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Quantification of the *push–pull* effect in 2-alkylidene-4-oxothiazolidines by using NMR spectral data and barriers to rotation around the C=C bond†

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Supplementary Information

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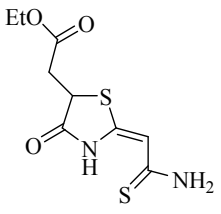
Figure S1. The facile *E* to *Z* isomerization of (*E*)-(5-ethoxycarbonylmethyl-4-oxothiazolidin-2-ylidene)ethanthioamide **9a** at 298 K illustrated by the three ^{1}H NMR spectra recorded 5, 170 and 1380 minutes after its dissolution (DMSO-d_6)



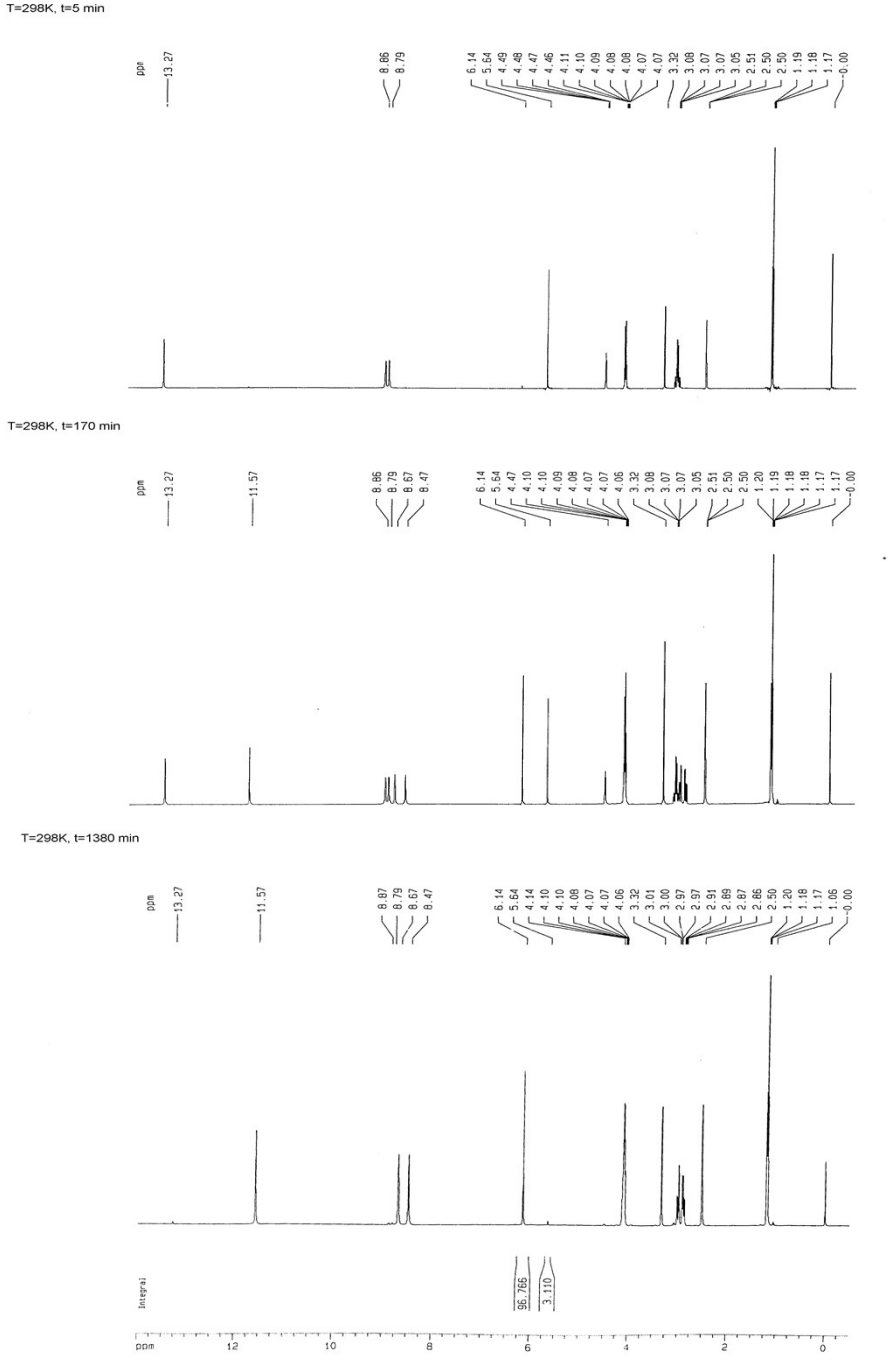
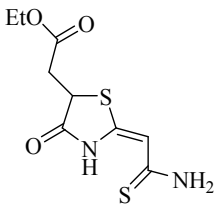


Figure S2. The facile *E* to *Z* isomerization of (*E*)-(5-ethoxycarbonylmethyl-4-oxothiazolidin-2-ylidene)ethanthioamide **9a** at 303 K illustrated by the three ^{1}H NMR spectra recorded 5, 75 and 930 minutes after its dissolution (DMSO-d_6)



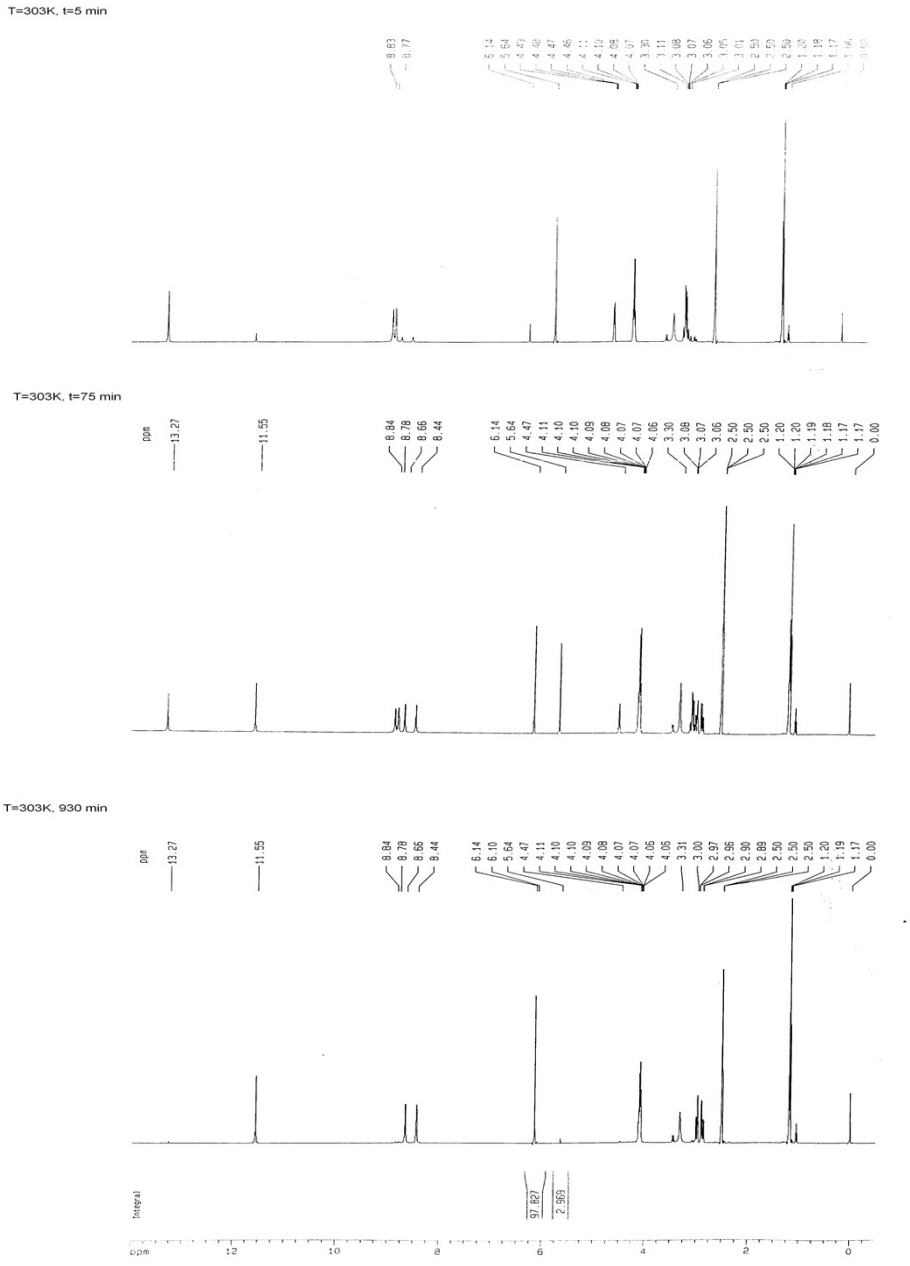
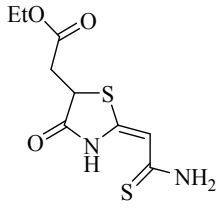
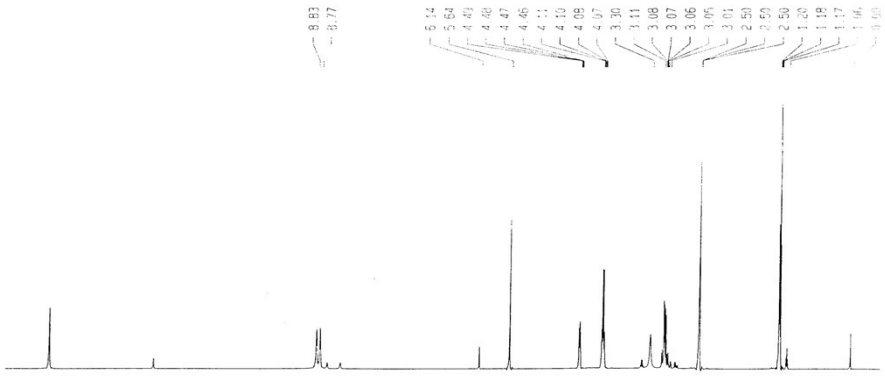


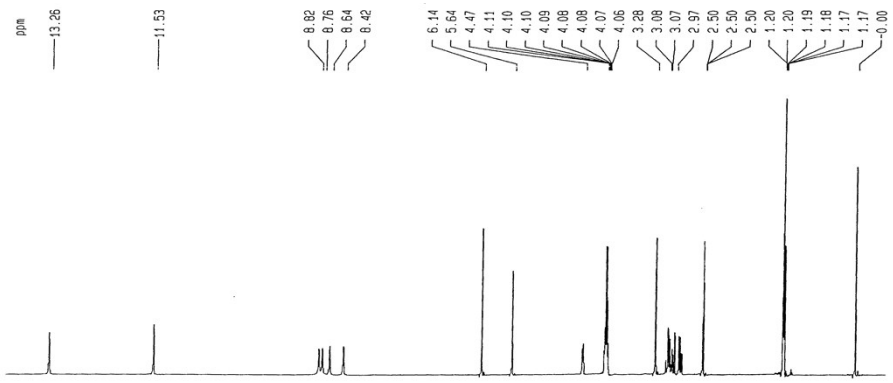
Figure S3. The facile *E* to *Z* isomerization of (*E*)-(5-ethoxycarbonylmethyl-4-oxothiazolidin-2-ylidene)ethanthioamide **9a** at 308 K illustrated by the three ^{1}H NMR spectra recorded 5, 65 and 930 minutes after its dissolution (DMSO-d_6)



T=308K, t=5 min



T=308K, t=65 min



T=308K, 930 min

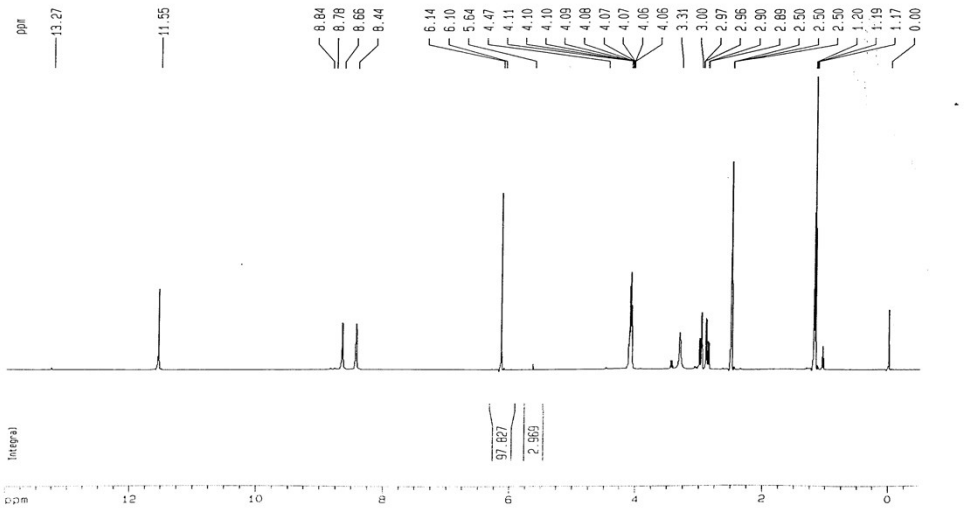


Table S1. The concentration ratio of (*E*)- and (*Z*)-(5-ethoxycarbonylmethyl-4-oxothiazolidin-2-ylidene)ethanthioamide **9a** at 298, 303 i 308 K (DMSO-d_6)

t min	T = 303K		T = 308K		T = 298K	
	Z	***E***	***Z***	***E***	***Z***	***E***
0	0	100	0	100	0	100
5	1.944	98.055	4.350	95.650	2.431	97.655
10	8.796	91.240	12.423	87.577	4.444	95.153
15	13.128	86.486	19.567	80.533	6.512	93.465
20	17.330	82.670	19.706	80.294	8.142	91.129
25	21.132	78.474	22.960	77.040	9.760	90.155
30	24.545	75.453	26.253	73.747	11.821	88.283
35	28.675	71.331	29.301	70.699	13.146	86.818
40	31.702	68.191	31.920	68.080	14.894	85.161
45	34.712	65.288	35.095	64.905	15.781	83.211
50	37.030	62.970	38.346	61.627	17.297	81.267
55	40.820	59.180	41.118	58.339	18.245	81.850
60	42.628	57.372	43.328	56.185	19.996	80.003
65	44.863	55.137	46.682	53.322	22.573	77.109
70	47.072	52.928	49.047	50.430	24.315	75.458
75	49.489	50.511	51.205	48.795	25.297	74.087
80	50.839	49.161	53.052	45.983	26.066	73.934
85	52.757	47.243	55.922	44.078	26.890	71.789
90	53.701	46.299			29.393	70.092
95	55.792	44.208	59.913	40.042	31.221	68.746
100	57.973	44.027			32.209	67.653
105	59.433	40.567	63.987	36.009	34.008	65.938
110	61.770	38.230			35.302	64.305
115	63.208	36.792	67.465	32.527	36.628	63.193
120	64.009	35.879			37.654	62.098
125	65.787	34.218	68.649	30.751	38.512	60.968
130	67.050	32.950			40.360	59.742
135	68.348	31.665	74.685	25.388	41.493	58.086
140	69.742	30.258			43.540	56.168
145	71.058	28.942	75.728	24.208	45.045	54.953
150	72.355	27.645			46.042	53.657
155	73.480	26.520	77.062	22.709	46.877	53.121
160					47.553	52.469
165	75.498	24.501	79.433	20.277	48.514	51.485
170					49.632	50.383
175	77.795	22.203	81.902	18.175	50.636	49.361
180						
185			82.445	17.649	51.760	48.239
190						
195						
200						
205	81.530	17.970	85.282	14.196	55.485	44.511
210						
215						
220						

225			86.444	13.632		
230						
235						
240					62.223	37.787
245			89.338	10.004		
250						
255	87.006	12.966				
260						
265			90.052	9.755		
270						
275						
280						
285			93.009	6.905		
290						
295						
300					70.103	29.832
305	90.303	9.401	94.452	6.624		
310						
315						
320						
325						
330						
335			95.687	4.749		
340						
345						
350	92.374	7.626				
355			96.232	3.768		
360					75.910	24.063
365			96.580	3.464		
370						
375						
380						
385						
390						
395						
400	92.948	7.052	96.717	3.287		
405						
410						
415						
420					81.773	18.232
425						
430						
435						
440						
445	93.164	6.314				
450						
455						
460						
465						
470						

475					
480				85.478	14.522
485					
490	93.932	5.939			
495					
500					
505					
510					
515					
520					
525					
530					
535					
540	94.812	5.047		88.415	11.500
545					
550					
555					
560					
565					
570					
575					
580					
585					
590	95.095	4.827			
595					
600				91.228	8.686
605					
610					
615					
620					
625					
630					
635					
640	95.774	4.270			
645					
650					
655					
660					
665				91.957	8.183
670					
675					
680					
685					
690	96.233	3.697			
700					
705					
710					
715					
720				93.292	6.747
725					

730						
735						
740	96.541	3.438				
745						
750						
755						
760						
765						
770						
775						
780					93.944	6.100
785						
790	97.004	3.192				
795						
800						
805						
810						
815						
820						
825						
830						
835						
840	97.091	2.923			94.695	5.364
845						
850						
855						
860						
865						
870						
875						
880						
885						
890	97.312	2.677				
895						
900					95.346	4.646
905						
910						
915						
920						
925						
930	97.827	2.173	96.840	3.102		
935						
940						
945						
950						
960					95.498	4.519
965						
970						
980						
985						

990				
995				
1000				
1005				
1010				
1015				
1020			95.737	4.256
1025				
1030				
1035				
1040				
1045				
1050				
1055				
1060				
1065				
1070				
1075				
1080				
1085				
1090				
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1100				
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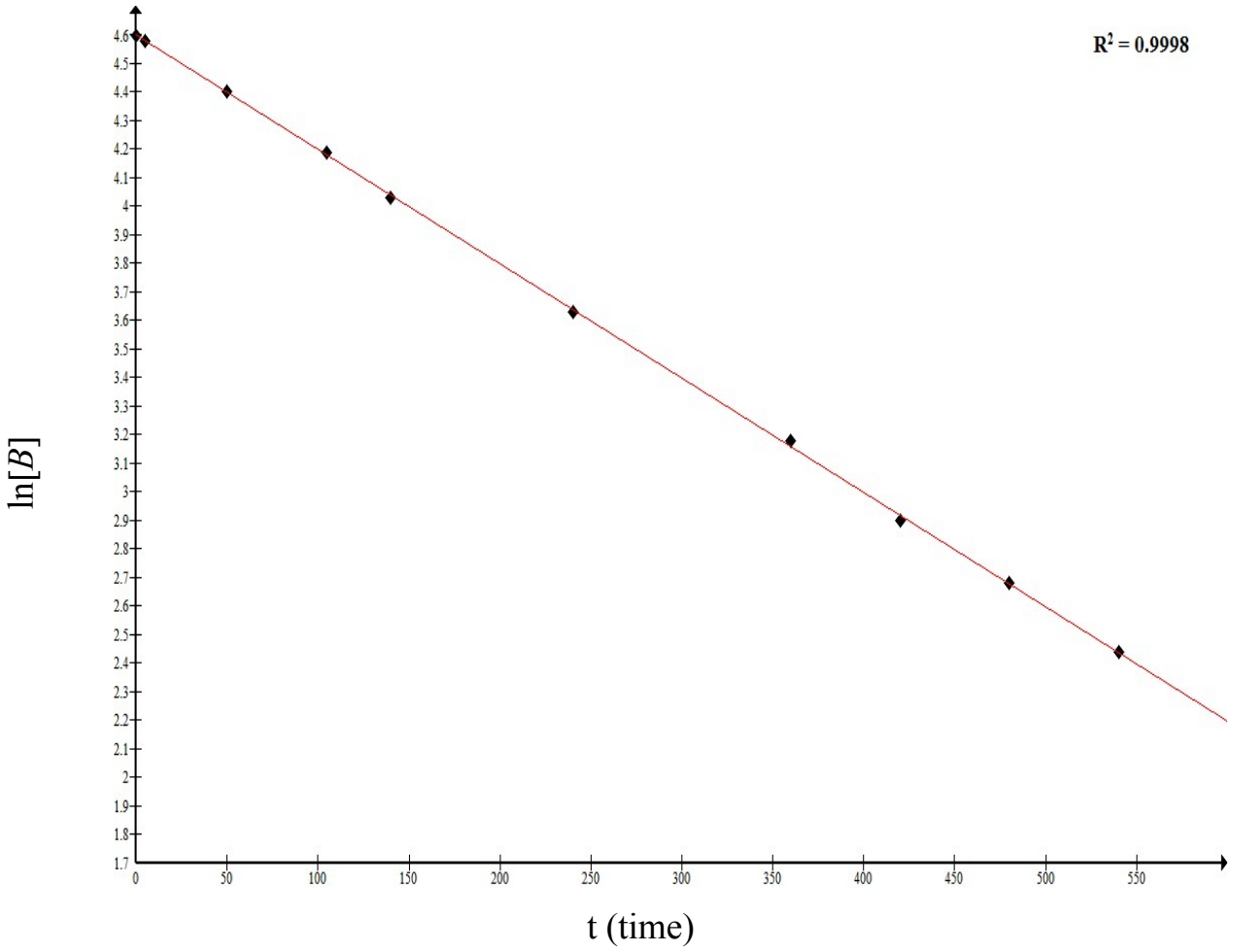
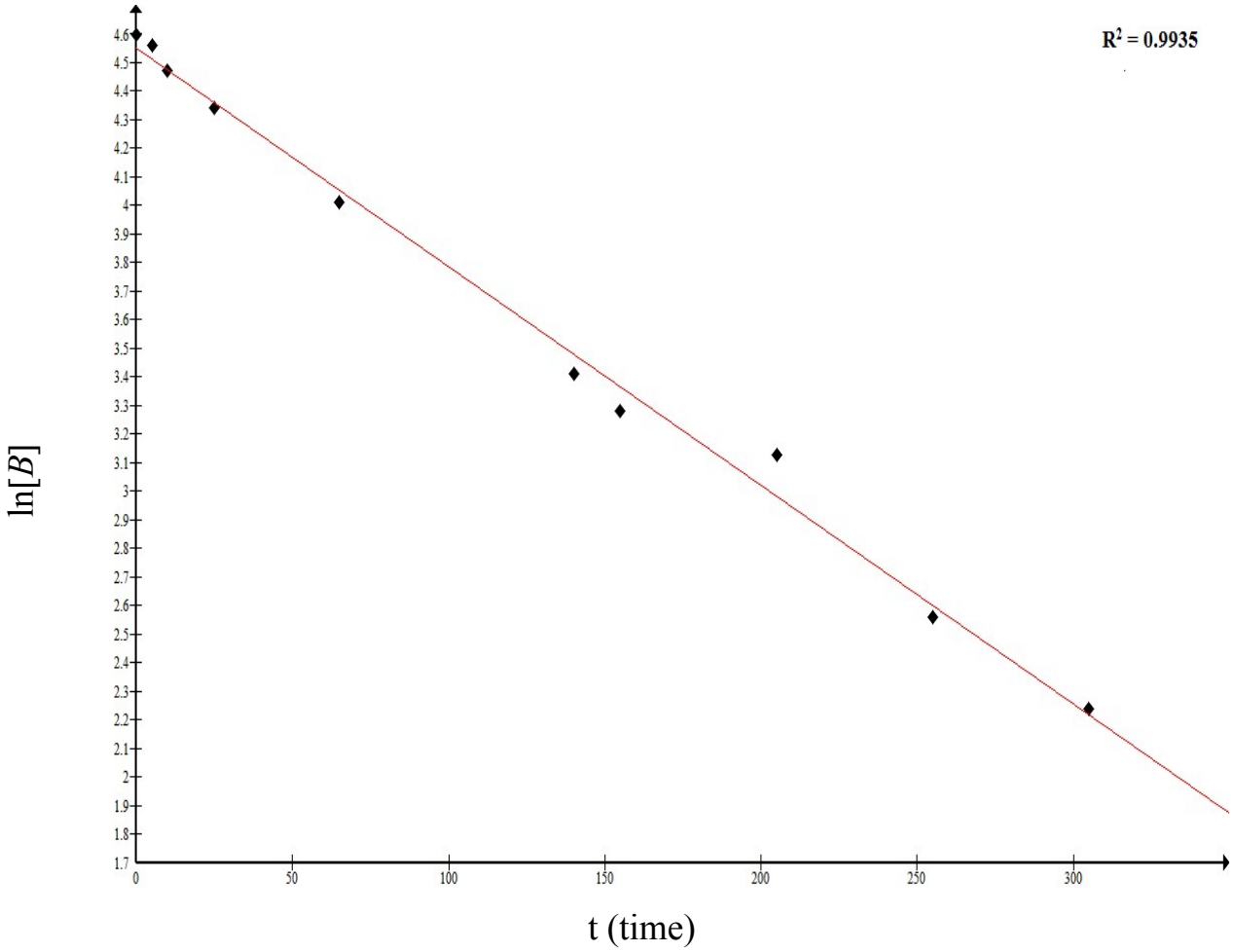
1295				
1300				
1305				
1310				
1315				
1320				
1325				
1330				
1335				
1340				
1345				
1350				
1355				
1360				
1365				
1370				
1375				
1380			96.766	3.110

Figure S4. The ln[*B*] plot against time (t) of the straight line fitted through the ten points for the configurational isomerization (*E*)-**9a** ⇌ (*Z*)-**9a** (**B** ⇌ **C**) determined at 298 K



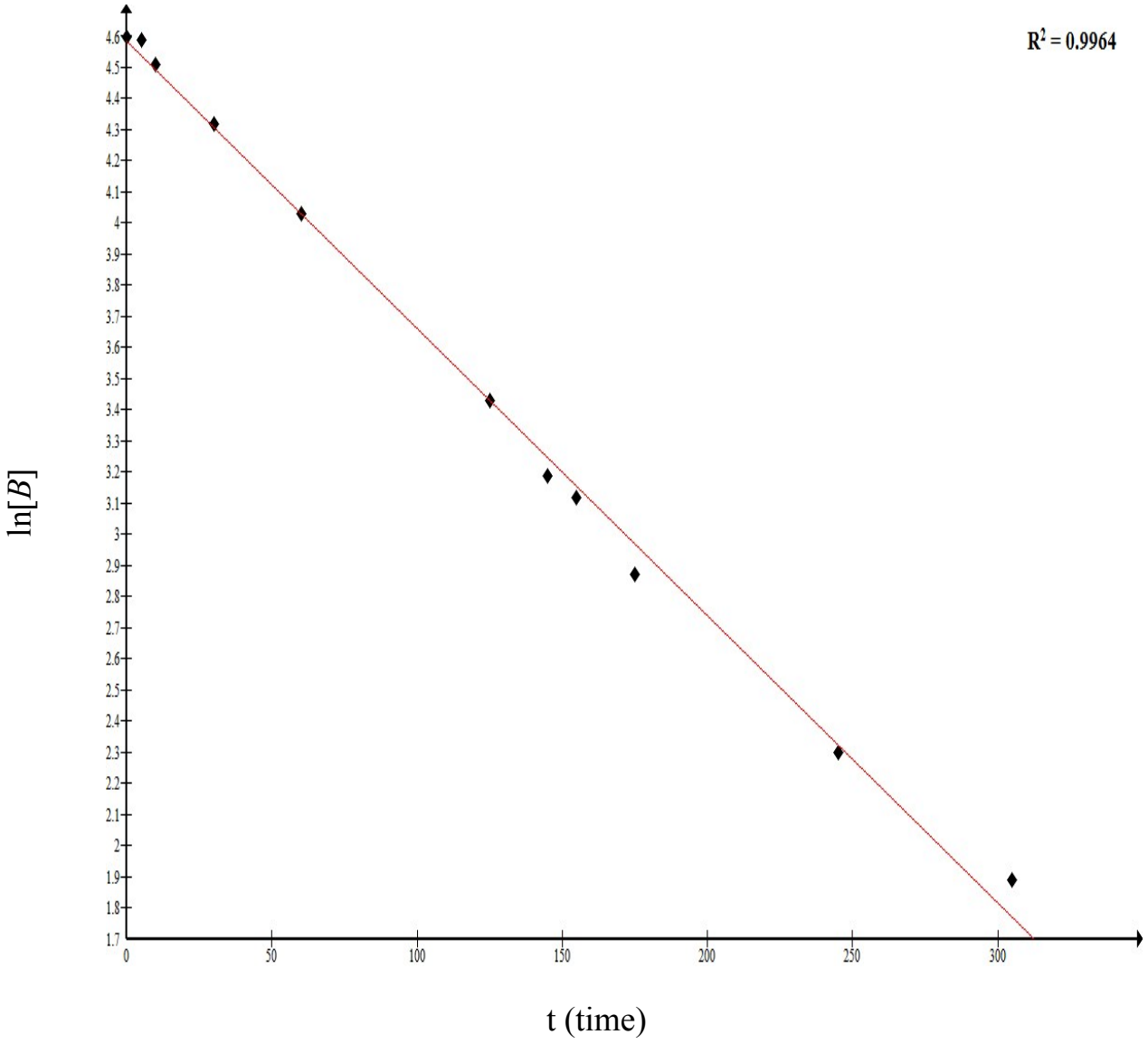
The plot of ln[*B*] versus t (time) determined for the configutational izomerization (*E*)-**9a** ⇌ (*Z*)-**9a** is in the great agreement with equation of the first order kinetics: ln[*B*] = ln[B_0]–*kt*. This plot yields a straight line of slope –*k* = –0.00435 min^{-1}, *k* = $7.26 \cdot 10^{-5}$ s^{-1}, where *k* is the overall rate constant.

Figure S5. The ln[*B*] plot against time (t) of the straight line fitted through the ten points for the configurational isomerization (*E*)-**9a** ⇌ (*Z*)-**9a** (**B** ⇌ **C**) determined at 303 K



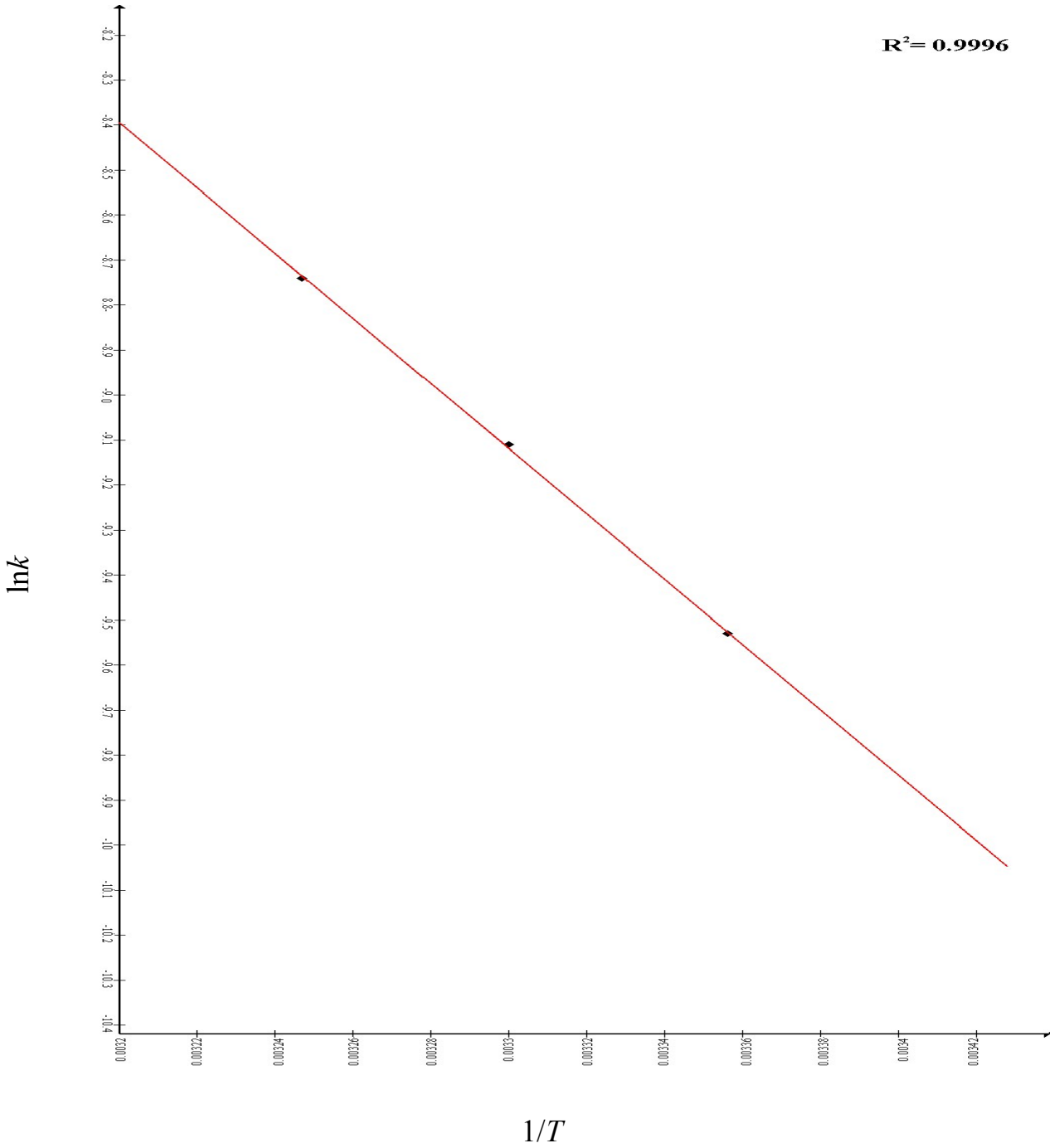
The plot of ln[*B*] versus t (time) determined for the configutational izomerization (*E*)-**9a** ⇌ (*Z*)-**9a** is in the great agreement with equation of the first order kinetics: ln[*B*] = ln[B_0]–*kt*. This plot yields a straight line of slope $-k = -0.00666$ min^{-1}, $k = 1.11 \cdot 10^{-4}$ s^{-1}, where *k* is the overall rate constant.

Figure S6. The ln[*B*] plot against time (t) of the straight line fitted through the ten points for the configurational isomerization (*E*)-**9a** ⇌ (*Z*)-**9a** (**B** ⇌ **C**) determined at 308 K



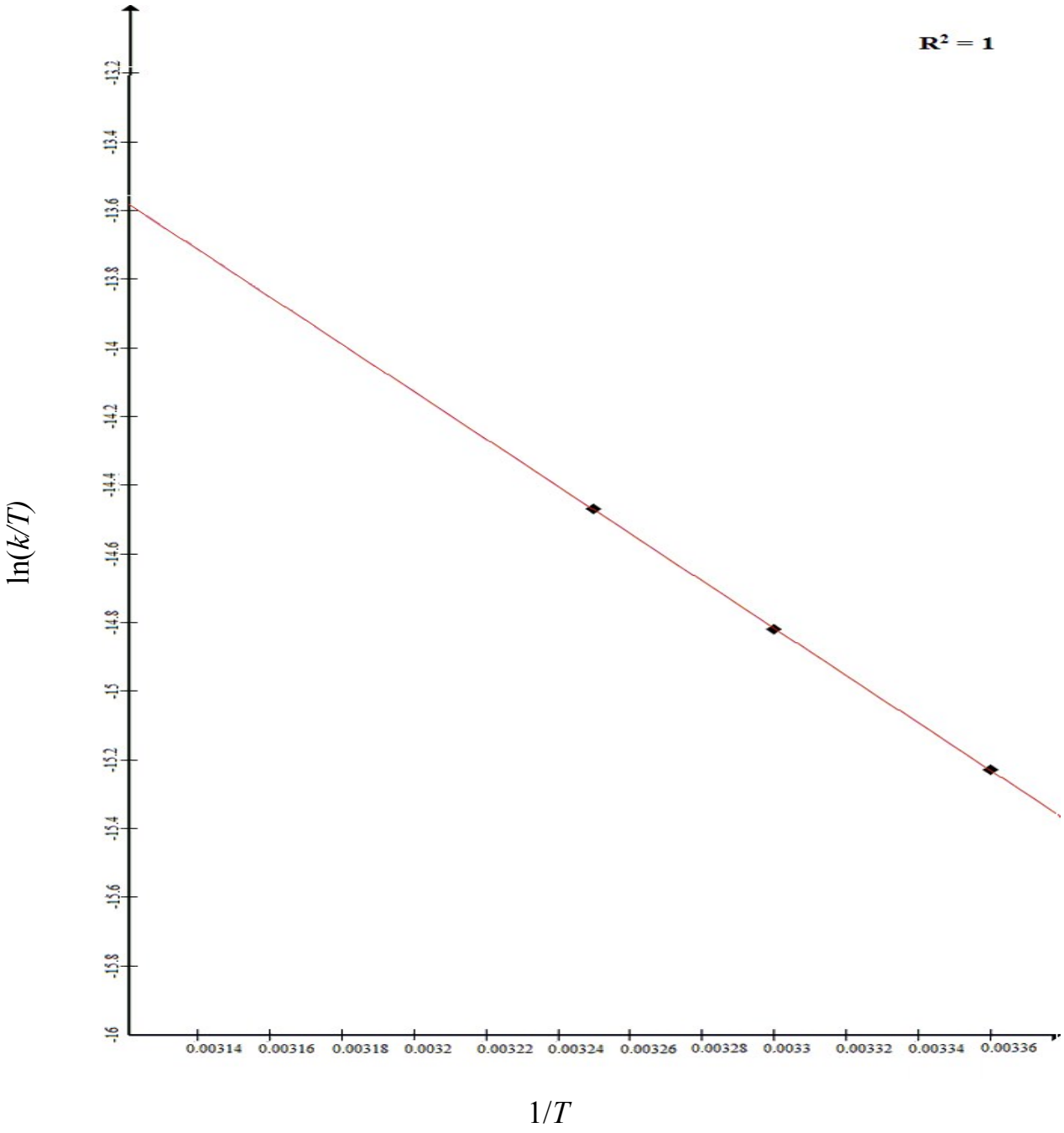
The plot of ln[*B*] versus t (time) determined for the configutational izomerization (*E*)-**9a** ⇌ (*Z*)-**9a** is in the great agreement with equation of the first order kinetics: ln[*B*] = ln[B_0]–*kt*. This plot yields a straight line of slope –*k* = –0.0096 min^{-1}, *k* = $1.60 \cdot 10^{-4}$ s^{-1}, where *k* is the overall rate constant.

Figure S7. The Arrhenius plot of the configurational isomerization (*E*)-**9a** ⇌ (*Z*)-**9a**



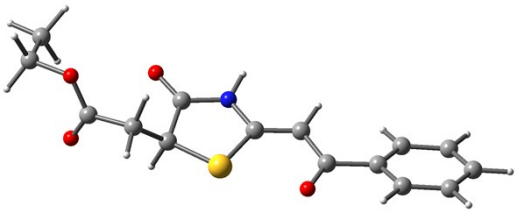
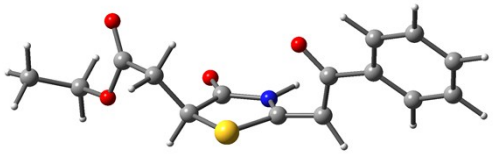
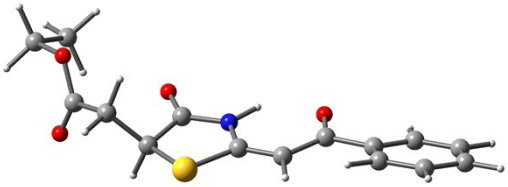
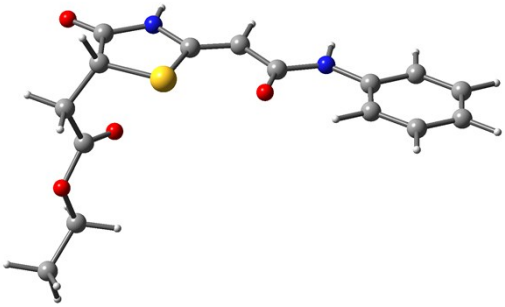
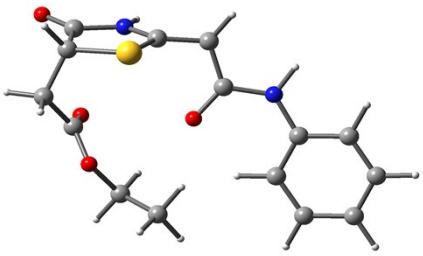
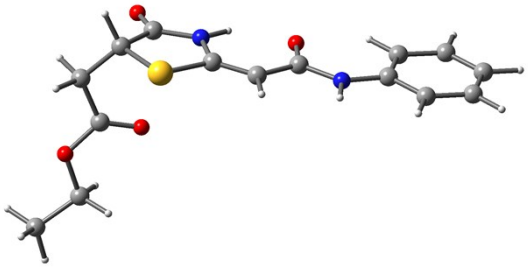
From the slope of this line equal to −7253.21, $-7253.21 = -E_A/R$, E_A = 60.3 kJmol^{-1} and from its interception of y axis equal to 14.80, lnA = 14.80.

Figure S8. The Eyring plot of the configurational isomerization (*E*)-**9a** ⇌ (*Z*)-**9a**

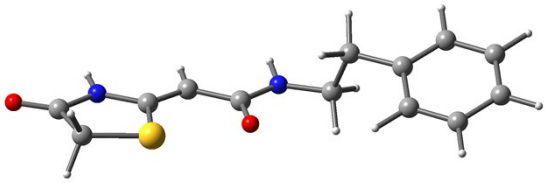


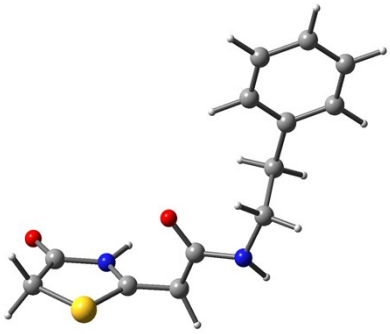
From the slope of this line equal to –6907.03, –6907.03 = $-\Delta H^{\ddagger}/R$, $\Delta H^{\ddagger}$ = 57.4 kJmol^{-1} and from its interception of y axis equal to 7.98, $\Delta S^{\ddagger}$ = –131.2 J/mol K. From the equation $\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger}$, $\Delta G^{\ddagger}$ = 96.5 kJmol^{-1}.

Figure S9. Depiction of the ground and transition structures (for restricted rotation about the partial C=C double bond) in compounds **1b**, **1d**, **1e**, **1g**, **7**, **8a**, **9a** and **9c**.

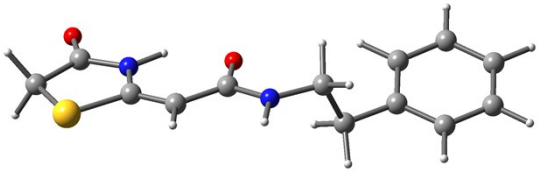
Compd.	ground state	transition state
(*Z*)-**1b**		
(*E*)-**1b**		
(*Z*)-**1d**		
(*E*)-**1d**		

(*Z*)-**1e**

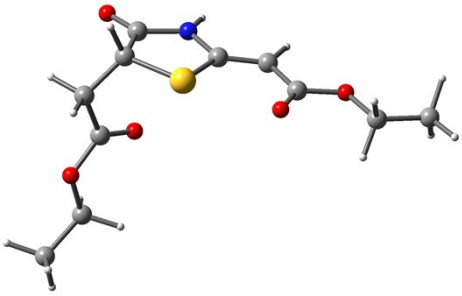


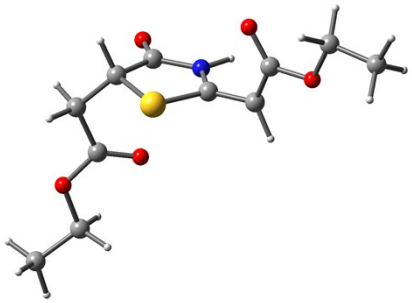


(*E*)-**1e**

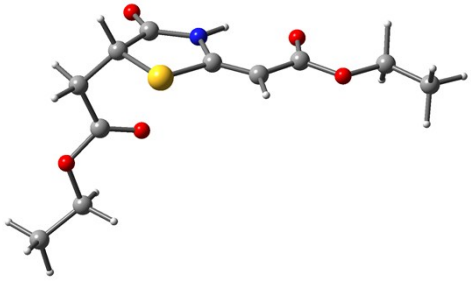


(*Z*)-**1g**



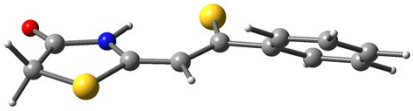


(*E*)-**1g**



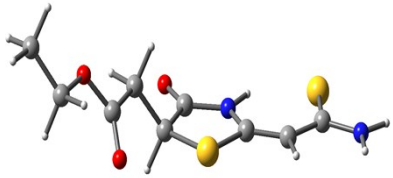
(*Z*)-**8a**

(*E*)-**8a**

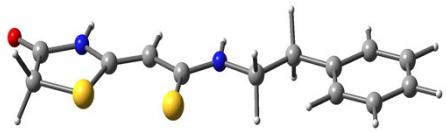


(*Z*)-**9a**

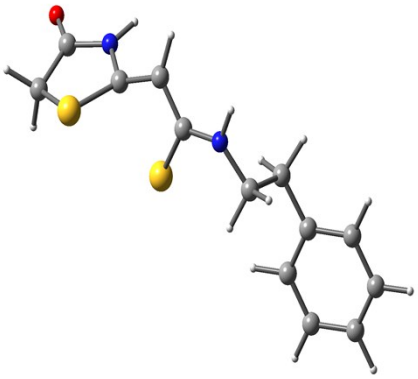
(*E*)-**9a**

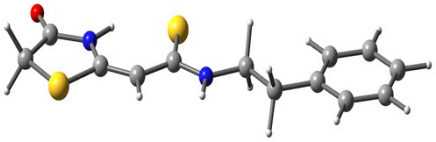


(*Z*)-**9c**



(*E*)-**9c**





Coordinates x,y,z (Å) and computed total energies (E_h) for the ground states (GS) and transition states (TS) of compounds 1b, 1d, 1e, 1g, 7, 8a, 9a and 9c

1b-*Z*

E = -1334.35766481

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.577049	1.831356	-0.476851
2	6	0	2.024269	0.725253	-0.383643
3	6	0	1.486771	-0.671321	-0.064785
4	7	0	0.110888	-0.680677	-0.048911
5	6	0	-0.554955	0.501384	-0.230010
6	6	0	3.048102	1.160120	0.664425
7	1	0	2.499947	0.677472	-1.363405
8	8	0	2.188267	-1.621283	0.149658
9	1	0	-0.443761	-1.520473	0.117230
10	6	0	-1.900110	0.655857	-0.218063
11	6	0	4.262961	0.250934	0.691249
12	1	0	2.613860	1.161593	1.663847
13	1	0	3.394970	2.171983	0.438736
14	8	0	4.790483	-0.137004	1.693119
15	8	0	4.686283	-0.024026	-0.549007
16	1	0	7.168537	0.054775	0.614594
17	6	0	5.763488	-0.974081	-0.651176
18	1	0	5.578319	-1.776922	0.063142
19	1	0	5.683374	-1.365453	-1.663934
20	6	0	7.105422	-0.310625	-0.410088
21	1	0	7.246903	0.523560	-1.099324
22	1	0	7.908927	-1.031825	-0.571570
23	6	0	-2.790135	-0.480803	-0.008094
24	1	0	-2.300140	1.641088	-0.401333
25	6	0	-7.039196	0.079433	0.085848
26	6	0	-6.486525	-1.181457	-0.123146
27	6	0	-5.108966	-1.339327	-0.146998
28	6	0	-4.269391	-0.236316	0.021933
29	6	0	-4.828986	1.024051	0.236576
30	6	0	-6.209755	1.179235	0.272603
31	1	0	-8.115380	0.203232	0.108446
32	1	0	-7.131746	-2.040080	-0.264072
33	1	0	-4.655390	-2.311498	-0.294238
34	1	0	-4.197358	1.887184	0.405032
35	1	0	-6.637285	2.158596	0.449554
36	8	0	-2.370126	-1.625715	0.124917

1b-*E*

E = -1334.36320592

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.233189	-1.050233	-0.340194
2	6	0	-1.900112	-0.292785	-0.310186
3	6	0	-1.729320	1.171272	0.063287
4	7	0	-0.391804	1.491001	0.140458

5	6	0	0.548242	0.493455	-0.025170
6	6	0	-2.849061	-0.990510	0.664664
7	1	0	-2.323658	-0.325525	-1.314988
8	8	0	-2.627326	1.942101	0.272022
9	1	0	-0.123283	2.434432	0.385320
10	6	0	1.880238	0.708091	0.057566
11	6	0	-4.241896	-0.390456	0.646896
12	1	0	-2.477062	-0.932399	1.687327
13	1	0	-2.935925	-2.045935	0.392626
14	8	0	-4.892583	-0.167861	1.627034
15	8	0	-4.660354	-0.177941	-0.607858
16	1	0	-7.099419	-0.894937	0.420500
17	6	0	-5.929629	0.486623	-0.744775
18	1	0	-5.978969	1.284578	-0.003136
19	1	0	-5.901308	0.921067	-1.742716
20	6	0	-7.079864	-0.489431	-0.590769
21	1	0	-6.981799	-1.308477	-1.305204
22	1	0	-8.026452	0.021062	-0.778533
23	6	0	2.817819	-0.397034	-0.103433
24	1	0	2.229125	1.706675	0.281124
25	6	0	7.050963	0.260698	0.062484
26	6	0	6.515826	-1.014439	0.225513
27	6	0	5.143285	-1.203102	0.165513
28	6	0	4.290501	-0.117513	-0.043227
29	6	0	4.832465	1.157054	-0.211194
30	6	0	6.209147	1.343917	-0.162510
31	1	0	8.123432	0.408907	0.105777
32	1	0	7.171023	-1.859959	0.396674
33	1	0	4.702707	-2.186189	0.276123
34	1	0	4.191328	2.007448	-0.408084
35	1	0	6.624298	2.334440	-0.303536
36	8	0	2.421262	-1.540489	-0.265865

1b-TS

E = -1334.28799723

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.322966	-0.838042	1.575952
2	6	0	-1.919087	-0.682636	0.707523
3	6	0	-1.659764	-1.133229	-0.723957
4	7	0	-0.279662	-1.360883	-0.906674
5	6	0	0.540111	-1.215551	0.134868
6	6	0	-2.403306	0.775356	0.690848
7	1	0	-2.670731	-1.331389	1.155769
8	8	0	-2.470786	-1.229048	-1.591628
9	1	0	0.113839	-1.527959	-1.827445
10	6	0	1.963080	-1.248561	0.055248
11	6	0	-3.721042	0.917637	-0.049654
12	1	0	-1.663891	1.421307	0.215205
13	1	0	-2.550832	1.115498	1.718540
14	8	0	-3.951751	1.767358	-0.858797
15	8	0	-4.589881	-0.023403	0.341399
16	1	0	-6.417808	1.996581	0.020967
17	6	0	-5.852584	-0.047162	-0.354660
18	1	0	-5.659509	0.112070	-1.416009
19	1	0	-6.225361	-1.058375	-0.201415
20	6	0	-6.803711	0.993637	0.201939

21	1	0	-6.942072	0.848505	1.274513
22	1	0	-7.775602	0.903465	-0.286749
23	6	0	2.491057	0.057375	-0.091569
24	1	0	2.505990	-2.151070	0.283733
25	6	0	6.743938	0.700975	-0.111274
26	6	0	5.853638	1.765424	-0.010699
27	6	0	4.484630	1.530731	-0.012730
28	6	0	3.990180	0.230422	-0.104191
29	6	0	4.887340	-0.831324	-0.213760
30	6	0	6.257417	-0.598128	-0.217572
31	1	0	7.812409	0.882195	-0.113061
32	1	0	6.227923	2.779599	0.066515
33	1	0	3.766833	2.339007	0.052191
34	1	0	4.520965	-1.845675	-0.318595
35	1	0	6.946383	-1.429700	-0.308569
36	8	0	1.765565	1.058970	-0.214256

1d-*z*

E = -1389.72598030

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.959843	-0.815041	1.320803
2	6	0	2.653634	-1.461436	1.078747
3	6	0	2.672326	-2.223917	-0.240319
4	7	0	1.411472	-2.261632	-0.786850
5	6	0	0.406157	-1.523628	-0.196402
6	1	0	2.865370	-2.186034	1.867079
7	8	0	3.647719	-2.736918	-0.717174
8	1	0	1.293405	-2.667882	-1.704394
9	6	0	-0.829042	-1.402229	-0.720178
10	6	0	-1.857249	-0.616586	-0.033595
11	1	0	-1.048564	-1.895097	-1.659755
12	6	0	-6.669258	1.360210	0.271361
13	6	0	-5.593219	1.439498	1.146459
14	6	0	-4.379069	0.823862	0.863272
15	6	0	-4.238935	0.108461	-0.329987
16	6	0	-5.321689	0.027348	-1.213161
17	6	0	-6.524329	0.647485	-0.914286
18	1	0	-7.607604	1.845851	0.507807
19	1	0	-5.691739	1.991329	2.073877
20	1	0	-3.548321	0.890585	1.547195
21	1	0	-5.214953	-0.527352	-2.140134
22	1	0	-7.349817	0.572233	-1.611948
23	8	0	-1.657425	-0.074801	1.040559
24	7	0	-3.056423	-0.550424	-0.706615
25	1	0	-3.096846	-1.028362	-1.593176
26	6	0	3.729833	-0.382479	1.090263
27	6	0	3.549215	0.608048	-0.038265
28	8	0	2.888600	0.407944	-1.021258
29	8	0	4.244582	1.724696	0.180370
30	6	0	4.175166	2.716337	-0.861591
31	6	0	5.018067	3.889054	-0.417241
32	1	0	4.703356	-0.862645	0.946630
33	1	0	3.760059	0.149603	2.041334
34	1	0	3.129021	2.990264	-1.009748
35	1	0	4.540370	2.271477	-1.789318
36	1	0	6.052483	3.580034	-0.262538

37	1	0	4.635208	4.302871	0.516294
38	1	0	4.998285	4.670631	-1.178254

1d-*E*

E = -1389.73152585

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.610770	1.170924	-0.754417
2	6	0	6.920645	1.081094	0.598551
3	6	0	5.947368	0.639509	1.485885
4	6	0	4.674322	0.286756	1.051645
5	6	0	4.368400	0.378836	-0.309309
6	6	0	5.347426	0.823434	-1.205211
7	7	0	3.113732	0.047624	-0.851046
8	6	0	1.990519	-0.411519	-0.207747
9	8	0	1.948875	-0.602693	1.001671
10	6	0	0.852060	-0.649962	-1.101630
11	6	0	-0.327645	-1.094064	-0.622076
12	16	0	-1.730521	-1.417452	-1.647387
13	6	0	-2.766569	-1.865414	-0.216322
14	6	0	-1.887583	-1.711112	1.030510
15	7	0	-0.601462	-1.378734	0.689156
16	6	0	-4.044067	-1.048788	-0.077750
17	6	0	-3.762810	0.422695	0.129128
18	8	0	-4.870916	1.150453	-0.023011
19	6	0	-4.723524	2.564026	0.210472
20	6	0	-6.081404	3.193816	0.003978
21	8	0	-2.297282	-1.888379	2.144283
22	8	0	-2.691076	0.878880	0.418260
23	1	0	-3.022648	-2.923062	-0.293856
24	1	0	0.123848	-1.190792	1.379620
25	1	0	0.942534	-0.461762	-2.162867
26	1	0	7.906849	1.351748	0.954033
27	1	0	6.174649	0.564991	2.542769
28	1	0	3.924723	-0.054513	1.746918
29	1	0	5.111681	0.895431	-2.262347
30	1	0	7.353982	1.512813	-1.464687
31	1	0	3.034705	0.168287	-1.848775
32	1	0	-4.578129	-1.404136	0.809387
33	1	0	-4.707205	-1.177472	-0.933710
34	1	0	-3.975813	2.954007	-0.482696
35	1	0	-4.348275	2.711028	1.224964
36	1	0	-6.807494	2.774143	0.701122
37	1	0	-6.434222	3.018473	-1.013010
38	1	0	-6.021006	4.270337	0.170691

1d-TS

E = -1389.65189800

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.888299	-1.324254	0.225106
2	6	0	-7.309076	-0.129243	-0.348559
3	6	0	-6.352733	0.818942	-0.694148

4	6	0	-4.996991	0.600403	-0.481527
5	6	0	-4.574851	-0.603410	0.099673
6	6	0	-5.540598	-1.559133	0.447564
7	7	0	-3.239021	-0.920121	0.348322
8	6	0	-2.107703	-0.112064	0.208080
9	8	0	-2.174084	1.029470	-0.257549
10	6	0	-0.889514	-0.699830	0.657538
11	6	0	0.251779	0.099903	0.362730
12	16	0	1.021176	0.146060	-1.182549
13	6	0	2.199031	1.448284	-0.685138
14	6	0	1.934257	1.702956	0.795539
15	7	0	0.823561	0.945381	1.216113
16	6	0	3.667018	1.127359	-0.932902
17	6	0	4.113738	-0.063245	-0.111633
18	8	0	5.303988	-0.504384	-0.499766
19	6	0	5.842187	-1.610479	0.256655
20	6	0	7.182996	-1.952566	-0.348211
21	8	0	2.545780	2.449605	1.493014
22	8	0	3.473614	-0.529808	0.792959
23	1	0	1.920887	2.362326	-1.215493
24	1	0	0.453597	1.015618	2.158352
25	1	0	-0.746864	-1.733724	0.936235
26	1	0	-8.361564	0.058409	-0.521317
27	1	0	-6.662847	1.755954	-1.143013
28	1	0	-4.258996	1.339025	-0.751066
29	1	0	-5.222927	-2.494315	0.898118
30	1	0	-7.612215	-2.081144	0.504373
31	1	0	-3.082186	-1.821668	0.770546
32	1	0	4.270017	1.986069	-0.621710
33	1	0	3.873020	0.948971	-1.988623
34	1	0	5.137018	-2.441664	0.200204
35	1	0	5.921341	-1.304353	1.301510
36	1	0	7.858945	-1.099120	-0.290794
37	1	0	7.069757	-2.237995	-1.394536
38	1	0	7.630580	-2.786961	0.193082

1e-*Z*

E = -1161.86142401

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.955763	1.337974	-0.059239
2	6	0	4.755273	1.450522	0.216502
3	6	0	5.324951	0.045563	0.268014
4	7	0	4.309757	-0.872003	0.100909
5	6	0	3.012975	-0.427178	-0.077787
6	1	0	4.975600	1.949522	1.159651
7	8	0	6.479286	-0.240660	0.430195
8	1	0	4.533360	-1.857330	0.113545
9	6	0	1.962189	-1.251630	-0.241451
10	6	0	0.611688	-0.710543	-0.426255
11	1	0	2.126552	-2.322808	-0.241064
12	6	0	-6.256718	0.973560	-0.070997
13	6	0	-5.102028	1.717859	-0.294909
14	6	0	-3.854278	1.158439	-0.050963
15	6	0	-3.739929	-0.150945	0.421484
16	6	0	-4.902464	-0.888418	0.638927
17	6	0	-6.154197	-0.331169	0.396670

18	1	0	-7.230490	1.410147	-0.257725
19	1	0	-5.174949	2.736811	-0.656429
20	1	0	-2.951271	1.737230	-0.221228
21	1	0	-4.826187	-1.905893	1.009283
22	1	0	-7.049017	-0.915446	0.576460
23	8	0	0.384051	0.492151	-0.454496
24	1	0	5.240379	1.993412	-0.593907
25	7	0	-0.384427	-1.629155	-0.578177
26	6	0	-1.762686	-1.193429	-0.707678
27	6	0	-2.374615	-0.751552	0.630608
28	1	0	-0.178771	-2.605899	-0.451530
29	1	0	-2.346718	-2.004923	-1.146114
30	1	0	-1.781648	-0.351778	-1.402540
31	1	0	-1.703171	-0.012668	1.073960
32	1	0	-2.430865	-1.608240	1.307760

1e-*E*

E = -1161.86836355

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.146608	-0.295263	0.340682
2	6	0	-6.243020	1.013161	-0.118137
3	6	0	-5.086037	1.761385	-0.314558
4	6	0	-3.841840	1.202038	-0.052311
5	6	0	-3.733654	-0.110753	0.411410
6	6	0	-4.898608	-0.852155	0.601503
7	6	0	-2.372315	-0.713673	0.639678
8	6	0	-1.749258	-1.166903	-0.689163
9	7	0	-0.381117	-1.628613	-0.537396
10	6	0	0.635474	-0.738307	-0.389381
11	8	0	0.423037	0.473841	-0.425045
12	6	0	1.970012	-1.321454	-0.199013
13	6	0	3.053755	-0.535796	-0.047670
14	16	0	4.693630	-1.158083	0.188276
15	6	0	5.388390	0.517125	0.279395
16	6	0	4.237576	1.506910	0.111845
17	7	0	3.048407	0.836082	-0.053493
18	8	0	4.367138	2.698731	0.124401
19	1	0	6.112055	0.684595	-0.516618
20	1	0	2.151458	1.304391	-0.187224
21	1	0	2.094708	-2.395794	-0.183345
22	1	0	-7.214026	1.449489	-0.319165
23	1	0	-5.154269	2.783186	-0.668768
24	1	0	-2.937541	1.784491	-0.201530
25	1	0	-4.827184	-1.872435	0.965055
26	1	0	-7.043402	-0.882628	0.499138
27	1	0	5.862761	0.692356	1.243552
28	1	0	-0.192784	-2.611751	-0.435425
29	1	0	-2.340239	-1.969783	-1.133857
30	1	0	-1.743781	-0.326517	-1.385712
31	1	0	-1.702837	0.025090	1.086051
32	1	0	-2.438627	-1.566100	1.321122

1e-TS

E = -1161.78363142

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.992523	0.174723	0.383834
2	6	0	-5.929143	1.287074	-0.446666
3	6	0	-4.688927	1.774536	-0.850307
4	6	0	-3.523052	1.152363	-0.423612
5	6	0	-3.574771	0.035698	0.415019
6	6	0	-4.821664	-0.446079	0.809246
7	6	0	-2.293778	-0.643483	0.819606
8	6	0	-1.723278	-1.485730	-0.334924
9	7	0	-0.384505	-1.981489	-0.083720
10	6	0	0.660827	-1.066260	-0.087076
11	8	0	0.491609	0.070767	-0.545733
12	6	0	1.906457	-1.511966	0.464770
13	6	0	2.967223	-0.600959	0.207004
14	16	0	3.757575	-0.420403	-1.321737
15	6	0	4.796752	0.953243	-0.746292
16	6	0	4.460816	1.173139	0.718416
17	7	0	3.453237	0.262087	1.102542
18	8	0	4.946823	1.975998	1.450480
19	1	0	4.570092	1.865580	-1.298922
20	1	0	3.042036	0.279431	2.030247
21	1	0	2.153591	-2.555868	0.606346
22	1	0	-6.839490	1.773003	-0.777007
23	1	0	-4.631824	2.642567	-1.496796
24	1	0	-2.552077	1.526383	-0.735307
25	1	0	-4.875139	-1.312681	1.460652
26	1	0	-6.954128	-0.209910	0.703438
27	1	0	5.857874	0.725470	-0.844000
28	1	0	-0.294571	-2.751622	0.561186
29	1	0	-2.379798	-2.333260	-0.546751
30	1	0	-1.677903	-0.866899	-1.231427
31	1	0	-1.541949	0.106552	1.076548
32	1	0	-2.456127	-1.278408	1.695746

1g-*Z*

E = -1257.19103270

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.134093	-0.722069	1.304071
2	6	0	1.381528	-1.668236	0.917278
3	6	0	1.206505	-2.269049	-0.473119
4	7	0	-0.051389	-1.997316	-0.955396
5	6	0	-0.869757	-1.146647	-0.242364
6	1	0	1.457202	-2.503422	1.615882
7	8	0	2.045209	-2.908953	-1.046419
8	1	0	-0.281962	-2.272991	-1.899878
9	6	0	-2.073981	-0.733826	-0.681760
10	6	0	-2.894842	0.154586	0.127406
11	1	0	-2.447696	-1.053875	-1.644594
12	8	0	-2.600522	0.572034	1.224313
13	8	0	-4.047485	0.468091	-0.490362

14	6	0	2.659018	-0.840959	0.987853
15	6	0	2.661468	0.283310	-0.023719
16	8	0	1.942926	0.337162	-0.984473
17	8	0	3.588593	1.196284	0.268949
18	6	0	3.704454	2.287874	-0.663139
19	6	0	4.797749	3.196472	-0.150949
20	1	0	3.505955	-1.492597	0.749237
21	1	0	2.824946	-0.434643	1.985836
22	1	0	2.739506	2.794336	-0.725018
23	1	0	3.932944	1.879609	-1.649550
24	1	0	5.743818	2.657786	-0.086108
25	1	0	4.545611	3.577066	0.839472
26	1	0	4.924929	4.043246	-0.827103
27	6	0	-4.919653	1.340480	0.240580
28	6	0	-6.144892	1.564626	-0.616486
29	1	0	-4.390822	2.271996	0.453568
30	1	0	-5.166373	0.874188	1.196885
31	1	0	-6.646179	0.617648	-0.820612
32	1	0	-5.866996	2.021166	-1.567299
33	1	0	-6.845033	2.226078	-0.103627

1g-*E*

E = -1257.19597171

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.404855	-1.131407	1.725042
2	6	0	1.463126	-1.883170	0.445349
3	6	0	0.696927	-1.780421	-0.878149
4	7	0	-0.554268	-1.251713	-0.682964
5	6	0	-0.874278	-0.774398	0.561107
6	1	0	1.570223	-2.946136	0.666679
7	8	0	1.149738	-2.146207	-1.927289
8	1	0	-1.195213	-1.068121	-1.452100
9	6	0	-2.016532	-0.136864	0.888932
10	6	0	-3.041070	0.115227	-0.115398
11	1	0	-2.185091	0.204026	1.899027
12	8	0	-2.983877	-0.205536	-1.286467
13	8	0	-4.095715	0.762137	0.401540
14	6	0	2.844466	-1.255670	0.317973
15	6	0	2.775188	0.201550	-0.080577
16	8	0	1.799051	0.742451	-0.522224
17	8	0	3.952222	0.805095	0.094206
18	6	0	4.009464	2.186307	-0.310077
19	6	0	5.414408	2.671877	-0.038943
20	1	0	3.384154	-1.782863	-0.475388
21	1	0	3.425859	-1.357028	1.234781
22	1	0	3.261254	2.744638	0.255617
23	1	0	3.745807	2.249592	-1.367526
24	1	0	6.137805	2.084993	-0.606065
25	1	0	5.651362	2.584951	1.022077
26	1	0	5.509103	3.718504	-0.332114
27	6	0	-5.155949	1.057559	-0.519363
28	6	0	-6.231348	1.780361	0.259452
29	1	0	-5.518426	0.122624	-0.951790
30	1	0	-4.756719	1.666525	-1.333120
31	1	0	-5.837680	2.703126	0.687349
32	1	0	-6.602174	1.152809	1.070793

33	1	0	-7.065829	2.029191	-0.398108

1g-*TS*

E = -1257.11630176

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.039526	0.042468	1.265581
2	6	0	-1.119723	1.392555	0.861462
3	6	0	-0.795112	1.801932	-0.572074
4	7	0	0.329200	1.087303	-1.027466
5	6	0	0.867173	0.150086	-0.249134
6	1	0	-0.869144	2.245419	1.496776
7	8	0	-1.377737	2.622480	-1.209151
8	1	0	0.727480	1.247574	-1.946730
9	6	0	2.007278	-0.628661	-0.585796
10	6	0	3.220393	-0.119334	-0.064326
11	1	0	1.889114	-1.621867	-0.990170
12	8	0	3.356914	0.949820	0.520972
13	8	0	4.282891	-0.946042	-0.293343
14	6	0	-2.595781	1.047587	1.011665
15	6	0	-3.002032	-0.051741	0.053499
16	8	0	-2.327145	-0.414308	-0.872983
17	8	0	-4.200117	-0.540492	0.350757
18	6	0	-4.698379	-1.565060	-0.536472
19	6	0	-6.058990	-1.974086	-0.024041
20	1	0	-3.188263	1.933978	0.764671
21	1	0	-2.845417	0.761174	2.033570
22	1	0	-3.987820	-2.393366	-0.538109
23	1	0	-4.740135	-1.154193	-1.546725
24	1	0	-6.738951	-1.121588	-0.019372
25	1	0	-5.984358	-2.366621	0.990599
26	1	0	-6.478098	-2.749573	-0.666684
27	6	0	5.537569	-0.456314	0.172042
28	6	0	6.578394	-1.495319	-0.187655
29	1	0	5.488875	-0.290061	1.251097
30	1	0	5.750925	0.508317	-0.295331
31	1	0	6.606344	-1.646902	-1.267812
32	1	0	6.342122	-2.449452	0.286025
33	1	0	7.567321	-1.174981	0.146108

7-(2*Z*,5*Z*)

E = -1255.96344354

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.073480	-0.116402	-0.002265
2	6	0	1.208862	1.081096	-0.000460
3	6	0	0.673498	2.483293	0.000225
4	7	0	-0.702098	2.416888	-0.000087
5	6	0	-1.297812	1.171776	-0.000843
6	6	0	2.528162	0.872068	0.000514
7	8	0	1.321324	3.494257	0.001032
8	1	0	-1.246188	3.268227	0.000837
9	6	0	-2.630078	0.989119	-0.000338

10	6	0	-3.207228	-0.353167	-0.000826
11	1	0	-3.300685	1.838035	0.000930
12	8	0	-2.574024	-1.381724	-0.002741
13	6	0	3.079664	-0.493437	-0.000186
14	8	0	2.404424	-1.492834	-0.001820
15	8	0	4.415234	-0.492068	0.001082
16	6	0	5.035828	-1.789416	0.000139
17	6	0	6.530609	-1.568020	0.002470
18	1	0	3.196065	1.724760	0.001567
19	1	0	4.699011	-2.336002	-0.883110
20	1	0	4.696667	-2.338436	0.880944
21	1	0	6.832905	-1.009928	0.889308
22	1	0	6.835179	-1.006802	-0.881611
23	1	0	7.048811	-2.528139	0.001463
24	8	0	-4.548289	-0.311320	0.001201
25	6	0	-5.204337	-1.588817	0.000752
26	6	0	-6.692641	-1.324611	0.002973
27	1	0	-4.883320	-2.149035	0.881355
28	1	0	-4.885661	-2.147136	-0.881911
29	1	0	-6.980840	-0.754938	-0.881343
30	1	0	-6.978697	-0.757346	0.889532
31	1	0	-7.239409	-2.268827	0.002336

7-(2*E*,5*Z*)

E = -1255.96840173

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.209541	-0.743281	-0.006624
2	6	0	1.179955	0.710118	-0.002090
3	6	0	0.316639	1.945760	0.000313
4	7	0	-1.007166	1.560726	-0.000851
5	6	0	-1.280317	0.221387	-0.003321
6	6	0	2.510825	0.805958	-0.000268
7	8	0	0.721383	3.073948	0.002996
8	1	0	-1.786801	2.216666	0.000656
9	6	0	-2.507018	-0.345331	-0.003311
10	6	0	-3.708433	0.497391	-0.000771
11	1	0	-2.567018	-1.422413	-0.005414
12	8	0	-3.670872	1.707654	-0.000343
13	6	0	3.351313	-0.403603	-0.002259
14	8	0	2.909874	-1.527381	-0.007377
15	8	0	4.651825	-0.110107	0.002382
16	6	0	5.544651	-1.238591	0.000320
17	6	0	6.953123	-0.691819	0.010493
18	1	0	2.968054	1.787690	0.002857
19	1	0	5.340077	-1.841711	-0.886594
20	1	0	5.331347	-1.852042	0.878004
21	1	0	7.121112	-0.084937	0.900816
22	1	0	7.129473	-0.073246	-0.870112
23	1	0	7.670669	-1.513648	0.008430
24	8	0	-4.913103	-0.098390	0.001006
25	6	0	-5.045887	-1.521845	0.003352
26	6	0	-6.528406	-1.821737	0.007848
27	1	0	-4.562145	-1.936183	0.892929
28	1	0	-4.567079	-1.938765	-0.887684
29	1	0	-7.001303	-1.394362	-0.876544
30	1	0	-6.996540	-1.391284	0.893278

31	1	0	-6.693860	-2.900249	0.010170

7-TS

E = -1255.88053446

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.010423	-0.425709	-0.439872
2	6	0	1.133779	0.896456	-0.144188
3	6	0	0.394080	2.197248	-0.058425
4	7	0	-0.974462	1.926610	-0.273945
5	6	0	-1.350027	0.662467	-0.456019
6	6	0	2.458968	0.854171	-0.007520
7	8	0	0.846993	3.280645	0.145989
8	1	0	-1.684925	2.648307	-0.205857
9	6	0	-2.699770	0.232492	-0.604646
10	6	0	-3.236974	-0.185082	0.645570
11	1	0	-3.104361	0.086406	-1.593151
12	8	0	-2.637157	-0.070457	1.704803
13	6	0	3.193513	-0.432201	-0.097841
14	8	0	2.660363	-1.486475	-0.328178
15	8	0	4.495025	-0.264900	0.105762
16	6	0	5.295220	-1.464626	0.047811
17	6	0	6.726206	-1.058666	0.308702
18	1	0	3.007017	1.771266	0.176860
19	1	0	5.162643	-1.918199	-0.936244
20	1	0	4.917111	-2.164900	0.794919
21	1	0	6.820015	-0.595855	1.291523
22	1	0	7.067156	-0.348964	-0.445707
23	1	0	7.370746	-1.938096	0.275495
24	8	0	-4.492558	-0.718392	0.680307
25	6	0	-5.216212	-0.874501	-0.528051
26	6	0	-6.562774	-1.469183	-0.172633
27	1	0	-4.667924	-1.535860	-1.208896
28	1	0	-5.337897	0.098345	-1.018179
29	1	0	-7.097059	-0.806349	0.508906
30	1	0	-6.428739	-2.432607	0.320440
31	1	0	-7.166711	-1.613247	-1.070547

8a-*Z*

E = -1350.84298815

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.386879	1.242352	0.204949
2	6	0	-4.017131	0.414005	0.146692
3	6	0	-3.798456	-1.052281	-0.165246
4	7	0	-2.443365	-1.300804	-0.263824
5	6	0	-1.547611	-0.267733	-0.086761
6	1	0	-4.641196	0.855593	-0.629094
7	8	0	-4.652036	-1.883220	-0.302042
8	1	0	-2.129150	-2.241850	-0.458791
9	6	0	-0.202886	-0.480895	-0.148553
10	6	0	0.828333	0.499297	0.009224
11	1	0	0.103780	-1.498777	-0.364671

12	6	0	4.845641	-0.998608	-0.018921
13	6	0	4.546884	0.216939	-0.627709
14	6	0	3.248847	0.705713	-0.612848
15	6	0	2.222633	-0.026755	-0.009882
16	6	0	2.531224	-1.249460	0.595543
17	6	0	3.836129	-1.726101	0.600568
18	1	0	5.861833	-1.374146	-0.023462
19	1	0	5.329626	0.787566	-1.112701
20	1	0	3.011271	1.656371	-1.073543
21	1	0	1.754463	-1.811041	1.101484
22	1	0	4.064286	-2.664039	1.092344
23	16	0	0.544985	2.117484	0.203342
24	1	0	-4.526403	0.499610	1.106228

8a-*E*

E = -1350.84806139

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.567593	-1.868548	0.311122
2	6	0	4.073043	-0.875636	0.116345
3	6	0	3.644061	0.570336	-0.111388
4	7	0	2.261469	0.667085	-0.104729
5	6	0	1.529559	-0.459477	0.094548
6	1	0	4.653119	-1.209501	-0.742649
7	8	0	4.394356	1.487391	-0.271147
8	1	0	1.766095	1.557392	-0.218561
9	6	0	0.168153	-0.561335	0.134828
10	6	0	-0.778166	0.500726	-0.021526
11	1	0	-0.222730	-1.551283	0.333387
12	6	0	-4.893529	-0.700373	-0.005335
13	6	0	-4.506631	0.479125	0.624030
14	6	0	-3.176771	0.873161	0.613355
15	6	0	-2.207685	0.078111	-0.005053
16	6	0	-2.604440	-1.108671	-0.630391
17	6	0	-3.940488	-1.488468	-0.640140
18	1	0	-5.934301	-1.001173	-0.004391
19	1	0	-5.244800	1.096219	1.121746
20	1	0	-2.871121	1.795704	1.090451
21	1	0	-1.870843	-1.717322	-1.145966
22	1	0	-4.236685	-2.398867	-1.146998
23	16	0	-0.414945	2.114612	-0.211875
24	1	0	4.691123	-0.921892	1.011659

8a-TS

E = -1350.81397759

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.336072	1.578231	-0.285538
2	6	0	3.882108	0.708344	0.095480
3	6	0	3.636186	-0.778206	-0.139391
4	7	0	2.299697	-1.011491	-0.343627
5	6	0	1.366372	0.041819	-0.166936
6	1	0	4.183409	0.848767	1.134239

7	8	0	4.493027	-1.620614	-0.136573
8	1	0	1.974811	-1.968344	-0.378547
9	6	0	0.123297	0.032487	-1.010825
10	6	0	-0.814517	-0.051147	-0.065783
11	1	0	0.060052	0.116440	-2.087964
12	6	0	-5.069157	-0.083580	-0.129309
13	6	0	-4.383302	1.123046	-0.035646
14	6	0	-2.994353	1.135486	-0.012958
15	6	0	-2.285341	-0.064095	-0.088101
16	6	0	-2.975212	-1.273607	-0.176562
17	6	0	-4.364396	-1.280563	-0.199620
18	1	0	-6.152262	-0.091012	-0.146538
19	1	0	-4.930454	2.056302	0.019255
20	1	0	-2.450928	2.070175	0.062219
21	1	0	-2.417938	-2.201717	-0.228065
22	1	0	-4.896669	-2.221154	-0.272616
23	16	0	0.237408	-0.120023	1.381448
24	1	0	4.682095	1.044660	-0.560660

9a-*Z*

E = -1481.66666481

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.084970	2.533077	-0.434967
2	7	0	1.251833	2.231295	-0.317823
3	6	0	1.638591	0.913509	-0.144160
4	16	0	0.235108	-0.146357	-0.140047
5	6	0	-0.913115	1.261115	-0.411133
6	8	0	-0.526927	3.646589	-0.531208
7	6	0	2.945372	0.586516	-0.007605
8	6	0	3.486928	-0.740941	0.183602
9	16	0	2.580306	-2.137225	0.299792
10	7	0	4.832754	-0.784887	0.270069
11	1	0	5.277462	-1.678038	0.404694
12	1	0	5.402765	0.041412	0.195722
13	1	0	3.652526	1.410777	-0.047349
14	1	0	1.925912	2.984760	-0.316182
15	6	0	-2.004030	1.369767	0.647770
16	6	0	-2.972759	0.207130	0.690963
17	8	0	-2.649400	-0.748516	-0.191131
18	8	0	-3.910456	0.144374	1.432633
19	6	0	-3.474211	-1.928852	-0.180218
20	6	0	-2.876179	-2.896268	-1.175203
21	1	0	-3.485837	-2.330430	0.834522
22	1	0	-4.494612	-1.639542	-0.439126
23	1	0	-2.867463	-2.461798	-2.175644
24	1	0	-3.465371	-3.814206	-1.200342
25	1	0	-1.851689	-3.146531	-0.896446
26	1	0	-2.582321	2.281033	0.473866
27	1	0	-1.566170	1.456002	1.645737
28	1	0	-1.363446	1.139117	-1.397749

9a-*E*

E = -1481.67344929

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.360549	1.716668	-0.556554
2	7	0	1.507344	0.984668	-0.340748
3	6	0	1.388049	-0.341215	-0.038552
4	16	0	-0.308142	-0.837930	-0.014097
5	6	0	-0.884307	0.835216	-0.449428
6	8	0	0.322712	2.892897	-0.786294
7	6	0	2.389909	-1.217093	0.218942
8	6	0	3.807908	-0.929138	0.232276
9	16	0	4.529280	0.559608	-0.069025
10	7	0	4.583048	-1.991547	0.519510
11	1	0	4.194124	-2.901040	0.707467
12	1	0	5.582143	-1.868151	0.548290
13	1	0	2.088054	-2.235610	0.437307
14	1	0	2.444883	1.397207	-0.373453
15	6	0	-1.855394	1.435700	0.558805
16	6	0	-3.184591	0.722435	0.677118
17	8	0	-3.254889	-0.353261	-0.122344
18	8	0	-4.069691	1.072609	1.402660
19	6	0	-4.480969	-1.105581	-0.056450
20	6	0	-4.339122	-2.273530	-1.004639
21	1	0	-4.635111	-1.424203	0.976068
22	1	0	-5.306185	-0.445433	-0.329887
23	1	0	-4.171555	-1.922365	-2.023555
24	1	0	-5.248812	-2.875644	-0.990358
25	1	0	-3.499330	-2.905202	-0.712043
26	1	0	-2.057638	2.472369	0.276138
27	1	0	-1.411886	1.459735	1.557385
28	1	0	-1.346899	0.790905	-1.436036

9a-TS

E = -1481.61222280

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.328551	2.301484	-0.355869
2	7	0	1.590430	1.741688	-0.562825
3	6	0	1.689376	0.394140	-0.672062
4	16	0	0.095555	-0.298294	-0.970259
5	6	0	-0.736275	1.213553	-0.387830
6	8	0	0.133906	3.460188	-0.134059
7	6	0	2.929369	-0.246997	-1.025231
8	6	0	3.338555	-1.068776	-0.003023
9	16	0	2.391110	-0.898707	1.434557
10	7	0	4.423479	-1.879294	-0.044273
11	1	0	4.780859	-2.185423	-0.934372
12	1	0	4.588480	-2.473974	0.751118
13	1	0	3.500788	0.075360	-1.887256
14	1	0	2.421413	2.298182	-0.400587
15	6	0	-1.345825	1.062845	1.005850
16	6	0	-2.521394	0.110808	1.076853
17	8	0	-2.840301	-0.394494	-0.124406
18	8	0	-3.102345	-0.154186	2.088571
19	6	0	-3.927788	-1.338715	-0.136203
20	6	0	-4.089796	-1.815884	-1.560708
21	1	0	-3.684064	-2.152400	0.549035

22	1	0	-4.822795	-0.839629	0.239909
23	1	0	-4.316416	-0.979441	-2.223173
24	1	0	-4.907556	-2.535654	-1.619700
25	1	0	-3.176294	-2.299830	-1.908884
26	1	0	-1.691971	2.038907	1.357910
27	1	0	-0.596613	0.706825	1.718373
28	1	0	-1.498556	1.495512	-1.112966

9c-*Z*

E = -1484.80803152

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.803175	1.268141	0.005171
2	6	0	5.530103	0.666550	0.012084
3	6	0	5.511760	-0.847966	0.003843
4	7	0	4.206820	-1.291401	-0.002775
5	6	0	3.169628	-0.375109	-0.002515
6	1	0	6.053068	1.007875	0.904717
7	8	0	6.472604	-1.567217	0.003536
8	1	0	4.030704	-2.286491	-0.008358
9	6	0	1.879653	-0.780353	-0.007364
10	6	0	0.701962	0.064917	-0.007015
11	1	0	1.718061	-1.855392	-0.011070
12	6	0	-6.927629	0.362618	0.008163
13	6	0	-5.884338	1.277279	0.003083
14	6	0	-4.562001	0.838353	-0.001538
15	6	0	-4.266659	-0.523289	-0.001138
16	6	0	-5.326045	-1.434688	0.004004
17	6	0	-6.643315	-1.000559	0.008573
18	1	0	-7.955040	0.705721	0.011864
19	1	0	-6.093674	2.340333	0.002685
20	1	0	-3.766288	1.573819	-0.005327
21	1	0	-5.109102	-2.498485	0.004607
22	1	0	-7.449794	-1.724204	0.012646
23	16	0	0.740278	1.735693	-0.008222
24	1	0	6.063775	1.017777	-0.870259
25	7	0	-0.461868	-0.615219	-0.005873
26	6	0	-1.769166	0.014334	-0.003370
27	6	0	-2.849790	-1.055873	-0.006320
28	1	0	-0.428936	-1.624209	-0.001763
29	1	0	-1.852613	0.663365	-0.880554
30	1	0	-1.852678	0.658254	0.877707
31	1	0	-2.715181	-1.700376	0.870176
32	1	0	-2.718030	-1.692539	-0.888940

9c-*E*

E = -1484.81491294

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.652129	-0.851578	-0.004542
2	6	0	-6.897955	0.519086	-0.002931
3	6	0	-5.829408	1.404079	0.000358
4	6	0	-4.519961	0.928081	0.002155

5	6	0	-4.263154	-0.441354	0.000567
6	6	0	-5.347664	-1.322711	-0.002873
7	6	0	-2.861946	-1.014140	0.003083
8	6	0	-1.752624	0.026144	0.000808
9	7	0	-0.462179	-0.639689	0.000881
10	6	0	0.721421	-0.000715	0.001728
11	16	0	0.778858	1.681780	0.004127
12	6	0	1.867061	-0.892030	0.001424
13	6	0	3.172879	-0.537751	0.000054
14	16	0	4.461086	-1.753464	0.001187
15	6	0	5.756585	-0.484013	-0.000924
16	6	0	5.066967	0.877472	-0.003383
17	7	0	3.695536	0.723234	-0.002253
18	8	0	5.643385	1.926953	-0.005735
19	1	0	6.380013	-0.558539	0.888605
20	1	0	3.049988	1.518127	-0.002699
21	1	0	1.663776	-1.957803	0.002836
22	1	0	-7.915310	0.890945	-0.004474
23	1	0	-6.008684	2.472606	0.001725
24	1	0	-3.704198	1.641286	0.004751
25	1	0	-5.160824	-2.392189	-0.004363
26	1	0	-7.478654	-1.552228	-0.007190
27	1	0	6.380616	-0.561885	-0.889741
28	1	0	-0.458500	-1.649587	-0.002289
29	1	0	-1.818242	0.673164	-0.879246
30	1	0	-1.816718	0.675201	0.879382
31	1	0	-2.747120	-1.655444	0.884647
32	1	0	-2.746261	-1.660575	-0.874614

9c-TS

E = -1484.75647795

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.153023	0.021088	0.374919
2	6	0	-6.129669	-1.197871	-0.291993
3	6	0	-4.909160	-1.798758	-0.587193
4	6	0	-3.721141	-1.182534	-0.215809
5	6	0	-3.733789	0.040931	0.458092
6	6	0	-4.960846	0.635812	0.745290
7	6	0	-2.430998	0.710783	0.808716
8	6	0	-1.802621	1.365618	-0.431548
9	7	0	-0.469009	1.883856	-0.179952
10	6	0	0.634360	1.106883	-0.112458
11	16	0	0.669729	-0.541897	-0.657175
12	6	0	1.840928	1.504326	0.421617
13	6	0	2.841568	0.505762	0.164464
14	16	0	3.811905	0.431499	-1.314011
15	6	0	4.826043	-0.912453	-0.643004
16	6	0	4.599275	-0.930623	0.858432
17	7	0	3.510364	-0.110425	1.170039
18	8	0	5.214267	-1.563329	1.663435
19	1	0	5.881892	-0.756243	-0.853834
20	1	0	3.113801	-0.133325	2.101414
21	1	0	2.030618	2.331832	1.094899
22	1	0	-7.056809	-1.679129	-0.579260
23	1	0	-4.884078	-2.750322	-1.105011
24	1	0	-2.766868	-1.649247	-0.443357

25	1	0	-4.982731	1.585703	1.270042
26	1	0	-7.099537	0.493598	0.609971
27	1	0	4.511767	-1.878503	-1.044914
28	1	0	-0.390789	2.815294	0.200118
29	1	0	-1.736723	0.637065	-1.240236
30	1	0	-2.428906	2.187465	-0.784934
31	1	0	-2.584698	1.467488	1.583205
32	1	0	-1.722270	-0.026474	1.195645