

Sterically controlled diastereoselectivity in thio-Staudinger cycloadditions of alkyl/alkenyl/aryl-substituted thioketenes

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Electronic Supplementary Information

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1. Details of calculations

DFT calculations on representative reactions were performed using Gaussian 09 program package.^[1] The optimization of the minima and transition states were performed at B3LYP/6-31+g(d,p) level. Frequency calculations were carried out based on the optimized structures at the same level of theory to verify if real minima or transition states were obtained, and to produce zero-point energies. IRC calculations were performed at the same level of theory to confirm the calculated transition states connect the correct reactants and products.

[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

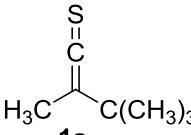
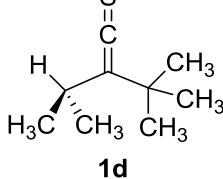
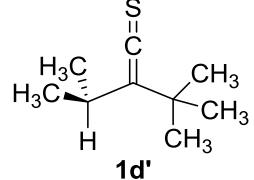
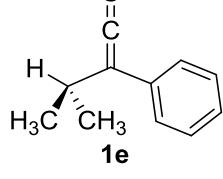
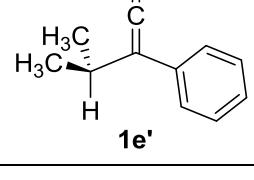
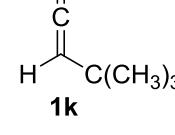
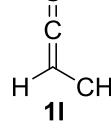
Table S1. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.) calculated at B3LYP/6-31+g(d,p) level in the gas phase.

Structure	E	H	G
5	-402.990272	-402.981983	-403.022171
1a	-671.981690	-671.970505	-672.017736
<i>exo-1a-TS1</i>	-1074.948526	-1074.929407	-1074.996388
E-1a	-1074.963660	-1074.944811	-1075.009324
<i>exo-1a-TS2</i>	-1074.945492	-1074.927447	-1074.989141
7a	-1075.002070	-1074.984017	-1075.045604
<i>endo-1a-TS3</i>	-1074.941963	-1074.922899	-1074.988497
F-1a	-1074.960991	-1074.942215	-1075.006465
<i>endo-1a-TS4</i>	-1074.937827	-1074.919604	-1074.981630
8a	-1074.986388	-1074.968078	-1075.030433
1d	-750.550847	-750.537277	-750.588967
<i>exo-1d-TS1</i>	-1153.514181	-1153.492438	-1153.563916
E-1d	-1153.527579	-1153.505927	-1153.576326
<i>exo-1d-TS2</i>	-1153.509288	-1153.488602	-1153.555634
7d	-1153.559330	-1153.538808	-1153.605209
<i>endo-1d-TS3</i>	-1153.508092	-1153.486552	-1153.556890

F-1d	-1153. 524010	-1153. 502779	-1153. 571977
<i>endo-1d-TS4</i>	-1153. 500506	-1153. 479736	-1153. 479736
8d	-1153. 548467	-1153. 527666	-1153. 594878
1d'	-750. 557467	-750. 543630	-750. 596477
<i>exo-1d'-TS1</i>	-1153. 512496	-1153. 490916	-1153. 561690
E-1d'	-1153. 526219	-1153. 504858	-1153. 574154
<i>exo-1d'-TS2</i>	-1153. 509217	-1153. 488367	-1153. 555792
7d'	-1153. 561130	-1153. 540612	-1153. 606677
<i>endo-1d'-TS3</i>	-1153. 514472	-1153. 492764	-1153. 563866
F-1d'	-1153. 529181	-1153. 507734	-1153. 577413
<i>endo-1d'-TS4</i>	-1153. 504893	-1153. 484156	-1153. 551218
8d'	-1153. 552647	-1153. 531645	-1153. 599589
1e	-824. 386651	-824. 373655	-824. 427415
<i>exo-1e-TS1</i>	-1227. 358249	-1227. 336952	-1227. 410787
E-1e	-1227. 374246	-1227. 353193	-1227. 424888
<i>exo-1e-TS2</i>	-1227. 351675	-1227. 331712	-1227. 399227
7e	-1227. 401178	-1227. 381172	-1227. 448454
<i>endo-1e-TS3</i>	-1227. 362297	-1227. 341080	-1227. 414315
F-1e	-1227. 381135	-1227. 360262	-1227. 430875
<i>endo-1e-TS4</i>	-1227. 351518	-1227. 331116	-1227. 400039
8e	-1227. 394912	-1227. 374582	-1227. 443087
1e'	-824. 389321	-824. 376496	-824. 428909
<i>exo-1e'-TS1</i>	-1227. 352454	-1227. 331397	-1227. 403140
E-1e'	-1227. 369512	-1227. 348616	-1227. 419207
<i>exo-1e'-TS2</i>	-1227. 353437	-1227. 333539	-1227. 400319
7e'	-1227. 394524	-1227. 374535	-1227. 441588
<i>endo-1e'-TS3</i>	-1227. 363293	-1227. 342246	-1227. 413943
F-1e'	-1227. 378580	-1227. 357692	-1227. 427943
<i>endo-1e'-TS4</i>	-1227. 354657	-1227. 334392	-1227. 402397
8e'	-1227. 397712	-1227. 377608	-1227. 445009
1k	-632. 693023	-632. 683385	-632. 726497
<i>exo-1k-TS1</i>	-1035. 669843	-1035. 652177	-1035. 716301
E-1k	-1035. 685501	-1035. 668083	-1035. 729579
<i>exo-1k-TS2</i>	-1035. 665571	-1035. 648771	-1035. 708504
7k	-1035. 716923	-1035. 700211	-1035. 759647
<i>endo-1k-TS3</i>	-1035. 659094	-1035. 641265	-1035. 704655
F-1k	-1035. 676073	-1035. 658652	-1035. 720439
<i>endo-1k-TS4</i>	-1035. 647998	-1035. 631122	-1035. 690874
8k	-1035. 701912	-1035. 685125	-1035. 744500
1l	-514. 824194	-514. 818303	-514. 852066
<i>exo-1l-TS1</i>	-917. 802991	-917. 789018	-917. 844692
E-1l	-917. 821971	-917. 808328	-917. 862083
<i>exo-1l-TS2</i>	-917. 800879	-917. 788032	-917. 839380

7I	-917.851191	-917.838469	-917.889559
<i>endo</i> - 1I-TS3	-917.800197	-917.786316	-917.841104
F-1I	-917.816238	-917.802730	-917.855692
<i>endo</i> - 1I-TS4	-917.785391	-917.772525	-917.823855
8I	-917.846576	-917.833901	-917.884771

Table S2. Calculated Gibbs free energies change at 298 K (ΔG , in kcal/mol) for the reactions of **5** and different thioketenes

Thioketenes	TS1	E	TS2	7	TS3	F	TS4	8
 1a	27.3	19.2	31.9	-3.6	32.3	21.0	36.6	5.9
 1d	34.3	26.6	39.5	8.4	38.8	29.3	44.9	14.9
 1d'	35.7	27.9	39.4	7.5	34.4	25.9	42.3	12.0
 1e	25.3	16.4	32.5	1.6	23.1	12.7	32.0	5.0
 1e'	30.1	20.0	31.9	6.0	23.3	14.5	30.5	3.8
 1k	20.3	12.0	25.2	-6.9	27.6	17.7	36.3	2.6
 1l	18.5	7.6	21.9	-9.6	20.8	11.6	31.6	-6.6

3. Intrinsic reaction coordinate (IRC) analysis

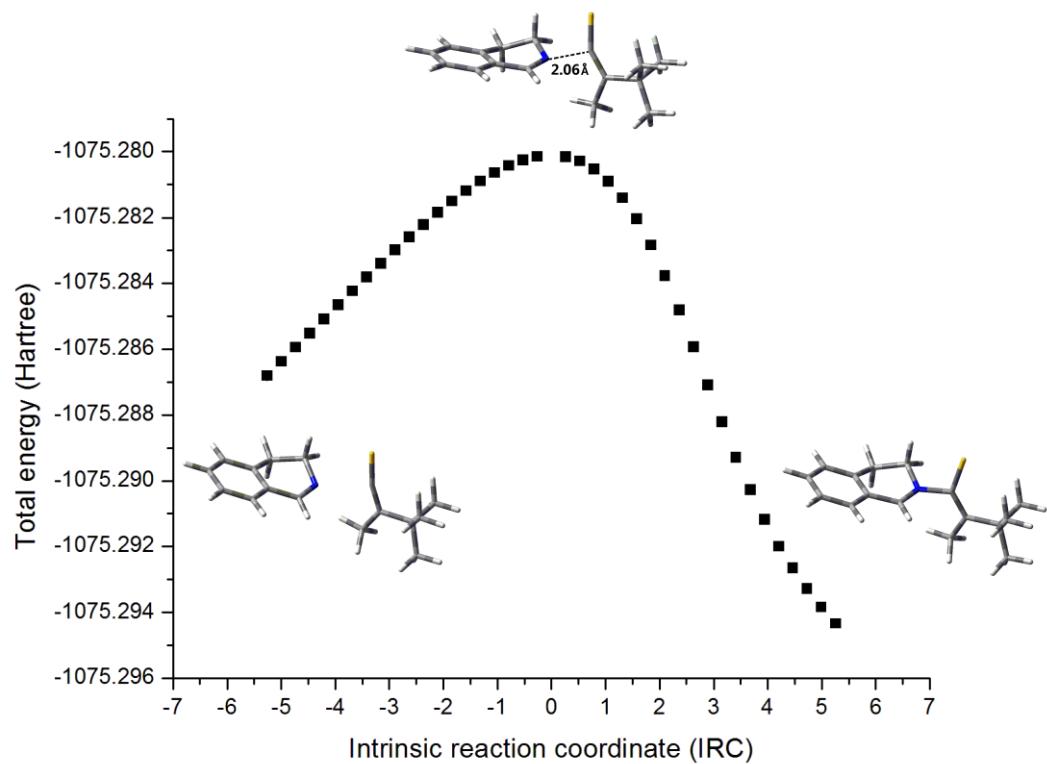


Figure S1. The intrinsic reaction coordinate (IRC) analysis of **TS1** of **1a** and **5**.

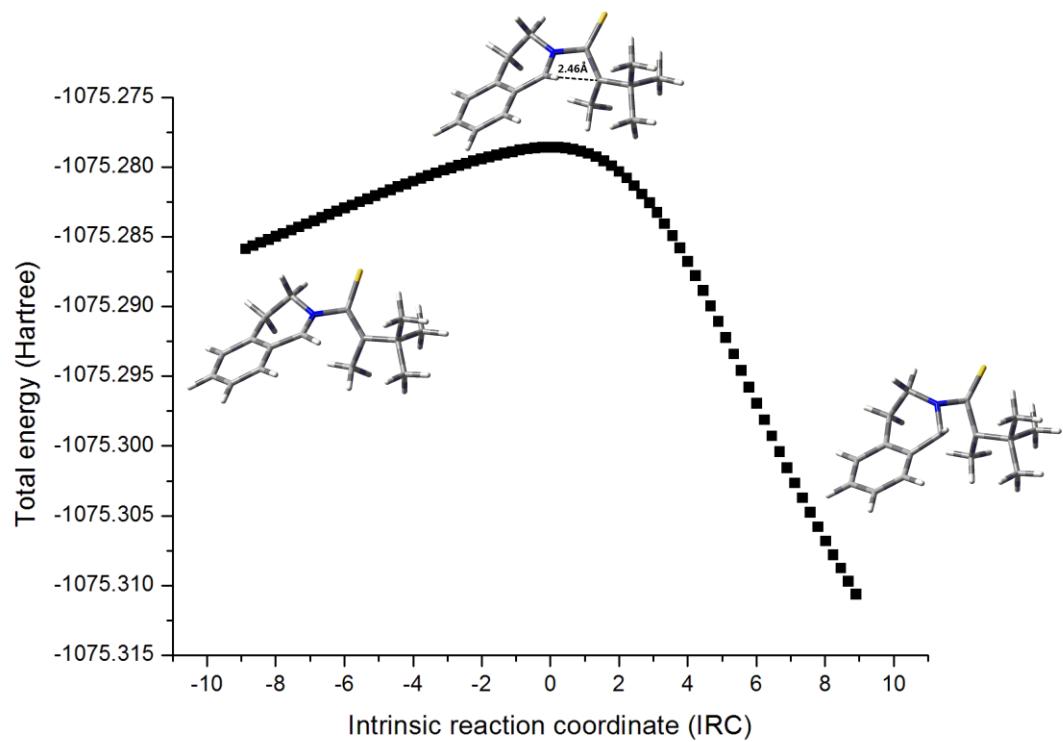


Figure S2. The intrinsic reaction coordinate (IRC) analysis of **TS2** of **1a** and **5**.

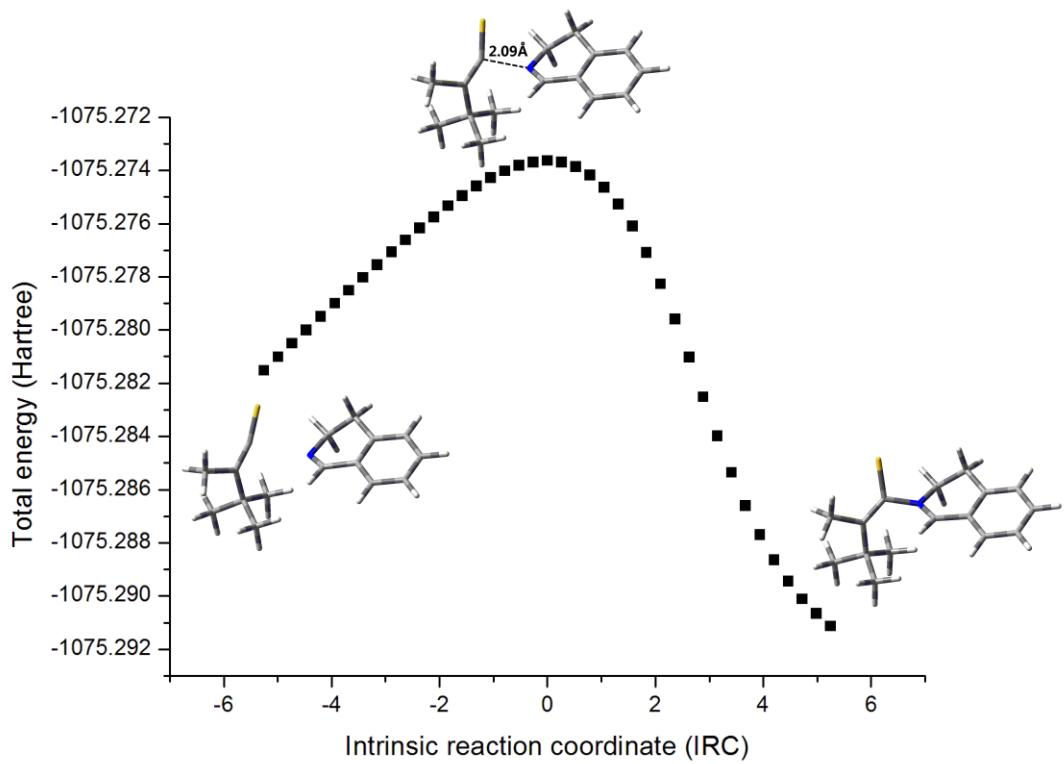


Figure S3. The intrinsic reaction coordinate (IRC) analysis of **TS3** of **1a** and **5**.

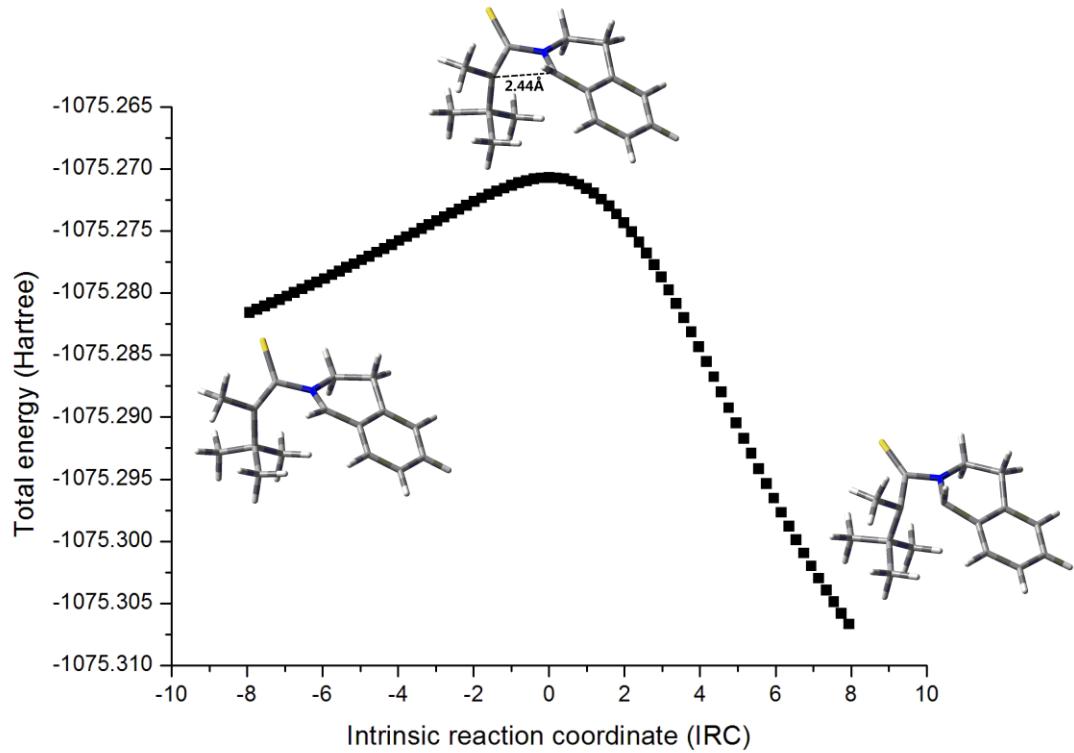


Figure S4. The intrinsic reaction coordinate (IRC) analysis of **TS4** of **1a** and **5**.

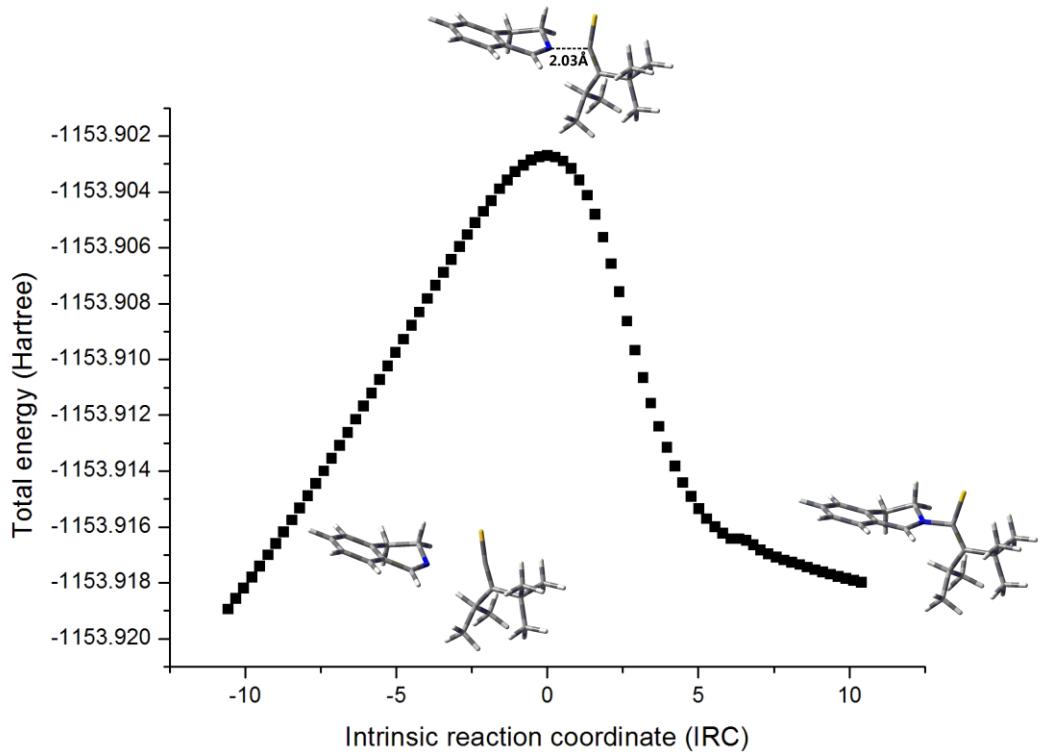


Figure S5. The intrinsic reaction coordinate (IRC) analysis of **TS1** of **1d** and **5**.

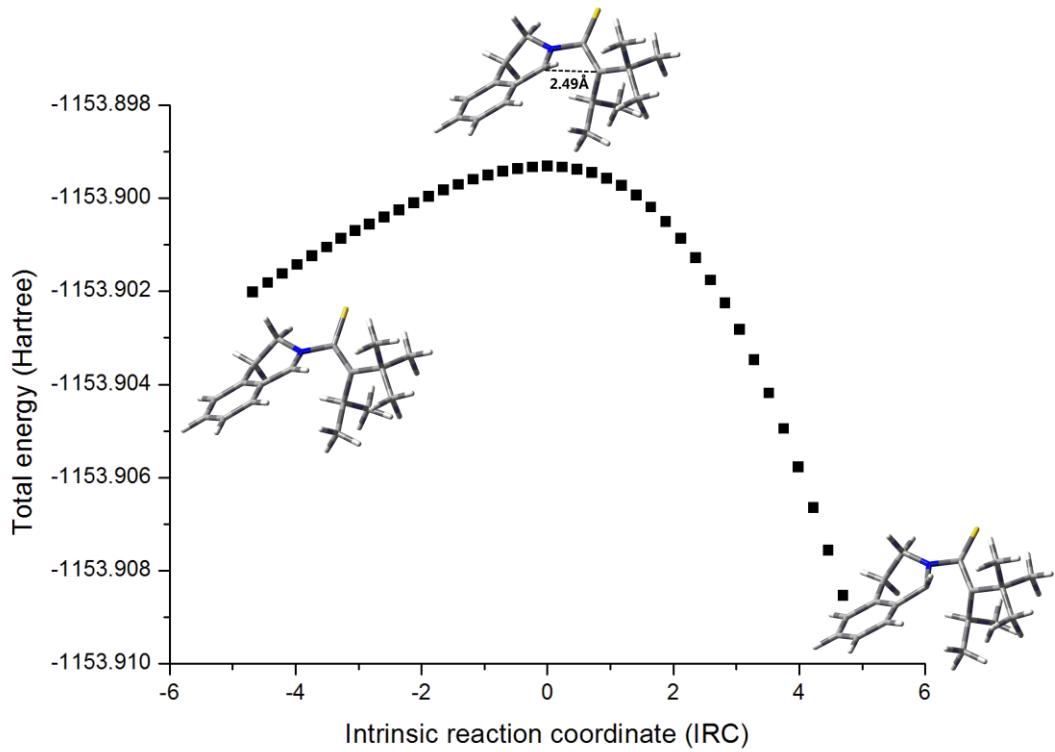


Figure S6. The intrinsic reaction coordinate (IRC) analysis of **TS2** of **1d** and **5**.

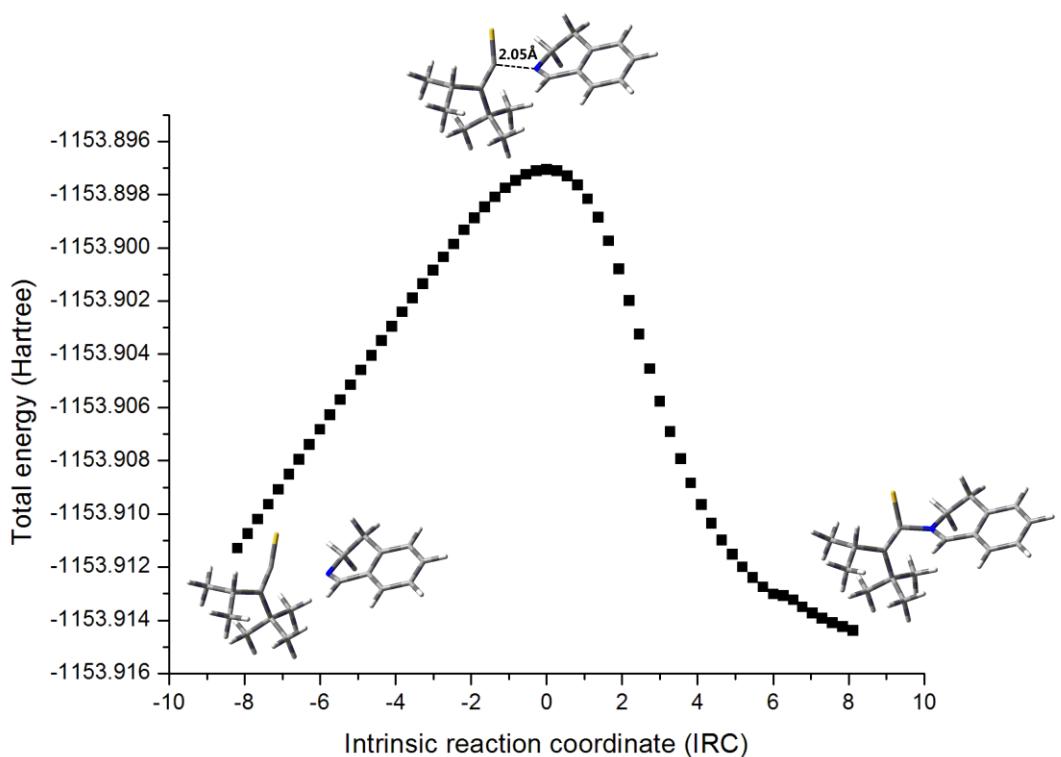


Figure S7. The intrinsic reaction coordinate (IRC) analysis of **TS3** of **1d** and **5**.

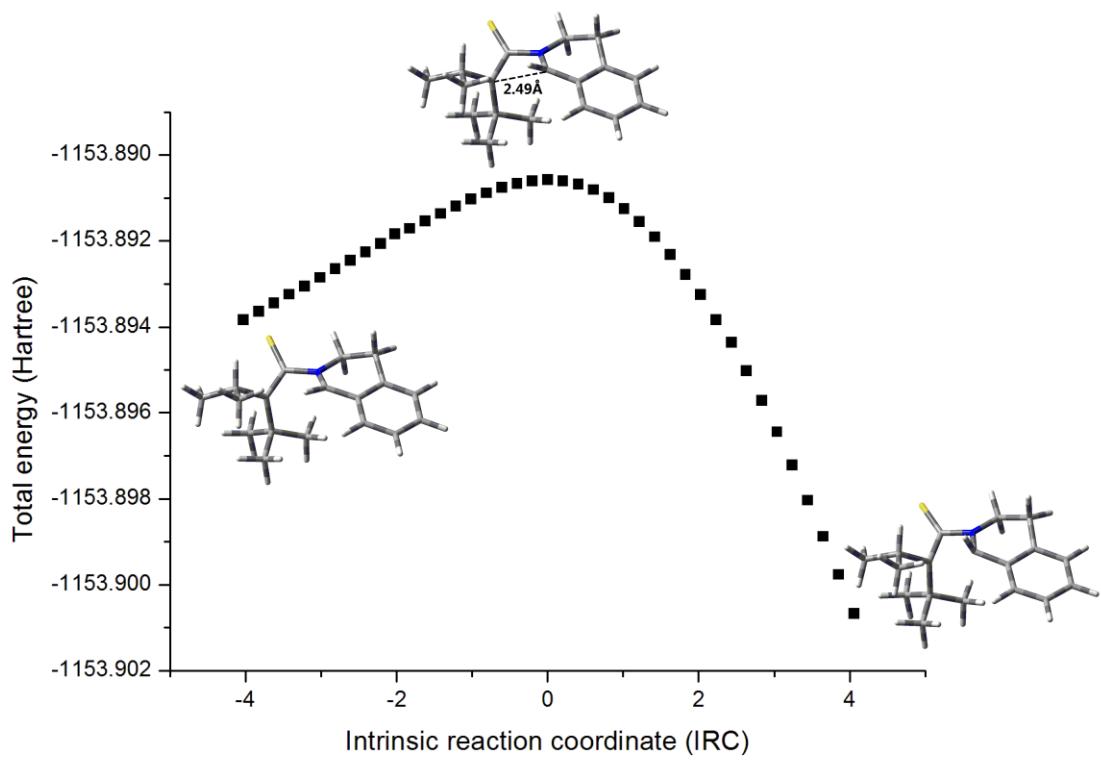


Figure S8. The intrinsic reaction coordinate (IRC) analysis of **TS4** of **1d** and **5**.

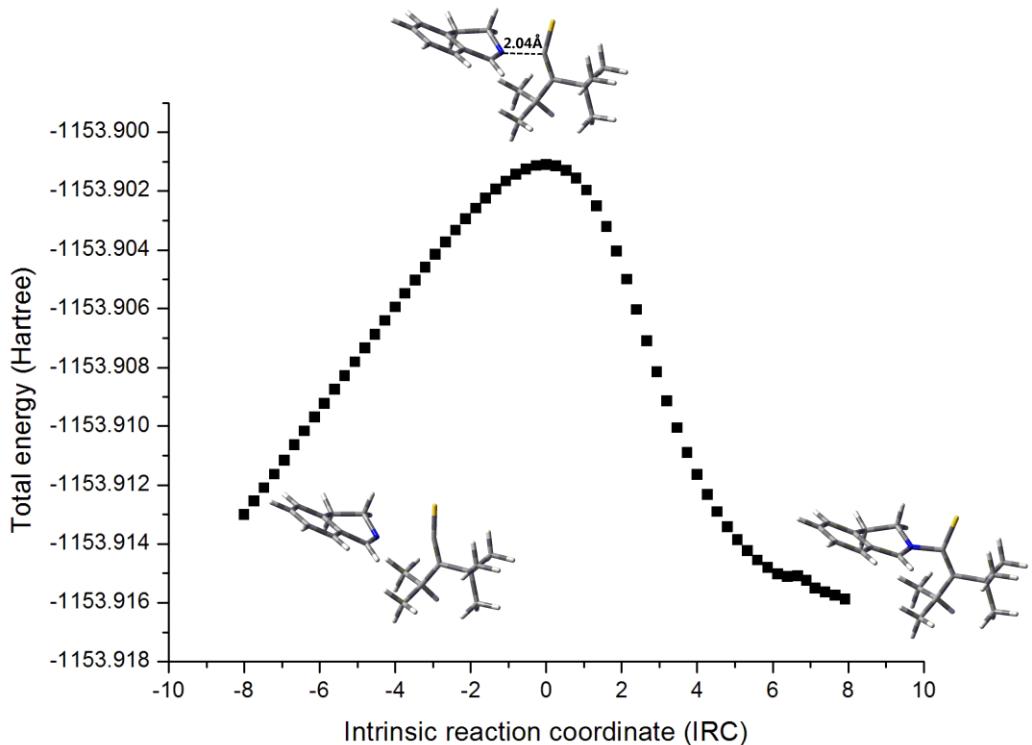


Figure S9. The intrinsic reaction coordinate (IRC) analysis of **TS1** of **1d'** and **5**.

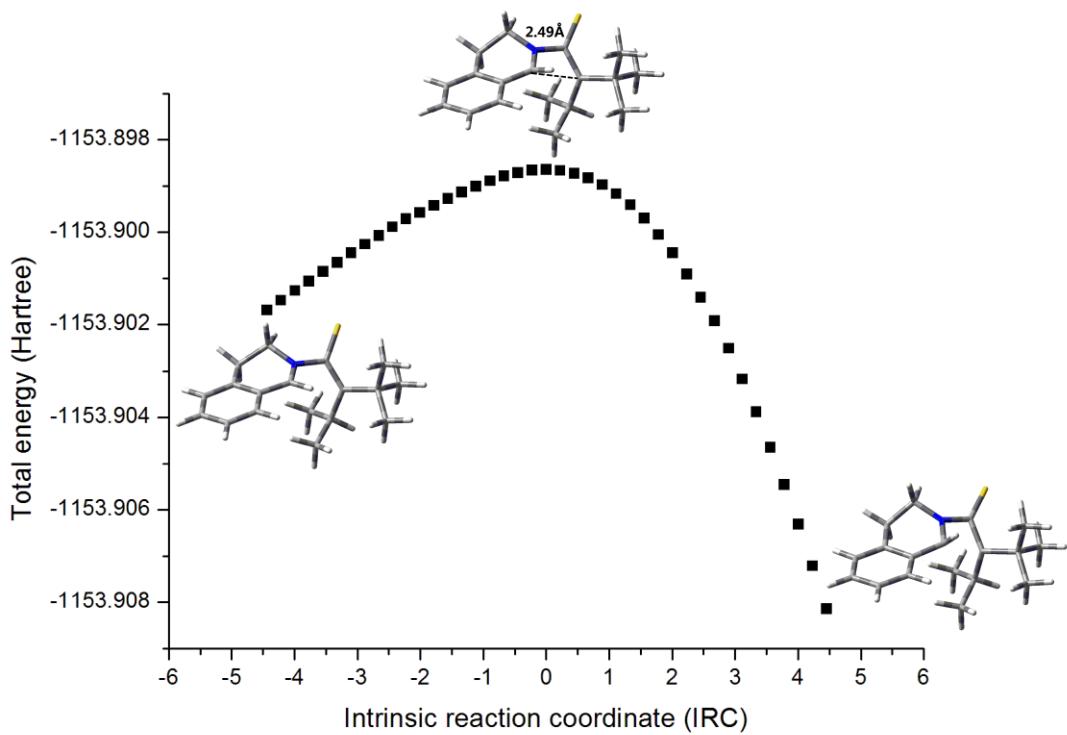


Figure S10. The intrinsic reaction coordinate (IRC) analysis of **TS2** of **1d'** and **5**.

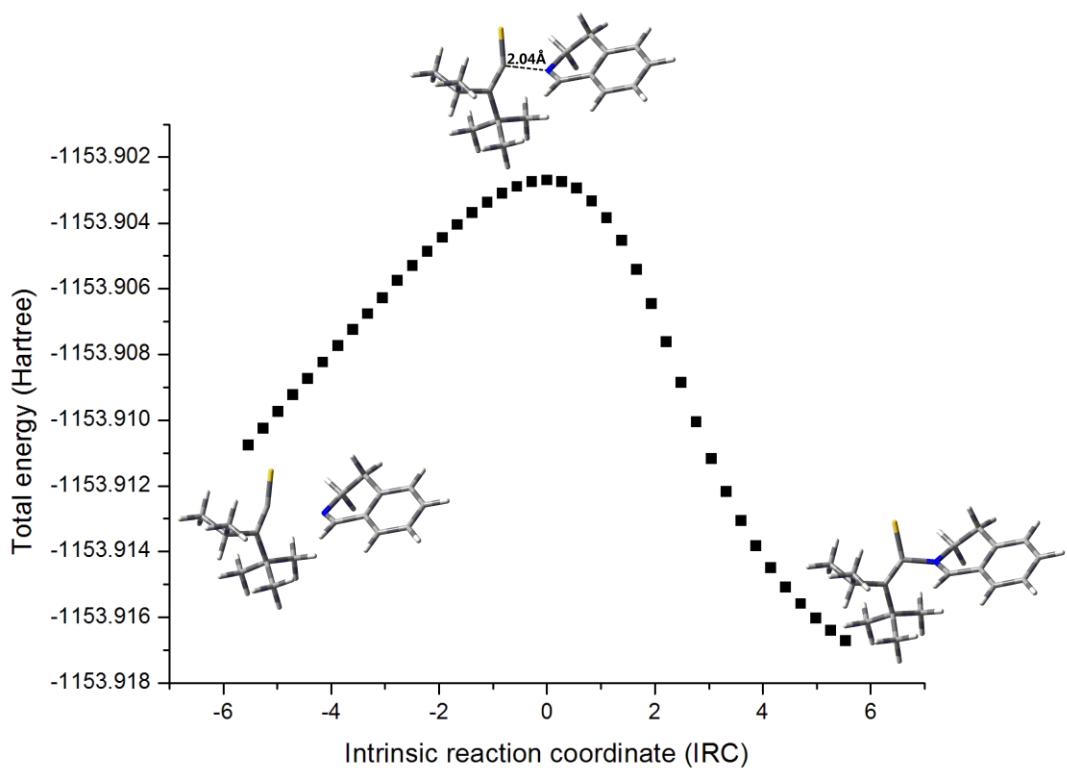


Figure S11. The intrinsic reaction coordinate (IRC) analysis of **TS3** of **1d'** and **5**.

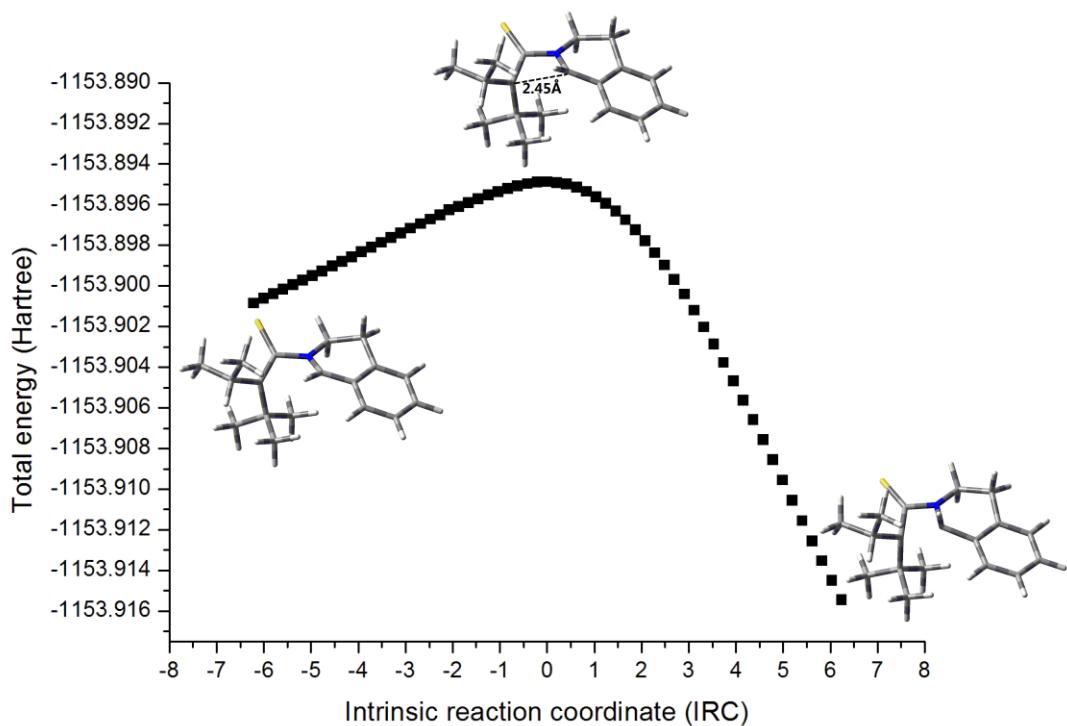


Figure S12. The intrinsic reaction coordinate (IRC) analysis of **TS4** of **1d'** and **5**.

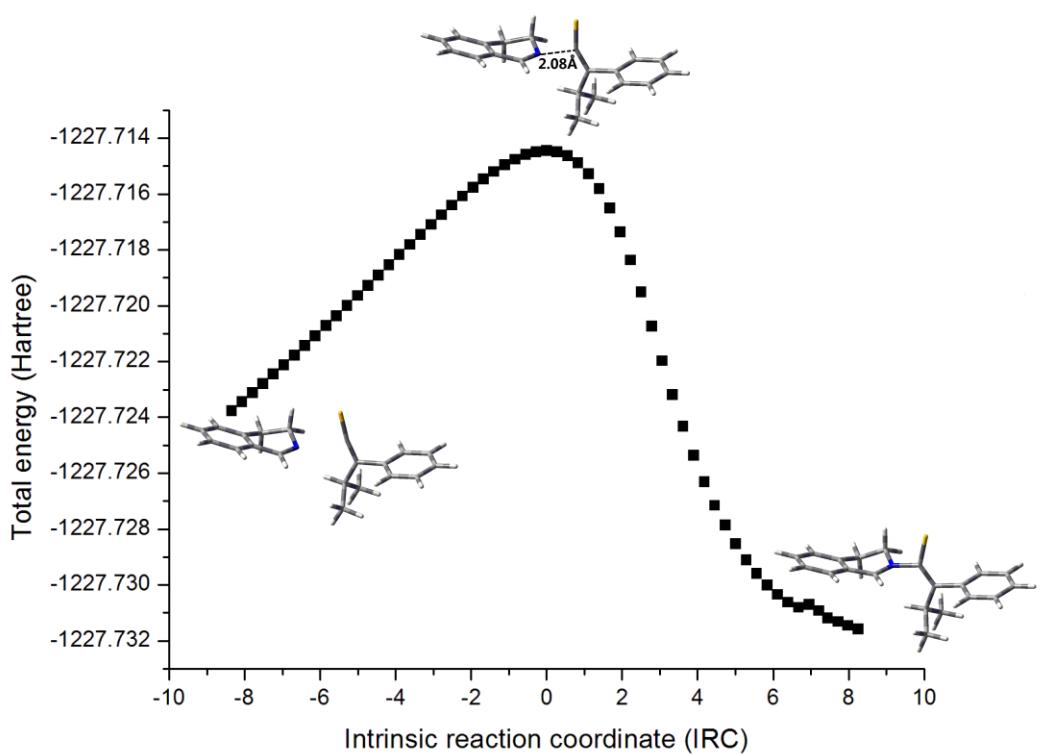


Figure S13. The intrinsic reaction coordinate (IRC) analysis of **TS1** of **1e** and **5**.

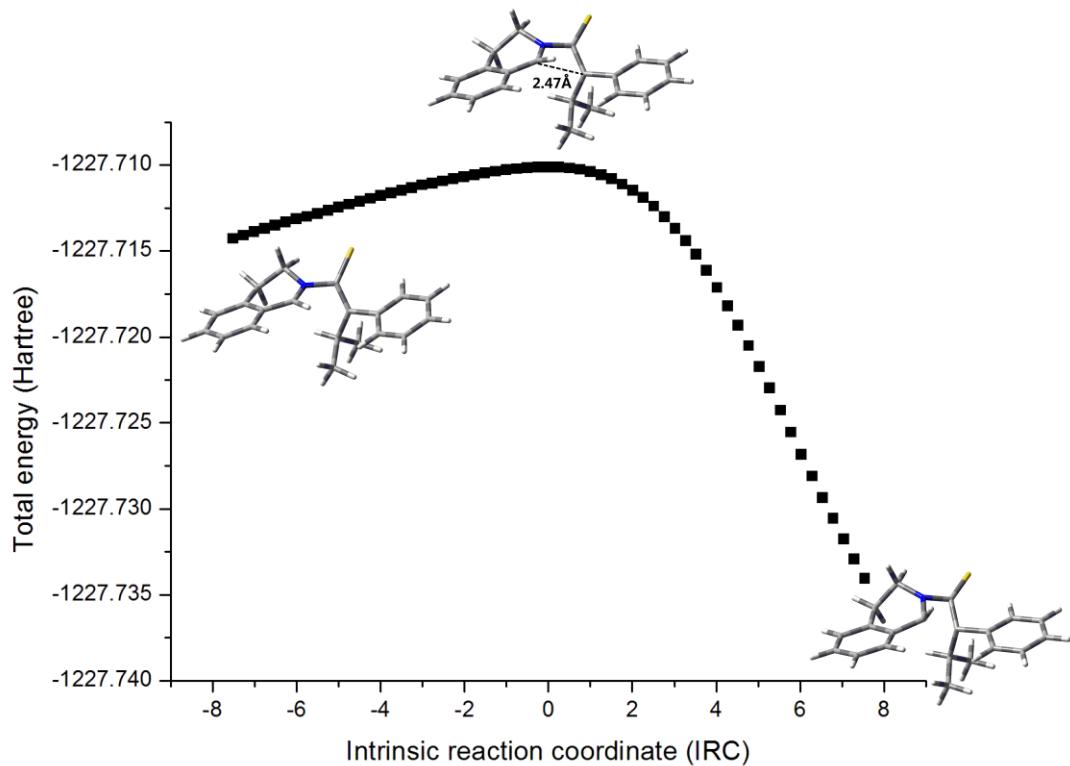


Figure S14. The intrinsic reaction coordinate (IRC) analysis of **TS2** of **1e** and **5**.

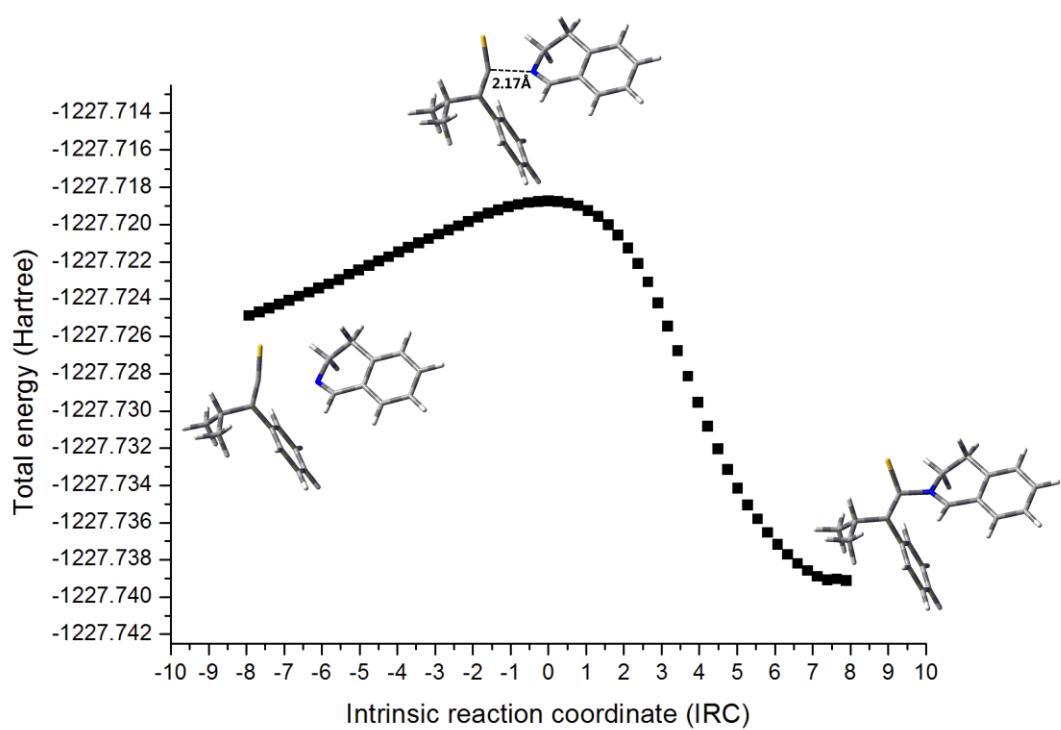


Figure S15. The intrinsic reaction coordinate (IRC) analysis of **TS3** of **1e** and **5**.

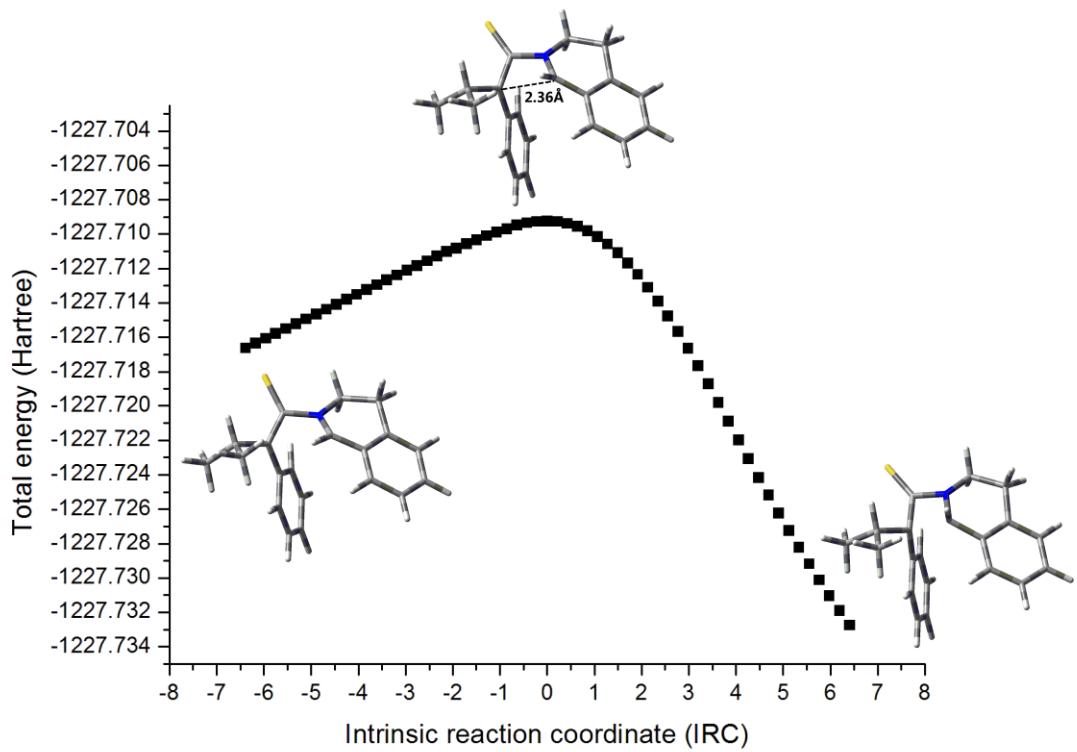


Figure S16. The intrinsic reaction coordinate (IRC) analysis of **TS4** of **1e** and **5**.

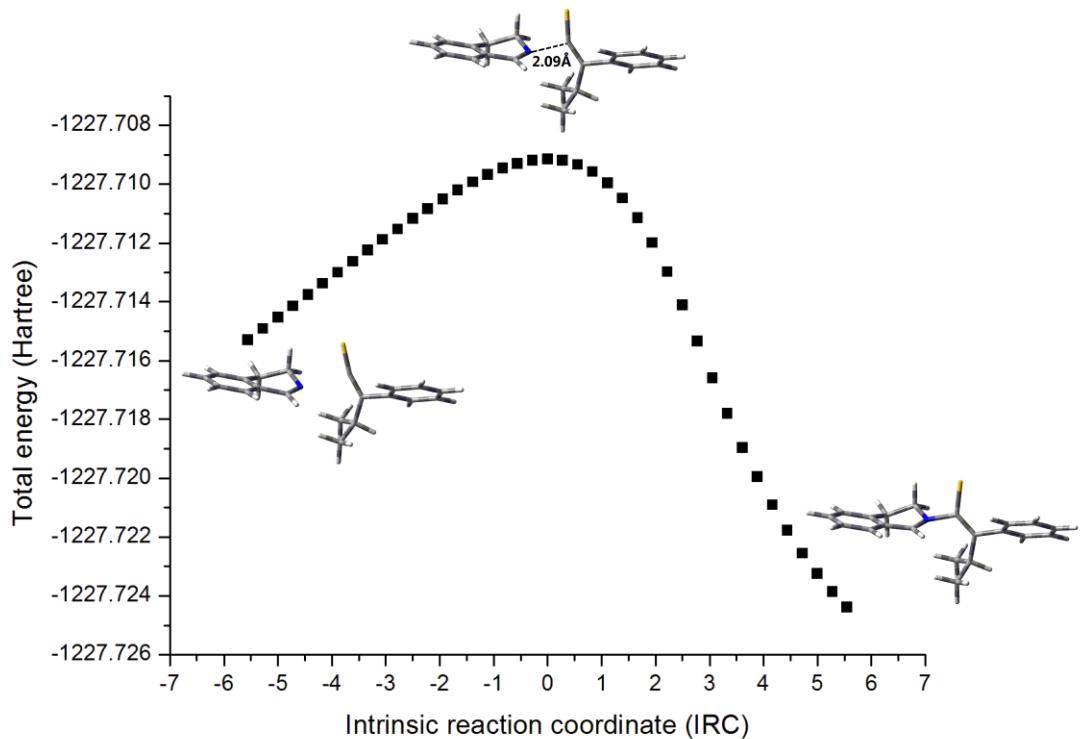


Figure S17. The intrinsic reaction coordinate (IRC) analysis of **TS1** of **1e'** and **5**.

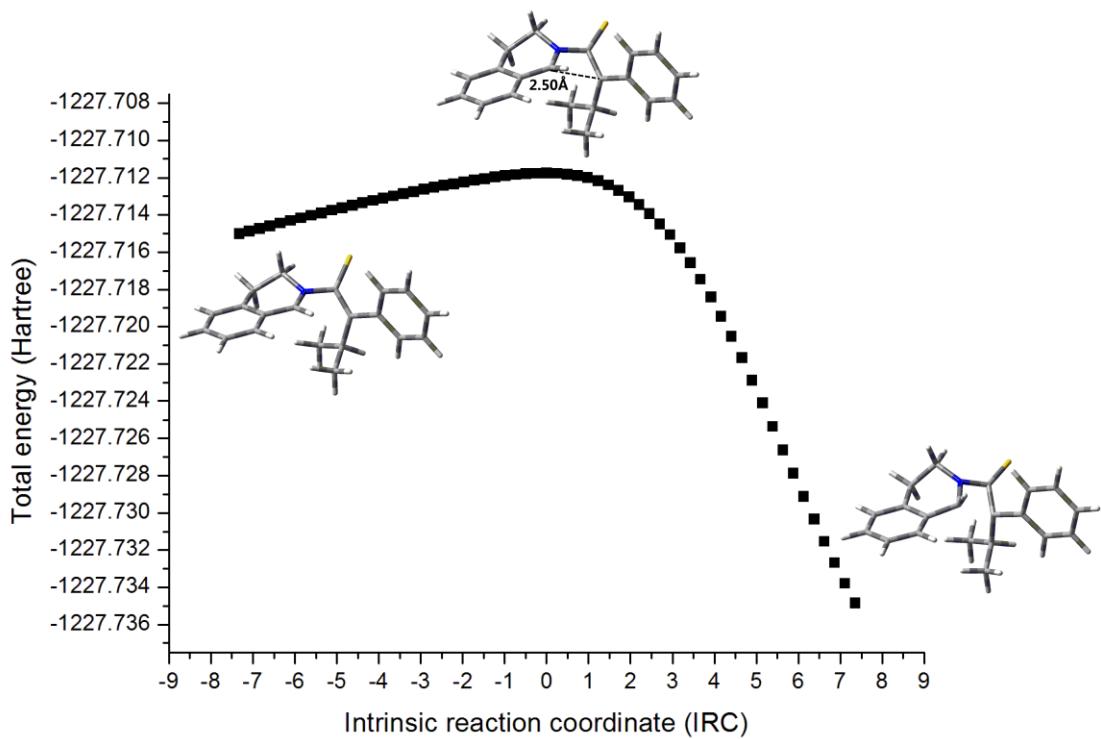


Figure S18. The intrinsic reaction coordinate (IRC) analysis of **TS2** of **1e'** and **5**.

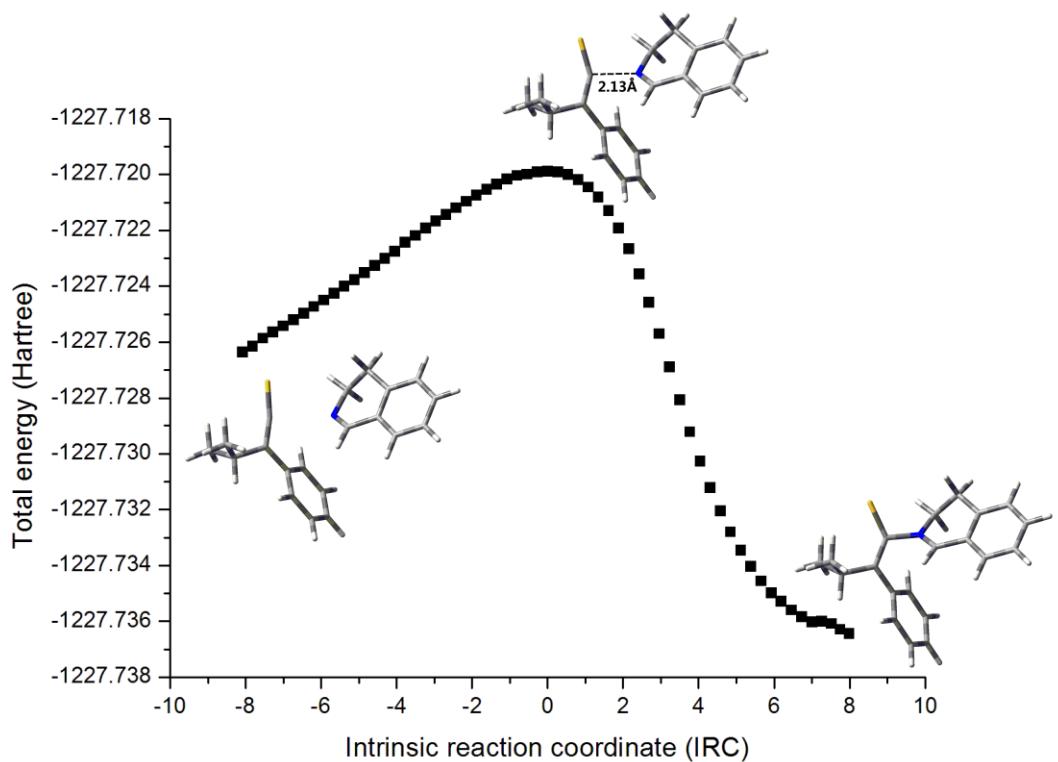


Figure S19. The intrinsic reaction coordinate (IRC) analysis of **TS3** of **1e'** and **5**.

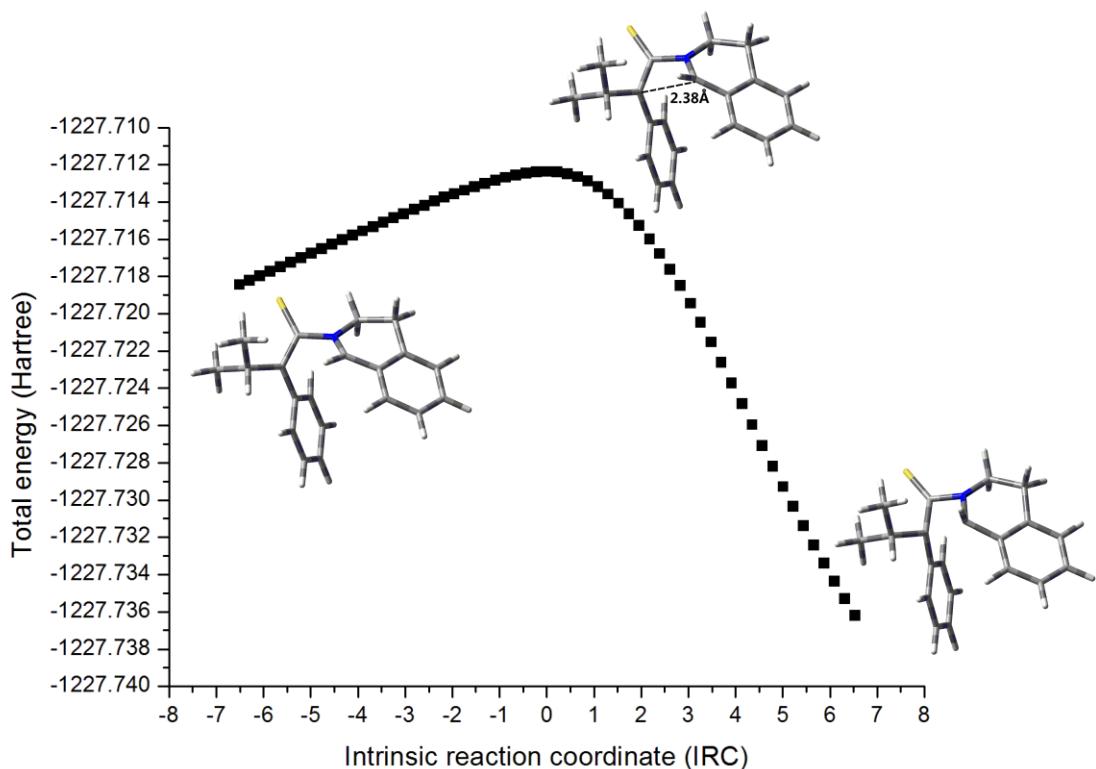


Figure S20. The intrinsic reaction coordinate (IRC) analysis of **TS4** of **1e'** and **5**.

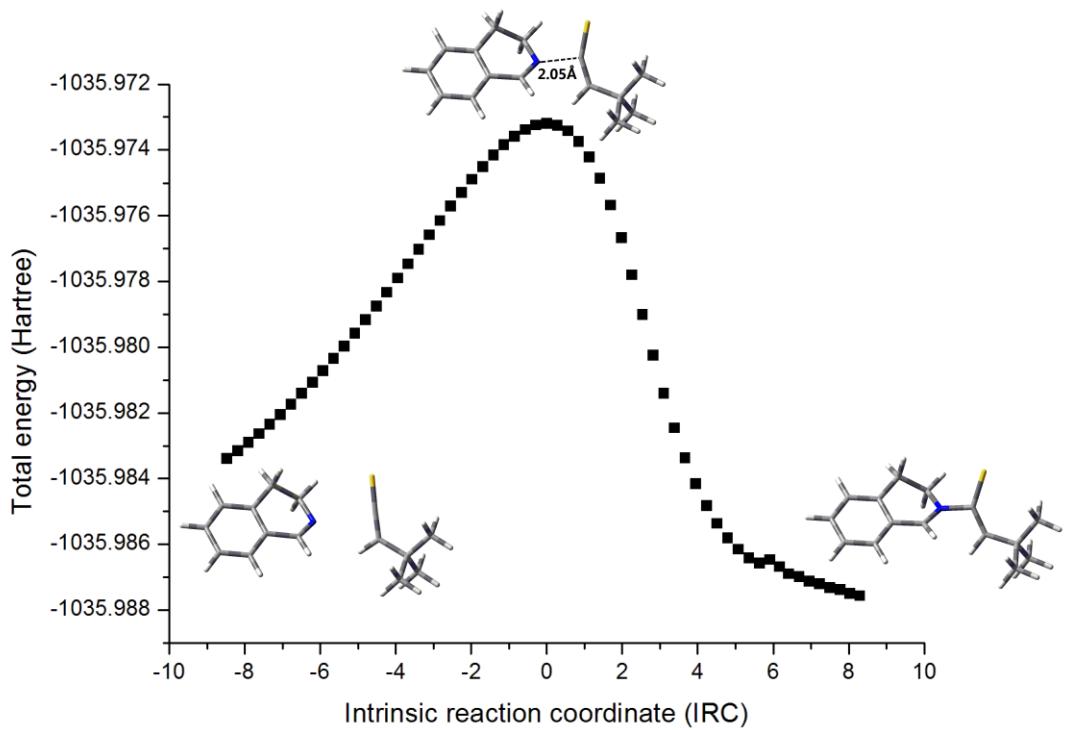


Figure S21. The intrinsic reaction coordinate (IRC) analysis of **TS1** of **1k** and **5**.

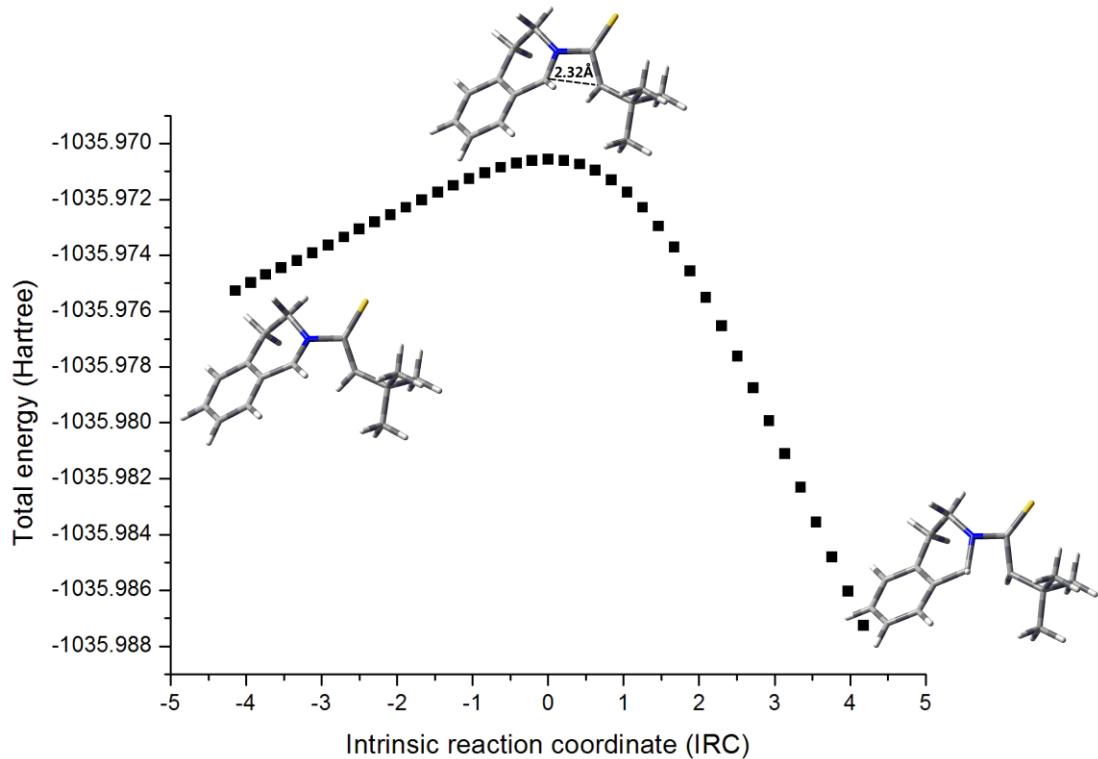


Figure S22. The intrinsic reaction coordinate (IRC) analysis of **TS2** of **1k** and **5**.

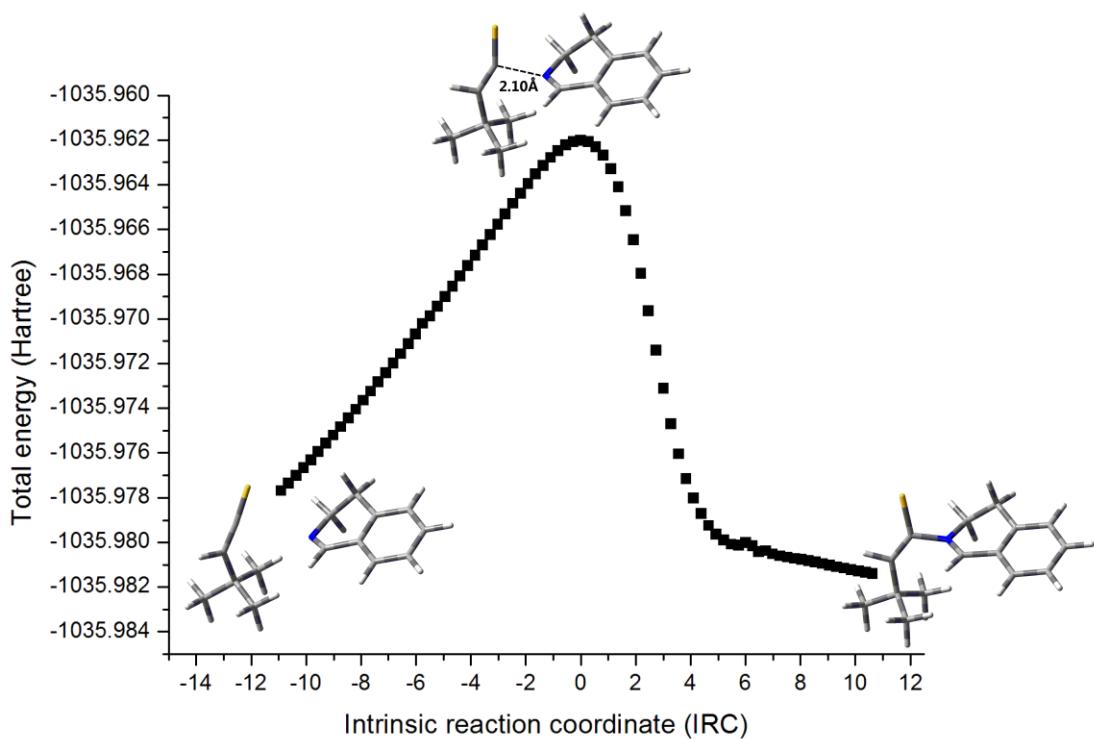


Figure S23. The intrinsic reaction coordinate (IRC) analysis of **TS3** of **1k** and **5**.

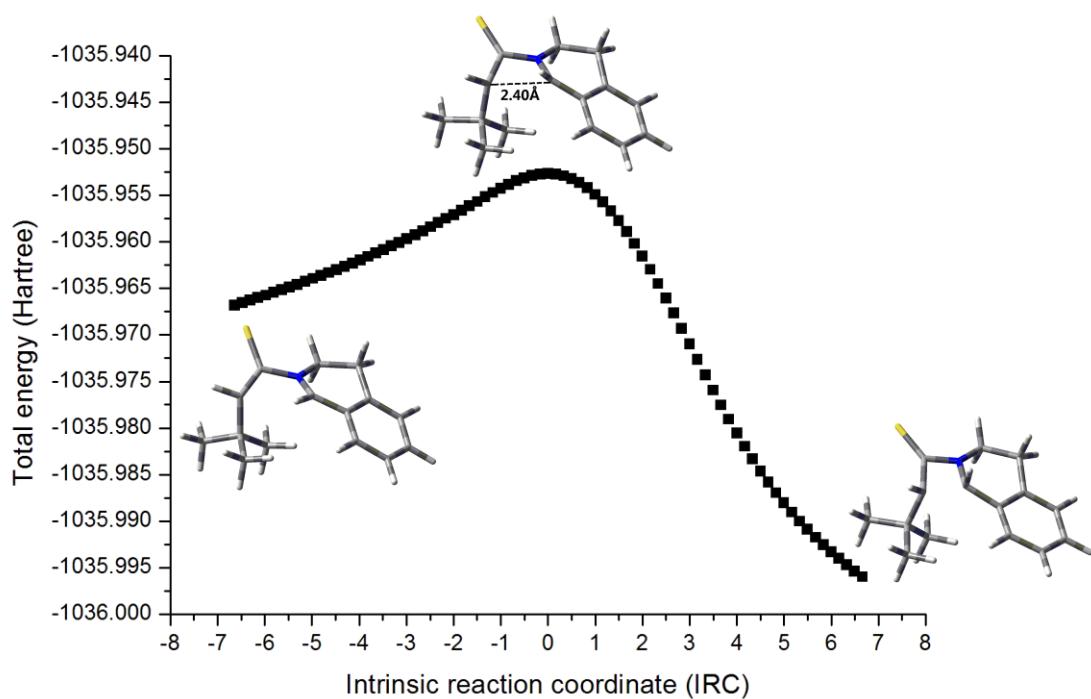


Figure S24. The intrinsic reaction coordinate (IRC) analysis of **TS4** of **1k** and **5**.

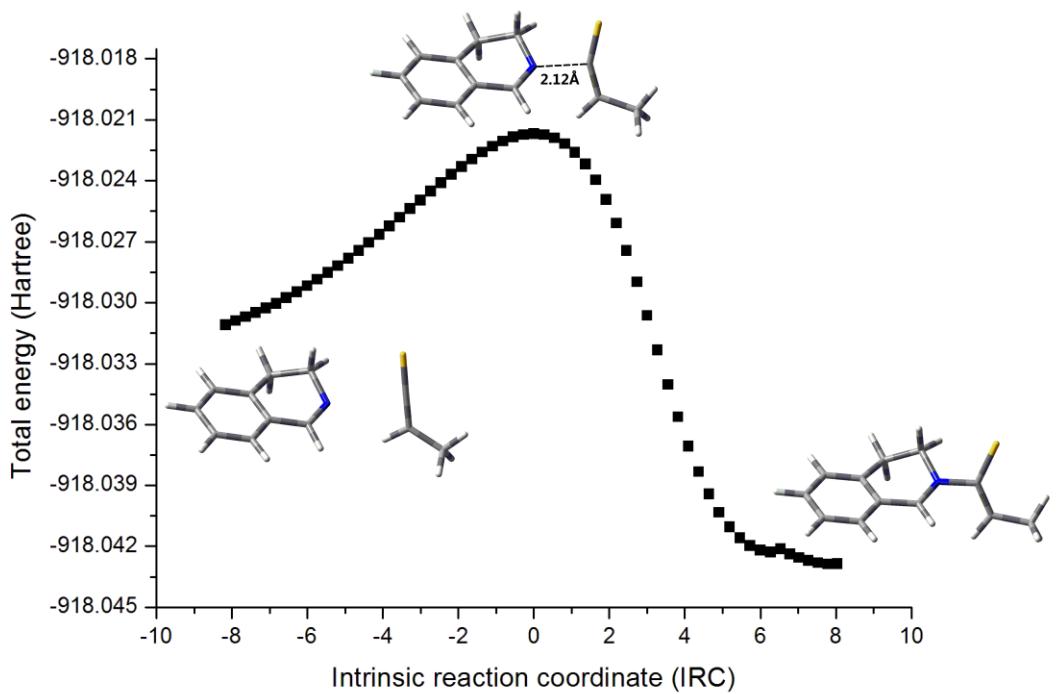


Figure S25. The intrinsic reaction coordinate (IRC) analysis of **TS1** of **1l** and **5**.

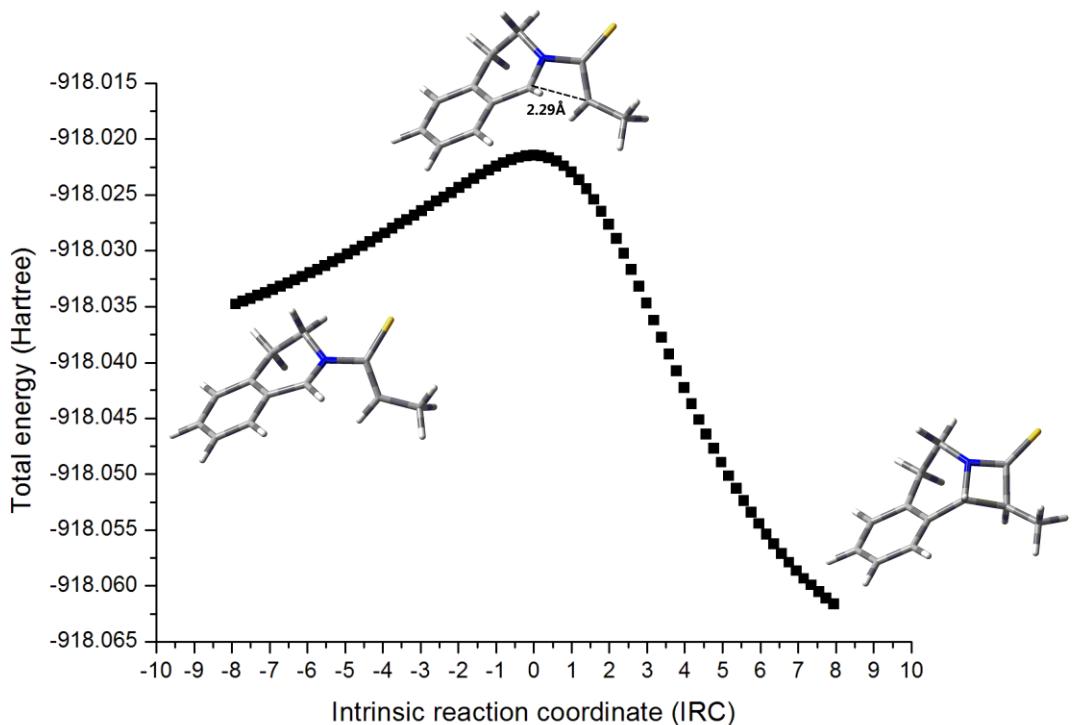


Figure S26. The intrinsic reaction coordinate (IRC) analysis of **TS2** of **1l** and **5**.

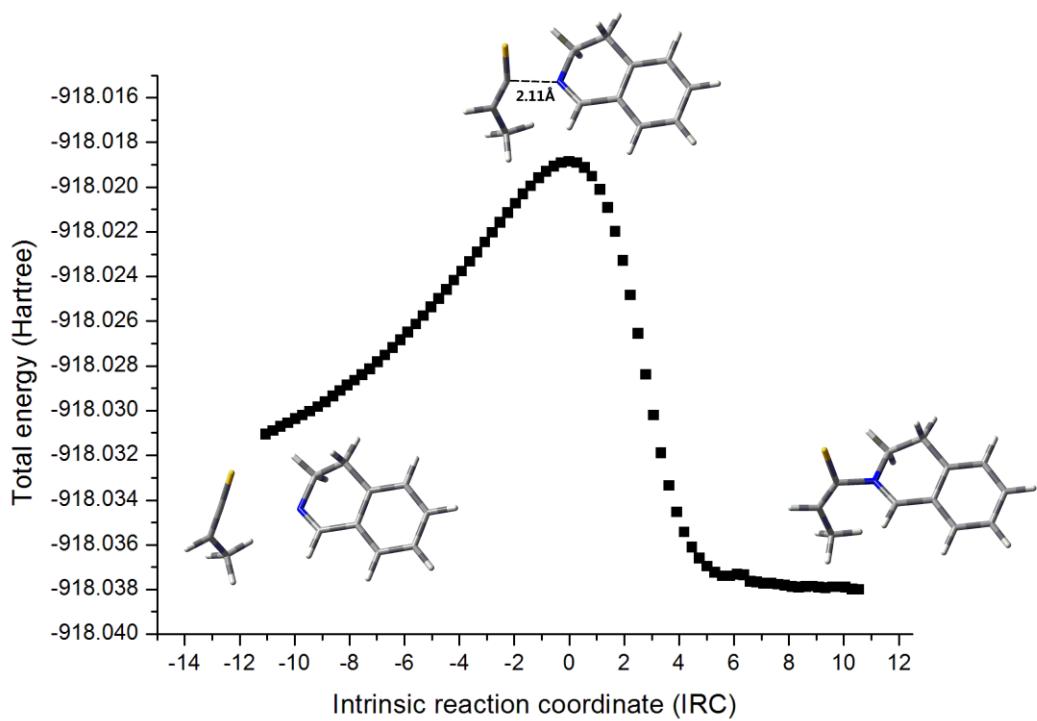


Figure S27. The intrinsic reaction coordinate (IRC) analysis of **TS3** of **1l** and **5**.

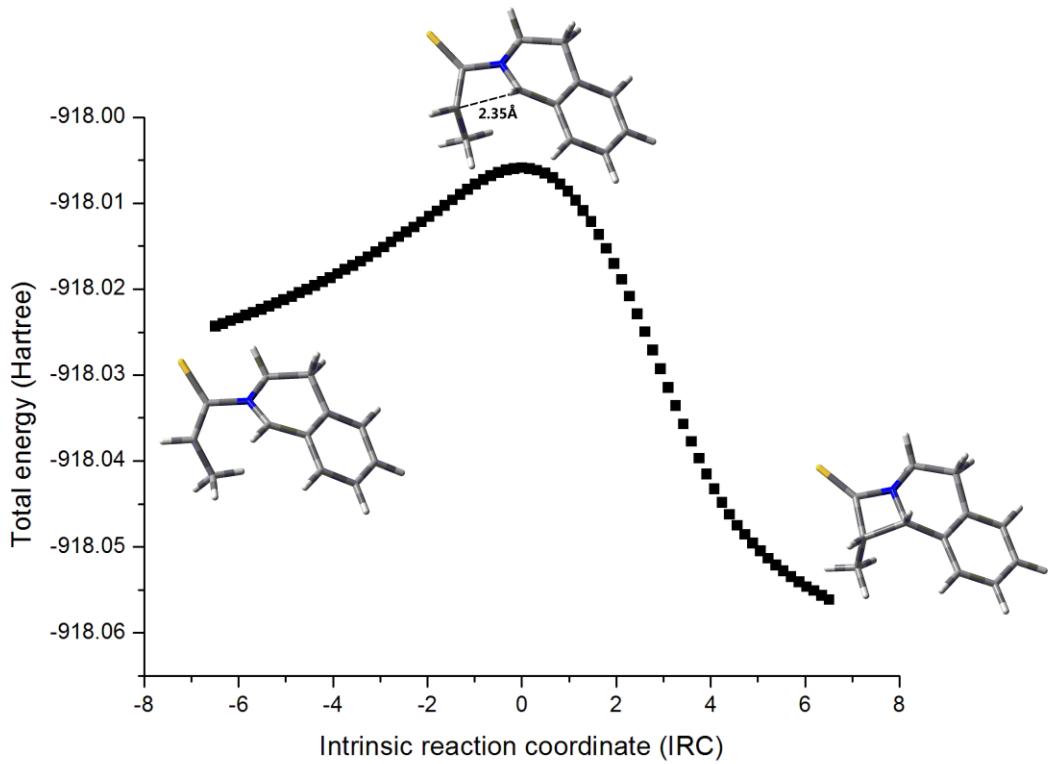
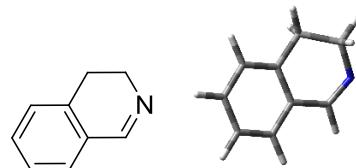


Figure S28. The intrinsic reaction coordinate (IRC) analysis of **TS4** of **1l** and **5**.

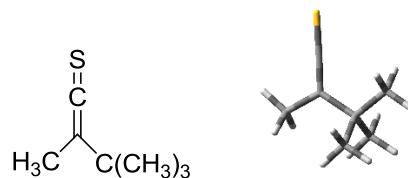
4. Coordinates of all stationary points (in gas phase)

5



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.294407	1.390616	0.006576
2	6	0	0.078725	0.700041	-0.087196
3	6	0	0.062909	-0.709028	-0.102801
4	6	0	1.270294	-1.403584	-0.013262
5	6	0	2.482013	-0.710751	0.091215
6	6	0	2.496579	0.687415	0.099064
7	1	0	1.293373	2.478100	0.013379
8	1	0	1.267172	-2.490890	-0.025858
9	1	0	3.414293	-1.263461	0.164466
10	1	0	3.437811	1.223427	0.176380
11	6	0	-1.283001	-1.373478	-0.279920
12	1	0	-1.491824	-1.471899	-1.356158
13	1	0	-1.279232	-2.388033	0.133767
14	6	0	-1.210777	1.412221	-0.164709
15	1	0	-1.176717	2.483764	-0.380926
16	7	0	-2.364377	0.890345	0.027372
17	6	0	-2.393177	-0.538090	0.371033
18	1	0	-3.376522	-0.930324	0.095215
19	1	0	-2.325546	-0.605278	1.468131

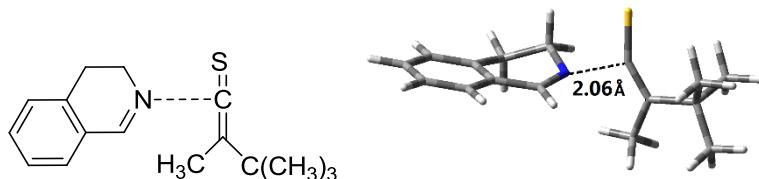
1a



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

1	6	0	1.284804	0.175005	-0.000010
2	16	0	2.779470	-0.323844	-0.000367
3	6	0	0.050076	0.626264	0.000002
4	6	0	-0.156997	2.134543	0.000317
5	1	0	-0.716796	2.455424	-0.885636
6	1	0	-0.716979	2.455021	0.886302
7	1	0	0.798609	2.663651	0.000536
8	6	0	-1.169325	-0.323982	0.000060
9	6	0	-2.021288	-0.061177	-1.262705
10	1	0	-2.880897	-0.741209	-1.282974
11	1	0	-2.411255	0.961190	-1.288390
12	1	0	-1.435426	-0.226960	-2.172946
13	6	0	-2.020963	-0.061380	1.263088
14	1	0	-1.434895	-0.227414	2.173150
15	1	0	-2.410824	0.961020	1.289091
16	1	0	-2.880632	-0.741335	1.283418
17	6	0	-0.721913	-1.798018	-0.000118
18	1	0	-1.599066	-2.454053	-0.000081
19	1	0	-0.124959	-2.035595	-0.886719
20	1	0	-0.124770	-2.035757	0.886312

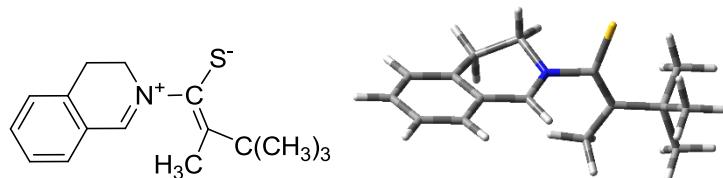
exo-1a-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.273858	1.676270	-0.643580
2	6	0	-2.580867	0.610715	-0.050925
3	6	0	-3.280994	-0.497209	0.469566
4	6	0	-4.672311	-0.523595	0.371465
5	6	0	-5.361113	0.534980	-0.232058
6	6	0	-4.664677	1.637234	-0.737972
7	1	0	-2.719503	2.523709	-1.038695
8	1	0	-5.223768	-1.371997	0.768656
9	1	0	-6.444188	0.499021	-0.305090
10	1	0	-5.202934	2.456987	-1.203524
11	6	0	-2.468721	-1.561288	1.172380
12	1	0	-2.371540	-1.286238	2.233328

13	1	0	-2.982634	-2.527926	1.145463
14	6	0	-1.118824	0.613114	0.040428
15	1	0	-0.581719	1.534804	-0.190271
16	7	0	-0.407826	-0.411122	0.340968
17	6	0	-1.072570	-1.704186	0.554971
18	1	0	-0.424080	-2.309558	1.194537
19	1	0	-1.122083	-2.207336	-0.418118
20	6	0	1.514420	-0.468984	-0.389741
21	16	0	1.376689	-1.313396	-1.779466
22	6	0	2.276755	0.193640	0.489296
23	6	0	1.865760	0.536910	1.903560
24	1	0	0.857119	0.189582	2.117810
25	1	0	2.540706	0.058188	2.625413
26	1	0	1.906211	1.614695	2.103345
27	6	0	3.767643	0.471322	0.090287
28	6	0	4.394689	1.531896	1.025363
29	1	0	5.427627	1.717906	0.711442
30	1	0	3.857371	2.485435	0.973760
31	1	0	4.424434	1.210642	2.070385
32	6	0	3.896448	1.016045	-1.348046
33	1	0	3.522132	0.312151	-2.092763
34	1	0	3.339944	1.953771	-1.458874
35	1	0	4.950396	1.219142	-1.571864
36	6	0	4.569941	-0.843608	0.225006
37	1	0	5.626217	-0.678862	-0.022377
38	1	0	4.522044	-1.230419	1.249753
39	1	0	4.175676	-1.611047	-0.447630

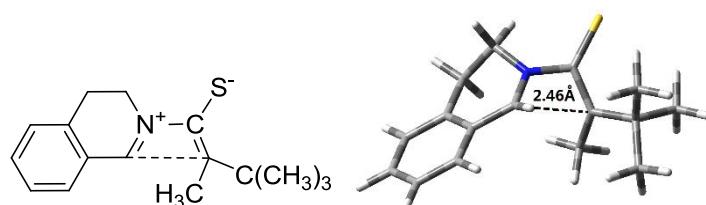
E-1a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.266685	-1.142973	-1.291928
2	6	0	2.448831	-0.411460	-0.411188
3	6	0	3.019701	0.294447	0.673284
4	6	0	4.402737	0.269565	0.842338
5	6	0	5.214185	-0.446795	-0.045383

6	6	0	4.647017	-1.155553	-1.110887
7	1	0	2.815441	-1.684368	-2.118928
8	1	0	4.852405	0.808790	1.671937
9	1	0	6.290696	-0.453728	0.097005
10	1	0	5.280234	-1.711134	-1.795253
11	6	0	2.069164	0.985295	1.623244
12	1	0	1.760281	0.275351	2.404285
13	1	0	2.562301	1.819601	2.131955
14	6	0	1.011621	-0.396170	-0.577573
15	1	0	0.527046	-1.084842	-1.262800
16	7	0	0.231421	0.435270	0.054841
17	6	0	0.840469	1.513705	0.884297
18	1	0	0.064063	1.866401	1.563536
19	1	0	1.102388	2.335183	0.213423
20	6	0	-1.216810	0.489922	-0.234042
21	16	0	-1.506115	1.889913	-1.215058
22	6	0	-1.997343	-0.487330	0.316667
23	6	0	-1.433304	-1.520466	1.275357
24	1	0	-0.365231	-1.400130	1.458784
25	1	0	-1.930827	-1.457428	2.251685
26	1	0	-1.589746	-2.545983	0.918691
27	6	0	-3.529808	-0.527307	0.069467
28	6	0	-4.196462	-1.763284	0.720064
29	1	0	-5.268995	-1.740254	0.499578
30	1	0	-3.803556	-2.706045	0.323715
31	1	0	-4.091622	-1.777929	1.809619
32	6	0	-3.836948	-0.606198	-1.446422
33	1	0	-3.431462	0.251153	-1.985428
34	1	0	-3.409291	-1.519418	-1.878364
35	1	0	-4.921968	-0.637611	-1.604994
36	6	0	-4.190016	0.731015	0.684752
37	1	0	-5.271978	0.716158	0.503912
38	1	0	-4.032500	0.756861	1.770061
39	1	0	-3.778098	1.645403	0.252349

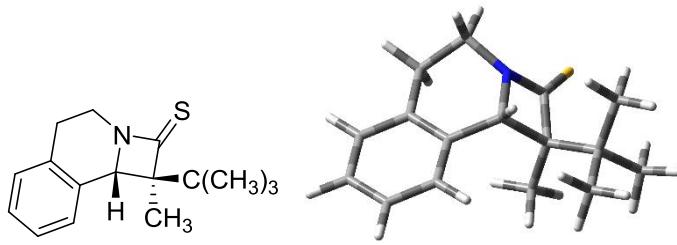
exo-1a-TS2



Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	2. 632796	-1. 610062	-0. 825493
2	6	0	2. 024162	-0. 402886	-0. 420403
3	6	0	2. 792546	0. 570871	0. 272808
4	6	0	4. 133037	0. 301090	0. 548675
5	6	0	4. 721483	-0. 907393	0. 159924
6	6	0	3. 967731	-1. 864507	-0. 530648
7	1	0	2. 042335	-2. 344551	-1. 367170
8	1	0	4. 729919	1. 047325	1. 067683
9	1	0	5. 766623	-1. 096447	0. 385883
10	1	0	4. 424218	-2. 799780	-0. 840017
11	6	0	2. 136495	1. 877253	0. 685503
12	1	0	1. 790072	1. 799850	1. 725972
13	1	0	2. 869389	2. 690961	0. 661995
14	6	0	0. 637958	-0. 139738	-0. 713127
15	1	0	0. 107072	-0. 752430	-1. 427014
16	7	0	0. 093885	1. 059093	-0. 351011
17	6	0	0. 953162	2. 241562	-0. 218107
18	1	0	0. 341772	3. 045080	0. 194361
19	1	0	1. 297649	2. 548403	-1. 213135
20	6	0	-1. 266397	0. 984854	-0. 112224
21	16	0	-2. 332066	2. 267348	-0. 397540
22	6	0	-1. 549201	-0. 344679	0. 399491
23	6	0	-0. 863185	-0. 741080	1. 695954
24	1	0	0. 001230	-0. 112114	1. 911746
25	1	0	-1. 573826	-0. 608138	2. 526816
26	1	0	-0. 542130	-1. 786163	1. 719248
27	6	0	-2. 827470	-1. 111571	0. 041584
28	6	0	-4. 022976	-0. 616845	0. 904836
29	1	0	-4. 912884	-1. 210668	0. 663303
30	1	0	-3. 823120	-0. 737492	1. 975041
31	1	0	-4. 233076	0. 435954	0. 706687
32	6	0	-2. 628582	-2. 623733	0. 314559
33	1	0	-1. 751303	-3. 016618	-0. 212819
34	1	0	-2. 515597	-2. 844814	1. 379709
35	1	0	-3. 506129	-3. 172406	-0. 042817
36	6	0	-3. 180625	-0. 949030	-1. 454089
37	1	0	-4. 087647	-1. 519662	-1. 682457
38	1	0	-3. 356932	0. 094800	-1. 718458
39	1	0	-2. 377370	-1. 336935	-2. 092308

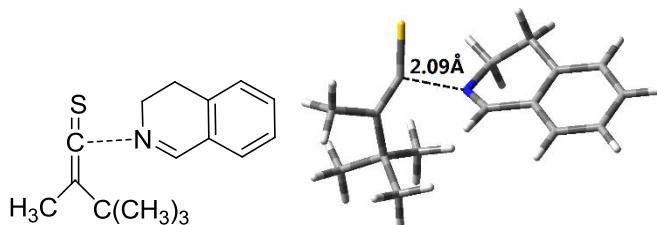
7a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.080090	-1.743347	0.150069
2	6	0	-1.572820	-0.441854	0.282380
3	6	0	-2.424507	0.662471	0.068959
4	6	0	-3.761319	0.421472	-0.285225
5	6	0	-4.252518	-0.874404	-0.434676
6	6	0	-3.406018	-1.965650	-0.215389
7	1	0	-1.423230	-2.589854	0.334279
8	1	0	-4.424533	1.268622	-0.444168
9	1	0	-5.290716	-1.032856	-0.711523
10	1	0	-3.778671	-2.980217	-0.321494
11	6	0	-1.931444	2.096908	0.196735
12	1	0	-1.628040	2.466988	-0.791642
13	1	0	-2.749719	2.741906	0.536576
14	6	0	-0.140610	-0.234765	0.719324
15	1	0	0.029375	-0.763156	1.664820
16	7	0	0.217531	1.185192	0.812610
17	6	0	-0.727516	2.233157	1.144709
18	1	0	-0.227505	3.197254	1.028471
19	1	0	-1.032466	2.116812	2.191037
20	6	0	1.214954	1.155808	-0.104006
21	16	0	2.102801	2.367402	-0.788846
22	6	0	1.083426	-0.376302	-0.298079
23	6	0	0.668480	-0.694531	-1.739836
24	1	0	-0.224865	-0.132438	-2.023924
25	1	0	1.466096	-0.412211	-2.430216
26	1	0	0.445159	-1.757324	-1.871923
27	6	0	2.284704	-1.241735	0.229487
28	6	0	3.453618	-1.208080	-0.780918
29	1	0	4.320318	-1.727446	-0.356495
30	1	0	3.199579	-1.710038	-1.719338
31	1	0	3.750602	-0.180400	-1.010423
32	6	0	1.836868	-2.706668	0.427630
33	1	0	1.042951	-2.795237	1.178029
34	1	0	1.478874	-3.159518	-0.502360

35	1	0	2. 683386	-3. 307939	0. 777634
36	6	0	2. 809792	-0. 700065	1. 578188
37	1	0	3. 624572	-1. 337802	1. 937575
38	1	0	3. 201578	0. 316072	1. 475544
39	1	0	2. 039733	-0. 690482	2. 356684

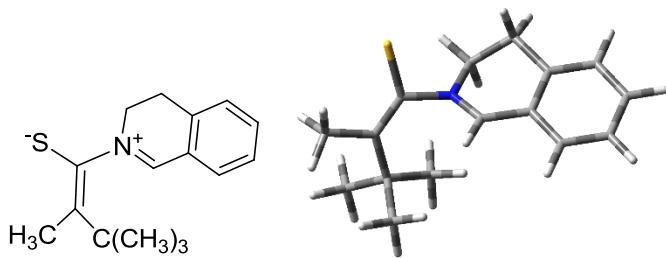
endo-1a-TS3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2. 938347	-1. 466688	-1. 095657
2	6	0	-2. 259907	-0. 466255	-0. 385236
3	6	0	-2. 970183	0. 439700	0. 429555
4	6	0	-4. 355871	0. 314458	0. 527463
5	6	0	-5. 030212	-0. 694344	-0. 171273
6	6	0	-4. 324168	-1. 584664	-0. 985706
7	1	0	-2. 377527	-2. 152606	-1. 725687
8	1	0	-4. 915399	1. 008887	1. 149092
9	1	0	-6. 109143	-0. 781519	-0. 081450
10	1	0	-4. 850356	-2. 362252	-1. 530730
11	6	0	-2. 177375	1. 543846	1. 093218
12	1	0	-2. 119535	2. 399804	0. 407039
13	1	0	-2. 680411	1. 895250	2. 000487
14	6	0	-0. 801382	-0. 335456	-0. 462832
15	1	0	-0. 271663	-0. 864938	-1. 256180
16	7	0	-0. 091393	0. 357024	0. 348767
17	6	0	-0. 753765	1. 087434	1. 434756
18	1	0	-0. 126606	1. 950943	1. 672227
19	1	0	-0. 755170	0. 422044	2. 309725
20	6	0	1. 715244	1. 100930	-0. 388979
21	16	0	1. 300393	2. 635763	-0. 751512
22	6	0	2. 649041	0. 143640	-0. 422041
23	6	0	3. 758656	0. 451982	-1. 433580
24	1	0	3. 427556	1. 188713	-2. 166227
25	1	0	4. 659212	0. 846566	-0. 947126
26	1	0	4. 046633	-0. 457221	-1. 975739

27	6	0	2. 836766	-1. 135762	0. 426753
28	6	0	4. 342031	-1. 275167	0. 782944
29	1	0	4. 485669	-2. 157752	1. 415734
30	1	0	4. 975218	-1. 399141	-0. 099222
31	1	0	4. 698486	-0. 400766	1. 338326
32	6	0	2. 416115	-2. 388968	-0. 379216
33	1	0	1. 340576	-2. 387592	-0. 579160
34	1	0	2. 939136	-2. 442017	-1. 340039
35	1	0	2. 652182	-3. 303031	0. 179588
36	6	0	2. 079435	-1. 118701	1. 772025
37	1	0	2. 421865	-1. 956042	2. 391228
38	1	0	2. 273584	-0. 191362	2. 321272
39	1	0	1. 002689	-1. 223254	1. 646508

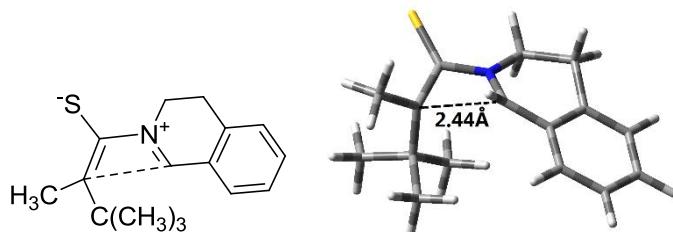
F-1a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2. 782863	-1. 359757	-1. 160740
2	6	0	-2. 094301	-0. 365457	-0. 443165
3	6	0	-2. 785411	0. 465082	0. 470050
4	6	0	-4. 151866	0. 268908	0. 655688
5	6	0	-4. 831003	-0. 735223	-0. 046634
6	6	0	-4. 148017	-1. 548557	-0. 956425
7	1	0	-2. 242982	-1. 982364	-1. 869167
8	1	0	-4. 694907	0. 904510	1. 350145
9	1	0	-5. 895347	-0. 877920	0. 114728
10	1	0	-4. 678110	-2. 321099	-1. 504350
11	6	0	-1. 997798	1. 567937	1. 143095
12	1	0	-2. 015615	2. 467616	0. 514928
13	1	0	-2. 445146	1. 833118	2. 106596
14	6	0	-0. 679737	-0. 145489	-0. 660629
15	1	0	-0. 183163	-0. 562172	-1. 531451
16	7	0	0. 053994	0. 587627	0. 127191
17	6	0	-0. 548252	1. 145150	1. 366474

18	1	0	0.075311	1.985111	1.665722
19	1	0	-0.490219	0.350700	2.121224
20	6	0	1.412029	1.001776	-0.272011
21	16	0	1.303201	2.663671	-0.772834
22	6	0	2.470131	0.142196	-0.247666
23	6	0	3.748038	0.687193	-0.858923
24	1	0	3.519947	1.439775	-1.615274
25	1	0	4.384635	1.173552	-0.107188
26	1	0	4.342140	-0.105533	-1.325263
27	6	0	2.575753	-1.285781	0.341506
28	6	0	3.905221	-1.397158	1.139682
29	1	0	3.989509	-2.397014	1.580411
30	1	0	4.785960	-1.238974	0.513972
31	1	0	3.934376	-0.664523	1.953770
32	6	0	2.604556	-2.328577	-0.805917
33	1	0	1.650978	-2.347249	-1.345471
34	1	0	3.393179	-2.110407	-1.532249
35	1	0	2.785453	-3.335052	-0.408542
36	6	0	1.465023	-1.694530	1.334222
37	1	0	1.727845	-2.656974	1.786908
38	1	0	1.370456	-0.968233	2.148159
39	1	0	0.487517	-1.825271	0.865759

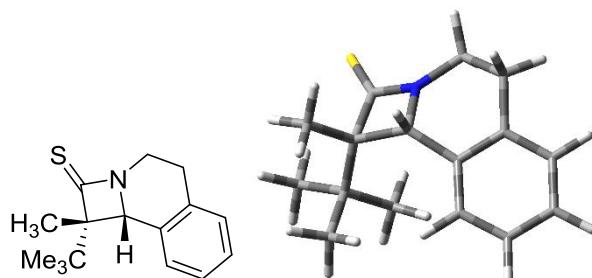
endo-1a-TS4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.424303	-1.362216	-0.930107
2	6	0	-1.815646	-0.153713	-0.544160
3	6	0	-2.573627	0.817127	0.157654
4	6	0	-3.892461	0.528155	0.510873
5	6	0	-4.476466	-0.694080	0.161980
6	6	0	-3.743725	-1.632661	-0.573143
7	1	0	-1.849874	-2.094799	-1.490327
8	1	0	-4.477194	1.274368	1.043463
9	1	0	-5.502394	-0.905529	0.447970

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
10	1	0	-4.199110	-2.575340	-0.861447
11	6	0	-1.956829	2.186770	0.339489
12	1	0	-2.089405	2.748677	-0.596328
13	1	0	-2.475619	2.751695	1.120134
14	6	0	-0.441436	0.175331	-0.888850
15	1	0	-0.077850	-0.039818	-1.882850
16	7	0	0.219727	1.125746	-0.153239
17	6	0	-0.462221	2.130881	0.668909
18	1	0	0.032620	3.090311	0.486831
19	1	0	-0.298244	1.868579	1.721751
20	6	0	1.585402	0.994977	-0.257600
21	16	0	2.682170	2.275236	-0.209177
22	6	0	1.903923	-0.399239	-0.526336
23	6	0	2.929261	-0.653787	-1.602654
24	1	0	2.753416	0.002072	-2.461435
25	1	0	3.946327	-0.431634	-1.254717
26	1	0	2.914610	-1.694459	-1.938283
27	6	0	1.780329	-1.472886	0.580556
28	6	0	3.211334	-1.655777	1.176233
29	1	0	3.168149	-2.357399	2.016784
30	1	0	3.911669	-2.061465	0.441276
31	1	0	3.610142	-0.704409	1.542307
32	6	0	1.307479	-2.832416	0.017727
33	1	0	0.282266	-2.762128	-0.357527
34	1	0	1.945755	-3.192170	-0.794302
35	1	0	1.327488	-3.590529	0.808935
36	6	0	0.857494	-1.080203	1.750723
37	1	0	0.922433	-1.848079	2.528836
38	1	0	1.161026	-0.129496	2.199912
39	1	0	-0.190064	-1.010025	1.450765

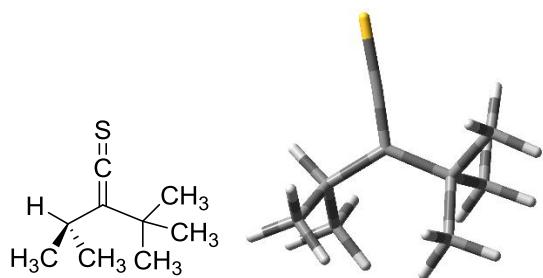
8a



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

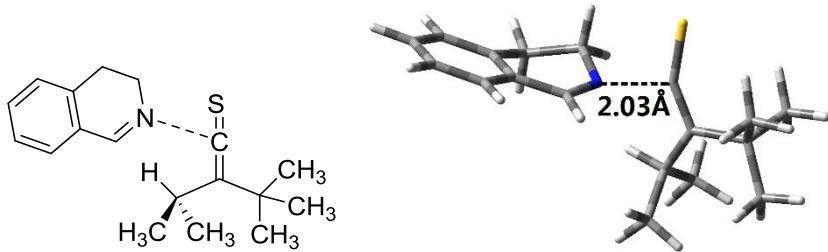
1	6	0	2. 021979	-1. 551650	0. 354141
2	6	0	1. 548128	-0. 235504	0. 397763
3	6	0	2. 428827	0. 816707	0. 048584
4	6	0	3. 715194	0. 511887	-0. 413603
5	6	0	4. 159654	-0. 808160	-0. 494849
6	6	0	3. 313175	-1. 841549	-0. 091241
7	1	0	1. 381445	-2. 366760	0. 663768
8	1	0	4. 381065	1. 323723	-0. 696090
9	1	0	5. 160559	-1. 025424	-0. 855855
10	1	0	3. 650584	-2. 873264	-0. 125794
11	6	0	2. 025373	2. 261630	0. 279752
12	1	0	2. 140336	2. 485231	1. 350471
13	1	0	2. 704437	2. 936165	-0. 249853
14	6	0	0. 189013	0. 193662	0. 926241
15	1	0	0. 294978	0. 327105	2. 014763
16	7	0	-0. 240971	1. 450900	0. 294950
17	6	0	0. 578130	2. 567002	-0. 129501
18	1	0	0. 220994	3. 500529	0. 321398
19	1	0	0. 484051	2. 670809	-1. 217693
20	6	0	-1. 510383	1. 109061	0. 036644
21	16	0	-2. 726324	2. 008153	-0. 636907
22	6	0	-1. 331640	-0. 312469	0. 644103
23	6	0	-2. 083284	-0. 423960	1. 982585
24	1	0	-1. 886309	0. 453356	2. 606805
25	1	0	-3. 162350	-0. 469633	1. 823755
26	1	0	-1. 773555	-1. 311838	2. 542423
27	6	0	-1. 648695	-1. 499997	-0. 338724
28	6	0	-3. 153352	-1. 494749	-0. 714086
29	1	0	-3. 345004	-2. 323523	-1. 405290
30	1	0	-3. 799744	-1. 643165	0. 155928
31	1	0	-3. 449651	-0. 563912	-1. 200679
32	6	0	-1. 364716	-2. 867090	0. 325978
33	1	0	-0. 368726	-2. 937419	0. 766934
34	1	0	-2. 089714	-3. 087410	1. 115432
35	1	0	-1. 449726	-3. 662414	-0. 422663
36	6	0	-0. 853006	-1. 371484	-1. 656374
37	1	0	-1. 163431	-2. 162102	-2. 348335
38	1	0	-1. 052996	-0. 412522	-2. 145399
39	1	0	0. 224361	-1. 464295	-1. 512638

1d



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.403878	-0.273223	0.049813
2	16	0	2.970293	-0.448196	0.087974
3	6	0	0.091849	-0.179236	0.022387
4	6	0	-0.634958	-1.546706	0.113457
5	1	0	0.143872	-2.265901	0.395525
6	6	0	-0.579928	1.219908	-0.055183
7	6	0	-0.991985	1.683101	1.364472
8	1	0	-1.416610	2.693396	1.317992
9	1	0	-1.742769	1.027511	1.811339
10	1	0	-0.124019	1.710371	2.030982
11	6	0	-1.822112	1.210002	-0.971791
12	1	0	-1.564676	0.905002	-1.990765
13	1	0	-2.609646	0.548515	-0.602202
14	1	0	-2.241070	2.221549	-1.020783
15	6	0	0.415680	2.254693	-0.625142
16	1	0	-0.065433	3.237120	-0.684985
17	1	0	1.301297	2.358375	0.009411
18	1	0	0.747968	1.976139	-1.630370
19	6	0	-1.705700	-1.627705	1.217214
20	1	0	-2.570162	-0.990602	1.007369
21	1	0	-2.070929	-2.658404	1.291657
22	1	0	-1.298726	-1.344536	2.192451
23	6	0	-1.184467	-2.031593	-1.244830
24	1	0	-0.411781	-1.989202	-2.018490
25	1	0	-1.516443	-3.072827	-1.155596
26	1	0	-2.039105	-1.440822	-1.583500

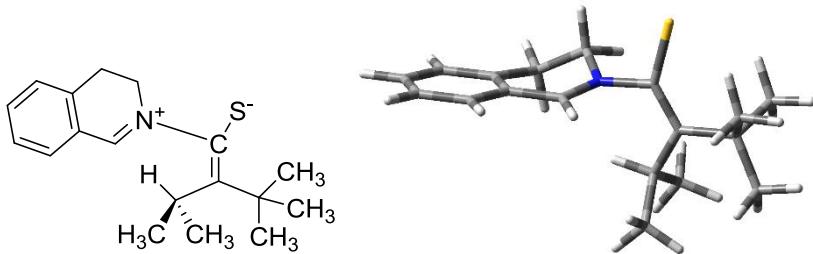
exo-1d-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.220855	-0.822918	-0.334846
2	16	0	-0.959843	-2.382828	-0.755126
3	6	0	-2.082502	0.135890	0.048680
4	6	0	-1.753548	1.626632	-0.123021
5	1	0	-0.728340	1.633099	-0.493580
6	6	0	-3.511842	-0.377772	0.472672
7	6	0	-4.295116	-0.809021	-0.791044
8	1	0	-5.278951	-1.206622	-0.511929
9	1	0	-4.455033	0.038375	-1.465622
10	1	0	-3.756818	-1.587153	-1.339473
11	6	0	-4.340086	0.695994	1.215521
12	1	0	-3.881730	0.972518	2.169459
13	1	0	-4.499660	1.603609	0.631213
14	1	0	-5.327987	0.277054	1.437492
15	6	0	-3.420393	-1.573129	1.450847
16	1	0	-4.430021	-1.872962	1.755340
17	1	0	-2.931169	-2.440948	1.008081
18	1	0	-2.865497	-1.292603	2.353479
19	6	0	-2.578753	2.317343	-1.233465
20	1	0	-3.635460	2.433356	-0.978406
21	1	0	-2.178147	3.321969	-1.418353
22	1	0	-2.521453	1.753258	-2.169926
23	6	0	-1.719306	2.482186	1.163641
24	1	0	-1.174477	1.971094	1.964676
25	1	0	-1.201282	3.427032	0.957176
26	1	0	-2.711544	2.735777	1.542070
27	7	0	0.627179	0.002523	-0.481923
28	6	0	1.346874	0.005055	0.580738
29	6	0	1.288253	-0.065897	-1.793627
30	6	0	2.810755	0.005707	0.589061
31	1	0	0.816919	-0.029927	1.533692
32	6	0	2.640799	0.655312	-1.813852
33	1	0	0.606436	0.364342	-2.532453

34	1	0	1.402222	-1.127821	-2.040722
35	6	0	3.530436	-0.268611	1.761316
36	6	0	3.486482	0.283632	-0.617157
37	1	0	2.473651	1.742755	-1.802481
38	1	0	3.163794	0.428390	-2.748823
39	6	0	4.924617	-0.285617	1.735636
40	1	0	2.994771	-0.479884	2.683214
41	6	0	4.881173	0.266358	-0.629439
42	6	0	5.597357	-0.020343	0.538588
43	1	0	5.483971	-0.505821	2.639546
44	1	0	5.413876	0.478473	-1.552942
45	1	0	6.683081	-0.034574	0.513242

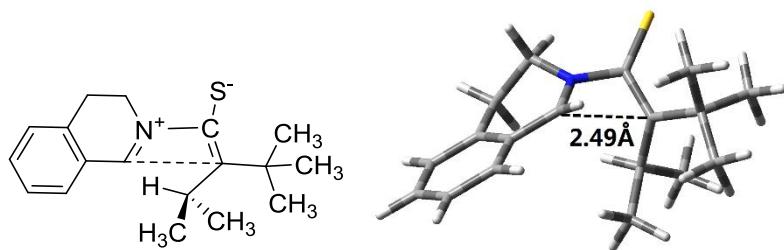
E-1d



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.988818	-0.837148	0.064962
2	16	0	1.104366	-2.567305	0.117750
3	6	0	1.869588	0.204788	-0.078273
4	6	0	1.383995	1.635325	0.228338
5	1	0	0.310795	1.555496	0.410114
6	6	0	3.370321	-0.107662	-0.370825
7	6	0	4.007722	-0.769342	0.879053
8	1	0	5.047164	-1.049699	0.667366
9	1	0	4.014996	-0.074713	1.726928
10	1	0	3.462441	-1.670414	1.169327
11	6	0	4.225772	1.132939	-0.723810
12	1	0	3.921806	1.583128	-1.673052
13	1	0	4.220761	1.906516	0.046161
14	1	0	5.265000	0.806649	-0.841292
15	6	0	3.514199	-1.049731	-1.594381
16	1	0	4.578084	-1.222670	-1.797888
17	1	0	3.032199	-2.013235	-1.432954
18	1	0	3.073602	-0.588606	-2.486622

19	6	0	1. 943239	2. 201423	1. 557090
20	1	0	3. 017767	2. 394273	1. 523479
21	1	0	1. 448554	3. 152294	1. 792558
22	1	0	1. 759115	1. 509383	2. 385620
23	6	0	1. 500759	2. 675928	-0. 911095
24	1	0	1. 195535	2. 249246	-1. 872622
25	1	0	0. 839774	3. 525084	-0. 696832
26	1	0	2. 509103	3. 076034	-1. 028232
27	7	0	-0. 443376	-0. 514097	0. 283676
28	6	0	-1. 220851	-0. 228683	-0. 723311
29	6	0	-1. 054360	-0. 795535	1. 615114
30	6	0	-2. 650469	-0. 049974	-0. 591607
31	1	0	-0. 740365	-0. 147586	-1. 693422
32	6	0	-2. 243477	0. 130473	1. 865309
33	1	0	-0. 265882	-0. 670526	2. 357619
34	1	0	-1. 359311	-1. 844350	1. 618414
35	6	0	-3. 475765	-0. 002228	-1. 730100
36	6	0	-3. 204899	0. 108254	0. 699659
37	1	0	-1. 891862	1. 160354	2. 023437
38	1	0	-2. 742606	-0. 177820	2. 789365
39	6	0	-4. 848740	0. 178907	-1. 586724
40	1	0	-3. 036422	-0. 121692	-2. 716660
41	6	0	-4. 580510	0. 291844	0. 826102
42	6	0	-5. 400213	0. 323043	-0. 308368
43	1	0	-5. 488337	0. 205397	-2. 463181
44	1	0	-5. 017935	0. 414576	1. 813415
45	1	0	-6. 470978	0. 462696	-0. 193594

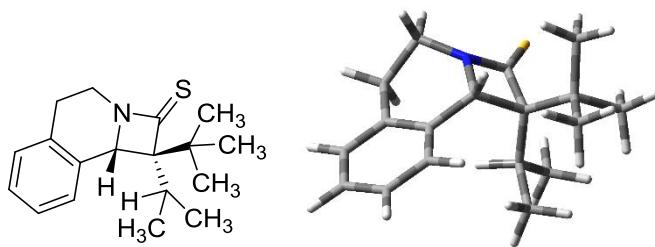
exo-1d-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1. 125761	1. 149631	-0. 162540
2	16	0	-2. 113863	2. 518052	-0. 294198
3	6	0	-1. 491978	-0. 241098	0. 101467

4	6	0	-0. 914272	-0. 789485	1. 427260
5	1	0	-0. 089502	-0. 113858	1. 673895
6	6	0	-2. 726841	-0. 850434	-0. 594434
7	6	0	-4. 075332	-0. 327366	-0. 014312
8	1	0	-4. 897506	-0. 786447	-0. 577240
9	1	0	-4. 199256	-0. 598468	1. 036621
10	1	0	-4. 146356	0. 757050	-0. 102825
11	6	0	-2. 751373	-2. 393411	-0. 494538
12	1	0	-1. 822502	-2. 845702	-0. 856109
13	1	0	-2. 932611	-2. 741853	0. 524991
14	1	0	-3. 569638	-2. 772557	-1. 116108
15	6	0	-2. 685037	-0. 495935	-2. 103853
16	1	0	-3. 568245	-0. 908699	-2. 603597
17	1	0	-2. 676534	0. 583099	-2. 269302
18	1	0	-1. 802796	-0. 931708	-2. 588290
19	6	0	-1. 931869	-0. 628433	2. 587453
20	1	0	-2. 742841	-1. 359843	2. 522566
21	1	0	-1. 418344	-0. 792538	3. 542360
22	1	0	-2. 370013	0. 373630	2. 604011
23	6	0	-0. 312243	-2. 210599	1. 459440
24	1	0	0. 360809	-2. 382480	0. 615511
25	1	0	0. 272633	-2. 322571	2. 380043
26	1	0	-1. 067479	-2. 998319	1. 462998
27	7	0	0. 245969	1. 211840	-0. 311386
28	6	0	0. 789907	0. 075530	-0. 840587
29	6	0	1. 114998	2. 349880	0. 017266
30	6	0	2. 174662	-0. 232787	-0. 579680
31	1	0	0. 276586	-0. 407730	-1. 658078
32	6	0	2. 276812	1. 838146	0. 875380
33	1	0	0. 502675	3. 088236	0. 535847
34	1	0	1. 481200	2. 801828	-0. 912667
35	6	0	2. 789813	-1. 354128	-1. 176694
36	6	0	2. 937246	0. 613533	0. 268056
37	1	0	1. 907599	1. 596282	1. 882389
38	1	0	3. 011812	2. 640942	0. 997954
39	6	0	4. 122584	-1. 653468	-0. 918022
40	1	0	2. 205187	-1. 989631	-1. 837040
41	6	0	4. 276085	0. 302236	0. 507110
42	6	0	4. 869463	-0. 825331	-0. 070520
43	1	0	4. 583244	-2. 523382	-1. 376209
44	1	0	4. 867834	0. 953739	1. 145818
45	1	0	5. 912857	-1. 049610	0. 129814

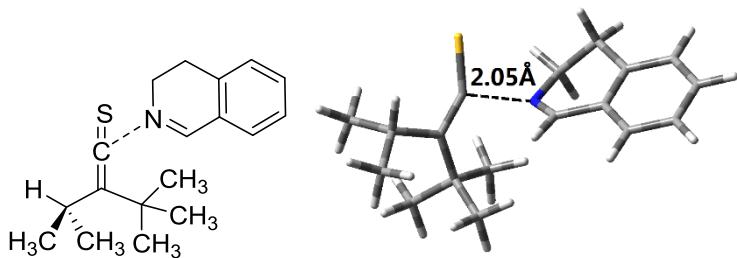
7d



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.158871	1.272341	-0.037646
2	16	0	-2.179014	2.433701	0.555807
3	6	0	-1.019028	-0.283409	0.010021
4	6	0	-0.646741	-0.739255	1.471497
5	1	0	0.274289	-0.180247	1.684646
6	6	0	-2.145003	-1.048154	-0.796958
7	6	0	-3.418131	-1.243014	0.054557
8	1	0	-4.219894	-1.641710	-0.577720
9	1	0	-3.262824	-1.954279	0.869360
10	1	0	-3.763148	-0.296498	0.479789
11	6	0	-1.664077	-2.432077	-1.296087
12	1	0	-0.779228	-2.353024	-1.937265
13	1	0	-1.434557	-3.122795	-0.484567
14	1	0	-2.456352	-2.889379	-1.899434
15	6	0	-2.559021	-0.234506	-2.050945
16	1	0	-3.298871	-0.806068	-2.621433
17	1	0	-3.012108	0.722817	-1.781630
18	1	0	-1.718669	-0.035365	-2.724144
19	6	0	-1.630501	-0.350797	2.596859
20	1	0	-2.515573	-0.991178	2.615786
21	1	0	-1.119725	-0.478779	3.558542
22	1	0	-1.963252	0.684860	2.525546
23	6	0	-0.288330	-2.228822	1.638081
24	1	0	0.413674	-2.592611	0.886763
25	1	0	0.179888	-2.369757	2.618706
26	1	0	-1.180098	-2.862408	1.615079
27	7	0	-0.048167	1.412125	-0.791868
28	6	0	0.304276	-0.003666	-0.880306
29	6	0	0.902167	2.501573	-0.882716
30	6	0	1.730472	-0.266743	-0.445701
31	1	0	0.180376	-0.379751	-1.902084
32	6	0	2.017510	2.213139	0.136981
33	1	0	0.375469	3.432621	-0.662659

34	1	0	1.301478	2.551467	-1.902333
35	6	0	2.294491	-1.540598	-0.615704
36	6	0	2.544134	0.790476	0.019245
37	1	0	1.609841	2.382897	1.142558
38	1	0	2.841155	2.923821	0.005675
39	6	0	3.619542	-1.798305	-0.271370
40	1	0	1.684233	-2.339258	-1.029139
41	6	0	3.880029	0.517985	0.352286
42	6	0	4.415950	-0.762550	0.226116
43	1	0	4.030639	-2.795241	-0.399929
44	1	0	4.509094	1.330911	0.707342
45	1	0	5.452338	-0.946833	0.493464

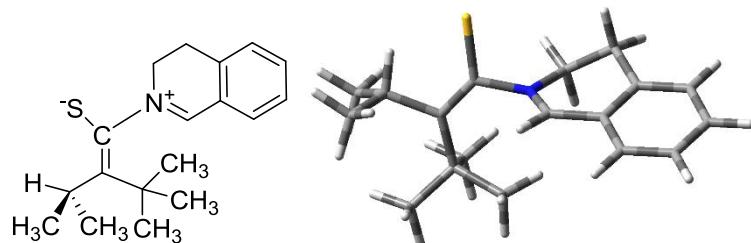
endo-1d-TS3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.264876	-0.999485	-0.149191
2	16	0	-0.913285	-2.534841	-0.596044
3	6	0	-2.198794	-0.037162	-0.091067
4	6	0	-3.333558	-0.343358	-1.123820
5	1	0	-2.884982	-1.060709	-1.815449
6	6	0	-2.275340	1.164901	0.890058
7	6	0	-1.480590	0.926074	2.197947
8	1	0	-1.765830	1.684389	2.936271
9	1	0	-1.703573	-0.058647	2.621108
10	1	0	-0.404378	1.003678	2.053019
11	6	0	-3.738306	1.399218	1.351573
12	1	0	-4.420430	1.624031	0.531451
13	1	0	-4.125296	0.529867	1.891665
14	1	0	-3.760435	2.253707	2.037323
15	6	0	-1.760797	2.476818	0.244052
16	1	0	-1.849743	3.307403	0.955675
17	1	0	-0.706861	2.392190	-0.034174
18	1	0	-2.327547	2.743573	-0.651221

19	6	0	-4.561371	-1.071568	-0.536396
20	1	0	-5.190610	-0.425949	0.080648
21	1	0	-5.184972	-1.453234	-1.354302
22	1	0	-4.245468	-1.927537	0.067945
23	6	0	-3.742619	0.851655	-2.010062
24	1	0	-2.871479	1.298729	-2.500193
25	1	0	-4.417860	0.494710	-2.796808
26	1	0	-4.269673	1.641383	-1.467868
27	7	0	0.572720	-0.343650	0.466478
28	6	0	1.230904	0.364256	-0.375962
29	6	0	1.306272	-1.131109	1.465531
30	6	0	2.693006	0.457245	-0.415189
31	1	0	0.651353	0.929587	-1.106825
32	6	0	2.678937	-1.612164	0.981403
33	1	0	0.676208	-1.984611	1.728541
34	1	0	1.408385	-0.498080	2.357938
35	6	0	3.336532	1.470834	-1.139632
36	6	0	3.443921	-0.502235	0.295452
37	1	0	2.536030	-2.437385	0.270680
38	1	0	3.247669	-2.013225	1.827189
39	6	0	4.729431	1.547993	-1.146737
40	1	0	2.743668	2.198506	-1.688116
41	6	0	4.835928	-0.418207	0.274834
42	6	0	5.476674	0.603217	-0.437124
43	1	0	5.229311	2.335732	-1.701812
44	1	0	5.426466	-1.154527	0.814092
45	1	0	6.561446	0.657889	-0.439449

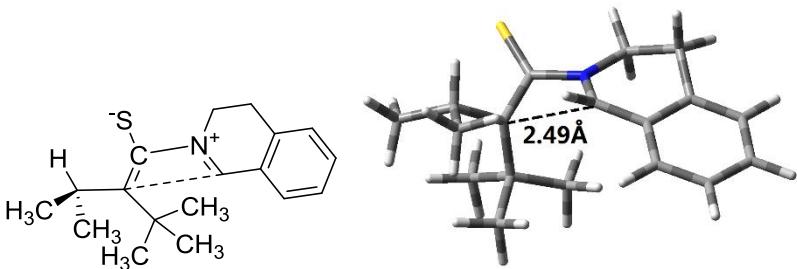
F-1d



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.994315	-0.867264	-0.143806
2	16	0	-0.908487	-2.577257	-0.483060
3	6	0	-2.048920	0.003117	-0.071022
4	6	0	-3.392357	-0.670870	-0.425815

5	1	0	-3.152344	-1.737631	-0.426210
6	6	0	-2.012696	1.483139	0.412916
7	6	0	-2.330962	1.537614	1.934270
8	1	0	-2.302940	2.575804	2.288833
9	1	0	-3.317287	1.133688	2.165782
10	1	0	-1.594060	0.964830	2.507495
11	6	0	-3.053330	2.351947	-0.340507
12	1	0	-2.815549	2.412856	-1.407455
13	1	0	-4.073004	1.982492	-0.242747
14	1	0	-3.034493	3.370512	0.063949
15	6	0	-0.672907	2.238207	0.220805
16	1	0	-0.827211	3.288767	0.490580
17	1	0	0.133525	1.871454	0.857436
18	1	0	-0.337471	2.216718	-0.820559
19	6	0	-4.547966	-0.540107	0.587846
20	1	0	-4.962385	0.468661	0.677847
21	1	0	-5.367978	-1.193709	0.267746
22	1	0	-4.240077	-0.872207	1.584784
23	6	0	-3.863420	-0.380440	-1.869559
24	1	0	-3.044709	-0.542433	-2.578302
25	1	0	-4.672452	-1.071356	-2.136371
26	1	0	-4.242115	0.635959	-2.008426
27	7	0	0.396818	-0.470155	0.152069
28	6	0	1.193518	-0.010527	-0.769632
29	6	0	0.928653	-0.751706	1.510217
30	6	0	2.612683	0.178450	-0.559573
31	1	0	0.745544	0.200194	-1.735186
32	6	0	2.359248	-1.282875	1.455406
33	1	0	0.251332	-1.470286	1.967963
34	1	0	0.884822	0.193807	2.067121
35	6	0	3.379820	0.920335	-1.475596
36	6	0	3.227328	-0.422563	0.564011
37	1	0	2.342472	-2.308913	1.066986
38	1	0	2.764144	-1.324951	2.471823
39	6	0	4.746835	1.088486	-1.265929
40	1	0	2.898189	1.366760	-2.341342
41	6	0	4.596095	-0.250480	0.755313
42	6	0	5.353659	0.505191	-0.149021
43	1	0	5.337410	1.667424	-1.968867
44	1	0	5.079861	-0.712274	1.612019
45	1	0	6.419049	0.633113	0.017613

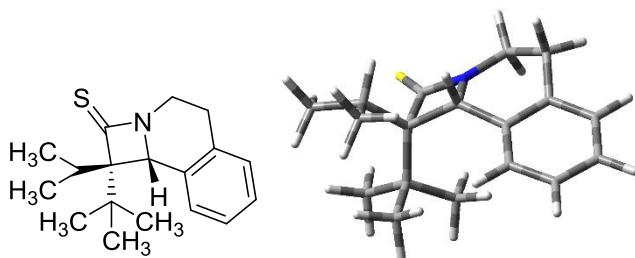
endo-1d-TS4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.111636	1.202547	-0.146443
2	16	0	2.065206	2.594847	-0.181828
3	6	0	1.629659	-0.167090	-0.129359
4	6	0	2.663615	-0.477503	-1.225883
5	1	0	2.634707	0.403321	-1.875599
6	6	0	1.557740	-0.949207	1.206917
7	6	0	2.770905	-0.490561	2.083487
8	1	0	2.677147	-0.940042	3.078776
9	1	0	3.728134	-0.802617	1.668324
10	1	0	2.786013	0.597233	2.196206
11	6	0	1.643579	-2.478127	1.014688
12	1	0	0.804257	-2.852478	0.419713
13	1	0	2.573849	-2.785671	0.532274
14	1	0	1.607461	-2.969549	1.993425
15	6	0	0.302046	-0.653755	2.055388
16	1	0	0.393540	-1.180647	3.010847
17	1	0	0.201249	0.410995	2.283506
18	1	0	-0.614065	-0.998663	1.573637
19	6	0	4.148546	-0.631457	-0.827208
20	1	0	4.341408	-1.544070	-0.254521
21	1	0	4.751489	-0.687349	-1.741071
22	1	0	4.492263	0.230525	-0.250982
23	6	0	2.241089	-1.676919	-2.115126
24	1	0	1.219637	-1.573337	-2.493274
25	1	0	2.907593	-1.722944	-2.983658
26	1	0	2.310268	-2.634820	-1.595360
27	7	0	-0.258645	1.191658	-0.199685
28	6	0	-0.763250	0.049791	-0.773037
29	6	0	-1.110805	2.264450	0.327756
30	6	0	-2.132846	-0.339995	-0.490218
31	1	0	-0.274195	-0.329102	-1.655552
32	6	0	-2.560448	2.099724	-0.138730
33	1	0	-0.679193	3.214159	-0.005378

34	1	0	-1.042097	2.238386	1.422667
35	6	0	-2.590790	-1.660678	-0.657741
36	6	0	-3.040721	0.666744	-0.076730
37	1	0	-2.634399	2.441984	-1.181099
38	1	0	-3.203733	2.757815	0.453634
39	6	0	-3.911970	-1.990506	-0.363911
40	1	0	-1.897000	-2.427701	-0.991321
41	6	0	-4.359212	0.317823	0.219190
42	6	0	-4.796011	-1.004866	0.090570
43	1	0	-4.251660	-3.015423	-0.479934
44	1	0	-5.058283	1.090125	0.531257
45	1	0	-5.823746	-1.261792	0.328877

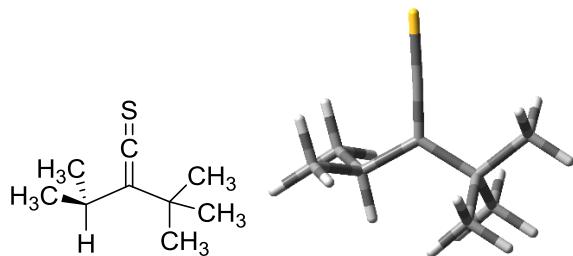
8d



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.207980	1.307598	-0.072838
2	16	0	-2.315536	2.420080	-0.606419
3	6	0	-1.142554	-0.228101	0.225338
4	6	0	-1.994107	-0.572672	1.501155
5	1	0	-1.778236	0.270019	2.174197
6	6	0	-1.317928	-1.084263	-1.099197
7	6	0	-2.719964	-0.884514	-1.735673
8	1	0	-2.737017	-1.415291	-2.694448
9	1	0	-3.522821	-1.297391	-1.125332
10	1	0	-2.941226	0.166745	-1.925660
11	6	0	-1.162774	-2.603713	-0.862611
12	1	0	-0.252383	-2.871778	-0.325576
13	1	0	-2.011831	-3.013578	-0.309822
14	1	0	-1.133861	-3.114270	-1.831868
15	6	0	-0.298461	-0.633730	-2.175565
16	1	0	-0.484171	-1.193264	-3.098595
17	1	0	-0.412475	0.428695	-2.412779
18	1	0	0.737222	-0.814192	-1.887201

19	6	0	-3.524612	-0.575504	1.342727
20	1	0	-3.889184	-1.496265	0.878020
21	1	0	-3.982726	-0.515475	2.336832
22	1	0	-3.876173	0.277565	0.757967
23	6	0	-1.542834	-1.838900	2.259461
24	1	0	-0.454643	-1.903883	2.366162
25	1	0	-1.969239	-1.825659	3.268830
26	1	0	-1.886179	-2.756675	1.777010
27	7	0	0.062061	1.504623	0.299966
28	6	0	0.361033	0.141183	0.748889
29	6	0	0.973102	2.618610	0.144310
30	6	0	1.755653	-0.289627	0.336564
31	1	0	0.335666	0.102553	1.848280
32	6	0	2.355181	2.166429	0.637462
33	1	0	0.612709	3.490935	0.702256
34	1	0	1.000473	2.897716	-0.916717
35	6	0	2.172127	-1.616409	0.178806
36	6	0	2.716979	0.744662	0.244637
37	1	0	2.371687	2.231340	1.735215
38	1	0	3.115636	2.865704	0.277655
39	6	0	3.494911	-1.923734	-0.145022
40	1	0	1.460299	-2.422712	0.303534
41	6	0	4.036596	0.424590	-0.099182
42	6	0	4.428626	-0.898612	-0.305803
43	1	0	3.789971	-2.960751	-0.275328
44	1	0	4.768759	1.223713	-0.186790
45	1	0	5.455932	-1.127188	-0.573646

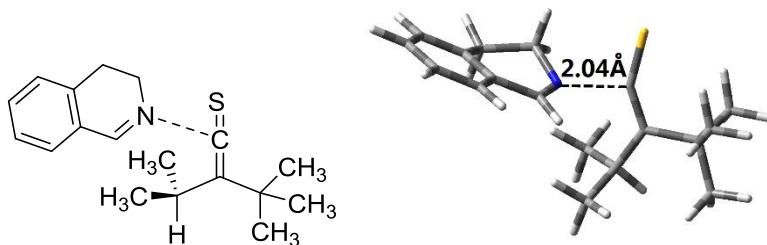
1d'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.955989	0.805294	-0.000078
2	16	0	2.138582	1.847507	-0.000058
3	6	0	0.002415	-0.097392	-0.000032

4	6	0	0.401524	-1.589984	0.000039
5	1	0	-0.536896	-2.155128	0.000190
6	6	0	-1.492059	0.309831	0.000027
7	6	0	-2.176950	-0.257106	1.265061
8	1	0	-3.241663	0.004450	1.262480
9	1	0	-2.107085	-1.348132	1.319527
10	1	0	-1.727057	0.158805	2.172459
11	6	0	-2.177184	-0.257355	-1.264772
12	1	0	-1.727379	0.158290	-2.172338
13	1	0	-2.107493	-1.348403	-1.319004
14	1	0	-3.241864	0.004343	-1.262107
15	6	0	-1.650785	1.842049	-0.000147
16	1	0	-2.713885	2.106502	-0.000115
17	1	0	-1.192987	2.292784	0.886342
18	1	0	-1.193086	2.292548	-0.886805
19	6	0	1.177366	-1.980782	-1.270340
20	1	0	2.136185	-1.453371	-1.321559
21	1	0	1.383858	-3.057355	-1.278096
22	1	0	0.611552	-1.734684	-2.174233
23	6	0	1.177652	-1.980576	1.270321
24	1	0	0.612033	-1.734361	2.174304
25	1	0	1.384171	-3.057145	1.278189
26	1	0	2.136468	-1.453129	1.321226

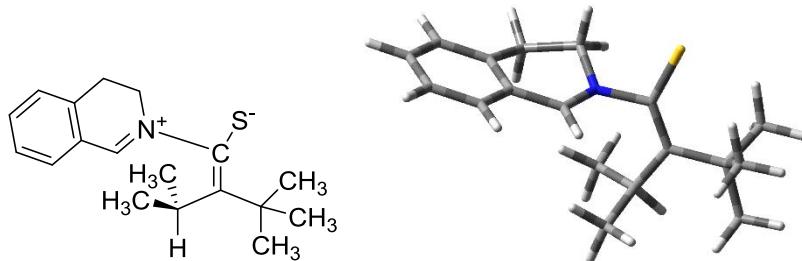
exo-1d'-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.329456	-0.667512	-0.481738
2	16	0	-1.084514	-2.176144	-1.066928
3	6	0	-2.188413	0.231055	0.021221
4	6	0	-2.010836	1.756858	0.067056
5	1	0	-3.028159	2.149004	0.112707
6	6	0	-3.585638	-0.364299	0.470791
7	6	0	-4.384307	-0.823445	-0.771237

8	1	0	-5.358173	-1.229391	-0.469864
9	1	0	-4.567085	0.019781	-1.447663
10	1	0	-3.849074	-1.596658	-1.327721
11	6	0	-4.457230	0.668591	1.226233
12	1	0	-3.939260	1.105336	2.086243
13	1	0	-4.812826	1.481215	0.585234
14	1	0	-5.346526	0.154761	1.606942
15	6	0	-3.388656	-1.550345	1.443305
16	1	0	-4.362198	-1.971154	1.721536
17	1	0	-2.790105	-2.350147	1.004527
18	1	0	-2.892024	-1.216156	2.361786
19	6	0	-1.307887	2.292658	1.334440
20	1	0	-0.235369	2.082252	1.318746
21	1	0	-1.428190	3.381156	1.401644
22	1	0	-1.726339	1.853053	2.245084
23	6	0	-1.410466	2.397863	-1.199742
24	1	0	-1.871248	1.989963	-2.105020
25	1	0	-1.591759	3.479719	-1.184785
26	1	0	-0.331160	2.250654	-1.267742
27	7	0	0.545421	0.128138	-0.529571
28	6	0	1.229143	-0.005454	0.549164
29	6	0	1.259252	0.095267	-1.817988
30	6	0	2.689276	-0.097100	0.603516
31	1	0	0.668825	-0.091038	1.480615
32	6	0	2.644109	0.746511	-1.741539
33	1	0	0.633795	0.594106	-2.562011
34	1	0	1.338990	-0.956840	-2.114379
35	6	0	3.347519	-0.507458	1.772379
36	6	0	3.425058	0.238783	-0.551521
37	1	0	2.531471	1.837381	-1.652147
38	1	0	3.187497	0.562176	-2.674309
39	6	0	4.738528	-0.603220	1.792068
40	1	0	2.766137	-0.761728	2.654910
41	6	0	4.816227	0.143320	-0.518293
42	6	0	5.470222	-0.279045	0.644986
43	1	0	5.250045	-0.929482	2.692246
44	1	0	5.394595	0.398971	-1.402463
45	1	0	6.553739	-0.353762	0.655133

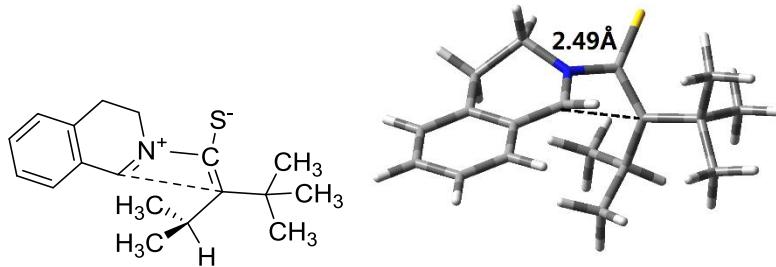
E-1d'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.096901	-0.754470	0.000814
2	16	0	-1.225395	-2.445250	0.381333
3	6	0	-1.982578	0.283322	-0.090374
4	6	0	-1.620595	1.699157	-0.583541
5	1	0	-2.564661	2.123008	-0.925792
6	6	0	-3.483467	0.034996	0.287103
7	6	0	-4.111750	-0.999651	-0.680512
8	1	0	-5.158414	-1.182009	-0.406277
9	1	0	-4.096950	-0.618736	-1.709103
10	1	0	-3.576861	-1.950361	-0.654920
11	6	0	-4.369929	1.302660	0.200527
12	1	0	-4.005058	2.124726	0.825782
13	1	0	-4.490686	1.671492	-0.823987
14	1	0	-5.371072	1.043975	0.561490
15	6	0	-3.593275	-0.459963	1.752173
16	1	0	-4.640903	-0.673612	1.997064
17	1	0	-3.010948	-1.367123	1.916843
18	1	0	-3.239168	0.312504	2.446180
19	6	0	-1.129487	2.649665	0.534114
20	1	0	-0.105262	2.413353	0.842888
21	1	0	-1.131191	3.689111	0.182651
22	1	0	-1.766332	2.592596	1.421791
23	6	0	-0.702878	1.813677	-1.818669
24	1	0	-0.987755	1.096325	-2.595153
25	1	0	-0.793643	2.819553	-2.245990
26	1	0	0.353268	1.669742	-1.581237
27	7	0	0.344204	-0.493828	-0.261322
28	6	0	1.101527	0.005383	0.673734
29	6	0	0.986267	-1.154824	-1.439464
30	6	0	2.543261	0.079713	0.581321
31	1	0	0.597160	0.331181	1.577211
32	6	0	2.283243	-0.454652	-1.846620
33	1	0	0.249508	-1.151600	-2.242899

34	1	0	1. 169676	-2. 192133	-1. 154508
35	6	0	3. 310165	0. 418998	1. 711546
36	6	0	3. 172577	-0. 182223	-0. 656461
37	1	0	2. 063282	0. 494704	-2. 352469
38	1	0	2. 799033	-1. 085277	-2. 578029
39	6	0	4. 697635	0. 480390	1. 618390
40	1	0	2. 812793	0. 618432	2. 656808
41	6	0	4. 562689	-0. 116441	-0. 733462
42	6	0	5. 322881	0. 209597	0. 395698
43	1	0	5. 291182	0. 733010	2. 491205
44	1	0	5. 058295	-0. 317679	-1. 679570
45	1	0	6. 405283	0. 253608	0. 320031

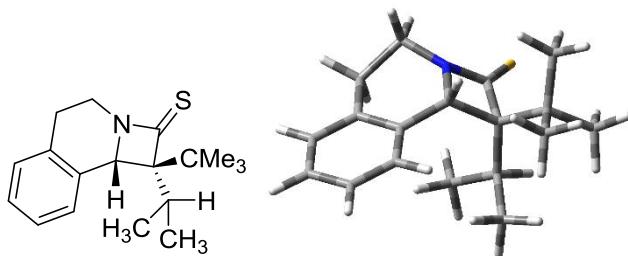
exo-1d'-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1. 199580	1. 057355	-0. 215061
2	16	0	-2. 194384	2. 402426	-0. 471721
3	6	0	-1. 586923	-0. 292960	0. 187045
4	6	0	-1. 219226	-0. 775586	1. 614141
5	1	0	-2. 175071	-1. 151579	2. 004977
6	6	0	-2. 811978	-0. 966078	-0. 464358
7	6	0	-4. 132011	-0. 485345	0. 205813
8	1	0	-4. 980936	-0. 998605	-0. 262022
9	1	0	-4. 152602	-0. 719439	1. 275602
10	1	0	-4. 256434	0. 592074	0. 084643
11	6	0	-2. 740333	-2. 507493	-0. 318555
12	1	0	-1. 840858	-2. 916275	-0. 791341
13	1	0	-2. 763804	-2. 840035	0. 722713
14	1	0	-3. 607994	-2. 949429	-0. 819631
15	6	0	-2. 883452	-0. 660497	-1. 978752
16	1	0	-3. 737376	-1. 186920	-2. 419131
17	1	0	-3. 002243	0. 405738	-2. 176437
18	1	0	-1. 982051	-1. 010417	-2. 496394

19	6	0	-0.223143	-1.949578	1.731813
20	1	0	0.797080	-1.605903	1.541600
21	1	0	-0.255914	-2.364920	2.746590
22	1	0	-0.439537	-2.758099	1.031618
23	6	0	-0.798786	0.352465	2.574448
24	1	0	-1.503833	1.187964	2.553066
25	1	0	-0.755464	-0.036166	3.597972
26	1	0	0.195068	0.739800	2.332289
27	7	0	0.164502	1.093312	-0.373185
28	6	0	0.704735	-0.106811	-0.761018
29	6	0	1.023595	2.283439	-0.290699
30	6	0	2.112211	-0.348919	-0.548114
31	1	0	0.180101	-0.686564	-1.505216
32	6	0	2.270077	1.937426	0.530113
33	1	0	0.433493	3.081101	0.161793
34	1	0	1.293974	2.595663	-1.307091
35	6	0	2.714928	-1.541441	-1.004094
36	6	0	2.913749	0.638416	0.083055
37	1	0	1.998860	1.866264	1.592608
38	1	0	2.987847	2.760724	0.447941
39	6	0	4.071525	-1.771918	-0.807731
40	1	0	2.101075	-2.286951	-1.503083
41	6	0	4.275918	0.393171	0.261386
42	6	0	4.857135	-0.804044	-0.168357
43	1	0	4.520934	-2.697498	-1.154652
44	1	0	4.894737	1.152676	0.733524
45	1	0	5.918928	-0.974819	-0.018570

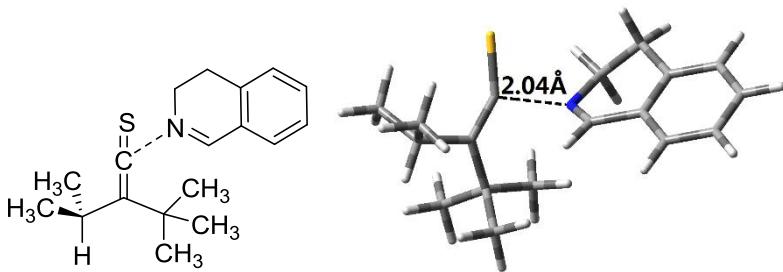
7d'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.233125	1.252733	0.040879
2	16	0	-2.238951	2.384993	0.704858
3	6	0	-1.100066	-0.298684	0.091114

4	6	0	-0. 910338	-0. 743127	1. 582822
5	1	0	-1. 879138	-0. 512571	2. 041425
6	6	0	-2. 251810	-1. 043827	-0. 710719
7	6	0	-3. 509407	-1. 224141	0. 169302
8	1	0	-4. 323392	-1. 632904	-0. 439942
9	1	0	-3. 347186	-1. 916226	0. 999909
10	1	0	-3. 844365	-0. 266438	0. 578825
11	6	0	-1. 790265	-2. 424023	-1. 239299
12	1	0	-0. 957680	-2. 332231	-1. 945524
13	1	0	-1. 485539	-3. 111501	-0. 450153
14	1	0	-2. 617518	-2. 895344	-1. 781975
15	6	0	-2. 685440	-0. 215983	-1. 948476
16	1	0	-3. 434705	-0. 780790	-2. 513478
17	1	0	-3. 133001	0. 738725	-1. 661724
18	1	0	-1. 8555864	-0. 010710	-2. 633227
19	6	0	-0. 622969	-2. 237379	1. 829560
20	1	0	0. 280395	-2. 571925	1. 311023
21	1	0	-0. 455957	-2. 393021	2. 901207
22	1	0	-1. 448205	-2. 889492	1. 539214
23	6	0	0. 129662	0. 079846	2. 374983
24	1	0	-0. 009414	1. 156752	2. 258662
25	1	0	0. 014244	-0. 144072	3. 440853
26	1	0	1. 154696	-0. 178117	2. 097547
27	7	0	-0. 140409	1. 379612	-0. 737614
28	6	0	0. 200650	-0. 040308	-0. 818754
29	6	0	0. 787577	2. 464229	-0. 971790
30	6	0	1. 646653	-0. 312689	-0. 465265
31	1	0	0. 035701	-0. 422415	-1. 833297
32	6	0	2. 040374	2. 200042	-0. 116968
33	1	0	0. 296484	3. 400525	-0. 697117
34	1	0	1. 040894	2. 499674	-2. 038563
35	6	0	2. 154663	-1. 618086	-0. 538329
36	6	0	2. 524645	0. 759257	-0. 194174
37	1	0	1. 800484	2. 444823	0. 926052
38	1	0	2. 846096	2. 877288	-0. 421888
39	6	0	3. 500891	-1. 883551	-0. 295340
40	1	0	1. 483579	-2. 434787	-0. 790847
41	6	0	3. 880288	0. 477027	0. 033570
42	6	0	4. 369754	-0. 827997	-0. 003023
43	1	0	3. 871363	-2. 903291	-0. 343947
44	1	0	4. 560688	1. 299623	0. 241340
45	1	0	5. 422999	-1. 018777	0. 180627

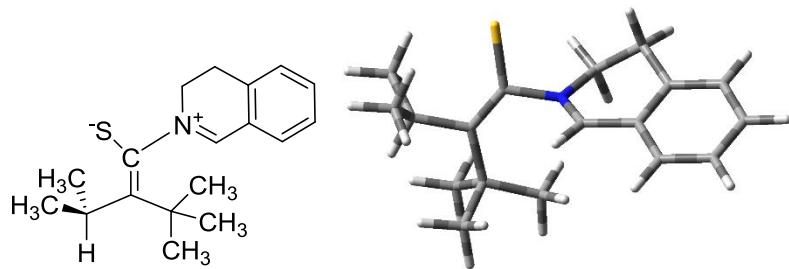
endo-1d'-TS3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.355142	-0.890095	-0.110000
2	16	0	1.092043	-2.501192	0.010555
3	6	0	2.219463	0.119783	0.047269
4	6	0	3.405333	-0.207217	1.007019
5	1	0	3.939585	0.738864	1.143100
6	6	0	2.270120	1.509701	-0.638329
7	6	0	1.264488	1.708860	-1.793333
8	1	0	1.537909	2.612983	-2.349580
9	1	0	1.288306	0.867024	-2.492542
10	1	0	0.240123	1.840348	-1.446625
11	6	0	3.674052	1.693398	-1.283416
12	1	0	4.492336	1.633451	-0.562310
13	1	0	3.847213	0.938214	-2.057174
14	1	0	3.729937	2.680355	-1.756687
15	6	0	2.052364	2.637224	0.400671
16	1	0	2.165451	3.620883	-0.071184
17	1	0	1.046546	2.584837	0.830673
18	1	0	2.772672	2.580356	1.222930
19	6	0	2.941973	-0.633414	2.411366
20	1	0	2.393883	-1.579628	2.385177
21	1	0	3.809162	-0.764310	3.069568
22	1	0	2.290481	0.125709	2.858356
23	6	0	4.414007	-1.216440	0.427280
24	1	0	4.806798	-0.883217	-0.538071
25	1	0	5.260935	-1.341249	1.113002
26	1	0	3.947360	-2.194873	0.281620
27	7	0	-0.511095	-0.219029	-0.571490
28	6	0	-1.175663	0.299978	0.393479
29	6	0	-1.230146	-0.820302	-1.698361
30	6	0	-2.638963	0.342391	0.459992
31	1	0	-0.598780	0.740926	1.208064
32	6	0	-2.587617	-1.418671	-1.310350

33	1	0	-0.581548	-1.593247	-2.119266
34	1	0	-1.350372	-0.030125	-2.453005
35	6	0	-3.300959	1.178554	1.370325
36	6	0	-3.372635	-0.482071	-0.418742
37	1	0	-2.417991	-2.361121	-0.772181
38	1	0	-3.154808	-1.664439	-2.214556
39	6	0	-4.695302	1.213774	1.400621
40	1	0	-2.721429	1.802303	2.046316
41	6	0	-4.766021	-0.442123	-0.374245
42	6	0	-5.425522	0.403818	0.525829
43	1	0	-5.209232	1.864750	2.101082
44	1	0	-5.342979	-1.076094	-1.042770
45	1	0	-6.511244	0.426677	0.545178

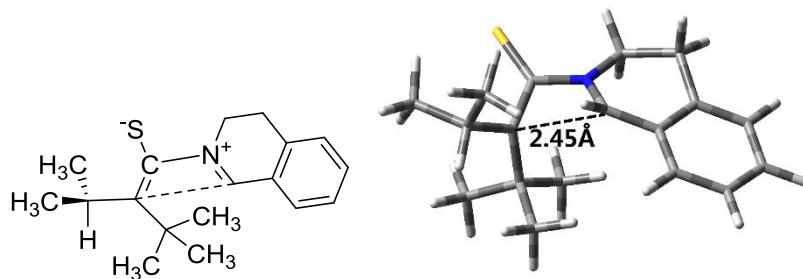
F-1d'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.074061	-0.766323	0.035519
2	16	0	1.055271	-2.467509	0.410456
3	6	0	2.060653	0.175540	0.020851
4	6	0	3.461145	-0.242233	0.524604
5	1	0	4.085668	0.654146	0.482876
6	6	0	1.996726	1.649885	-0.476079
7	6	0	3.068597	1.849250	-1.587575
8	1	0	3.074855	2.896415	-1.911889
9	1	0	4.079978	1.604534	-1.257614
10	1	0	2.840038	1.226545	-2.459234
11	6	0	2.303278	2.614468	0.701063
12	1	0	1.532855	2.538227	1.476776
13	1	0	3.268871	2.411249	1.170975
14	1	0	2.321653	3.651894	0.345618
15	6	0	0.675410	2.138450	-1.110578
16	1	0	0.838375	3.142031	-1.518013
17	1	0	0.356252	1.505588	-1.943303

Center Number	Atomic Number	Atomic Type	X	Y	Z
18	1	0	-0.145882	2.220565	-0.395505
19	6	0	3.473752	-0.670836	2.007023
20	1	0	2.905497	-1.589491	2.165247
21	1	0	4.506801	-0.841402	2.334137
22	1	0	3.045803	0.111757	2.644610
23	6	0	4.164457	-1.280780	-0.374921
24	1	0	4.241071	-0.921419	-1.406942
25	1	0	5.181419	-1.462776	-0.005984
26	1	0	3.624367	-2.229648	-0.382979
27	7	0	-0.337163	-0.428509	-0.271474
28	6	0	-1.091746	0.158780	0.611989
29	6	0	-0.955242	-0.944540	-1.521608
30	6	0	-2.531084	0.254171	0.483726
31	1	0	-0.590499	0.546605	1.493581
32	6	0	-2.342762	-1.526969	-1.264194
33	1	0	-0.273159	-1.691241	-1.922567
34	1	0	-1.020377	-0.092489	-2.209886
35	6	0	-3.268610	1.114724	1.316113
36	6	0	-3.191662	-0.566163	-0.460536
37	1	0	-2.237869	-2.471448	-0.715928
38	1	0	-2.817528	-1.756003	-2.223965
39	6	0	-4.655162	1.182091	1.197020
40	1	0	-2.750316	1.729958	2.046799
41	6	0	-4.579141	-0.494108	-0.559564
42	6	0	-5.309302	0.378437	0.258022
43	1	0	-5.223773	1.852167	1.834005
44	1	0	-5.098441	-1.124686	-1.276440
45	1	0	-6.390065	0.425568	0.163411

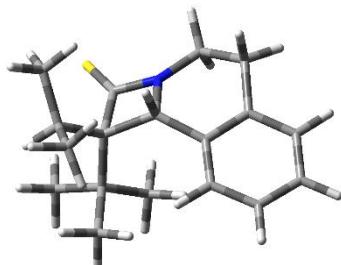
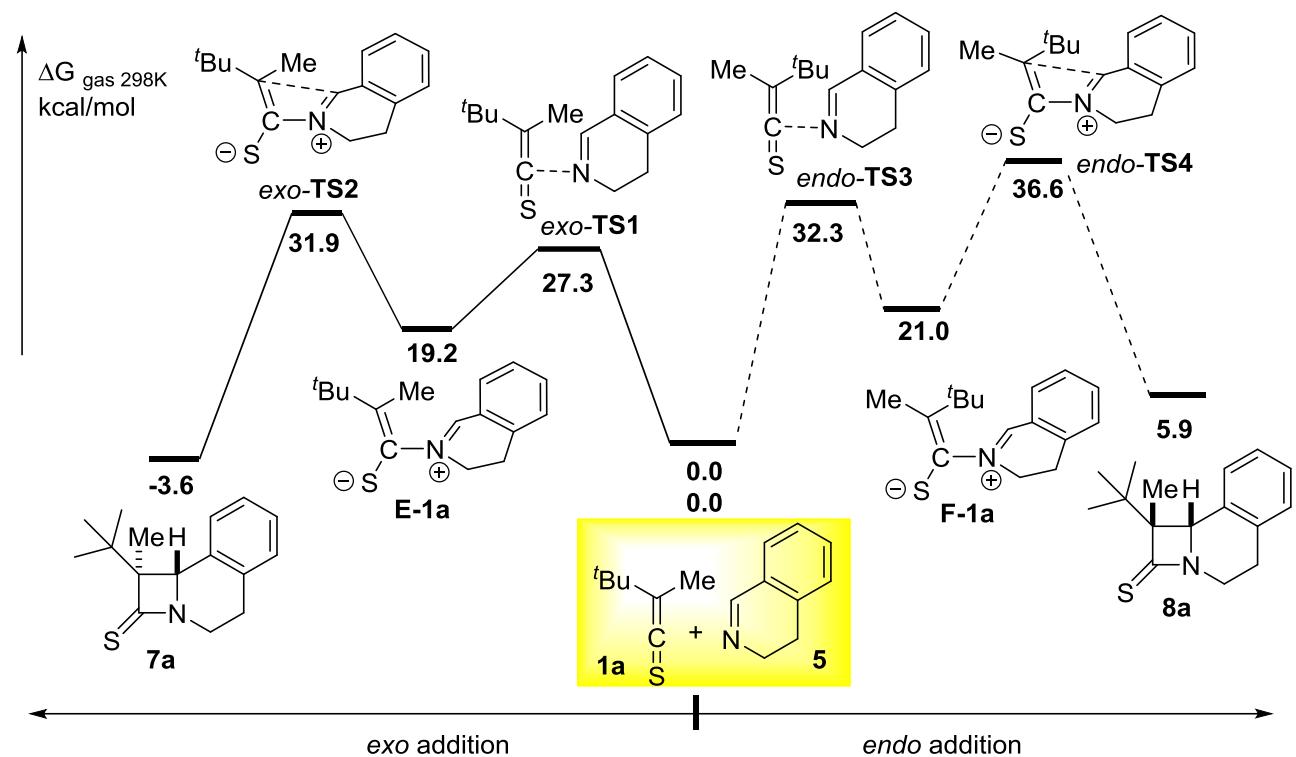
endo-1d'-TS4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.238349	1.044445	-0.039972
2	16	0	-2.271602	2.360683	-0.271072

3	6	0	-1.608546	-0.364154	0.096219
4	6	0	-2.703826	-0.773838	1.084459
5	1	0	-2.796303	-1.862693	1.009290
6	6	0	-1.323342	-1.338787	-1.081449
7	6	0	-2.667425	-1.545414	-1.845456
8	1	0	-2.485248	-2.173219	-2.725163
9	1	0	-3.417860	-2.049640	-1.231567
10	1	0	-3.080313	-0.591464	-2.186911
11	6	0	-0.829479	-2.721149	-0.594866
12	1	0	0.166865	-2.642896	-0.151784
13	1	0	-1.499045	-3.169284	0.144732
14	1	0	-0.769781	-3.413725	-1.442406
15	6	0	-0.313558	-0.802500	-2.116319
16	1	0	-0.262164	-1.502879	-2.956702
17	1	0	-0.623138	0.168471	-2.515181
18	1	0	0.695088	-0.713198	-1.709110
19	6	0	-2.287017	-0.458103	2.538803
20	1	0	-2.100004	0.613186	2.671691
21	1	0	-3.090429	-0.741750	3.227313
22	1	0	-1.389925	-1.010688	2.838614
23	6	0	-4.127775	-0.200401	0.846339
24	1	0	-4.452839	-0.294652	-0.190655
25	1	0	-4.835136	-0.749702	1.480206
26	1	0	-4.165769	0.858413	1.105724
27	7	0	0.125935	1.158888	0.057669
28	6	0	0.693292	0.132065	0.775383
29	6	0	0.908104	2.211896	-0.600038
30	6	0	2.090883	-0.197399	0.552841
31	1	0	0.223210	-0.155414	1.701529
32	6	0	2.365111	2.196205	-0.128471
33	1	0	0.419137	3.167049	-0.382778
34	1	0	0.838636	2.049617	-1.682881
35	6	0	2.640188	-1.442909	0.913157
36	6	0	2.933327	0.800684	0.001141
37	1	0	2.420818	2.679800	0.857542
38	1	0	2.967539	2.805544	-0.809407
39	6	0	3.983188	-1.719864	0.667835
40	1	0	2.001820	-2.198171	1.363229
41	6	0	4.274724	0.504224	-0.244553
42	6	0	4.800494	-0.752855	0.071232
43	1	0	4.391989	-2.690062	0.934007
44	1	0	4.921768	1.271206	-0.663535
45	1	0	5.845206	-0.969876	-0.130046

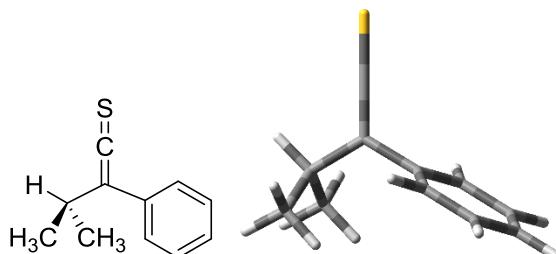
8d'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.371043	1.156250	-0.145093
2	16	0	-2.542314	2.153282	-0.765060
3	6	0	-1.163732	-0.364277	0.189102
4	6	0	-2.043572	-0.926658	1.359855
5	1	0	-2.909576	-1.413022	0.901151
6	6	0	-1.255605	-1.222517	-1.151425
7	6	0	-2.705138	-1.181483	-1.704152
8	1	0	-2.730837	-1.727155	-2.654171
9	1	0	-3.419937	-1.670369	-1.035128
10	1	0	-3.050926	-0.163220	-1.884582
11	6	0	-0.916587	-2.718593	-0.963922
12	1	0	0.094612	-2.890036	-0.594316

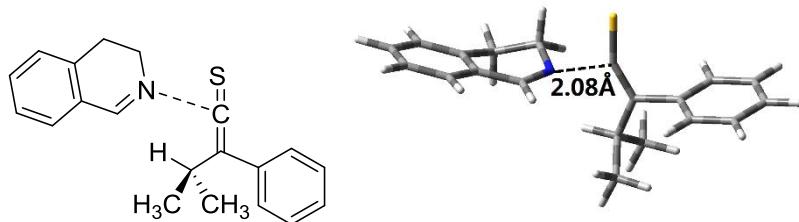
13	1	0	-1.623449	-3.221695	-0.298697
14	1	0	-0.989138	-3.214507	-1.938475
15	6	0	-0.328580	-0.649767	-2.249662
16	1	0	-0.458601	-1.231945	-3.168384
17	1	0	-0.574648	0.389281	-2.486756
18	1	0	0.726857	-0.704468	-1.974644
19	6	0	-1.319398	-1.989258	2.216947
20	1	0	-0.569921	-1.532795	2.873230
21	1	0	-2.045495	-2.490485	2.866518
22	1	0	-0.820988	-2.759212	1.626872
23	6	0	-2.598282	0.161970	2.299037
24	1	0	-3.243946	0.866566	1.771535
25	1	0	-3.182151	-0.305377	3.099777
26	1	0	-1.794265	0.734962	2.778268
27	7	0	-0.128215	1.474005	0.236995
28	6	0	0.273516	0.153736	0.733281
29	6	0	0.700841	2.634228	-0.015628
30	6	0	1.696731	-0.192033	0.346647
31	1	0	0.230502	0.150267	1.831709
32	6	0	2.124327	2.315384	0.461814
33	1	0	0.294766	3.515236	0.494909
34	1	0	0.679017	2.843863	-1.092735
35	6	0	2.207228	-1.494391	0.300265
36	6	0	2.579829	0.897372	0.163451
37	1	0	2.168459	2.462017	1.550830
38	1	0	2.821705	3.037936	0.027542
39	6	0	3.546318	-1.732693	-0.013913
40	1	0	1.558042	-2.333481	0.518997
41	6	0	3.916676	0.644666	-0.170482
42	6	0	4.401058	-0.659951	-0.274487
43	1	0	3.917004	-2.752666	-0.055721
44	1	0	4.589656	1.483817	-0.329463
45	1	0	5.440254	-0.835965	-0.536094

1e



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1. 657235	-0. 903655	-0. 000133
2	16	0	2. 637004	-2. 134680	-0. 000099
3	6	0	0. 845085	0. 129967	0. 000196
4	6	0	1. 412347	1. 562022	0. 000299
5	1	0	2. 504681	1. 465656	0. 000069
6	6	0	1. 004495	2. 329691	-1. 269713
7	1	0	-0. 081714	2. 458376	-1. 323997
8	1	0	1. 460111	3. 326473	-1. 268598
9	1	0	1. 333206	1. 807132	-2. 173698
10	6	0	1. 004988	2. 329269	1. 270728
11	1	0	1. 334124	1. 806447	2. 174405
12	1	0	1. 460524	3. 326087	1. 269737
13	1	0	-0. 081209	2. 457841	1. 325520
14	6	0	-0. 637544	-0. 127572	-0. 000034
15	6	0	-1. 341966	-0. 250607	1. 208211
16	6	0	-1. 341943	-0. 248614	-1. 208494
17	6	0	-2. 721235	-0. 473911	1. 207946
18	1	0	-0. 803391	-0. 177506	2. 148125
19	6	0	-2. 721213	-0. 471903	-1. 208619
20	1	0	-0. 803358	-0. 174003	-2. 148282
21	6	0	-3. 414643	-0. 582772	-0. 000433
22	1	0	-3. 251194	-0. 568575	2. 151466
23	1	0	-3. 251157	-0. 565007	-2. 152303
24	1	0	-4. 486325	-0. 759524	-0. 000590

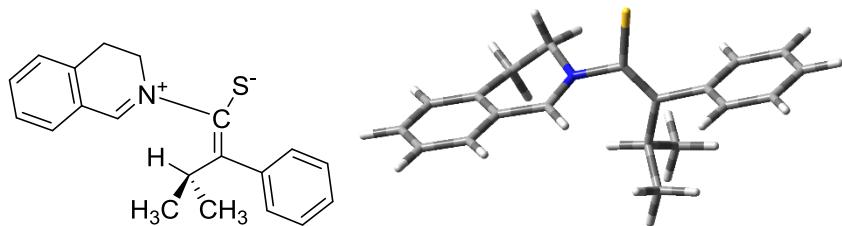
exo-1e-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0. 829388	-0. 650631	-0. 427236
2	16	0	-0. 631025	-2. 149410	-1. 022952
3	6	0	-1. 640497	0. 313646	0. 025854
4	6	0	-1. 280988	1. 736592	0. 445290

5	1	0	-0.210758	1.853454	0.260938
6	6	0	-2.019478	2.794201	-0.399587
7	1	0	-3.103135	2.740963	-0.251861
8	1	0	-1.692186	3.801146	-0.114521
9	1	0	-1.819200	2.662023	-1.468280
10	6	0	-1.523857	1.989388	1.947200
11	1	0	-0.967010	1.277728	2.566292
12	1	0	-1.201147	3.001606	2.218943
13	1	0	-2.585212	1.899864	2.202079
14	7	0	1.095000	0.138054	-0.340440
15	6	0	1.861570	-0.193879	0.632450
16	6	0	1.692611	0.455500	-1.644345
17	6	0	3.324414	-0.236167	0.559998
18	1	0	1.378372	-0.504153	1.560397
19	6	0	3.077903	1.102910	-1.531301
20	1	0	1.000052	1.113964	-2.175952
21	1	0	1.739208	-0.484177	-2.209426
22	6	0	4.082374	-0.868154	1.556397
23	6	0	3.957461	0.365480	-0.547190
24	1	0	2.965681	2.143227	-1.191160
25	1	0	3.546357	1.145429	-2.520233
26	6	0	5.471838	-0.920338	1.448170
27	1	0	3.579219	-1.326882	2.403737
28	6	0	5.347892	0.308638	-0.643203
29	6	0	6.101773	-0.333568	0.346111
30	1	0	6.060212	-1.415927	2.214103
31	1	0	5.847852	0.768054	-1.492122
32	1	0	7.183406	-0.373760	0.256018
33	6	0	-3.091195	-0.099141	0.084246
34	6	0	-3.917875	0.023553	-1.043713
35	6	0	-3.647633	-0.609597	1.267735
36	6	0	-5.265603	-0.338780	-0.987495
37	1	0	-3.494328	0.393322	-1.972814
38	6	0	-4.995917	-0.972122	1.327174
39	1	0	-3.014752	-0.736739	2.141019
40	6	0	-5.810312	-0.835201	0.200131
41	1	0	-5.887599	-0.239457	-1.872905
42	1	0	-5.406626	-1.368784	2.251715
43	1	0	-6.857556	-1.120704	0.244235

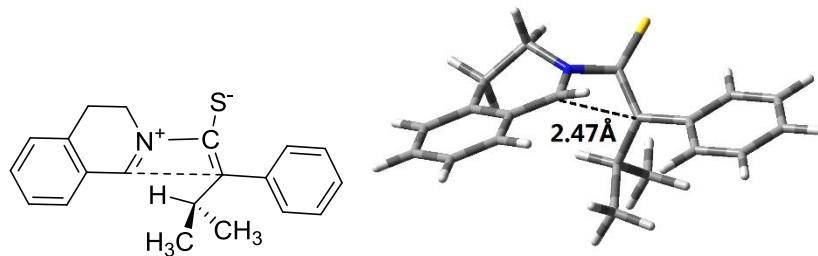
E-1e



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.566495	-0.783630	-0.107741
2	16	0	0.893494	-2.380076	-0.666788
3	6	0	1.378422	0.280366	0.157386
4	6	0	0.922363	1.621616	0.737306
5	1	0	-0.156614	1.564557	0.917779
6	6	0	1.582392	1.920564	2.100774
7	1	0	2.667108	2.027899	2.003144
8	1	0	1.187888	2.855834	2.515666
9	1	0	1.388397	1.119597	2.822285
10	6	0	1.159521	2.801534	-0.229357
11	1	0	0.646635	2.647817	-1.185496
12	1	0	0.787488	3.735264	0.209112
13	1	0	2.225621	2.932107	-0.440334
14	7	0	-0.879135	-0.619594	0.126215
15	6	0	-1.625767	0.048270	-0.709949
16	6	0	-1.530199	-1.442061	1.184973
17	6	0	-3.063147	0.141120	-0.582124
18	1	0	-1.112684	0.528887	-1.536956
19	6	0	-2.754479	-0.717645	1.742501
20	1	0	-0.774058	-1.632828	1.946775
21	1	0	-1.804302	-2.398878	0.734097
22	6	0	-3.846198	0.651981	-1.633850
23	6	0	-3.670032	-0.260529	0.630726
24	1	0	-2.436929	0.155682	2.330648
25	1	0	-3.279440	-1.388123	2.430097
26	6	0	-5.227968	0.742693	-1.491406
27	1	0	-3.366912	0.960775	-2.558815
28	6	0	-5.054182	-0.161071	0.758100
29	6	0	-5.831072	0.333474	-0.296276
30	1	0	-5.834583	1.127158	-2.305118
31	1	0	-5.531881	-0.467290	1.685019
32	1	0	-6.908903	0.401727	-0.183197
33	6	0	2.846192	0.096746	-0.086247
34	6	0	3.681060	-0.442275	0.905945

35	6	0	3.425341	0.468319	-1.309774
36	6	0	5.051824	-0.594063	0.688065
37	1	0	3.246072	-0.762896	1.847913
38	6	0	4.796893	0.319556	-1.531466
39	1	0	2.791755	0.859897	-2.100351
40	6	0	5.616160	-0.209614	-0.531415
41	1	0	5.677231	-1.020149	1.467890
42	1	0	5.222319	0.609031	-2.488598
43	1	0	6.682112	-0.329801	-0.703490

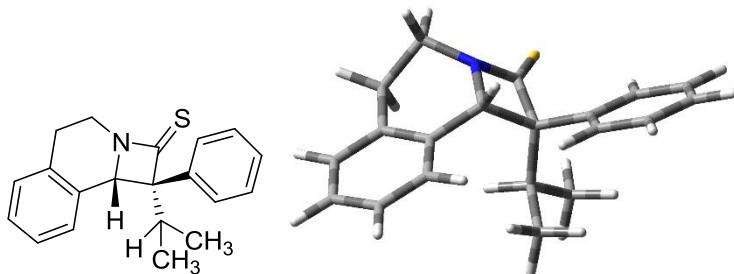
exo-1e-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.595106	1.415397	-0.260868
2	16	0	-1.409355	2.844384	-0.635171
3	6	0	-1.096981	0.176931	0.325652
4	6	0	-0.512662	-0.200983	1.700355
5	1	0	0.480405	0.256651	1.761170
6	6	0	-1.383031	0.470722	2.793631
7	1	0	-2.386675	0.033704	2.819816
8	1	0	-0.922861	0.322923	3.777877
9	1	0	-1.484728	1.546070	2.619245
10	6	0	-0.351393	-1.696855	2.013618
11	1	0	0.274422	-2.201411	1.270838
12	1	0	0.131644	-1.809960	2.990824
13	1	0	-1.315415	-2.211324	2.064337
14	7	0	0.751686	1.226895	-0.520155
15	6	0	1.070711	-0.064192	-0.825103
16	6	0	1.802020	2.253900	-0.507661
17	6	0	2.414903	-0.532953	-0.596111
18	1	0	0.403245	-0.622393	-1.465585
19	6	0	2.960110	1.749737	0.359821
20	1	0	1.356469	3.171403	-0.122107
21	1	0	2.132532	2.439881	-1.536826

22	6	0	2.797333	-1.839421	-0.969140
23	6	0	3.371945	0.334935	-0.006336
24	1	0	2.665439	1.783955	1.418311
25	1	0	3.811256	2.430387	0.250751
26	6	0	4.090768	-2.292679	-0.736074
27	1	0	2.064768	-2.492533	-1.436438
28	6	0	4.667191	-0.135392	0.210581
29	6	0	5.029382	-1.440225	-0.141050
30	1	0	4.372576	-3.302028	-1.019939
31	1	0	5.407375	0.528037	0.651496
32	1	0	6.043224	-1.786030	0.036818
33	6	0	-2.412469	-0.386626	-0.062717
34	6	0	-2.504458	-1.772235	-0.328698
35	6	0	-3.581330	0.387560	-0.225851
36	6	0	-3.701773	-2.354575	-0.742573
37	1	0	-1.618337	-2.391755	-0.247873
38	6	0	-4.781106	-0.203167	-0.628205
39	1	0	-3.539131	1.450771	-0.028374
40	6	0	-4.851174	-1.572770	-0.889990
41	1	0	-3.733245	-3.419457	-0.956151
42	1	0	-5.666279	0.417569	-0.736498
43	1	0	-5.786090	-2.025513	-1.207568

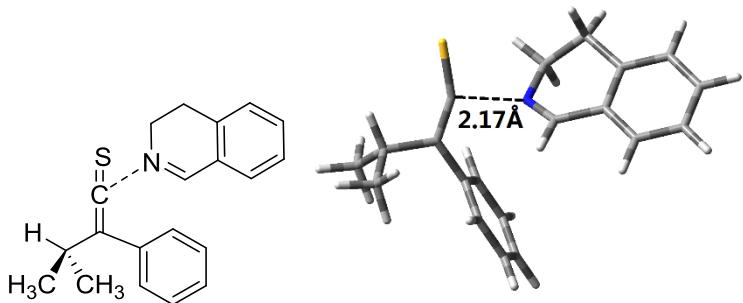
7e



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.440238	1.635744	-0.179889
2	16	0	-1.004932	3.128768	0.253590
3	6	0	-0.670770	0.146210	0.222740
4	6	0	-0.348508	-0.132568	1.731607
5	1	0	0.662434	0.262871	1.900611
6	6	0	-1.303779	0.590612	2.697440
7	1	0	-2.321176	0.193242	2.615648
8	1	0	-0.966752	0.424006	3.726672

9	1	0	-1.340879	1.666178	2.518164
10	6	0	-0.336794	-1.631343	2.077445
11	1	0	0.343157	-2.209689	1.450305
12	1	0	-0.011653	-1.758077	3.115762
13	1	0	-1.338709	-2.062720	1.988482
14	7	0	0.529475	1.309240	-1.062554
15	6	0	0.540029	-0.133992	-0.807632
16	6	0	1.692626	2.072161	-1.471831
17	6	0	1.916250	-0.632758	-0.418185
18	1	0	0.188038	-0.695988	-1.680475
19	6	0	2.810297	1.766413	-0.460213
20	1	0	1.421346	3.129808	-1.475217
21	1	0	1.981536	1.774186	-2.485804
22	6	0	2.164364	-2.011550	-0.331225
23	6	0	2.991294	0.270063	-0.261401
24	1	0	2.547578	2.248667	0.490787
25	1	0	3.754353	2.212432	-0.792379
26	6	0	3.430110	-2.503171	-0.020713
27	1	0	1.352772	-2.710291	-0.517141
28	6	0	4.262970	-0.239757	0.043355
29	6	0	4.485530	-1.608787	0.180240
30	1	0	3.594630	-3.574090	0.052435
31	1	0	5.092167	0.453722	0.161653
32	1	0	5.479241	-1.976988	0.417824
33	6	0	-2.002866	-0.441383	-0.227559
34	6	0	-2.078475	-1.747895	-0.737240
35	6	0	-3.193635	0.294416	-0.116593
36	6	0	-3.299984	-2.304076	-1.123852
37	1	0	-1.177058	-2.346499	-0.831026
38	6	0	-4.416422	-0.259728	-0.504135
39	1	0	-3.159915	1.310281	0.261801
40	6	0	-4.476844	-1.560608	-1.008582
41	1	0	-3.329041	-3.317319	-1.514836
42	1	0	-5.322650	0.332576	-0.414077
43	1	0	-5.427769	-1.989286	-1.311417

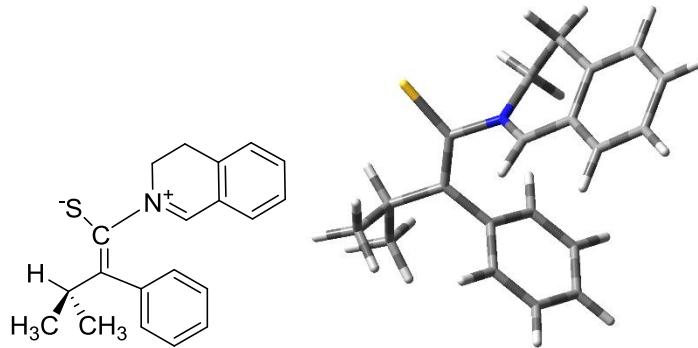
endo-1e-TS3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.349518	-1.591560	-0.099785
2	16	0	-1.015122	-3.172624	-0.149093
3	6	0	-2.196147	-0.563926	-0.204574
4	6	0	-3.637499	-0.936916	-0.631258
5	1	0	-3.649489	-2.024334	-0.751070
6	6	0	-4.652784	-0.576523	0.468995
7	1	0	-4.689710	0.504743	0.640783
8	1	0	-5.657549	-0.905717	0.178962
9	1	0	-4.398095	-1.062599	1.416453
10	6	0	-4.049483	-0.324558	-1.982984
11	1	0	-3.327860	-0.571183	-2.768974
12	1	0	-5.026150	-0.719999	-2.286274
13	1	0	-4.141410	0.764901	-1.924135
14	7	0	0.569157	-0.683848	0.344349
15	6	0	1.218584	-0.024936	-0.540701
16	6	0	1.301981	-1.275603	1.466344
17	6	0	2.673469	0.175618	-0.525340
18	1	0	0.642005	0.433439	-1.345149
19	6	0	2.729215	-1.708159	1.110662
20	1	0	0.722552	-2.133503	1.819054
21	1	0	1.310353	-0.523574	2.268539
22	6	0	3.282202	1.144223	-1.335364
23	6	0	3.451058	-0.633808	0.328230
24	1	0	2.684252	-2.622027	0.501494
25	1	0	3.277913	-1.962950	2.023807
26	6	0	4.665004	1.324906	-1.290267
27	1	0	2.668987	1.757549	-1.990769
28	6	0	4.833195	-0.447753	0.360560
29	6	0	5.438072	0.528693	-0.439879
30	1	0	5.137306	2.078680	-1.912716
31	1	0	5.443764	-1.068280	1.011745
32	1	0	6.514957	0.665076	-0.400351

33	6	0	-1.905031	0.850273	0.173649
34	6	0	-1.735153	1.202974	1.524159
35	6	0	-1.831091	1.872420	-0.788163
36	6	0	-1.484813	2.524203	1.899950
37	1	0	-1.801747	0.426988	2.280864
38	6	0	-1.580806	3.196767	-0.415079
39	1	0	-1.951132	1.627026	-1.838667
40	6	0	-1.405756	3.528579	0.930557
41	1	0	-1.356032	2.770006	2.950653
42	1	0	-1.520839	3.967937	-1.178486
43	1	0	-1.212408	4.557253	1.221011

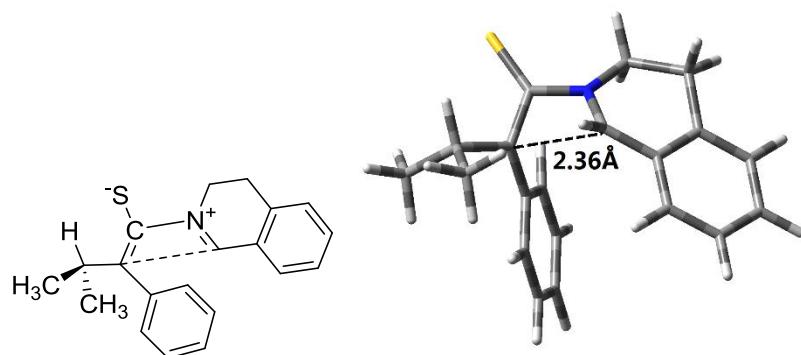
F-1e



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.980947	-1.436519	0.042097
2	16	0	-0.998047	-3.155011	-0.118702
3	6	0	-1.974358	-0.500250	-0.029912
4	6	0	-3.395208	-0.988260	-0.314250
5	1	0	-3.415983	-2.026935	0.037931
6	6	0	-4.473460	-0.205108	0.453080
7	1	0	-4.542411	0.836152	0.118887
8	1	0	-5.453425	-0.670272	0.297766
9	1	0	-4.273045	-0.197593	1.530035
10	6	0	-3.711060	-1.038999	-1.824720
11	1	0	-2.953446	-1.620839	-2.358353
12	1	0	-4.683480	-1.517858	-1.991867
13	1	0	-3.761185	-0.035972	-2.265035
14	7	0	0.403400	-0.960914	0.241742
15	6	0	1.030149	-0.279455	-0.671106
16	6	0	1.118128	-1.335127	1.488834
17	6	0	2.437169	0.052466	-0.578540

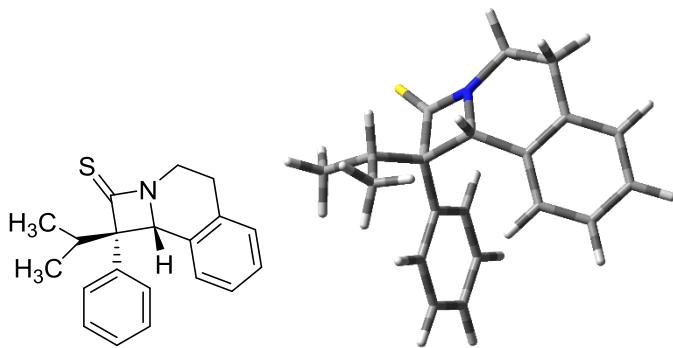
18	1	0	0.449617	0.018732	-1.538255
19	6	0	2.574933	-1.691811	1.208645
20	1	0	0.573015	-2.172858	1.920069
21	1	0	1.048942	-0.462874	2.151803
22	6	0	3.004173	1.003204	-1.445023
23	6	0	3.240880	-0.626099	0.366763
24	1	0	2.612549	-2.653633	0.680308
25	1	0	3.100936	-1.823635	2.159620
26	6	0	4.362693	1.299657	-1.359518
27	1	0	2.374677	1.510626	-2.170806
28	6	0	4.599525	-0.325832	0.431747
29	6	0	5.158261	0.635317	-0.420482
30	1	0	4.800740	2.040630	-2.020562
31	1	0	5.230012	-0.844096	1.149336
32	1	0	6.218023	0.862310	-0.351847
33	6	0	-1.733072	0.954755	0.207330
34	6	0	-1.318328	1.425320	1.467861
35	6	0	-1.947745	1.912089	-0.803867
36	6	0	-1.098750	2.785427	1.702105
37	1	0	-1.191419	0.713161	2.278558
38	6	0	-1.736146	3.273183	-0.571603
39	1	0	-2.272966	1.583007	-1.785972
40	6	0	-1.304830	3.717390	0.681957
41	1	0	-0.780685	3.117396	2.686903
42	1	0	-1.906619	3.987334	-1.372898
43	1	0	-1.140920	4.775710	0.863014

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.279677	-1.506945	0.164179
2	16	0	-2.332847	-2.655654	0.785236

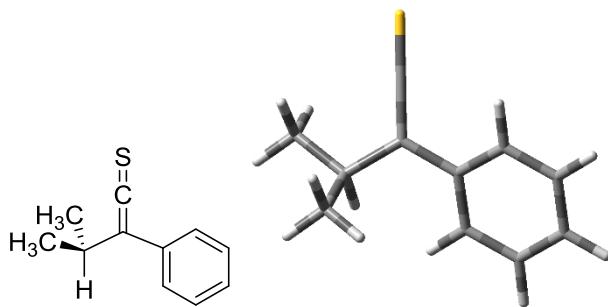
3	6	0	-1.608299	-0.175664	-0.360518
4	6	0	-2.852049	-0.058080	-1.245830
5	1	0	-3.203839	-1.087273	-1.369865
6	6	0	-4.003660	0.727002	-0.585454
7	1	0	-3.754511	1.783727	-0.447128
8	1	0	-4.898441	0.668803	-1.215821
9	1	0	-4.249498	0.301804	0.391836
10	6	0	-2.558400	0.477385	-2.667107
11	1	0	-1.759283	-0.087294	-3.158814
12	1	0	-3.459747	0.376052	-3.281593
13	1	0	-2.280233	1.535158	-2.672703
14	7	0	0.081539	-1.657995	0.037158
15	6	0	0.559736	-0.865452	-0.982013
16	6	0	0.938161	-2.400225	0.966677
17	6	0	1.890992	-0.307774	-0.858374
18	1	0	0.078857	-0.929755	-1.947287
19	6	0	2.405343	-2.333471	0.522282
20	1	0	0.578825	-3.433746	1.012306
21	1	0	0.805371	-1.961995	1.962992
22	6	0	2.289157	0.850954	-1.548570
23	6	0	2.808506	-0.974645	-0.008644
24	1	0	2.564376	-3.070964	-0.277215
25	1	0	3.044806	-2.635410	1.357317
26	6	0	3.566382	1.374556	-1.357347
27	1	0	1.583477	1.351352	-2.205164
28	6	0	4.082706	-0.436477	0.170508
29	6	0	4.459862	0.739201	-0.488278
30	1	0	3.863113	2.280636	-1.876903
31	1	0	4.794578	-0.948793	0.813108
32	1	0	5.453351	1.149625	-0.334038
33	6	0	-1.111197	0.988741	0.407696
34	6	0	-0.767642	0.843001	1.770723
35	6	0	-1.012181	2.285549	-0.147001
36	6	0	-0.317726	1.927171	2.526931
37	1	0	-0.903690	-0.120194	2.251604
38	6	0	-0.573221	3.366808	0.613015
39	1	0	-1.260497	2.447125	-1.189051
40	6	0	-0.216298	3.196467	1.955601
41	1	0	-0.067420	1.778799	3.573880
42	1	0	-0.502932	4.348434	0.152217
43	1	0	0.125134	4.041732	2.545587



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.799300	-1.665300	-0.559795
2	16	0	1.675251	-2.429192	-1.733556
3	6	0	1.019692	-0.494036	0.454399
4	6	0	2.008191	-0.948066	1.580716
5	1	0	1.746098	-2.003470	1.740694
6	6	0	3.479648	-0.923384	1.134892
7	1	0	3.844987	0.099603	1.002060
8	1	0	4.103921	-1.404535	1.896414
9	1	0	3.617331	-1.457511	0.191566
10	6	0	1.836311	-0.263468	2.955261
11	1	0	0.786944	-0.099367	3.222094
12	1	0	2.274325	-0.902104	3.730351
13	1	0	2.351083	0.698778	3.017701
14	7	0	-0.459085	-1.874564	-0.138329
15	6	0	-0.503729	-0.799623	0.865252
16	6	0	-1.589573	-2.570637	-0.722706
17	6	0	-1.688545	0.106215	0.626308
18	1	0	-0.554122	-1.213918	1.882266
19	6	0	-2.868669	-2.028146	-0.058620
20	1	0	-1.498676	-3.653610	-0.577647
21	1	0	-1.587550	-2.381952	-1.803352
22	6	0	-1.706969	1.474673	0.914432
23	6	0	-2.854684	-0.522423	0.135141
24	1	0	-2.980872	-2.508509	0.924162
25	1	0	-3.738106	-2.330269	-0.649936
26	6	0	-2.861779	2.229053	0.693992
27	1	0	-0.815231	1.958968	1.296059
28	6	0	-3.999948	0.248735	-0.093845
29	6	0	-4.007568	1.618223	0.180519
30	1	0	-2.860464	3.292428	0.914376
31	1	0	-4.896389	-0.230294	-0.480269

32	1	0	-4. 904250	2. 203025	-0. 002881
33	6	0	1. 264559	0. 854443	-0. 219175
34	6	0	0. 877700	1. 060307	-1. 554958
35	6	0	1. 826714	1. 946905	0. 462721
36	6	0	1. 041117	2. 298056	-2. 179577
37	1	0	0. 455599	0. 242702	-2. 127606
38	6	0	1. 995943	3. 186728	-0. 159127
39	1	0	2. 135633	1. 846592	1. 493767
40	6	0	1. 602764	3. 370887	-1. 485591
41	1	0	0. 732073	2. 417455	-3. 214060
42	1	0	2. 438481	4. 006983	0. 399327
43	1	0	1. 735912	4. 333197	-1. 971325

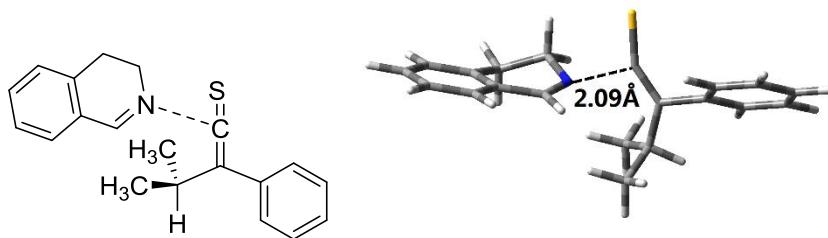
1e'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1. 415074	0. 933956	0. 088029
2	16	0	2. 317186	2. 217606	0. 077789
3	6	0	0. 655467	-0. 147635	0. 111856
4	6	0	1. 318210	-1. 537288	0. 147264
5	1	0	0. 805994	-2. 103098	0. 936485
6	6	0	1. 104984	-2. 272794	-1. 189804
7	1	0	1. 640467	-1. 760572	-1. 996853
8	1	0	1. 487644	-3. 297915	-1. 124312
9	1	0	0. 047541	-2. 321308	-1. 464340
10	6	0	2. 806886	-1. 499949	0. 520358
11	1	0	2. 970373	-1. 002439	1. 481336
12	1	0	3. 194771	-2. 521020	0. 596238
13	1	0	3. 399000	-0. 977381	-0. 238990
14	6	0	-0. 826852	-0. 010303	0. 079407
15	6	0	-1. 436917	1. 159774	-0. 416701
16	6	0	-1. 665518	-1. 037519	0. 551599
17	6	0	-2. 822973	1. 301215	-0. 426443

18	1	0	-0.817298	1.960463	-0.809242
19	6	0	-3.054770	-0.895593	0.535006
20	1	0	-1.240281	-1.953973	0.945514
21	6	0	-3.643462	0.273521	0.049501
22	1	0	-3.263672	2.214446	-0.816335
23	1	0	-3.676459	-1.704773	0.907960
24	1	0	-4.723845	0.381559	0.037489

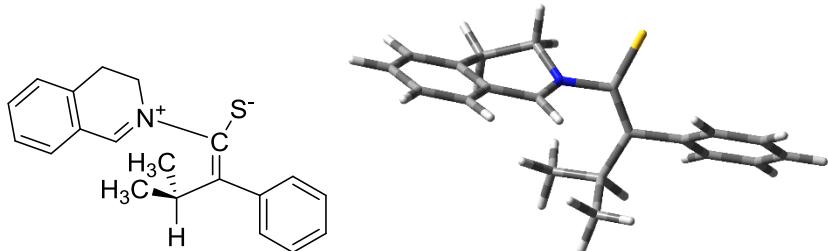
exo-1e'-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.674888	-0.742631	-0.176396
2	16	0	-1.015207	-2.424429	0.014160
3	6	0	-1.491771	0.354601	-0.224889
4	6	0	-1.134259	1.817371	-0.536217
5	1	0	-2.032487	2.208511	-1.028593
6	6	0	-0.973307	2.664195	0.746988
7	1	0	-0.053061	2.404324	1.283711
8	1	0	-0.922435	3.731945	0.501432
9	1	0	-1.816107	2.512337	1.427885
10	6	0	0.017306	2.096535	-1.519228
11	1	0	-0.038524	1.445500	-2.398166
12	1	0	-0.049767	3.133245	-1.868582
13	1	0	1.004702	1.982220	-1.063712
14	7	0	0.776496	-0.557251	-0.321596
15	6	0	1.488579	-0.064049	0.655833
16	6	0	1.476557	-1.223602	-1.460541
17	6	0	2.931861	0.009311	0.626623
18	1	0	0.940514	0.274797	1.528519
19	6	0	2.764180	-0.481140	-1.817277
20	1	0	0.770458	-1.255564	-2.290436
21	1	0	1.684486	-2.251632	-1.156919
22	6	0	3.654513	0.331567	1.791175
23	6	0	3.610000	-0.224291	-0.592312
24	1	0	2.527162	0.477547	-2.297958

25	1	0	3.316072	-1.075204	-2.552704
26	6	0	5.043894	0.401481	1.751183
27	1	0	3.121280	0.511825	2.720648
28	6	0	5.001502	-0.150133	-0.615264
29	6	0	5.716822	0.157568	0.547978
30	1	0	5.602636	0.640969	2.650313
31	1	0	5.533361	-0.329418	-1.545950
32	1	0	6.800982	0.208995	0.514343
33	6	0	-2.948828	0.137967	0.034519
34	6	0	-3.917043	0.503072	-0.917957
35	6	0	-3.396465	-0.403940	1.252133
36	6	0	-5.280327	0.334143	-0.665673
37	1	0	-3.601592	0.901862	-1.878697
38	6	0	-4.757993	-0.561678	1.513085
39	1	0	-2.665400	-0.712095	1.991970
40	6	0	-5.707501	-0.194154	0.555086
41	1	0	-6.006693	0.611050	-1.425016
42	1	0	-5.077319	-0.979454	2.463987
43	1	0	-6.767412	-0.323312	0.755450

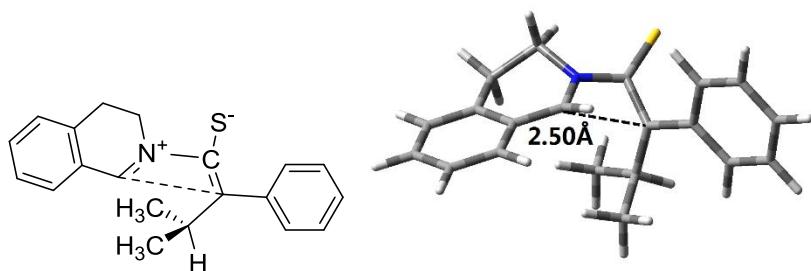
E-1e'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.674876	-0.742607	0.176537
2	16	0	1.015104	-2.424474	-0.013545
3	6	0	1.491780	0.354616	0.224745
4	6	0	1.134341	1.817482	0.535636
5	1	0	2.032701	2.208777	1.027655
6	6	0	0.973079	2.663867	-0.747829
7	1	0	0.052738	2.403701	-1.284243
8	1	0	0.922163	3.731687	-0.502601
9	1	0	1.815754	2.511850	-1.428845
10	6	0	-0.017000	2.096988	1.518816
11	1	0	0.038987	1.446210	2.397940

12	1	0	0.050167	3.133799	1.867853
13	1	0	-1.004485	1.982567	1.063537
14	7	0	-0.776512	-0.557164	0.321692
15	6	0	-1.488622	-0.064350	-0.655908
16	6	0	-1.476508	-1.222864	1.461059
17	6	0	-2.931904	0.009049	-0.626662
18	1	0	-0.940592	0.274125	-1.528762
19	6	0	-2.764086	-0.480185	1.817466
20	1	0	-0.770356	-1.254320	2.290932
21	1	0	-1.684457	-2.251072	1.158060
22	6	0	-3.654611	0.330757	-1.791329
23	6	0	-3.609984	-0.223959	0.592421
24	1	0	-2.527015	0.478756	2.297613
25	1	0	-3.315954	-1.073831	2.553250
26	6	0	-5.043994	0.400678	-1.751307
27	1	0	-3.121425	0.510565	-2.720917
28	6	0	-5.001481	-0.149784	0.615407
29	6	0	-5.716859	0.157352	-0.547953
30	1	0	-5.602772	0.639719	-2.650534
31	1	0	-5.533301	-0.328611	1.546204
32	1	0	-6.801018	0.208791	-0.514283
33	6	0	2.948859	0.137860	-0.034573
34	6	0	3.917019	0.503049	0.917913
35	6	0	3.396536	-0.404096	-1.252143
36	6	0	5.280316	0.334114	0.665694
37	1	0	3.601490	0.901917	1.878602
38	6	0	4.758076	-0.561832	-1.513040
39	1	0	2.665492	-0.712308	-1.991984
40	6	0	5.707539	-0.194242	-0.555017
41	1	0	6.006655	0.611088	1.425044
42	1	0	5.077447	-0.979648	-2.463912
43	1	0	6.767464	-0.323384	-0.755330

exo-1e'-TS2

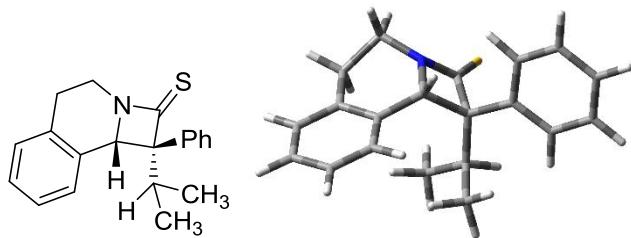


Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	-0.655443	1.407782	-0.036143
2	16	0	-1.437041	2.889599	-0.214941
3	6	0	-1.241742	0.198846	0.556548
4	6	0	-0.806568	-0.247460	1.958743
5	1	0	-1.694667	-0.047940	2.582135
6	6	0	-0.498193	-1.755779	2.071365
7	1	0	0.471966	-1.971262	1.612151
8	1	0	-0.449951	-2.057312	3.124274
9	1	0	-1.250860	-2.374576	1.576892
10	6	0	0.327759	0.565916	2.598041
11	1	0	0.139429	1.641918	2.540726
12	1	0	0.413582	0.293076	3.655137
13	1	0	1.291297	0.350054	2.128941
14	7	0	0.637227	1.151236	-0.409544
15	6	0	0.916011	-0.174999	-0.650436
16	6	0	1.685133	2.156699	-0.640523
17	6	0	2.275429	-0.636750	-0.568379
18	1	0	0.177964	-0.769604	-1.168933
19	6	0	2.969811	1.715423	0.068401
20	1	0	1.308400	3.110435	-0.269258
21	1	0	1.847089	2.250719	-1.721494
22	6	0	2.599394	-1.980077	-0.868434
23	6	0	3.315355	0.265856	-0.214303
24	1	0	2.858937	1.864663	1.151209
25	1	0	3.789806	2.367121	-0.252256
26	6	0	3.911592	-2.429524	-0.786802
27	1	0	1.804352	-2.663302	-1.155965
28	6	0	4.627043	-0.203666	-0.147844
29	6	0	4.932150	-1.541342	-0.421488
30	1	0	4.144915	-3.465956	-1.011439
31	1	0	5.425622	0.487574	0.111515
32	1	0	5.960421	-1.885145	-0.363503
33	6	0	-2.510742	-0.301067	0.028298
34	6	0	-3.447181	-1.027083	0.802875
35	6	0	-2.805624	-0.136267	-1.349444
36	6	0	-4.608034	-1.548817	0.234870
37	1	0	-3.284931	-1.166125	1.865396
38	6	0	-3.958344	-0.666230	-1.916222
39	1	0	-2.120939	0.430593	-1.971762
40	6	0	-4.871001	-1.377141	-1.126962
41	1	0	-5.313918	-2.087053	0.861198
42	1	0	-4.151256	-0.520485	-2.975179

43	1	0	-5.776018	-1.785545	-1.566893
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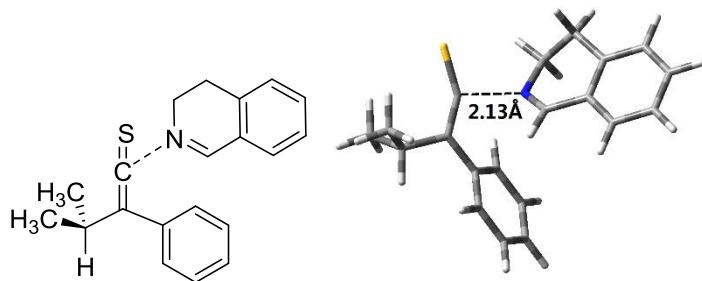
7e'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.565816	1.543202	0.183152
2	16	0	-1.205362	2.893384	0.874771
3	6	0	-0.738565	0.008897	0.383917
4	6	0	-0.430433	-0.459350	1.835297
5	1	0	-1.306448	-0.137174	2.410744
6	6	0	-0.292194	-1.990547	1.970196
7	1	0	0.697033	-2.322928	1.645374
8	1	0	-0.400918	-2.279396	3.021746
9	1	0	-1.039020	-2.542280	1.394158
10	6	0	0.776108	0.219564	2.510402
11	1	0	0.687878	1.308419	2.508488
12	1	0	0.821551	-0.103457	3.556330
13	1	0	1.723345	-0.063271	2.044083
14	7	0	0.351532	1.373007	-0.797199
15	6	0	0.421091	-0.091855	-0.733821
16	6	0	1.433686	2.226359	-1.245185
17	6	0	1.836139	-0.594630	-0.539750
18	1	0	0.029215	-0.559010	-1.644484
19	6	0	2.696186	1.818967	-0.466464
20	1	0	1.151098	3.263535	-1.051806
21	1	0	1.576164	2.094258	-2.324112
22	6	0	2.098996	-1.972085	-0.586444
23	6	0	2.914104	0.314029	-0.461452
24	1	0	2.591878	2.181031	0.564903
25	1	0	3.574611	2.318451	-0.890169
26	6	0	3.399353	-2.462736	-0.490563
27	1	0	1.269941	-2.665597	-0.701134
28	6	0	4.219045	-0.195345	-0.378935
29	6	0	4.467321	-1.567202	-0.379053
30	1	0	3.579668	-3.533370	-0.515425

31	1	0	5.052157	0.501179	-0.320643
32	1	0	5.487100	-1.934774	-0.312535
33	6	0	-2.116255	-0.437365	-0.139926
34	6	0	-3.092104	-1.026144	0.679815
35	6	0	-2.476323	-0.172408	-1.474989
36	6	0	-4.353326	-1.367812	0.181513
37	1	0	-2.890398	-1.222917	1.724978
38	6	0	-3.731782	-0.512886	-1.977417
39	1	0	-1.782242	0.337607	-2.135900
40	6	0	-4.679525	-1.121659	-1.151381
41	1	0	-5.080822	-1.824063	0.846936
42	1	0	-3.971656	-0.289082	-3.013039
43	1	0	-5.659303	-1.386314	-1.537921

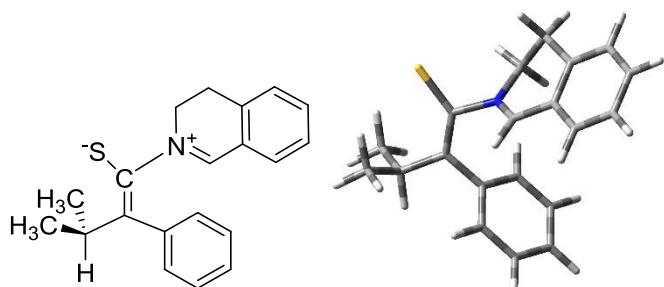
endo-1e'-TS3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.457011	-1.349592	-0.126359
2	16	0	1.319379	-2.954006	-0.275450
3	6	0	2.188980	-0.268753	0.174096
4	6	0	3.571332	-0.517008	0.838017
5	1	0	3.942195	0.479745	1.102248
6	6	0	3.499776	-1.337444	2.135516
7	1	0	3.142150	-2.354333	1.948190
8	1	0	4.494443	-1.408737	2.590819
9	1	0	2.825313	-0.872122	2.862796
10	6	0	4.576518	-1.120730	-0.160314
11	1	0	4.667205	-0.494456	-1.054116
12	1	0	5.568793	-1.203294	0.299018
13	1	0	4.263196	-2.121023	-0.475496
14	7	0	-0.514028	-0.628503	-0.493685
15	6	0	-1.141849	-0.006287	0.432459
16	6	0	-1.277743	-1.280898	-1.556837

17	6	0	-2.603693	0.094155	0.515873
18	1	0	-0.540178	0.494762	1.191967
19	6	0	-2.638230	-1.813381	-1.093384
20	1	0	-0.661841	-2.096868	-1.947301
21	1	0	-1.400915	-0.539388	-2.359699
22	6	0	-3.220943	1.030180	1.357288
23	6	0	-3.379294	-0.781776	-0.271809
24	1	0	-2.479599	-2.711185	-0.479281
25	1	0	-3.230547	-2.122864	-1.961097
26	6	0	-4.612789	1.112084	1.408569
27	1	0	-2.608199	1.695579	1.960118
28	6	0	-4.769884	-0.695076	-0.206305
29	6	0	-5.384736	0.249290	0.624676
30	1	0	-5.092887	1.840843	2.054341
31	1	0	-5.379207	-1.367406	-0.805044
32	1	0	-6.468700	0.308783	0.660659
33	6	0	1.853661	1.133147	-0.180241
34	6	0	1.433321	1.480261	-1.478473
35	6	0	1.996624	2.172126	0.760268
36	6	0	1.145594	2.803749	-1.815359
37	1	0	1.349629	0.700276	-2.228340
38	6	0	1.707464	3.496723	0.425607
39	1	0	2.321970	1.938373	1.770434
40	6	0	1.277158	3.820304	-0.864459
41	1	0	0.830408	3.043580	-2.827445
42	1	0	1.817750	4.275992	1.174986
43	1	0	1.057470	4.850900	-1.127730

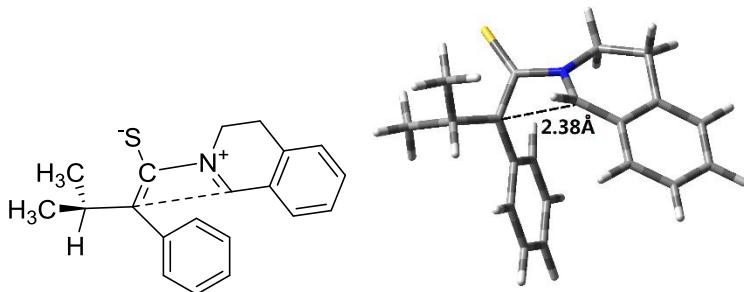
F-1e'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.123182	-1.235715	0.022983
2	16	0	-1.234017	-2.951730	-0.106579
3	6	0	-2.024135	-0.214588	-0.099321

4	6	0	-3.493113	-0.467266	-0.473644
5	1	0	-3.956901	0.524153	-0.540928
6	6	0	-3.679337	-1.140683	-1.847472
7	1	0	-3.252286	-2.146087	-1.856901
8	1	0	-4.747416	-1.213558	-2.085230
9	1	0	-3.198049	-0.558424	-2.642374
10	6	0	-4.247862	-1.225786	0.638509
11	1	0	-4.186208	-0.685955	1.590192
12	1	0	-5.307777	-1.323635	0.374612
13	1	0	-3.832138	-2.226457	0.781592
14	7	0	0.298726	-0.859956	0.249461
15	6	0	0.990862	-0.251913	-0.666803
16	6	0	0.975525	-1.293583	1.498681
17	6	0	2.423673	-0.057406	-0.574586
18	1	0	0.443849	0.094387	-1.538245
19	6	0	2.389769	-1.795891	1.222794
20	1	0	0.350931	-2.069292	1.937685
21	1	0	0.997055	-0.413344	2.154047
22	6	0	3.080459	0.829765	-1.444913
23	6	0	3.157420	-0.807634	0.373263
24	1	0	2.333968	-2.761802	0.703961
25	1	0	2.899776	-1.968948	2.175941
26	6	0	4.461614	0.991769	-1.360916
27	1	0	2.503465	1.393642	-2.172672
28	6	0	4.539300	-0.643673	0.435207
29	6	0	5.189022	0.254679	-0.420894
30	1	0	4.969667	1.684061	-2.024612
31	1	0	5.116297	-1.219453	1.153956
32	1	0	6.266166	0.375792	-0.354404
33	6	0	-1.667858	1.207861	0.176458
34	6	0	-1.146790	1.617741	1.418741
35	6	0	-1.899625	2.208165	-0.790435
36	6	0	-0.838722	2.956954	1.673839
37	1	0	-1.016175	0.879397	2.204555
38	6	0	-1.593422	3.546418	-0.539067
39	1	0	-2.317028	1.927984	-1.754116
40	6	0	-1.055233	3.928953	0.694346
41	1	0	-0.446578	3.242218	2.646554
42	1	0	-1.776086	4.292770	-1.307648
43	1	0	-0.821524	4.970921	0.892453

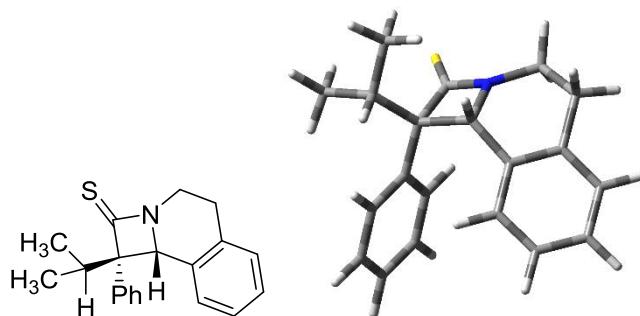
endo-1e'-TS4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.381143	-1.234543	-0.304782
2	16	0	2.518862	-2.190620	-1.087830
3	6	0	1.592963	0.044706	0.379920
4	6	0	2.755228	0.241250	1.343562
5	1	0	2.460728	1.071672	1.998715
6	6	0	3.029215	-0.971775	2.248329
7	1	0	3.365178	-1.836067	1.669317
8	1	0	3.811563	-0.722853	2.973312
9	1	0	2.137822	-1.266809	2.814326
10	6	0	4.046542	0.695385	0.617890
11	1	0	3.868482	1.585742	0.007505
12	1	0	4.820022	0.935415	1.356773
13	1	0	4.414763	-0.101323	-0.033362
14	7	0	0.041416	-1.531805	-0.200732
15	6	0	-0.526592	-0.920493	0.891487
16	6	0	-0.731714	-2.248725	-1.221052
17	6	0	-1.910993	-0.507484	0.817627
18	1	0	-0.026052	-1.006622	1.844657
19	6	0	-2.194117	-2.407029	-0.785733
20	1	0	-0.253535	-3.219296	-1.389289
21	1	0	-0.655003	-1.678782	-2.154716
22	6	0	-2.435233	0.514477	1.630211
23	6	0	-2.750631	-1.172869	-0.110484
24	1	0	-2.260792	-3.243287	-0.075318
25	1	0	-2.796258	-2.686719	-1.655587
26	6	0	-3.763571	0.909620	1.486171
27	1	0	-1.788062	1.013932	2.345307
28	6	0	-4.077587	-0.764343	-0.240685
29	6	0	-4.582630	0.279988	0.542393
30	1	0	-4.159140	1.712273	2.101196
31	1	0	-4.729268	-1.277469	-0.943717
32	1	0	-5.616553	0.590923	0.426006

33	6	0	0. 997817	1. 249600	-0. 234592
34	6	0	0. 631811	1. 252503	-1. 600030
35	6	0	0. 822792	2. 454669	0. 485419
36	6	0	0. 088066	2. 388353	-2. 201787
37	1	0	0. 823814	0. 369677	-2. 201053
38	6	0	0. 288086	3. 588037	-0. 121278
39	1	0	1. 086536	2. 500236	1. 537363
40	6	0	-0. 089501	3. 563470	-1. 469088
41	1	0	-0. 176255	2. 358551	-3. 255343
42	1	0	0. 158498	4. 495020	0. 463004
43	1	0	-0. 504749	4. 449576	-1. 939697

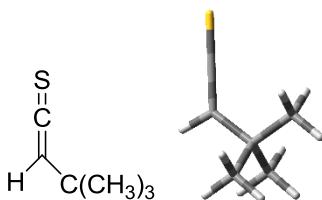
8e'



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0. 956733	-1. 429087	-0. 634662
2	16	0	1. 883325	-1. 980565	-1. 886648
3	6	0	1. 057397	-0. 325325	0. 455232
4	6	0	2. 129639	-0. 665276	1. 546804
5	1	0	1. 902158	-0. 030387	2. 414426
6	6	0	2. 085360	-2. 126700	2. 034253
7	1	0	2. 354114	-2. 820258	1. 231093
8	1	0	2. 812833	-2. 257932	2. 841890
9	1	0	1. 110236	-2. 425386	2. 430179
10	6	0	3. 559771	-0. 346632	1. 070482
11	1	0	3. 684777	0. 701130	0. 789819
12	1	0	4. 272985	-0. 568842	1. 871960
13	1	0	3. 821003	-0. 959295	0. 202527
14	7	0	-0. 245670	-1. 840916	-0. 194545
15	6	0	-0. 423785	-0. 814380	0. 847861
16	6	0	-1. 282169	-2. 637185	-0. 825443
17	6	0	-1. 706149	-0. 042760	0. 613906
18	1	0	-0. 446272	-1. 252889	1. 854378

19	6	0	-2.621171	-2.276148	-0.160087
20	1	0	-1.065235	-3.707029	-0.724270
21	1	0	-1.288662	-2.401844	-1.896799
22	6	0	-1.898191	1.300440	0.954215
23	6	0	-2.784366	-0.787137	0.083177
24	1	0	-2.684202	-2.800673	0.804319
25	1	0	-3.443839	-2.657116	-0.772416
26	6	0	-3.132167	1.918783	0.738956
27	1	0	-1.081486	1.874725	1.374601
28	6	0	-4.010993	-0.150931	-0.139512
29	6	0	-4.188419	1.196468	0.181226
30	1	0	-3.261753	2.964918	1.000180
31	1	0	-4.837569	-0.720579	-0.557459
32	1	0	-5.146329	1.675851	0.001594
33	6	0	1.146786	1.109447	-0.058590
34	6	0	0.877992	1.426612	-1.398079
35	6	0	1.449708	2.168563	0.815568
36	6	0	0.908265	2.749630	-1.848277
37	1	0	0.657831	0.635647	-2.105585
38	6	0	1.482296	3.490758	0.369535
39	1	0	1.664219	1.969686	1.860863
40	6	0	1.210399	3.789305	-0.968376
41	1	0	0.698271	2.961676	-2.892739
42	1	0	1.723381	4.286350	1.069176
43	1	0	1.238403	4.817034	-1.318687

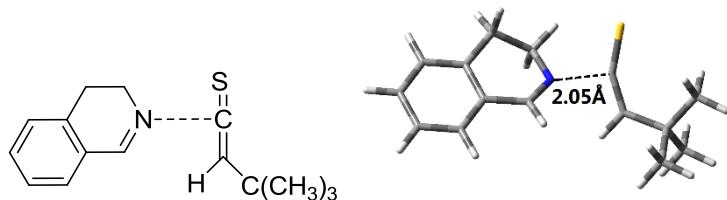
1k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.296541	-0.428107	-0.000109
2	16	0	-2.788717	0.068154	-0.000191
3	6	0	-0.054336	-0.849321	0.000118
4	6	0	1.210703	0.017580	0.000089
5	6	0	2.032267	-0.327092	-1.261878
6	1	0	2.968074	0.244341	-1.275207
7	1	0	2.288020	-1.392332	-1.289740

8	1	0	1.472155	-0.089480	-2.171894
9	6	0	2.032026	-0.326645	1.262335
10	1	0	1.471737	-0.088715	2.172160
11	1	0	2.287778	-1.391874	1.290621
12	1	0	2.967828	0.244797	1.275644
13	6	0	0.863377	1.516321	-0.000210
14	1	0	1.781773	2.113286	-0.000230
15	1	0	0.282932	1.791785	-0.887016
16	1	0	0.282766	1.792100	0.886390
17	1	0	0.091427	-1.930790	0.000251

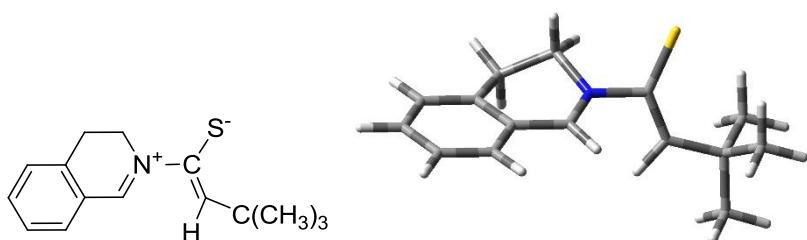
exo-1k-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.041802	-1.859493	-0.334886
2	6	0	2.392950	-0.638535	-0.103250
3	6	0	3.137425	0.539420	0.116286
4	6	0	4.530327	0.465891	0.110306
5	6	0	5.176876	-0.757107	-0.105613
6	6	0	4.435467	-1.920989	-0.330375
7	1	0	2.453278	-2.756663	-0.509857
8	1	0	5.116646	1.366566	0.273342
9	1	0	6.262193	-0.799165	-0.101232
10	1	0	4.940423	-2.866439	-0.502370
11	6	0	2.363320	1.829721	0.275036
12	1	0	2.197136	2.268727	-0.719050
13	1	0	2.936852	2.562484	0.852315
14	6	0	0.929116	-0.545053	-0.086810
15	1	0	0.345010	-1.375620	-0.488025
16	7	0	0.277954	0.452369	0.383171
17	6	0	1.007572	1.587741	0.947013
18	1	0	0.360810	2.464673	0.844368
19	1	0	1.130305	1.384089	2.020352
20	6	0	-1.697285	0.746141	-0.092032
21	16	0	-1.804661	2.233224	-0.740837
22	6	0	-2.231450	-0.410685	0.301372

23	6	0	-3.680541	-0.868715	0.114676
24	6	0	-4.308063	-1.045252	1.518064
25	1	0	-5.330575	-1.435112	1.438306
26	1	0	-4.345782	-0.088922	2.049767
27	1	0	-3.727045	-1.747693	2.127316
28	6	0	-4.539123	0.108682	-0.705351
29	1	0	-4.124240	0.265357	-1.705472
30	1	0	-4.612902	1.085867	-0.220594
31	1	0	-5.551916	-0.296585	-0.814785
32	6	0	-3.653172	-2.239976	-0.601712
33	1	0	-4.667321	-2.646665	-0.698619
34	1	0	-3.052871	-2.968148	-0.042825
35	1	0	-3.225729	-2.147431	-1.605989
36	1	0	-1.606696	-1.118231	0.837884

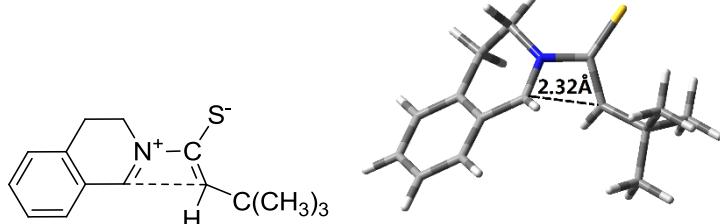
E-1k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.092144	1.498649	-0.922731
2	6	0	-2.308561	0.528359	-0.271860
3	6	0	-2.910822	-0.416261	0.590907
4	6	0	-4.292455	-0.380807	0.770639
5	6	0	-5.070067	0.578550	0.111478
6	6	0	-4.471236	1.520300	-0.733335
7	1	0	-2.615831	2.220680	-1.580404
8	1	0	-4.767261	-1.101927	1.430645
9	1	0	-6.145700	0.592227	0.260061
10	1	0	-5.078620	2.263108	-1.240485
11	6	0	-1.993643	-1.375483	1.313806
12	1	0	-1.660162	-0.916370	2.255815
13	1	0	-2.522790	-2.295687	1.580525
14	6	0	-0.872710	0.496512	-0.454674
15	1	0	-0.360164	1.313414	-0.952197
16	7	0	-0.129012	-0.497828	-0.053484
17	6	0	-0.781605	-1.734070	0.455588

18	1	0	-0.023368	-2.288578	1.007963
19	1	0	-1.068617	-2.335701	-0.411334
20	6	0	1.326618	-0.505255	-0.289617
21	16	0	1.818299	-1.796300	-1.311754
22	6	0	1.976808	0.499352	0.363844
23	6	0	3.472356	0.788137	0.364053
24	6	0	3.722612	2.030926	1.244048
25	1	0	4.790815	2.273060	1.274078
26	1	0	3.190775	2.907472	0.853416
27	1	0	3.387359	1.862127	2.274809
28	6	0	3.978639	1.082586	-1.068103
29	1	0	3.812891	0.225839	-1.725416
30	1	0	3.459111	1.948868	-1.494671
31	1	0	5.052239	1.307828	-1.048977
32	6	0	4.254860	-0.409222	0.954490
33	1	0	5.331087	-0.196410	0.950729
34	1	0	3.950302	-0.598570	1.990426
35	1	0	4.077199	-1.316836	0.371869
36	1	0	1.369141	1.147419	0.994404

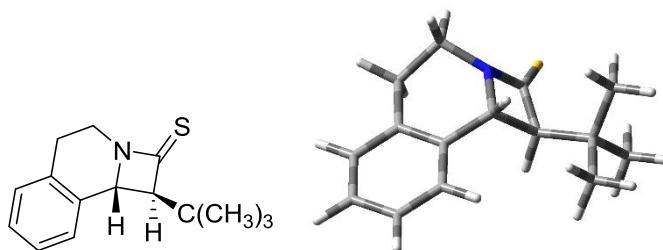
exo-1k-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.541721	-1.576816	-0.804088
2	6	0	1.914470	-0.383997	-0.392296
3	6	0	2.643320	0.567843	0.367156
4	6	0	3.968977	0.287147	0.703047
5	6	0	4.576102	-0.909346	0.308512
6	6	0	3.860040	-1.843522	-0.449548
7	1	0	1.978902	-2.293378	-1.396837
8	1	0	4.538624	1.016621	1.273749
9	1	0	5.608224	-1.106724	0.582376
10	1	0	4.331883	-2.769250	-0.764295
11	6	0	1.973272	1.866824	0.784450
12	1	0	1.553538	1.754914	1.794026

13	1	0	2.715615	2.670347	0.841178
14	6	0	0.537933	-0.106410	-0.753201
15	1	0	0.078478	-0.662420	-1.559777
16	7	0	0.001468	1.108181	-0.412814
17	6	0	0.857106	2.274079	-0.185297
18	1	0	0.224417	3.068819	0.213032
19	1	0	1.273657	2.611264	-1.142159
20	6	0	-1.352637	0.979374	-0.135289
21	16	0	-2.501774	2.194966	-0.340214
22	6	0	-1.494781	-0.375926	0.324441
23	6	0	-2.714880	-1.266924	0.262053
24	6	0	-3.702826	-0.841427	1.384212
25	1	0	-4.572863	-1.509848	1.380198
26	1	0	-3.230630	-0.905408	2.371115
27	1	0	-4.042625	0.185236	1.229534
28	6	0	-2.259035	-2.719803	0.526634
29	1	0	-1.564482	-3.067004	-0.246894
30	1	0	-1.757704	-2.810096	1.497492
31	1	0	-3.122842	-3.393364	0.531190
32	6	0	-3.420250	-1.194352	-1.107642
33	1	0	-4.290711	-1.860223	-1.116586
34	1	0	-3.759230	-0.179339	-1.326885
35	1	0	-2.747713	-1.513334	-1.912712
36	1	0	-0.767626	-0.653994	1.086507

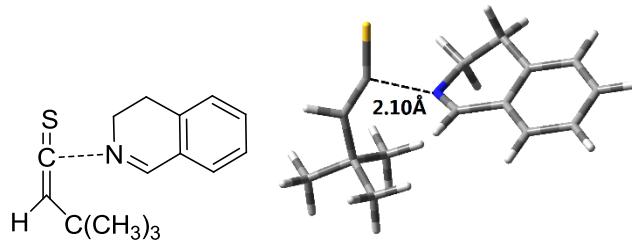
7k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.006566	-1.773685	0.075606
2	6	0	-1.512504	-0.470014	0.234466
3	6	0	-2.362358	0.631197	-0.000627
4	6	0	-3.684687	0.384388	-0.402709
5	6	0	-4.163414	-0.913064	-0.575267
6	6	0	-3.318343	-2.001034	-0.334856

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
7	1	0	-1.351468	-2.617918	0.274958
8	1	0	-4.346491	1.228836	-0.580710
9	1	0	-5.190725	-1.075554	-0.888022
10	1	0	-3.681186	-3.017010	-0.459671
11	6	0	-1.883858	2.068912	0.147412
12	1	0	-1.573680	2.450151	-0.834505
13	1	0	-2.712525	2.702807	0.483122
14	6	0	-0.091582	-0.257087	0.708336
15	1	0	0.075124	-0.783572	1.656514
16	7	0	0.262478	1.166447	0.795193
17	6	0	-0.693054	2.210050	1.111343
18	1	0	-0.196585	3.176796	1.001589
19	1	0	-1.010291	2.092599	2.153710
20	6	0	1.243321	1.131368	-0.145388
21	16	0	2.116649	2.340864	-0.849754
22	6	0	1.106963	-0.394027	-0.310052
23	6	0	2.302898	-1.318874	0.023352
24	6	0	1.800958	-2.775108	0.104846
25	1	0	2.643491	-3.457021	0.266127
26	1	0	1.099580	-2.919606	0.934684
27	1	0	1.300369	-3.077608	-0.822408
28	6	0	2.967381	-0.925585	1.357884
29	1	0	3.366380	0.092779	1.319058
30	1	0	2.267847	-0.985371	2.199408
31	1	0	3.799152	-1.604200	1.576636
32	6	0	3.338940	-1.205991	-1.115204
33	1	0	4.198953	-1.853747	-0.909234
34	1	0	2.906890	-1.516752	-2.073795
35	1	0	3.697305	-0.178861	-1.225920
36	1	0	0.739562	-0.624380	-1.316686

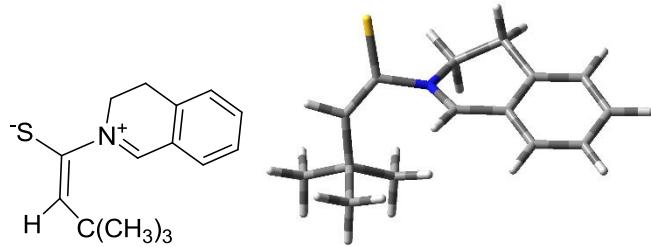
endo-1k-TS3



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

1	6	0	-2.799463	-1.465669	-1.059184
2	6	0	-2.068109	-0.485094	-0.373770
3	6	0	-2.714402	0.398669	0.515111
4	6	0	-4.089615	0.272280	0.710657
5	6	0	-4.815826	-0.716897	0.036380
6	6	0	-4.173635	-1.585840	-0.850859
7	1	0	-2.288475	-2.133982	-1.747813
8	1	0	-4.600198	0.950278	1.389871
9	1	0	-5.885571	-0.805487	0.202324
10	1	0	-4.740452	-2.348019	-1.376515
11	6	0	-1.871285	1.482650	1.148652
12	1	0	-1.861096	2.358612	0.485725
13	1	0	-2.303755	1.807911	2.100980
14	6	0	-0.620195	-0.348575	-0.561464
15	1	0	-0.162035	-0.849641	-1.415113
16	7	0	0.153861	0.322531	0.210361
17	6	0	-0.429397	1.011809	1.370821
18	1	0	0.216256	1.862244	1.602210
19	1	0	-0.376605	0.311683	2.216517
20	6	0	1.890219	1.194710	-0.589683
21	16	0	1.363237	2.659719	-1.056273
22	6	0	2.891485	0.321748	-0.486259
23	6	0	3.153678	-1.014971	0.211433
24	6	0	2.514641	-2.196842	-0.554859
25	1	0	2.819837	-3.151239	-0.107651
26	1	0	1.423936	-2.148931	-0.522223
27	1	0	2.827593	-2.198117	-1.604491
28	6	0	2.674404	-1.026311	1.678884
29	1	0	3.105936	-0.188007	2.235836
30	1	0	1.587470	-0.960633	1.748337
31	1	0	2.986276	-1.957469	2.167825
32	6	0	4.687538	-1.218797	0.210786
33	1	0	4.949751	-2.164554	0.697618
34	1	0	5.082944	-1.245008	-0.811272
35	1	0	5.192175	-0.408511	0.748458
36	1	0	3.756966	0.718414	-1.022643

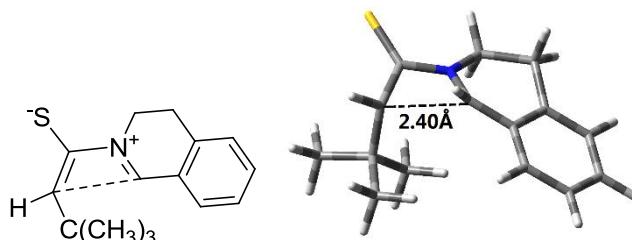
F-1k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.547529	-1.438087	-1.082649
2	6	0	-1.876879	-0.391600	-0.424903
3	6	0	-2.568001	0.438884	0.488236
4	6	0	-3.916571	0.191160	0.733687
5	6	0	-4.576987	-0.863971	0.090967
6	6	0	-3.894278	-1.677693	-0.818771
7	1	0	-2.007879	-2.060898	-1.791017
8	1	0	-4.460300	0.825811	1.428426
9	1	0	-5.627099	-1.046449	0.298749
10	1	0	-4.410633	-2.490017	-1.320252
11	6	0	-1.806113	1.597895	1.093243
12	1	0	-1.890317	2.473405	0.436591
13	1	0	-2.228750	1.877289	2.063752
14	6	0	-0.480991	-0.122272	-0.701050
15	1	0	0.004088	-0.553874	-1.571141
16	7	0	0.245155	0.669487	0.033647
17	6	0	-0.330400	1.251092	1.272974
18	1	0	0.264768	2.130972	1.510062
19	1	0	-0.199341	0.493713	2.056552
20	6	0	1.591181	1.100952	-0.398587
21	16	0	1.484658	2.725019	-0.987460
22	6	0	2.647072	0.258546	-0.300453
23	6	0	2.856642	-1.154125	0.243959
24	6	0	2.814270	-2.175045	-0.921834
25	1	0	3.082388	-3.179749	-0.570898
26	1	0	1.814365	-2.230135	-1.366566
27	1	0	3.515054	-1.893783	-1.714971
28	6	0	1.866614	-1.595497	1.341665
29	1	0	1.853278	-0.879356	2.170571
30	1	0	0.845096	-1.717506	0.971348
31	1	0	2.176454	-2.565202	1.747680
32	6	0	4.277374	-1.185749	0.861086
33	1	0	4.515446	-2.188073	1.236268
34	1	0	5.035532	-0.914630	0.118265

35	1	0	4.358132	-0.479524	1.694485
36	1	0	3.556691	0.704367	-0.699498

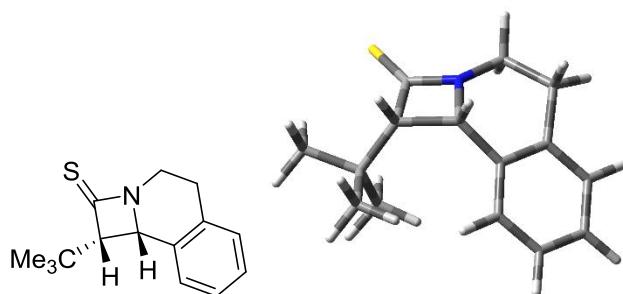
endo-1k-TS4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.327797	1.289755	-0.934059
2	6	0	1.671071	0.103466	-0.559741
3	6	0	2.356942	-0.861655	0.219323
4	6	0	3.654048	-0.586711	0.655740
5	6	0	4.284697	0.614513	0.316013
6	6	0	3.624252	1.546158	-0.492812
7	1	0	1.805682	2.017713	-1.548783
8	1	0	4.185389	-1.327487	1.248324
9	1	0	5.292285	0.815222	0.667477
10	1	0	4.117252	2.472404	-0.772161
11	6	0	1.702796	-2.214986	0.397924
12	1	0	1.888317	-2.807124	-0.509689
13	1	0	2.156960	-2.764121	1.228402
14	6	0	0.314329	-0.207317	-0.986057
15	1	0	0.027028	-0.030087	-2.011950
16	7	0	-0.409407	-1.125913	-0.266237
17	6	0	0.190231	-2.123003	0.623230
18	1	0	-0.311814	-3.077420	0.430378
19	1	0	-0.039251	-1.833452	1.656395
20	6	0	-1.762740	-0.923711	-0.426656
21	16	0	-2.956959	-2.106179	-0.374736
22	6	0	-1.973103	0.475631	-0.717950
23	6	0	-1.916386	1.605300	0.311027
24	6	0	-3.377397	1.765460	0.829167
25	1	0	-3.420654	2.568128	1.575416
26	1	0	-4.061637	2.021727	0.013635
27	1	0	-3.735240	0.840550	1.291139
28	6	0	-1.498414	2.918431	-0.384646

29	1	0	-0.453908	2.873650	-0.708250
30	1	0	-2.119447	3.115510	-1.265888
31	1	0	-1.609220	3.767550	0.299672
32	6	0	-1.007546	1.335934	1.520860
33	1	0	-1.107889	2.154042	2.242424
34	1	0	-1.289691	0.409552	2.031976
35	1	0	0.046110	1.272072	1.240158
36	1	0	-2.736530	0.668234	-1.477425

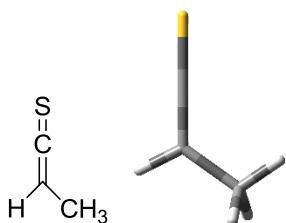
8k



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.793741	-1.635002	-0.228105
2	6	0	-1.425259	-0.298428	-0.416329
3	6	0	-2.357036	0.717427	-0.093651
4	6	0	-3.591156	0.367109	0.466935
5	6	0	-3.932990	-0.968977	0.680680
6	6	0	-3.034404	-1.972642	0.317714
7	1	0	-1.112256	-2.428300	-0.504254
8	1	0	-4.296430	1.152910	0.726197
9	1	0	-4.894686	-1.222607	1.116710
10	1	0	-3.291331	-3.017998	0.461378
11	6	0	-2.050984	2.163518	-0.434102
12	1	0	-2.203993	2.311593	-1.513080
13	1	0	-2.753118	2.832313	0.072107
14	6	0	-0.130559	0.177671	-1.056791
15	1	0	-0.294167	0.245022	-2.143885
16	7	0	0.258290	1.487395	-0.497509
17	6	0	-0.612597	2.569203	-0.083461
18	1	0	-0.329080	3.505531	-0.578330
19	1	0	-0.489394	2.716344	0.996768
20	6	0	1.515223	1.164021	-0.146196
21	16	0	2.649036	2.065505	0.651682

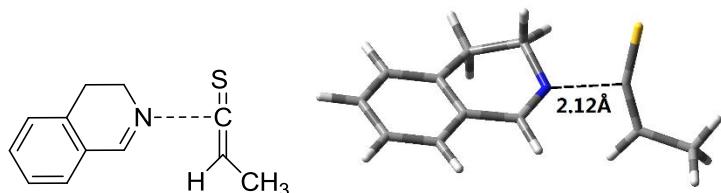
22	6	0	1. 391701	-0. 245907	-0. 770375
23	6	0	1. 910231	-1. 490748	-0. 004265
24	6	0	1. 645266	-2. 761001	-0. 841543
25	1	0	2. 041655	-3. 640901	-0. 322515
26	1	0	0. 585563	-2. 943133	-1. 032103
27	1	0	2. 147842	-2. 697171	-1. 813936
28	6	0	1. 312923	-1. 618302	1. 410590
29	1	0	1. 528248	-0. 724484	2. 004822
30	1	0	0. 231120	-1. 765804	1. 398846
31	1	0	1. 761603	-2. 474988	1. 926239
32	6	0	3. 447359	-1. 350011	0. 122627
33	1	0	3. 856916	-2. 243760	0. 607429
34	1	0	3. 920300	-1. 257427	-0. 862318
35	1	0	3. 725895	-0. 474311	0. 711816
36	1	0	1. 908852	-0. 240246	-1. 738605

1l



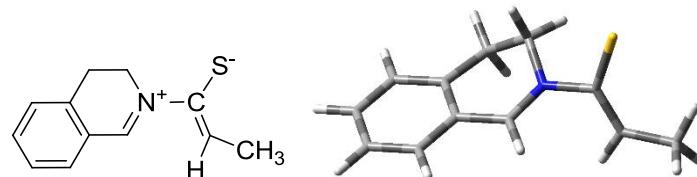
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0. 196566	0. 256753	0. 000046
2	16	0	-1. 715905	-0. 143786	-0. 000008
3	6	0	1. 074832	0. 584807	-0. 000022
4	1	0	1. 308604	1. 649440	-0. 000013
5	6	0	2. 219941	-0. 405374	-0. 000002
6	1	0	2. 851078	-0. 265509	-0. 885197
7	1	0	2. 851013	-0. 265550	0. 885248
8	1	0	1. 854550	-1. 434920	-0. 000038

exo-1l-TS1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.421705	1.619451	-0.526097
2	6	0	-1.609089	0.595901	-0.017985
3	6	0	-2.172477	-0.632524	0.384766
4	6	0	-3.549572	-0.817407	0.257541
5	6	0	-4.357304	0.200921	-0.261786
6	6	0	-3.796442	1.421016	-0.652664
7	1	0	-1.972309	2.561750	-0.829400
8	1	0	-3.996737	-1.759223	0.565263
9	1	0	-5.427210	0.041208	-0.359170
10	1	0	-4.426801	2.209001	-1.052926
11	6	0	-1.238827	-1.653594	0.994924
12	1	0	-1.169644	-1.469665	2.077593
13	1	0	-1.632917	-2.667918	0.872767
14	6	0	-0.157402	0.766579	0.112218
15	1	0	0.261278	1.769019	0.000175
16	7	0	0.668300	-0.188948	0.327304
17	6	0	0.160712	-1.563960	0.376507
18	1	0	0.880813	-2.167360	0.935126
19	1	0	0.156774	-1.947667	-0.652017
20	6	0	2.732105	0.011907	-0.104350
21	16	0	3.106246	-1.110126	-1.206676
22	6	0	3.039640	1.026425	0.701920
23	6	0	4.421585	1.639223	0.716855
24	1	0	2.300367	1.422556	1.388235
25	1	0	4.380392	2.710194	0.478490
26	1	0	4.881345	1.543782	1.709299
27	1	0	5.079269	1.155347	-0.008847

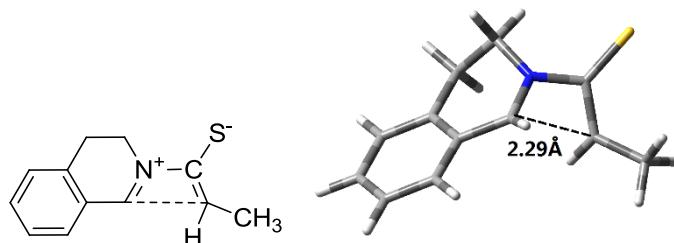
E-11



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.390971	1.548159	-0.588188

2	6	0	-1.501173	0.558830	-0.130102
3	6	0	-1.994920	-0.658559	0.394063
4	6	0	-3.372300	-0.867995	0.430606
5	6	0	-4.253418	0.114108	-0.037204
6	6	0	-3.764073	1.323779	-0.543912
7	1	0	-1.998696	2.480283	-0.985771
8	1	0	-3.763507	-1.800194	0.829474
9	1	0	-5.323996	-0.064571	-0.003527
10	1	0	-4.451294	2.082938	-0.903576
11	6	0	-0.981160	-1.638012	0.938460
12	1	0	-0.784791	-1.405064	1.995092
13	1	0	-1.369854	-2.660693	0.906664
14	6	0	-0.071773	0.778588	-0.168299
15	1	0	0.331330	1.760845	-0.391501
16	7	0	0.798073	-0.174152	0.041914
17	6	0	0.324085	-1.580513	0.146128
18	1	0	1.127197	-2.151334	0.611789
19	1	0	0.192392	-1.960996	-0.870635
20	6	0	2.238420	0.084993	-0.031536
21	16	0	3.040442	-0.815599	-1.254907
22	6	0	2.691081	0.977597	0.893413
23	6	0	4.127936	1.379106	1.010948
24	1	0	1.982149	1.397604	1.604987
25	1	0	4.317313	2.348141	0.526019
26	1	0	4.427806	1.479171	2.060766
27	1	0	4.769982	0.642017	0.519066

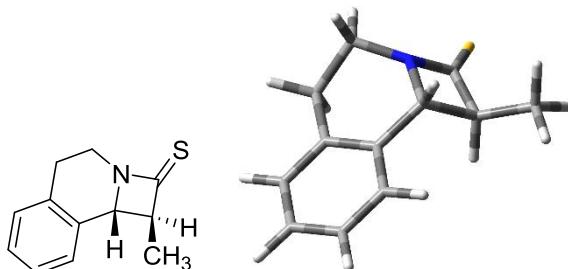
exo-1l-TS2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.264176	1.458286	-0.639127
2	6	0	-1.354107	0.428642	-0.327954
3	6	0	-1.824071	-0.768150	0.273063
4	6	0	-3.185743	-0.886467	0.558641

5	6	0	-4.077799	0.150401	0.267430
6	6	0	-3.615311	1.326038	-0.335908
7	1	0	-1.895481	2.364801	-1.112372
8	1	0	-3.556936	-1.804691	1.007449
9	1	0	-5.132373	0.036389	0.500076
10	1	0	-4.307515	2.128548	-0.571623
11	6	0	-0.846662	-1.891650	0.580628
12	1	0	-0.503301	-1.803101	1.620821
13	1	0	-1.351832	-2.860185	0.498312
14	6	0	0.057704	0.568433	-0.631015
15	1	0	0.374205	1.311539	-1.352451
16	7	0	0.885619	-0.501313	-0.394352
17	6	0	0.368705	-1.868702	-0.355545
18	1	0	1.176903	-2.513859	-0.007131
19	1	0	0.088718	-2.182217	-1.368544
20	6	0	2.132108	-0.040192	0.002323
21	16	0	3.612796	-0.784926	-0.269491
22	6	0	1.865149	1.228537	0.619684
23	6	0	2.855433	2.342200	0.700697
24	1	0	1.072329	1.221183	1.364448
25	1	0	3.533697	2.190467	1.553839
26	1	0	2.350889	3.301942	0.858312
27	1	0	3.479252	2.392944	-0.196322

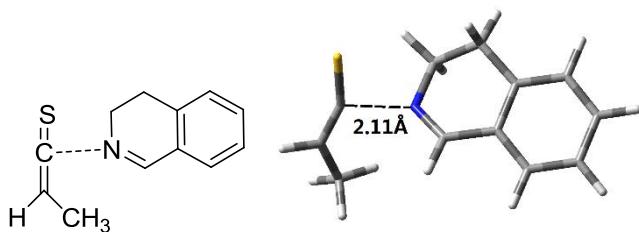
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.089241	1.481550	0.128698
2	6	0	1.158243	0.440414	0.260787
3	6	0	1.548500	-0.886774	-0.013921
4	6	0	2.869080	-1.124218	-0.427176
5	6	0	3.784122	-0.083049	-0.574090
6	6	0	3.392337	1.230384	-0.295340
7	1	0	1.784530	2.499335	0.362508

8	1	0	3.180030	-2.145352	-0.635429
9	1	0	4.799418	-0.294745	-0.896514
10	1	0	4.098723	2.048559	-0.400135
11	6	0	0.578180	-2.055077	0.101280
12	1	0	0.151227	-2.268151	-0.887769
13	1	0	1.119172	-2.956812	0.410279
14	6	0	-0.240503	0.744233	0.743269
15	1	0	-0.208290	1.276483	1.704129
16	7	0	-1.091357	-0.453314	0.799669
17	6	0	-0.583647	-1.783089	1.073337
18	1	0	-1.398273	-2.498314	0.939012
19	1	0	-0.246853	-1.825685	2.115452
20	6	0	-2.009644	-0.020884	-0.106426
21	16	0	-3.313351	-0.750168	-0.799483
22	6	0	-1.311444	1.340446	-0.247211
23	6	0	-2.084599	2.582464	0.174784
24	1	0	-0.907443	1.451208	-1.259180
25	1	0	-2.454793	2.487622	1.201267
26	1	0	-1.455661	3.477409	0.114617
27	1	0	-2.947868	2.725928	-0.482129

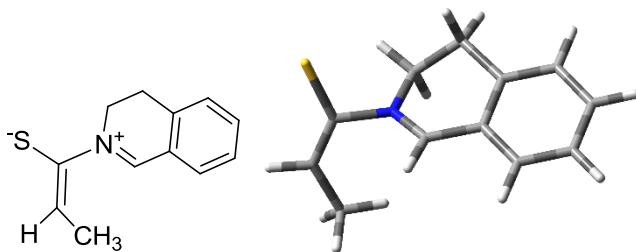
endo-1I-TS3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.372769	1.468946	-0.691602
2	6	0	1.459486	0.515366	-0.220065
3	6	0	1.912212	-0.721856	0.284103
4	6	0	3.283426	-0.975460	0.314744
5	6	0	4.194731	-0.016664	-0.144334
6	6	0	3.742175	1.205852	-0.649582
7	1	0	2.007315	2.415034	-1.083240
8	1	0	3.645382	-1.926762	0.696504
9	1	0	5.259688	-0.227361	-0.109622
10	1	0	4.451118	1.945228	-1.009102
11	6	0	0.862107	-1.729291	0.697986

12	1	0	0.586739	-2.335070	-0.176561
13	1	0	1.257828	-2.419697	1.450570
14	6	0	0.015306	0.772757	-0.235324
15	1	0	-0.356783	1.612619	-0.825178
16	7	0	-0.850552	0.083202	0.410663
17	6	0	-0.394870	-1.037680	1.238622
18	1	0	-1.222227	-1.748858	1.305973
19	1	0	-0.216314	-0.633339	2.245602
20	6	0	-2.835540	-0.017234	-0.298067
21	16	0	-2.935802	-1.472560	-1.005210
22	6	0	-3.372141	1.149949	0.051536
23	6	0	-2.877482	2.270815	0.921490
24	1	0	-4.375256	1.271129	-0.362186
25	1	0	-2.714251	3.191469	0.343938
26	1	0	-3.623238	2.511280	1.689505
27	1	0	-1.946385	2.009862	1.425477

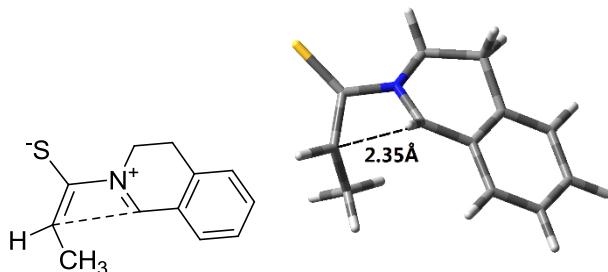
F-11



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.275419	1.370864	-0.814635
2	6	0	1.348991	0.438066	-0.315942
3	6	0	1.795058	-0.742232	0.323784
4	6	0	3.164763	-0.954915	0.461564
5	6	0	4.084892	-0.015061	-0.020594
6	6	0	3.641756	1.147072	-0.660139
7	1	0	1.918796	2.267645	-1.314136
8	1	0	3.520706	-1.860656	0.945342
9	1	0	5.149048	-0.194313	0.100449
10	1	0	4.357612	1.870019	-1.038098
11	6	0	0.745251	-1.740680	0.760317
12	1	0	0.530801	-2.429707	-0.067027
13	1	0	1.106058	-2.344311	1.599308
14	6	0	-0.074440	0.651756	-0.482128

15	1	0	-0.444460	1.399792	-1.177422
16	7	0	-0.971783	-0.049728	0.146660
17	6	0	-0.547317	-1.038680	1.168562
18	1	0	-1.370523	-1.741763	1.281500
19	1	0	-0.411851	-0.476740	2.102773
20	6	0	-2.411879	0.061659	-0.171031
21	16	0	-2.929461	-1.330490	-1.048840
22	6	0	-3.060004	1.168337	0.262334
23	6	0	-2.525445	2.323565	1.064476
24	1	0	-4.117547	1.200878	0.011312
25	1	0	-2.593488	3.268536	0.506914
26	1	0	-3.113137	2.465205	1.981423
27	1	0	-1.480437	2.192842	1.363072

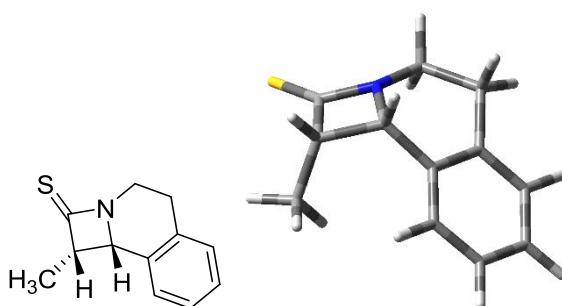
endo-11-TS4



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.168061	1.343296	-0.654533
2	6	0	1.259232	0.284472	-0.481009
3	6	0	1.703072	-0.947083	0.062328
4	6	0	3.033536	-1.070193	0.464273
5	6	0	3.924582	-0.000401	0.323549
6	6	0	3.493529	1.202147	-0.246980
7	1	0	1.822853	2.279532	-1.084557
8	1	0	3.383648	-2.015080	0.872510
9	1	0	4.955695	-0.110597	0.645712
10	1	0	4.188083	2.027910	-0.367896
11	6	0	0.741064	-2.115878	0.024481
12	1	0	0.751215	-2.532993	-0.992522
13	1	0	1.068804	-2.916345	0.694611
14	6	0	-0.141638	0.394755	-0.846968
15	1	0	-0.431203	0.876254	-1.770242
16	7	0	-1.045185	-0.439986	-0.240341
17	6	0	-0.698165	-1.720459	0.378489

18	1	0	-1.419595	-2.469151	0.033291
19	1	0	-0.827348	-1.617271	1.463281
20	6	0	-2.263990	0.207440	-0.116242
21	16	0	-3.781804	-0.508926	-0.138065
22	6	0	-1.970784	1.613024	-0.006818
23	6	0	-1.219414	2.196488	1.165323
24	1	0	-2.712898	2.288116	-0.438775
25	1	0	-1.939536	2.470310	1.951793
26	1	0	-0.690609	3.115692	0.887498
27	1	0	-0.498462	1.500680	1.601363

8I



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.875642	1.451812	0.288724
2	6	0	-1.095204	0.302287	0.454131
3	6	0	-1.603668	-0.952902	0.055523
4	6	0	-2.866119	-1.016005	-0.545949
5	6	0	-3.631618	0.137725	-0.728502
6	6	0	-3.139693	1.372758	-0.300263
7	1	0	-1.496839	2.414128	0.617876
8	1	0	-3.256965	-1.979380	-0.864309
9	1	0	-4.609387	0.071204	-1.196533
10	1	0	-3.734108	2.272611	-0.428055
11	6	0	-0.809589	-2.209886	0.359696
12	1	0	-0.938664	-2.456589	1.423448
13	1	0	-1.206251	-3.059763	-0.203732
14	6	0	0.268270	0.304662	1.103186
15	1	0	0.167873	0.206278	2.194129
16	7	0	1.125800	-0.762044	0.538036
17	6	0	0.695723	-2.068252	0.069309
18	1	0	1.264423	-2.866305	0.560486
19	1	0	0.902516	-2.128288	-1.006365

20	6	0	2.115471	0.056137	0.114432
21	16	0	3.471471	-0.227113	-0.777514
22	6	0	1.427419	1.300649	0.699795
23	6	0	1.193716	2.430897	-0.295992
24	1	0	1.953359	1.678266	1.583283
25	1	0	0.676583	3.276394	0.168606
26	1	0	2.164927	2.781853	-0.658207
27	1	0	0.614013	2.098413	-1.161197