Substituent Effect of Group 14 Elements on the Ring-Opening Reaction of Cyclobutene

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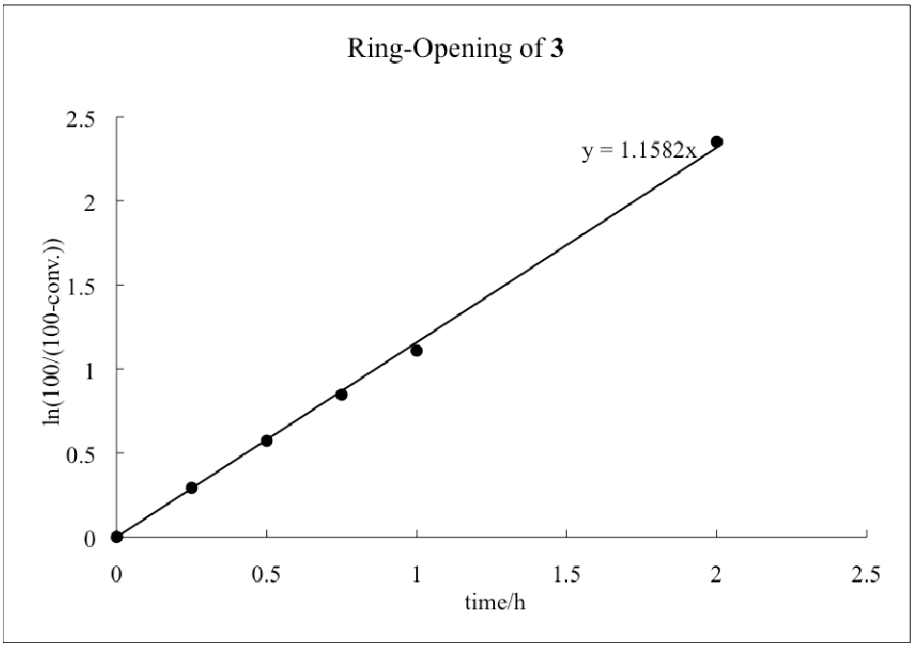
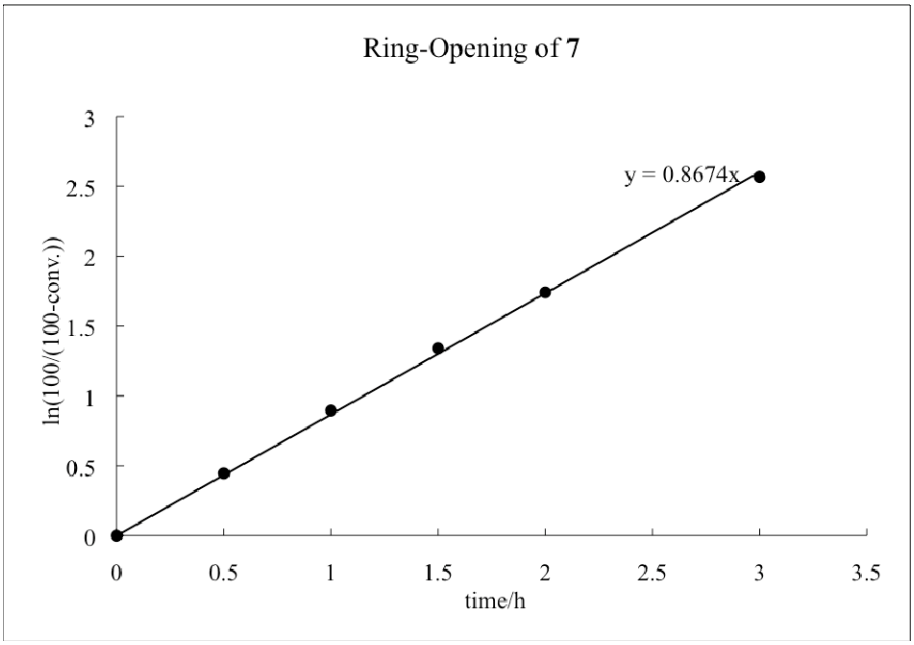
Ring-Opening Reaction of 3

Time (h)	Conversion (%)	ln(100/(100-conv.)	Ratio (*Z*/*E*)	
			Z	*E*
0	0.0	0	0	100
0.25	25.4	0.2926	0	100
0.5	43.6	0.5726	0	100
0.75	57.1	0.8467	0	100
1	67.0	1.1084	0	100
2	90.5	2.3507	0	100



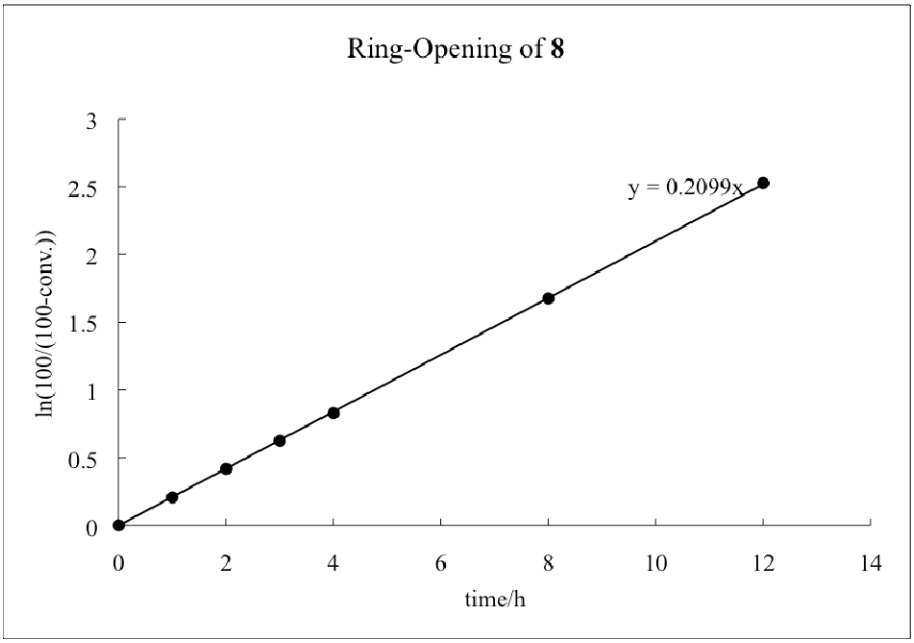
Ring-Opening Reaction of 7

Time (h)	Conversion (%)	ln(100/(100-conv.)	Ratio (*Z*/*E*)	
			Z	*E*
0	0.0	0		
0.5	36.0	0.4457	76.5	23.5
1	59.2	0.8955	76.5	23.5
1.5	73.8	1.3408	75.6	24.4
2	82.5	1.7413	75.5	24.5
3	92.3	2.5664	75.7	24.3



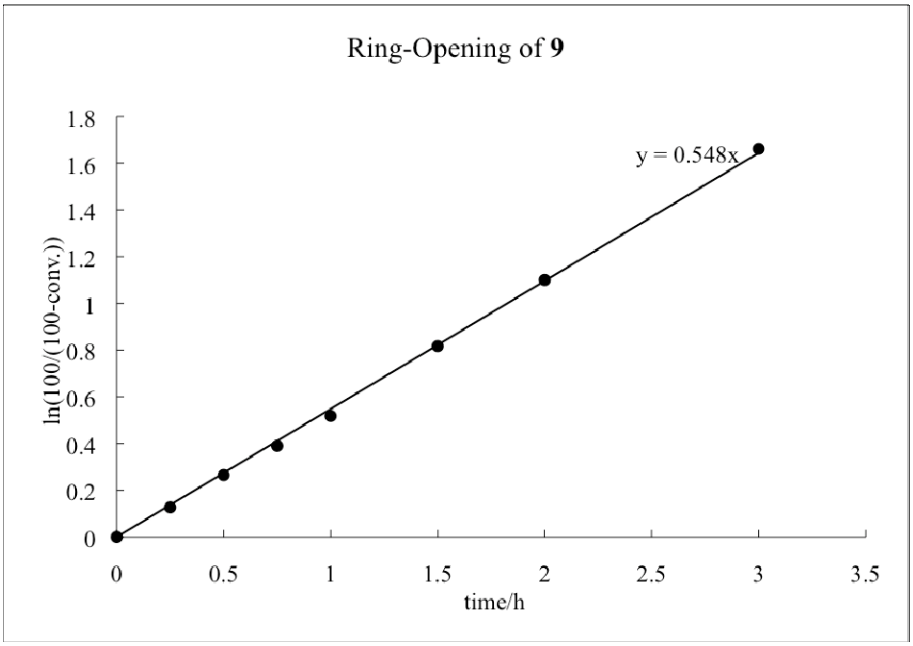
Ring-Opening Reaction of 8

Time (h)	Conversion (%)	ln(100/(100-conv.)	Ratio (*Z*/*E*)	
			Z	*E*
0	0.0	0		
1	18.7	0.2069	46.5	53.5
2	34.1	0.4178	46.7	53.3
3	46.4	0.6244	46.6	53.4
4	56.3	0.8282	46.7	53.3
8	81.3	1.6759	46.5	53.5
12	92.0	2.5268	46.7	53.3



Ring-Opening Reaction of 9

Time (h)	Conversion (%)	ln(100/(100-conv.)	Ratio (*Z*/*E*)	
			Z	*E*
0	0.0	0		
0.25	11.9	0.1268	70.1	29.9
0.5	23.3	0.2650	70.3	29.7
0.75	32.3	0.3899	71.0	29.0
1	40.4	0.5178	71.0	29.0
1.5	55.8	0.8170	70.7	29.3
2	66.7	1.1002	70.6	29.4
3	81.0	1.6613	70.8	29.2



Optimized Cartesian Coordinates and Energies

Ring-Opening Reaction of **17**

Cyclobutene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.891428	1.054643	-0.184207
2	6	0	-2.712669	-0.150354	0.230273
3	6	0	-1.843473	-1.03887	-0.264971
4	6	0	-0.842357	0.005532	-0.740348
5	14	0	0.902997	-0.002697	0.015594
6	6	0	1.819165	1.555629	-0.540799
7	6	0	1.825558	-1.53301	-0.604812
8	6	0	0.809864	-0.050025	1.902604
9	1	0	-1.540569	1.699679	0.62784
10	1	0	-2.338388	1.686085	-0.958006
11	1	0	-3.661255	-0.240528	0.747155
12	1	0	-1.834149	-2.122631	-0.312338
13	1	0	-0.744377	0.052798	-1.833481
14	1	0	1.906222	1.598432	-1.630828
15	1	0	2.832081	1.587634	-0.127394
16	1	0	1.30122	2.462483	-0.214308
17	1	0	2.842135	-1.572964	-0.201154
18	1	0	1.903855	-1.537542	-1.696347
19	1	0	1.316597	-2.454247	-0.305297
20	1	0	1.814083	-0.079038	2.336966
21	1	0	0.269818	-0.93365	2.253816
22	1	0	0.302805	0.829984	2.30862

Sum of electronic and zero-point Energies = -564.565175

Sum of electronic and thermal Energies = -564.553653

Z-butadiene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.583205	-0.999657	-0.195858
2	6	0	2.577973	0.261671	0.240057
3	6	0	1.671321	1.3271	-0.208087
4	6	0	0.338995	1.275762	-0.381267
5	14	0	-0.959722	-0.039884	0.015027
6	6	0	-1.211422	-1.219658	-1.443708
7	6	0	-2.569857	0.918001	0.282259
8	6	0	-0.576235	-1.016895	1.584092
9	1	0	3.301253	-1.722077	0.175333
10	1	0	1.88889	-1.341234	-0.954979
11	1	0	3.346832	0.569033	0.948011
12	1	0	2.176176	2.275644	-0.401143
13	1	0	-0.100269	2.201431	-0.759534
14	1	0	-1.409097	-0.669526	-2.368438
15	1	0	-2.065819	-1.879474	-1.260698
16	1	0	-0.336082	-1.851625	-1.615291
17	1	0	-3.400038	0.239065	0.500107
18	1	0	-2.842882	1.498287	-0.604762
19	1	0	-2.483683	1.615499	1.120949
20	1	0	-1.417946	-1.673372	1.828029
21	1	0	-0.42169	-0.345063	2.43334
22	1	0	0.31658	-1.636166	1.483763

Sum of electronic and zero-point Energies = -564.581953

Sum of electronic and thermal Energies = -564.569728

E-butadiene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.707362	-0.690381	-0.0514
2	6	0	-3.03878	0.455596	0.101818
3	6	0	-1.585808	0.634445	-0.033307
4	6	0	-0.639625	-0.288677	0.209346
5	14	0	1.211666	-0.047002	0.004797
6	6	0	2.060564	-0.348255	1.667394
7	6	0	1.581937	1.705666	-0.593295
8	6	0	1.859286	-1.3029	-1.252576
9	1	0	-3.205257	-1.612907	-0.323383
10	1	0	-4.782374	-0.736912	0.076974
11	1	0	-3.603901	1.359772	0.320555
12	1	0	-1.280934	1.633348	-0.343846
13	1	0	-0.980819	-1.261615	0.569803
14	1	0	1.719605	0.366939	2.421449
15	1	0	3.147106	-0.249673	1.578671
16	1	0	1.849946	-1.35331	2.04563
17	1	0	2.660401	1.847534	-0.713923
18	1	0	1.230015	2.458769	0.11783
19	1	0	1.113819	1.911433	-1.560284
20	1	0	2.94314	-1.212402	-1.376315
21	1	0	1.396681	-1.157246	-2.232901
22	1	0	1.647977	-2.328664	-0.935303

Sum of electronic and zero-point Energies = -564.587913

Sum of electronic and thermal Energies = -564.575570

Inward TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.961822	1.064421	-0.273298
2	6	0	-2.481929	-0.113509	0.341771
3	6	0	-1.846671	-1.148423	-0.294694
4	6	0	-0.677387	-0.582633	-0.898326
5	14	0	0.85911	0.005971	0.021129
6	6	0	1.601984	1.506943	-0.855837
7	6	0	2.119349	-1.408999	-0.079809
8	6	0	0.543164	0.386427	1.841582
9	1	0	-1.820999	2.001274	0.270263
10	1	0	-2.101998	1.198037	-1.337365
11	1	0	-3.180214	-0.141134	1.172917
12	1	0	-2.187183	-2.17226	-0.427034
13	1	0	-0.423581	-0.922578	-1.915538
14	1	0	1.765917	1.304812	-1.919052
15	1	0	2.56961	1.777156	-0.42124
16	1	0	0.945828	2.378698	-0.78232
17	1	0	3.068733	-1.127646	0.387598
18	1	0	2.332364	-1.682775	-1.117953
19	1	0	1.751069	-2.304996	0.429172
20	1	0	1.500576	0.510368	2.358033
21	1	0	0.005429	-0.43008	2.330513
22	1	0	-0.033218	1.302174	1.987863

Sum of electronic and zero-point Energies = -564.517578

Sum of electronic and thermal Energies = -564.506348

Outward TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.531136	-1.026745	0.033262
2	6	0	2.925012	0.347565	-0.011099
3	6	0	1.747658	1.035166	-0.11925
4	6	0	0.779093	0.067752	-0.570594
5	14	0	-1.026664	-0.02382	-0.012376
6	6	0	-2.06089	-0.83878	-1.367192
7	6	0	-1.655209	1.729066	0.324962
8	6	0	-1.160847	-1.041403	1.57694
9	1	0	1.923603	-1.364146	0.861268
10	1	0	3.108816	-1.822707	-0.442502
11	1	0	3.945743	0.719121	-0.039543
12	1	0	1.533447	2.064542	0.155524
13	1	0	1.003575	-0.385163	-1.531321
14	1	0	-2.035615	-0.254725	-2.292039
15	1	0	-3.107968	-0.937526	-1.064754
16	1	0	-1.689054	-1.841879	-1.598348
17	1	0	-2.697007	1.707447	0.660125
18	1	0	-1.607039	2.351207	-0.573247
19	1	0	-1.069483	2.222701	1.105951
20	1	0	-2.194079	-1.074244	1.937081
21	1	0	-0.545009	-0.613973	2.374022
22	1	0	-0.832344	-2.072901	1.418868

Sum of electronic and zero-point Energies = -564.516079

Sum of electronic and thermal Energies = -564.504589

Ring-Opening Reaction of 18

Cyclobutene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.128852	-1.054952	-0.195011
2	6	0	2.941063	0.15139	0.235962
3	6	0	2.078851	1.038276	-0.276391
4	6	0	1.09616	-0.006773	-0.772009
5	32	0	-0.733069	0.001795	0.011036
6	6	0	-1.711743	-1.600578	-0.60979
7	6	0	-1.68276	1.627023	-0.595309
8	6	0	-0.629738	-0.00048	1.984047
9	1	0	1.758779	-1.696531	0.611258
10	1	0	2.593337	-1.689561	-0.956048
11	1	0	3.878695	0.243336	0.772146
12	1	0	2.06683	2.122023	-0.323252
13	1	0	0.996187	-0.053293	-1.862867
14	1	0	-1.797125	-1.602884	-1.699015
15	1	0	-2.719485	-1.621296	-0.187869
16	1	0	-1.19452	-2.513024	-0.304249
17	1	0	-2.696221	1.652707	-0.187552
18	1	0	-1.752512	1.651027	-1.685413
19	1	0	-1.159368	2.527233	-0.264866
20	1	0	-1.630955	0.089975	2.412108
21	1	0	-0.025033	0.836087	2.339805
22	1	0	-0.184512	-0.926677	2.353662

Sum of electronic and zero-point Energies = -2352.039226

Sum of electronic and thermal Energies = -2352.027019

Z-butadiene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.759462	-1.01635	-0.200301
2	6	0	2.797874	0.244722	0.234709
3	6	0	1.930553	1.34165	-0.216079
4	6	0	0.600985	1.333266	-0.396956
5	32	0	-0.766744	-0.02766	0.012016
6	6	0	-1.009536	-1.299231	-1.483883
7	6	0	-2.447616	0.992527	0.225015
8	6	0	-0.4043	-1.00413	1.687764
9	1	0	3.447663	-1.764364	0.176642
10	1	0	2.058958	-1.332419	-0.964701
11	1	0	3.571697	0.523982	0.948797
12	1	0	2.464426	2.276097	-0.40107
13	1	0	0.172556	2.264759	-0.767746
14	1	0	-1.141567	-0.762993	-2.42612
15	1	0	-1.897209	-1.912617	-1.309524
16	1	0	-0.148968	-1.963434	-1.583353
17	1	0	-3.281064	0.317759	0.434498
18	1	0	-2.681065	1.550025	-0.6855
19	1	0	-2.365788	1.702901	1.050987
20	1	0	-1.266241	-1.627414	1.938991
21	1	0	-0.236822	-0.299848	2.505244
22	1	0	0.474701	-1.642033	1.596731

Sum of electronic and zero-point Energies = -2352.055591

Sum of electronic and thermal Energies = -2352.042709

E-butadiene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.013503	-0.692729	-0.050466
2	6	0	-3.340376	0.450046	0.105625
3	6	0	-1.886033	0.623365	-0.029813
4	6	0	-0.947738	-0.300185	0.228275
5	32	0	0.981221	-0.034329	0.003743
6	6	0	1.88016	-0.299731	1.743492
7	6	0	1.33228	1.79016	-0.662361
8	6	0	1.669138	-1.364664	-1.286273
9	1	0	-3.514809	-1.615993	-0.326258
10	1	0	-5.088443	-0.735859	0.079822
11	1	0	-3.901388	1.355972	0.328171
12	1	0	-1.576212	1.616698	-0.353062
13	1	0	-1.278299	-1.269814	0.602028
14	1	0	1.528134	0.433613	2.472014
15	1	0	2.961896	-0.189861	1.635115
16	1	0	1.674847	-1.298674	2.135322
17	1	0	2.407271	1.940071	-0.787248
18	1	0	0.963387	2.540979	0.03995
19	1	0	0.850885	1.952377	-1.629157
20	1	0	2.748861	-1.252	-1.410762
21	1	0	1.192148	-1.236433	-2.26017
22	1	0	1.469089	-2.380106	-0.936427

Sum of electronic and zero-point Energies = -2352.060664

Sum of electronic and thermal Energies = -2352.047612

Inward TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.185214	1.062611	-0.2798
2	6	0	-2.6921	-0.115538	0.343552
3	6	0	-2.073702	-1.149681	-0.313616
4	6	0	-0.918405	-0.584996	-0.938261
5	32	0	0.702504	0.005512	0.018558
6	6	0	1.474014	1.585205	-0.882361
7	6	0	2.007595	-1.481938	-0.115803
8	6	0	0.355005	0.378024	1.922096
9	1	0	-2.026799	1.997081	0.263542
10	1	0	-2.348603	1.200086	-1.339984
11	1	0	-3.366948	-0.145163	1.193845
12	1	0	-2.423572	-2.170165	-0.45035
13	1	0	-0.668414	-0.923633	-1.954982
14	1	0	1.639549	1.380771	-1.942926
15	1	0	2.434175	1.85123	-0.433407
16	1	0	0.80211	2.441888	-0.79861
17	1	0	2.958071	-1.200461	0.344905
18	1	0	2.197477	-1.737141	-1.161268
19	1	0	1.628433	-2.372022	0.39158
20	1	0	1.307644	0.458501	2.451582
21	1	0	-0.22336	-0.430988	2.371586
22	1	0	-0.193048	1.311504	2.055789

Sum of electronic and zero-point Energies = -2351.989711

Sum of electronic and thermal Energies = -2351.977723

Outward TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.80681	-1.02722	0.037788
2	6	0	3.194964	0.347179	-0.013379
3	6	0	2.01337	1.030299	-0.124357
4	6	0	1.058279	0.056695	-0.576091
5	32	0	-0.833797	-0.017375	-0.009777
6	6	0	-1.922678	-0.809542	-1.455123
7	6	0	-1.4586	1.816274	0.391802
8	6	0	-1.008171	-1.12183	1.621032
9	1	0	2.197379	-1.361977	0.865601
10	1	0	3.39076	-1.823624	-0.429478
11	1	0	4.213841	0.723462	-0.048444
12	1	0	1.790375	2.056989	0.153426
13	1	0	1.268955	-0.398688	-1.537254
14	1	0	-1.873077	-0.194603	-2.356573
15	1	0	-2.968844	-0.889857	-1.150482
16	1	0	-1.561437	-1.810821	-1.701784
17	1	0	-2.5003	1.79299	0.720721
18	1	0	-1.390222	2.451741	-0.493565
19	1	0	-0.859983	2.265184	1.187499
20	1	0	-2.046146	-1.136682	1.962386
21	1	0	-0.387705	-0.719061	2.424858
22	1	0	-0.695929	-2.15017	1.425914

Sum of electronic and zero-point Energies = -2351.989849

Sum of electronic and thermal Energies = -2351.977661

Ring-Opening Reaction of 19

Cyclobutene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.392193	-1.056528	-0.210489
2	6	0	3.196915	0.151927	0.247858
3	6	0	2.338288	1.045287	-0.292985
4	6	0	1.366005	-0.005708	-0.811177
5	50	0	-0.641295	0.001412	0.008488
6	6	0	-1.717028	-1.711081	-0.732478
7	6	0	-1.649017	1.801921	-0.60733
8	6	0	-0.547248	-0.071526	2.156374
9	1	0	2.007157	-1.70788	0.588997
10	1	0	2.879474	-1.687326	-0.968299
11	1	0	4.120054	0.243851	0.820679
12	1	0	2.326056	2.135521	-0.339704
13	1	0	1.293519	-0.051607	-1.910231
14	1	0	-1.78732	-1.685976	-1.828649
15	1	0	-2.737975	-1.734273	-0.326721
16	1	0	-1.215561	-2.645058	-0.444187
17	1	0	-2.671184	1.832665	-0.205231
18	1	0	-1.712995	1.862336	-1.702519
19	1	0	-1.115914	2.692465	-0.24717
20	1	0	-1.556797	-0.007252	2.585566
21	1	0	0.045931	0.764161	2.550874
22	1	0	-0.090318	-1.007968	2.503557

Sum of electronic and zero-point Energies= -278.351606

Sum of electronic and thermal Energies= -278.338457

Z-butadiene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.882183	-1.051564	-0.209236
2	6	0	3.01255	0.217525	0.223303
3	6	0	2.213377	1.371452	-0.238309
4	6	0	0.873614	1.419652	-0.435435
5	50	0	-0.655403	-0.019054	0.013013
6	6	0	-0.380395	-0.882568	1.960795
7	6	0	-0.796666	-1.569981	-1.475144
8	6	0	-2.48342	1.114685	-0.023305
9	1	0	3.51427	-1.850542	0.178759
10	1	0	2.165881	-1.321904	-0.984419
11	1	0	3.805523	0.445156	0.943192
12	1	0	2.801691	2.282582	-0.408728
13	1	0	0.492583	2.379431	-0.806735
14	1	0	0.536368	-1.483628	2.000075
15	1	0	-1.231897	-1.529731	2.212876
16	1	0	-0.309178	-0.095453	2.723387
17	1	0	-1.776568	-2.064015	-1.416374
18	1	0	-0.02174	-2.33407	-1.329659
19	1	0	-0.684516	-1.153996	-2.485556
20	1	0	-3.346285	0.477094	0.213576
21	1	0	-2.649888	1.553973	-1.016857
22	1	0	-2.453547	1.932588	0.709804

Sum of electronic and zero-point Energies= -278.366886

Sum of electronic and thermal Energies= -278.353175

E-butadiene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.329975	-0.716143	-0.043127
2	6	0	-3.652388	0.43954	0.104226
3	6	0	-2.187516	0.607908	-0.017656
4	6	0	-1.247515	-0.335025	0.233071
5	50	0	0.852846	-0.025837	0.001883
6	6	0	1.832174	-0.328538	1.892975
7	6	0	1.170402	1.983244	-0.692282
8	6	0	1.626577	-1.442498	-1.420355
9	1	0	-3.826104	-1.649433	-0.296585
10	1	0	-5.412852	-0.755649	0.072444
11	1	0	-4.218853	1.354186	0.304043
12	1	0	-1.87412	1.612187	-0.322882
13	1	0	-1.604699	-1.309988	0.586789
14	1	0	1.641194	-1.341938	2.271992
15	1	0	1.467906	0.389274	2.640126
16	1	0	2.919049	-0.2013	1.794483
17	1	0	2.243533	2.181785	-0.81849
18	1	0	0.772377	2.715069	0.023761
19	1	0	0.678959	2.1472	-1.660808
20	1	0	2.71105	-1.317264	-1.544576
21	1	0	1.150261	-1.311539	-2.401247
22	1	0	1.439447	-2.471684	-1.084322

Sum of electronic and zero-point Energies= -278.370582

Sum of electronic and thermal Energies= -278.356702

Inward TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.365873	1.071203	-0.276343
2	6	0	-2.907938	-0.106184	0.341049
3	6	0	-2.337495	-1.152847	-0.361934
4	6	0	-1.173199	-0.610348	-1.010233
5	50	0	0.611002	0.001363	0.017893
6	6	0	1.425506	1.752535	-0.928651
7	6	0	2.040844	-1.601616	-0.185922
8	6	0	0.212706	0.344572	2.097488
9	1	0	-2.157468	1.992544	0.285423
10	1	0	-2.55821	1.241416	-1.332926
11	1	0	-3.558958	-0.129645	1.216782
12	1	0	-2.729256	-2.162227	-0.514909
13	1	0	-0.975732	-0.936009	-2.050001
14	1	0	1.580716	1.577138	-2.002249
15	1	0	2.394823	2.020984	-0.485992
16	1	0	0.747551	2.609294	-0.817311
17	1	0	2.995818	-1.334892	0.28861
18	1	0	2.237574	-1.818134	-1.245183
19	1	0	1.66871	-2.520842	0.286807
20	1	0	1.156473	0.377667	2.659294
21	1	0	-0.40551	-0.463561	2.509346
22	1	0	-0.313965	1.294242	2.254928

Sum of electronic and zero-point Energies= -278.303698

Sum of electronic and thermal Energies= -278.290753

Outward TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.088045	-1.036462	0.046155
2	6	0	3.493469	0.341321	-0.014147
3	6	0	2.306752	1.035894	-0.140999
4	6	0	1.343405	0.057846	-0.593563
5	50	0	-0.729919	-0.011996	-0.007299
6	6	0	-1.874236	-0.952569	-1.56674
7	6	0	-1.424808	1.996773	0.33748
8	6	0	-0.933703	-1.144996	1.811424
9	1	0	2.463507	-1.359806	0.874896
10	1	0	3.670351	-1.84698	-0.412798
11	1	0	4.521812	0.70962	-0.045585
12	1	0	2.086854	2.068601	0.1411
13	1	0	1.577931	-0.41125	-1.549879
14	1	0	-1.811866	-0.377079	-2.50033
15	1	0	-2.932925	-1.030916	-1.283623
16	1	0	-1.500115	-1.966513	-1.764789
17	1	0	-2.475017	1.989011	0.660339
18	1	0	-1.35131	2.600057	-0.577241
19	1	0	-0.832487	2.487899	1.121439
20	1	0	-1.979433	-1.154424	2.148588
21	1	0	-0.320979	-0.709955	2.612779
22	1	0	-0.61391	-2.185332	1.662397

Sum of electronic and zero-point Energies= -278.302653

Sum of electronic and thermal Energies= -278.289562