 058499	-0. 714660
44	6	0	-2. 385478	4. 188521	0. 321835
45	1	0	-3. 353193	4. 683821	0. 162876
46	1	0	-2. 358941	3. 786228	1. 338246
47	1	0	-1. 597841	4. 946419	0. 231638
48	6	0	-2. 185238	3. 677838	-2. 127889

49	1	0	-2.037510	2.910203	-2.899783
50	1	0	-3.140472	4.177368	-2.330237
51	1	0	-1.386778	4.422278	-2.240204
52	6	0	-3.343086	2.052737	-0.613250
53	1	0	-3.273807	1.299727	-1.410234
54	1	0	-3.330462	1.541211	0.352788
55	1	0	-4.306370	2.567495	-0.728516

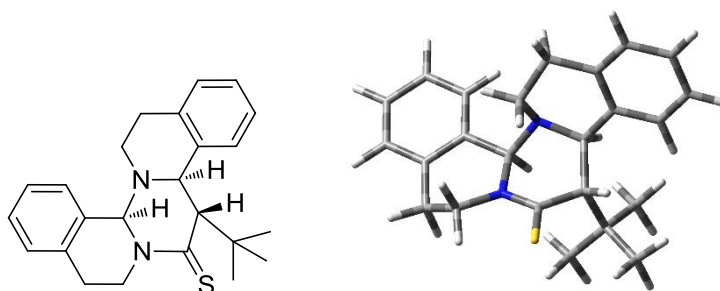
7n



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.999368	-1.220540	-0.602393
2	6	0	0.099245	-1.636830	0.567451
3	16	0	0.571678	-2.391138	1.987344
4	7	0	-1.201090	-1.291186	0.327583
5	6	0	-1.406100	-0.129361	-0.598664
6	6	0	-2.267963	-1.677950	1.254413
7	6	0	-2.821556	0.432665	-0.564945
8	6	0	-3.616207	-1.671059	0.537924
9	1	0	-2.024296	-2.672265	1.631894
10	1	0	-2.285075	-1.003717	2.122667
11	6	0	-3.057485	1.693665	-1.128776
12	6	0	-3.895400	-0.320116	-0.070460
13	1	0	-3.614038	-2.451144	-0.237154
14	1	0	-4.402477	-1.940386	1.252256
15	6	0	-4.350068	2.208471	-1.193902
16	1	0	-2.213698	2.265578	-1.501593
17	6	0	-5.189821	0.209515	-0.136507
18	6	0	-5.422096	1.463502	-0.696406
19	1	0	-4.520016	3.189477	-1.629112
20	1	0	-6.019362	-0.370799	0.261351
21	1	0	-6.432593	1.860920	-0.739347
22	1	0	0.390051	-1.504042	-1.470303
23	1	0	-1.236653	-0.480526	-1.625158

24	7	0	-0.390164	0.878215	-0.324849
25	6	0	0.944991	0.409563	-0.767123
26	6	0	-0.444369	1.309838	1.087800
27	6	0	2.046813	1.343604	-0.236213
28	1	0	0.960483	0.542050	-1.856321
29	6	0	0.407928	2.546601	1.279856
30	1	0	-1.489198	1.527055	1.325360
31	1	0	-0.101570	0.524429	1.776546
32	6	0	3.317732	1.342657	-0.837562
33	6	0	1.795385	2.334681	0.731580
34	1	0	-0.057629	3.395918	0.759979
35	1	0	0.448836	2.809269	2.344200
36	6	0	4.329049	2.212663	-0.442692
37	1	0	3.530121	0.653528	-1.642979
38	6	0	2.821895	3.200411	1.136029
39	6	0	4.089222	3.140876	0.570907
40	1	0	5.298162	2.166796	-0.932028
41	1	0	2.602276	3.943807	1.899577
42	1	0	4.871217	3.820702	0.898129
43	6	0	2.297984	-2.065318	-0.883248
44	6	0	1.929331	-3.572214	-0.856995
45	1	0	2.761137	-4.152478	-1.274304
46	1	0	1.737374	-3.932158	0.153802
47	1	0	1.043335	-3.779043	-1.471950
48	6	0	2.731131	-1.799654	-2.349161
49	1	0	2.905599	-0.749301	-2.588253
50	1	0	3.658346	-2.342516	-2.565211
51	1	0	1.967922	-2.164951	-3.048746
52	6	0	3.474679	-1.850248	0.089213
53	1	0	3.863987	-0.831831	0.072268
54	1	0	3.172152	-2.082386	1.112317
55	1	0	4.295395	-2.525515	-0.185289

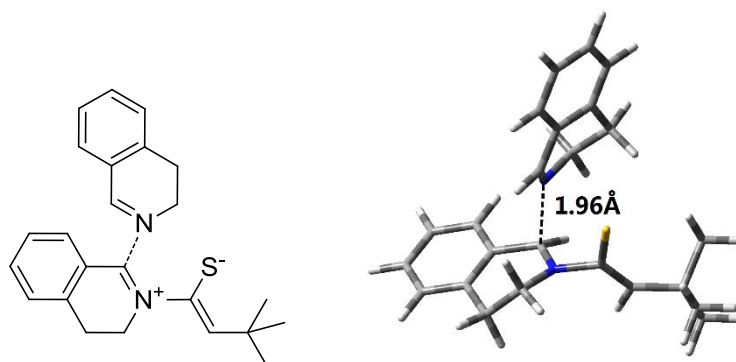
4n



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.212797	1.203729	-0.088350
2	6	0	-0.130574	1.496154	0.952250
3	16	0	-0.495897	2.382910	2.331831
4	7	0	1.106214	1.020981	0.673002
5	6	0	1.216611	-0.027312	-0.394508
6	6	0	2.240088	1.284932	1.564835
7	6	0	2.587128	-0.689882	-0.454265
8	6	0	3.553797	1.255894	0.787778
9	1	0	2.070725	2.259089	2.025134
10	1	0	2.255382	0.543105	2.375883
11	6	0	2.721532	-1.906837	-1.135256
12	6	0	3.724156	-0.056639	0.066801
13	1	0	3.566171	2.092316	0.073923
14	1	0	4.383660	1.424961	1.483266
15	6	0	3.973452	-2.499236	-1.285947
16	1	0	1.831824	-2.381195	-1.536829
17	6	0	4.976373	-0.663595	-0.084776
18	6	0	5.106581	-1.876217	-0.757980
19	1	0	4.063799	-3.445415	-1.812472
20	1	0	5.854319	-0.176384	0.333547
21	1	0	6.085639	-2.334951	-0.866999
22	1	0	1.068361	0.482043	-1.356235
23	7	0	0.128160	-0.972587	-0.275852
24	6	0	-1.133393	-0.292999	-0.629931
25	6	0	0.093379	-1.695373	1.003463
26	6	0	-2.358511	-1.118596	-0.233830
27	1	0	-1.131447	-0.248824	-1.722368
28	6	0	-0.890371	-2.850886	0.875741
29	1	0	1.100359	-2.069666	1.207218
30	1	0	-0.199962	-1.047652	1.846239
31	6	0	-3.637304	-0.665500	-0.594487
32	6	0	-2.246898	-2.341970	0.448191
33	1	0	-0.503222	-3.568556	0.138995
34	1	0	-0.971171	-3.384162	1.830876
35	6	0	-4.780433	-1.403328	-0.301207
36	1	0	-3.745044	0.283573	-1.111074
37	6	0	-3.403929	-3.075194	0.744888
38	6	0	-4.664817	-2.620778	0.372422
39	1	0	-5.756758	-1.026887	-0.594129
40	1	0	-3.304118	-4.014914	1.284254
41	1	0	-5.549653	-3.203858	0.612994

42	1	0	-2.147868	1.281742	0.463605
43	6	0	-1.285290	2.386166	-1.190734
44	6	0	-2.356777	3.383605	-0.696053
45	1	0	-2.417219	4.248384	-1.368271
46	1	0	-3.348050	2.914463	-0.664907
47	1	0	-2.123652	3.742443	0.310864
48	6	0	0.038342	3.164249	-1.361130
49	1	0	0.363485	3.627035	-0.425096
50	1	0	0.853258	2.535897	-1.737750
51	1	0	-0.110307	3.967476	-2.092615
52	6	0	-1.705436	1.890008	-2.590842
53	1	0	-2.625799	1.297140	-2.576802
54	1	0	-1.892090	2.759896	-3.231482
55	1	0	-0.926353	1.295221	-3.081540

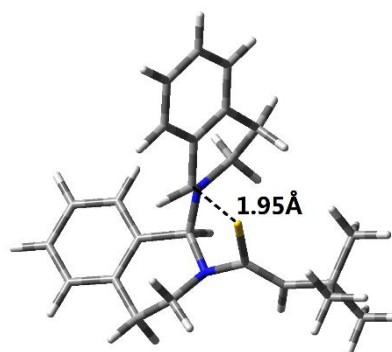
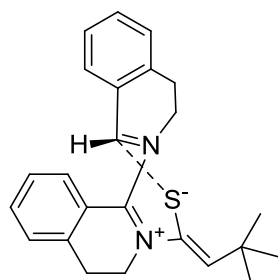
TS1-exo-n



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.109230	2.879538	0.152394
2	6	0	0.001196	1.741665	-0.570265
3	16	0	1.320871	1.054667	-1.488062
4	7	0	-1.207320	0.898970	-0.586515
5	6	0	-1.476165	0.114248	0.466565
6	6	0	-1.841353	0.621031	-1.888973
7	6	0	-2.721621	-0.700357	0.447461
8	6	0	-3.346627	0.461391	-1.691770
9	1	0	-1.607894	1.464432	-2.539695
10	1	0	-1.414189	-0.274704	-2.353380
11	6	0	-3.004576	-1.583311	1.498623
12	6	0	-3.646845	-0.537833	-0.598329
13	1	0	-3.781260	1.436125	-1.426050
14	1	0	-3.812882	0.152832	-2.634593

15	6	0	-4.190770	-2.309157	1.513213
16	1	0	-2.282053	-1.707526	2.300387
17	6	0	-4.835106	-1.276375	-0.574755
18	6	0	-5.108747	-2.157031	0.469472
19	1	0	-4.399424	-2.993213	2.330814
20	1	0	-5.550441	-1.155576	-1.384972
21	1	0	-6.035116	-2.724974	0.470773
22	1	0	-1.094632	3.079561	0.575768
23	1	0	-1.190567	0.547139	1.421110
24	7	0	-0.040106	-1.198162	0.684396
25	6	0	0.596733	-1.544327	-0.394784
26	6	0	0.688305	-1.208610	1.959810
27	6	0	1.944148	-2.117281	-0.384783
28	1	0	0.030952	-1.579414	-1.319191
29	6	0	2.193734	-0.964081	1.797093
30	1	0	0.248831	-0.444337	2.611368
31	1	0	0.508614	-2.181346	2.442128
32	6	0	2.411317	-2.904914	-1.444111
33	6	0	2.757171	-1.882360	0.741197
34	1	0	2.350835	0.075572	1.477478
35	1	0	2.700554	-1.098419	2.759398
36	6	0	3.683502	-3.469625	-1.382865
37	1	0	1.777346	-3.069794	-2.311877
38	6	0	4.028477	-2.448359	0.789636
39	6	0	4.490254	-3.242126	-0.265184
40	1	0	4.047047	-4.081303	-2.203603
41	1	0	4.665338	-2.266176	1.652145
42	1	0	5.483263	-3.680582	-0.214630
43	6	0	0.955381	3.934244	0.436921
44	6	0	0.329086	5.017118	1.340127
45	1	0	1.058503	5.803224	1.569212
46	1	0	-0.532641	5.490708	0.852625
47	1	0	-0.015703	4.591127	2.291369
48	6	0	1.433150	4.598365	-0.874846
49	1	0	0.594968	5.075702	-1.396926
50	1	0	2.183981	5.371187	-0.662258
51	1	0	1.875353	3.857820	-1.547139
52	6	0	2.165746	3.317051	1.172317
53	1	0	1.857052	2.882225	2.131840
54	1	0	2.626396	2.531194	0.566726
55	1	0	2.922859	4.084766	1.380017

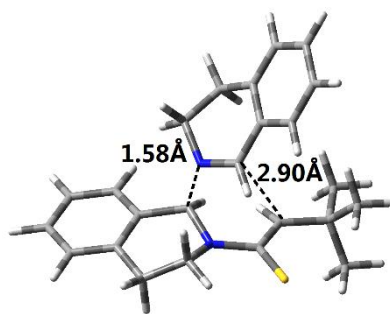
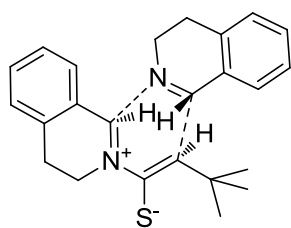
C-exo-n



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.196964	-2.106367	0.219536
2	6	0	-1.209273	-1.330264	-0.260009
3	16	0	-1.437700	0.225289	-1.148809
4	7	0	0.146642	-1.769381	-0.132379
5	6	0	0.977541	-0.934453	0.755954
6	6	0	0.743142	-2.249631	-1.384855
7	6	0	2.478690	-1.120442	0.502011
8	6	0	2.013949	-3.029847	-1.066201
9	1	0	0.000858	-2.896756	-1.860885
10	1	0	0.972346	-1.439231	-2.098486
11	6	0	3.376559	-0.269202	1.160406
12	6	0	2.978956	-2.145745	-0.315259
13	1	0	1.746400	-3.910691	-0.465757
14	1	0	2.474454	-3.396364	-1.991701
15	6	0	4.752094	-0.435134	1.026060
16	1	0	2.985689	0.538832	1.771469
17	6	0	4.365313	-2.299858	-0.451073
18	6	0	5.251047	-1.459525	0.217370
19	1	0	5.432509	0.235318	1.544280
20	1	0	4.747060	-3.086208	-1.098909
21	1	0	6.323194	-1.593600	0.099946
22	1	0	-1.838407	-3.030521	0.672472
23	1	0	0.778648	-1.273067	1.782705
24	7	0	0.603626	0.491811	0.751644
25	6	0	0.233986	1.012004	-0.517745
26	6	0	-0.013256	1.040178	1.969997
27	6	0	0.075648	2.505720	-0.519496
28	1	0	0.975000	0.702754	-1.258191
29	6	0	-1.003296	2.186090	1.693271
30	1	0	-0.537025	0.244152	2.515827
31	1	0	0.783130	1.410373	2.633032

32	6	0	0.508314	3.291221	-1.589638
33	6	0	-0.515054	3.105686	0.603469
34	1	0	-1.965207	1.756802	1.386204
35	1	0	-1.178815	2.736725	2.624313
36	6	0	0.357401	4.678458	-1.547285
37	1	0	0.968531	2.817737	-2.453844
38	6	0	-0.649018	4.494203	0.644561
39	6	0	-0.218501	5.279829	-0.427377
40	1	0	0.696358	5.286657	-2.381393
41	1	0	-1.097546	4.963459	1.517474
42	1	0	-0.329951	6.360085	-0.385439
43	6	0	-3.712637	-1.922705	0.209424
44	6	0	-4.340766	-3.168963	0.869535
45	1	0	-5.433716	-3.087919	0.891006
46	1	0	-4.081363	-4.081693	0.319084
47	1	0	-3.991321	-3.288556	1.902418
48	6	0	-4.254227	-1.809670	-1.234054
49	1	0	-3.972464	-2.686817	-1.828122
50	1	0	-5.349774	-1.744819	-1.224605
51	1	0	-3.869456	-0.920552	-1.742999
52	6	0	-4.128055	-0.675518	1.022699
53	1	0	-3.779651	-0.752163	2.059529
54	1	0	-3.716493	0.239622	0.587942
55	1	0	-5.221215	-0.581575	1.040928

TS2-Re-n

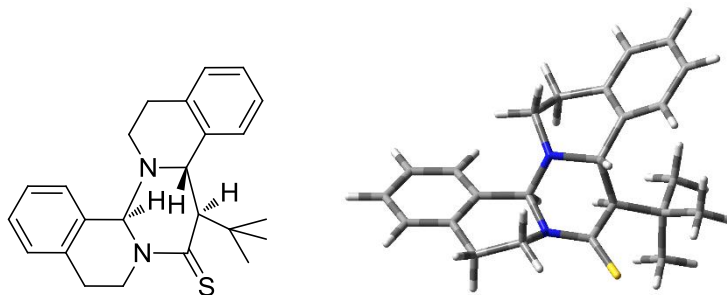


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.852962	-1.695163	0.886826
2	6	0	-0.109885	-1.953353	-0.253054
3	16	0	-0.611208	-2.977567	-1.546422
4	7	0	1.145289	-1.229014	-0.414187
5	6	0	1.402591	-0.065531	0.353856

6	6	0	1. 802362	-1. 197234	-1. 733682
7	6	0	2. 864252	0. 367624	0. 358688
8	6	0	3. 315132	-1. 160975	-1. 589365
9	1	0	1. 474211	-2. 079691	-2. 279773
10	1	0	1. 468958	-0. 313323	-2. 301778
11	6	0	3. 354043	1. 164636	1. 406234
12	6	0	3. 768154	-0. 116194	-0. 600979
13	1	0	3. 668262	-2. 142721	-1. 242860
14	1	0	3. 772378	-0. 991133	-2. 572243
15	6	0	4. 685938	1. 569763	1. 447294
16	1	0	2. 699565	1. 442959	2. 228223
17	6	0	5. 104761	0. 299009	-0. 554996
18	6	0	5. 563009	1. 152257	0. 445051
19	1	0	5. 038672	2. 191205	2. 265481
20	1	0	5. 795573	-0. 073609	-1. 308070
21	1	0	6. 603903	1. 463749	0. 461870
22	1	0	1. 109024	-0. 217333	1. 392678
23	6	0	-0. 707525	0. 726411	-0. 693746
24	6	0	-1. 879698	1. 573217	-0. 735365
25	7	0	0. 412698	1. 091195	-0. 080898
26	6	0	-2. 882801	1. 349923	-1. 697011
27	6	0	-2. 025947	2. 608850	0. 214549
28	6	0	0. 422529	2. 393242	0. 616011
29	6	0	-4. 012768	2. 160358	-1. 721442
30	1	0	-2. 764724	0. 540330	-2. 411967
31	6	0	-3. 163823	3. 408290	0. 180519
32	6	0	-0. 932239	2. 733790	1. 244936
33	1	0	1. 205592	2. 383167	1. 368879
34	1	0	0. 697423	3. 157565	-0. 122761
35	6	0	-4. 152214	3. 190471	-0. 785490
36	1	0	-4. 786100	1. 990260	-2. 464492
37	1	0	-3. 284033	4. 205544	0. 910175
38	1	0	-1. 132328	2. 045498	2. 080066
39	1	0	-0. 892684	3. 744463	1. 666136
40	1	0	-5. 033679	3. 825250	-0. 805329
41	1	0	-0. 685929	-0. 141654	-1. 338807
42	1	0	-0. 368962	-1. 143489	1. 689499
43	6	0	-2. 173699	-2. 314118	1. 345645
44	6	0	-2. 002230	-3. 832937	1. 594008
45	1	0	-2. 938096	-4. 265557	1. 973154
46	1	0	-1. 727902	-4. 344911	0. 668632
47	1	0	-1. 217295	-4. 020727	2. 336977
48	6	0	-2. 552573	-1. 643848	2. 685103
49	1	0	-3. 494054	-2. 051047	3. 072182

50	1	0	-1.779471	-1.808859	3.447126
51	1	0	-2.681885	-0.560076	2.562545
52	6	0	-3.332849	-2.080079	0.352793
53	1	0	-4.255320	-2.532913	0.739610
54	1	0	-3.517519	-1.007660	0.216082
55	1	0	-3.109495	-2.519934	-0.621192

8n



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.979781	1.056815	0.490334
2	6	0	-0.100901	2.000719	-0.071642
3	16	0	0.162480	3.535531	-0.683328
4	7	0	-1.307993	1.366808	-0.197226
5	6	0	-1.369602	-0.037485	0.226581
6	6	0	-2.215607	1.716205	-1.305820
7	6	0	-2.801534	-0.574936	0.258788
8	6	0	-3.668167	1.471361	-0.940377
9	1	0	-2.040760	2.759074	-1.559568
10	1	0	-1.927638	1.093728	-2.165510
11	6	0	-3.069167	-1.730675	1.012872
12	6	0	-3.879903	0.115450	-0.314279
13	1	0	-4.001159	2.244986	-0.233895
14	1	0	-4.286469	1.584460	-1.839420
15	6	0	-4.355490	-2.251563	1.114383
16	1	0	-2.259516	-2.221991	1.546428
17	6	0	-5.173069	-0.416090	-0.208841
18	6	0	-5.415469	-1.598742	0.481355
19	1	0	-4.530698	-3.152919	1.694931
20	1	0	-5.999594	0.123857	-0.665791
21	1	0	-6.424855	-1.995319	0.548433
22	1	0	-1.068948	-0.061205	1.283543
23	6	0	0.958997	-0.077530	-0.653390

24	6	0	2.097514	-1.087089	-0.635684
25	7	0	-0.402688	-0.747390	-0.643462
26	6	0	3.264859	-0.832503	-1.366578
27	6	0	1.984482	-2.308204	0.054808
28	6	0	-0.364231	-2.206241	-0.552672
29	6	0	4.350537	-1.705887	-1.318211
30	1	0	3.323544	0.060665	-1.981941
31	6	0	3.074272	-3.182530	0.096799
32	6	0	0.610395	-2.706107	0.533070
33	1	0	-1.377795	-2.573064	-0.400827
34	1	0	-0.033616	-2.606702	-1.519304
35	6	0	4.265963	-2.874423	-0.559327
36	1	0	5.252431	-1.480259	-1.880553
37	1	0	2.974234	-4.127538	0.626535
38	1	0	0.352704	-2.259450	1.504852
39	1	0	0.548077	-3.794459	0.655044
40	1	0	5.106073	-3.562216	-0.514371
41	1	0	1.048716	0.464853	-1.603384
42	1	0	0.566391	0.572617	1.379733
43	6	0	2.305483	1.676801	1.079215
44	6	0	1.888515	2.726059	2.141903
45	1	0	2.780819	3.081497	2.670640
46	1	0	1.389772	3.589012	1.699820
47	1	0	1.218108	2.285674	2.892299
48	6	0	3.083338	0.584607	1.855588
49	1	0	3.886811	1.061864	2.428946
50	1	0	2.436855	0.063414	2.574099
51	1	0	3.543131	-0.162395	1.208275
52	6	0	3.268694	2.339160	0.074550
53	1	0	4.114437	2.770301	0.624859
54	1	0	3.682832	1.615377	-0.630697
55	1	0	2.783077	3.138693	-0.485666
