Supporting Information

COMPUTATIONAL STUDIES ON THE RACEMIZATION BARRIERS OF WINDING VINE-SHAPED HETEROBIARYLS WITH MOLECULAR ASYMMETRY‡

Atsunori Mori,[a]* Shiomi Ashida,[a] Yukiko Ito,[a] Jiaqiang Cheng,[a] Toyoko Suzuki,[a] Kentaro Okano,[a] Takayoshi Hashimoto[b]

[a]Department of Chemical Science and Engineering, Kobe University, 1-1 Rokkodai, Nada, Kobe 657-8501, Japan and [b]Research Facility Center for Science and Technology, Kobe University, 1-1 Rokkodai, Nada, Kobe 657-8501, Japan
E-mail: amori@kobe-u.ac.jp

Calculation results of 1 to 19:

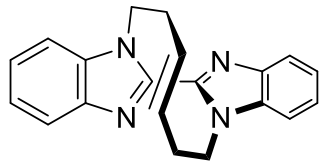	
1 GS	**1'** TS
−992.00877 au	−991.95598 au

Fig s1. Calculation studies on the isomerization of **1**

Cartesian coordinate of **1** (GS)

C	3.864315	0.872828	−1.828243
H	3.768226	1.572736	−2.652704
C	5.105598	0.488122	−1.334728
H	6.009557	0.894860	−1.779436
C	5.218445	−0.422904	−0.263875
H	6.205664	−0.699489	0.096011
C	4.095293	−0.979488	0.341510
H	4.192249	−1.683191	1.163445
C	2.849634	−0.591847	−0.161105
C	2.720423	0.329438	−1.228446
N	1.383379	0.547071	−1.512444
C	0.729539	−0.214788	−0.660085
C	1.158495	−1.637369	1.405386
H	1.906780	−2.409309	1.608673
H	0.206672	−2.135186	1.211123
N	1.553296	−0.945167	0.182958
C	1.046057	−0.670014	2.616846
H	2.011991	−0.170976	2.759179
H	0.852774	−1.277685	3.510441
C	−0.046787	0.338267	2.392881
H	−1.068089	−0.014077	2.547249
C	0.146556	1.550153	1.860241
H	1.167447	1.889623	1.677098
C	−0.952043	2.414499	1.306216
H	−0.740653	3.480366	1.460802
H	−1.906191	2.190351	1.797638
C	−1.117276	2.182332	−0.222605
H	−0.181151	2.365808	−0.753596
H	−1.871264	2.864296	−0.627178
C	−0.733965	−0.306780	−0.589613
N	−1.540603	0.819067	−0.529236
N	−1.403370	−1.441105	−0.583252
C	−2.733467	−1.066819	−0.505653
C	−3.887798	−1.860639	−0.472817

H	−3.807860	−2.942482	−0.518555
C	−2.842097	0.344066	−0.457696
C	−4.076636	0.992984	−0.362104
H	−4.158201	2.075471	−0.323053
C	−5.210271	0.185950	−0.323253
H	−6.189391	0.651246	−0.250496
C	−5.118040	−1.220267	−0.379702
H	−6.029367	−1.811022	−0.350287

Cartesian coordinate of **1'** (TS)

Atom	X	Y	Z
1 N	N1	−1.3681631	−1.6716324	0.0879941
2 C	C1	−0.8034158	−0.5065507	−0.1797443
3 N	N2	−1.7822855	0.4861064	−0.4317343
4 C	C2	−3.0133522	−0.1462595	−0.2652236
5 C	C3	−2.7207166	−1.4864919	0.0465528
6 C	C4	−3.7524430	−2.4132860	0.2639422
7 H	H2	−3.5140733	−3.4458543	0.4987434
8 C	C5	−5.0607697	−1.9603647	0.1709873
9 H	H1	−5.8839880	−2.6501827	0.3347014
10 C	C6	−5.3442795	−0.6114453	−0.1306468
11 H	H7	−6.3794162	−0.2867863	−0.1912196
12 C	C7	−4.3319979	0.3184145	−0.3502151
13 H	H6	−4.5785255	1.3522378	−0.5718556
14 C	C8	0.7004726	−0.5497876	−0.2053395
15 N	N3	1.7309160	0.3975848	−0.4363587
16 N	N4	1.2064394	−1.7291142	0.1104797
17 C	C9	2.5668609	−1.6024225	0.1121232
18 C	C10	2.9254839	−0.2841545	−0.2195793
19 C	C11	3.5530903	−2.5644535	0.3784716
20 H	H9	3.2673260	−3.5803065	0.6325994
21 C	C12	4.8817572	−2.1685440	0.3024278
22 H	H5	5.6708175	−2.8874240	0.5047858
23 C	C13	5.2302030	−0.8436041	−0.0341980
24 H	H11	6.2796896	−0.5665537	−0.0830170
25 C	C14	4.2630516	0.1217799	−0.3027714
26 H	H10	4.5536488	1.1372539	−0.5547523
27 C	C15	−1.7816353	1.9437072	−0.5438327
28 H	H3	−0.9919812	2.2679554	−1.2221104
29 H	H12	−2.7273637	2.2082588	−1.0234996
30 C	C16	1.8424483	1.7599480	−0.9585229
31 H	H8	2.6839681	1.7522620	−1.6592312
32 H	H14	0.9567039	2.0034239	−1.5464669
33 C	C17	2.0720035	2.8210828	0.1667815
34 H	H15	2.7093319	3.6266753	−0.2152166
35 H	H16	2.6003428	2.3441578	0.9985126
36 C	C18	−1.6386522	2.6859077	0.8141209
37 H	H4	−1.9272251	3.7325237	0.6515259
38 H	H18	−2.3295060	2.2556019	1.5463296
39 C	C19	−0.1904086	2.5851763	1.2056838
40 H	H19	0.1248140	1.7159898	1.7813253
41 C	C20	0.7084290	3.3164778	0.5407513
42 H	H20	0.3403133	4.1493734	−0.0644329

Point Group = C1 Order = 1 Nsymop = 1

Frequency calculation of **1'**

SPARTAN '14 Quantum Mechanics Driver: (Win/64b) Release 1.1.2

Job type : Geometry optimization.
Applying : Constraints
Method : B3LYP
Basis set : 6-31G*
With Options : PRINTMO THERMO PRINTFREQ

Charge : neutral (singlet)

Energy : -991.934823 hartrees
Solvation : -55.55 kJ/mol (SM54/AM1)

uncorrected Intensity
cm^{-1}
1 -41 0.01
2 39 0.66
3 72 0.25
4 76 0.35
5 110 0.43
6 130 0.11
7 159 0.53
8 200 2.22
9 210 0.89
10 246 0.82
11 254 0.51
12 263 0.69
13 269 1.02
14 297 1.44
15 327 2.22
16 336 1.15
17 377 1.17
18 408 1.37
19 447 5.88
20 451 0.50
21 487 1.89
22 498 0.81
23 524 0.58
24 551 2.42
25 570 3.34
26 574 4.48
27 584 2.21
28 597 2.98
29 599 0.13
30 622 1.71
31 633 0.69
32 668 3.55
33 704 6.05
34 714 1.46
35 726 4.37

36 752 52.20
37 755 57.81
38 771 0.25
39 775 4.81
40 792 8.68
41 822 0.12
42 848 8.06
43 854 1.77
44 859 0.98
45 872 0.42
46 892 8.13
47 916 0.57
48 921 2.71
49 924 9.40
50 927 1.17
51 929 2.04
52 973 0.10
53 974 0.07
54 980 1.32
55 998 34.64
56 1034 31.40
57 1040 7.32
58 1042 9.25
59 1057 5.05
60 1077 33.19
61 1090 4.43
62 1134 2.23
63 1139 0.12
64 1146 5.69
65 1170 9.12
66 1178 0.32
67 1184 0.30
68 1193 8.05
69 1197 19.47
70 1243 1.82
71 1261 12.01
72 1289 5.59
73 1296 13.40
74 1327 27.60
75 1332 10.54
76 1339 11.90
77 1344 26.44
78 1352 52.45
79 1359 42.19
80 1365 158.75
81 1368 55.72
82 1373 26.61
83 1376 5.18
84 1396 8.06
85 1404 15.19
86 1407 9.57
87 1408 19.55
88 1462 6.62
89 1471 35.17

90 1504 8.53
91 1510 4.50
92 1514 10.46
93 1515 3.82
94 1528 1.33
95 1530 2.01
96 1534 7.53
97 1552 19.72
98 1639 1.17
99 1642 0.50
100 1661 0.50
101 1662 2.85
102 1733 2.93
103 3054 22.47
104 3066 16.68
105 3079 41.88
106 3102 20.55
107 3108 8.04
108 3114 14.41
109 3125 33.70
110 3148 27.77
111 3159 23.69
112 3174 11.71
113 3186 0.15
114 3187 0.56
115 3197 17.13
116 3198 17.27
117 3209 41.36
118 3210 25.87
119 3222 17.35
120 3222 16.28

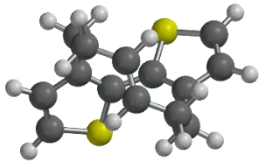	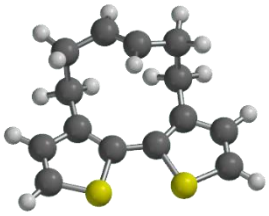
2 GS	**2'** TS
-17025916.61 (KJ/mol)	-17025809.7 (KJ/mol)

Fig s2. Calculation studies on the isomerization of **2**

Cartesian coordinate of **2** (GS)

S	−1.486338	−1.364399	−1.633667
C	−0.731105	−0.062566	−0.722691
C	−3.070555	−0.838960	−1.177591
H	−3.945403	−1.376593	−1.518686
C	−3.017493	0.275234	−0.389803
H	−3.901295	0.769585	0.002114

C	−1.686759	0.736782	−0.123870
C	0.731105	0.062566	−0.722691
C	1.686759	−0.736782	−0.123870
C	3.017493	−0.275234	−0.389803
H	3.901295	−0.769585	0.002114
C	3.070555	0.838960	−1.177591
H	3.945403	1.376593	−1.518686
S	1.486338	1.364399	−1.633667
C	−1.404644	1.912876	0.778924
H	−2.227595	2.634173	0.698803
H	−0.495942	2.431657	0.455739
C	−1.239974	1.503761	2.276477
H	−1.190292	2.420378	2.878821
H	−2.131544	0.950370	2.595983
C	1.404644	−1.912876	0.778924
H	0.495942	−2.431657	0.455739
H	2.227595	−2.634173	0.698803
C	1.239974	−1.503761	2.276477
H	2.131544	−0.950370	2.595983
H	1.190292	−2.420378	2.878821
C	0.006333	−0.667800	2.455459
H	−0.944557	−1.204011	2.435238
C	−0.006333	0.667800	2.455459
H	0.944557	1.204011	2.435238

Cartesian coordinate of **2'** (TS)

S	0.394969	2.659665	−0.270290
C	0.380628	0.932321	0.196798
C	2.103986	2.786097	−0.153986
H	2.601829	3.724993	−0.356191
C	2.643499	1.600442	0.227280
H	3.708431	1.454213	0.379445
C	1.700372	0.536106	0.446002
C	−0.984698	0.338813	0.183744
C	−1.590267	−0.895742	0.441635
C	−3.018154	−0.854200	0.287859
H	−3.632610	−1.733941	0.452052
C	−3.525385	0.352193	−0.075886
H	−4.555902	0.631330	−0.249684
S	−2.266557	1.508120	−0.249657
C	2.342791	−0.751267	0.926655
H	1.680316	−1.326552	1.577427
H	3.193731	−0.459470	1.554106
C	2.864367	−1.673446	−0.239446
H	3.046959	−1.065320	−1.131973
H	3.816923	−2.130965	0.051112
C	−1.028633	−2.268670	0.742089
H	−0.159576	−2.231358	1.402139
H	−1.804594	−2.827538	1.280129
C	−0.629133	−3.069388	−0.542632
H	−1.453092	−3.056083	−1.265210
H	−0.452472	−4.113423	−0.253195
C	0.631549	−2.439075	−1.056241

H	0.534224	-1.554799	-1.685620
C	1.792833	-2.697800	-0.450206
H	1.834821	-3.554901	0.227800

Frequency calculation of **2'**
Method: RB3LYP
Basis set: 6-31G(D)

Reason for exit: Successful completion
Quantum Calculation CPU Time : 36:09.47
Quantum Calculation Wall Time: 52:02.66

SPARTAN '14 Semi-Empirical Program: (Win/64b) Release 1.1.2
Semi-empirical Property Calculation

M0001

Guess from Archive
Energy Due to Solvation
Solvation Energy SM5.4/A -19.930
Memory Used: 3.016 Mb

Reason for exit: Successful completion
Semi-Empirical Program CPU Time : .08
Semi-Empirical Program Wall Time: .20

SPARTAN '14 Properties Program: (Win/64b) Release 1.1.2

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 21 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
1*	i 50.276	0.0000	1.2395	8.3144	4.1572	0.00	0.01
2*	49.082	0.2936	1.2395	8.3144	4.1572	21.09	0.24
3*	103.259	0.6176	1.2395	8.3144	4.1572	39.24	0.62
4*	109.962	0.6577	1.2395	8.3144	4.1572	41.18	0.25
5*	120.796	0.7225	1.2395	8.3144	4.1572	44.17	0.20
6*	168.190	1.0060	1.2395	8.3144	4.1572	55.59	3.34
7*	197.057	1.1787	1.2395	8.3144	4.1572	61.36	0.53
8*	242.335	1.4495	1.2395	7.4711	4.1572	68.95	1.12
9*	258.986	1.5491	1.2395	6.9813	4.1572	71.34	0.05
10*	265.425	1.5876	1.2213	6.8023	4.1572	72.22	0.87
11*	295.399	1.7669	1.1183	6.0367	4.1572	75.96	2.77
12*	326.155	1.9508	1.0199	5.3515	4.1572	79.28	0.09
13*	375.619	2.2467	0.8765	4.4214	4.1572	83.68	0.02
14*	392.195	2.3458	0.8323	4.1496	4.1572	84.93	1.57
15*	444.360	2.6579	0.7053	3.4016	4.1572	88.29	1.78
16*	466.829	2.7923	0.6559	3.1233	4.1572	89.49	2.21

17*	488.282	2.9206	0.6115	2.8789	4.1572	90.52	0.06
18*	506.133	3.0273	0.5766	2.6901	4.1572	91.31	1.76
19*	542.368	3.2441	0.5109	2.3439	4.1572	92.70	2.08
20*	548.812	3.2826	0.5000	2.2871	4.1572	92.92	8.35
21*	567.218	3.3927	0.4698	2.1322	4.1572	93.53	3.77
22	633.460	3.7889	0.3740	1.6550	4.0239	95.30	13.85
23	650.511	3.8909	0.3524	1.5500	3.8779	95.67	3.99
24	687.234	4.1106	0.3095	1.3454	3.5725	96.37	26.89
25	697.700	4.1732	0.2982	1.2921	3.4879	96.55	2.40
26	732.507	4.3814	0.2632	1.1289	3.2145	97.08	40.30
27	742.649	4.4420	0.2538	1.0853	3.1373	97.22	5.22
28	785.202	4.6965	0.2173	0.9191	2.8260	97.74	13.13
29	814.572	4.8722	0.1951	0.8191	2.6234	98.04	6.31
30	832.685	4.9806	0.1824	0.7627	2.5035	98.20	13.42
31	852.385	5.0984	0.1695	0.7057	2.3776	98.36	17.36
32	867.169	5.1868	0.1604	0.6656	2.2861	98.48	18.25
33	872.155	5.2166	0.1574	0.6525	2.2558	98.51	1.52
34	879.320	5.2595	0.1532	0.6343	2.2128	98.56	10.77
35	906.078	5.4196	0.1385	0.5703	2.0577	98.74	0.31
36	907.369	5.4273	0.1379	0.5673	2.0504	98.75	9.69
37	920.013	5.5029	0.1314	0.5394	1.9802	98.82	8.53
38	958.346	5.7322	0.1135	0.4628	1.7786	99.02	0.76
39	1000.521	5.9844	0.0965	0.3906	1.5758	99.20	0.94
40	1004.502	6.0083	0.0951	0.3843	1.5577	99.22	0.70
41	1036.197	6.1978	0.0841	0.3381	1.4193	99.33	7.91
42	1041.037	6.2268	0.0825	0.3315	1.3991	99.34	24.89
43	1083.831	6.4827	0.0698	0.2786	1.2305	99.46	2.44
44	1099.498	6.5765	0.0656	0.2614	1.1732	99.50	0.02
45	1111.513	6.6483	0.0626	0.2489	1.1308	99.53	0.48
46	1133.024	6.7770	0.0575	0.2279	1.0581	99.58	7.94
47	1163.092	6.9568	0.0510	0.2014	0.9633	99.63	0.79
48	1178.121	7.0467	0.0480	0.1893	0.9188	99.66	9.01
49	1204.889	7.2068	0.0431	0.1695	0.8438	99.70	4.59
50	1221.754	7.3077	0.0403	0.1581	0.7994	99.72	0.18
51	1247.240	7.4601	0.0364	0.1423	0.7363	99.76	0.65
52	1269.546	7.5936	0.0332	0.1297	0.6846	99.78	4.78
53	1295.213	7.7471	0.0300	0.1165	0.6293	99.81	0.71
54	1338.901	8.0084	0.0251	0.0971	0.5442	99.84	6.65
55	1355.823	8.1096	0.0234	0.0905	0.5142	99.86	10.96
56	1365.004	8.1645	0.0225	0.0870	0.4985	99.86	0.87
57	1385.779	8.2888	0.0207	0.0798	0.4647	99.88	7.51
58	1388.122	8.3028	0.0205	0.0790	0.4610	99.88	0.76
59	1390.276	8.3157	0.0203	0.0783	0.4576	99.88	0.18
60	1394.052	8.3383	0.0200	0.0770	0.4518	99.88	5.12
61	1397.608	8.3595	0.0197	0.0759	0.4463	99.88	25.82
62	1426.796	8.5341	0.0175	0.0671	0.4039	99.90	2.98
63	1457.685	8.7189	0.0154	0.0589	0.3631	99.91	3.14
64	1518.616	9.0833	0.0119	0.0455	0.2936	99.93	0.05
65	1521.278	9.0993	0.0118	0.0450	0.2909	99.94	7.21
66	1522.093	9.1041	0.0118	0.0448	0.2900	99.94	6.66
67	1525.349	9.1236	0.0116	0.0442	0.2867	99.94	7.24
68	1558.372	9.3211	0.0101	0.0384	0.2551	99.95	9.36
69	1568.679	9.3828	0.0097	0.0368	0.2460	99.95	7.62
70	1783.135	10.6655	0.0039	0.0146	0.1128	99.98	3.84

```
71 3024.677 18.0916 0.0000 0.0001 0.0008 100.00 48.65
72 3035.262 18.1549 0.0000 0.0001 0.0008 100.00 17.83
73 3047.787 18.2298 0.0000 0.0001 0.0007 100.00 60.07
74 3050.466 18.2458 0.0000 0.0001 0.0007 100.00 53.72
75 3081.085 18.4290 0.0000 0.0000 0.0006 100.00 25.34
76 3087.408 18.4668 0.0000 0.0000 0.0006 100.00 12.74
77 3091.853 18.4934 0.0000 0.0000 0.0006 100.00 19.04
78 3099.417 18.5386 0.0000 0.0000 0.0006 100.00 11.45
79 3129.861 18.7207 0.0000 0.0000 0.0005 100.00 6.98
80 3135.606 18.7551 0.0000 0.0000 0.0005 100.00 51.86
81 3208.859 19.1932 0.0000 0.0000 0.0004 100.00 16.37
82 3209.301 19.1959 0.0000 0.0000 0.0004 100.00 8.63
83 3267.818 19.5459 0.0000 0.0000 0.0003 100.00 0.43
84 3269.892 19.5583 0.0000 0.0000 0.0003 100.00 0.35
-- ---------- ------- ------- ------- ----
Total Vibrations 633.6298 25.0330 138.2560 156.0758

Ideal Gas 2.4789
Translation 3.7184 177.4261 12.4716
Rotation 3.7184 138.0281 12.4716
---------- ------- ------- -------
Totals 668.5785 453.7103 181.0191

Vibrational(v) Corrections:
Temp. Correction Hv 668.5785
Entropy Correction (Hv-TSv) 533.3048

Reason for exit: Successful completion
Properties CPU Time : .95
Properties Wall Time: 1.05
```

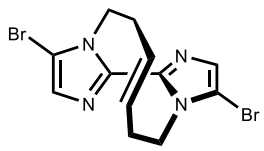	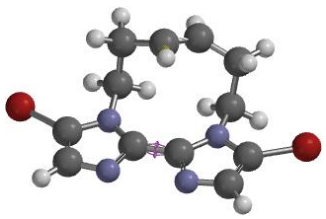
3 GS	**3'** TS
-5831.243256 au	-5831.185460 au

Fig s3. Calculation studies on the isomerization of **3**

Cartesian coordinate of **3** (GS)

N	-1.045945	-1.444907	-1.382909
C	-0.684088	-0.260152	-0.914486
N	-1.753822	0.445583	-0.402956
C	-2.844583	-0.386983	-0.566710
C	-2.396078	-1.533023	-1.173912
H	-2.974069	-2.392739	-1.481577

C	0.684088	0.260152	−0.914486
N	1.045945	1.444907	−1.382909
C	2.844583	0.386983	−0.566710
C	2.396078	1.533023	−1.173912
H	2.974069	2.392739	−1.481577
N	1.753822	−0.445583	−0.402956
C	−1.684013	1.659689	0.413779
H	−0.891253	2.280979	−0.005880
H	−2.631424	2.193001	0.305088
C	−1.414402	1.341150	1.910690
H	−2.227547	0.710659	2.289082
H	−1.455600	2.291215	2.458353
C	1.684013	−1.659689	0.413779
H	0.891253	−2.280979	−0.005880
H	2.631424	−2.193001	0.305088
C	1.414402	−1.341150	1.910690
H	1.455600	−2.291215	2.458353
H	2.227547	−0.710659	2.289082
C	0.084078	−0.663382	2.087112
H	−0.797088	−1.307081	2.069797
C	−0.084078	0.663382	2.087112
H	0.797088	1.307081	2.069797
Br	−4.603163	0.100876	−0.074858
Br	4.603163	−0.100876	−0.074858

Cartesian coordinate of 3' (TS)

N	−1.333094	2.172855	−0.403013
C	−0.787214	1.026178	−0.006736
N	−1.797694	0.102673	0.303628
C	−2.991193	0.772980	0.044579
C	−2.678372	2.031485	−0.379699
H	−3.350623	2.831673	−0.656836
C	0.715416	1.054826	0.042085
N	1.239303	2.204685	−0.373520
C	2.925433	0.855166	0.116029
C	2.586889	2.097340	−0.334681
H	3.242200	2.906208	−0.626791
N	1.746277	0.159425	0.374939
C	−1.821436	−1.333103	0.599782
H	−1.020962	−1.569000	1.299863
H	−2.763524	−1.525376	1.115882
C	−1.698806	−2.229650	−0.662784
H	−2.406360	−1.894374	−1.427776
H	−1.979961	−3.248893	−0.368678
C	1.830230	−1.179344	0.971683
H	2.669785	−1.156741	1.669046
H	0.934538	−1.354217	1.567809
C	2.025809	−2.312174	−0.087412
H	2.518576	−1.893428	−0.970204
H	2.685760	−3.082445	0.325587
C	0.653158	−2.837378	−0.375469
H	0.298906	−3.606069	0.317040
C	−0.258866	−2.173816	−1.090806

H	0.045767	-1.367432	-1.757032
Br	-4.709917	0.014192	0.262333
Br	4.657300	0.148816	0.394033

Frequency calculation of **3'**

Term	ZPE cm-1	Enthalpy kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	**i 58.541**	**0.0000**	**1.2395**	**8.3144**	**4.1572**	**0.00**	**0.02**
2*	27.539	0.1647	1.2395	8.3144	4.1572	12.44	0.01
3*	55.194	0.3301	1.2395	8.3144	4.1572	23.38	0.04
4*	90.501	0.5413	1.2395	8.3144	4.1572	35.39	0.16
5*	119.839	0.7168	1.2395	8.3144	4.1572	43.92	0.05
6*	135.089	0.8080	1.2395	8.3144	4.1572	47.89	0.29
7*	166.657	0.9968	1.2395	8.3144	4.1572	55.26	0.58
8*	201.049	1.2025	1.2395	8.3144	4.1572	62.10	0.26
9*	205.619	1.2299	1.2395	8.3144	4.1572	62.93	0.27
10*	233.005	1.3937	1.2395	7.7641	4.1572	67.52	1.18
11*	237.530	1.4207	1.2395	7.6202	4.1572	68.22	3.18
12*	260.175	1.5562	1.2395	6.9479	4.1572	71.51	2.09
13*	286.316	1.7125	1.1488	6.2577	4.1572	74.88	1.19
14*	298.473	1.7853	1.1081	5.9640	4.1572	76.32	1.22
15*	350.774	2.0981	0.9463	4.8647	4.1572	81.60	3.43
16*	369.743	2.2116	0.8926	4.5222	4.1572	83.21	0.38
17*	381.072	2.2793	0.8618	4.3300	4.1572	84.10	1.81
18*	407.843	2.4394	0.7924	3.9089	4.1572	86.03	4.18
19*	468.948	2.8049	0.6514	3.0982	4.1572	89.60	1.84
20*	491.865	2.9420	0.6044	2.8400	4.1572	90.69	1.82
21*	540.862	3.2351	0.5135	2.3574	4.1572	92.65	1.87
22*	558.341	3.3396	0.4841	2.2056	4.1572	93.24	3.00
23*	569.854	3.4085	0.4656	2.1109	4.1572	93.61	4.30
24	619.953	3.7081	0.3920	1.7430	4.1412	94.98	1.65
25	627.317	3.7522	0.3821	1.6944	4.0770	95.16	0.94
26	668.666	3.9995	0.3306	1.4454	3.7254	96.03	4.75
27	683.547	4.0885	0.3136	1.3647	3.6026	96.31	4.90
28	690.966	4.1329	0.3054	1.3262	3.5422	96.44	11.37
29	714.430	4.2732	0.2809	1.2110	3.3549	96.82	0.67
30	830.450	4.9672	0.1839	0.7695	2.5181	98.18	5.05
31	847.313	5.0681	0.1728	0.7199	2.4096	98.32	4.02
32	847.614	5.0699	0.1726	0.7191	2.4077	98.33	19.00
33	850.955	5.0898	0.1704	0.7096	2.3866	98.35	9.56
34	887.872	5.3107	0.1484	0.6131	2.1623	98.62	8.66
35	902.764	5.3997	0.1403	0.5778	2.0764	98.72	36.88
36	916.500	5.4819	0.1332	0.5471	1.9995	98.80	21.55
37	923.028	5.5209	0.1299	0.5330	1.9637	98.84	20.94
38	976.717	5.8421	0.1058	0.4298	1.6879	99.10	1.62
39	991.802	5.9323	0.0998	0.4045	1.6162	99.17	46.85
40	1013.942	6.0647	0.0916	0.3700	1.5154	99.25	34.30
41	1040.154	6.2215	0.0828	0.3327	1.4027	99.34	9.28
42	1071.766	6.4106	0.0731	0.2926	1.2762	99.43	2.54
43	1089.244	6.5151	0.0683	0.2725	1.2104	99.48	3.99
44	1112.891	6.6566	0.0622	0.2475	1.1260	99.53	10.23
45	1130.864	6.7641	0.0579	0.2299	1.0652	99.57	0.66
46	1170.026	6.9983	0.0496	0.1958	0.9425	99.65	0.71

```
47 1181.178 7.0650 0.0474 0.1870 0.9099 99.67 0.37
48 1212.340 7.2514 0.0419 0.1644 0.8240 99.71 21.99
49 1216.532 7.2765 0.0412 0.1616 0.8130 99.72 2.74
50 1242.819 7.4337 0.0370 0.1449 0.7469 99.75 0.06
51 1270.191 7.5974 0.0332 0.1293 0.6832 99.78 18.06
52 1297.985 7.7637 0.0296 0.1152 0.6235 99.81 0.11
53 1324.960 7.9250 0.0265 0.1029 0.5701 99.83 1.99
54 1335.232 7.9865 0.0255 0.0986 0.5509 99.84 18.05
55 1342.363 8.0291 0.0247 0.0957 0.5379 99.85 53.95
56 1354.062 8.0991 0.0236 0.0911 0.5172 99.85 85.34
57 1360.963 8.1404 0.0229 0.0885 0.5053 99.86 20.67
58 1376.152 8.2312 0.0215 0.0831 0.4801 99.87 9.51
59 1378.107 8.2429 0.0214 0.0824 0.4769 99.87 11.85
60 1395.815 8.3488 0.0199 0.0765 0.4491 99.88 9.12
61 1396.374 8.3522 0.0198 0.0763 0.4482 99.88 10.24
62 1403.701 8.3960 0.0192 0.0740 0.4372 99.89 4.41
63 1418.315 8.4834 0.0181 0.0696 0.4159 99.89 1.20
64 1436.339 8.5912 0.0168 0.0645 0.3909 99.90 12.54
65 1452.903 8.6903 0.0157 0.0601 0.3692 99.91 1.25
66 1508.049 9.0201 0.0125 0.0476 0.3047 99.93 4.68
67 1510.904 9.0372 0.0123 0.0470 0.3016 99.93 2.81
68 1524.100 9.1161 0.0117 0.0444 0.2880 99.94 0.85
69 1547.082 9.2536 0.0106 0.0403 0.2655 99.94 23.19
70 1548.586 9.2626 0.0105 0.0401 0.2641 99.94 129.77
71 1555.792 9.3057 0.0102 0.0388 0.2575 99.95 7.97
72 1732.836 10.3647 0.0048 0.0182 0.1358 99.98 2.47
73 3058.237 18.2923 0.0000 0.0001 0.0007 100.00 20.51
74 3075.879 18.3978 0.0000 0.0000 0.0007 100.00 24.65
75 3107.992 18.5899 0.0000 0.0000 0.0006 100.00 7.66
76 3111.738 18.6123 0.0000 0.0000 0.0006 100.00 9.07
77 3116.305 18.6396 0.0000 0.0000 0.0006 100.00 4.10
78 3122.667 18.6777 0.0000 0.0000 0.0005 100.00 18.06
79 3129.013 18.7157 0.0000 0.0000 0.0005 100.00 34.73
80 3161.609 18.9106 0.0000 0.0000 0.0005 100.00 18.09
81 3167.431 18.9454 0.0000 0.0000 0.0004 100.00 10.42
82 3174.352 18.9868 0.0000 0.0000 0.0004 100.00 14.61
83 3272.953 19.5766 0.0000 0.0000 0.0003 100.00 6.44
84 3273.099 19.5775 0.0000 0.0000 0.0003 100.00 5.46
-- ---------- ------- ------- ------- ----
Total Vibrations 605.0712 27.8685 158.6130 160.3982

Ideal Gas 2.4789
Translation 3.7184 182.5664 12.4716
Rotation 3.7184 146.1479 12.4716
---------- ------- ------- -------
Totals 642.8554 487.3273 185.3415

Vibrational(v) Corrections:
Temp. Correction Hv 642.8554
Entropy Correction (Hv-TSv) 497.5588

Reason for exit: Successful completion
Properties CPU Time : 1.14
Properties Wall Time: 1.27
```

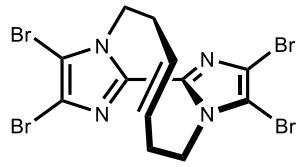	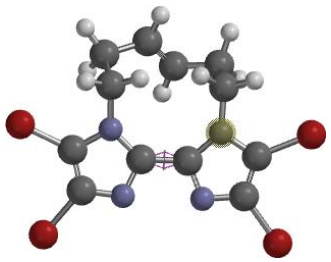
4 GS	**4'** TS
-10977.797017 au	-10977.739209 au

Fig s4. Calculation studies on the isomerization of **4**

Cartesian coordinate of **4** (GS)

N	1.437837	-1.053292	0.872603
C	0.730787	-0.034199	0.403123
N	1.530988	0.962329	-0.105470
C	2.830254	0.512828	0.054217
C	2.736376	-0.720860	0.659346
C	-0.730787	0.034199	0.403123
N	-1.437837	1.053292	0.872603
N	-1.530988	-0.962329	-0.105470
C	-2.736376	0.720860	0.659346
C	-2.830254	-0.512828	0.054217
C	1.095232	2.096136	-0.926326
H	0.147123	2.444428	-0.513899
H	1.832095	2.893521	-0.810958
C	0.949790	1.703422	-2.422742
H	0.710958	2.619535	-2.977114
H	1.917879	1.341319	-2.787937
C	-1.095232	-2.096136	-0.926326
H	-0.147123	-2.444428	-0.513899
H	-1.832095	-2.893521	-0.810958
C	-0.949790	-1.703422	-2.422742
H	-1.917879	-1.341319	-2.787937
H	-0.710958	-2.619535	-2.977114
C	0.116827	-0.658655	-2.601495
H	1.149059	-1.012576	-2.587526
C	-0.116827	0.658655	-2.601495
H	-1.149059	1.012576	-2.587526
Br	-4.154345	1.852631	1.171447
Br	-4.333657	-1.517754	-0.449341
Br	4.154345	-1.852631	1.171447
Br	4.333657	1.517754	-0.449341

Cartesian coordinate of **4'** (TS)

N	-1.253227	-1.265462	0.010988
C	-0.736842	-0.065554	0.270991

N	−1.770767	0.855193	0.484040
C	−2.952158	0.131811	0.322649
C	−2.587156	−1.157184	0.039363
C	0.764277	−0.040696	0.215079
N	1.304990	−1.233159	−0.028647
N	1.776407	0.909108	0.396072
C	2.636615	−1.089761	−0.027126
C	2.973378	0.213071	0.227560
C	−1.854151	2.266657	0.883804
H	−2.693405	2.340990	1.577630
H	−0.957720	2.518672	1.449848
C	−2.047971	3.234730	−0.329042
H	−2.532640	2.691078	−1.145558
H	−2.714062	4.051719	−0.032974
C	1.799498	2.374204	0.488250
H	0.998579	2.702610	1.149494
H	2.741815	2.635275	0.971515
C	1.676781	3.081659	−0.887996
H	2.384438	2.642280	−1.598026
H	1.958331	4.131873	−0.740426
C	0.236798	2.964940	−1.303777
H	−0.066896	2.077372	−1.857821
C	−0.675509	3.718180	−0.684619
H	−0.323260	4.572902	−0.100998
Br	3.802070	−2.541460	−0.331563
Br	4.683898	0.989869	0.357385
Br	−3.723789	−2.630288	−0.277654
Br	−4.675507	0.864506	0.512256

Frequency calculation of 4'

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 15 low frequency terms

Term	ZPE	Correction	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1*	**i 25.372**	**0.0000**	**1.2395**	**0.0000**	**8.3144 0.00 0.01**
2*	30.177	0.1805	1.2395	24.3414	8.2997 13.55 0.09
3*	52.645	0.3149	1.2395	19.7294	8.2698 22.43 0.03
4*	66.122	0.3955	1.2395	17.8471	8.2442 27.32 0.17
5*	75.057	0.4489	1.2395	16.8034	8.2241 30.39 0.57
6*	104.884	0.6273	1.2395	14.0642	8.1392 39.72 0.14
7*	113.618	0.6796	1.2395	13.4143	8.1092 42.21 0.17
8*	130.829	0.7825	1.2395	12.2750	8.0437 46.81 0.30
9*	150.513	0.9003	1.2395	11.1533	7.9583 51.63 0.14
10*	154.283	0.9228	1.2395	10.9566	7.9408 52.50 0.96
11*	162.102	0.9696	1.2395	10.5650	7.9031 54.26 1.36
12*	180.092	1.0772	1.2395	9.7380	7.8103 58.07 0.12
13*	188.299	1.1263	1.2395	9.3909	7.7652 59.69 0.13
14*	243.562	1.4568	1.2395	7.4336	7.4199 69.13 0.71
15*	260.225	1.5565	1.2395	6.9464	7.3028 71.51 3.37
16	280.574	1.6782	1.1684	6.4021	7.1527 74.18 2.27
17	289.595	1.7322	1.1377	6.1769	7.0838 75.28 1.78

18	294.712	1.7628	1.1206	6.0531	7.0441	75.88	2.01
19	319.028	1.9082	1.0420	5.5022	6.8499	78.55	0.72
20	361.302	2.1611	0.9162	4.6713	6.4934	82.51	0.14
21	400.209	2.3938	0.8117	4.0245	6.1490	85.50	2.48
22	420.407	2.5146	0.7615	3.7262	5.9658	86.85	1.04
23	427.570	2.5574	0.7443	3.6259	5.9004	87.30	5.36
24	485.466	2.9037	0.6172	2.9098	5.3650	90.39	3.51
25	491.659	2.9408	0.6048	2.8422	5.3075	90.68	0.75
26	500.639	2.9945	0.5871	2.7469	5.2241	91.07	0.11
27	570.158	3.4103	0.4651	2.1084	4.5848	93.62	4.61
28	577.068	3.4516	0.4543	2.0536	4.5223	93.83	0.97
29	609.723	3.6470	0.4061	1.8126	4.2309	94.73	3.51
30	638.445	3.8187	0.3676	1.6236	3.9810	95.41	1.52
31	643.146	3.8469	0.3616	1.5945	3.9407	95.51	0.34
32	683.813	4.0901	0.3133	1.3633	3.6004	96.31	7.48
33	689.491	4.1241	0.3070	1.3337	3.5542	96.41	3.61
34	697.341	4.1710	0.2986	1.2939	3.4907	96.54	0.97
35	708.567	4.2382	0.2869	1.2388	3.4011	96.73	0.65
36	842.795	5.0410	0.1757	0.7329	2.4383	98.29	1.98
37	858.160	5.1329	0.1659	0.6897	2.3415	98.41	4.96
38	899.547	5.3805	0.1420	0.5853	2.0948	98.70	15.14
39	924.198	5.5279	0.1293	0.5305	1.9574	98.84	8.22
40	961.373	5.7503	0.1122	0.4572	1.7634	99.03	11.12
41	968.978	5.7958	0.1090	0.4434	1.7256	99.07	38.50
42	984.684	5.8897	0.1026	0.4163	1.6497	99.14	60.84
43	996.570	5.9608	0.0980	0.3968	1.5940	99.18	39.99
44	1032.852	6.1778	0.0852	0.3427	1.4334	99.32	19.53
45	1048.503	6.2714	0.0801	0.3217	1.3683	99.37	30.45
46	1073.591	6.4215	0.0726	0.2905	1.2692	99.44	10.65
47	1091.830	6.5306	0.0676	0.2697	1.2009	99.49	2.92
48	1118.179	6.6882	0.0609	0.2422	1.1078	99.55	6.41
49	1168.037	6.9864	0.0500	0.1974	0.9485	99.64	26.74
50	1179.406	7.0544	0.0478	0.1883	0.9150	99.66	5.29
51	1188.650	7.1097	0.0460	0.1813	0.8886	99.68	0.91
52	1241.314	7.4247	0.0373	0.1458	0.7505	99.75	2.09
53	1254.968	7.5064	0.0353	0.1378	0.7180	99.77	18.47
54	1297.368	7.7600	0.0297	0.1155	0.6248	99.81	16.75
55	1326.884	7.9365	0.0263	0.1021	0.5665	99.83	2.43
56	1336.562	7.9944	0.0253	0.0981	0.5485	99.84	22.83
57	1347.394	8.0592	0.0242	0.0937	0.5289	99.85	196.01
58	1351.286	8.0825	0.0238	0.0922	0.5221	99.85	1.53
59	1360.520	8.1377	0.0230	0.0887	0.5061	99.86	81.63
60	1365.592	8.1681	0.0225	0.0868	0.4975	99.86	13.75
61	1376.002	8.2303	0.0215	0.0831	0.4803	99.87	12.43
62	1384.216	8.2794	0.0208	0.0803	0.4671	99.87	14.32
63	1386.171	8.2911	0.0207	0.0796	0.4640	99.88	33.61
64	1394.815	8.3428	0.0199	0.0768	0.4506	99.88	2.13
65	1402.764	8.3904	0.0193	0.0743	0.4386	99.89	10.12
66	1423.395	8.5138	0.0177	0.0681	0.4087	99.90	7.85
67	1458.730	8.7251	0.0153	0.0586	0.3618	99.91	10.79
68	1505.394	9.0043	0.0126	0.0481	0.3075	99.93	4.60
69	1508.038	9.0201	0.0125	0.0476	0.3047	99.93	3.40
70	1523.580	9.1130	0.0117	0.0445	0.2885	99.94	2.59
71	1534.377	9.1776	0.0112	0.0425	0.2777	99.94	298.15

```
72 1543.116 9.2299 0.0108 0.0410 0.2693 99.94 30.76
73 1545.701 9.2453 0.0107 0.0405 0.2668 99.94 10.20
74 1737.971 10.3954 0.0047 0.0178 0.1333 99.98 2.57
75 3060.570 18.3063 0.0000 0.0001 0.0007 100.00 19.55
76 3077.684 18.4086 0.0000 0.0000 0.0007 100.00 22.30
77 3112.272 18.6155 0.0000 0.0000 0.0006 100.00 5.05
78 3114.920 18.6314 0.0000 0.0000 0.0006 100.00 8.05
79 3116.998 18.6438 0.0000 0.0000 0.0006 100.00 3.51
80 3125.878 18.6969 0.0000 0.0000 0.0005 100.00 16.26
81 3132.318 18.7354 0.0000 0.0000 0.0005 100.00 38.60
82 3164.145 18.9258 0.0000 0.0000 0.0005 100.00 15.92
83 3170.116 18.9615 0.0000 0.0000 0.0004 100.00 10.10
84 3175.344 18.9928 0.0000 0.0000 0.0004 100.00 12.43
-- ---------- ------- ------- ------- ----
Total Vibrations 551.4489 33.3657 255.8122 258.4704 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 186.9757 12.4716
Rotation 3.7184 154.6307 12.4716
---------- ------- ------- -------
Totals 594.7304 597.4186 283.4136

Vibrational(v) Corrections:
Temp. Correction Hv 594.7304
Entropy Correction (Hv-TSv) 416.6101

Reason for exit: Successful completion
Properties CPU Time : 2.92
Properties Wall Time: 2.92
```

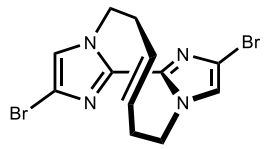	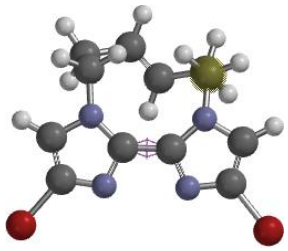
5 GS	**5'** TS
-5831.249227 au	-5831.194495 au

Fig s5. Calculation studies on the isomerization of **5**

Cartesian coordinate of **5** (GS)

N	−1.693051	0.562801	0.725755
C	−0.706909	−0.188966	0.250328
N	−1.170477	−1.377066	−0.262732
C	−2.540884	−1.361809	−0.106856
H	−3.169051	−2.182976	−0.415028
C	−2.819057	−0.162928	0.502832
C	0.706909	0.188966	0.250328

N	1.693051	−0.562801	0.725755
N	1.170477	1.377066	−0.262732
C	2.819057	0.162928	0.502832
C	2.540884	1.361809	−0.106856
H	3.169051	2.182976	−0.415028
C	−0.424820	−2.330347	−1.085660
H	0.584413	−2.402376	−0.676029
H	−0.905038	−3.307403	−0.977808
C	0.424820	2.330347	−1.085660
H	−0.584413	2.402376	−0.676029
H	0.905038	3.307403	−0.977808
C	−0.396491	−1.908582	−2.581318
H	0.103921	−2.710026	−3.139426
H	−1.428511	−1.847295	−2.946888
C	0.396491	1.908582	−2.581318
H	1.428511	1.847295	−2.946888
H	−0.103921	2.710026	−3.139426
C	−0.309230	0.593010	−2.757941
H	−1.399965	0.621539	−2.740393
C	0.309230	−0.593010	−2.757941
H	1.399965	−0.621539	−2.740393
Br	4.531732	−0.461782	1.028314
Br	−4.531732	0.461782	1.028314

Cartesian coordinate of **5'** (TS)

N	1.368421	−0.877544	−0.012982
C	0.755976	0.274787	0.263540
N	1.712370	1.280063	0.444041
C	2.947122	0.683038	0.250662
H	3.866034	1.243464	0.324369
C	2.687338	−0.629521	−0.024441
C	−0.734728	0.176049	0.354607
N	−1.218800	−1.037098	0.084586
N	−1.796261	1.053956	0.609519
C	−2.555589	−0.954162	0.153732
C	−2.957557	0.311311	0.471883
H	−3.930759	0.746172	0.637671
C	1.693994	2.745329	0.530678
H	0.924809	3.068748	1.233475
H	2.659478	3.029925	0.959090
C	−1.970337	2.453068	1.025946
H	−2.818965	2.456612	1.716191
H	−1.100895	2.773840	1.601618
C	1.483099	3.445788	−0.838489
H	1.716050	4.509780	−0.702996
H	2.183617	3.037358	−1.574218
C	−2.233231	3.419600	−0.173163
H	−2.923146	4.209230	0.144205
H	−2.715437	2.856813	−0.979077
C	−0.892808	3.965325	−0.559813
H	−0.567899	4.838169	0.012728
C	0.037524	3.255207	−1.202561
H	−0.238767	2.353160	−1.746820
Br	−3.679640	−2.449767	−0.152202

Br 3.963328 -1.982281 -0.378999

Frequency calculation of 5'

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 11 low frequency terms

	Enthalpy Term	ZPE	Correction	Entropy	Cv	% in
	cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
1*	**i 35.295**	**0.0000**	**1.2395**	**0.0000**	**8.3144**	**0.00 0.05**
2*	61.904	0.3703	1.2395	18.3909	8.2529	25.82 0.04
3*	70.729	0.4231	1.2395	17.2922	8.2342	28.92 0.64
4*	88.996	0.5323	1.2395	15.4054	8.1878	34.91 3.26
5*	101.822	0.6090	1.2395	14.3055	8.1491	38.82 0.50
6*	141.484	0.8463	1.2395	11.6469	7.9988	49.48 1.36
7*	155.019	0.9272	1.2395	10.9189	7.9373	52.67 0.04
8*	169.245	1.0123	1.2395	10.2250	7.8673	55.81 0.13
9*	206.212	1.2334	1.2395	8.6899	7.6610	63.03 0.23
10*	221.779	1.3265	1.2395	8.1358	7.5643	65.71 2.16
11*	244.343	1.4615	1.2395	7.4099	7.4145	69.25 2.64
12	270.188	1.6161	1.2045	6.6734	7.2303	72.85 2.90
13	286.230	1.7120	1.1490	6.2598	7.1097	74.87 0.22
14	290.336	1.7366	1.1352	6.1588	7.0781	75.37 0.28
15	362.519	2.1683	0.9128	4.6495	6.4828	82.61 0.97
16	372.651	2.2289	0.8846	4.4720	6.3943	83.44 0.12
17	394.225	2.3580	0.8271	4.1175	6.2028	85.08 0.23
18	443.815	2.6546	0.7066	3.4087	5.7510	88.25 0.85
19	477.483	2.8560	0.6335	2.9994	5.4391	90.02 10.19
20	492.176	2.9439	0.6037	2.8366	5.3027	90.70 1.43
21	496.670	2.9707	0.5949	2.7886	5.2609	90.90 0.93
22	562.939	3.3671	0.4766	2.1673	4.6503	93.39 3.56
23	572.491	3.4243	0.4614	2.0897	4.5636	93.69 1.01
24	628.818	3.7612	0.3801	1.6847	4.0640	95.19 1.28
25	645.784	3.8626	0.3582	1.5785	3.9181	95.57 13.94
26	677.295	4.0511	0.3206	1.3981	3.6539	96.19 4.12
27	688.514	4.1182	0.3081	1.3388	3.5621	96.39 9.37
28	695.826	4.1620	0.3002	1.3015	3.5029	96.52 2.98
29	702.916	4.2044	0.2927	1.2663	3.4461	96.64 2.96
30	717.554	4.2919	0.2778	1.1964	3.3303	96.87 27.33
31	731.402	4.3748	0.2643	1.1338	3.2230	97.07 0.82
32	842.560	5.0396	0.1758	0.7336	2.4398	98.29 4.74
33	856.932	5.1256	0.1667	0.6931	2.3492	98.40 4.48
34	898.309	5.3731	0.1427	0.5882	2.1019	98.69 9.79
35	923.607	5.5244	0.1296	0.5318	1.9606	98.84 12.01
36	962.123	5.7548	0.1119	0.4558	1.7596	99.04 53.95
37	969.043	5.7962	0.1090	0.4433	1.7253	99.07 21.30
38	978.264	5.8513	0.1052	0.4272	1.6804	99.11 54.92
39	987.008	5.9036	0.1017	0.4124	1.6387	99.15 3.55
40	1029.744	6.1592	0.0862	0.3471	1.4466	99.31 14.62
41	1046.973	6.2623	0.0806	0.3237	1.3746	99.36 25.04
42	1056.761	6.3208	0.0776	0.3111	1.3350	99.39 32.22
43	1091.502	6.5286	0.0677	0.2700	1.2021	99.48 0.98
44	1103.974	6.6032	0.0644	0.2566	1.1572	99.51 6.77
45	1153.515	6.8996	0.0530	0.2095	0.9927	99.62 6.12

```
46 1170.121 6.9989 0.0496 0.1957 0.9423 99.65 11.43
47 1177.424 7.0426 0.0482 0.1899 0.9208 99.66 20.81
48 1188.823 7.1107 0.0460 0.1812 0.8881 99.68 0.41
49 1198.153 7.1665 0.0443 0.1743 0.8622 99.69 0.99
50 1243.620 7.4385 0.0369 0.1444 0.7450 99.75 13.26
51 1255.462 7.5093 0.0352 0.1375 0.7168 99.77 16.94
52 1293.631 7.7376 0.0302 0.1173 0.6326 99.81 50.41
53 1329.528 7.9523 0.0261 0.1010 0.5615 99.84 1.84
54 1336.746 7.9955 0.0253 0.0980 0.5482 99.84 206.26
55 1343.654 8.0368 0.0246 0.0952 0.5356 99.85 110.73
56 1359.689 8.1327 0.0230 0.0890 0.5075 99.86 18.81
57 1367.510 8.1795 0.0223 0.0861 0.4943 99.86 25.16
58 1370.823 8.1993 0.0220 0.0849 0.4888 99.87 1.78
59 1382.995 8.2721 0.0209 0.0807 0.4691 99.87 15.91
60 1386.214 8.2914 0.0207 0.0796 0.4640 99.88 49.26
61 1393.850 8.3371 0.0200 0.0771 0.4521 99.88 11.86
62 1404.374 8.4000 0.0192 0.0738 0.4362 99.89 30.43
63 1412.022 8.4458 0.0186 0.0714 0.4249 99.89 6.62
64 1445.121 8.6437 0.0162 0.0621 0.3792 99.91 14.84
65 1475.212 8.8237 0.0143 0.0547 0.3417 99.92 8.57
66 1508.282 9.0215 0.0125 0.0475 0.3044 99.93 4.47
67 1509.813 9.0307 0.0124 0.0472 0.3028 99.93 2.80
68 1526.312 9.1294 0.0116 0.0440 0.2857 99.94 3.05
69 1544.154 9.2361 0.0107 0.0408 0.2683 99.94 22.09
70 1560.392 9.3332 0.0100 0.0381 0.2533 99.95 151.87
71 1572.556 9.4060 0.0095 0.0362 0.2426 99.95 16.01
72 1738.377 10.3978 0.0047 0.0178 0.1331 99.98 2.43
73 3056.810 18.2838 0.0000 0.0001 0.0007 100.00 21.26
74 3070.322 18.3646 0.0000 0.0000 0.0007 100.00 21.79
75 3088.850 18.4754 0.0000 0.0000 0.0006 100.00 27.57
76 3093.406 18.5027 0.0000 0.0000 0.0006 100.00 34.63
77 3111.495 18.6109 0.0000 0.0000 0.0006 100.00 8.47
78 3114.334 18.6278 0.0000 0.0000 0.0006 100.00 8.78
79 3127.275 18.7053 0.0000 0.0000 0.0005 100.00 34.87
80 3145.647 18.8151 0.0000 0.0000 0.0005 100.00 25.88
81 3153.519 18.8622 0.0000 0.0000 0.0005 100.00 19.36
82 3174.750 18.9892 0.0000 0.0000 0.0004 100.00 10.60
83 3296.521 19.7176 0.0000 0.0000 0.0003 100.00 0.75
84 3297.252 19.7219 0.0000 0.0000 0.0003 100.00 0.58
-- ---------- ------- ------- ------- ----
Total Vibrations 604.6925 27.8332 190.4089 224.5186 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 182.5664 12.4716
Rotation 3.7184 148.5778 12.4716
---------- ------- ------- -------
Totals 642.4414 521.5531 249.4618

Vibrational(v) Corrections:
Temp. Correction Hv 642.4414
Entropy Correction (Hv-TSv) 486.9404

Reason for exit: Successful completion
Properties CPU Time : 1.50
```

Properties Wall Time: 1.47

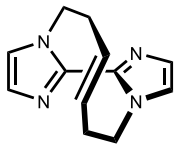	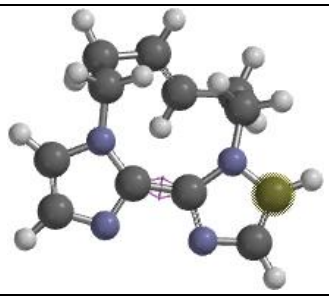
6 GS	**6'** TS
-684.690020 au	-684.634892 au

Fig s6. Calculation studies on the isomerization of **6**

Cartesian coordinate of **6** (GS)

N	-1.056457	1.445008	1.431853
C	-2.409210	1.514699	1.207608
H	-2.985973	2.378958	1.509129
C	-2.857486	0.365206	0.605590
H	-3.839773	0.042595	0.291806
N	-1.751319	-0.447025	0.460289
C	-0.685026	0.259145	0.971395
C	0.685026	-0.259145	0.971395
N	1.056457	-1.445008	1.431853
N	1.751319	0.447025	0.460289
C	2.857486	-0.365206	0.605590
H	3.839773	-0.042595	0.291806
C	2.409210	-1.514699	1.207608
H	2.985973	-2.378958	1.509129
C	-1.687866	-1.655536	-0.358529
H	-0.901235	-2.291943	0.051371
H	-2.641754	-2.181925	-0.253521
C	1.687866	1.655536	-0.358529
H	0.901235	2.291943	0.051371
H	2.641754	2.181925	-0.253521
C	1.420202	1.334326	-1.856197
H	2.229132	0.692484	-2.226224
H	1.470160	2.279919	-2.411479
C	-1.420202	-1.334326	-1.856197
H	-2.229132	-0.692484	-2.226224
H	-1.470160	-2.279919	-2.411479
C	0.087014	0.662898	-2.034256
H	-0.791114	1.310441	-2.013752
C	-0.087014	-0.662898	-2.034256
H	0.791114	-1.310441	-2.013752

Cartesian coordinate of **6'** (TS)

N	-0.650642	-2.488018	-0.375339
C	-1.997692	-2.658210	-0.380390

H	−2.447913	−3.587329	−0.705044
C	−2.613499	−1.528651	0.074227
H	−3.651090	−1.278488	0.242595
N	−1.611304	−0.619642	0.377033
C	−0.399187	−1.261625	0.075264
C	1.050590	−0.882615	0.076741
N	1.881816	−1.852476	−0.297561
N	1.790804	0.251536	0.442473
C	3.123368	−0.082426	0.255034
H	3.904115	0.636160	0.457847
C	3.147591	−1.371017	−0.194389
H	4.005675	−1.984071	−0.437654
C	−2.047355	0.635294	1.000500
H	−2.887058	0.375764	1.652957
H	−1.260367	1.021309	1.650272
C	1.491484	1.668936	0.665860
H	0.662972	1.776293	1.367574
H	2.378202	2.087704	1.151365
C	1.169944	2.455351	−0.634692
H	1.933772	2.243605	−1.390089
H	1.219243	3.525660	−0.394606
C	−0.220559	2.060289	−1.047997
H	−0.333887	1.195738	−1.700217
C	−2.485063	1.711795	−0.043424
H	−2.889336	1.200583	−0.923442
H	−3.284543	2.326972	0.384423
C	−1.258317	2.518138	−0.342951
H	−1.081036	3.355885	0.336869

Frequency calculation of 6'

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 17 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1* i	**53.914**	**0.0000**	**1.2395**	**8.3144**	**4.1572 0.00 0.07**
2*	84.262	0.5040	1.2395	8.3144	4.1572 33.41 2.25
3*	110.843	0.6630	1.2395	8.3144	4.1572 41.43 0.29
4*	145.911	0.8727	1.2395	8.3144	4.1572 50.55 0.71
5*	170.221	1.0181	1.2395	8.3144	4.1572 56.02 2.37
6*	190.665	1.1404	1.2395	8.3144	4.1572 60.15 0.54
7*	240.587	1.4390	1.2395	7.5250	4.1572 68.68 2.55
8*	258.404	1.5456	1.2395	6.9978	4.1572 71.26 2.43
9*	277.012	1.6569	1.1806	6.4937	4.1572 73.73 0.91
10*	330.261	1.9754	1.0073	5.2668	4.1572 79.68 1.00
11*	352.096	2.1060	0.9425	4.8400	4.1572 81.72 1.13
12*	383.235	2.2923	0.8560	4.2943	4.1572 84.27 0.69
13*	442.369	2.6460	0.7099	3.4275	4.1572 88.17 4.81
14*	471.069	2.8176	0.6469	3.0734	4.1572 89.70 3.62
15*	496.830	2.9717	0.5946	2.7869	4.1572 90.91 0.89
16*	520.392	3.1126	0.5499	2.5482	4.1572 91.88 1.77
17*	563.876	3.3727	0.4751	2.1595	4.1572 93.42 2.81
18	626.666	3.7483	0.3830	1.6987	4.0827 95.14 1.92
19	641.179	3.8351	0.3641	1.6066	3.9575 95.47 1.22

20	664.703	3.9758	0.3352	1.4676	3.7584	95.95	3.95
21	680.511	4.0704	0.3170	1.3808	3.6275	96.25	0.89
22	689.326	4.1231	0.3072	1.3346	3.5555	96.41	37.64
23	702.171	4.1999	0.2935	1.2699	3.4520	96.62	2.72
24	723.593	4.3280	0.2718	1.1687	3.2833	96.96	27.16
25	734.452	4.3930	0.2614	1.1204	3.1996	97.11	1.10
26	839.428	5.0209	0.1779	0.7427	2.4599	98.26	5.36
27	854.962	5.1138	0.1679	0.6985	2.3614	98.38	3.81
28	857.414	5.1285	0.1664	0.6918	2.3462	98.40	12.62
29	859.192	5.1391	0.1653	0.6869	2.3351	98.42	2.00
30	895.995	5.3592	0.1439	0.5936	2.1152	98.68	11.06
31	908.592	5.4346	0.1372	0.5646	2.0435	98.75	0.19
32	921.090	5.5093	0.1309	0.5371	1.9743	98.83	14.41
33	925.237	5.5341	0.1288	0.5283	1.9517	98.85	0.61
34	969.794	5.8007	0.1087	0.4420	1.7216	99.07	0.57
35	985.474	5.8944	0.1023	0.4150	1.6459	99.14	3.78
36	1024.720	6.1292	0.0879	0.3542	1.4682	99.29	16.04
37	1041.362	6.2287	0.0824	0.3311	1.3977	99.34	28.22
38	1047.574	6.2659	0.0804	0.3229	1.3721	99.36	45.27
39	1088.847	6.5127	0.0684	0.2730	1.2119	99.48	0.19
40	1097.377	6.5638	0.0661	0.2636	1.1808	99.50	4.22
41	1111.618	6.6490	0.0625	0.2487	1.1304	99.53	0.43
42	1135.698	6.7930	0.0569	0.2254	1.0494	99.58	2.38
43	1153.795	6.9012	0.0529	0.2093	0.9918	99.62	34.49
44	1179.347	7.0541	0.0478	0.1884	0.9152	99.66	6.51
45	1184.471	7.0847	0.0468	0.1844	0.9005	99.67	7.81
46	1212.550	7.2527	0.0418	0.1643	0.8234	99.71	15.51
47	1220.524	7.3004	0.0405	0.1589	0.8026	99.72	0.20
48	1245.454	7.4495	0.0366	0.1433	0.7405	99.75	0.68
49	1276.105	7.6328	0.0324	0.1262	0.6701	99.79	23.02
50	1295.662	7.7498	0.0299	0.1163	0.6283	99.81	3.74
51	1323.915	7.9188	0.0267	0.1034	0.5721	99.83	77.96
52	1332.780	7.9718	0.0257	0.0996	0.5555	99.84	21.37
53	1336.475	7.9939	0.0253	0.0981	0.5486	99.84	51.79
54	1360.609	8.1382	0.0229	0.0887	0.5060	99.86	3.56
55	1363.173	8.1536	0.0227	0.0877	0.5016	99.86	7.49
56	1368.134	8.1833	0.0222	0.0859	0.4933	99.86	15.97
57	1382.469	8.2690	0.0210	0.0809	0.4699	99.87	13.92
58	1393.694	8.3361	0.0200	0.0772	0.4523	99.88	14.01
59	1396.598	8.3535	0.0198	0.0762	0.4479	99.88	3.05
60	1405.920	8.4093	0.0190	0.0733	0.4339	99.89	15.41
61	1443.708	8.6353	0.0163	0.0625	0.3811	99.91	31.45
62	1471.652	8.8024	0.0145	0.0555	0.3460	99.92	8.74
63	1473.184	8.8116	0.0144	0.0552	0.3441	99.92	4.84
64	1509.996	9.0318	0.0124	0.0472	0.3026	99.93	3.02
65	1512.011	9.0438	0.0123	0.0468	0.3005	99.93	3.31
66	1525.525	9.1247	0.0116	0.0442	0.2865	99.94	1.82
67	1538.060	9.1996	0.0110	0.0419	0.2741	99.94	13.11
68	1568.436	9.3813	0.0097	0.0368	0.2462	99.95	36.04
69	1576.612	9.4302	0.0094	0.0355	0.2391	99.95	2.74
70	1737.963	10.3953	0.0047	0.0178	0.1333	99.98	2.65
71	3050.704	18.2473	0.0000	0.0001	0.0007	100.00	23.47
72	3064.872	18.3320	0.0000	0.0000	0.0007	100.00	21.14
73	3080.885	18.4278	0.0000	0.0000	0.0006	100.00	42.75

```
74 3088.753 18.4748 0.0000 0.0000 0.0006 100.00 33.80
75 3105.949 18.5777 0.0000 0.0000 0.0006 100.00 8.35
76 3109.107 18.5966 0.0000 0.0000 0.0006 100.00 9.61
77 3122.379 18.6760 0.0000 0.0000 0.0005 100.00 36.31
78 3139.353 18.7775 0.0000 0.0000 0.0005 100.00 25.20
79 3150.348 18.8433 0.0000 0.0000 0.0005 100.00 24.45
80 3178.175 19.0097 0.0000 0.0000 0.0004 100.00 9.62
81 3251.855 19.4504 0.0000 0.0000 0.0003 100.00 13.28
82 3252.689 19.4554 0.0000 0.0000 0.0003 100.00 11.81
83 3278.273 19.6084 0.0000 0.0000 0.0003 100.00 7.13
84 3280.421 19.6213 0.0000 0.0000 0.0003 100.00 6.07
-- ---------- ------- ------- ------- ----
Total Vibrations 657.9914 22.0161 120.8720 143.6685

Ideal Gas 2.4789
Translation 3.7184 175.6839 12.4716
Rotation 3.7184 134.1345 12.4716
---------- ------- ------- -------
Totals 689.9233 430.6905 168.6117

Vibrational(v) Corrections:
Temp. Correction Hv 689.9233
Entropy Correction (Hv-TSv) 561.5129

Reason for exit: Successful completion
Properties CPU Time : 1.61
Properties Wall Time: 2.44
```

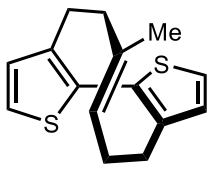	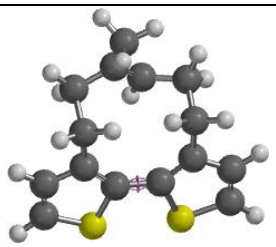
7 GS	**7'** TS
-1377.579018 au	-1377.539100 au

Fig s7. Calculation studies on the isomerization of **7**

Cartesian coordinate of **7**(GS)

C	−3.478143	0.372571	−0.562183
H	−4.462555	0.506124	−0.990947
C	−3.071258	−0.565461	0.342567
H	−3.731744	−1.323902	0.752089
C	−1.688396	−0.462545	0.707089
C	−1.054349	0.574443	0.048867
S	−2.180725	1.431169	−0.997647
C	0.335826	1.038141	0.131037
C	1.347246	0.956987	−0.807871
C	2.559650	1.566585	−0.347467

H	3.466371	1.596819	−0.944183
C	2.468883	2.101809	0.905685
H	3.236583	2.611150	1.473053
S	0.885357	1.887539	1.570065
C	−1.035977	−1.444185	1.649992
H	−1.780805	−1.776140	2.384538
H	−0.236567	−0.954529	2.216420
C	−0.453282	−2.702744	0.931571
H	−1.234196	−3.139330	0.297811
H	−0.204157	−3.448332	1.698712
C	1.245025	0.248969	−2.136712
H	1.920237	0.729318	−2.856083
H	0.231038	0.348270	−2.538964
C	1.595794	−1.270123	−2.055487
H	2.624951	−1.384660	−1.698891
H	1.564674	−1.676540	−3.075603
C	0.611227	−1.978754	−1.171990
H	−0.390844	−2.062871	−1.595572
C	0.765166	−2.343378	0.110539
C	2.066315	−2.311123	0.874938
H	2.295215	−3.308913	1.275195
H	2.006507	−1.635574	1.739423
H	2.917289	−1.992128	0.269117

Cartesian coordinate of 7' (TS)

C	1.354414	3.367619	0.089005
H	1.842169	4.318319	0.257912
C	0.062815	3.119779	−0.247704
H	−0.674743	3.903217	−0.391582
C	−0.269585	1.732184	−0.427107
C	0.821038	0.885810	−0.196422
S	2.238500	1.899313	0.207832
C	1.119576	−0.572576	−0.175169
C	0.449240	−1.781047	−0.394211
C	1.306264	−2.923679	−0.237413
H	0.935552	−3.934767	−0.373828
C	2.594391	−2.640461	0.086841
H	3.419389	−3.320602	0.250864
S	2.823751	−0.943110	0.217804
C	−1.708577	1.493576	−0.836495
H	−1.814178	0.597925	−1.451625
H	−1.991054	2.332011	−1.484684
C	−1.000835	−2.117594	−0.670529
H	−1.014910	−3.076392	−1.203548
H	−1.480402	−1.393091	−1.331508
C	−1.864977	−2.252089	0.630625
H	−1.324102	−2.850807	1.372012
H	−2.785375	−2.791064	0.381726
C	−2.715713	1.415704	0.375918
H	−3.606882	2.016845	0.158813
H	−2.243985	1.836462	1.269668
C	−2.126562	−0.849115	1.091649
H	−1.304287	−0.377055	1.630172
C	−3.049624	−0.046409	0.540514

C	-4.238391	-0.519582	-0.258737
H	-4.130144	-0.272567	-1.325800
H	-5.148437	-0.007779	0.082884
H	-4.411889	-1.595348	-0.179961

Frequency calculation of **7'**

Term	ZPE	Enthalpy	Entropy	Cv	% in	
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
1*	**i 48.329**	**0.0000**	**1.2395**	**8.3144**	**4.1572**	**0.00**	**0.00**
2*	87.789	0.5251	1.2395	8.3144	4.1572	34.53	0.07
3*	99.545	0.5954	1.2395	8.3144	4.1572	38.14	0.01
4*	107.273	0.6416	1.2395	8.3144	4.1572	40.41	0.06
5*	137.226	0.8208	1.2395	8.3144	4.1572	48.43	1.52
6*	164.536	0.9841	1.2395	8.3144	4.1572	54.80	0.31
7*	183.985	1.1005	1.2395	8.3144	4.1572	58.85	0.20
8*	196.474	1.1752	1.2395	8.3144	4.1572	61.25	0.31
9*	197.910	1.1838	1.2395	8.3144	4.1572	61.52	0.12
10*	267.412	1.5995	1.2143	6.7482	4.1572	72.49	0.53
11*	290.293	1.7363	1.1353	6.1598	4.1572	75.36	1.39
12*	291.104	1.7412	1.1326	6.1401	4.1572	75.46	0.63
13*	359.454	2.1500	0.9214	4.7047	4.1572	82.35	0.44
14*	372.985	2.2309	0.8837	4.4663	4.1572	83.47	0.56
15*	398.561	2.3839	0.8159	4.0498	4.1572	85.39	0.27
16*	413.328	2.4722	0.7788	3.8280	4.1572	86.39	0.24
17*	417.767	2.4988	0.7679	3.7638	4.1572	86.68	1.73
18*	462.969	2.7692	0.6642	3.1694	4.1572	89.29	0.85
19*	511.733	3.0608	0.5660	2.6335	4.1572	91.54	0.39
20*	521.603	3.1199	0.5477	2.5365	4.1572	91.93	0.68
21*	534.373	3.1963	0.5248	2.4163	4.1572	92.41	3.60
22*	551.323	3.2976	0.4957	2.2653	4.1572	93.01	1.21
23*	560.801	3.3543	0.4801	2.1850	4.1572	93.32	2.15
24*	583.060	3.4875	0.4451	2.0071	4.1572	94.00	11.48
25	657.328	3.9317	0.3440	1.5099	3.8203	95.81	1.12
26	660.985	3.9536	0.3396	1.4888	3.7895	95.88	45.45
27	689.936	4.1267	0.3066	1.3315	3.5506	96.42	1.42
28	706.276	4.2245	0.2892	1.2499	3.4193	96.69	4.04
29	735.523	4.3994	0.2604	1.1158	3.1914	97.13	35.33
30	743.818	4.4490	0.2527	1.0803	3.1285	97.24	1.30
31	774.297	4.6313	0.2262	0.9592	2.9038	97.62	1.54
32	819.793	4.9034	0.1913	0.8024	2.5885	98.09	4.85
33	837.589	5.0099	0.1791	0.7481	2.4718	98.24	7.08
34	865.910	5.1793	0.1612	0.6689	2.2938	98.47	29.38
35	871.220	5.2110	0.1580	0.6550	2.2615	98.51	4.37
36	879.564	5.2610	0.1531	0.6336	2.2114	98.57	6.93
37	890.507	5.3264	0.1469	0.6067	2.1469	98.64	2.52
38	892.247	5.3368	0.1460	0.6025	2.1368	98.65	1.44
39	897.173	5.3663	0.1433	0.5908	2.1084	98.68	5.15
40	912.416	5.4575	0.1353	0.5560	2.0222	98.78	8.03
41	934.139	5.5874	0.1245	0.5099	1.9039	98.90	16.87
42	961.657	5.7520	0.1121	0.4566	1.7620	99.03	4.80
43	978.739	5.8542	0.1050	0.4264	1.6781	99.11	1.24
44	988.325	5.9115	0.1012	0.4102	1.6325	99.15	0.23
45	1022.611	6.1166	0.0886	0.3572	1.4773	99.28	11.18

46	1039.605	6.2182	0.0829	0.3335	1.4050	99.34	4.76
47	1075.654	6.4338	0.0720	0.2881	1.2613	99.44	2.21
48	1095.981	6.5554	0.0665	0.2652	1.1858	99.50	0.08
49	1104.428	6.6059	0.0643	0.2562	1.1556	99.52	4.06
50	1138.283	6.8084	0.0563	0.2230	1.0410	99.59	7.86
51	1143.792	6.8414	0.0551	0.2180	1.0233	99.60	0.57
52	1170.228	6.9995	0.0496	0.1956	0.9419	99.65	1.55
53	1189.487	7.1147	0.0459	0.1807	0.8863	99.68	1.33
54	1215.407	7.2697	0.0414	0.1623	0.8159	99.72	1.93
55	1235.684	7.3910	0.0381	0.1493	0.7643	99.74	1.16
56	1259.897	7.5359	0.0346	0.1350	0.7066	99.77	4.15
57	1265.298	7.5682	0.0338	0.1320	0.6942	99.78	12.43
58	1272.917	7.6137	0.0328	0.1279	0.6771	99.79	2.09
59	1336.585	7.9945	0.0253	0.0980	0.5484	99.84	2.77
60	1345.221	8.0462	0.0244	0.0946	0.5328	99.85	0.41
61	1361.021	8.1407	0.0229	0.0885	0.5052	99.86	7.15
62	1367.353	8.1786	0.0223	0.0862	0.4946	99.86	8.19
63	1402.816	8.3907	0.0193	0.0743	0.4385	99.89	2.08
64	1407.385	8.4180	0.0189	0.0728	0.4317	99.89	0.06
65	1415.636	8.4674	0.0183	0.0703	0.4197	99.89	0.53
66	1445.468	8.6458	0.0162	0.0620	0.3788	99.91	6.07
67	1450.198	8.6741	0.0159	0.0608	0.3727	99.91	0.24
68	1476.638	8.8323	0.0142	0.0544	0.3400	99.92	6.50
69	1510.195	9.0330	0.0124	0.0472	0.3024	99.93	4.58
70	1512.240	9.0452	0.0123	0.0467	0.3002	99.93	2.98
71	1520.618	9.0953	0.0118	0.0451	0.2915	99.93	2.71
72	1525.195	9.1227	0.0116	0.0442	0.2869	99.94	0.23
73	1537.582	9.1968	0.0110	0.0420	0.2746	99.94	5.35
74	1546.537	9.2503	0.0106	0.0404	0.2661	99.94	10.50
75	1583.242	9.4699	0.0091	0.0345	0.2335	99.95	1.28
76	1590.664	9.5143	0.0088	0.0335	0.2274	99.95	10.96
77	1735.457	10.3803	0.0048	0.0180	0.1345	99.98	2.25
78	3020.439	18.0662	0.0000	0.0001	0.0008	100.00	24.81
79	3048.888	18.2364	0.0000	0.0001	0.0007	100.00	17.19
80	3053.442	18.2636	0.0000	0.0001	0.0007	100.00	26.74
81	3061.190	18.3100	0.0000	0.0001	0.0007	100.00	75.06
82	3065.442	18.3354	0.0000	0.0000	0.0007	100.00	38.42
83	3065.604	18.3364	0.0000	0.0000	0.0007	100.00	31.05
84	3102.898	18.5594	0.0000	0.0000	0.0006	100.00	17.71
85	3106.679	18.5821	0.0000	0.0000	0.0006	100.00	23.13
86	3125.989	18.6976	0.0000	0.0000	0.0005	100.00	20.49
87	3137.869	18.7686	0.0000	0.0000	0.0005	100.00	27.97
88	3142.398	18.7957	0.0000	0.0000	0.0005	100.00	23.38
89	3155.417	18.8736	0.0000	0.0000	0.0005	100.00	18.09
90	3210.618	19.2038	0.0000	0.0000	0.0004	100.00	18.33
91	3211.141	19.2069	0.0000	0.0000	0.0004	100.00	7.95
92	3269.471	19.5558	0.0000	0.0000	0.0003	100.00	0.35
93	3271.815	19.5698	0.0000	0.0000	0.0003	100.00	0.31
--	----------	-------	-------	-------	----		
Total Vibrations	710.3278	27.4566	152.4442	171.6182			

Ideal Gas	2.4789		
Translation	3.7184	178.1167	12.4716
Rotation	3.7184	139.1290	12.4716

```
---------- ------- ------- -------
Totals 747.7001 469.6899 196.5615

Vibrational(v) Corrections:
Temp. Correction Hv 747.7001
Entropy Correction (Hv-TSv) 607.6621

Reason for exit: Successful completion
Properties CPU Time : 2.08
Properties Wall Time: 3.35
```

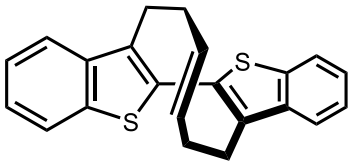	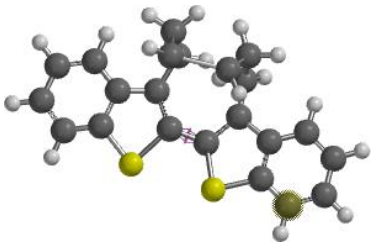
8 GS	**8'** TS
-1645.565075 au	-1645.023303 au

Fig s8. Calculation studies on the isomerization of **8**

Cartesian coordinate of **8** (GS)

C	-3.111741	0.708691	0.966737
C	-3.002589	-0.449936	0.159496
C	-1.627841	-0.833965	-0.092968
C	-0.733668	0.024235	0.495558
S	-1.531382	1.316159	1.414871
C	-4.352564	1.244003	1.326480
H	-4.414415	2.132886	1.947821
C	-5.504394	0.612182	0.871583
H	-6.477830	1.011966	1.141775
C	-5.420226	-0.538289	0.067545
H	-6.331386	-1.017924	-0.279210
C	-4.186830	-1.067283	-0.288121
H	-4.135987	-1.957376	-0.909500
C	0.733668	-0.024235	0.495558
C	1.627841	0.833965	-0.092968
C	3.002589	0.449936	0.159496
C	3.111741	-0.708691	0.966737
S	1.531382	-1.316159	1.414871
C	4.352564	-1.244003	1.326480
H	4.414415	-2.132886	1.947821
C	5.504394	-0.612182	0.871583
H	6.477830	-1.011966	1.141775
C	5.420226	0.538289	0.067545
H	6.331386	1.017924	-0.279210
C	4.186830	1.067283	-0.288121
H	4.135987	1.957376	-0.909500

C	−1.257723	−1.990351	−0.986358
H	−2.010736	−2.782124	−0.892210
H	−0.305898	−2.425835	−0.665211
C	−1.137000	−1.580686	−2.489280
H	−2.065154	−1.087468	−2.802701
H	−1.032884	−2.496113	−3.086248
C	1.257723	1.990351	−0.986358
H	2.010736	2.782124	−0.892210
H	0.305898	2.425835	−0.665211
C	1.137000	1.580686	−2.489280
H	2.065154	1.087468	−2.802701
H	1.032884	2.496113	−3.086248
C	−0.038235	0.666901	−2.678690
H	−1.022815	1.137538	−2.659591
C	0.038235	−0.666901	−2.678690
H	1.022815	−1.137538	−2.659591

Cartesian coordinate of **8'** (TS)

C	3.089401	−1.332090	−0.076989
C	2.936993	0.061907	0.231953
C	1.609317	0.472537	0.690472
C	0.650217	−0.613477	0.000530
S	1.578632	−2.314213	−0.093742
C	4.342072	−1.938092	−0.151700
H	4.428392	−2.999362	−0.380336
C	5.485427	−1.171271	0.066783
H	6.465712	−1.629554	−0.026053
C	5.370374	0.184144	0.398648
H	6.268409	0.774905	0.560036
C	4.120538	0.786542	0.499497
H	4.053077	1.834346	0.786543
C	−0.757355	−0.709961	0.436077
C	−1.589138	0.579016	0.604510
C	−2.992806	0.122874	0.200027
C	−3.166419	−1.235007	−0.190534
S	−1.643336	−2.157590	−0.492770
C	−4.431213	−1.831869	−0.278283
H	−4.530864	−2.877570	−0.566488
C	−5.559525	−1.057250	−0.028775
H	−6.548847	−1.489115	−0.157564
C	−5.423056	0.282006	0.371985
H	−6.314307	0.876494	0.555313
C	−4.164150	0.857873	0.510573
H	−4.083657	1.887647	0.854549
C	1.268171	1.975526	0.708676
H	1.723168	2.220880	1.651653
H	0.284242	2.086593	1.067183
C	1.596454	2.884554	−0.456705
H	2.644729	3.150909	−0.372335
H	0.999636	3.803615	−0.366789
C	−1.331171	1.890940	0.928888
H	−0.406644	1.607830	1.173264
H	−1.892766	2.128228	1.814697
C	−1.294413	2.926818	−0.167606

H	−0.663687	3.785809	0.109047
H	−2.324470	3.302722	−0.239165
C	−0.884601	2.340270	−1.487445
H	−1.584406	1.688335	−2.005499
C	1.289093	2.159413	−1.725415
H	2.036833	2.261531	−2.537314

Frequency calculation of **8'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 32 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1* i	**45.067**	**0.0000**	**1.2395**	**8.3144**	**4.1572**	**0.00**	**0.00**
2*	41.596	0.2488	1.2395	8.3144	4.1572	18.19	0.32
3*	67.821	0.4057	1.2395	8.3144	4.1572	27.91	0.03
4*	88.466	0.5291	1.2395	8.3144	4.1572	34.75	0.34
5*	109.336	0.6540	1.2395	8.3144	4.1572	41.00	0.29
6*	119.103	0.7124	1.2395	8.3144	4.1572	43.72	0.04
7*	149.726	0.8956	1.2395	8.3144	4.1572	51.45	0.21
8*	167.590	1.0024	1.2395	8.3144	4.1572	55.46	0.08
9*	180.856	1.0818	1.2395	8.3144	4.1572	58.22	0.11
10*	208.258	1.2457	1.2395	8.3144	4.1572	63.40	0.10
11*	229.190	1.3709	1.2395	7.8879	4.1572	66.91	0.14
12*	235.906	1.4110	1.2395	7.6715	4.1572	67.97	1.54
13*	250.325	1.4973	1.2395	7.2311	4.1572	70.12	0.52
14*	285.536	1.7079	1.1514	6.2771	4.1572	74.79	0.36
15*	293.427	1.7551	1.1248	6.0839	4.1572	75.73	0.55
16*	323.087	1.9325	1.0294	5.4158	4.1572	78.97	0.76
17*	359.053	2.1476	0.9225	4.7120	4.1572	82.32	2.02
18*	382.131	2.2857	0.8589	4.3124	4.1572	84.18	0.96
19*	426.531	2.5512	0.7468	3.6403	4.1572	87.23	0.86
20*	427.616	2.5577	0.7442	3.6253	4.1572	87.30	0.03
21*	436.791	2.6126	0.7227	3.5009	4.1572	87.85	3.60
22*	444.752	2.6602	0.7044	3.3965	4.1572	88.31	0.82
23*	469.146	2.8061	0.6510	3.0959	4.1572	89.61	0.62
24*	489.711	2.9291	0.6087	2.8633	4.1572	90.59	2.52
25*	502.994	3.0086	0.5826	2.7224	4.1572	91.17	1.19
26*	503.428	3.0112	0.5818	2.7179	4.1572	91.19	0.59
27*	516.581	3.0898	0.5569	2.5854	4.1572	91.73	0.07
28*	530.250	3.1716	0.5321	2.4545	4.1572	92.26	4.87
29*	540.293	3.2317	0.5145	2.3625	4.1572	92.63	3.47
30*	553.614	3.3113	0.4919	2.2456	4.1572	93.09	0.36
31*	559.116	3.3443	0.4829	2.1991	4.1572	93.27	3.13
32*	577.688	3.4553	0.4533	2.0487	4.1572	93.84	0.72
33	623.513	3.7294	0.3872	1.7193	4.1101	95.07	0.97
34	664.155	3.9725	0.3359	1.4707	3.7630	95.94	0.56
35	684.698	4.0954	0.3123	1.3587	3.5932	96.33	0.06
36	722.774	4.3231	0.2726	1.1724	3.2896	96.94	9.22
37	731.083	4.3728	0.2646	1.1352	3.2254	97.06	3.85
38	740.300	4.4280	0.2559	1.0952	3.1551	97.19	2.11
39	742.265	4.4397	0.2541	1.0869	3.1402	97.22	37.06
40	773.921	4.6291	0.2265	0.9606	2.9065	97.61	1.38
41	775.576	4.6390	0.2251	0.9544	2.8946	97.63	53.58

42	777.947	4.6532	0.2232	0.9456	2.8776	97.66	0.53
43	786.582	4.7048	0.2162	0.9142	2.8163	97.75	10.01
44	823.215	4.9239	0.1889	0.7917	2.5657	98.12	2.90
45	838.467	5.0151	0.1785	0.7455	2.4661	98.25	3.55
46	863.106	5.1625	0.1629	0.6763	2.3110	98.45	1.41
47	865.753	5.1783	0.1613	0.6693	2.2947	98.47	0.05
48	872.108	5.2164	0.1575	0.6527	2.2561	98.51	3.63
49	886.193	5.3006	0.1493	0.6172	2.1722	98.61	23.68
50	912.302	5.4568	0.1353	0.5563	2.0228	98.78	17.54
51	934.885	5.5919	0.1242	0.5083	1.9000	98.90	10.99
52	940.176	5.6235	0.1217	0.4977	1.8721	98.93	0.64
53	941.486	5.6313	0.1211	0.4951	1.8652	98.94	0.88
54	970.669	5.8059	0.1083	0.4404	1.7173	99.08	3.76
55	980.543	5.8649	0.1043	0.4233	1.6694	99.12	0.09
56	980.646	5.8656	0.1042	0.4231	1.6690	99.12	0.09
57	1003.011	5.9993	0.0956	0.3867	1.5645	99.21	4.17
58	1020.307	6.1028	0.0894	0.3606	1.4874	99.27	22.03
59	1034.727	6.1890	0.0845	0.3401	1.4255	99.32	1.66
60	1046.516	6.2596	0.0807	0.3243	1.3765	99.36	13.33
61	1060.790	6.3449	0.0764	0.3060	1.3190	99.40	8.16
62	1065.522	6.3732	0.0750	0.3002	1.3004	99.42	0.50
63	1085.082	6.4902	0.0694	0.2772	1.2258	99.47	0.09
64	1086.550	6.4990	0.0690	0.2755	1.2204	99.47	3.33
65	1092.890	6.5369	0.0673	0.2685	1.1970	99.49	4.61
66	1125.871	6.7342	0.0591	0.2347	1.0818	99.56	4.72
67	1158.683	6.9305	0.0519	0.2051	0.9768	99.63	1.43
68	1167.983	6.9861	0.0500	0.1974	0.9486	99.64	5.94
69	1174.141	7.0229	0.0488	0.1925	0.9304	99.65	0.44
70	1183.222	7.0772	0.0471	0.1854	0.9041	99.67	5.67
71	1190.992	7.1237	0.0456	0.1796	0.8820	99.68	9.95
72	1204.615	7.2052	0.0432	0.1697	0.8446	99.70	0.12
73	1205.983	7.2134	0.0430	0.1688	0.8409	99.70	0.18
74	1218.333	7.2872	0.0409	0.1604	0.8083	99.72	1.11
75	1241.586	7.4263	0.0372	0.1457	0.7499	99.75	3.40
76	1291.344	7.7240	0.0304	0.1184	0.6373	99.80	4.36
77	1296.548	7.7551	0.0298	0.1159	0.6265	99.81	9.80
78	1324.053	7.9196	0.0266	0.1033	0.5719	99.83	1.91
79	1326.892	7.9366	0.0263	0.1021	0.5665	99.83	1.41
80	1336.766	7.9956	0.0253	0.0980	0.5481	99.84	0.66
81	1342.702	8.0311	0.0247	0.0956	0.5373	99.85	4.69
82	1349.313	8.0707	0.0240	0.0930	0.5255	99.85	5.37
83	1355.757	8.1092	0.0234	0.0905	0.5143	99.86	2.78
84	1373.280	8.2140	0.0218	0.0841	0.4848	99.87	7.25
85	1375.664	8.2283	0.0216	0.0832	0.4809	99.87	15.04
86	1380.431	8.2568	0.0212	0.0816	0.4732	99.87	4.02
87	1383.792	8.2769	0.0209	0.0804	0.4678	99.87	7.03
88	1462.888	8.7500	0.0150	0.0576	0.3566	99.91	2.42
89	1473.439	8.8131	0.0144	0.0551	0.3438	99.92	7.48
90	1498.625	8.9638	0.0130	0.0495	0.3149	99.93	3.00
91	1499.474	8.9688	0.0129	0.0493	0.3140	99.93	6.19
92	1514.110	9.0564	0.0122	0.0464	0.2983	99.93	3.24
93	1519.498	9.0886	0.0119	0.0453	0.2927	99.93	3.27
94	1525.009	9.1216	0.0116	0.0443	0.2871	99.94	9.81
95	1529.354	9.1476	0.0114	0.0435	0.2827	99.94	2.32

```
96 1534.357 9.1775 0.0112 0.0426 0.2778 99.94 7.79
97 1558.314 9.3208 0.0101 0.0384 0.2552 99.95 14.82
98 1614.372 9.6561 0.0080 0.0302 0.2089 99.96 0.12
99 1615.909 9.6653 0.0079 0.0300 0.2078 99.96 0.11
100 1646.732 9.8496 0.0070 0.0263 0.1859 99.96 0.45
101 1648.022 9.8574 0.0069 0.0262 0.1851 99.96 0.70
102 1735.768 10.3822 0.0048 0.0180 0.1344 99.98 2.90
103 3051.505 18.2520 0.0000 0.0001 0.0007 100.00 31.33
104 3060.987 18.3088 0.0000 0.0001 0.0007 100.00 23.55
105 3075.627 18.3963 0.0000 0.0000 0.0007 100.00 57.61
106 3080.068 18.4229 0.0000 0.0000 0.0006 100.00 35.17
107 3104.539 18.5693 0.0000 0.0000 0.0006 100.00 14.18
108 3106.231 18.5794 0.0000 0.0000 0.0006 100.00 5.35
109 3121.758 18.6723 0.0000 0.0000 0.0005 100.00 41.70
110 3141.193 18.7885 0.0000 0.0000 0.0005 100.00 17.79
111 3158.917 18.8945 0.0000 0.0000 0.0005 100.00 24.70
112 3167.524 18.9460 0.0000 0.0000 0.0004 100.00 13.74
113 3188.826 19.0734 0.0000 0.0000 0.0004 100.00 2.63
114 3189.187 19.0756 0.0000 0.0000 0.0004 100.00 2.37
115 3198.627 19.1320 0.0000 0.0000 0.0004 100.00 4.68
116 3199.442 19.1369 0.0000 0.0000 0.0004 100.00 5.15
117 3209.495 19.1970 0.0000 0.0000 0.0004 100.00 25.00
118 3210.580 19.2035 0.0000 0.0000 0.0004 100.00 26.63
119 3216.771 19.2406 0.0000 0.0000 0.0004 100.00 45.74
120 3217.517 19.2450 0.0000 0.0000 0.0004 100.00 21.74
-- ---------- ------- ------- ------- ----
Total Vibrations 884.5203 35.9936 198.9321 227.0555

Ideal Gas 2.4789
Translation 3.7184 181.6789 12.4716
Rotation 3.7184 147.1630 12.4716
---------- ------- ------- -------
Totals 930.4297 527.7739 251.9988

Vibrational(v) Corrections:
Temp. Correction Hv 930.4297
Entropy Correction (Hv-TSv) 773.0739

Reason for exit: Successful completion
Properties CPU Time : 4.56
Properties Wall Time: 5.56
```

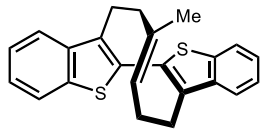	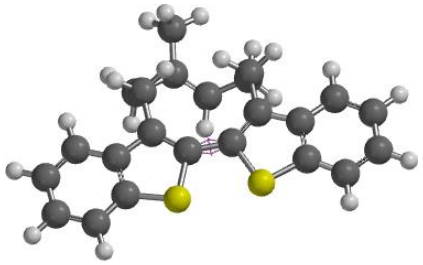
9 GS	**9'** TS
-1684.880756 au	-1684.837631 au

Fig s9. Calculation studies on the isomerization of **9**

Cartesian coordinate of **9** (GS)

C	−3.035822	−1.032616	0.827152
C	−2.924199	−0.498670	−0.479961
C	−1.549604	−0.293477	−0.890896
C	−0.657431	−0.651164	0.088593
S	−1.456079	−1.283627	1.541290
C	−4.277597	−1.300494	1.411644
H	−4.341849	−1.711567	2.415077
C	−5.427607	−1.028534	0.678882
H	−6.401860	−1.230291	1.115374
C	−5.340699	−0.496364	−0.619745
H	−6.250634	−0.290391	−1.176688
C	−4.106378	−0.231909	−1.197195
H	−4.052436	0.179636	−2.201080
C	0.810316	−0.615387	0.058163
C	1.676621	0.180781	0.764107
C	3.062705	−0.104415	0.448018
C	3.209759	−1.144421	−0.501762
S	1.650585	−1.770033	−0.995794
C	4.466744	−1.569142	−0.943067
H	4.558022	−2.369753	−1.671515
C	5.596449	−0.943166	−0.428285
H	6.582107	−1.259513	−0.758390
C	5.474552	0.093672	0.513583
H	6.368890	0.571562	0.903729
C	4.225089	0.512467	0.950050
H	4.144507	1.314917	1.677849
C	−1.173870	0.347540	−2.203282
H	−1.906081	0.072290	−2.972170
H	−0.206844	−0.036841	−2.543746
C	−1.083152	1.905061	−2.121576
H	−2.054137	2.308183	−1.815996
H	−0.883798	2.280459	−3.134394
C	1.274227	1.293435	1.699239
H	2.020008	1.378475	2.498863
H	0.325925	1.048459	2.187500
C	1.134121	2.677585	0.986402

H	2.043173	2.870972	0.404958
H	1.070367	3.453985	1.760440
C	−0.089644	2.694883	0.097525
C	0.017995	2.302090	−1.181688
H	1.021408	2.095275	−1.557433
C	−1.385800	3.038983	0.790718
H	−1.328671	4.047445	1.223557
H	−1.593367	2.352902	1.623871
H	−2.250176	3.011778	0.123591

Cartesian coordinate of **9'** (TS)

C	3.143727	−1.552236	−0.079001
C	3.145376	−0.172535	0.206845
C	1.813783	0.394781	0.372547
C	0.797727	−0.538051	0.185033
S	1.522392	−2.153893	−0.165162
C	4.318438	−2.287503	−0.266318
H	4.277560	−3.351308	−0.481794
C	5.534178	−1.622373	−0.172433
H	6.461337	−2.170764	−0.313572
C	5.568996	−0.243925	0.101407
H	6.525924	0.266240	0.167739
C	4.397289	0.475880	0.288120
H	4.458144	1.540058	0.491694
C	−0.692043	−0.585651	0.210047
C	−1.763726	0.279521	0.413536
C	−3.056861	−0.362171	0.217526
C	−2.973523	−1.734571	−0.086640
S	−1.318306	−2.241346	−0.151084
C	−4.103350	−2.530928	−0.297760
H	−4.001986	−3.588066	−0.525649
C	−5.355156	−1.934016	−0.213354
H	−6.248692	−2.530131	−0.376244
C	−5.470242	−0.563737	0.078285
H	−6.454845	−0.108037	0.135760
C	−4.342359	0.216133	0.293536
H	−4.461391	1.272672	0.510825
C	1.771003	1.883377	0.620611
H	2.665878	2.153665	1.190922
H	0.928029	2.167588	1.249770
C	1.719638	2.733158	−0.698588
H	2.426627	2.327803	−1.430434
H	2.036856	3.755086	−0.465713
C	−1.836750	1.734019	0.813728
H	−0.961072	2.032350	1.389699
H	−2.680935	1.835505	1.504277
C	−2.029373	2.721415	−0.405272
H	−2.821529	3.445318	−0.177891
H	−2.346025	2.155448	−1.286962
C	−0.691487	3.388567	−0.605318
C	0.294402	2.666290	−1.159719
H	0.016095	1.750092	−1.680994
C	−0.487333	4.661148	0.179637
H	0.500806	5.102962	0.031129

H	-0.622702	4.498602	1.260037
H	-1.236165	5.408769	-0.114151

Frequency calculation of 9'

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 14 low frequency terms

Term	ZPE	Enthalpy Correction	Entropy	Cv	% in Ground	IR Int.
	cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K		
1*	**i 46.481**	**0.0000**	**1.2395**	**0.0000**	**8.3144**	**0.00**	**0.01**
2*	40.811	0.2441	1.2395	21.8374	8.2876	17.88	0.33
3*	64.023	0.3829	1.2395	18.1131	8.2486	26.58	0.03
4*	72.554	0.4340	1.2395	17.0825	8.2300	29.54	0.14
5*	94.558	0.5656	1.2395	14.9095	8.1716	36.64	0.22
6*	108.783	0.6507	1.2395	13.7674	8.1261	40.84	0.26
7*	117.014	0.6999	1.2395	13.1757	8.0970	43.15	0.15
8*	140.491	0.8403	1.2395	11.7033	8.0031	49.24	0.11
9*	172.204	1.0300	1.2395	10.0887	7.8520	56.44	0.12
10*	173.354	1.0369	1.2395	10.0365	7.8460	56.68	0.19
11*	182.726	1.0929	1.2395	9.6247	7.7960	58.60	0.01
12*	206.958	1.2379	1.2395	8.6622	7.6565	63.16	0.10
13*	229.858	1.3749	1.2395	7.8661	7.5119	67.02	0.09
14*	237.167	1.4186	1.2395	7.6317	7.4633	68.16	1.21
15	276.016	1.6509	1.1841	6.5196	7.1870	73.60	0.07
16	298.089	1.7830	1.1094	5.9730	7.0177	76.27	0.26
17	326.501	1.9529	1.0188	5.3443	6.7885	79.31	0.82
18	338.464	2.0245	0.9825	5.1018	6.6887	80.47	1.25
19	372.696	2.2292	0.8845	4.4713	6.3939	83.45	1.08
20	390.982	2.3386	0.8355	4.1689	6.2318	84.84	0.56
21	423.017	2.5302	0.7552	3.6893	5.9420	87.01	0.72
22	427.885	2.5593	0.7435	3.6216	5.8975	87.32	0.84
23	435.719	2.6062	0.7252	3.5152	5.8256	87.79	2.49
24	437.679	2.6179	0.7206	3.4891	5.8075	87.90	2.11
25	457.182	2.7346	0.6768	3.2398	5.6275	88.99	0.44
26	494.048	2.9551	0.6000	2.8165	5.2853	90.78	2.72
27	503.326	3.0106	0.5819	2.7190	5.1991	91.19	0.03
28	515.833	3.0854	0.5583	2.5928	5.0832	91.70	0.88
29	518.793	3.1031	0.5528	2.5638	5.0558	91.82	1.65
30	531.272	3.1777	0.5303	2.4450	4.9405	92.30	3.32
31	538.020	3.2181	0.5184	2.3830	4.8783	92.55	2.22
32	542.071	3.2423	0.5114	2.3465	4.8411	92.69	6.85
33	552.870	3.3069	0.4932	2.2520	4.7421	93.06	0.45
34	572.052	3.4216	0.4621	2.0932	4.5676	93.67	4.12
35	583.887	3.4924	0.4438	2.0008	4.4609	94.03	7.25
36	621.991	3.7203	0.3892	1.7294	4.1234	95.03	1.56
37	663.565	3.9690	0.3366	1.4741	3.7679	95.93	0.66
38	686.530	4.1064	0.3103	1.3491	3.5783	96.36	0.17
39	722.807	4.3233	0.2726	1.1723	3.2894	96.94	9.59
40	730.057	4.3667	0.2656	1.1397	3.2333	97.05	4.65
41	740.374	4.4284	0.2559	1.0949	3.1545	97.19	0.21
42	741.592	4.4357	0.2547	1.0897	3.1453	97.21	37.51
43	767.651	4.5916	0.2317	0.9844	2.9519	97.54	14.75
44	774.931	4.6351	0.2257	0.9568	2.8993	97.62	8.77

45 776.934 4.6471 0.2240 0.9494 2.8849 97.65 28.29
46 781.480 4.6743 0.2203 0.9326 2.8524 97.70 4.36
47 793.440 4.7458 0.2109 0.8899 2.7682 97.83 9.69
48 850.798 5.0889 0.1705 0.7101 2.3876 98.35 4.06
49 859.139 5.1388 0.1653 0.6871 2.3355 98.42 9.98
50 864.811 5.1727 0.1618 0.6718 2.3005 98.46 1.51
51 865.391 5.1762 0.1615 0.6703 2.2970 98.46 0.68
52 877.020 5.2457 0.1546 0.6401 2.2266 98.55 3.85
53 928.213 5.5519 0.1274 0.5221 1.9357 98.87 30.46
54 934.631 5.5903 0.1243 0.5089 1.9013 98.90 11.60
55 938.859 5.6156 0.1223 0.5003 1.8790 98.92 2.52
56 940.811 5.6273 0.1214 0.4964 1.8687 98.93 1.98
57 941.892 5.6338 0.1209 0.4943 1.8631 98.94 2.19
58 977.102 5.8444 0.1057 0.4292 1.6860 99.10 4.92
59 979.946 5.8614 0.1045 0.4243 1.6723 99.12 0.06
60 980.624 5.8654 0.1042 0.4231 1.6691 99.12 0.09
61 1004.067 6.0057 0.0952 0.3850 1.5597 99.21 1.83
62 1019.734 6.0994 0.0896 0.3614 1.4899 99.27 7.97
63 1045.191 6.2516 0.0812 0.3260 1.3819 99.36 1.65
64 1054.543 6.3076 0.0783 0.3139 1.3439 99.38 2.15
65 1064.678 6.3682 0.0752 0.3012 1.3037 99.41 7.07
66 1065.917 6.3756 0.0748 0.2997 1.2988 99.42 0.96
67 1078.441 6.4505 0.0713 0.2848 1.2507 99.45 1.04
68 1085.241 6.4912 0.0694 0.2770 1.2252 99.47 0.05
69 1105.665 6.6133 0.0640 0.2549 1.1512 99.52 2.23
70 1111.403 6.6477 0.0626 0.2490 1.1312 99.53 9.67
71 1157.004 6.9204 0.0522 0.2065 0.9819 99.62 1.69
72 1163.214 6.9576 0.0510 0.2013 0.9630 99.64 5.61
73 1176.126 7.0348 0.0484 0.1909 0.9246 99.66 0.11
74 1183.194 7.0771 0.0471 0.1854 0.9041 99.67 4.30
75 1193.237 7.1371 0.0452 0.1779 0.8758 99.68 7.90
76 1202.706 7.1938 0.0435 0.1711 0.8497 99.70 3.50
77 1205.233 7.2089 0.0431 0.1693 0.8429 99.70 0.22
78 1212.070 7.2498 0.0419 0.1646 0.8247 99.71 0.77
79 1224.571 7.3246 0.0399 0.1563 0.7922 99.73 1.38
80 1261.701 7.5466 0.0343 0.1340 0.7024 99.77 8.07
81 1291.544 7.7251 0.0304 0.1183 0.6369 99.80 5.01
82 1296.999 7.7578 0.0297 0.1157 0.6256 99.81 9.15
83 1331.406 7.9636 0.0259 0.1002 0.5580 99.84 4.25
84 1333.426 7.9757 0.0256 0.0994 0.5543 99.84 1.14
85 1335.513 7.9881 0.0254 0.0985 0.5504 99.84 1.01
86 1344.854 8.0440 0.0245 0.0947 0.5335 99.85 8.58
87 1358.112 8.1233 0.0232 0.0896 0.5102 99.86 0.89
88 1363.164 8.1535 0.0227 0.0877 0.5016 99.86 1.70
89 1377.348 8.2384 0.0214 0.0826 0.4781 99.87 25.54
90 1381.054 8.2605 0.0211 0.0814 0.4722 99.87 1.31
91 1412.773 8.4503 0.0185 0.0712 0.4238 99.89 0.54
92 1443.187 8.6322 0.0163 0.0626 0.3818 99.91 6.79
93 1463.353 8.7528 0.0150 0.0575 0.3561 99.91 2.79
94 1474.087 8.8170 0.0144 0.0550 0.3430 99.92 6.23
95 1498.749 8.9645 0.0130 0.0495 0.3148 99.93 6.38
96 1498.989 8.9659 0.0130 0.0495 0.3145 99.93 4.39
97 1508.691 9.0240 0.0124 0.0475 0.3040 99.93 3.62
98 1511.529 9.0409 0.0123 0.0469 0.3010 99.93 2.14

```
99 1517.910 9.0791 0.0120 0.0456 0.2943 99.93 2.67
100 1525.399 9.1239 0.0116 0.0442 0.2867 99.94 3.88
101 1526.864 9.1327 0.0115 0.0439 0.2852 99.94 0.74
102 1530.730 9.1558 0.0113 0.0432 0.2813 99.94 19.20
103 1536.268 9.1889 0.0111 0.0422 0.2759 99.94 6.47
104 1553.456 9.2917 0.0103 0.0392 0.2596 99.94 12.68
105 1614.573 9.6573 0.0080 0.0302 0.2088 99.96 0.12
106 1616.036 9.6660 0.0079 0.0300 0.2077 99.96 0.19
107 1646.778 9.8499 0.0070 0.0263 0.1859 99.96 0.40
108 1648.124 9.8580 0.0069 0.0262 0.1850 99.96 0.60
109 1732.233 10.3611 0.0049 0.0182 0.1361 99.98 2.60
110 3018.507 18.0547 0.0000 0.0001 0.0008 100.00 24.72
111 3053.534 18.2642 0.0000 0.0001 0.0007 100.00 27.59
112 3066.525 18.3419 0.0000 0.0000 0.0007 100.00 19.45
113 3069.879 18.3619 0.0000 0.0000 0.0007 100.00 35.77
114 3072.693 18.3788 0.0000 0.0000 0.0007 100.00 47.92
115 3080.697 18.4267 0.0000 0.0000 0.0006 100.00 38.09
116 3109.496 18.5989 0.0000 0.0000 0.0006 100.00 16.40
117 3111.012 18.6080 0.0000 0.0000 0.0006 100.00 21.09
118 3140.072 18.7818 0.0000 0.0000 0.0005 100.00 24.39
119 3141.535 18.7905 0.0000 0.0000 0.0005 100.00 13.03
120 3156.464 18.8798 0.0000 0.0000 0.0005 100.00 11.08
121 3158.978 18.8949 0.0000 0.0000 0.0005 100.00 31.46
122 3188.903 19.0739 0.0000 0.0000 0.0004 100.00 2.62
123 3189.062 19.0748 0.0000 0.0000 0.0004 100.00 2.02
124 3198.703 19.1325 0.0000 0.0000 0.0004 100.00 5.30
125 3199.536 19.1375 0.0000 0.0000 0.0004 100.00 5.72
126 3209.916 19.1996 0.0000 0.0000 0.0004 100.00 25.94
127 3210.667 19.2040 0.0000 0.0000 0.0004 100.00 28.42
128 3217.045 19.2422 0.0000 0.0000 0.0004 100.00 47.03
129 3217.579 19.2454 0.0000 0.0000 0.0004 100.00 18.89
-- ---------- ------- ------- ------- ----
Total Vibrations 958.3006 38.8586 265.3934 327.3106 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 182.1738 12.4716
Rotation 3.7184 148.5334 12.4716
---------- ------- ------- -------
Totals 1007.0749 596.1006 352.2538

Vibrational(v) Corrections:
Temp. Correction Hv 1007.0749
Entropy Correction (Hv-TSv) 829.3475

Reason for exit: Successful completion
Properties CPU Time : 3.28
Properties Wall Time: 3.22
```

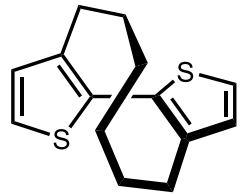	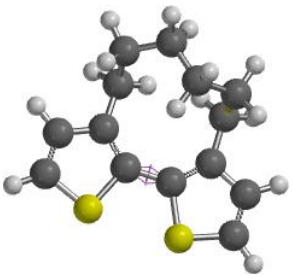
10 GS	**10'** TS
-1339.488595 au	-1339.468232 au

Fig s10. Calculation studies on the isomerization of **10**

Cartesian coordinate of **10** (GS)

C	−0. 731153	0. 061609	0. 818733
C	−1. 664707	−0. 700086	0. 142801
C	−3. 001181	−0. 230914	0. 363082
H	−3. 872046	−0. 701134	−0. 083486
C	−3. 076707	0. 855320	1. 187711
H	−3. 960345	1. 389393	1. 511452
S	−1. 509899	1. 342800	1. 736568
C	0. 731153	−0. 061609	0. 818733
C	1. 664707	0. 700086	0. 142801
C	3. 001181	0. 230914	0. 363082
H	3. 872046	0. 701134	−0. 083486
C	3. 076707	−0. 855320	1. 187711
H	3. 960345	−1. 389393	1. 511452
S	1. 509899	−1. 342800	1. 736568
C	−1. 350136	−1. 891025	−0. 735769
H	−0. 450702	−2. 391180	−0. 359118
H	−2. 170662	−2. 613576	−0. 635097
C	1. 350136	1. 891025	−0. 735769
H	2. 170662	2. 613576	−0. 635097
C	−1. 142499	−1. 599324	−2. 242158
H	−1. 068594	−2. 572674	−2. 744756
H	−2. 035680	−1. 109620	−2. 655103
C	1. 142499	1. 599324	−2. 242158
H	2. 035680	1. 109620	−2. 655103
H	1. 068594	2. 572674	−2. 744756
C	0. 113377	−0. 763892	−2. 562531
H	0. 499908	−1. 054598	−3. 548742
H	0. 900569	−1. 027589	−1. 847280
H	0. 450702	2. 391180	−0. 359118
C	−0. 113377	0. 763892	−2. 562531
H	−0. 499908	1. 054598	−3. 548742
H	−0. 900569	1. 027589	−1. 847280

Cartesian coordinate of **10'** (TS)

C	1. 114247	0. 043075	−0. 177723
C	1. 078625	1. 404184	−0. 479706
C	2. 360097	2. 033237	−0. 320163
H	2. 504998	3. 091204	−0. 516239

C	3.358825	1.207861	0.091474
H	4.398178	1.441662	0.278925
S	2.772544	-0.395611	0.306102
C	0.156929	-1.084562	-0.189169
C	-1.194830	-1.259955	-0.480171
C	-1.631795	-2.610185	-0.258582
H	-2.656481	-2.917291	-0.445027
C	-0.665042	-3.463310	0.171419
H	-0.740389	-4.520562	0.387463
S	0.842062	-2.646226	0.328118
C	-0.066702	2.335925	-0.820008
H	-0.814262	1.873177	-1.461644
H	0.352532	3.157040	-1.414389
C	-2.245840	-0.315829	-1.028590
H	-2.821967	-0.900821	-1.756002
H	-1.805132	0.490897	-1.610577
C	-0.735678	2.945633	0.434006
H	-1.310304	3.832083	0.129088
H	0.054760	3.304024	1.105700
C	-3.244841	0.253969	0.019710
H	-3.251700	-0.396181	0.903879
H	-4.256139	0.199845	-0.404031
C	-1.667847	1.989889	1.195256
H	-1.886634	2.434475	2.174130
H	-1.136395	1.054231	1.409149
C	-2.999809	1.707901	0.452290
H	-3.841653	2.011878	1.087554
H	-3.061351	2.349560	-0.438473

Frequency calculation of **10'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 21 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1*	**i 45.346**	**0.0000**	**1.2395**	**8.3144**	**4.1572 0.00 0.01**
2*	88.567	0.5297	1.2395	8.3144	4.1572 34.78 0.15
3*	96.381	0.5765	1.2395	8.3144	4.1572 37.19 0.03
4*	116.876	0.6991	1.2395	8.3144	4.1572 43.11 0.30
5*	134.920	0.8070	1.2395	8.3144	4.1572 47.85 0.69
6*	173.150	1.0357	1.2395	8.3144	4.1572 56.64 0.64
7*	187.910	1.1239	1.2395	8.3144	4.1572 59.62 0.38
8*	204.574	1.2236	1.2395	8.3144	4.1572 62.74 1.59
9*	220.859	1.3210	1.2395	8.1672	4.1572 65.55 0.21
10*	257.080	1.5377	1.2395	7.0354	4.1572 71.08 0.88
11*	335.587	2.0073	0.9912	5.1590	4.1572 80.20 0.24
12*	347.090	2.0761	0.9570	4.9344	4.1572 81.27 0.79
13*	381.054	2.2792	0.8618	4.3303	4.1572 84.10 0.83
14*	395.235	2.3640	0.8244	4.1016	4.1572 85.15 0.41
15*	421.611	2.5218	0.7586	3.7091	4.1572 86.93 0.17
16*	430.197	2.5732	0.7381	3.5898	4.1572 87.46 0.77
17*	462.448	2.7661	0.6653	3.1757	4.1572 89.26 0.65
18*	478.151	2.8600	0.6321	2.9918	4.1572 90.05 0.57
19*	521.389	3.1186	0.5481	2.5386	4.1572 91.92 0.02

20*	554.347	3.3157	0.4907	2.2394	4.1572	93.11	0.39
21*	567.247	3.3929	0.4697	2.1320	4.1572	93.53	3.40
22	652.784	3.9045	0.3496	1.5365	3.8587	95.72	16.22
23	655.901	3.9232	0.3458	1.5182	3.8323	95.78	14.31
24	684.706	4.0954	0.3123	1.3586	3.5931	96.33	1.78
25	699.562	4.1843	0.2962	1.2828	3.4729	96.58	15.12
26	730.996	4.3723	0.2647	1.1356	3.2261	97.06	43.69
27	737.561	4.4116	0.2585	1.1070	3.1759	97.15	0.28
28	763.580	4.5672	0.2352	1.0002	2.9816	97.49	1.46
29	781.942	4.6770	0.2199	0.9309	2.8491	97.70	1.12
30	818.525	4.8959	0.1922	0.8065	2.5969	98.07	3.27
31	837.272	5.0080	0.1793	0.7490	2.4738	98.24	5.23
32	841.744	5.0347	0.1764	0.7359	2.4450	98.28	6.40
33	870.797	5.2085	0.1582	0.6561	2.2640	98.50	31.11
34	875.238	5.2351	0.1556	0.6446	2.2373	98.54	5.43
35	890.976	5.3292	0.1467	0.6056	2.1442	98.64	2.04
36	895.290	5.3550	0.1443	0.5953	2.1192	98.67	0.90
37	913.279	5.4626	0.1348	0.5541	2.0174	98.78	3.69
38	922.719	5.5191	0.1301	0.5336	1.9654	98.84	0.97
39	954.451	5.7089	0.1152	0.4700	1.7983	99.00	0.57
40	971.640	5.8117	0.1079	0.4387	1.7126	99.08	1.08
41	1019.927	6.1005	0.0895	0.3611	1.4890	99.27	3.39
42	1031.790	6.1715	0.0855	0.3442	1.4379	99.31	2.05
43	1073.278	6.4196	0.0727	0.2909	1.2704	99.44	0.51
44	1086.039	6.4960	0.0692	0.2761	1.2222	99.47	0.79
45	1099.671	6.5775	0.0656	0.2612	1.1725	99.50	1.34
46	1112.242	6.6527	0.0624	0.2481	1.1282	99.53	0.10
47	1136.639	6.7986	0.0566	0.2245	1.0463	99.59	6.13
48	1157.357	6.9225	0.0522	0.2062	0.9808	99.62	2.03
49	1190.159	7.1187	0.0458	0.1802	0.8844	99.68	0.24
50	1198.505	7.1687	0.0443	0.1741	0.8612	99.69	0.44
51	1231.849	7.3681	0.0387	0.1517	0.7739	99.74	1.54
52	1251.815	7.4875	0.0357	0.1396	0.7254	99.76	0.26
53	1258.821	7.5294	0.0347	0.1356	0.7090	99.77	4.77
54	1281.916	7.6676	0.0316	0.1232	0.6574	99.79	1.70
55	1308.641	7.8274	0.0284	0.1102	0.6019	99.82	1.54
56	1330.309	7.9570	0.0260	0.1007	0.5601	99.84	3.72
57	1354.235	8.1001	0.0235	0.0911	0.5169	99.85	1.05
58	1363.943	8.1582	0.0226	0.0874	0.5003	99.86	9.82
59	1380.775	8.2589	0.0211	0.0815	0.4726	99.87	3.47
60	1390.301	8.3158	0.0203	0.0783	0.4576	99.88	5.81
61	1397.857	8.3610	0.0197	0.0758	0.4460	99.88	4.59
62	1407.666	8.4197	0.0189	0.0728	0.4313	99.89	0.26
63	1412.986	8.4515	0.0185	0.0711	0.4235	99.89	0.20
64	1414.655	8.4615	0.0184	0.0706	0.4211	99.89	3.36
65	1461.163	8.7397	0.0152	0.0580	0.3588	99.91	0.38
66	1491.723	8.9225	0.0134	0.0510	0.3226	99.93	9.27
67	1506.649	9.0118	0.0125	0.0479	0.3062	99.93	1.06
68	1515.585	9.0652	0.0121	0.0461	0.2967	99.93	2.91
69	1517.082	9.0742	0.0120	0.0458	0.2952	99.93	3.16
70	1527.991	9.1394	0.0115	0.0437	0.2841	99.94	5.15
71	1532.232	9.1648	0.0113	0.0429	0.2798	99.94	4.12
72	1556.341	9.3090	0.0102	0.0387	0.2570	99.95	10.43
73	1584.910	9.4799	0.0090	0.0343	0.2321	99.95	0.43

```
74 1594.708 9.5385 0.0087 0.0329 0.2242 99.95 7.53
75 3022.979 18.0814 0.0000 0.0001 0.0008 100.00 11.14
76 3027.323 18.1074 0.0000 0.0001 0.0008 100.00 38.89
77 3035.811 18.1582 0.0000 0.0001 0.0008 100.00 24.89
78 3045.261 18.2147 0.0000 0.0001 0.0007 100.00 6.53
79 3055.052 18.2733 0.0000 0.0001 0.0007 100.00 25.94
80 3057.706 18.2891 0.0000 0.0001 0.0007 100.00 46.29
81 3063.561 18.3242 0.0000 0.0000 0.0007 100.00 62.43
82 3072.686 18.3787 0.0000 0.0000 0.0007 100.00 15.82
83 3080.373 18.4247 0.0000 0.0000 0.0006 100.00 65.23
84 3087.639 18.4682 0.0000 0.0000 0.0006 100.00 58.78
85 3160.212 18.9023 0.0000 0.0000 0.0005 100.00 12.46
86 3197.712 19.1266 0.0000 0.0000 0.0004 100.00 25.87
87 3211.093 19.2066 0.0000 0.0000 0.0004 100.00 14.33
88 3213.715 19.2223 0.0000 0.0000 0.0004 100.00 12.10
89 3270.691 19.5631 0.0000 0.0000 0.0003 100.00 0.28
90 3270.809 19.5638 0.0000 0.0000 0.0003 100.00 0.37
-- ---------- ------- ------- ------- ----
Total Vibrations 699.3727 25.3726 141.6771 160.1213

Ideal Gas 2.4789
Translation 3.7184 177.5278 12.4716
Rotation 3.7184 137.7405 12.4716
---------- ------- ------- -------
Totals 734.6611 456.9453 185.0646

Vibrational(v) Corrections:
Temp. Correction Hv 734.6611
Entropy Correction (Hv-TSv) 598.4228

Reason for exit: Successful completion
Properties CPU Time : 1.97
Properties Wall Time: 6.81
```

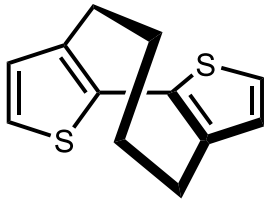	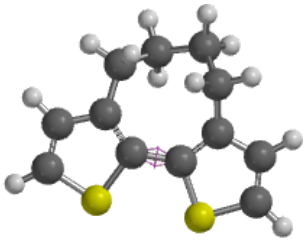
11 GS	**11'** TS
-1260.870147 au	-1260.856200 au

Fig s11. Calculation studies on the isomerization of **11**

Cartesian coordinate of **11** (GS)

S	−1.658920	0.673661	1.899476
C	−0.726622	−0.007413	0.575147

C	−3.150678	0.299399	1.102832
H	−4.094662	0.534798	1.576120
C	−2.937674	−0.300693	−0.105699
H	−3.742144	−0.625056	−0.758692
C	−1.552965	−0.491528	−0.420245
C	0.726622	0.007413	0.575147
C	1.552965	0.491528	−0.420245
C	2.937674	0.300693	−0.105699
H	3.742144	0.625056	−0.758692
C	3.150678	−0.299399	1.102832
H	4.094662	−0.534798	1.576120
S	1.658920	−0.673661	1.899476
C	−1.078456	−1.200715	−1.666775
H	−1.878674	−1.879884	−1.986456
H	−0.215333	−1.833866	−1.425199
C	−0.711410	−0.288576	−2.863595
H	−0.828305	−0.875821	−3.784139
H	−1.440832	0.530428	−2.927129
C	1.078456	1.200715	−1.666775
H	0.215333	1.833866	−1.425199
H	1.878674	1.879884	−1.986456
C	0.711410	0.288576	−2.863595
H	1.440832	−0.530428	−2.927129
H	0.828305	0.875821	−3.784139

Cartesian coordinate of **11'** (TS)

C	0.795769	−0.359920	−0.090603
C	1.636815	0.738428	−0.248734
C	3.019082	0.363369	−0.246510
H	3.815079	1.094314	−0.349937
C	3.247982	−0.968237	−0.068550
H	4.193472	−1.489767	−0.006796
S	1.763825	−1.829493	0.106878
C	−0.661451	−0.519713	−0.096328
C	−1.709982	0.385031	−0.225785
S	−1.306852	−2.148413	0.151110
C	−2.938890	−1.587872	0.124455
H	−3.757363	−2.285180	0.241038
C	−2.988794	−0.241116	−0.080828
H	−3.917869	0.314861	−0.160140
C	−1.630432	1.826555	−0.684538
H	−2.629564	2.120274	−1.027743
H	−0.992628	1.873918	−1.574755
C	1.287308	2.217325	−0.223410
H	0.945565	2.567718	−1.205701
H	2.225876	2.753076	−0.044695
C	0.266772	2.612640	0.873530
H	0.612562	3.518621	1.385858
H	0.239175	1.824521	1.634303
C	−1.149994	2.867862	0.337239
H	−1.855609	2.917690	1.176713
H	−1.181418	3.850898	−0.153798

Frequency calculation of **11'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 17 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1*	**i 37.750**	**0.0000**	**1.2395**	**8.3144**	**4.1572 0.00 0.01**
2*	103.891	0.6214	1.2395	8.3144	4.1572 39.43 0.78
3*	144.438	0.8639	1.2395	8.3144	4.1572 50.19 0.26
4*	152.883	0.9144	1.2395	8.3144	4.1572 52.18 0.94
5*	184.796	1.1053	1.2395	8.3144	4.1572 59.01 0.41
6*	204.529	1.2234	1.2395	8.3144	4.1572 62.73 0.73
7*	251.488	1.5042	1.2395	7.1969	4.1572 70.29 0.17
8*	318.203	1.9033	1.0446	5.5200	4.1572 78.47 1.97
9*	326.214	1.9512	1.0197	5.3503	4.1572 79.28 0.31
10*	350.306	2.0953	0.9477	4.8735	4.1572 81.56 0.17
11*	393.161	2.3516	0.8298	4.1343	4.1572 85.00 0.42
12*	456.822	2.7324	0.6775	3.2443	4.1572 88.97 0.73
13*	475.775	2.8458	0.6371	3.0189	4.1572 89.93 0.45
14*	489.269	2.9265	0.6095	2.8681	4.1572 90.57 0.42
15*	516.966	3.0921	0.5562	2.5816	4.1572 91.75 0.40
16*	539.076	3.2244	0.5166	2.3734	4.1572 92.58 0.33
17*	562.084	3.3620	0.4780	2.1743	4.1572 93.36 2.41
18	634.280	3.7938	0.3729	1.6498	4.0168 95.32 19.00
19	652.119	3.9005	0.3504	1.5405	3.8643 95.70 5.23
20	680.549	4.0706	0.3170	1.3806	3.6272 96.25 5.34
21	690.654	4.1310	0.3058	1.3278	3.5447 96.43 7.89
22	713.325	4.2666	0.2820	1.2162	3.3636 96.80 50.40
23	737.244	4.4097	0.2588	1.1083	3.1783 97.15 3.92
24	779.695	4.6636	0.2218	0.9392	2.8651 97.68 2.40
25	827.898	4.9519	0.1857	0.7772	2.5348 98.16 3.86
26	830.758	4.9690	0.1837	0.7685	2.5161 98.18 10.26
27	851.880	5.0954	0.1698	0.7071	2.3808 98.36 13.68
28	884.378	5.2898	0.1504	0.6216	2.1829 98.60 7.60
29	888.220	5.3127	0.1482	0.6122	2.1603 98.62 0.10
30	902.070	5.3956	0.1407	0.5794	2.0804 98.71 16.64
31	919.720	5.5011	0.1316	0.5401	1.9818 98.82 2.33
32	935.392	5.5949	0.1239	0.5073	1.8973 98.90 4.36
33	957.212	5.7254	0.1140	0.4649	1.7843 99.01 0.48
34	962.606	5.7577	0.1117	0.4549	1.7572 99.04 0.92
35	1061.787	6.3509	0.0761	0.3048	1.3151 99.40 0.55
36	1082.950	6.4775	0.0700	0.2796	1.2338 99.46 0.90
37	1100.025	6.5796	0.0655	0.2608	1.1713 99.51 0.66
38	1107.985	6.6272	0.0634	0.2525	1.1431 99.52 0.12
39	1135.870	6.7940	0.0568	0.2252	1.0488 99.58 7.31
40	1171.011	7.0042	0.0494	0.1950	0.9396 99.65 0.49
41	1210.649	7.2413	0.0422	0.1656	0.8284 99.71 1.89
42	1219.176	7.2923	0.0407	0.1598	0.8061 99.72 0.79
43	1247.732	7.4631	0.0363	0.1420	0.7351 99.76 1.36
44	1269.458	7.5930	0.0333	0.1297	0.6848 99.78 4.00
45	1279.783	7.6548	0.0319	0.1243	0.6621 99.79 9.68
46	1326.267	7.9328	0.0264	0.1024	0.5677 99.83 4.76

```
47 1369.362 8.1906 0.0221 0.0855 0.4912 99.87 1.32
48 1388.621 8.3058 0.0205 0.0788 0.4602 99.88 10.03
49 1401.215 8.3811 0.0194 0.0748 0.4409 99.88 0.55
50 1403.929 8.3974 0.0192 0.0739 0.4368 99.89 4.09
51 1421.038 8.4997 0.0179 0.0688 0.4120 99.89 1.00
52 1428.772 8.5460 0.0173 0.0666 0.4012 99.90 1.27
53 1458.144 8.7216 0.0153 0.0588 0.3626 99.91 0.66
54 1490.263 8.9138 0.0134 0.0513 0.3242 99.92 7.62
55 1513.633 9.0535 0.0122 0.0465 0.2988 99.93 2.74
56 1515.947 9.0674 0.0121 0.0460 0.2964 99.93 2.35
57 1529.014 9.1455 0.0114 0.0435 0.2830 99.94 2.16
58 1539.025 9.2054 0.0110 0.0417 0.2732 99.94 10.02
59 1577.532 9.4357 0.0093 0.0354 0.2383 99.95 1.67
60 1588.917 9.5038 0.0089 0.0337 0.2288 99.95 3.89
61 3027.375 18.1077 0.0000 0.0001 0.0008 100.00 37.35
62 3040.497 18.1862 0.0000 0.0001 0.0008 100.00 8.29
63 3050.879 18.2483 0.0000 0.0001 0.0007 100.00 29.41
64 3059.671 18.3009 0.0000 0.0001 0.0007 100.00 43.39
65 3068.055 18.3510 0.0000 0.0000 0.0007 100.00 23.16
66 3081.381 18.4307 0.0000 0.0000 0.0006 100.00 44.76
67 3090.841 18.4873 0.0000 0.0000 0.0006 100.00 24.22
68 3098.994 18.5361 0.0000 0.0000 0.0006 100.00 49.60
69 3211.974 19.2119 0.0000 0.0000 0.0004 100.00 17.11
70 3212.886 19.2173 0.0000 0.0000 0.0004 100.00 10.57
71 3271.221 19.5662 0.0000 0.0000 0.0003 100.00 0.27
72 3271.789 19.5696 0.0000 0.0000 0.0003 100.00 0.26
-- ---------- ------- ------- ------- ----
Total Vibrations 548.1382 20.3636 111.5650 132.4987

Ideal Gas 2.4789
Translation 3.7184 176.0332 12.4716
Rotation 3.7184 134.2001 12.4716
---------- ------- ------- -------
Totals 578.4175 421.7983 157.4419

Vibrational(v) Corrections:
Temp. Correction Hv 578.4175
Entropy Correction (Hv-TSv) 452.6584

Reason for exit: Successful completion
Properties CPU Time : 1.33
Properties Wall Time: 3.87
```

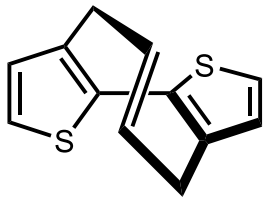	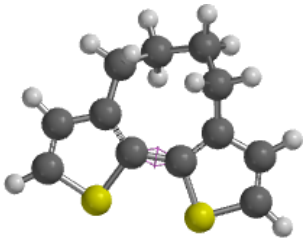
12 GS	**12'** TS
-1259.602957 au	-1259.597082 au

Fig s12. Calculation studies on the isomerization of **12**

Cartesian coordinate of **12** (GS)

C	0.743108	0.060050	0.272348
C	1.738320	0.524370	-0.590112
C	3.039722	0.513345	0.006388
H	3.924112	0.844616	-0.529781
C	3.070594	0.038663	1.283579
H	3.925798	-0.082895	1.935236
S	1.494814	-0.417861	1.810134
C	-0.743108	-0.060050	0.272348
C	-1.738320	-0.524370	-0.590112
C	-3.039722	-0.513345	0.006388
H	-3.924112	-0.844616	-0.529781
C	-3.070594	-0.038663	1.283579
H	-3.925798	0.082895	1.935236
S	-1.494814	0.417861	1.810134
C	-1.598362	-0.958779	-2.049294
H	-2.352975	-0.418029	-2.638391
H	-1.832714	-2.026147	-2.152333
C	1.598362	0.958779	-2.049294
H	1.832714	2.026147	-2.152333
H	2.352975	0.418029	-2.638391
C	-0.205872	-0.634234	-2.496454
H	0.532532	-1.435179	-2.454245
C	0.205872	0.634234	-2.496454
H	-0.532532	1.435179	-2.454245

Cartesian coordinate of **12** ' (TS)

C	0.752910	0.002190	0.223856
C	1.828643	0.007435	-0.680029
C	3.111550	0.011903	-0.041240
H	4.033363	0.009240	-0.614662
C	3.071188	0.015472	1.316570
H	3.892053	0.013703	2.021376
S	1.446252	0.008068	1.874077
C	-0.752910	-0.002190	0.223856
C	-1.828643	-0.007435	-0.680029
C	-3.111550	-0.011903	-0.041240

H	-4.033363	-0.009240	-0.614662
C	-3.071188	-0.015472	1.316570
H	-3.892053	-0.013703	2.021376
S	-1.446252	-0.008068	1.874077
C	1.844089	0.021941	-2.206781
H	2.047477	1.045250	-2.554817
H	2.672089	-0.605807	-2.558737
C	-1.844089	-0.021941	-2.206781
H	-2.672089	0.605807	-2.558737
H	-2.047477	-1.045250	-2.554817
C	0.506473	-0.431121	-2.669445
H	0.301854	-1.501897	-2.627947
C	-0.506473	0.431121	-2.669445
H	-0.301854	1.501897	-2.627947

Frequency calculation of **12'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 18 low frequency terms

Term		ZPE	Enthalpy	Entropy	Cv	% in
		cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
1*	A	i 62.813	0.0000	1.2395	8.3144	4.1572	0.00	0.05
2*	B	111.517	0.6670	1.2395	8.3144	4.1572	41.62	0.85
3*	A	144.743	0.8658	1.2395	8.3144	4.1572	50.27	0.29
4*	B	170.585	1.0203	1.2395	8.3144	4.1572	56.10	0.44
5*	B	225.120	1.3465	1.2395	8.0228	4.1572	66.26	1.93
6*	A	227.577	1.3612	1.2395	7.9411	4.1572	66.65	0.39
7*	B	288.735	1.7270	1.1406	6.1979	4.1572	75.18	2.60
8*	A	304.781	1.8230	1.0875	5.8178	4.1572	77.03	0.19
9*	B	309.888	1.8535	1.0710	5.7024	4.1572	77.58	1.08
10*	A	331.816	1.9847	1.0026	5.2351	4.1572	79.84	0.16
11*	B	425.967	2.5478	0.7481	3.6481	4.1572	87.20	1.19
12*	A	436.364	2.6100	0.7237	3.5066	4.1572	87.82	0.04
13*	B	461.280	2.7591	0.6678	3.1898	4.1572	89.20	0.93
14*	???	522.074	3.1227	0.5468	2.5320	4.1572	91.95	0.00
15*	B	522.284	3.1239	0.5465	2.5300	4.1572	91.96	0.20
16*	A	571.989	3.4213	0.4622	2.0937	4.1572	93.67	1.42
17*	A	579.150	3.4641	0.4511	2.0373	4.1572	93.89	5.07
18*	B	612.316	3.6625	0.4025	1.7947	4.1572	94.79	14.39
19	A	633.479	3.7890	0.3740	1.6548	4.0237	95.30	0.05
20	B	681.890	4.0786	0.3154	1.3735	3.6162	96.28	5.96
21	B	715.045	4.2769	0.2803	1.2081	3.3500	96.83	65.55
22	A	715.517	4.2797	0.2798	1.2059	3.3463	96.83	0.34
23	A	731.364	4.3745	0.2643	1.1340	3.2233	97.07	0.01
24	B	830.666	4.9685	0.1838	0.7688	2.5167	98.18	19.44
25	A	842.460	5.0390	0.1759	0.7339	2.4405	98.28	5.80
26	B	851.382	5.0924	0.1702	0.7085	2.3839	98.36	10.67
27	A	862.879	5.1612	0.1630	0.6770	2.3124	98.45	27.66
28	B	884.580	5.2910	0.1502	0.6211	2.1817	98.60	1.55
29	???	886.228	5.3008	0.1493	0.6171	2.1720	98.61	0.03
30	B	905.130	5.4139	0.1390	0.5724	2.0630	98.73	6.75
31	A	926.921	5.5442	0.1280	0.5248	1.9426	98.86	0.32
32	B	950.863	5.6874	0.1168	0.4768	1.8166	98.98	3.08
33	B	973.023	5.8200	0.1073	0.4363	1.7058	99.09	6.03

```
34 A 1012.393 6.0555 0.0922 0.3723 1.5223 99.24 36.86
35 A 1087.498 6.5047 0.0688 0.2745 1.2168 99.47 0.00
36 A 1109.154 6.6342 0.0631 0.2513 1.1390 99.53 1.07
37 B 1126.576 6.7384 0.0589 0.2340 1.0795 99.56 4.67
38 B 1137.486 6.8037 0.0564 0.2237 1.0436 99.59 4.38
39 A 1178.535 7.0492 0.0479 0.1890 0.9176 99.66 1.87
40 B 1181.860 7.0691 0.0473 0.1864 0.9080 99.67 1.40
41 A 1209.445 7.2341 0.0424 0.1664 0.8316 99.71 0.35
42 ??? 1209.829 7.2364 0.0423 0.1661 0.8306 99.71 15.55
43 A 1244.839 7.4458 0.0367 0.1437 0.7420 99.75 8.56
44 B 1328.982 7.9491 0.0261 0.1012 0.5626 99.84 0.25
45 A 1329.604 7.9528 0.0260 0.1010 0.5614 99.84 6.27
46 B 1364.311 8.1604 0.0226 0.0873 0.4997 99.86 1.25
47 A 1366.987 8.1764 0.0224 0.0863 0.4952 99.86 0.52
48 A 1406.482 8.4126 0.0190 0.0731 0.4330 99.89 2.47
49 B 1413.684 8.4557 0.0184 0.0709 0.4225 99.89 0.12
50 B 1424.808 8.5222 0.0176 0.0677 0.4067 99.90 0.81
51 A 1451.425 8.6814 0.0158 0.0605 0.3711 99.91 1.76
52 ??? 1508.249 9.0213 0.0125 0.0475 0.3045 99.93 4.00
53 A 1508.431 9.0224 0.0125 0.0475 0.3043 99.93 2.89
54 B 1578.642 9.4424 0.0093 0.0352 0.2374 99.95 1.45
55 A 1585.280 9.4821 0.0090 0.0342 0.2318 99.95 15.49
56 A 1764.501 10.5541 0.0042 0.0159 0.1209 99.98 4.11
57 B 3023.376 18.0838 0.0000 0.0001 0.0008 100.00 41.64
58 A 3024.430 18.0901 0.0000 0.0001 0.0008 100.00 18.40
59 B 3069.275 18.3583 0.0000 0.0000 0.0007 100.00 53.31
60 A 3070.135 18.3635 0.0000 0.0000 0.0007 100.00 2.48
61 A 3145.886 18.8166 0.0000 0.0000 0.0005 100.00 3.65
62 B 3150.332 18.8432 0.0000 0.0000 0.0005 100.00 33.61
63 B 3210.947 19.2057 0.0000 0.0000 0.0004 100.00 23.99
64 A 3211.175 19.2071 0.0000 0.0000 0.0004 100.00 2.83
65 ??? 3268.575 19.5504 0.0000 0.0000 0.0003 100.00 0.49
66 ??? 3268.607 19.5506 0.0000 0.0000 0.0003 100.00 0.42
-- ---------- ------- ------- ------- ----
Total Vibrations 482.1509 20.0562 109.2562 129.1116

Ideal Gas 2.4789
Translation 3.7184 175.9186 12.4716
Rotation 3.7184 128.0373 12.4716
---------- ------- ------- -------
Totals 512.1229 413.2120 154.0548

Vibrational(v) Corrections:
Temp. Correction Hv 512.1229
Entropy Correction (Hv-TSv) 388.9237

Reason for exit: Successful completion
Properties CPU Time : 1.33
Properties Wall Time: 4.57
```

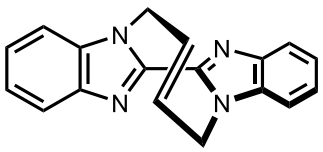	
13 GS	**13'** TS
-913.315680 au	-913.307907 au

Fig s13. Calculation studies on the isomerization of **13**

Cartesian coordinate of **13** (GS)

H	4.398912	-1.226528	1.467186
C	4.214542	-0.706391	0.531452
C	3.753986	0.638903	-1.953720
C	2.925690	-0.364863	0.107599
C	5.263469	-0.361180	-0.316394
C	5.037511	0.301313	-1.541296
C	2.683755	0.299029	-1.115156
H	6.280753	-0.612672	-0.029017
H	5.886689	0.547878	-2.172538
H	3.568466	1.146761	-2.895137
N	1.332947	0.518342	-1.276124
N	1.684441	-0.532933	0.692943
C	0.748813	0.026309	-0.203734
C	-0.748813	-0.026309	-0.203734
N	-1.332947	-0.518342	-1.276124
C	-2.683755	-0.299029	-1.115156
C	-5.263469	0.361180	-0.316394
C	-3.753986	-0.638903	-1.953720
C	-2.925690	0.364863	0.107599
C	-4.214542	0.706391	0.531452
C	-5.037511	-0.301313	-1.541296
H	-3.568466	-1.146761	-2.895137
H	-4.398912	1.226528	1.467186
H	-5.886689	-0.547878	-2.172538
H	-6.280753	0.612672	-0.029017
N	-1.684441	0.532933	0.692943
C	1.524441	-1.053944	2.064969
H	2.317417	-0.606093	2.677539
H	1.665593	-2.140201	2.071070
C	-1.524441	1.053944	2.064969
H	-2.317417	0.606093	2.677539
H	-1.665593	2.140201	2.071070
C	0.156416	-0.648732	2.518622
H	-0.631224	-1.399851	2.485992
C	-0.156416	0.648732	2.518622
H	0.631224	1.399851	2.485992

Cartesian coordinate of 13' (TS)

H	3.378370	0.009895	3.258530
C	3.648733	0.005961	2.207225
C	4.321547	−0.001835	−0.575452
C	2.647833	−0.000175	1.223764
C	4.971779	0.006976	1.785476
C	5.302017	0.003246	0.413213
C	2.991087	−0.004928	−0.140421
H	5.771497	0.011830	2.520875
H	6.348061	0.007101	0.119009
H	4.593281	0.003596	−1.626945
N	1.287703	−0.003683	1.363356
C	0.759354	−0.008574	0.151688
N	1.791559	−0.011411	−0.832519
C	−0.759354	0.008574	0.151688
N	−1.287703	0.003683	1.363356
C	−2.647833	0.000175	1.223764
C	−5.302017	−0.003246	0.413213
C	−3.648733	−0.005961	2.207225
C	−2.991087	0.004928	−0.140421
C	−4.321547	0.001835	−0.575452
C	−4.971779	−0.006976	1.785476
H	−3.378370	−0.009895	3.258530
H	−4.593281	−0.003596	−1.626945
H	−5.771497	−0.011830	2.520875
H	−6.348061	−0.007101	0.119009
N	−1.791559	0.011411	−0.832519
C	1.835133	−0.084376	−2.305339
H	2.130657	0.892451	−2.709743
H	2.604653	−0.814202	−2.576713
C	−1.835133	0.084376	−2.305339
H	−2.130657	−0.892451	−2.709743
H	−2.604653	0.814202	−2.576713
C	0.472265	−0.468008	−2.742420
H	0.203584	−1.523022	−2.704454
C	−0.472265	0.468008	−2.742420
H	−0.203584	1.523022	−2.704454

Frequency calculation of 13'

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 8 low frequency terms

Term	ZPE	Correction	Entropy	Cv	% in	
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
--	----------	-------	-------	-------	----	
1* A	**i 47.499**	**0.0000**	**1.2395**	**0.0000**	**8.3144**	**0.00 0.03**
2* B	49.681	0.2972	1.2395	20.2087	8.2747	21.32 0.71
3* B	98.308	0.5880	1.2395	14.5919	8.1602	37.77 1.66
4* A	99.701	0.5963	1.2395	14.4771	8.1559	38.19 0.05
5* A	126.846	0.7587	1.2395	12.5239	8.0596	45.78 0.05
6* A	144.221	0.8626	1.2395	11.4938	7.9868	50.14 0.00
7* B	199.022	1.1904	1.2395	8.9625	7.7037	61.73 2.81
8* B	246.087	1.4719	1.2395	7.3572	7.4025	69.50 0.14
9 B	261.314	1.5630	1.2360	6.9160	7.2950	71.66 0.28

10	A	261.862	1.5663	1.2341	6.9007	7.2910	71.74	0.12
11	A	267.897	1.6024	1.2126	6.7351	7.2471	72.55	0.66
12	B	276.503	1.6539	1.1824	6.5069	7.1833	73.67	1.91
13	B	300.736	1.7988	1.1007	5.9111	6.9968	76.57	0.65
14	B	356.464	2.1321	0.9299	4.7592	6.5353	82.10	4.41
15	A	365.346	2.1853	0.9048	4.5993	6.4582	82.85	0.23
16	A	383.725	2.2952	0.8547	4.2862	6.2965	84.30	0.12
17	B	445.552	2.6650	0.7026	3.3862	5.7350	88.35	4.92
18	A	465.159	2.7823	0.6595	3.1431	5.5535	89.40	0.00
19	A	497.609	2.9764	0.5930	2.7787	5.2522	90.94	1.13
20	B	553.247	3.3092	0.4925	2.2488	4.7387	93.07	0.26
21	A	565.272	3.3811	0.4729	2.1481	4.6291	93.46	6.43
22	B	575.637	3.4431	0.4565	2.0648	4.5352	93.78	7.44
23	A	583.572	3.4905	0.4443	2.0032	4.4637	94.02	0.06
24	B	585.370	3.5013	0.4416	1.9895	4.4476	94.07	0.11
25	A	624.305	3.7342	0.3861	1.7141	4.1032	95.08	0.04
26	B	636.897	3.8095	0.3695	1.6333	3.9943	95.37	1.06
27	A	658.949	3.9414	0.3421	1.5005	3.8067	95.84	0.12
28	B	661.477	3.9565	0.3390	1.4860	3.7854	95.89	1.60
29	A	712.239	4.2601	0.2831	1.2213	3.3721	96.78	0.09
30	A	732.415	4.3808	0.2633	1.1293	3.2152	97.08	9.95
31	B	732.911	4.3838	0.2628	1.1272	3.2114	97.09	12.45
32	B	757.234	4.5293	0.2407	1.0253	3.0283	97.41	103.69
33	A	757.707	4.5321	0.2403	1.0234	3.0248	97.42	0.11
34	A	769.999	4.6056	0.2298	0.9755	2.9349	97.57	0.08
35	B	774.284	4.6312	0.2262	0.9593	2.9039	97.62	13.41
36	B	800.587	4.7886	0.2054	0.8653	2.7186	97.90	2.70
37	A	858.201	5.1332	0.1659	0.6896	2.3413	98.41	0.01
38	B	858.822	5.1369	0.1655	0.6879	2.3374	98.41	1.12
39	B	874.345	5.2297	0.1561	0.6469	2.2426	98.53	20.71
40	A	878.846	5.2567	0.1535	0.6354	2.2157	98.56	0.02
41	A	923.101	5.5214	0.1299	0.5328	1.9633	98.84	2.65
42	B	929.830	5.5616	0.1266	0.5187	1.9270	98.87	3.43
43	A	929.850	5.5617	0.1266	0.5187	1.9269	98.87	0.29
44	B	931.835	5.5736	0.1256	0.5146	1.9162	98.89	0.39
45	A	976.258	5.8393	0.1060	0.4306	1.6901	99.10	0.46
46	B	976.647	5.8416	0.1058	0.4300	1.6882	99.10	0.16
47	A	982.121	5.8744	0.1036	0.4206	1.6619	99.13	4.13
48	B	1003.170	6.0003	0.0955	0.3864	1.5638	99.21	1.62
49	A	1014.897	6.0704	0.0913	0.3685	1.5111	99.25	42.13
50	B	1038.583	6.2121	0.0833	0.3349	1.4093	99.33	10.91
51	A	1038.828	6.2136	0.0832	0.3345	1.4083	99.33	0.01
52	B	1080.417	6.4623	0.0707	0.2825	1.2433	99.46	29.11
53	A	1135.032	6.7890	0.0570	0.2260	1.0516	99.58	2.77
54	B	1137.191	6.8019	0.0565	0.2240	1.0445	99.59	15.98
55	B	1146.200	6.8558	0.0545	0.2159	1.0156	99.60	5.70
56	A	1157.015	6.9205	0.0522	0.2065	0.9819	99.62	2.99
57	A	1171.444	7.0068	0.0493	0.1946	0.9383	99.65	17.47
58	B	1186.052	7.0942	0.0465	0.1832	0.8960	99.67	1.06
59	A	1190.281	7.1195	0.0457	0.1801	0.8840	99.68	12.45
60	B	1192.405	7.1322	0.0454	0.1785	0.8781	99.68	17.49
61	B	1234.657	7.3849	0.0383	0.1499	0.7669	99.74	3.01
62	A	1260.132	7.5373	0.0345	0.1349	0.7060	99.77	113.66
63	A	1268.187	7.5854	0.0334	0.1304	0.6877	99.78	27.69

```
64 A 1309.647 7.8334 0.0283 0.1097 0.5999 99.82 29.88
65 B 1313.526 7.8566 0.0278 0.1080 0.5923 99.82 3.06
66 B 1337.173 7.9981 0.0253 0.0978 0.5474 99.84 57.00
67 A 1341.668 8.0250 0.0248 0.0960 0.5392 99.85 9.88
68 A 1356.661 8.1146 0.0233 0.0901 0.5127 99.86 11.77
69 B 1357.538 8.1199 0.0232 0.0898 0.5112 99.86 4.83
70 A 1364.227 8.1599 0.0226 0.0873 0.4998 99.86 12.25
71 B 1365.670 8.1685 0.0225 0.0868 0.4974 99.86 10.60
72 A 1386.978 8.2960 0.0206 0.0794 0.4628 99.88 98.35
73 B 1396.072 8.3504 0.0198 0.0764 0.4487 99.88 36.82
74 B 1419.176 8.4886 0.0180 0.0693 0.4146 99.89 38.23
75 A 1432.266 8.5669 0.0171 0.0656 0.3964 99.90 1.87
76 A 1451.080 8.6794 0.0158 0.0606 0.3715 99.91 6.23
77 B 1467.359 8.7768 0.0148 0.0565 0.3512 99.92 30.21
78 B 1505.724 9.0062 0.0126 0.0481 0.3072 99.93 7.67
79 A 1512.445 9.0464 0.0122 0.0467 0.3000 99.93 11.70
80 B 1530.488 9.1544 0.0114 0.0433 0.2816 99.94 1.44
81 A 1531.931 9.1630 0.0113 0.0430 0.2801 99.94 3.37
82 B 1544.385 9.2375 0.0107 0.0408 0.2681 99.94 2.83
83 A 1546.031 9.2473 0.0106 0.0405 0.2665 99.94 0.22
84 B 1640.151 9.8103 0.0072 0.0271 0.1904 99.96 2.95
85 A 1641.627 9.8191 0.0071 0.0269 0.1894 99.96 0.85
86 B 1661.788 9.9397 0.0065 0.0247 0.1761 99.97 0.08
87 A 1662.786 9.9457 0.0065 0.0246 0.1754 99.97 2.65
88 A 1765.182 10.5581 0.0042 0.0158 0.1206 99.98 1.89
89 B 3044.178 18.2082 0.0000 0.0001 0.0007 100.00 22.64
90 A 3044.634 18.2110 0.0000 0.0001 0.0007 100.00 46.88
91 B 3099.817 18.5410 0.0000 0.0000 0.0006 100.00 33.75
92 A 3100.193 18.5433 0.0000 0.0000 0.0006 100.00 1.77
93 A 3168.404 18.9513 0.0000 0.0000 0.0004 100.00 1.88
94 B 3173.039 18.9790 0.0000 0.0000 0.0004 100.00 16.60
95 B 3186.933 19.0621 0.0000 0.0000 0.0004 100.00 0.16
96 A 3186.993 19.0624 0.0000 0.0000 0.0004 100.00 0.09
97 B 3198.546 19.1315 0.0000 0.0000 0.0004 100.00 4.67
98 A 3198.598 19.1319 0.0000 0.0000 0.0004 100.00 24.03
99 B 3208.715 19.1924 0.0000 0.0000 0.0004 100.00 53.14
100 A 3208.842 19.1931 0.0000 0.0000 0.0004 100.00 12.87
101 ??? 3220.749 19.2643 0.0000 0.0000 0.0004 100.00 20.59
102 ??? 3220.768 19.2645 0.0000 0.0000 0.0004 100.00 19.69
-- ---------- ------- ------- ------- ----
Total Vibrations 752.4777 29.0293 181.9643 247.0187 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 179.2998 12.4716
Rotation 3.7184 137.2917 12.4716
---------- ------- ------- -------
Totals 791.4228 498.5558 271.9620

Vibrational(v) Corrections:
Temp. Correction Hv 791.4228
Entropy Correction (Hv-TSv) 642.7784

Reason for exit: Successful completion
Properties CPU Time : 2.05
```

Properties Wall Time: 2.06

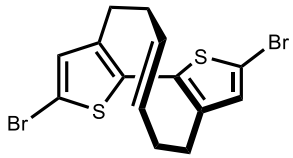	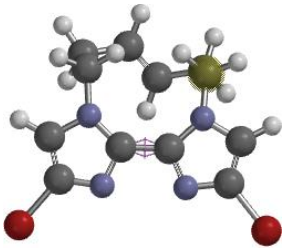
14 GS	**14'** TS
-6484.814944 au	-6484.774056 au

Fig s14. Calculation studies on the isomerization of **14**

Cartesian coordinate of **14** (GS)

S	−1.838099	0.829753	1.019806
C	−0.711479	−0.175445	0.107980
C	−3.167476	−0.184981	0.557707
C	−2.772698	−1.231356	−0.224209
H	−3.457368	−1.976738	−0.613109
C	−1.363239	−1.240410	−0.484778
C	0.711479	0.175445	0.107980
C	1.363239	1.240410	−0.484778
C	2.772698	1.231356	−0.224209
H	3.457368	1.976738	−0.613109
C	3.167476	0.184981	0.557707
S	1.838099	−0.829753	1.019806
C	−0.728060	−2.266189	−1.392556
H	−1.283585	−3.208623	−1.313098
H	0.297839	−2.475730	−1.071891
C	−0.703863	−1.817211	−2.887264
H	−0.369857	−2.668979	−3.493713
H	−1.724542	−1.569760	−3.203878
C	0.728060	2.266189	−1.392556
H	−0.297839	2.475730	−1.071891
H	1.283585	3.208623	−1.313098
C	0.703863	1.817211	−2.887264
H	1.724542	1.569760	−3.203878
H	0.369857	2.668979	−3.493713
C	−0.204683	0.635633	−3.060561
H	−1.275799	0.846053	−3.044661
C	0.204683	−0.635633	−3.060561
H	1.275799	−0.846053	−3.044661
Br	4.935433	−0.200884	1.113685
Br	−4.935433	0.200884	1.113685

Cartesian coordinate of **14'** (TS)

S	−1.398025	−1.316559	−0.011964
C	−0.730857	0.311155	0.339613
C	−3.026725	−0.760995	0.081012
C	−3.081876	0.562702	0.370900

H	-4.012220	1.106218	0.490980
C	-1.799810	1.194439	0.533943
C	0.755819	0.337626	0.315168
C	1.789625	1.261678	0.501370
C	3.095523	0.675009	0.381577
H	4.003344	1.255857	0.497014
C	3.090722	-0.654518	0.110049
S	1.484399	-1.266850	-0.013650
C	-1.899179	2.660901	0.906643
H	-1.059483	2.984350	1.525240
H	-2.789718	2.763999	1.537865
C	-2.037541	3.620198	-0.336122
H	-2.440988	3.061415	-1.187310
H	-2.742844	4.425275	-0.102093
C	1.796940	2.763866	0.687207
H	0.984818	3.108813	1.329716
H	2.731115	3.025677	1.199032
C	1.722147	3.550865	-0.663222
H	2.471483	3.166318	-1.364019
H	1.961649	4.601895	-0.457378
C	0.311569	3.413162	-1.156486
H	0.057583	2.516686	-1.721077
C	-0.656881	4.139553	-0.593381
H	-0.363423	4.995668	0.020372
Br	4.585292	-1.786228	-0.120528
Br	-4.478143	-1.939651	-0.175598

Frequency calculation of **14'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 13 low frequency terms

Term	ZPE	Enthalpy Correction	Entropy	Cv	% in Ground	IR Int.
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K		
1* i	**45.618**	**0.0000**	**1.2395**	**0.0000**	**8.3144**	**0.00**	**0.02**
2*	49.568	0.2965	1.2395	20.2276	8.2749	21.27	0.22
3*	68.569	0.4101	1.2395	17.5477	8.2390	28.17	0.03
4*	78.179	0.4676	1.2395	16.4684	8.2165	31.43	0.00
5*	99.565	0.5955	1.2395	14.4883	8.1563	38.15	0.02
6*	116.945	0.6995	1.2395	13.1805	8.0972	43.13	0.00
7*	131.812	0.7884	1.2395	12.2148	8.0397	47.06	0.18
8*	157.170	0.9401	1.2395	10.8095	7.9270	53.16	0.31
9*	196.806	1.1772	1.2395	9.0489	7.7167	61.32	0.27
10*	206.671	1.2362	1.2395	8.6728	7.6582	63.11	0.75
11*	229.819	1.3746	1.2395	7.8673	7.5122	67.01	1.10
12*	241.503	1.4445	1.2395	7.4967	7.4340	68.82	0.43
13*	251.387	1.5036	1.2395	7.1999	7.3656	70.27	0.44
14	281.475	1.6836	1.1653	6.3792	7.1459	74.29	0.57
15	322.672	1.9300	1.0307	5.4246	6.8201	78.93	0.20
16	329.916	1.9733	1.0084	5.2738	6.7602	79.65	2.73
17	356.241	2.1308	0.9306	4.7633	6.5372	82.08	0.19
18	370.236	2.2145	0.8913	4.5137	6.4155	83.25	0.58
19	417.818	2.4991	0.7677	3.7631	5.9895	86.68	0.30
20	454.661	2.7195	0.6823	3.2710	5.6508	88.85	0.22

21	463.590	2.7729	0.6628	3.1619	5.5681	89.32	7.43
22	478.207	2.8603	0.6320	2.9912	5.4324	90.05	6.78
23	491.654	2.9407	0.6048	2.8422	5.3075	90.68	0.24
24	516.596	3.0899	0.5569	2.5853	5.0761	91.73	0.73
25	537.599	3.2156	0.5192	2.3868	4.8822	92.53	0.06
26	555.578	3.3231	0.4887	2.2289	4.7174	93.15	1.08
27	570.944	3.4150	0.4639	2.1021	4.5776	93.64	3.43
28	675.912	4.0428	0.3222	1.4055	3.6653	96.17	6.62
29	683.670	4.0893	0.3135	1.3641	3.6016	96.31	0.16
30	713.615	4.2684	0.2817	1.2148	3.3613	96.81	7.36
31	721.911	4.3180	0.2735	1.1764	3.2963	96.93	9.40
32	812.808	4.8617	0.1964	0.8248	2.6353	98.02	6.04
33	828.659	4.9565	0.1852	0.7749	2.5298	98.17	0.91
34	846.585	5.0637	0.1732	0.7220	2.4142	98.32	9.06
35	851.031	5.0903	0.1704	0.7094	2.3861	98.35	21.66
36	855.236	5.1154	0.1677	0.6977	2.3597	98.39	3.93
37	876.152	5.2406	0.1551	0.6423	2.2318	98.54	8.08
38	897.315	5.3671	0.1432	0.5905	2.1076	98.68	17.07
39	918.177	5.4919	0.1323	0.5434	1.9903	98.81	10.42
40	940.344	5.6245	0.1216	0.4974	1.8712	98.93	27.68
41	969.837	5.8009	0.1086	0.4419	1.7214	99.07	4.44
42	982.201	5.8749	0.1036	0.4205	1.6615	99.13	2.49
43	986.937	5.9032	0.1017	0.4125	1.6390	99.15	7.69
44	1005.291	6.0130	0.0948	0.3831	1.5541	99.22	5.61
45	1028.401	6.1512	0.0866	0.3490	1.4524	99.30	21.24
46	1033.130	6.1795	0.0851	0.3423	1.4322	99.32	37.37
47	1079.480	6.4567	0.0710	0.2836	1.2468	99.45	3.62
48	1092.349	6.5337	0.0675	0.2691	1.1990	99.49	6.22
49	1139.956	6.8185	0.0559	0.2215	1.0356	99.59	1.74
50	1165.046	6.9685	0.0506	0.1998	0.9574	99.64	0.43
51	1183.384	7.0782	0.0470	0.1853	0.9036	99.67	2.22
52	1216.147	7.2742	0.0412	0.1618	0.8140	99.72	2.68
53	1239.411	7.4133	0.0375	0.1470	0.7552	99.75	1.13
54	1247.582	7.4622	0.0363	0.1421	0.7354	99.76	23.27
55	1258.768	7.5291	0.0347	0.1356	0.7092	99.77	1.37
56	1329.614	7.9529	0.0260	0.1010	0.5614	99.84	2.73
57	1333.103	7.9737	0.0257	0.0995	0.5549	99.84	2.13
58	1342.068	8.0273	0.0248	0.0958	0.5385	99.85	2.35
59	1345.859	8.0500	0.0244	0.0943	0.5317	99.85	9.82
60	1362.057	8.1469	0.0228	0.0881	0.5035	99.86	9.50
61	1374.646	8.2222	0.0217	0.0836	0.4825	99.87	2.66
62	1382.017	8.2663	0.0210	0.0810	0.4706	99.87	0.51
63	1389.542	8.3113	0.0204	0.0785	0.4588	99.88	1.26
64	1450.080	8.6734	0.0159	0.0608	0.3728	99.91	29.78
65	1470.603	8.7962	0.0146	0.0558	0.3472	99.92	31.83
66	1515.267	9.0633	0.0121	0.0461	0.2971	99.93	3.18
67	1524.617	9.1192	0.0116	0.0444	0.2875	99.94	3.60
68	1527.359	9.1356	0.0115	0.0438	0.2847	99.94	0.41
69	1552.085	9.2835	0.0104	0.0395	0.2609	99.94	11.34
70	1583.233	9.4698	0.0091	0.0345	0.2335	99.95	42.56
71	1591.052	9.5166	0.0088	0.0334	0.2271	99.95	50.96
72	1739.931	10.4071	0.0047	0.0176	0.1323	99.98	2.42
73	3048.750	18.2356	0.0000	0.0001	0.0007	100.00	17.36
74	3056.451	18.2816	0.0000	0.0001	0.0007	100.00	17.17

```
75 3060.668 18.3069 0.0000 0.0001 0.0007 100.00 67.16
76 3069.011 18.3568 0.0000 0.0000 0.0007 100.00 54.96
77 3100.843 18.5472 0.0000 0.0000 0.0006 100.00 13.92
78 3104.977 18.5719 0.0000 0.0000 0.0006 100.00 6.61
79 3121.035 18.6679 0.0000 0.0000 0.0005 100.00 28.21
80 3125.261 18.6932 0.0000 0.0000 0.0005 100.00 29.84
81 3140.175 18.7824 0.0000 0.0000 0.0005 100.00 28.02
82 3168.945 18.9545 0.0000 0.0000 0.0004 100.00 15.23
83 3230.334 19.3217 0.0000 0.0000 0.0003 100.00 3.08
84 3233.168 19.3386 0.0000 0.0000 0.0003 100.00 3.06
-- ---------- ------- ------- ------- ----
Total Vibrations 583.1630 30.4612 213.2662 242.6509 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 183.5992 12.4716
Rotation 3.7184 150.4069 12.4716
---------- ------- ------- -------
Totals 623.5400 547.2723 267.5942

Vibrational(v) Corrections:
Temp. Correction Hv 623.5400
Entropy Correction (Hv-TSv) 460.3707

Reason for exit: Successful completion
Properties CPU Time : 1.66
Properties Wall Time: 1.67
```

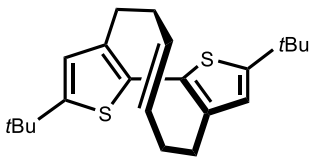	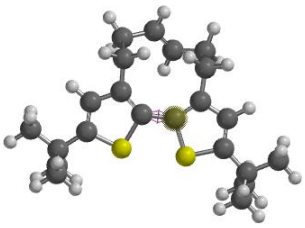
15 GS	**15'** TS
-1652.780359 au	-1652.741629 au

Fig s15. Calculation studies on the isomerization of **15**

Cartesian coordinate of **15** (GS)

S	−1.838253	0.840662	1.030426
C	−0.713617	−0.168248	0.129050
C	−3.211218	−0.149787	0.579403
C	−2.785141	−1.189995	−0.203121
H	−3.458209	−1.941044	−0.603314
C	−1.376506	−1.221769	−0.465577
C	0.713617	0.168248	0.129050
C	1.376506	1.221769	−0.465577
C	2.785141	1.189995	−0.203121
H	3.458209	1.941044	−0.603314
C	3.211218	0.149787	0.579403
S	1.838253	−0.840662	1.030426

C	−0.751177	−2.254497	−1.371429
H	−1.315576	−3.192375	−1.292957
H	0.272999	−2.473454	−1.050796
C	−0.721274	−1.810376	−2.867470
H	−0.395488	−2.665938	−3.473893
H	−1.739707	−1.553212	−3.184154
C	0.751177	2.254497	−1.371429
H	−0.272999	2.473454	−1.050796
H	1.315576	3.192375	−1.292957
C	0.721274	1.810376	−2.867470
H	1.739707	1.553212	−3.184154
H	0.395488	2.665938	−3.473893
C	−0.198023	0.637637	−3.043767
H	−1.267213	0.857849	−3.025441
C	0.198023	−0.637637	−3.043767
H	1.267213	−0.857849	−3.025441
C	−4.615029	0.182261	1.064357
C	−5.631068	−0.800113	0.449872
H	−5.623881	−0.752922	−0.644745
H	−6.641554	−0.549222	0.791407
H	−5.424594	−1.833050	0.751283
C	−4.679333	0.065405	2.605997
H	−3.993506	0.769211	3.089974
H	−4.409418	−0.944850	2.932670
H	−5.693892	0.281545	2.962694
C	−4.997629	1.621070	0.644836
H	−4.968872	1.732003	−0.444817
H	−4.314209	2.361063	1.075676
H	−6.011427	1.861242	0.987196
C	4.615029	−0.182261	1.064357
C	4.997629	−1.621070	0.644836
H	6.011427	−1.861242	0.987196
H	4.968872	−1.732003	−0.444817
H	4.314209	−2.361063	1.075676
C	4.679333	−0.065405	2.605997
H	5.693892	−0.281545	2.962694
H	3.993506	−0.769211	3.089974
H	4.409418	0.944850	2.932670
C	5.631068	0.800113	0.449872
H	6.641554	0.549222	0.791407
H	5.424594	1.833050	0.751283
H	5.623881	0.752922	−0.644745

Cartesian coordinate of **15'** (TS)

S	−1.391315	−1.334489	0.007800
C	−0.734689	0.293582	0.349161
C	−3.050485	−0.824328	0.085346
C	−3.082891	0.507641	0.367085
H	−4.009854	1.060253	0.480099
C	−1.813243	1.163547	0.533318
C	0.751324	0.333521	0.330181
C	1.776524	1.264056	0.513193
C	3.083328	0.678129	0.399207
H	3.975178	1.284373	0.517521

C	3.128645	-0.657612	0.132880
S	1.502045	-1.257566	0.015205
C	-1.930502	2.630497	0.896917
H	-1.098356	2.969414	1.518027
H	-2.826789	2.728589	1.521373
C	-2.072044	3.583459	-0.350469
H	-2.465756	3.015259	-1.200092
H	-2.786451	4.383660	-0.125507
C	1.769830	2.766317	0.692499
H	0.953395	3.109770	1.330993
H	2.701520	3.040273	1.203409
C	1.690540	3.548334	-0.660557
H	2.445341	3.166805	-1.357462
H	1.918808	4.603303	-0.460317
C	0.282971	3.394468	-1.157618
H	0.039062	2.488438	-1.711254
C	-0.695752	4.115946	-0.605843
H	-0.413289	4.979866	0.002450
C	4.323792	-1.575606	-0.070560
C	4.359510	-2.069666	-1.537048
H	4.446908	-1.226840	-2.231474
H	3.450654	-2.623907	-1.795159
H	5.218116	-2.734459	-1.692460
C	5.629148	-0.814671	0.231098
H	5.764156	0.036805	-0.445010
H	6.486559	-1.484153	0.099145
H	5.646162	-0.442694	1.261416
C	4.228778	-2.795786	0.874742
H	3.329362	-3.390372	0.679258
H	4.199573	-2.479593	1.923165
H	5.099090	-3.447902	0.735174
C	-4.190408	-1.808690	-0.124344
C	-4.069076	-2.468071	-1.518515
H	-4.895180	-3.171799	-1.676766
H	-3.129774	-3.022584	-1.619102
H	-4.101342	-1.715340	-2.313890
C	-5.542678	-1.075613	-0.036500
H	-6.359437	-1.787551	-0.200376
H	-5.623508	-0.290717	-0.796544
H	-5.690088	-0.617879	0.948005
C	-4.144115	-2.908060	0.964239
H	-4.973797	-3.611629	0.826422
H	-4.225295	-2.470566	1.965264
H	-3.208229	-3.475443	0.919573

Frequency calculation of **15'**

```
Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 45 low frequency terms
Term  ZPE      Enthalpy  Entropy   Cv        % in
cm-1  kJ/mol   kJ/mol    J/mol.K   J/mol.K   Ground IR Int.
--  ----------  -------  -------  -------  ----
```
1* i 41.178 0.0000 1.2395 8.3144 4.1572 0.00 0.01
2* i 19.626 0.0000 1.2395 8.3144 4.1572 0.00 0.00

3* 39.022 0.2334 1.2395 8.3144 4.1572 17.16 0.00
4* 46.177 0.2762 1.2395 8.3144 4.1572 19.98 0.91
5* 71.152 0.4256 1.2395 8.3144 4.1572 29.06 0.06
6* 73.839 0.4417 1.2395 8.3144 4.1572 29.98 0.18
7* 101.708 0.6083 1.2395 8.3144 4.1572 38.79 0.04
8* 114.210 0.6831 1.2395 8.3144 4.1572 42.37 0.01
9* 131.569 0.7870 1.2395 8.3144 4.1572 47.00 0.17
10* 149.887 0.8965 1.2395 8.3144 4.1572 51.49 0.09
11* 163.418 0.9775 1.2395 8.3144 4.1572 54.55 0.03
12* 201.491 1.2052 1.2395 8.3144 4.1572 62.18 0.05
13* 211.685 1.2662 1.2395 8.3144 4.1572 64.00 0.42
14* 218.941 1.3096 1.2395 8.2333 4.1572 65.23 0.40
15* 220.733 1.3203 1.2395 8.1715 4.1572 65.53 0.08
16* 234.947 1.4053 1.2395 7.7019 4.1572 67.82 0.36
17* 239.091 1.4301 1.2395 7.5714 4.1572 68.46 0.23
18* 262.375 1.5694 1.2322 6.8864 4.1572 71.81 0.48
19* 269.229 1.6103 1.2079 6.6991 4.1572 72.73 0.30
20* 277.619 1.6605 1.1785 6.4780 4.1572 73.81 0.28
21* 288.472 1.7254 1.1415 6.2044 4.1572 75.14 0.04
22* 291.599 1.7442 1.1310 6.1281 4.1572 75.52 0.74
23* 293.111 1.7532 1.1259 6.0916 4.1572 75.69 0.11
24* 301.680 1.8044 1.0976 5.8892 4.1572 76.68 0.02
25* 317.224 1.8974 1.0477 5.5411 4.1572 78.36 0.06
26* 326.674 1.9539 1.0183 5.3407 4.1572 79.33 0.05
27* 331.813 1.9847 1.0026 5.2351 4.1572 79.84 0.05
28* 346.537 2.0728 0.9586 4.9450 4.1572 81.22 0.15
29* 362.767 2.1698 0.9121 4.6451 4.1572 82.63 0.40
30* 371.246 2.2205 0.8885 4.4962 4.1572 83.33 0.39
31* 397.380 2.3769 0.8189 4.0682 4.1572 85.30 0.39
32* 400.395 2.3949 0.8112 4.0216 4.1572 85.52 0.04
33* 421.959 2.5239 0.7577 3.7042 4.1572 86.95 0.17
34* 429.226 2.5673 0.7404 3.6031 4.1572 87.40 2.20
35* 466.602 2.7909 0.6564 3.1259 4.1572 89.48 0.59
36* 470.670 2.8152 0.6478 3.0780 4.1572 89.68 0.49
37* 489.187 2.9260 0.6097 2.8690 4.1572 90.56 1.30
38* 499.813 2.9895 0.5887 2.7555 4.1572 91.04 0.18
39* 531.358 3.1782 0.5301 2.4442 4.1572 92.30 0.78
40* 540.878 3.2352 0.5135 2.3572 4.1572 92.65 0.50
41* 554.243 3.3151 0.4909 2.2403 4.1572 93.11 2.48
42* 566.618 3.3891 0.4707 2.1371 4.1572 93.51 1.19
43* 589.381 3.5253 0.4356 1.9593 4.1572 94.18 1.20
44* 598.630 3.5806 0.4219 1.8912 4.1572 94.44 6.81
45* 600.289 3.5905 0.4195 1.8792 4.1572 94.48 0.07
46 681.853 4.0784 0.3155 1.3737 3.6165 96.28 4.92
47 687.501 4.1122 0.3092 1.3440 3.5703 96.38 0.34
48 725.486 4.3394 0.2700 1.1601 3.2686 96.98 0.03
49 732.231 4.3797 0.2635 1.1301 3.2166 97.08 0.63
50 812.838 4.8619 0.1963 0.8247 2.6351 98.02 0.91
51 815.590 4.8783 0.1943 0.8158 2.6166 98.05 4.53
52 825.663 4.9386 0.1872 0.7841 2.5495 98.14 5.58
53 836.925 5.0059 0.1796 0.7501 2.4760 98.24 3.25
54 853.634 5.1059 0.1687 0.7022 2.3698 98.37 12.96
55 862.273 5.1575 0.1634 0.6786 2.3161 98.44 10.99
56 864.648 5.1717 0.1619 0.6722 2.3015 98.46 7.05

57	879.285	5.2593	0.1533	0.6343	2.2130	98.56	9.51
58	904.617	5.4108	0.1393	0.5736	2.0659	98.73	18.04
59	925.627	5.5365	0.1286	0.5275	1.9496	98.85	1.08
60	933.915	5.5860	0.1246	0.5103	1.9051	98.90	0.66
61	934.396	5.5889	0.1244	0.5093	1.9026	98.90	0.67
62	945.491	5.6553	0.1193	0.4872	1.8443	98.96	1.37
63	950.575	5.6857	0.1170	0.4774	1.8181	98.98	1.12
64	956.597	5.7217	0.1143	0.4660	1.7874	99.01	8.58
65	973.032	5.8200	0.1073	0.4363	1.7058	99.09	1.93
66	974.074	5.8263	0.1069	0.4344	1.7007	99.09	0.02
67	974.318	5.8277	0.1068	0.4340	1.6995	99.09	0.02
68	1000.637	5.9851	0.0965	0.3904	1.5753	99.20	1.60
69	1018.456	6.0917	0.0901	0.3633	1.4955	99.27	1.15
70	1033.835	6.1837	0.0848	0.3414	1.4292	99.32	33.55
71	1036.840	6.2017	0.0838	0.3372	1.4166	99.33	0.85
72	1039.867	6.2198	0.0829	0.3331	1.4039	99.34	7.70
73	1058.386	6.3306	0.0771	0.3090	1.3285	99.39	0.12
74	1062.164	6.3531	0.0760	0.3043	1.3136	99.41	0.24
75	1068.501	6.3911	0.0741	0.2966	1.2888	99.42	0.52
76	1075.160	6.4309	0.0722	0.2886	1.2632	99.44	4.95
77	1081.100	6.4664	0.0705	0.2817	1.2407	99.46	1.42
78	1093.283	6.5393	0.0672	0.2681	1.1956	99.49	6.46
79	1145.528	6.8518	0.0547	0.2165	1.0178	99.60	0.19
80	1169.407	6.9946	0.0497	0.1963	0.9444	99.65	1.77
81	1187.278	7.1015	0.0463	0.1823	0.8925	99.68	3.02
82	1220.602	7.3008	0.0405	0.1589	0.8024	99.72	1.02
83	1235.952	7.3926	0.0381	0.1491	0.7637	99.74	3.52
84	1237.851	7.4040	0.0378	0.1479	0.7590	99.75	1.52
85	1238.826	7.4098	0.0376	0.1473	0.7566	99.75	3.80
86	1241.928	7.4284	0.0372	0.1454	0.7490	99.75	2.76
87	1246.036	7.4530	0.0366	0.1430	0.7391	99.76	11.23
88	1263.336	7.5564	0.0341	0.1331	0.6987	99.77	40.52
89	1269.913	7.5958	0.0332	0.1295	0.6838	99.78	2.70
90	1287.497	7.7009	0.0309	0.1204	0.6455	99.80	65.84
91	1291.837	7.7269	0.0304	0.1182	0.6363	99.80	22.98
92	1330.138	7.9560	0.0260	0.1007	0.5604	99.84	3.06
93	1333.722	7.9774	0.0256	0.0992	0.5537	99.84	1.68
94	1342.829	8.0319	0.0247	0.0955	0.5371	99.85	2.52
95	1347.058	8.0572	0.0243	0.0938	0.5295	99.85	12.37
96	1365.353	8.1666	0.0225	0.0869	0.4979	99.86	14.06
97	1377.057	8.2366	0.0214	0.0827	0.4786	99.87	3.82
98	1384.298	8.2799	0.0208	0.0803	0.4670	99.87	2.16
99	1392.460	8.3288	0.0201	0.0776	0.4542	99.88	2.24
100	1419.088	8.4880	0.0180	0.0693	0.4148	99.89	6.56
101	1423.391	8.5138	0.0177	0.0681	0.4087	99.90	4.97
102	1425.158	8.5243	0.0176	0.0676	0.4062	99.90	6.85
103	1427.557	8.5387	0.0174	0.0669	0.4029	99.90	5.18
104	1454.887	8.7022	0.0156	0.0596	0.3667	99.91	0.50
105	1456.631	8.7126	0.0154	0.0592	0.3645	99.91	0.66
106	1473.747	8.8150	0.0144	0.0550	0.3434	99.92	2.36
107	1491.526	8.9213	0.0134	0.0510	0.3228	99.93	5.70
108	1507.213	9.0151	0.0125	0.0478	0.3056	99.93	0.06
109	1507.698	9.0180	0.0125	0.0477	0.3051	99.93	0.46
110	1511.395	9.0401	0.0123	0.0469	0.3011	99.93	0.12

111	1515.651	9.0656	0.0121	0.0461	0.2967	99.93	2.45
112	1516.650	9.0716	0.0120	0.0459	0.2956	99.93	0.54
113	1516.724	9.0720	0.0120	0.0459	0.2955	99.93	0.31
114	1518.382	9.0819	0.0119	0.0455	0.2938	99.93	0.59
115	1525.127	9.1223	0.0116	0.0443	0.2869	99.94	2.41
116	1526.614	9.1312	0.0115	0.0440	0.2854	99.94	0.18
117	1528.863	9.1446	0.0114	0.0436	0.2832	99.94	6.70
118	1530.585	9.1549	0.0114	0.0432	0.2815	99.94	6.36
119	1532.171	9.1644	0.0113	0.0429	0.2799	99.94	7.06
120	1535.947	9.1870	0.0111	0.0423	0.2762	99.94	6.25
121	1545.954	9.2469	0.0106	0.0405	0.2666	99.94	7.48
122	1551.125	9.2778	0.0104	0.0396	0.2618	99.94	5.15
123	1551.417	9.2795	0.0104	0.0396	0.2615	99.94	11.00
124	1609.784	9.6286	0.0081	0.0308	0.2124	99.96	11.04
125	1617.400	9.6742	0.0079	0.0299	0.2066	99.96	16.33
126	1739.754	10.4060	0.0047	0.0176	0.1324	99.98	2.97
127	3043.469	18.2040	0.0000	0.0001	0.0008	100.00	10.51
128	3043.506	18.2042	0.0000	0.0001	0.0008	100.00	28.95
129	3043.663	18.2051	0.0000	0.0001	0.0007	100.00	20.75
130	3045.100	18.2137	0.0000	0.0001	0.0007	100.00	19.66
131	3046.275	18.2208	0.0000	0.0001	0.0007	100.00	21.34
132	3050.890	18.2484	0.0000	0.0001	0.0007	100.00	19.22
133	3052.344	18.2571	0.0000	0.0001	0.0007	100.00	49.22
134	3052.757	18.2595	0.0000	0.0001	0.0007	100.00	25.30
135	3055.424	18.2755	0.0000	0.0001	0.0007	100.00	74.16
136	3064.598	18.3304	0.0000	0.0000	0.0007	100.00	65.25
137	3096.669	18.5222	0.0000	0.0000	0.0006	100.00	15.21
138	3101.596	18.5517	0.0000	0.0000	0.0006	100.00	6.88
139	3111.268	18.6095	0.0000	0.0000	0.0006	100.00	3.17
140	3111.641	18.6117	0.0000	0.0000	0.0006	100.00	4.76
141	3113.533	18.6231	0.0000	0.0000	0.0006	100.00	0.84
142	3114.295	18.6276	0.0000	0.0000	0.0006	100.00	3.72
143	3117.109	18.6444	0.0000	0.0000	0.0006	100.00	27.02
144	3119.055	18.6561	0.0000	0.0000	0.0005	100.00	27.70
145	3119.833	18.6607	0.0000	0.0000	0.0005	100.00	81.54
146	3120.870	18.6669	0.0000	0.0000	0.0005	100.00	87.54
147	3121.169	18.6687	0.0000	0.0000	0.0005	100.00	41.21
148	3121.293	18.6695	0.0000	0.0000	0.0005	100.00	23.60
149	3123.745	18.6841	0.0000	0.0000	0.0005	100.00	38.94
150	3124.840	18.6907	0.0000	0.0000	0.0005	100.00	47.47
151	3125.811	18.6965	0.0000	0.0000	0.0005	100.00	28.67
152	3126.026	18.6978	0.0000	0.0000	0.0005	100.00	27.15
153	3134.909	18.7509	0.0000	0.0000	0.0005	100.00	33.69
154	3169.177	18.9559	0.0000	0.0000	0.0004	100.00	15.26
155	3215.213	19.2312	0.0000	0.0000	0.0004	100.00	17.52
156	3216.208	19.2372	0.0000	0.0000	0.0004	100.00	13.19
--	----------	-------	-------	-------	----		
Total Vibrations	1228.5961	49.5812	279.7059	275.8970			

Ideal Gas	2.4789		
Translation	3.7184	182.1068	12.4716
Rotation	3.7184	149.1814	12.4716
----------	-------	-------	-------
Totals	1288.0931	610.9941	300.8402

```
Vibrational(v) Corrections:
Temp. Correction Hv 1288.0931
Entropy Correction (Hv-TSv) 1105.9253

Reason for exit: Successful completion
Properties CPU Time : 2.55
Properties Wall Time: 2.66
```

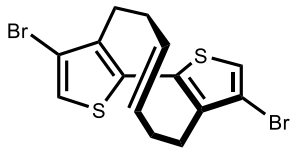	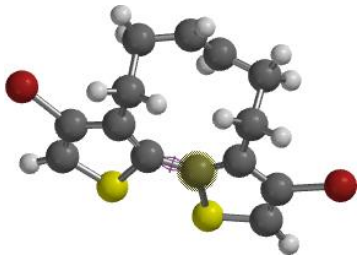
16a GS	**16a'** TS
-6484.821998 au	-6484.777294 au

Fig s16a. Calculation studies on the isomerization of **16a**

Cartesian coordinate of **16a** (GS)

S	−1. 146550	−1. 646370	−1. 728678
C	−0. 701289	−0. 216336	−0. 810108
C	−2. 810971	−1. 476471	−1. 298057
H	−3. 554573	−2. 181152	−1. 641573
C	−2. 993071	−0. 375402	−0. 514502
C	−1. 803231	0. 375035	−0. 219914
C	0. 701289	0. 216336	−0. 810108
C	1. 803231	−0. 375035	−0. 219914
C	2. 993071	0. 375402	−0. 514502
C	2. 810971	1. 476471	−1. 298057
H	3. 554573	2. 181152	−1. 641573
S	1. 146550	1. 646370	−1. 728678
C	−1. 764222	1. 583895	0. 680124
H	−2. 709400	2. 130583	0. 595736
H	−0. 971120	2. 263440	0. 351813
C	−1. 520128	1. 218177	2. 178082
H	−1. 657387	2. 129782	2. 773661
H	−2. 281018	0. 498612	2. 502007
C	1. 764222	−1. 583895	0. 680124
H	0. 971120	−2. 263440	0. 351813
H	2. 709400	−2. 130583	0. 595736
C	1. 520128	−1. 218177	2. 178082
H	2. 281018	−0. 498612	2. 502007
H	1. 657387	−2. 129782	2. 773661
C	0. 142020	−0. 652614	2. 354208
H	−0. 679847	−1. 371111	2. 336794
C	−0. 142020	0. 652614	2. 354208
H	0. 679847	1. 371111	2. 336794

Br	4.726933	−0.113056	0.126480
Br	−4.726933	0.113056	0.126480

Cartesian coordinate of **16a'** (TS)

S	1.392193	2.506549	−0.317405
C	0.724409	0.893447	0.067647
C	3.019024	1.978195	−0.228808
H	3.840295	2.658818	−0.399140
C	3.061001	0.659930	0.083909
C	1.786395	0.003468	0.281187
C	−0.771032	0.880869	0.045816
C	−1.816105	−0.029044	0.251876
C	−3.102899	0.612296	0.098438
C	−3.083754	1.934999	−0.199952
H	−3.916613	2.605392	−0.353270
S	−1.466215	2.485827	−0.319205
C	1.837904	−1.447958	0.696031
H	0.965527	−1.716768	1.292537
H	2.699109	−1.564153	1.360265
C	1.980901	−2.447582	−0.517478
H	2.377476	−1.917586	−1.389336
H	2.693863	−3.237240	−0.259147
C	−1.811203	−1.517112	0.500731
H	−0.971222	−1.815484	1.127466
H	−2.718606	−1.765662	1.058497
C	−1.772266	−2.367280	−0.815077
H	−2.532157	−2.011501	−1.518671
H	−2.018143	−3.403683	−0.552134
C	−0.368457	−2.267717	−1.334737
H	−0.112359	−1.392188	−1.931220
C	0.600712	−2.977898	−0.752155
H	0.307482	−3.809757	−0.105630
Br	−4.783864	−0.284153	0.291808
Br	4.755090	−0.214145	0.256334

Frequency calculation of **16a'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 12 low frequency terms

Term	ZPE	Enthalpy Correction	Entropy	Cv	% in Ground	IR Int.
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K		
--	----------	-------	-------	-------	----	
1* i	**52.475**	**0.0000**	**1.2395**	**0.0000**	**8.3144**	**0.00** **0.01**
2*	36.215	0.2166	1.2395	22.8280	8.2933	16.03 0.13
3*	68.828	0.4117	1.2395	17.5165	8.2384	28.26 0.01
4*	91.237	0.5457	1.2395	15.2019	8.1814	35.61 0.03
5*	123.763	0.7403	1.2395	12.7224	8.0716	44.97 0.72
6*	135.234	0.8089	1.2395	12.0089	8.0255	47.93 0.26
7*	165.708	0.9912	1.2395	10.3913	7.8852	55.05 0.30
8*	189.858	1.1356	1.2395	9.3269	7.7564	60.00 0.24
9*	191.514	1.1455	1.2395	9.2596	7.7471	60.31 0.07
10*	212.693	1.2722	1.2395	8.4534	7.6214	64.17 0.06
11*	237.746	1.4220	1.2395	7.6135	7.4594	68.25 0.31
12*	247.687	1.4815	1.2395	7.3093	7.3914	69.74 1.15

13	265.379	1.5873	1.2215	6.8036	7.2655	72.21	1.21
14	286.138	1.7115	1.1494	6.2621	7.1104	74.86	0.54
15	298.303	1.7842	1.1087	5.9680	7.0160	76.30	1.66
16	342.743	2.0501	0.9698	5.0180	6.6526	80.87	0.93
17	346.131	2.0703	0.9598	4.9527	6.6238	81.18	0.87
18	364.877	2.1824	0.9061	4.6076	6.4623	82.81	2.47
19	422.352	2.5262	0.7568	3.6987	5.9481	86.97	0.52
20	453.626	2.7133	0.6846	3.2839	5.6604	88.80	0.13
21	462.002	2.7634	0.6663	3.1810	5.5828	89.24	1.45
22	472.650	2.8271	0.6436	3.0550	5.4840	89.78	0.24
23	495.896	2.9661	0.5964	2.7968	5.2681	90.86	1.93
24	538.413	3.2204	0.5178	2.3794	4.8747	92.56	0.94
25	546.256	3.2673	0.5043	2.3095	4.8027	92.84	2.37
26	563.821	3.3724	0.4752	2.1600	4.6423	93.42	0.41
27	590.706	3.5332	0.4336	1.9494	4.3998	94.22	5.20
28	697.710	4.1732	0.2982	1.2920	3.4878	96.55	17.17
29	700.593	4.1905	0.2951	1.2777	3.4647	96.60	1.27
30	723.502	4.3275	0.2719	1.1691	3.2840	96.95	33.26
31	741.309	4.4340	0.2550	1.0909	3.1474	97.21	49.06
32	742.977	4.4440	0.2535	1.0839	3.1348	97.23	2.56
33	746.346	4.4641	0.2504	1.0697	3.1094	97.27	14.87
34	825.046	4.9349	0.1877	0.7860	2.5536	98.13	5.54
35	837.523	5.0095	0.1792	0.7483	2.4722	98.24	2.77
36	862.343	5.1580	0.1633	0.6784	2.3157	98.44	3.56
37	871.633	5.2135	0.1577	0.6539	2.2590	98.51	1.70
38	876.628	5.2434	0.1548	0.6411	2.2289	98.55	0.50
39	889.254	5.3189	0.1476	0.6097	2.1543	98.63	20.84
40	909.573	5.4405	0.1367	0.5624	2.0380	98.76	8.59
41	928.109	5.5513	0.1274	0.5223	1.9362	98.87	4.36
42	964.732	5.7704	0.1108	0.4510	1.7466	99.05	39.93
43	974.489	5.8287	0.1067	0.4337	1.6987	99.09	56.33
44	996.210	5.9587	0.0982	0.3974	1.5957	99.18	23.00
45	1017.442	6.0857	0.0904	0.3648	1.4999	99.26	0.14
46	1029.548	6.1581	0.0863	0.3473	1.4475	99.30	36.59
47	1080.164	6.4608	0.0708	0.2828	1.2442	99.46	12.08
48	1090.915	6.5251	0.0679	0.2707	1.2043	99.48	5.82
49	1107.721	6.6256	0.0635	0.2527	1.1440	99.52	4.29
50	1162.697	6.9545	0.0511	0.2017	0.9645	99.63	0.96
51	1177.106	7.0407	0.0482	0.1901	0.9217	99.66	0.34
52	1217.848	7.2843	0.0410	0.1607	0.8095	99.72	0.40
53	1220.030	7.2974	0.0406	0.1593	0.8039	99.72	7.98
54	1229.610	7.3547	0.0391	0.1531	0.7795	99.74	1.27
55	1244.278	7.4424	0.0368	0.1440	0.7434	99.75	2.41
56	1325.455	7.9280	0.0265	0.1027	0.5692	99.83	6.22
57	1328.207	7.9444	0.0262	0.1015	0.5640	99.84	4.98
58	1345.276	8.0465	0.0244	0.0945	0.5327	99.85	2.20
59	1346.623	8.0546	0.0243	0.0940	0.5303	99.85	8.07
60	1354.050	8.0990	0.0236	0.0911	0.5172	99.85	13.38
61	1363.304	8.1544	0.0227	0.0877	0.5014	99.86	20.14
62	1377.956	8.2420	0.0214	0.0824	0.4772	99.87	1.13
63	1383.245	8.2736	0.0209	0.0806	0.4687	99.87	7.21
64	1441.199	8.6203	0.0165	0.0632	0.3844	99.90	2.70
65	1462.447	8.7474	0.0151	0.0577	0.3572	99.91	0.48
66	1514.725	9.0601	0.0121	0.0463	0.2976	99.93	4.05

```
67 1518.790 9.0844 0.0119 0.0455 0.2934 99.93 0.93
68 1521.252 9.0991 0.0118 0.0450 0.2909 99.94 2.31
69 1547.326 9.2551 0.0106 0.0403 0.2653 99.94 15.83
70 1558.711 9.3232 0.0101 0.0384 0.2548 99.95 39.28
71 1567.467 9.3755 0.0097 0.0370 0.2470 99.95 0.34
72 1736.904 10.3890 0.0048 0.0179 0.1338 99.98 2.41
73 3056.026 18.2791 0.0000 0.0001 0.0007 100.00 32.19
74 3072.046 18.3749 0.0000 0.0000 0.0007 100.00 31.19
75 3090.987 18.4882 0.0000 0.0000 0.0006 100.00 12.89
76 3094.451 18.5089 0.0000 0.0000 0.0006 100.00 15.24
77 3107.407 18.5864 0.0000 0.0000 0.0006 100.00 9.80
78 3109.398 18.5983 0.0000 0.0000 0.0006 100.00 10.76
79 3125.018 18.6918 0.0000 0.0000 0.0005 100.00 38.37
80 3143.188 18.8004 0.0000 0.0000 0.0005 100.00 18.64
81 3159.992 18.9009 0.0000 0.0000 0.0005 100.00 17.14
82 3163.509 18.9220 0.0000 0.0000 0.0005 100.00 16.76
83 3289.723 19.6769 0.0000 0.0000 0.0003 100.00 6.33
84 3290.808 19.6834 0.0000 0.0000 0.0003 100.00 5.68
-- ---------- ------- ------- ------- ----
Total Vibrations 582.6447 30.5898 208.1784 243.6596 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 183.5992 12.4716
Rotation 3.7184 148.3315 12.4716
---------- ------- ------- -------
Totals 623.1502 540.1090 268.6028

Vibrational(v) Corrections:
Temp. Correction Hv 623.1502
Entropy Correction (Hv-TSv) 462.1167

Reason for exit: Successful completion
Properties CPU Time : 2.03
Properties Wall Time: 2.03
```

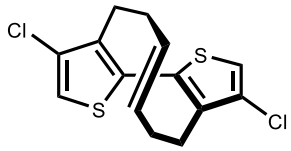	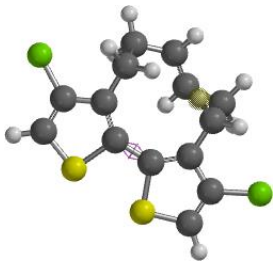
16b GS	**16b'** TS
-2257.451296 au	-2257.407604 au

Fig s16b. Calculation studies on the isomerization of **16b**

Cartesian coordinate of **16b** (GS)

S	−1.214967	−1.598999	−1.682887
C	−0.709200	−0.188067	−0.765545
C	−2.868227	−1.368894	−1.239571

H	−3.643297	−2.043995	−1.573346
C	−3.003209	−0.263389	−0.451800
C	−1.784052	0.442153	−0.167669
C	0.709200	0.188067	−0.765545
C	1.784052	−0.442153	−0.167669
C	3.003209	0.263389	−0.451800
C	2.868227	1.368894	−1.239571
H	3.643297	2.043995	−1.573346
S	1.214967	1.598999	−1.682887
C	−1.706981	1.649131	0.731941
H	−2.637782	2.220217	0.649163
H	−0.896573	2.307101	0.401717
C	−1.471495	1.276751	2.229443
H	−1.571389	2.193577	2.824382
H	−2.258971	0.587852	2.556471
C	1.706981	−1.649131	0.731941
H	0.896573	−2.307101	0.401717
H	2.637782	−2.220217	0.649163
C	1.471495	−1.276751	2.229443
H	2.258971	−0.587852	2.556471
H	1.571389	−2.193577	2.824382
C	0.115948	−0.657695	2.403285
H	−0.734122	−1.342436	2.385453
C	−0.115948	0.657695	2.403285
H	0.734122	1.342436	2.385453
Cl	4.559322	−0.246981	0.173676
Cl	−4.559322	0.246981	0.173676

Cartesian coordinate of **16b'** (TS)

S	1.372772	2.407904	−0.296470
C	0.717694	0.802081	0.138821
C	3.003984	1.901878	−0.168088
H	3.823384	2.580658	−0.354488
C	3.055610	0.595540	0.191964
C	1.786156	−0.066022	0.398742
C	−0.775582	0.768548	0.103589
C	−1.808315	−0.148531	0.332453
C	−3.102306	0.461085	0.126645
C	−3.100851	1.772071	−0.222194
H	−3.945503	2.416188	−0.418478
S	−1.491328	2.346755	−0.332756
C	1.858071	−1.502622	0.859989
H	0.990192	−1.763842	1.466509
H	2.722915	−1.585994	1.524054
C	2.010486	−2.538287	−0.321812
H	2.381416	−2.027580	−1.216180
H	2.745665	−3.302058	−0.047782
C	−1.794094	−1.619754	0.667955
H	−0.952814	−1.873771	1.312368
H	−2.701061	−1.839543	1.239129
C	−1.747398	−2.547684	−0.593930
H	−2.519354	−2.250585	−1.311547
H	−1.970453	−3.570851	−0.266655
C	−0.349180	−2.451006	−1.129822

H	-0.117209	-1.608147	-1.781221
C	0.639423	-3.106318	-0.516354
H	0.368330	-3.905051	0.179928
Cl	4.603266	-0.208798	0.394619
Cl	-4.618836	-0.407363	0.298842

Frequency calculation of **16b'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 11 low frequency terms

	Enthalpy				
Term	ZPE	Correction	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1* i	**53.857**	**0.0000**	**1.2395**	**0.0000**	**8.3144**	**0.00**	**0.00**
2*	45.172	0.2702	1.2395	20.9964	8.2816	19.59	0.23
3*	71.100	0.4253	1.2395	17.2491	8.2333	29.04	0.02
4*	115.896	0.6932	1.2395	13.2535	8.1010	42.84	0.05
5*	129.572	0.7750	1.2395	12.3527	8.0487	46.49	0.53
6*	150.935	0.9028	1.2395	11.1310	7.9564	51.73	0.51
7*	171.768	1.0274	1.2395	10.1086	7.8543	56.35	0.44
8*	213.649	1.2779	1.2395	8.4193	7.6155	64.34	0.04
9*	224.064	1.3402	1.2395	8.0583	7.5496	66.08	0.24
10*	238.263	1.4251	1.2395	7.5973	7.4559	68.33	0.79
11*	240.443	1.4382	1.2395	7.5294	7.4412	68.66	0.18
12	264.007	1.5791	1.2264	6.8413	7.2755	72.03	1.31
13	272.243	1.6284	1.1973	6.6187	7.2151	73.12	1.46
14	301.392	1.8027	1.0985	5.8959	6.9917	76.65	0.33
15	352.098	2.1060	0.9425	4.8399	6.5728	81.72	0.40
16	367.547	2.1984	0.8987	4.5605	6.4390	83.03	2.09
17	376.274	2.2506	0.8747	4.4103	6.3624	83.73	2.98
18	386.538	2.3120	0.8472	4.2403	6.2715	84.52	2.84
19	441.169	2.6388	0.7126	3.4431	5.7754	88.10	3.25
20	462.395	2.7657	0.6654	3.1763	5.5792	89.26	1.37
21	474.332	2.8371	0.6401	3.0355	5.4684	89.86	0.13
22	481.975	2.8829	0.6243	2.9487	5.3974	90.23	0.85
23	497.247	2.9742	0.5937	2.7825	5.2556	90.92	2.08
24	542.687	3.2460	0.5104	2.3410	4.8354	92.71	0.36
25	549.785	3.2884	0.4983	2.2786	4.7703	92.96	2.67
26	569.658	3.4073	0.4659	2.1124	4.5893	93.60	0.45
27	598.494	3.5798	0.4221	1.8922	4.3303	94.43	5.86
28	703.429	4.2074	0.2922	1.2637	3.4420	96.64	8.60
29	703.941	4.2105	0.2916	1.2612	3.4379	96.65	1.48
30	733.317	4.3862	0.2625	1.1254	3.2083	97.10	35.00
31	736.758	4.4068	0.2592	1.1104	3.1820	97.14	52.12
32	738.717	4.4185	0.2574	1.1020	3.1671	97.17	4.64
33	758.546	4.5371	0.2395	1.0201	3.0186	97.43	18.80
34	824.512	4.9317	0.1880	0.7877	2.5571	98.13	6.06
35	839.208	5.0196	0.1780	0.7433	2.4613	98.26	3.27
36	872.368	5.2179	0.1573	0.6520	2.2545	98.52	4.72
37	875.213	5.2349	0.1556	0.6447	2.2374	98.54	1.71
38	883.017	5.2816	0.1511	0.6250	2.1909	98.59	0.20
39	892.696	5.3395	0.1457	0.6014	2.1342	98.65	22.85
40	912.202	5.4562	0.1354	0.5565	2.0233	98.77	8.25
41	930.255	5.5642	0.1264	0.5178	1.9247	98.88	3.95

```
42 966.321 5.7799 0.1101 0.4482 1.7388 99.06 20.62
43 983.811 5.8845 0.1030 0.4178 1.6538 99.13 62.33
44 999.693 5.9795 0.0968 0.3919 1.5796 99.20 37.92
45 1020.064 6.1013 0.0895 0.3609 1.4884 99.27 5.40
46 1026.665 6.1408 0.0872 0.3514 1.4598 99.29 36.08
47 1083.162 6.4787 0.0700 0.2794 1.2330 99.46 11.26
48 1092.215 6.5329 0.0675 0.2693 1.1995 99.49 9.51
49 1113.061 6.6576 0.0622 0.2473 1.1254 99.54 5.85
50 1164.450 6.9650 0.0507 0.2003 0.9592 99.64 1.16
51 1177.198 7.0412 0.0482 0.1901 0.9215 99.66 0.15
52 1219.047 7.2915 0.0408 0.1599 0.8064 99.72 4.44
53 1219.987 7.2971 0.0406 0.1593 0.8040 99.72 2.35
54 1230.045 7.3573 0.0390 0.1528 0.7784 99.74 0.89
55 1244.935 7.4464 0.0367 0.1436 0.7418 99.75 2.44
56 1327.845 7.9423 0.0262 0.1017 0.5647 99.84 6.17
57 1330.542 7.9584 0.0259 0.1006 0.5596 99.84 7.03
58 1349.582 8.0723 0.0240 0.0929 0.5251 99.85 5.69
59 1352.282 8.0884 0.0237 0.0918 0.5203 99.85 0.27
60 1361.201 8.1418 0.0229 0.0884 0.5049 99.86 14.12
61 1368.321 8.1844 0.0222 0.0858 0.4930 99.86 30.80
62 1377.212 8.2376 0.0214 0.0827 0.4784 99.87 3.00
63 1386.854 8.2952 0.0206 0.0794 0.4630 99.88 9.51
64 1446.272 8.6506 0.0161 0.0618 0.3777 99.91 5.15
65 1468.321 8.7825 0.0147 0.0563 0.3500 99.92 0.31
66 1517.585 9.0772 0.0120 0.0457 0.2947 99.93 4.40
67 1520.516 9.0947 0.0118 0.0451 0.2916 99.93 1.73
68 1524.083 9.1160 0.0117 0.0445 0.2880 99.94 1.08
69 1552.121 9.2837 0.0104 0.0395 0.2608 99.94 14.62
70 1566.598 9.3703 0.0098 0.0371 0.2478 99.95 39.72
71 1575.391 9.4229 0.0094 0.0357 0.2402 99.95 0.60
72 1736.572 10.3870 0.0048 0.0179 0.1340 99.98 2.35
73 3056.044 18.2792 0.0000 0.0001 0.0007 100.00 33.09
74 3072.130 18.3754 0.0000 0.0000 0.0007 100.00 33.02
75 3091.291 18.4900 0.0000 0.0000 0.0006 100.00 12.37
76 3094.191 18.5074 0.0000 0.0000 0.0006 100.00 17.40
77 3106.068 18.5784 0.0000 0.0000 0.0006 100.00 8.92
78 3109.199 18.5971 0.0000 0.0000 0.0006 100.00 12.18
79 3124.749 18.6901 0.0000 0.0000 0.0005 100.00 39.76
80 3143.950 18.8050 0.0000 0.0000 0.0005 100.00 17.37
81 3158.009 18.8891 0.0000 0.0000 0.0005 100.00 13.81
82 3161.528 18.9101 0.0000 0.0000 0.0005 100.00 20.68
83 3288.742 19.6710 0.0000 0.0000 0.0003 100.00 5.42
84 3289.747 19.6771 0.0000 0.0000 0.0003 100.00 5.14
-- ---------- ------- ------- ------- ----
Total Vibrations 585.8140 29.9225 195.0036 240.3102 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 180.5009 12.4716
Rotation 3.7184 143.6277 12.4716
---------- ------- ------- -------
Totals 625.6523 519.1322 265.2535

Vibrational(v) Corrections:
Temp. Correction Hv 625.6523
```

```
Entropy Correction (Hv-TSv) 470.8730

Reason for exit: Successful completion
Properties CPU Time : 1.45
Properties Wall Time: 1.46
```

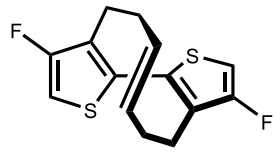	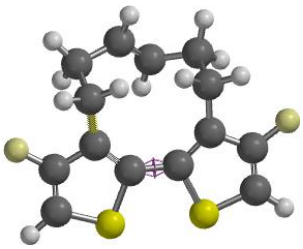
16c GS	**16c'** TS
-1536.722381 au	-1536.683960 au

Fig s16c. Calculation studies on the isomerization of **16c**

Cartesian coordinate of **16c** (GS)

S	−1.323258	−1.519275	−1.649198
C	−0.718965	−0.141028	−0.736904
C	−2.961719	−1.178997	−1.202280
H	−3.786843	−1.794830	−1.529174
C	−3.003417	−0.066475	−0.418679
C	−1.747908	0.556871	−0.138380
C	0.718965	0.141028	−0.736904
C	1.747908	−0.556871	−0.138380
C	3.003417	0.066475	−0.418679
C	2.961719	1.178997	−1.202280
H	3.786843	1.794830	−1.529174
S	1.323258	1.519275	−1.649198
C	−1.633540	1.748771	0.775497
H	−2.553968	2.338486	0.702585
H	−0.809351	2.393865	0.453386
C	−1.409902	1.346869	2.267043
H	−1.467148	2.258455	2.875622
H	−2.229134	0.690416	2.584290
C	1.633540	−1.748771	0.775497
H	0.809351	−2.393865	0.453386
H	2.553968	−2.338486	0.702585
C	1.409902	−1.346869	2.267043
H	2.229134	−0.690416	2.584290
H	1.467148	−2.258455	2.875622
C	0.084745	−0.662483	2.434394
H	−0.797144	−1.305724	2.416791
C	−0.084745	0.662483	2.434394
H	0.797144	1.305724	2.416791
F	4.146647	−0.441002	0.083593
F	−4.146647	0.441002	0.083593

Cartesian coordinate of **16c'** (TS)

S	1.309841	2.395802	-0.275748
C	0.684554	0.777530	0.163998
C	2.957703	1.919167	-0.146779
H	3.771887	2.604230	-0.330921
C	3.011913	0.615691	0.213613
C	1.766704	-0.068428	0.422224
C	-0.798517	0.698631	0.134957
C	-1.786281	-0.259105	0.373743
C	-3.096081	0.293793	0.180813
C	-3.175701	1.599457	-0.168968
H	-4.056309	2.196003	-0.355762
S	-1.586469	2.245050	-0.297163
C	1.925642	-1.498497	0.887766
H	1.093987	-1.807355	1.523582
H	2.821021	-1.526233	1.516204
C	2.098117	-2.527407	-0.293796
H	2.464743	-2.006465	-1.184361
H	2.845201	-3.279692	-0.018614
C	-1.758544	-1.735377	0.691040
H	-0.934937	-1.992455	1.358165
H	-2.686510	-1.969096	1.222935
C	-1.664885	-2.639801	-0.583059
H	-2.439265	-2.351855	-1.302568
H	-1.860085	-3.675486	-0.277483
C	-0.265431	-2.491034	-1.104726
H	-0.055960	-1.636588	-1.748149
C	0.739441	-3.123482	-0.493411
H	0.487979	-3.935844	0.194388
F	-4.189280	-0.479355	0.344827
F	4.176733	-0.040723	0.392632

Frequency calculation of **16c'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 9 low frequency terms

Term	ZPE	Correction	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1*	**i 54.357**	**0.0000**	**1.2395**	**0.0000**	**8.3144 0.00 0.00**
2*	60.449	0.3616	1.2395	18.5871	8.2557 25.30 0.20
3*	73.544	0.4399	1.2395	16.9710	8.2277 29.88 0.01
4*	119.125	0.7125	1.2395	13.0311	8.0892 43.72 0.16
5*	148.069	0.8856	1.2395	11.2837	7.9695 51.06 0.80
6*	156.918	0.9386	1.2395	10.8223	7.9283 53.10 0.29
7*	188.572	1.1279	1.2395	9.3797	7.7637 59.75 0.25
8*	236.669	1.4156	1.2395	7.6474	7.4667 68.09 1.07
9*	252.133	1.5081	1.2395	7.1781	7.3604 70.38 1.01
10	263.491	1.5760	1.2282	6.8555	7.2792 71.96 0.02
11	268.866	1.6082	1.2091	6.7089	7.2400 72.68 0.49
12	285.648	1.7086	1.1510	6.2743	7.1141 74.80 0.25
13	295.631	1.7683	1.1175	6.0312	7.0369 75.99 1.89
14	326.439	1.9525	1.0190	5.3456	6.7890 79.31 0.39
15	362.148	2.1661	0.9138	4.6562	6.4861 82.58 1.46
16	376.049	2.2493	0.8753	4.4141	6.3644 83.71 0.95

17	433.813	2.5948	0.7296	3.5408	5.8431	87.67	0.18
18	457.136	2.7343	0.6769	3.2404	5.6279	88.99	7.10
19	468.753	2.8038	0.6518	3.1005	5.5202	89.59	0.72
20	479.312	2.8669	0.6298	2.9786	5.4222	90.10	0.84
21	499.753	2.9892	0.5889	2.7561	5.2323	91.03	1.56
22	538.099	3.2185	0.5183	2.3823	4.8776	92.55	3.50
23	549.425	3.2863	0.4989	2.2818	4.7736	92.94	0.34
24	551.842	3.3007	0.4949	2.2609	4.7515	93.03	0.19
25	558.219	3.3389	0.4843	2.2066	4.6933	93.24	3.06
26	594.991	3.5588	0.4273	1.9177	4.3615	94.34	2.83
27	619.497	3.7054	0.3926	1.7460	4.1452	94.97	4.62
28	700.543	4.1902	0.2952	1.2779	3.4650	96.60	21.67
29	709.489	4.2437	0.2859	1.2344	3.3938	96.74	1.23
30	721.222	4.3139	0.2741	1.1795	3.3017	96.92	1.24
31	723.817	4.3294	0.2716	1.1677	3.2815	96.96	52.10
32	781.415	4.6739	0.2204	0.9329	2.8529	97.70	20.92
33	790.417	4.7277	0.2132	0.9006	2.7893	97.79	23.71
34	829.465	4.9613	0.1846	0.7725	2.5246	98.17	5.89
35	844.174	5.0493	0.1748	0.7289	2.4295	98.30	4.35
36	875.192	5.2348	0.1556	0.6447	2.2375	98.54	1.25
37	887.867	5.3106	0.1484	0.6131	2.1624	98.62	28.58
38	890.128	5.3241	0.1471	0.6076	2.1492	98.64	6.49
39	907.534	5.4283	0.1378	0.5670	2.0495	98.75	12.74
40	929.417	5.5591	0.1268	0.5196	1.9292	98.87	6.15
41	955.640	5.7160	0.1147	0.4678	1.7923	99.01	0.12
42	974.892	5.8312	0.1066	0.4330	1.6967	99.09	4.15
43	1008.922	6.0347	0.0934	0.3775	1.5378	99.23	12.21
44	1021.088	6.1075	0.0891	0.3594	1.4840	99.28	32.73
45	1058.690	6.3324	0.0770	0.3086	1.3273	99.40	3.02
46	1075.320	6.4318	0.0721	0.2884	1.2626	99.44	6.65
47	1090.032	6.5198	0.0681	0.2717	1.2075	99.48	2.56
48	1153.806	6.9013	0.0529	0.2093	0.9918	99.62	66.57
49	1166.942	6.9799	0.0502	0.1983	0.9517	99.64	6.84
50	1180.809	7.0628	0.0475	0.1873	0.9110	99.66	17.18
51	1183.500	7.0789	0.0470	0.1852	0.9033	99.67	15.05
52	1222.695	7.3133	0.0402	0.1575	0.7970	99.73	7.89
53	1226.056	7.3334	0.0396	0.1553	0.7885	99.73	10.72
54	1241.275	7.4245	0.0373	0.1458	0.7506	99.75	0.54
55	1247.514	7.4618	0.0363	0.1421	0.7356	99.76	1.77
56	1331.848	7.9662	0.0258	0.1000	0.5572	99.84	0.85
57	1337.869	8.0022	0.0252	0.0975	0.5461	99.84	2.82
58	1351.625	8.0845	0.0238	0.0921	0.5215	99.85	2.76
59	1354.331	8.1007	0.0235	0.0910	0.5168	99.85	4.91
60	1375.563	8.2277	0.0216	0.0833	0.4810	99.87	4.37
61	1381.502	8.2632	0.0211	0.0812	0.4715	99.87	14.05
62	1423.137	8.5122	0.0177	0.0682	0.4090	99.90	57.90
63	1429.490	8.5502	0.0173	0.0664	0.4002	99.90	80.46
64	1471.962	8.8043	0.0145	0.0555	0.3456	99.92	36.40
65	1496.928	8.9536	0.0131	0.0499	0.3168	99.93	0.64
66	1519.766	9.0902	0.0119	0.0453	0.2924	99.93	1.03
67	1519.994	9.0916	0.0119	0.0452	0.2922	99.93	4.93
68	1524.402	9.1179	0.0117	0.0444	0.2877	99.94	2.50
69	1544.207	9.2364	0.0107	0.0408	0.2683	99.94	12.19
70	1622.198	9.7029	0.0077	0.0292	0.2031	99.96	80.47

```
71 1630.418 9.7521 0.0075 0.0282 0.1972 99.96 27.20
72 1736.806 10.3884 0.0048 0.0179 0.1339 99.98 2.25
73 3053.138 18.2618 0.0000 0.0001 0.0007 100.00 36.47
74 3068.175 18.3518 0.0000 0.0000 0.0007 100.00 35.12
75 3083.544 18.4437 0.0000 0.0000 0.0006 100.00 20.35
76 3086.491 18.4613 0.0000 0.0000 0.0006 100.00 23.79
77 3103.052 18.5604 0.0000 0.0000 0.0006 100.00 15.13
78 3105.349 18.5741 0.0000 0.0000 0.0006 100.00 6.29
79 3122.047 18.6740 0.0000 0.0000 0.0005 100.00 43.35
80 3133.741 18.7439 0.0000 0.0000 0.0005 100.00 19.51
81 3152.333 18.8551 0.0000 0.0000 0.0005 100.00 18.20
82 3162.049 18.9132 0.0000 0.0000 0.0005 100.00 17.79
83 3292.365 19.6927 0.0000 0.0000 0.0003 100.00 4.99
84 3295.138 19.7093 0.0000 0.0000 0.0003 100.00 5.00
-- ---------- ------- ------- ------- ----
Total Vibrations 593.7778 28.6399 179.6677 232.8839 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 179.1260 12.4716
Rotation 3.7184 140.6396 12.4716
---------- ------- ------- -------
Totals 632.3335 499.4334 257.8272

Vibrational(v) Corrections:
Temp. Correction Hv 632.3335
Entropy Correction (Hv-TSv) 483.4274

Reason for exit: Successful completion
Properties CPU Time : 1.44
Properties Wall Time: 1.41
```

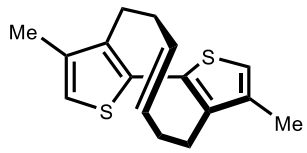	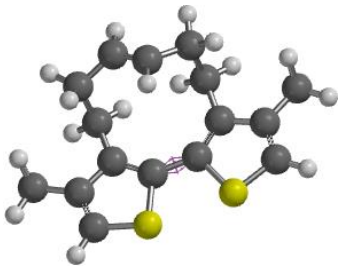
16d GS	**16d'** TS
-1416.899462 au	-1416.856100 au

Fig s16d. Calculation studies on the isomerization of **16d**

Cartesian coordinate of **16d** (GS)

S	−1.277802	−1.558399	−1.618373
C	−0.715549	−0.162416	−0.711093
C	−2.919678	−1.242553	−1.174407
H	−3.711955	−1.895807	−1.517285
C	−3.044327	−0.127367	−0.391749
C	−1.773537	0.504392	−0.124960

C	0.715549	0.162416	−0.711093
C	1.773537	−0.504392	−0.124960
C	3.044327	0.127367	−0.391749
C	2.919678	1.242553	−1.174407
H	3.711955	1.895807	−1.517285
S	1.277802	1.558399	−1.618373
C	−1.637088	1.713962	0.768855
H	−2.540243	2.331004	0.691176
H	−0.801879	2.339050	0.435921
C	−1.410408	1.343984	2.269136
H	−1.464061	2.266877	2.861365
H	−2.224848	0.691768	2.608336
C	1.637088	−1.713962	0.768855
H	0.801879	−2.339050	0.435921
H	2.540243	−2.331004	0.691176
C	1.410408	−1.343984	2.269136
H	2.224848	−0.691768	2.608336
H	1.464061	−2.266877	2.861365
C	0.085024	−0.662283	2.443445
H	−0.796199	−1.306074	2.421469
C	−0.085024	0.662283	2.443445
H	0.796199	1.306074	2.421469
C	4.364828	−0.383445	0.122840
H	5.187596	0.256737	−0.210005
H	4.570411	−1.400875	−0.233745
H	4.392614	−0.416819	1.219351
C	−4.364828	0.383445	0.122840
H	−4.392614	0.416819	1.219351
H	−5.187596	−0.256737	−0.210005
H	−4.570411	1.400875	−0.233745

Cartesian coordinate of **16d'** (TS)

S	1.543906	2.269340	−0.307419
C	0.793405	0.707743	0.127059
C	3.137483	1.658764	−0.144315
H	3.988353	2.302960	−0.324137
C	3.145401	0.346543	0.217655
C	1.817042	−0.213808	0.378350
C	−0.700059	0.763988	0.140812
C	−1.793387	−0.077201	0.388178
C	−3.074129	0.573742	0.175469
C	−2.964063	1.876689	−0.201251
H	−3.762353	2.578266	−0.405780
S	−1.327694	2.372225	−0.321283
C	1.765236	−1.691920	0.692601
H	0.916583	−1.947467	1.327884
H	2.661037	−1.949182	1.268070
C	1.708717	−2.602331	−0.582211
H	2.482865	−2.302970	−1.297730
H	1.916266	−3.635222	−0.274011
C	−1.883701	−1.514450	0.854047
H	−1.024652	−1.795430	1.465123
H	−2.750498	−1.592043	1.518561
C	−2.047426	−2.551007	−0.326306

H	−2.410924	−2.033723	−1.220654
H	−2.787831	−3.312331	−0.055536
C	−0.683588	−3.134850	−0.524900
H	−0.424976	−3.948752	0.158388
C	0.314603	−2.478938	−1.121921
H	0.095073	−1.618441	−1.753492
C	−4.414995	−0.089633	0.367375
H	−5.220339	0.604974	0.109407
H	−4.575774	−0.404567	1.406695
H	−4.534788	−0.980892	−0.260555
C	4.429703	−0.415831	0.427894
H	4.503740	−1.294989	−0.223625
H	4.534752	−0.769991	1.461529
H	5.289564	0.226254	0.213276

Frequency calculation of **16d'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
*Modifying values for 12 low frequency terms

Term	ZPE	Correction Enthalpy	Entropy	Cv	% in	
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
--	----------	-------	-------	-------	----	
1* i	**52.255**	**0.0000**	**1.2395**	**0.0000**	**8.3144**	**0.00 0.02**
2*	61.500	0.3679	1.2395	18.4449	8.2537	25.68 0.50
3*	83.969	0.5022	1.2395	15.8819	8.2016	33.32 0.04
4*	126.620	0.7574	1.2395	12.5383	8.0605	45.72 0.69
5*	157.475	0.9419	1.2395	10.7942	7.9256	53.23 0.54
6*	163.006	0.9750	1.2395	10.5210	7.8986	54.46 0.60
7*	174.840	1.0458	1.2395	9.9695	7.8382	56.99 0.15
8*	189.405	1.1329	1.2395	9.3455	7.7590	59.91 0.07
9*	209.398	1.2525	1.2395	8.5726	7.6416	63.60 0.20
10*	234.461	1.4024	1.2395	7.7174	7.4814	67.74 1.05
11*	248.461	1.4861	1.2395	7.2862	7.3861	69.85 0.19
12*	256.011	1.5313	1.2395	7.0659	7.3330	70.93 0.64
13	271.911	1.6264	1.1984	6.6275	7.2175	73.08 0.86
14	278.269	1.6644	1.1763	6.4612	7.1701	73.89 1.76
15	294.023	1.7586	1.1229	6.0696	7.0495	75.80 0.32
16	328.524	1.9650	1.0126	5.3025	6.7718	79.51 0.76
17	367.711	2.1994	0.8982	4.5577	6.4376	83.04 1.05
18	377.612	2.2586	0.8711	4.3878	6.3506	83.83 2.32
19	414.028	2.4764	0.7770	3.8178	6.0240	86.44 0.02
20	425.030	2.5422	0.7503	3.6611	5.9236	87.14 0.39
21	454.771	2.7201	0.6821	3.2696	5.6498	88.86 0.70
22	482.200	2.8842	0.6238	2.9461	5.3953	90.24 0.11
23	498.936	2.9843	0.5904	2.7647	5.2399	91.00 1.93
24	540.314	3.2318	0.5145	2.3623	4.8572	92.63 1.32
25	552.712	3.3059	0.4934	2.2534	4.7436	93.06 3.11
26	557.393	3.3340	0.4857	2.2136	4.7008	93.21 1.16
27	558.333	3.3396	0.4841	2.2056	4.6922	93.24 2.50
28	580.681	3.4732	0.4487	2.0254	4.4897	93.93 1.90
29	604.387	3.6150	0.4137	1.8500	4.2781	94.59 3.11
30	707.302	4.2306	0.2882	1.2449	3.4112	96.71 0.53
31	709.467	4.2436	0.2859	1.2345	3.3940	96.74 1.03
32	747.038	4.4683	0.2498	1.0669	3.1042	97.28 38.86

33	748.337	4.4760	0.2486	1.0615	3.0945	97.30	5.57
34	766.418	4.5842	0.2328	0.9892	2.9609	97.52	3.33
35	783.742	4.6878	0.2185	0.9244	2.8364	97.72	8.29
36	829.032	4.9587	0.1849	0.7738	2.5274	98.17	5.99
37	842.614	5.0399	0.1758	0.7334	2.4395	98.29	2.81
38	876.256	5.2412	0.1550	0.6420	2.2311	98.54	2.63
39	888.776	5.3161	0.1479	0.6109	2.1570	98.63	2.71
40	895.861	5.3584	0.1440	0.5939	2.1159	98.67	24.20
41	903.193	5.4023	0.1401	0.5768	2.0740	98.72	15.64
42	925.610	5.5364	0.1286	0.5275	1.9497	98.85	11.74
43	945.616	5.6560	0.1192	0.4870	1.8437	98.96	6.70
44	973.582	5.8233	0.1071	0.4353	1.7031	99.09	3.40
45	1004.088	6.0058	0.0952	0.3850	1.5596	99.21	7.68
46	1015.650	6.0749	0.0910	0.3674	1.5078	99.26	18.71
47	1025.264	6.1324	0.0877	0.3534	1.4658	99.29	27.42
48	1033.933	6.1843	0.0848	0.3412	1.4288	99.32	0.09
49	1058.188	6.3294	0.0771	0.3093	1.3293	99.39	5.68
50	1070.204	6.4012	0.0736	0.2945	1.2822	99.43	1.33
51	1073.344	6.4200	0.0727	0.2908	1.2701	99.44	2.10
52	1074.334	6.4259	0.0724	0.2896	1.2663	99.44	1.93
53	1092.210	6.5329	0.0675	0.2693	1.1995	99.49	3.75
54	1135.461	6.7916	0.0569	0.2256	1.0502	99.58	3.78
55	1167.570	6.9836	0.0501	0.1977	0.9499	99.64	0.45
56	1178.926	7.0515	0.0479	0.1887	0.9164	99.66	0.04
57	1191.159	7.1247	0.0456	0.1794	0.8816	99.68	0.81
58	1226.887	7.3384	0.0395	0.1548	0.7863	99.73	1.38
59	1230.979	7.3629	0.0388	0.1522	0.7760	99.74	1.99
60	1233.591	7.3785	0.0384	0.1506	0.7695	99.74	0.50
61	1245.942	7.4524	0.0366	0.1430	0.7394	99.76	2.86
62	1329.168	7.9502	0.0261	0.1011	0.5622	99.84	1.66
63	1334.806	7.9839	0.0255	0.0988	0.5517	99.84	1.99
64	1347.852	8.0619	0.0242	0.0935	0.5281	99.85	2.08
65	1350.520	8.0779	0.0239	0.0925	0.5234	99.85	2.78
66	1370.287	8.1961	0.0220	0.0851	0.4897	99.87	4.81
67	1378.193	8.2434	0.0213	0.0824	0.4768	99.87	8.97
68	1389.756	8.3126	0.0204	0.0784	0.4584	99.88	3.15
69	1398.118	8.3626	0.0197	0.0757	0.4456	99.88	2.08
70	1443.763	8.6356	0.0163	0.0625	0.3810	99.91	0.22
71	1444.855	8.6421	0.0162	0.0622	0.3796	99.91	0.65
72	1450.047	8.6732	0.0159	0.0608	0.3729	99.91	1.47
73	1471.926	8.8041	0.0145	0.0555	0.3456	99.92	2.62
74	1511.252	9.0393	0.0123	0.0469	0.3013	99.93	7.13
75	1514.882	9.0610	0.0121	0.0462	0.2975	99.93	6.84
76	1516.435	9.0703	0.0120	0.0459	0.2958	99.93	7.27
77	1518.136	9.0805	0.0120	0.0456	0.2941	99.93	7.17
78	1518.664	9.0836	0.0119	0.0455	0.2935	99.93	7.88
79	1525.829	9.1265	0.0116	0.0441	0.2862	99.94	1.24
80	1533.032	9.1696	0.0112	0.0428	0.2791	99.94	1.15
81	1558.797	9.3237	0.0101	0.0383	0.2547	99.95	10.38
82	1608.369	9.6202	0.0082	0.0310	0.2135	99.96	9.18
83	1614.444	9.6565	0.0080	0.0302	0.2089	99.96	3.06
84	1736.613	10.3872	0.0048	0.0179	0.1340	99.98	3.00
85	3038.549	18.1746	0.0000	0.0001	0.0008	100.00	34.63
86	3041.087	18.1897	0.0000	0.0001	0.0008	100.00	31.35

```
87 3047.552 18.2284 0.0000 0.0001 0.0007 100.00 36.01
88 3060.140 18.3037 0.0000 0.0001 0.0007 100.00 30.95
89 3076.251 18.4001 0.0000 0.0000 0.0007 100.00 60.10
90 3078.759 18.4151 0.0000 0.0000 0.0006 100.00 37.13
91 3089.418 18.4788 0.0000 0.0000 0.0006 100.00 19.83
92 3091.663 18.4922 0.0000 0.0000 0.0006 100.00 15.68
93 3098.805 18.5350 0.0000 0.0000 0.0006 100.00 22.75
94 3102.510 18.5571 0.0000 0.0000 0.0006 100.00 4.44
95 3118.755 18.6543 0.0000 0.0000 0.0005 100.00 45.91
96 3123.181 18.6808 0.0000 0.0000 0.0005 100.00 24.31
97 3123.945 18.6853 0.0000 0.0000 0.0005 100.00 24.18
98 3133.505 18.7425 0.0000 0.0000 0.0005 100.00 19.56
99 3150.215 18.8425 0.0000 0.0000 0.0005 100.00 20.82
100 3165.173 18.9319 0.0000 0.0000 0.0005 100.00 14.75
101 3257.562 19.4845 0.0000 0.0000 0.0003 100.00 0.63
102 3259.083 19.4936 0.0000 0.0000 0.0003 100.00 0.43
-- ---------- ------- ------- ------- ----
Total Vibrations 783.6403 31.6796 198.4920 256.4903 -Unscaled-

Ideal Gas 2.4789
Translation 3.7184 178.7709 12.4716
Rotation 3.7184 140.4301 12.4716
---------- ------- ------- -------
Totals 825.2356 517.6930 281.4336

Vibrational(v) Corrections:
Temp. Correction Hv 825.2356
Entropy Correction (Hv-TSv) 670.8855

Reason for exit: Successful completion
Properties CPU Time : 1.64
Properties Wall Time: 1.64
```

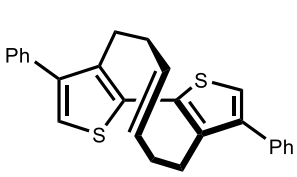	
16e GS	**16e'** TS
-1800.373199 au	-1800.328027 au

Fig s16e. Calculation studies on the isomerization of **16e**

Cartesian coordinate of **16e** (GS)

S	-1.049115	-1.736248	-1.741352
C	-0.689159	-0.251761	-0.872207
C	-2.718067	-1.638149	-1.314134
H	-3.417909	-2.388095	-1.658700
C	-3.004029	-0.519514	-0.572731

C	−1.832069	0.289065	−0.312641
C	0.689159	0.251761	−0.872207
C	1.832069	−0.289065	−0.312641
C	3.004029	0.519514	−0.572731
C	2.718067	1.638149	−1.314134
H	3.417909	2.388095	−1.658700
S	1.049115	1.736248	−1.741352
C	−1.844566	1.497587	0.594283
H	−2.813376	2.001347	0.528842
H	−1.086340	2.218740	0.272212
C	−1.583009	1.133383	2.090442
H	−1.773281	2.030127	2.694876
H	−2.304574	0.369021	2.402855
C	1.844566	−1.497587	0.594283
H	1.086340	−2.218740	0.272212
H	2.813376	−2.001347	0.528842
C	1.583009	−1.133383	2.090442
H	2.304574	−0.369021	2.402855
H	1.773281	−2.030127	2.694876
C	0.177903	−0.643650	2.269904
H	−0.603557	−1.405918	2.250494
C	−0.177903	0.643650	2.269904
H	0.603557	1.405918	2.250494
C	4.383631	0.217943	−0.108909
C	7.026827	−0.300158	0.716814
C	5.090165	1.149248	0.668741
C	5.029002	−0.977077	−0.468853
C	6.336457	−1.234580	−0.058205
C	6.400117	0.893968	1.075962
H	4.599636	2.074412	0.959091
H	4.507921	−1.695425	−1.096014
H	6.819688	−2.162638	−0.352322
H	6.929314	1.627748	1.678492
H	8.045984	−0.500695	1.036184
C	−4.383631	−0.217943	−0.108909
C	−7.026827	0.300158	0.716814
C	−5.029002	0.977077	−0.468853
C	−5.090165	−1.149248	0.668741
C	−6.400117	−0.893968	1.075962
C	−6.336457	1.234580	−0.058205
H	−4.507921	1.695425	−1.096014
H	−4.599636	−2.074412	0.959091
H	−6.929314	−1.627748	1.678492
H	−6.819688	2.162638	−0.352322
H	−8.045984	0.500695	1.036184

Cartesian coordinate of **16e'** (TS)

S	1.405352	2.595043	−0.644039
C	0.729399	1.028186	−0.110373
C	3.025968	2.068441	−0.474941
H	3.847257	2.738267	−0.692308
C	3.094310	0.783196	−0.028119
C	1.794380	0.169361	0.192859
C	−0.765715	1.016359	−0.131305

C	−1.816734	0.137227	0.156872
C	−3.126283	0.733133	−0.050224
C	−3.075039	2.022278	−0.492795
H	−3.906215	2.682179	−0.702523
S	−1.463085	2.573935	−0.660725
C	1.842797	−1.262428	0.680934
H	0.978839	−1.508230	1.300437
H	2.715182	−1.357244	1.332930
C	1.971474	−2.316613	−0.488303
H	2.344606	−1.819870	−1.389489
H	2.697780	−3.087930	−0.210102
C	−1.808209	−1.331110	0.516707
H	−0.965786	−1.591187	1.158247
H	−2.713517	−1.545349	1.091003
C	−1.783871	−2.274407	−0.734514
H	−2.560158	−1.972175	−1.446043
H	−2.018207	−3.291504	−0.395293
C	−0.390224	−2.204773	−1.284581
H	−0.149720	−1.370081	−1.943102
C	0.592917	−2.868504	−0.671157
H	0.314262	−3.655236	0.035987
C	−4.437446	0.059939	0.173279
C	−6.960179	−1.124492	0.576297
C	−4.876917	−0.274263	1.465010
C	−5.289209	−0.202293	−0.910544
C	−6.540150	−0.789006	−0.711179
C	−6.124761	−0.863758	1.664838
H	−4.238724	−0.054085	2.317046
H	−4.960979	0.054438	−1.914199
H	−7.184893	−0.985971	−1.563867
H	−6.448212	−1.112188	2.672323
H	−7.933057	−1.583225	0.731640
C	4.412516	0.119674	0.197876
C	6.935948	−1.060699	0.597607
C	5.159902	−0.359870	−0.887676
C	4.954243	0.003952	1.488130
C	6.203787	−0.583553	1.686879
C	6.411722	−0.945654	−0.690403
H	4.753275	−0.268437	−1.891280
H	4.393175	0.388446	2.336101
H	6.609052	−0.662055	2.692407
H	6.976710	−1.310811	−1.544096
H	7.910274	−1.516595	0.752416

Frequency calculation of **16e'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 37 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1* i	**49.540**	**0.0000**	**1.2395**	**8.3144**	**4.1572**	**0.00**	**0.01**
2*	24.628	0.1473	1.2395	8.3144	4.1572	11.21	0.06
3*	39.174	0.2343	1.2395	8.3144	4.1572	17.22	0.00
4*	43.168	0.2582	1.2395	8.3144	4.1572	18.80	0.15

5* 51.221 0.3064 1.2395 8.3144 4.1572 21.90 0.08
6* 56.507 0.3380 1.2395 8.3144 4.1572 23.87 0.02
7* 76.335 0.4566 1.2395 8.3144 4.1572 30.81 0.01
8* 113.248 0.6774 1.2395 8.3144 4.1572 42.10 0.39
9* 115.207 0.6891 1.2395 8.3144 4.1572 42.65 0.00
10* 140.118 0.8381 1.2395 8.3144 4.1572 49.14 0.20
11* 157.347 0.9411 1.2395 8.3144 4.1572 53.20 0.31
12* 172.894 1.0341 1.2395 8.3144 4.1572 56.58 0.44
13* 188.481 1.1274 1.2395 8.3144 4.1572 59.73 0.09
14* 202.007 1.2083 1.2395 8.3144 4.1572 62.27 0.09
15* 244.162 1.4604 1.2395 7.4154 4.1572 69.22 0.87
16* 260.672 1.5592 1.2384 6.9339 4.1572 71.58 1.06
17* 262.996 1.5731 1.2300 6.8692 4.1572 71.89 0.76
18* 289.397 1.7310 1.1383 6.1817 4.1572 75.26 0.36
19* 296.417 1.7730 1.1149 6.0126 4.1572 76.08 1.56
20* 321.517 1.9231 1.0343 5.4491 4.1572 78.81 0.03
21* 333.460 1.9945 0.9976 5.2018 4.1572 79.99 0.46
22* 342.586 2.0491 0.9703 5.0211 4.1572 80.86 0.27
23* 366.800 2.1940 0.9008 4.5736 4.1572 82.97 0.67
24* 376.428 2.2515 0.8743 4.4077 4.1572 83.74 1.92
25* 418.529 2.5034 0.7660 3.7529 4.1572 86.73 0.04
26* 419.040 2.5064 0.7648 3.7456 4.1572 86.76 0.02
27* 429.644 2.5698 0.7394 3.5974 4.1572 87.42 0.18
28* 453.122 2.7103 0.6857 3.2902 4.1572 88.77 0.92
29* 470.819 2.8161 0.6474 3.0763 4.1572 89.69 1.50
30* 491.506 2.9399 0.6051 2.8438 4.1572 90.67 0.63
31* 508.628 3.0423 0.5718 2.6647 4.1572 91.41 2.76
32* 532.912 3.1875 0.5274 2.4298 4.1572 92.36 4.52
33* 547.212 3.2731 0.5027 2.3011 4.1572 92.87 7.19
34* 574.126 3.4340 0.4589 2.0767 4.1572 93.74 3.26
35* 576.861 3.4504 0.4546 2.0552 4.1572 93.82 2.62
36* 589.667 3.5270 0.4351 1.9571 4.1572 94.19 0.18
37* 601.945 3.6004 0.4172 1.8674 4.1572 94.52 0.67
38 634.999 3.7981 0.3720 1.6452 4.0106 95.33 0.37
39 636.391 3.8065 0.3702 1.6365 3.9986 95.36 0.42
40 654.708 3.9160 0.3472 1.5252 3.8424 95.76 21.42
41 658.673 3.9397 0.3424 1.5021 3.8090 95.84 3.46
42 718.608 4.2982 0.2767 1.1915 3.3221 96.88 23.63
43 720.376 4.3088 0.2750 1.1834 3.3083 96.91 23.34
44 732.827 4.3833 0.2629 1.1275 3.2120 97.09 5.16
45 735.458 4.3990 0.2604 1.1160 3.1919 97.12 3.33
46 749.832 4.4850 0.2472 1.0553 3.0833 97.32 5.18
47 762.594 4.5613 0.2360 1.0041 2.9888 97.48 22.66
48 764.455 4.5725 0.2344 0.9968 2.9752 97.50 22.05
49 768.127 4.5944 0.2313 0.9826 2.9484 97.54 22.09
50 782.367 4.6796 0.2196 0.9294 2.8461 97.71 13.49
51 785.451 4.6980 0.2171 0.9182 2.8243 97.74 16.10
52 831.503 4.9735 0.1832 0.7663 2.5112 98.19 5.59
53 845.998 5.0602 0.1736 0.7237 2.4179 98.31 2.12
54 865.565 5.1772 0.1614 0.6698 2.2959 98.47 0.11
55 866.505 5.1829 0.1608 0.6673 2.2901 98.47 0.10
56 873.114 5.2224 0.1569 0.6501 2.2500 98.52 0.81
57 874.371 5.2299 0.1561 0.6468 2.2425 98.53 2.08
58 883.333 5.2835 0.1510 0.6242 2.1890 98.59 3.85

59	896.397	5.3616	0.1437	0.5927	2.1128	98.68	29.47
60	913.958	5.4667	0.1345	0.5526	2.0136	98.79	15.06
61	929.489	5.5596	0.1268	0.5194	1.9288	98.87	9.63
62	935.181	5.5936	0.1240	0.5077	1.8984	98.90	5.90
63	936.856	5.6036	0.1233	0.5043	1.8895	98.91	1.82
64	968.359	5.7921	0.1093	0.4445	1.7287	99.07	5.66
65	972.399	5.8162	0.1076	0.4374	1.7089	99.08	0.05
66	972.478	5.8167	0.1075	0.4372	1.7085	99.08	0.69
67	979.651	5.8596	0.1046	0.4248	1.6737	99.12	16.65
68	995.779	5.9561	0.0983	0.3981	1.5977	99.18	1.25
69	997.106	5.9640	0.0978	0.3960	1.5915	99.19	0.35
70	999.186	5.9765	0.0970	0.3927	1.5820	99.19	1.41
71	1016.925	6.0826	0.0906	0.3655	1.5022	99.26	4.22
72	1017.661	6.0870	0.0903	0.3644	1.4990	99.26	4.72
73	1018.179	6.0901	0.0902	0.3637	1.4967	99.27	0.94
74	1033.829	6.1837	0.0848	0.3414	1.4293	99.32	30.18
75	1057.878	6.3275	0.0772	0.3096	1.3306	99.39	1.13
76	1060.616	6.3439	0.0764	0.3062	1.3197	99.40	8.83
77	1077.368	6.4441	0.0716	0.2861	1.2548	99.45	4.25
78	1090.949	6.5253	0.0678	0.2707	1.2041	99.48	3.52
79	1096.068	6.5559	0.0665	0.2651	1.1855	99.50	0.31
80	1107.988	6.6272	0.0634	0.2525	1.1431	99.52	3.77
81	1108.782	6.6320	0.0632	0.2516	1.1403	99.53	3.68
82	1163.279	6.9580	0.0509	0.2013	0.9628	99.64	1.69
83	1173.896	7.0215	0.0488	0.1927	0.9311	99.65	3.38
84	1194.264	7.1433	0.0450	0.1771	0.8729	99.69	0.02
85	1194.343	7.1438	0.0450	0.1771	0.8727	99.69	0.00
86	1212.815	7.2542	0.0418	0.1641	0.8227	99.71	2.59
87	1212.942	7.2550	0.0418	0.1640	0.8224	99.71	0.80
88	1218.093	7.2858	0.0409	0.1605	0.8089	99.72	0.27
89	1220.449	7.2999	0.0405	0.1590	0.8028	99.72	5.50
90	1232.794	7.3737	0.0386	0.1511	0.7715	99.74	1.43
91	1245.090	7.4473	0.0367	0.1436	0.7414	99.75	0.88
92	1247.939	7.4643	0.0363	0.1419	0.7346	99.76	0.15
93	1250.571	7.4801	0.0359	0.1403	0.7283	99.76	1.63
94	1324.757	7.9238	0.0266	0.1030	0.5705	99.83	1.18
95	1328.239	7.9446	0.0262	0.1015	0.5640	99.84	0.78
96	1329.492	7.9521	0.0261	0.1010	0.5616	99.84	0.82
97	1331.335	7.9632	0.0259	0.1002	0.5582	99.84	0.18
98	1344.041	8.0391	0.0246	0.0950	0.5349	99.85	3.25
99	1349.837	8.0738	0.0240	0.0928	0.5246	99.85	6.35
100	1361.488	8.1435	0.0229	0.0883	0.5045	99.86	3.55
101	1362.331	8.1485	0.0228	0.0880	0.5030	99.86	0.31
102	1366.642	8.1743	0.0224	0.0864	0.4958	99.86	9.35
103	1374.548	8.2216	0.0217	0.0836	0.4827	99.87	4.24
104	1383.335	8.2742	0.0209	0.0806	0.4685	99.87	2.75
105	1389.138	8.3089	0.0204	0.0786	0.4594	99.88	0.65
106	1447.625	8.6587	0.0160	0.0615	0.3760	99.91	1.56
107	1469.036	8.7868	0.0147	0.0561	0.3491	99.92	1.52
108	1488.010	8.9003	0.0136	0.0518	0.3268	99.92	1.69
109	1488.087	8.9007	0.0136	0.0518	0.3267	99.92	6.57
110	1516.042	9.0679	0.0121	0.0460	0.2963	99.93	3.11
111	1521.369	9.0998	0.0118	0.0450	0.2908	99.94	0.62
112	1525.397	9.1239	0.0116	0.0442	0.2867	99.94	7.34

```
113 1539.053 9.2056 0.0110 0.0417 0.2732 99.94 21.37
114 1540.637 9.2151 0.0109 0.0414 0.2717 99.94 4.42
115 1550.845 9.2761 0.0104 0.0397 0.2620 99.94 8.42
116 1584.811 9.4793 0.0090 0.0343 0.2322 99.95 1.38
117 1591.558 9.5196 0.0088 0.0333 0.2267 99.95 4.12
118 1633.919 9.7730 0.0074 0.0278 0.1947 99.96 1.83
119 1634.390 9.7758 0.0073 0.0278 0.1944 99.96 1.75
120 1661.874 9.9402 0.0065 0.0247 0.1760 99.97 12.87
121 1662.549 9.9442 0.0065 0.0246 0.1756 99.97 5.10
122 1737.918 10.3951 0.0047 0.0178 0.1333 99.98 3.03
123 3051.180 18.2501 0.0000 0.0001 0.0007 100.00 36.22
124 3065.595 18.3363 0.0000 0.0000 0.0007 100.00 38.94
125 3089.094 18.4769 0.0000 0.0000 0.0006 100.00 21.03
126 3096.526 18.5213 0.0000 0.0000 0.0006 100.00 15.18
127 3104.499 18.5690 0.0000 0.0000 0.0006 100.00 16.59
128 3106.074 18.5784 0.0000 0.0000 0.0006 100.00 8.24
129 3122.148 18.6746 0.0000 0.0000 0.0005 100.00 40.06
130 3136.302 18.7592 0.0000 0.0000 0.0005 100.00 32.38
131 3155.122 18.8718 0.0000 0.0000 0.0005 100.00 16.98
132 3164.426 18.9275 0.0000 0.0000 0.0005 100.00 15.69
133 3180.311 19.0225 0.0000 0.0000 0.0004 100.00 3.09
134 3181.281 19.0283 0.0000 0.0000 0.0004 100.00 3.40
135 3186.604 19.0601 0.0000 0.0000 0.0004 100.00 0.77
136 3187.431 19.0651 0.0000 0.0000 0.0004 100.00 1.10
137 3195.590 19.1139 0.0000 0.0000 0.0004 100.00 20.40
138 3196.691 19.1205 0.0000 0.0000 0.0004 100.00 21.17
139 3202.211 19.1535 0.0000 0.0000 0.0004 100.00 33.20
140 3203.729 19.1625 0.0000 0.0000 0.0004 100.00 32.24
141 3210.526 19.2032 0.0000 0.0000 0.0004 100.00 24.10
142 3211.769 19.2106 0.0000 0.0000 0.0004 100.00 21.97
143 3265.781 19.5337 0.0000 0.0000 0.0003 100.00 0.13
144 3266.349 19.5371 0.0000 0.0000 0.0003 100.00 0.40
-- ---------- ------- ------- ------- ----
Total Vibrations 1061.0942 43.8816 244.4144 272.8158

Ideal Gas 2.4789
Translation 3.7184 183.4250 12.4716
Rotation 3.7184 151.7242 12.4716
---------- ------- ------- -------
Totals 1114.8916 579.5636 297.7591

Vibrational(v) Corrections:
Temp. Correction Hv 1114.8916
Entropy Correction (Hv-TSv) 942.0947

Reason for exit: Successful completion
Properties CPU Time : 3.05
Properties Wall
```

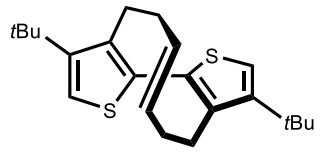	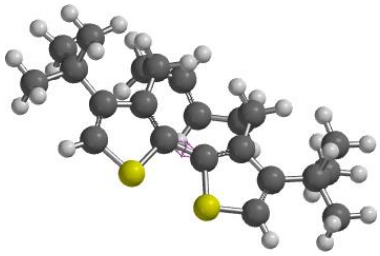
16f GS	**16f'** TS
-1652.761162 au	-1652.707794 au

Fig s16f. Calculation studies on the isomerization of **16f**

Cartesian coordinate of **16f** (GS)

S	−1.067762	1.699450	−1.387768
C	−0.693522	0.572989	−0.099541
C	−2.754070	1.377141	−1.234149
H	−3.441341	1.894012	−1.887156
C	−3.052587	0.478446	−0.240956
C	−1.843061	−0.003472	0.415768
C	0.706780	0.476157	0.341101
C	1.834910	0.048475	−0.340618
C	3.061682	0.273606	0.413783
C	2.797346	0.840011	1.635435
H	3.505964	1.110194	2.403931
S	1.122711	1.148884	1.904286
C	−1.778443	−1.073892	1.486636
H	−2.697834	−1.087468	2.077022
H	−0.969855	−0.842177	2.187521
C	−1.526667	−2.511516	0.923971
H	−1.634810	−3.222552	1.753912
H	−2.297716	−2.753293	0.184799
C	1.724584	−0.644592	−1.682479
H	0.917832	−0.188019	−2.264661
H	2.636177	−0.505864	−2.268480
C	1.429632	−2.178028	−1.578564
H	2.194292	−2.654588	−0.956142
H	1.516513	−2.605634	−2.586461
C	0.068298	−2.421492	−1.002428
H	−0.778860	−2.287270	−1.677338
C	−0.168236	−2.611165	0.298667
H	0.678851	−2.700593	0.980615
C	−4.510652	0.153557	0.134941
C	−4.805450	−1.364029	0.094917
H	−4.249386	−1.922116	0.850454
H	−4.560490	−1.783482	−0.887635
H	−5.872182	−1.539364	0.280125
C	−5.493650	0.825943	−0.848424
H	−5.413400	1.918245	−0.823790
H	−6.522049	0.566402	−0.573746
H	−5.330419	0.489839	−1.878820

C	−4.821112	0.712845	1.545570
H	−4.668498	1.797475	1.571790
H	−4.189509	0.270622	2.321341
H	−5.865816	0.508741	1.812630
C	4.506473	0.026021	−0.060477
C	5.515359	0.327752	1.069050
H	6.533341	0.144435	0.707951
H	5.350507	−0.312512	1.943211
H	5.467127	1.373316	1.392829
C	4.738923	−1.441697	−0.488721
H	5.802160	−1.602029	−0.705182
H	4.182353	−1.713914	−1.387521
H	4.451322	−2.133268	0.311382
C	4.838000	0.978246	−1.236317
H	5.871686	0.823174	−1.570089
H	4.734830	2.023439	−0.924444
H	4.184734	0.823722	−2.099839

Cartesian coordinate of **16f'** (TS)

S	1.365719	2.044819	−1.189054
C	0.732132	0.590191	−0.377355
C	2.990218	1.639150	−0.868575
H	3.758900	2.328668	−1.181561
C	3.128249	0.467270	−0.182624
C	1.829415	−0.172289	0.064196
C	−0.775391	0.565767	−0.400036
C	−1.850144	−0.231391	0.027140
C	−3.165466	0.376099	−0.200506
C	−3.062620	1.558997	−0.873938
H	−3.851031	2.229228	−1.180402
S	−1.449382	2.008707	−1.202161
C	1.834518	−1.543158	0.703622
H	0.941362	−1.700102	1.309533
H	2.667501	−1.599747	1.403997
C	1.959003	−2.722624	−0.345453
H	2.335632	−2.329785	−1.294411
H	2.675944	−3.468985	0.014273
C	−1.806500	−1.651879	0.539470
H	−0.938805	−1.832665	1.173271
H	−2.676711	−1.832622	1.169514
C	−1.787367	−2.713338	−0.617943
H	−2.552747	−2.474418	−1.361846
H	−2.031071	−3.693423	−0.186611
C	−0.394128	−2.709078	−1.170901
H	−0.152785	−1.971859	−1.935822
C	0.582316	−3.286653	−0.468095
H	0.294285	−3.967571	0.338400
C	−4.543695	−0.101425	0.320215
C	4.527122	0.046375	0.336378
C	−4.967649	−1.494050	−0.211183
H	−4.355992	−2.313770	0.168311
H	−4.928410	−1.521134	−1.306162
H	−6.002297	−1.699297	0.088848

C	-4.556516	-0.084534	1.870174
H	-3.816991	-0.755098	2.315329
H	-5.543313	-0.385653	2.243566
H	-4.349560	0.925582	2.241160
C	-5.654753	0.875817	-0.132683
H	-5.738876	0.920140	-1.224350
H	-5.487201	1.890118	0.244077
H	-6.618746	0.535128	0.260355
C	4.583907	0.195219	1.878552
H	5.584813	-0.064183	2.245924
H	3.866672	-0.444768	2.399670
H	4.374523	1.230318	2.170423
C	5.614260	0.990521	-0.232319
H	6.595171	0.676378	0.140036
H	5.464850	2.028675	0.082098
H	5.648309	0.960099	-1.327209
C	4.953706	-1.383053	-0.080087
H	6.011994	-1.532200	0.163987
H	4.837237	-1.530488	-1.159680
H	4.396164	-2.168819	0.429765

Frequency calculation of **16f'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 45 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1*	**i 57.203**	**0.0000**	**1.2395**	**8.3144**	**4.1572 0.00 0.01**
2*	38.981	0.2332	1.2395	8.3144	4.1572 17.15 0.17
3*	61.349	0.3669	1.2395	8.3144	4.1572 25.63 0.01
4*	78.579	0.4700	1.2395	8.3144	4.1572 31.56 0.01
5*	98.923	0.5917	1.2395	8.3144	4.1572 37.96 0.08
6*	119.810	0.7166	1.2395	8.3144	4.1572 43.91 0.38
7*	120.606	0.7214	1.2395	8.3144	4.1572 44.12 0.27
8*	140.002	0.8374	1.2395	8.3144	4.1572 49.12 0.26
9*	154.708	0.9254	1.2395	8.3144	4.1572 52.60 0.27
10*	173.807	1.0396	1.2395	8.3144	4.1572 56.77 0.00
11*	186.799	1.1173	1.2395	8.3144	4.1572 59.40 0.19
12*	194.076	1.1608	1.2395	8.3144	4.1572 60.80 0.07
13*	204.202	1.2214	1.2395	8.3144	4.1572 62.67 0.15
14*	212.567	1.2714	1.2395	8.3144	4.1572 64.15 0.09
15*	229.221	1.3710	1.2395	7.8869	4.1572 66.92 1.59
16*	245.114	1.4661	1.2395	7.3866	4.1572 69.36 0.91
17*	254.444	1.5219	1.2395	7.1110	4.1572 70.71 0.23
18*	259.578	1.5526	1.2395	6.9646	4.1572 71.43 0.15
19*	267.559	1.6004	1.2138	6.7442	4.1572 72.50 0.76
20*	286.162	1.7116	1.1493	6.2615	4.1572 74.87 0.67
21*	293.618	1.7562	1.1242	6.0794	4.1572 75.75 0.09
22*	311.699	1.8644	1.0652	5.6621	4.1572 77.78 0.53
23*	326.214	1.9512	1.0197	5.3503	4.1572 79.28 0.05
24*	335.650	2.0076	0.9910	5.1578	4.1572 80.21 0.02
25*	339.463	2.0304	0.9796	5.0821	4.1572 80.57 0.14

26*	350.746	2.0979	0.9464	4.8653	4.1572	81.60	0.07
27*	357.461	2.1381	0.9271	4.7409	4.1572	82.18	0.20
28*	362.815	2.1701	0.9119	4.6442	4.1572	82.64	0.08
29*	374.099	2.2376	0.8806	4.4473	4.1572	83.56	1.13
30*	388.427	2.3233	0.8422	4.2098	4.1572	84.66	1.11
31*	396.076	2.3691	0.8223	4.0885	4.1572	85.21	0.87
32*	417.291	2.4960	0.7690	3.7706	4.1572	86.65	0.12
33*	424.721	2.5404	0.7511	3.6655	4.1572	87.12	0.05
34*	428.429	2.5626	0.7423	3.6141	4.1572	87.35	1.64
35*	455.788	2.7262	0.6798	3.2570	4.1572	88.91	0.06
36*	482.455	2.8857	0.6233	2.9433	4.1572	90.25	2.20
37*	493.764	2.9534	0.6006	2.8195	4.1572	90.77	1.26
38*	497.212	2.9740	0.5938	2.7829	4.1572	90.92	0.30
39*	526.139	3.1470	0.5395	2.4932	4.1572	92.11	0.48
40*	548.456	3.2805	0.5006	2.2902	4.1572	92.91	1.25
41*	557.186	3.3327	0.4860	2.2153	4.1572	93.20	1.37
42*	573.413	3.4298	0.4600	2.0824	4.1572	93.72	3.72
43*	582.613	3.4848	0.4458	2.0106	4.1572	93.99	6.05
44*	599.537	3.5860	0.4206	1.8847	4.1572	94.46	0.39
45*	611.236	3.6560	0.4040	1.8021	4.1572	94.76	2.06
46	723.356	4.3266	0.2720	1.1698	3.2851	96.95	9.27
47	739.509	4.4232	0.2567	1.0986	3.1611	97.18	6.04
48	740.358	4.4283	0.2559	1.0950	3.1546	97.19	1.42
49	749.004	4.4800	0.2480	1.0587	3.0895	97.31	1.97
50	773.378	4.6258	0.2269	0.9627	2.9104	97.61	10.52
51	778.830	4.6584	0.2225	0.9423	2.8713	97.67	19.26
52	816.892	4.8861	0.1934	0.8116	2.6078	98.06	2.05
53	820.134	4.9055	0.1911	0.8014	2.5862	98.09	6.74
54	831.855	4.9756	0.1830	0.7652	2.5089	98.19	5.75
55	840.893	5.0297	0.1769	0.7384	2.4505	98.27	1.68
56	877.354	5.2477	0.1544	0.6392	2.2246	98.55	5.17
57	894.216	5.3486	0.1449	0.5978	2.1254	98.66	17.73
58	914.537	5.4701	0.1342	0.5514	2.0104	98.79	5.89
59	919.599	5.5004	0.1316	0.5403	1.9825	98.82	6.92
60	926.152	5.5396	0.1284	0.5264	1.9468	98.85	10.38
61	927.737	5.5491	0.1276	0.5231	1.9382	98.86	3.60
62	932.810	5.5794	0.1252	0.5126	1.9110	98.89	0.79
63	933.374	5.5828	0.1249	0.5114	1.9080	98.89	0.93
64	938.667	5.6145	0.1224	0.5007	1.8800	98.92	6.24
65	942.482	5.6373	0.1206	0.4931	1.8600	98.94	10.17
66	967.637	5.7878	0.1096	0.4458	1.7322	99.06	0.39
67	968.674	5.7940	0.1091	0.4440	1.7271	99.07	0.03
68	972.747	5.8183	0.1074	0.4368	1.7072	99.09	5.47
69	997.629	5.9671	0.0976	0.3951	1.5891	99.19	10.31
70	1015.483	6.0739	0.0911	0.3677	1.5086	99.26	19.99
71	1027.339	6.1449	0.0870	0.3505	1.4569	99.30	15.78
72	1039.854	6.2197	0.0829	0.3331	1.4040	99.34	10.86
73	1051.245	6.2878	0.0793	0.3181	1.3572	99.37	1.19
74	1054.095	6.3049	0.0784	0.3144	1.3457	99.38	0.27
75	1059.990	6.3401	0.0766	0.3070	1.3222	99.40	1.40
76	1060.999	6.3462	0.0763	0.3057	1.3182	99.40	1.12
77	1094.201	6.5448	0.0670	0.2671	1.1923	99.49	2.25
78	1096.483	6.5584	0.0664	0.2646	1.1840	99.50	6.67
79	1124.608	6.7266	0.0594	0.2359	1.0861	99.56	1.62

80 1164.146 6.9631 0.0508 0.2005 0.9601 99.64 1.36
81 1182.568 7.0733 0.0472 0.1859 0.9059 99.67 1.30
82 1213.992 7.2613 0.0416 0.1633 0.8196 99.71 1.00
83 1221.288 7.3049 0.0404 0.1584 0.8006 99.72 0.26
84 1226.993 7.3390 0.0395 0.1547 0.7861 99.73 1.10
85 1235.921 7.3924 0.0381 0.1491 0.7638 99.74 0.64
86 1236.455 7.3956 0.0380 0.1488 0.7624 99.74 6.44
87 1243.219 7.4361 0.0370 0.1447 0.7459 99.75 1.71
88 1248.536 7.4679 0.0362 0.1415 0.7332 99.76 4.35
89 1250.038 7.4769 0.0360 0.1406 0.7296 99.76 1.31
90 1267.267 7.5799 0.0336 0.1309 0.6898 99.78 83.70
91 1268.657 7.5883 0.0334 0.1302 0.6866 99.78 7.78
92 1329.015 7.9493 0.0261 0.1012 0.5625 99.84 4.28
93 1331.047 7.9614 0.0259 0.1003 0.5587 99.84 1.28
94 1338.825 8.0080 0.0251 0.0971 0.5444 99.84 5.56
95 1345.124 8.0456 0.0244 0.0946 0.5330 99.85 1.16
96 1353.819 8.0976 0.0236 0.0912 0.5176 99.85 8.01
97 1360.006 8.1346 0.0230 0.0889 0.5070 99.86 1.95
98 1378.838 8.2473 0.0213 0.0821 0.4757 99.87 1.13
99 1382.379 8.2685 0.0210 0.0809 0.4701 99.87 3.35
100 1422.239 8.5069 0.0178 0.0684 0.4103 99.90 0.99
101 1423.759 8.5160 0.0177 0.0680 0.4082 99.90 9.08
102 1425.431 8.5260 0.0176 0.0675 0.4058 99.90 2.50
103 1425.795 8.5281 0.0175 0.0674 0.4053 99.90 8.53
104 1427.456 8.5381 0.0174 0.0669 0.4030 99.90 0.17
105 1441.526 8.6222 0.0164 0.0631 0.3840 99.90 1.52
106 1457.414 8.7173 0.0154 0.0590 0.3635 99.91 14.21
107 1458.144 8.7216 0.0153 0.0588 0.3626 99.91 3.38
108 1510.563 9.0352 0.0123 0.0471 0.3020 99.93 1.18
109 1510.992 9.0377 0.0123 0.0470 0.3016 99.93 0.97
110 1513.170 9.0508 0.0122 0.0466 0.2993 99.93 3.57
111 1514.673 9.0598 0.0121 0.0463 0.2977 99.93 2.16
112 1517.836 9.0787 0.0120 0.0456 0.2944 99.93 0.05
113 1519.650 9.0895 0.0119 0.0453 0.2925 99.93 0.56
114 1520.573 9.0950 0.0118 0.0451 0.2916 99.93 1.28
115 1524.347 9.1176 0.0117 0.0444 0.2877 99.94 0.23
116 1527.529 9.1366 0.0115 0.0438 0.2845 99.94 2.15
117 1530.391 9.1538 0.0114 0.0433 0.2817 99.94 1.73
118 1536.787 9.1920 0.0111 0.0421 0.2754 99.94 1.08
119 1539.274 9.2069 0.0110 0.0417 0.2730 99.94 5.83
120 1544.992 9.2411 0.0107 0.0407 0.2675 99.94 0.67
121 1554.633 9.2988 0.0103 0.0390 0.2585 99.94 15.36
122 1557.392 9.3153 0.0102 0.0386 0.2560 99.95 7.57
123 1561.944 9.3425 0.0100 0.0378 0.2519 99.95 12.80
124 1566.384 9.3691 0.0098 0.0371 0.2480 99.95 6.01
125 1572.431 9.4052 0.0095 0.0362 0.2427 99.95 3.95
126 1743.440 10.4281 0.0046 0.0174 0.1306 99.98 2.57
127 3045.244 18.2146 0.0000 0.0001 0.0007 100.00 23.13
128 3047.027 18.2253 0.0000 0.0001 0.0007 100.00 39.30
129 3047.700 18.2293 0.0000 0.0001 0.0007 100.00 17.28
130 3049.237 18.2385 0.0000 0.0001 0.0007 100.00 15.51
131 3050.415 18.2455 0.0000 0.0001 0.0007 100.00 26.00
132 3057.283 18.2866 0.0000 0.0001 0.0007 100.00 55.20
133 3057.562 18.2883 0.0000 0.0001 0.0007 100.00 22.76

```
134 3062.304 18.3166 0.0000 0.0001 0.0007 100.00 61.34
135 3105.683 18.5761 0.0000 0.0000 0.0006 100.00 3.11
136 3108.052 18.5903 0.0000 0.0000 0.0006 100.00 15.05
137 3109.189 18.5971 0.0000 0.0000 0.0006 100.00 12.20
138 3110.135 18.6027 0.0000 0.0000 0.0006 100.00 7.75
139 3113.337 18.6219 0.0000 0.0000 0.0006 100.00 6.21
140 3114.805 18.6307 0.0000 0.0000 0.0006 100.00 15.74
141 3118.821 18.6547 0.0000 0.0000 0.0005 100.00 21.12
142 3119.548 18.6590 0.0000 0.0000 0.0005 100.00 82.73
143 3120.301 18.6635 0.0000 0.0000 0.0005 100.00 60.63
144 3121.407 18.6702 0.0000 0.0000 0.0005 100.00 27.30
145 3121.611 18.6714 0.0000 0.0000 0.0005 100.00 63.99
146 3125.004 18.6917 0.0000 0.0000 0.0005 100.00 3.36
147 3128.820 18.7145 0.0000 0.0000 0.0005 100.00 28.24
148 3134.930 18.7510 0.0000 0.0000 0.0005 100.00 64.61
149 3145.096 18.8118 0.0000 0.0000 0.0005 100.00 64.48
150 3159.701 18.8992 0.0000 0.0000 0.0005 100.00 42.62
151 3163.629 18.9227 0.0000 0.0000 0.0005 100.00 8.26
152 3174.134 18.9855 0.0000 0.0000 0.0004 100.00 20.70
153 3174.755 18.9892 0.0000 0.0000 0.0004 100.00 2.77
154 3181.381 19.0289 0.0000 0.0000 0.0004 100.00 20.66
155 3291.181 19.6856 0.0000 0.0000 0.0003 100.00 0.01
156 3294.287 19.7042 0.0000 0.0000 0.0003 100.00 0.01
-- ---------- ------- ------- ------- ----
Total Vibrations 1232.1091 48.9324 274.2314 277.2659

Ideal Gas 2.4789
Translation 3.7184 182.1068 12.4716
Rotation 3.7184 147.9170 12.4716
---------- ------- ------- -------
Totals 1290.9572 604.2552 302.2091

Vibrational(v) Corrections:
Temp. Correction Hv 1290.9572
Entropy Correction (Hv-TSv) 1110.7985

Reason for exit: Successful completion
Properties CPU Time : 5.27
Properties Wall Time: 8.86
```

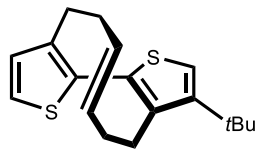	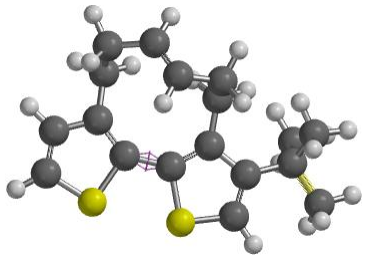
17 GS	**17'** TS
-1652.761162 au	-1652.707794 au

Fig s17. Calculation studies on the isomerization of **17**

Cartesian coordinate of **17** (GS)

S	−2.120713	−1.636226	1.512026
C	−1.644016	−0.685613	0.109158
C	−3.792202	−1.258095	1.272567
H	−4.542990	−1.638833	1.952375
C	−3.970270	−0.473062	0.169914
H	−4.944085	−0.126397	−0.162964
C	−2.753469	−0.142258	−0.512240
C	−0.228931	−0.652325	−0.283012
C	0.867572	−0.097772	0.356733
C	2.120679	−0.395935	−0.326679
C	1.903477	−1.136438	−1.461834
H	2.638868	−1.495422	−2.166090
S	0.244868	−1.523895	−1.725292
C	−2.726217	0.783139	−1.703794
H	−3.656823	0.666179	−2.273309
H	−1.905273	0.517012	−2.377847
C	−2.570656	2.282558	−1.294556
H	−2.698569	2.900942	−2.192262
H	−3.376074	2.545104	−0.597591
C	0.704613	0.777104	1.584941
H	−0.096506	0.376393	2.214987
H	1.608774	0.753291	2.197282
C	0.362827	2.268674	1.264160
H	1.118908	2.681134	0.587659
H	0.423608	2.833353	2.204660
C	−0.998649	2.394415	0.650403
H	−1.846996	2.256433	1.323380
C	−1.229158	2.504902	−0.660825
H	−0.381622	2.606480	−1.340960
C	3.544553	−0.039568	0.140038
C	4.593018	−0.489231	−0.900861
H	5.596377	−0.230856	−0.544870
H	4.444148	0.006773	−1.866770
H	4.572055	−1.572675	−1.060815
C	3.864682	−0.781455	1.461471
H	4.877065	−0.529190	1.801335
H	3.813964	−1.866375	1.317185
H	3.171488	−0.522811	2.266897
C	3.730628	1.483700	0.333977
H	4.779855	1.702268	0.567614
H	3.128188	1.882745	1.152190
H	3.467371	2.028863	−0.579519

Cartesian coordinate of **17'** (TS)

S	0.434142	−2.354623	0.388195
C	−0.172728	−0.748881	−0.074610
C	2.068052	−1.855606	0.317940
H	2.835625	−2.585503	0.523998
C	2.215311	−0.540106	−0.020152
C	0.921429	0.116816	−0.211347
C	−1.657893	−0.713101	−0.246439
C	−2.679059	0.187900	−0.580826

C	−3.988820	−0.402555	−0.489575
H	−4.883262	0.166950	−0.722854
C	−4.015404	−1.707678	−0.121589
H	−4.867557	−2.364295	−0.007880
S	−2.421837	−2.290582	0.136268
C	0.874262	1.617139	−0.377140
H	0.095735	1.918885	−1.078460
H	1.813061	1.957582	−0.810440
C	0.637959	2.395780	0.967569
H	1.249917	1.965876	1.766479
H	0.963535	3.433835	0.817546
C	−2.719017	1.625114	−1.068337
H	−1.807506	1.916231	−1.593512
H	−3.521670	1.679810	−1.814484
C	−3.013030	2.660728	0.080065
H	−3.595089	2.175575	0.870787
H	−3.611967	3.490126	−0.313170
C	−1.664676	3.114902	0.545418
H	−1.230024	3.933683	−0.034543
C	−0.833692	2.345483	1.253417
H	−1.216784	1.479168	1.791189
C	3.624772	0.060022	−0.237445
C	4.712673	−1.002570	0.045095
H	5.701479	−0.562713	−0.124607
H	4.623154	−1.869865	−0.617954
H	4.681768	−1.353585	1.082744
C	3.929602	1.244606	0.712265
H	4.974113	1.556427	0.590086
H	3.789495	0.946204	1.757471
H	3.308231	2.122115	0.528121
C	3.806381	0.482773	−1.717604
H	4.820485	0.870374	−1.875606
H	3.104722	1.257683	−2.036832
H	3.667248	−0.379815	−2.378759

Frequency calculation of **17'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm
Modifying values for 33 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1* i	**48.786**	**0.0000**	**1.2395**	**8.3144**	**4.1572 0.00 0.01**
2*	58.947	0.3526	1.2395	8.3144	4.1572 24.76 0.16
3*	86.635	0.5182	1.2395	8.3144	4.1572 34.17 0.03
4*	104.179	0.6231	1.2395	8.3144	4.1572 39.51 0.02
5*	123.519	0.7388	1.2395	8.3144	4.1572 44.90 0.45
6*	137.226	0.8208	1.2395	8.3144	4.1572 48.43 0.35
7*	163.275	0.9766	1.2395	8.3144	4.1572 54.52 0.46
8*	173.944	1.0404	1.2395	8.3144	4.1572 56.80 0.09
9*	202.354	1.2103	1.2395	8.3144	4.1572 62.34 0.34
10*	217.558	1.3013	1.2395	8.2814	4.1572 65.00 0.22
11*	235.051	1.4059	1.2395	7.6986	4.1572 67.83 0.12
12*	244.869	1.4646	1.2395	7.3940	4.1572 69.32 1.59
13*	254.520	1.5224	1.2395	7.1088	4.1572 70.72 0.34

14*	263.166	1.5741	1.2294	6.8645	4.1572	71.92	0.21
15*	291.482	1.7434	1.1313	6.1309	4.1572	75.50	1.06
16*	304.612	1.8220	1.0880	5.8217	4.1572	77.01	0.44
17*	322.819	1.9309	1.0302	5.4215	4.1572	78.94	0.05
18*	332.143	1.9867	1.0016	5.2284	4.1572	79.87	0.41
19*	353.500	2.1144	0.9384	4.8139	4.1572	81.84	0.28
20*	364.868	2.1824	0.9062	4.6077	4.1572	82.81	0.05
21*	385.423	2.3053	0.8502	4.2585	4.1572	84.43	1.04
22*	397.183	2.3757	0.8194	4.0712	4.1572	85.29	1.73
23*	413.366	2.4725	0.7787	3.8275	4.1572	86.40	0.82
24*	430.916	2.5775	0.7364	3.5800	4.1572	87.50	1.05
25*	441.917	2.6432	0.7109	3.4333	4.1572	88.15	0.15
26*	477.677	2.8571	0.6331	2.9972	4.1572	90.03	1.12
27*	487.118	2.9136	0.6139	2.8916	4.1572	90.47	1.47
28*	512.861	3.0676	0.5639	2.6222	4.1572	91.58	0.27
29*	537.604	3.2156	0.5192	2.3868	4.1572	92.53	0.08
30*	552.853	3.3068	0.4932	2.2522	4.1572	93.06	1.75
31*	560.133	3.3503	0.4812	2.1906	4.1572	93.30	1.04
32*	591.502	3.5380	0.4324	1.9434	4.1572	94.24	2.76
33*	603.595	3.6103	0.4148	1.8556	4.1572	94.57	5.23
34	658.311	3.9376	0.3428	1.5042	3.8120	95.83	22.99
35	698.906	4.1804	0.2969	1.2861	3.4782	96.57	5.04
36	732.851	4.3834	0.2629	1.1274	3.2119	97.09	8.22
37	738.627	4.4180	0.2575	1.1024	3.1678	97.17	9.36
38	742.064	4.4385	0.2543	1.0877	3.1417	97.22	7.15
39	775.240	4.6370	0.2254	0.9557	2.8970	97.63	15.47
40	816.858	4.8859	0.1934	0.8118	2.6081	98.06	3.50
41	820.465	4.9075	0.1909	0.8003	2.5840	98.09	6.17
42	838.216	5.0136	0.1787	0.7463	2.4677	98.25	5.53
43	854.194	5.1092	0.1684	0.7006	2.3662	98.38	5.36
44	876.377	5.2419	0.1550	0.6417	2.2304	98.54	6.43
45	881.760	5.2741	0.1518	0.6281	2.1983	98.58	16.47
46	893.669	5.3453	0.1452	0.5991	2.1286	98.66	4.17
47	908.163	5.4320	0.1374	0.5655	2.0459	98.75	13.83
48	914.698	5.4711	0.1341	0.5510	2.0095	98.79	12.56
49	930.157	5.5636	0.1264	0.5180	1.9252	98.88	3.73
50	936.157	5.5995	0.1236	0.5058	1.8932	98.91	1.24
51	945.495	5.6553	0.1193	0.4872	1.8443	98.96	1.98
52	959.736	5.7405	0.1129	0.4602	1.7716	99.03	5.63
53	967.665	5.7879	0.1096	0.4458	1.7321	99.06	0.11
54	979.277	5.8574	0.1048	0.4254	1.6755	99.11	9.80
55	1010.735	6.0455	0.0928	0.3748	1.5296	99.24	5.51
56	1024.761	6.1294	0.0879	0.3541	1.4680	99.29	10.33
57	1033.612	6.1824	0.0849	0.3417	1.4302	99.32	25.82
58	1061.777	6.3508	0.0761	0.3048	1.3151	99.40	1.18
59	1063.975	6.3640	0.0754	0.3021	1.3064	99.41	0.23
60	1076.140	6.4367	0.0719	0.2875	1.2594	99.44	5.18
61	1091.565	6.5290	0.0677	0.2700	1.2019	99.48	0.91
62	1115.885	6.6745	0.0615	0.2444	1.1157	99.54	9.47
63	1149.364	6.8747	0.0538	0.2131	1.0057	99.61	1.35
64	1170.126	6.9989	0.0496	0.1957	0.9422	99.65	0.75
65	1188.147	7.1067	0.0461	0.1817	0.8901	99.68	2.77
66	1222.337	7.3112	0.0402	0.1577	0.7979	99.73	0.55
67	1232.496	7.3720	0.0386	0.1512	0.7722	99.74	2.66

68	1237.996	7.4049	0.0378	0.1478	0.7586	99.75	3.19
69	1245.961	7.4525	0.0366	0.1430	0.7393	99.76	2.36
70	1258.598	7.5281	0.0348	0.1357	0.7096	99.77	3.11
71	1262.895	7.5538	0.0342	0.1333	0.6997	99.77	0.19
72	1273.309	7.6161	0.0327	0.1277	0.6763	99.79	44.23
73	1328.434	7.9458	0.0262	0.1014	0.5636	99.84	2.98
74	1334.913	7.9846	0.0255	0.0987	0.5515	99.84	0.96
75	1348.680	8.0669	0.0241	0.0932	0.5267	99.85	1.85
76	1354.614	8.1024	0.0235	0.0909	0.5163	99.86	8.36
77	1360.812	8.1395	0.0229	0.0886	0.5056	99.86	9.49
78	1375.395	8.2267	0.0216	0.0833	0.4813	99.87	0.37
79	1391.801	8.3248	0.0202	0.0778	0.4553	99.88	2.57
80	1400.496	8.3768	0.0195	0.0750	0.4420	99.88	1.23
81	1425.627	8.5271	0.0176	0.0674	0.4056	99.90	4.10
82	1429.875	8.5526	0.0173	0.0662	0.3997	99.90	5.21
83	1439.953	8.6128	0.0165	0.0635	0.3861	99.90	0.25
84	1459.307	8.7286	0.0153	0.0585	0.3611	99.91	8.38
85	1463.796	8.7554	0.0150	0.0574	0.3555	99.91	5.57
86	1512.168	9.0448	0.0123	0.0468	0.3003	99.93	0.28
87	1516.737	9.0721	0.0120	0.0459	0.2955	99.93	2.45
88	1519.887	9.0909	0.0119	0.0453	0.2923	99.93	0.69
89	1521.904	9.1030	0.0118	0.0449	0.2902	99.94	1.46
90	1524.576	9.1190	0.0116	0.0444	0.2875	99.94	0.99
91	1526.442	9.1301	0.0116	0.0440	0.2856	99.94	1.95
92	1535.960	9.1871	0.0111	0.0423	0.2762	99.94	3.62
93	1543.445	9.2319	0.0108	0.0409	0.2690	99.94	1.40
94	1555.497	9.3039	0.0102	0.0389	0.2577	99.95	10.38
95	1562.159	9.3438	0.0100	0.0378	0.2517	99.95	10.92
96	1569.079	9.3852	0.0097	0.0367	0.2456	99.95	2.69
97	1590.622	9.5140	0.0088	0.0335	0.2275	99.95	5.71
98	1734.478	10.3745	0.0048	0.0181	0.1350	99.98	3.09
99	3044.776	18.2118	0.0000	0.0001	0.0007	100.00	37.08
100	3047.389	18.2274	0.0000	0.0001	0.0007	100.00	17.05
101	3048.462	18.2338	0.0000	0.0001	0.0007	100.00	25.60
102	3049.947	18.2427	0.0000	0.0001	0.0007	100.00	20.67
103	3056.016	18.2790	0.0000	0.0001	0.0007	100.00	42.55
104	3064.370	18.3290	0.0000	0.0000	0.0007	100.00	67.01
105	3100.884	18.5474	0.0000	0.0000	0.0006	100.00	8.55
106	3105.799	18.5768	0.0000	0.0000	0.0006	100.00	15.90
107	3109.017	18.5960	0.0000	0.0000	0.0006	100.00	8.50
108	3111.535	18.6111	0.0000	0.0000	0.0006	100.00	5.87
109	3117.305	18.6456	0.0000	0.0000	0.0006	100.00	36.44
110	3119.616	18.6594	0.0000	0.0000	0.0005	100.00	77.12
111	3121.969	18.6735	0.0000	0.0000	0.0005	100.00	28.92
112	3122.677	18.6778	0.0000	0.0000	0.0005	100.00	16.28
113	3135.478	18.7543	0.0000	0.0000	0.0005	100.00	46.65
114	3143.536	18.8025	0.0000	0.0000	0.0005	100.00	44.62
115	3165.572	18.9343	0.0000	0.0000	0.0005	100.00	28.06
116	3171.531	18.9700	0.0000	0.0000	0.0004	100.00	13.97
117	3184.827	19.0495	0.0000	0.0000	0.0004	100.00	14.92
118	3210.169	19.2011	0.0000	0.0000	0.0004	100.00	13.74

```
119 3269.518 19.5561 0.0000 0.0000 0.0003 100.00 0.41
120 3291.102 19.6852 0.0000 0.0000 0.0003 100.00 0.02
-- ---------- ------- ------- ------- ----
Total Vibrations 935.0820 36.7010 204.0700 216.3715

Ideal Gas 2.4789
Translation 3.7184 179.9848 12.4716
Rotation 3.7184 143.2272 12.4716
---------- ------- ------- -------
Totals 981.6987 527.2819 241.3147

Vibrational(v) Corrections:
Temp. Correction Hv 981.6987
Entropy Correction (Hv-TSv) 824.4896

Reason for exit: Successful completion
Properties CPU Time : 3.09
Properties Wall Time: 10.34
```

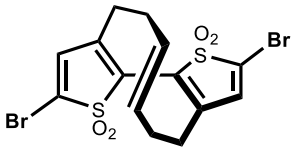	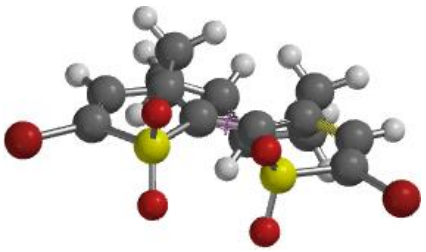
18 GS	**18'** TS
-6785.508121 au	-6785.452081 au

Fig s18. Calculation studies on the isomerization of **18**

Cartesian coordinate of **18** (GS)

C	0.703131	-0.180294	0.229131
C	3.256737	-0.265195	-0.314331
C	2.809553	-1.275829	0.437803
H	3.439516	-2.075402	0.813536
C	1.360203	-1.247870	0.745115
C	-0.703131	0.180294	0.229131
C	-1.360203	1.247870	0.745115
C	-2.809553	1.275829	0.437803

H	−3.439516	2.075402	0.813536
C	−3.256737	0.265195	−0.314331
C	0.784498	−2.283581	1.671360
H	1.382134	−3.200145	1.603261
H	−0.237346	−2.533240	1.375879
C	0.785583	−1.784552	3.157619
H	0.506567	−2.637771	3.787780
H	1.800683	−1.483287	3.443593
C	−0.784498	2.283581	1.671360
H	0.237346	2.533240	1.375879
H	−1.382134	3.200145	1.603261
C	−0.785583	1.784552	3.157619
H	−1.800683	1.483287	3.443593
H	−0.506567	2.637771	3.787780
C	0.174781	0.645189	3.323264
H	1.233463	0.910359	3.307942
C	−0.174781	−0.645189	3.323264
H	−1.233463	−0.910359	3.307942
Br	−4.987623	−0.091499	−0.925739
Br	4.987623	0.091499	−0.925739
S	1.885425	0.862503	−0.701874
O	1.596057	0.854246	−2.136534
O	2.097369	2.142944	−0.007697
S	−1.885425	−0.862503	−0.701874
O	−2.097369	−2.142944	−0.007697
O	−1.596057	−0.854246	−2.136534

Cartesian coordinate of **18'** (TS)

C	0.704144	−0.518711	0.335913
C	3.189445	0.409772	−0.005007
C	3.094904	−0.875502	0.320755
H	3.950256	−1.535470	0.417106
C	1.732200	−1.403370	0.573831
C	−0.761876	−0.528860	0.338679
C	−1.769053	−1.452461	0.511585
C	−3.145556	−0.909266	0.460620
H	−3.989351	−1.568441	0.631758
C	−3.268306	0.391986	0.213688
C	1.812143	−2.839412	1.033421
H	0.939978	−3.142612	1.611603
H	2.665384	−2.898006	1.720945
C	2.040647	−3.844256	−0.166582
H	2.519415	−3.323518	−1.002706
H	2.711241	−4.647877	0.154275
C	−1.777065	−2.953751	0.671554
H	−0.977904	−3.314666	1.317579
H	−2.719122	−3.229076	1.159482
C	−1.680402	−3.710359	−0.703109
H	−2.387773	−3.285506	−1.422807
H	−1.967377	−4.753760	−0.524346
C	−0.246948	−3.609803	−1.134020
H	0.051867	−2.729025	−1.700925
C	0.672963	−4.347580	−0.506157
H	0.328770	−5.186079	0.104864

Br	-4.793524	1.462031	0.085738
Br	4.688125	1.464020	-0.382447
S	1.554917	1.151382	0.023836
O	1.477242	1.989295	1.221481
O	1.245687	1.682778	-1.302573
S	-1.645450	1.093695	-0.097710
O	-1.567781	1.348639	-1.537510
O	-1.366483	2.143447	0.880777

Frequency calculation of **18'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 23 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in	
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
--	----------	-------	-------	-------	----	
1* i	**151.472**	**0.0000**	**1.2395**	**8.3144**	**4.1572**	**0.00**	**0.21**
2*	31.765	0.1900	1.2395	8.3144	4.1572	14.21	0.01
3*	38.661	0.2312	1.2395	8.3144	4.1572	17.02	0.01
4*	127.333	0.7616	1.2395	8.3144	4.1572	45.91	0.48
5*	178.792	1.0694	1.2395	8.3144	4.1572	57.80	0.27
6*	196.127	1.1731	1.2395	8.3144	4.1572	61.19	0.10
7*	211.836	1.2671	1.2395	8.3144	4.1572	64.02	1.59
8*	233.108	1.3943	1.2395	7.7607	4.1572	67.53	0.23
9*	263.220	1.5744	1.2292	6.8630	4.1572	71.92	1.49
10*	271.304	1.6228	1.2006	6.6436	4.1572	73.00	0.24
11*	323.377	1.9342	1.0285	5.4097	4.1572	79.00	0.44
12*	334.388	2.0001	0.9948	5.1831	4.1572	80.08	0.05
13*	385.421	2.3053	0.8502	4.2585	4.1572	84.43	0.52
14*	424.186	2.5372	0.7524	3.6729	4.1572	87.09	0.67
15*	446.562	2.6710	0.7004	3.3733	4.1572	88.41	4.49
16*	475.278	2.8428	0.6381	3.0246	4.1572	89.91	0.24
17*	496.519	2.9698	0.5952	2.7902	4.1572	90.89	1.39
18*	500.977	2.9965	0.5865	2.7433	4.1572	91.09	0.73
19*	521.955	3.1220	0.5471	2.5331	4.1572	91.94	1.30
20*	558.461	3.3403	0.4839	2.2046	4.1572	93.25	1.71
21*	577.705	3.4554	0.4533	2.0486	4.1572	93.84	0.12
22*	594.675	3.5569	0.4277	1.9200	4.1572	94.33	8.08
23*	611.417	3.6571	0.4037	1.8009	4.1572	94.77	1.13
24	637.071	3.8105	0.3693	1.6322	3.9928	95.38	7.49
25	676.740	4.0478	0.3213	1.4011	3.6585	96.18	0.18
26	715.105	4.2773	0.2802	1.2078	3.3496	96.83	3.14
27	739.360	4.4224	0.2568	1.0992	3.1622	97.18	10.09
28	757.285	4.5296	0.2406	1.0251	3.0279	97.41	68.19
29	763.646	4.5676	0.2351	1.0000	2.9811	97.49	2.64
30	788.533	4.7165	0.2147	0.9072	2.8025	97.77	0.65
31	807.423	4.8295	0.2003	0.8424	2.6718	97.97	0.14
32	838.876	5.0176	0.1783	0.7443	2.4635	98.25	13.79
33	851.502	5.0931	0.1701	0.7081	2.3831	98.36	2.13
34	857.276	5.1276	0.1664	0.6921	2.3470	98.40	0.78
35	862.314	5.1578	0.1633	0.6785	2.3159	98.44	2.58
36	889.042	5.3177	0.1477	0.6102	2.1555	98.63	8.14
37	920.937	5.5084	0.1310	0.5375	1.9751	98.83	2.02

38	935.071	5.5930	0.1241	0.5080	1.8990	98.90	0.81
39	949.751	5.6808	0.1173	0.4790	1.8223	98.98	0.64
40	967.521	5.7871	0.1096	0.4460	1.7328	99.06	14.79
41	974.372	5.8280	0.1068	0.4339	1.6992	99.09	2.10
42	978.823	5.8547	0.1050	0.4262	1.6777	99.11	5.34
43	980.786	5.8664	0.1042	0.4229	1.6683	99.12	4.17
44	998.496	5.9723	0.0973	0.3938	1.5851	99.19	8.93
45	1005.974	6.0171	0.0945	0.3821	1.5510	99.22	0.78
46	1033.541	6.1819	0.0849	0.3418	1.4305	99.32	32.30
47	1069.686	6.3981	0.0737	0.2951	1.2842	99.43	3.06
48	1080.403	6.4622	0.0707	0.2825	1.2433	99.46	3.07
49	1091.472	6.5285	0.0677	0.2701	1.2022	99.48	2.70
50	1101.817	6.5903	0.0650	0.2589	1.1649	99.51	2.62
51	1112.394	6.6536	0.0623	0.2480	1.1277	99.53	2.78
52	1148.786	6.8713	0.0540	0.2136	1.0075	99.61	10.22
53	1155.819	6.9133	0.0525	0.2075	0.9856	99.62	1.66
54	1167.958	6.9859	0.0500	0.1974	0.9487	99.64	3.15
55	1179.907	7.0574	0.0477	0.1879	0.9136	99.66	0.22
56	1208.894	7.2308	0.0425	0.1668	0.8331	99.71	0.81
57	1216.508	7.2763	0.0412	0.1616	0.8130	99.72	1.66
58	1218.182	7.2863	0.0409	0.1605	0.8087	99.72	0.96
59	1222.276	7.3108	0.0402	0.1578	0.7981	99.73	1.32
60	1245.823	7.4517	0.0366	0.1431	0.7397	99.76	2.64
61	1256.321	7.5145	0.0351	0.1370	0.7148	99.77	1.11
62	1306.290	7.8133	0.0286	0.1113	0.6066	99.82	1.36
63	1313.823	7.8584	0.0278	0.1078	0.5917	99.82	0.54
64	1322.612	7.9110	0.0268	0.1039	0.5746	99.83	2.12
65	1333.770	7.9777	0.0256	0.0992	0.5536	99.84	0.19
66	1340.552	8.0183	0.0249	0.0964	0.5412	99.84	2.46
67	1350.382	8.0771	0.0239	0.0925	0.5237	99.85	6.18
68	1352.578	8.0902	0.0237	0.0917	0.5198	99.85	0.13
69	1370.370	8.1966	0.0220	0.0851	0.4896	99.87	6.57
70	1382.329	8.2682	0.0210	0.0809	0.4701	99.87	4.88
71	1391.515	8.3231	0.0202	0.0779	0.4557	99.88	0.66
72	1472.613	8.8082	0.0145	0.0553	0.3448	99.92	13.50
73	1482.069	8.8647	0.0139	0.0531	0.3336	99.92	10.03
74	1515.616	9.0654	0.0121	0.0461	0.2967	99.93	6.97
75	1521.262	9.0992	0.0118	0.0450	0.2909	99.94	8.56
76	1524.278	9.1172	0.0117	0.0444	0.2878	99.94	0.92
77	1540.823	9.2162	0.0109	0.0414	0.2715	99.94	19.87
78	1550.939	9.2767	0.0104	0.0397	0.2619	99.94	4.12
79	1574.009	9.4147	0.0095	0.0359	0.2413	99.95	7.49
80	1625.380	9.7219	0.0076	0.0289	0.2008	99.96	0.59
81	1635.597	9.7830	0.0073	0.0276	0.1935	99.96	1.55
82	1658.683	9.9211	0.0066	0.0250	0.1780	99.97	0.86
83	1665.043	9.9592	0.0065	0.0243	0.1740	99.97	0.79
84	1727.452	10.3325	0.0050	0.0186	0.1386	99.98	5.24
85	3049.944	18.2427	0.0000	0.0001	0.0007	100.00	16.26
86	3050.008	18.2431	0.0000	0.0001	0.0007	100.00	33.59
87	3065.538	18.3360	0.0000	0.0000	0.0007	100.00	65.64
88	3078.272	18.4121	0.0000	0.0000	0.0006	100.00	39.46
89	3101.051	18.5484	0.0000	0.0000	0.0006	100.00	8.07
90	3104.892	18.5714	0.0000	0.0000	0.0006	100.00	14.82
91	3117.363	18.6460	0.0000	0.0000	0.0006	100.00	49.12

```
92 3163.510 18.9220 0.0000 0.0000 0.0005 100.00 16.81
93 3173.830 18.9837 0.0000 0.0000 0.0004 100.00 9.53
94 3176.919 19.0022 0.0000 0.0000 0.0004 100.00 14.79
95 3183.955 19.0443 0.0000 0.0000 0.0004 100.00 2.26
96 3189.581 19.0779 0.0000 0.0000 0.0004 100.00 16.06
97 3192.368 19.0946 0.0000 0.0000 0.0004 100.00 35.27
98 3200.222 19.1416 0.0000 0.0000 0.0004 100.00 19.15
99 3209.702 19.1983 0.0000 0.0000 0.0004 100.00 42.43
100 3211.532 19.2092 0.0000 0.0000 0.0004 100.00 28.81
101 3298.545 19.7297 0.0000 0.0000 0.0003 100.00 1.00
102 3354.390 20.0637 0.0000 0.0000 0.0002 100.00 13.44
-- ---------- ------- ------- ------- ----
Total Vibrations 813.9890 25.9785 141.8710 173.1021

Ideal Gas 2.4789
Translation 3.7184 176.8007 12.4716
Rotation 3.7184 138.0063 12.4716
---------- ------- ------- -------
Totals 849.8833 456.6781 198.0454

Vibrational(v) Corrections:
Temp. Correction Hv 849.8833
Entropy Correction (Hv-TSv) 713.7247

Reason for exit: Successful completion
Properties CPU Time : 2.34
Properties Wall Time: 5.20
```

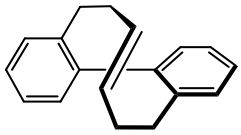	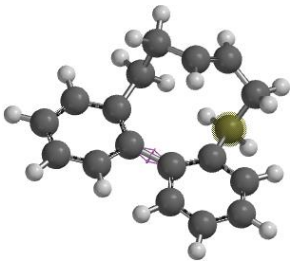
19 GS	**19'** TS
-696.747070 au	-696.663953 au

Fig s19. Calculation studies on the isomerization of **19**

Cartesian coordinate of **19** GS)

H	3.731963	−1.206151	0.135757
C	3.028995	−0.522233	−0.336130
C	1.246268	1.209044	−1.538133
C	1.655410	−0.782967	−0.210973
C	3.514268	0.577609	−1.039034
C	2.613371	1.452394	−1.645357
C	0.742268	0.108050	−0.824029
H	4.585250	0.744972	−1.118164
H	2.969886	2.310738	−2.208776

H	0.542468	1.874784	−2.031339
C	−0.742268	−0.108050	−0.824029
C	−3.514268	−0.577609	−1.039034
C	−1.246268	−1.209044	−1.538133
C	−1.655410	0.782967	−0.210973
C	−3.028995	0.522233	−0.336130
C	−2.613371	−1.452394	−1.645357
H	−0.542468	−1.874784	−2.031339
H	−3.731963	1.206151	0.135757
H	−2.969886	−2.310738	−2.208776
H	−4.585250	−0.744972	−1.118164
C	1.237360	−1.972534	0.632606
H	1.997303	−2.758753	0.540050
H	0.295435	−2.398690	0.274943
C	−1.237360	1.972534	0.632606
H	−1.997303	2.758753	0.540050
H	−0.295435	2.398690	0.274943
C	1.079541	−1.617108	2.143496
H	2.015500	−1.170462	2.501599
H	0.924969	−2.548055	2.704592
C	−1.079541	1.617108	2.143496
H	−2.015500	1.170462	2.501599
H	−0.924969	2.548055	2.704592
C	−0.064303	−0.664847	2.335093
H	−1.066256	−1.095735	2.311577
C	0.064303	0.664847	2.335093
H	1.066256	1.095735	2.311577

Cartesian coordinate of **19'** (TS)

H	−2.136618	−4.054526	−0.478357
C	−2.047739	−2.999797	−0.232093
C	−1.654116	−0.314202	0.529645
C	−0.787300	−2.441460	−0.110747
C	−3.167576	−2.206793	−0.023618
C	−2.932183	−0.907322	0.373699
C	−0.477732	−1.077672	0.191308
H	−0.001996	−3.161246	−0.240046
H	−4.178621	−2.592318	−0.119265
H	−3.790597	−0.286379	0.617197
C	1.053120	−0.734844	0.102403
C	3.973549	−0.724675	0.039737
C	1.878100	−1.834037	−0.283107
C	1.815222	0.475423	0.315166
C	3.229560	0.407310	0.316104
C	3.263876	−1.860805	−0.312929
H	1.438386	−2.754703	−0.616877
H	3.768594	1.326807	0.524393
H	3.767415	−2.775815	−0.613148
H	5.059371	−0.701427	0.063003
C	−1.872308	1.072293	1.143462
H	−0.977038	1.491384	1.597857
H	−2.571858	0.927504	1.975833
C	1.389947	1.935934	0.414877
H	2.237096	2.487619	0.834399

H	0.566247	2.109047	1.101707
C	-2.501352	2.102694	0.129463
H	-3.088244	1.564128	-0.621484
H	-3.185751	2.775514	0.659031
C	1.024812	2.596121	-0.962636
H	1.713806	2.252629	-1.741635
H	1.152719	3.681077	-0.855569
C	-1.341043	2.846282	-0.456970
H	-1.048203	3.747532	0.088606
C	-0.414605	2.258905	-1.220220
H	-0.636146	1.316890	-1.721191

Frequency calculation of **19'**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 23 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground IR Int.
--	----------	-------	-------	-------	----
1* i	**151.472**	**0.0000**	**1.2395**	**8.3144**	**4.1572 0.00 0.21**
2*	31.765	0.1900	1.2395	8.3144	4.1572 14.21 0.01
3*	38.661	0.2312	1.2395	8.3144	4.1572 17.02 0.01
4*	127.333	0.7616	1.2395	8.3144	4.1572 45.91 0.48
5*	178.792	1.0694	1.2395	8.3144	4.1572 57.80 0.27
6*	196.127	1.1731	1.2395	8.3144	4.1572 61.19 0.10
7*	211.836	1.2671	1.2395	8.3144	4.1572 64.02 1.59
8*	233.108	1.3943	1.2395	7.7607	4.1572 67.53 0.23
9*	263.220	1.5744	1.2292	6.8630	4.1572 71.92 1.49
10*	271.304	1.6228	1.2006	6.6436	4.1572 73.00 0.24
11*	323.377	1.9342	1.0285	5.4097	4.1572 79.00 0.44
12*	334.388	2.0001	0.9948	5.1831	4.1572 80.08 0.05
13*	385.421	2.3053	0.8502	4.2585	4.1572 84.43 0.52
14*	424.186	2.5372	0.7524	3.6729	4.1572 87.09 0.67
15*	446.562	2.6710	0.7004	3.3733	4.1572 88.41 4.49
16*	475.278	2.8428	0.6381	3.0246	4.1572 89.91 0.24
17*	496.519	2.9698	0.5952	2.7902	4.1572 90.89 1.39
18*	500.977	2.9965	0.5865	2.7433	4.1572 91.09 0.73
19*	521.955	3.1220	0.5471	2.5331	4.1572 91.94 1.30
20*	558.461	3.3403	0.4839	2.2046	4.1572 93.25 1.71
21*	577.705	3.4554	0.4533	2.0486	4.1572 93.84 0.12
22*	594.675	3.5569	0.4277	1.9200	4.1572 94.33 8.08
23*	611.417	3.6571	0.4037	1.8009	4.1572 94.77 1.13
24	637.071	3.8105	0.3693	1.6322	3.9928 95.38 7.49
25	676.740	4.0478	0.3213	1.4011	3.6585 96.18 0.18
26	715.105	4.2773	0.2802	1.2078	3.3496 96.83 3.14
27	739.360	4.4224	0.2568	1.0992	3.1622 97.18 10.09
28	757.285	4.5296	0.2406	1.0251	3.0279 97.41 68.19
29	763.646	4.5676	0.2351	1.0000	2.9811 97.49 2.64
30	788.533	4.7165	0.2147	0.9072	2.8025 97.77 0.65
31	807.423	4.8295	0.2003	0.8424	2.6718 97.97 0.14
32	838.876	5.0176	0.1783	0.7443	2.4635 98.25 13.79
33	851.502	5.0931	0.1701	0.7081	2.3831 98.36 2.13

34	857.276	5.1276	0.1664	0.6921	2.3470	98.40	0.78
35	862.314	5.1578	0.1633	0.6785	2.3159	98.44	2.58
36	889.042	5.3177	0.1477	0.6102	2.1555	98.63	8.14
37	920.937	5.5084	0.1310	0.5375	1.9751	98.83	2.02
38	935.071	5.5930	0.1241	0.5080	1.8990	98.90	0.81
39	949.751	5.6808	0.1173	0.4790	1.8223	98.98	0.64
40	967.521	5.7871	0.1096	0.4460	1.7328	99.06	14.79
41	974.372	5.8280	0.1068	0.4339	1.6992	99.09	2.10
42	978.823	5.8547	0.1050	0.4262	1.6777	99.11	5.34
43	980.786	5.8664	0.1042	0.4229	1.6683	99.12	4.17
44	998.496	5.9723	0.0973	0.3938	1.5851	99.19	8.93
45	1005.974	6.0171	0.0945	0.3821	1.5510	99.22	0.78
46	1033.541	6.1819	0.0849	0.3418	1.4305	99.32	32.30
47	1069.686	6.3981	0.0737	0.2951	1.2842	99.43	3.06
48	1080.403	6.4622	0.0707	0.2825	1.2433	99.46	3.07
49	1091.472	6.5285	0.0677	0.2701	1.2022	99.48	2.70
50	1101.817	6.5903	0.0650	0.2589	1.1649	99.51	2.62
51	1112.394	6.6536	0.0623	0.2480	1.1277	99.53	2.78
52	1148.786	6.8713	0.0540	0.2136	1.0075	99.61	10.22
53	1155.819	6.9133	0.0525	0.2075	0.9856	99.62	1.66
54	1167.958	6.9859	0.0500	0.1974	0.9487	99.64	3.15
55	1179.907	7.0574	0.0477	0.1879	0.9136	99.66	0.22
56	1208.894	7.2308	0.0425	0.1668	0.8331	99.71	0.81
57	1216.508	7.2763	0.0412	0.1616	0.8130	99.72	1.66
58	1218.182	7.2863	0.0409	0.1605	0.8087	99.72	0.96
59	1222.276	7.3108	0.0402	0.1578	0.7981	99.73	1.32
60	1245.823	7.4517	0.0366	0.1431	0.7397	99.76	2.64
61	1256.321	7.5145	0.0351	0.1370	0.7148	99.77	1.11
62	1306.290	7.8133	0.0286	0.1113	0.6066	99.82	1.36
63	1313.823	7.8584	0.0278	0.1078	0.5917	99.82	0.54
64	1322.612	7.9110	0.0268	0.1039	0.5746	99.83	2.12
65	1333.770	7.9777	0.0256	0.0992	0.5536	99.84	0.19
66	1340.552	8.0183	0.0249	0.0964	0.5412	99.84	2.46
67	1350.382	8.0771	0.0239	0.0925	0.5237	99.85	6.18
68	1352.578	8.0902	0.0237	0.0917	0.5198	99.85	0.13
69	1370.370	8.1966	0.0220	0.0851	0.4896	99.87	6.57
70	1382.329	8.2682	0.0210	0.0809	0.4701	99.87	4.88
71	1391.515	8.3231	0.0202	0.0779	0.4557	99.88	0.66
72	1472.613	8.8082	0.0145	0.0553	0.3448	99.92	13.50
73	1482.069	8.8647	0.0139	0.0531	0.3336	99.92	10.03
74	1515.616	9.0654	0.0121	0.0461	0.2967	99.93	6.97
75	1521.262	9.0992	0.0118	0.0450	0.2909	99.94	8.56
76	1524.278	9.1172	0.0117	0.0444	0.2878	99.94	0.92
77	1540.823	9.2162	0.0109	0.0414	0.2715	99.94	19.87
78	1550.939	9.2767	0.0104	0.0397	0.2619	99.94	4.12
79	1574.009	9.4147	0.0095	0.0359	0.2413	99.95	7.49
80	1625.380	9.7219	0.0076	0.0289	0.2008	99.96	0.59
81	1635.597	9.7830	0.0073	0.0276	0.1935	99.96	1.55
82	1658.683	9.9211	0.0066	0.0250	0.1780	99.97	0.86
83	1665.043	9.9592	0.0065	0.0243	0.1740	99.97	0.79
84	1727.452	10.3325	0.0050	0.0186	0.1386	99.98	5.24
85	3049.944	18.2427	0.0000	0.0001	0.0007	100.00	16.26
86	3050.008	18.2431	0.0000	0.0001	0.0007	100.00	33.59
87	3065.538	18.3360	0.0000	0.0000	0.0007	100.00	65.64

```
88 3078.272 18.4121 0.0000 0.0000 0.0006 100.00 39.46
89 3101.051 18.5484 0.0000 0.0000 0.0006 100.00 8.07
90 3104.892 18.5714 0.0000 0.0000 0.0006 100.00 14.82
91 3117.363 18.6460 0.0000 0.0000 0.0006 100.00 49.12
92 3163.510 18.9220 0.0000 0.0000 0.0005 100.00 16.81
93 3173.830 18.9837 0.0000 0.0000 0.0004 100.00 9.53
94 3176.919 19.0022 0.0000 0.0000 0.0004 100.00 14.79
95 3183.955 19.0443 0.0000 0.0000 0.0004 100.00 2.26
96 3189.581 19.0779 0.0000 0.0000 0.0004 100.00 16.06
97 3192.368 19.0946 0.0000 0.0000 0.0004 100.00 35.27
98 3200.222 19.1416 0.0000 0.0000 0.0004 100.00 19.15
99 3209.702 19.1983 0.0000 0.0000 0.0004 100.00 42.43
100 3211.532 19.2092 0.0000 0.0000 0.0004 100.00 28.81
101 3298.545 19.7297 0.0000 0.0000 0.0003 100.00 1.00
102 3354.390 20.0637 0.0000 0.0000 0.0002 100.00 13.44
-- ---------- ------- ------- ------- ----
Total Vibrations 813.9890 25.9785 141.8710 173.1021

Ideal Gas 2.4789
Translation 3.7184 176.8007 12.4716
Rotation 3.7184 138.0063 12.4716
---------- ------- ------- -------
Totals 849.8833 456.6781 198.0454

Vibrational(v) Corrections:
Temp. Correction Hv 849.8833
Entropy Correction (Hv-TSv) 713.7247

Reason for exit: Successful completion
Properties CPU Time : 2.34
Properties Wall Time: 5.20
```