Electronic Supporting Information (ESI)

Captodative substitution induced acceleration effect towards 4π electrocyclic ring–opening of substituted cyclobutenes

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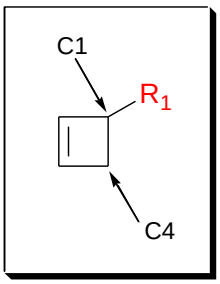
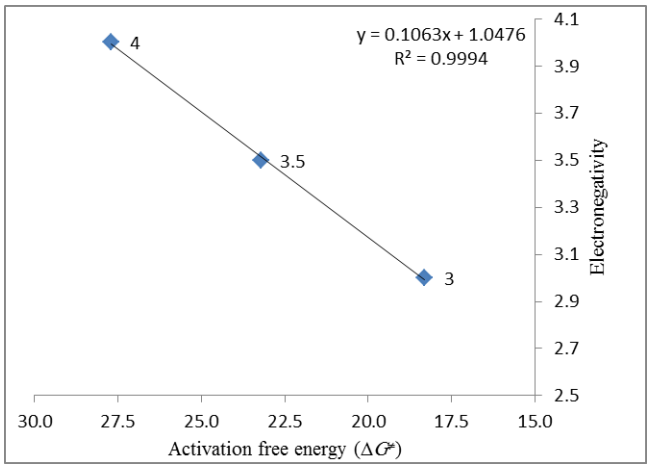
1. Complete citation for the reference 28

GAUSSIAN09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaor, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

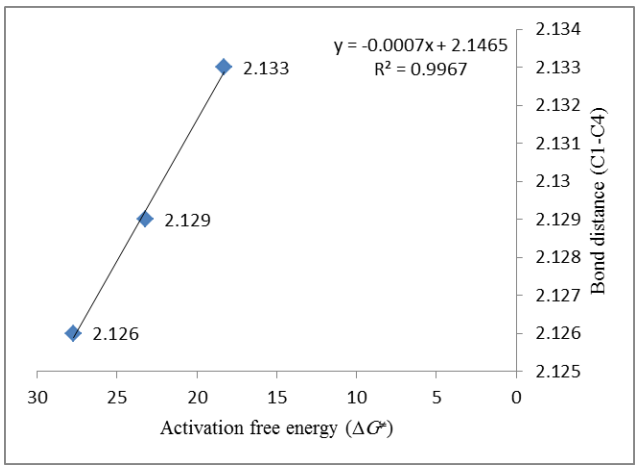
2. Linear free energy relationships for monosubstituted cyclobutenes



a)



b)



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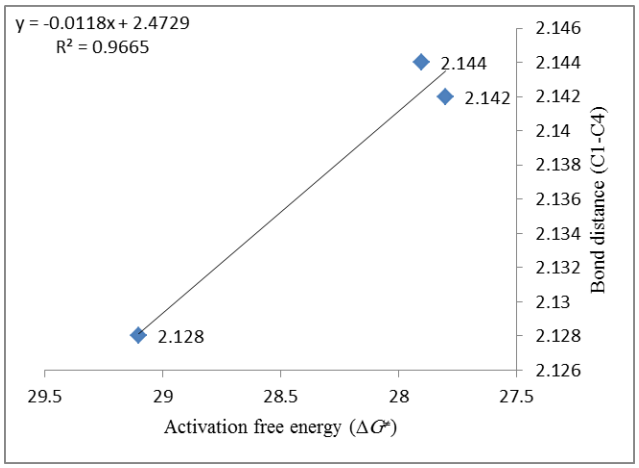


Fig. 1 Correlations involving linear free energy relationships between the activation free energy ($\Delta G^{\neq}$) of
a) NH_2, OH and F substituted cyclobutenes at C1 positions against the electronegativity values of N, O, and F atoms;
b) NH_2, OH and F substituted cyclobutenes at C1 positions against their corresponding C1–C4 bond distances in the transition states;
c) $C(O)CH_3$, CN and NO_2 substituted cyclobutenes at C1 positions against their corresponding C1–C4 bond distances in the transition states.

Note: By plotting the calculated bond lengths against corresponding barriers for all C1 substituted cyclobutenes, poor/no free energy linear relationships were obtained. Also, poor correlations were observed between the energy barriers and corresponding Hammett constants of the substituents.

3. Graphical description of torquoselectivity for monosubstituted cyclobutens

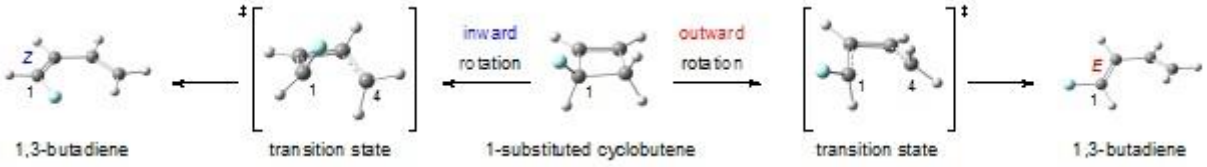
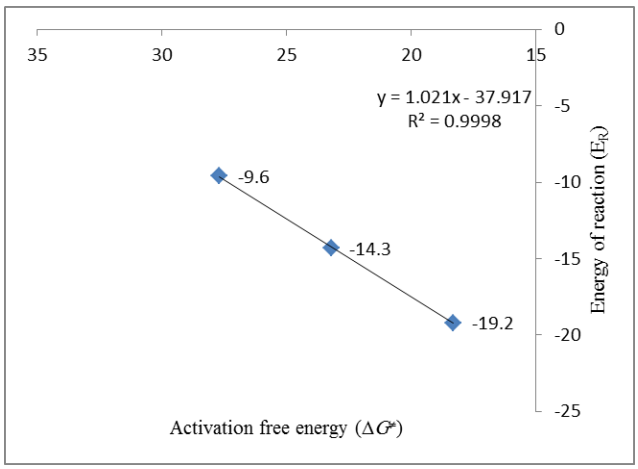
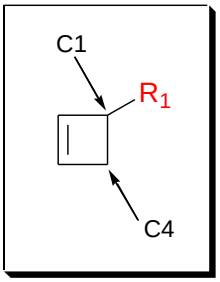


Fig. 2 Representative pictorial description of inward and outward rotations of F substituent located at C1 position of cyclobutene.

4 Linear free energy relationships for activation free energy and reaction exothermicity for monosubstituted cyclobutenes

a)





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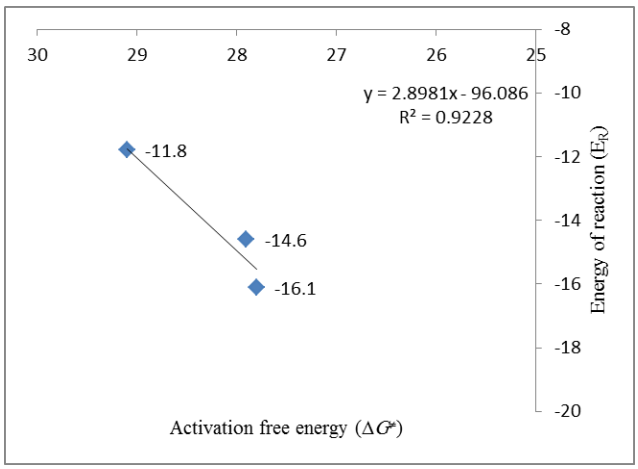
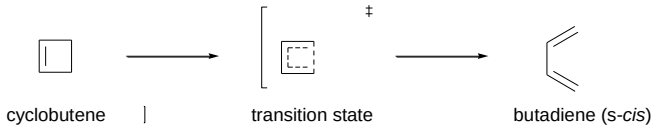


Fig. 3 Correlations involving linear free energy relationships between the activation free energy ($\Delta G^{\neq}$) and energy of reaction (E_R) for
a) NH_2, OH and F substituted cyclobutenes at C1 positions;
b) $C(O)CH_3$, CN and NO_2 substituted cyclobutenes at C1 positions.

Note: Poor/ no correlations were observed by plotting free energy barriers against corresponding energies of reactions and the bond distance (C1–C4) for all C1 substitued cyclobutenes.

5. Energies for

5.1 Butadiene



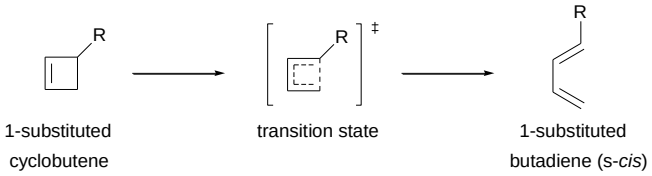
Butadiene [Product], (Hartree)		
Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
-155.9953673	-155.9102480	-155.9369670

Transition State, (Hartree)		
Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
-155.9252189	-155.8412880	-155.8669580

Cyclobutene [Starting Material], (Hartree)		
Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
-155.9797476	-155.8931250	-155.9187460

5.2 Monosubstituted butadienes

5.2.1 1-Substituted butadienes (outward rotation of substituents)

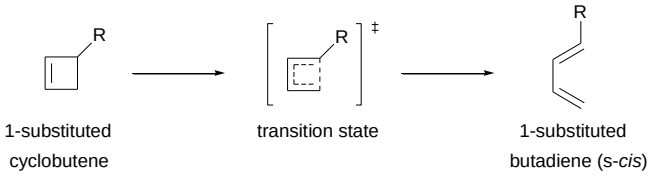


Entry	R	Butadiene [Product], (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-195.3158192	-195.2024940	-195.2315610
2	NH_2	-211.3559655	-211.2533510	-211.2819880
3	OH	-231.2159875	-231.1262220	-231.1548460
4	F	-255.2359958	-255.1583410	-255.1867290
5	$C(O)CH_3$	-308.6513638	-308.5281220	-308.5609210
6	CN	-248.2444639	-248.1601200	-248.1900280
7	NO_2	-360.5084487	-360.4199600	-360.4516760

Entry	R	Transition State, (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-195.2461315	-195.1344540	-195.1633160
2	NH_2	-211.2962231	-211.1947410	-211.2221940
3	OH	-231.1566367	-231.0676610	-231.0949870
4	F	-255.1766898	-255.0999920	-255.1272450
5	$C(O)CH_3$	-308.5822332	-308.4606370	-308.4925980
6	CN	-248.1764687	-248.0933730	-248.1221450
7	NO_2	-360.4433421	-360.3561030	-360.3865830

Entry	R	Cyclobutene [Starting Material], (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-195.2970650	-195.1822290	-195.2098920
2	NH_2	-211.3275257	-211.2237190	-211.2514100
3	OH	-231.1954838	-231.1045130	-231.1319910
4	F	-255.2234064	-255.1441800	-255.1714380
5	$C(O)CH_3$	-308.6278294	-308.5036480	-308.5353200
6	CN	-248.2236211	-248.1379740	-248.1666860
7	NO_2	-360.4910476	-360.4012970	-360.4328970

5.2.2 1-Substituted butadienes (inward rotation of substituents)

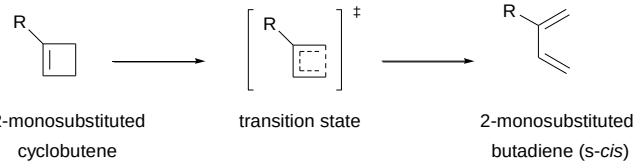


Entry	R	Butadiene [Product], (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-195.3132946	-195.1994960	-195.2284890
2	NH_2	-211.3578934	-211.2544640	-211.2828080
3	OH	-231.2179292	-231.1274420	-231.1559300
4	F	-255.2373343	-255.1591770	-255.1877000
5	$C(O)CH_3$	-308.6462229	-308.5225380	-308.5557270
6	CN	-248.2437889	-248.1589680	-248.1891530
7	NO_2	-360.5011987	-360.4122020	-360.4453190

Entry	R	Transition State, (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-195.2361213	-195.1239790	-195.1515930
2	NH_2	-211.2662339	-211.1653100	-211.1928830
3	OH	-231.1294267	-231.0414460	-231.0689100
4	F	-255.1530871	-255.0770170	-255.1043250
5	$C(O)CH_3$	-308.5779420	-308.4565000	-308.4880700
6	CN	-248.1689824	-248.0860140	-248.1146860
7	NO_2	-360.4332191	-360.3461360	-360.3763630

Entry	R	Cyclobutene [Starting Material], (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-195.2970649	-195.1822290	-195.2098910
2	NH_2	-211.3298002	-211.2257750	-211.2533310
3	OH	-231.1954836	-231.1045140	-231.1319930
4	F	-255.2234064	-255.1441800	-255.1714380
5	$C(O)CH_3$	-308.6276575	-308.5037310	-308.5356460
6	CN	-248.2236212	-248.1379750	-248.1666860
7	NO_2	-360.4910476	-360.4012970	-360.4328970

5.2.3 2-Substituted butadienes



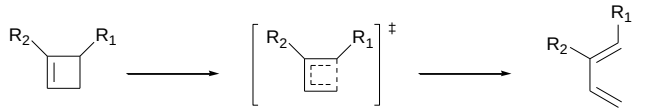
Entry	R	Butadiene [Product], (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-155.9953673	-155.9102480	-155.9369670
2	NH_2	-195.3148461	-195.2015800	-195.2304830
3	OH	-211.3550116	-211.2525740	-211.2810100
4	F	-231.219649	-231.130029	-231.158549
5	$C(O)CH_3$	-255.2402055	-255.1629350	-255.1914090
6	CN	-308.6474341	-308.5243420	-308.5567410
7	NO_2	-248.2399994	-248.1559100	-248.1857340

Entry	R	Transition State, (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-155.9252189	-155.8412880	-155.8669580
2	NH_2	-195.2462215	-195.1344830	-195.1628600
3	OH	-211.2883990	-211.1873420	-211.2148290
4	F	-231.1511044	-231.062468	-231.089808
5	$C(O)CH_3$	-255.1704014	-255.0940470	-255.1212990
6	CN	-308.5831243	-308.4616620	-308.4934700
7	NO_2	-248.1751392	-248.0921800	-248.1209230

Entry	R	Cyclobutene [Starting Material], (Hartree)		
		Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	-155.9797476	-155.8931250	-155.9187460
2	NH_2	-195.3036595	-195.1890470	-195.2170370
3	OH	-211.3436203	-211.2396740	-211.2672100
4	F	-231.2058093	-231.114602	-231.142144
5	$C(O)CH_3$	-255.2258948	-255.1465510	-255.1737800
6	CN	-308.6378058	-308.5136590	-308.5463100
7	NO_2	-248.2310472	-248.1452950	-248.1740470

5.3 Energies for disubstituted butadienes

5.3.1 1,2-Disubstituted butadienes



1,2-disubstituted cyclobutene — transition state — 1,2-disubstituted butadiene (s-*cis*)

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6319655	-234.4904790	-234.5218560
2		NH_2	-250.6710463	-250.5408260	-250.5722010
3		OH	-270.5369862	-270.4192610	-270.4506810
4		F	-294.5599033	-294.4543960	-294.4853380
5		$C(O)CH_3$	-347.9598784	-347.8084610	-347.8433550
6		CN	-287.5623944	-287.4501070	-287.4821240
7		NO_2	-399.8225912	-399.7062730	-399.7401580

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.5665524	-234.4269190	-234.4575280
2		NH_2	-250.6083347	-250.4791770	-250.5089560
3		OH	-270.4717467	-270.3552400	-270.3850500
4		F	-294.4915834	-294.3873500	-294.4171760
5		$C(O)CH_3$	-347.9050317	-347.7555620	-347.7893950
6		CN	-287.4978808	-287.3871020	-287.4184610
7		NO_2	-399.7625175	-399.6475330	-399.6798700

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6207264	-234.4779700	-234.5079240
2		NH_2	-250.6607603	-250.5286940	-250.5582170
3		OH	-270.5229359	-270.4036090	-270.4331630
4		F	-294.5433240	-294.4357850	-294.4649980
5		$C(O)CH_3$	-347.9551309	-347.8028520	-347.8371870
6		CN	-287.5489776	-287.4350970	-287.4658260
7		NO_2	-399.8115851	-399.6936700	-399.7259750

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6726036	-250.5420480	-250.5730520
2		NH_2	-266.7104499	-266.5906120	-266.6212120
3		OH	-286.5763658	-286.4688560	-286.4991720
4		F	-310.5985978	-310.5037440	-310.5339790
5		$C(O)CH_3$	-364.0093457	-363.8687810	-363.9028840
6		CN	-303.6100840	-303.5085140	-303.5402090
7		NO_2	-415.8816326	-415.7754680	-415.8079480

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6159733	-250.4865490	-250.5162560
2		NH_2	-266.6560200	-266.5371430	-266.5662970
3		OH	-286.5175885	-286.4118430	-286.4409670
4		F	-310.5380930	-310.4447030	-310.4737750
5		$C(O)CH_3$	-363.9573134	-363.8181580	-363.8516180
6		CN	-303.5493927	-303.4490480	-303.4795280
7		NO_2	-415.8139481	-415.7094630	-415.7413880

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6515052	-250.5197200	-250.5496560
2		NH_2	-266.6908384	-266.5697820	-266.5994970
3		OH	-286.5590150	-286.4500540	-286.4792060
4		F	-310.5731863	-310.4767020	-310.5059200
5		$C(O)CH_3$	-363.9876557	-363.8462460	-363.8807100
6		CN	-303.5793002	-303.4764660	-303.5071910
7		NO_2	-415.8430584	-415.7360390	-415.7681570

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.5349183	-270.4169570	-270.4477490
2		NH_2	-286.5732258	-286.4662010	-286.4965790
3		OH	-306.4307729	-306.3368150	-306.3672390
4		F	-330.4531007	-330.3711180	-330.4013410
5		$C(O)CH_3$	-383.8690168	-383.7408660	-383.7745340
6		CN	-323.4622866	-323.3732840	-323.4047300
7		NO_2	-435.7211642	-435.6279080	-435.6610720

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.4775159	-270.3606430	-270.3903090
2		NH_2	-286.5151231	-286.4092090	-286.4383420
3		OH	-306.3773052	-306.2839690	-306.3129870
4		F	-330.3970573	-330.3157610	-330.3445910
5		$C(O)CH_3$	-383.8138828	-383.6871950	-383.7200810
6		CN	-323.4066769	-323.3186580	-323.3489200
7		NO_2	-435.6685527	-435.5766470	-435.6084310

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.5200494	-270.4011110	-270.4309010
2		NH_2	-286.5609380	-286.4525630	-286.4818410
3		OH	-306.4210657	-306.3254580	-306.3546640
4		F	-330.4390287	-330.3555140	-330.3845900
5		$C(O)CH_3$	-383.8517692	-383.7233210	-383.7567160
6		CN	-323.4449877	-323.3551760	-323.3858630
7		NO_2	-435.6685527	-435.5766470	-435.6084310

Entry	R_1	R_2	1,3-Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.5556334	-294.4497920	-294.4803420
2		NH_2	-310.5941462	-310.4990730	-310.5290730
3		OH	-330.4514227	-330.3693850	-330.3994600
4		F	-354.4714732	-354.4015260	-354.4314490
5		$C(O)CH_3$	-407.8858411	-407.7702010	-407.8039200
6		CN	-347.4772336	-347.4005900	-347.4319000
7		NO_2	-459.7344641	-459.6538930	-459.6873000

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.4982975	-294.3937250	-294.4234230
2		NH_2	-310.5387408	-310.4447310	-310.4736870
3		OH	-330.3977579	-330.3164940	-330.3453530
4		F	-354.4156299	-354.3465130	-354.3752310
5		$C(O)CH_3$	-407.8296920	-407.7155410	-407.7486050
6		CN	-347.4226784	-347.3470330	-347.3772380
7		NO_2	-459.6834206	-459.6038620	-459.6356380

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.5478951	-294.4407190	-294.4703220
2		NH_2	-310.5881720	-310.4916480	-310.5207410
3		OH	-330.4484469	-330.3645230	-330.3934370
4		F	-354.4653120	-354.3935180	-354.4223120
5		$C(O)CH_3$	-407.8778259	-407.7612160	-407.7946280
6		CN	-347.4706341	-347.3924620	-347.4227550
7		NO_2	-459.7308218	-459.6487320	-459.6807050

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9635844	-347.8119750	-347.8470650
2		NH_2	-364.0116132	-363.8707280	-363.9044720
3		OH	-383.8745303	-383.7463400	-383.7804360
4		F	-407.8938486	-407.7784870	-407.8128000
5		$C(O)CH_3$	-461.2895212	-461.1292680	-461.1676670
6		CN	-400.8892038	-400.7672390	-400.8025530
7		NO_2	-513.1466437	-513.0215450	-513.0590600

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9032526	-347.7537840	-347.7879690
2		NH_2	-363.9497372	-363.8106480	-363.8440240
3		OH	-383.8053623	-383.6792760	-383.7126470
4		F	-407.8230982	-407.7092160	-407.7424420
5		$C(O)CH_3$	-461.2313200	-461.0722140	-461.1092740
6		CN	-400.8270336	-400.7066920	-400.7413890
7		NO_2	-513.0898076	-512.9655160	-513.0016640

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9518105	-347.7997030	-347.8336730
2		NH_2	-363.9930521	-363.8515130	-363.8847750
3		OH	-383.8538143	-383.7250920	-383.7586270
4		F	-407.8726209	-407.7559150	-407.7889600
5		$C(O)CH_3$	-461.2822382	-461.1208140	-461.1585560
6		CN	-400.8763869	-400.7534030	-400.7880580
7		NO_2	-513.1389257	-513.0119740	-513.0480150

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.5655841	-287.4532220	-287.4851940
2		NH_2	-303.6127084	-303.5110330	-303.5424930
3		OH	-323.4677805	-323.3789190	-323.4103430
4		F	-347.4857252	-347.4092940	-347.4409050
5		$C(O)CH_3$	-400.8897269	-400.7678770	-400.8031690
6		CN	-340.4812936	-340.3983900	-340.4311750
7		NO_2	-452.7401778	-452.6533940	-452.6882500

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.4991006	-287.3882230	-287.4194520
2		NH_2	-303.5433766	-303.4431640	-303.4736420
3		OH	-323.4019116	-323.3142160	-323.3445320
4		F	-347.4180351	-347.3426380	-347.3728680
5		$C(O)CH_3$	-400.8283886	-400.7080750	-400.7426480
6		CN	-340.4198538	-340.3380600	-340.3697720
7		NO_2	-452.6814320	-452.5957610	-452.6289840

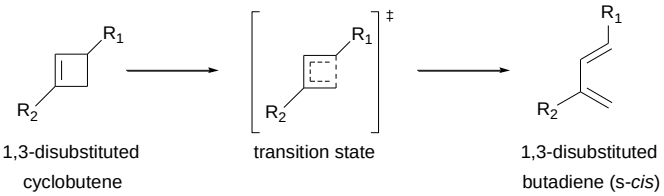
Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.5487916	-287.4351690	-287.4661320
2		NH_2	-303.5886930	-303.4858390	-303.5163930
3		OH	-323.4494611	-323.3591240	-323.3894530
4		F	-347.4652915	-347.3870830	-347.4173020
5		$C(O)CH_3$	-400.8784590	-400.7554470	-400.7901780
6		CN	-340.4687163	-340.3842240	-340.4159590
7		NO_2	-452.7295205	-452.6410870	-452.6743970

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.8252618	-399.7086610	-399.7423990
2		NH_2	-415.8827811	-415.7767560	-415.8093490
3		OH	-435.7253746	-435.6322680	-435.6654910
4		F	-459.7413522	-459.6608010	-459.6942770
5		$C(O)CH_3$	-513.1499682	-513.0245460	-513.0614760
6		CN	-452.7389122	-452.6519800	-452.6864810
7		NO_2	-564.9971149	-564.9063610	-564.9434730

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.7651843	-399.6500470	-399.6827220
2		NH_2	-415.8108911	-415.7063060	-415.7382930
3		OH	-435.6653758	-435.5737240	-435.6057530
4		F	-459.6807272	-459.6012630	-459.6331890
5		$C(O)CH_3$	-513.0939988	-512.9694440	-513.0052960
6		CN	-452.6829277	-452.5971270	-452.6305450
7		NO_2	-564.9425995	-564.8529750	-564.8877650

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.8163703	-399.6986310	-399.7321700
2		NH_2	-415.8576339	-415.7505180	-415.7830830
3		OH	-435.7166248	-435.6221520	-435.6545560
4		F	-459.7318108	-459.6494980	-459.6819200
5		$C(O)CH_3$	-513.1448585	-513.0177950	-513.0546620
6		CN	-452.7349975	-452.6464350	-452.6808270
7		NO_2	-564.9965162	-564.9039820	-564.9394240

5.3.2 1,3-Disubstituted butadienes



Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6351908	-234.4937380	-234.5248950
2		NH_2	-250.6756023	-250.5449710	-250.5756790
3		OH	-270.5385510	-270.4208630	-270.4516150
4		F	-294.5614371	-294.4559890	-294.4867130
5		$C(O)CH_3$	-347.9681674	-347.8169590	-347.8516930
6		CN	-287.5613741	-287.4491240	-287.4812360
7		NO_2	-399.8265229	-399.7103010	-399.7442770

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.5671286	-234.4277270	-234.4590450
2		NH_2	-250.6096221	-250.4808650	-250.5112620
3		OH	-270.4728879	-270.3566000	-270.3868830
4		F	-294.4926520	-294.3886620	-294.4190520
5		$C(O)CH_3$	-347.9043304	-347.7551400	-347.7896710
6		CN	-287.4970919	-287.3863920	-287.4178630
7		NO_2	-399.7627305	-399.6480610	-399.6811070

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6209556	-234.4782170	-234.5081490
2		NH_2	-250.6611474	-250.5291700	-250.5586750
3		OH	-270.5234144	-270.4040940	-270.4335680
4		F	-294.5433697	-294.4359390	-294.4651210
5		$C(O)CH_3$	-347.9550356	-347.8027150	-347.8371340
6		CN	-287.5484949	-287.4345790	-287.4653030
7		NO_2	-399.8113344	-399.6934170	-399.7257930

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6743788	-250.5438220	-250.5747150
2		NH_2	-266.7139827	-266.5944470	-266.6249320
3		OH	-286.5792110	-286.4723330	-286.5026780
4		F	-310.6022493	-310.5077540	-310.5381080
5		$C(O)CH_3$	-364.0093873	-363.8687920	-363.9029290
6		CN	-303.6024046	-303.5011840	-303.5330610
7		NO_2	-415.8690381	-415.7635320	-415.7970180

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6177641	-250.4885540	-250.5184120
2		NH_2	-266.6620638	-266.5434220	-266.5725670
3		OH	-286.5257290	-286.4196450	-286.4486710
4		F	-310.5452982	-310.4515100	-310.4804520
5		$C(O)CH_3$	-363.9536681	-363.8147370	-363.8481030
6		CN	-303.5479449	-303.4475950	-303.4780030
7		NO_2	-415.8136075	-415.7092540	-415.7412710

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6519972	-250.5202680	-250.5502180
2		NH_2	-266.6936481	-266.5726780	-266.6022860
3		OH	-286.5553354	-286.4470020	-286.4764990
4		F	-310.5745104	-310.4781010	-310.5072610
5		$C(O)CH_3$	-363.9849403	-363.8436760	-363.8779870
6		CN	-303.5780884	-303.4752840	-303.5060350
7		NO_2	-415.8408927	-415.7340620	-415.7664390

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.5354428	-270.4175670	-270.4482970
2		NH_2	-286.5744392	-286.4677230	-286.4981750
3		OH	-306.4393926	-306.3451280	-306.3753590
4		F	-330.4615823	-330.3795990	-330.4097510
5		$C(O)CH_3$	-383.8680011	-383.7403780	-383.7746080
6		CN	-323.4612478	-323.3725000	-323.4040740
7		NO_2	-435.7265513	-435.6338350	-435.6672350

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.4782233	-270.3615260	-270.3913580
2		NH_2	-286.5226133	-286.4164420	-286.4454520
3		OH	-306.3852559	-306.2915850	-306.3204590
4		F	-330.4041907	-330.3228320	-330.3516200
5		$C(O)CH_3$	-383.8134235	-383.6870770	-383.7203990
6		CN	-323.4064838	-323.3186020	-323.3488590
7		NO_2	-435.6716083	-435.5797460	-435.6116180

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.5201120	-270.4012450	-270.4309940
2		NH_2	-286.5625024	-286.4542780	-286.4835360
3		OH	-306.4232291	-306.3276720	-306.3568640
4		F	-330.4416790	-330.3581720	-330.3871550
5		$C(O)CH_3$	-383.8521961	-383.7238690	-383.7581220
6		CN	-323.4449196	-323.3550120	-323.3855540
7		NO_2	-435.7067893	-435.6129450	-435.6452350

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.5557640	-294.4499600	-294.4804480
2		NH_2	-310.5959178	-310.5009750	-310.5310290
3		OH	-330.4580367	-330.3760220	-330.4061110
4		F	-354.4797227	-354.4099160	-354.4398980
5		$C(O)CH_3$	-407.8876594	-407.7722000	-407.8062210
6		CN	-347.4789608	-347.4023690	-347.4337530
7		NO_2	-459.7439990	-459.6634690	-459.6966180

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.4984205	-294.3940250	-294.4239310
2		NH_2	-310.5426794	-310.4490510	-310.4780430
3		OH	-330.4044046	-330.3230630	-330.3518700
4		F	-354.4220857	-354.3530610	-354.3817840
5		$C(O)CH_3$	-407.8317468	-407.7177000	-407.7508450
6		CN	-347.4232778	-347.3477580	-347.3779530
7		NO_2	-459.6874727	-459.6079810	-459.6397890

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.5486126	-294.4415020	-294.4710480
2		NH_2	-310.5923519	-310.4959500	-310.5250140
3		OH	-330.4521014	-330.3682720	-330.3972410
4		F	-354.4691166	-354.3973740	-354.4261510
5		$C(O)CH_3$	-407.8786328	-407.7620670	-407.7959560
6		CN	-347.4705715	-347.3924260	-347.4227310
7		NO_2	-459.7316707	-459.6496070	-459.6816940

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9707245	-347.8194590	-347.8543180
2		NH_2	-364.0103554	-363.8699850	-363.9043660
3		OH	-383.8716473	-383.7443400	-383.7787900
4		F	-407.8946946	-407.7795460	-407.8143550
5		$C(O)CH_3$	-461.3032763	-461.1422120	-461.1804420
6		CN	-400.8934783	-400.7714820	-400.8072250
7		NO_2	-513.1585711	-513.0326300	-513.0702640

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9036599	-347.7543230	-347.7887600
2		NH_2	-363.9450862	-363.8065640	-363.8401820
3		OH	-383.8068871	-383.6807710	-383.7142270
4		F	-407.8255605	-407.7116880	-407.7450300
5		$C(O)CH_3$	-461.2389562	-461.0800820	-461.1178570
6		CN	-400.8292578	-400.7088580	-400.7435840
7		NO_2	-513.0936766	-512.9694280	-513.0057710

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9524293	-347.8003780	-347.8343200
2		NH_2	-363.9937242	-363.8523570	-363.8858060
3		OH	-383.8547417	-383.7261080	-383.7595690
4		F	-407.8733119	-407.7566520	-407.7898210
5		$C(O)CH_3$	-461.2842875	-461.1227420	-461.1607400
6		CN	-400.8763526	-400.7533290	-400.7880950
7		NO_2	-513.1386180	-513.0117250	-513.0482200

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.5640992	-287.4516550	-287.4836400
2		NH_2	-303.6035560	-303.5020410	-303.5335380
3		OH	-323.4643834	-323.3759020	-323.4074630
4		F	-347.4860808	-347.4098020	-347.4414820
5		$C(O)CH_3$	-400.8949129	-400.7728350	-400.8083590
6		CN	-340.4843911	-340.4013120	-340.4342290
7		NO_2	-452.7489284	-452.6619270	-452.6967180

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.4982895	-287.3874880	-287.4187910
2		NH_2	-303.5412310	-303.4410270	-303.4714860
3		OH	-323.4014525	-323.3138620	-323.3442060
4		F	-347.4187581	-347.3434450	-347.3736880
5		$C(O)CH_3$	-400.8313075	-400.7109690	-400.7456760
6		CN	-340.4209493	-340.3391630	-340.3708710
7		NO_2	-452.6845620	-452.5988520	-452.6321530

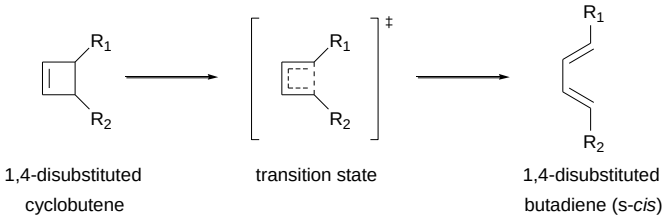
Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.5486733	-287.4351290	-287.4661070
2		NH_2	-303.5901698	-303.4873720	-303.5179010
3		OH	-323.4499610	-323.3598590	-323.3903380
4		F	-347.4673490	-347.3891980	-347.4193960
5		$C(O)CH_3$	-400.8787470	-400.7557870	-400.7908910
6		CN	-340.4694074	-340.3848970	-340.4166330
7		NO_2	-452.7305820	-452.6421350	-452.6755590

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.8283259	-399.7117770	-399.7455370
2		NH_2	-415.8674566	-415.7618960	-415.7951900
3		OH	-435.7279735	-435.6354590	-435.6688400
4		F	-459.7489933	-459.6686350	-459.7022010
5		$C(O)CH_3$	-513.1582463	-513.0321040	-513.0693630
6		CN	-452.7469382	-452.6597600	-452.6944470
7		NO_2	-565.0113259	-564.9202620	-564.9568420

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.7655721	-399.6506580	-399.6837690
2		NH_2	-415.8091387	-415.7048640	-415.7370330
3		OH	-435.6682931	-435.5766090	-435.6086900
4		F	-459.6845946	-459.6052020	-459.6371830
5		$C(O)CH_3$	-513.0972073	-512.9727740	-513.0090870
6		CN	-452.6857820	-452.5999250	-452.6333800
7		NO_2	-564.9486505	-564.8589190	-564.8939920

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.8169404	-399.6993360	-399.7334270
2		NH_2	-415.8605987	-415.7536960	-415.7868070
3		OH	-435.7194144	-435.6250960	-435.6580490
4		F	-459.7354378	-459.6531550	-459.6859010
5		$C(O)CH_3$	-513.1458424	-513.0188070	-513.0563550
6		CN	-452.7358868	-452.6473420	-452.6819460
7		NO_2	-564.9966542	-564.9041820	-564.9402660

5.3.3 1,4-Disubstituted butadienes



Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6359154	-234.4944140	-234.5257440
2		NH_2	-250.6743842	-250.5437670	-250.5748620
3		OH	-270.5357303	-270.4178030	-270.4487060
4		F	-294.5564868	-294.4506260	-294.4812810
5		$C(O)CH_3$	-347.9729971	-347.8215760	-347.8566650
6		CN	-287.5662949	-287.4537750	-287.4860150
7		NO_2	-399.8309940	-399.7143050	-399.7483130

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.5664067	-234.4269700	-234.4586200
2		NH_2	-250.6148278	-250.4855690	-250.5158600
3		OH	-270.4760230	-270.3593210	-270.3895020
4		F	-294.4973344	-294.3928450	-294.4228590
5		$C(O)CH_3$	-347.9039227	-347.7545100	-347.7888810
6		CN	-287.4994660	-287.3885760	-287.4199800
7		NO_2	-399.7673586	-399.6523190	-399.6852420

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6142553	-234.4712700	-234.5009170
2		NH_2	-250.6447713	-250.5128970	-250.5426150
3		OH	-270.5129943	-270.3939440	-270.4234540
4		F	-294.5411196	-294.4338460	-294.4631530
5		$C(O)CH_3$	-347.9455098	-347.7932180	-347.8268420
6		CN	-287.5417026	-287.4279430	-287.4586160
7		NO_2	-399.8094494	-399.6915910	-399.7246140

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6743842	-250.5437650	-250.5748660
2		NH_2	-266.7117593	-266.5919130	-266.6226040
3		OH	-286.5741956	-286.4670610	-286.4975820
4		F	-310.5952335	-310.5003690	-310.5307860
5		$C(O)CH_3$	-364.0167708	-363.8761250	-363.9109890
6		CN	-303.6102383	-303.5084570	-303.5404020
7		NO_2	-415.8772863	-415.7715520	-415.8056590

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6148278	-250.4855690	-250.5158590
2		NH_2	-266.6567673	-266.5380440	-266.5673000
3		OH	-286.5200684	-286.4141080	-286.4432770
4		F	-310.5452323	-310.4510880	-310.4800670
5		$C(O)CH_3$	-363.9599183	-363.8206350	-363.8542160
6		CN	-303.5544130	-303.4536060	-303.4840440
7		NO_2	-415.8246861	-415.7196490	-415.7516050

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	CH_3	-250.6447713	-250.5128990	-250.5426220
2		NH_2	-266.6785216	-266.5573480	-266.5869070
3		OH	-286.5473053	-286.4389220	-286.4682510
4		F	-310.5723749	-310.4761920	-310.5056040
5		$C(O)CH_3$	-363.9755424	-363.8344210	-363.8682130
6		CN	-303.5725979	-303.4701430	-303.5011570
7		NO_2	-415.8405217	-415.7339220	-415.7674850

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.5357303	-270.4178020	-270.4487050
2		NH_2	-286.5741956	-286.4670610	-286.4975820
3		OH	-306.4369030	-306.3423520	-306.3727520
4		F	-330.4561876	-330.3739480	-330.4041940
5		$C(O)CH_3$	-383.8759720	-383.7476320	-383.7822370
6		CN	-323.4674960	-323.3783230	-323.4100330
7		NO_2	-435.7329974	-435.6395940	-435.6732060

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.4760230	-270.3593210	-270.3895030
2		NH_2	-286.5200684	-286.4141080	-286.4432770
3		OH	-306.3839123	-306.2902280	-306.3192400
4		F	-330.4062238	-330.3246290	-330.3534740
5		$C(O)CH_3$	-383.8171419	-383.6902890	-383.7235670
6		CN	-323.4114136	-323.3230790	-323.3533490
7		NO_2	-435.6799311	-435.5874170	-435.6192710

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	CH_3	-270.5129944	-270.3939450	-270.4234560
2		NH_2	-286.5473053	-286.4389230	-286.4682530
3		OH	-306.4128641	-306.3176540	-306.3470230
4		F	-330.4408012	-330.3573100	-330.3863320
5		$C(O)CH_3$	-383.8439441	-383.7155730	-383.7492860
6		CN	-323.4402195	-323.3503150	-323.3807500
7		NO_2	-435.7086370	-435.6146100	-435.6474180

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.5564868	-294.4506260	-294.4812800
2		NH_2	-310.5952335	-310.5003690	-310.5307860
3		OH	-330.4561876	-330.3739480	-330.4041940
4		F	-354.4759562	-354.4058010	-354.4358150
5		$C(O)CH_3$	-407.8916602	-407.7759090	-407.8102450
6		CN	-347.4841328	-347.4072710	-347.4387660
7		NO_2	-459.7481700	-459.6671560	-459.7004280

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.4973344	-294.3928450	-294.4228600
2		NH_2	-310.5452322	-310.4510860	-310.4800630
3		OH	-330.4062237	-330.3246300	-330.3534740
4		F	-354.4257427	-354.3564150	-354.3851460
5		$C(O)CH_3$	-407.8311977	-407.7168870	-407.7501140
6		CN	-347.4265294	-347.3507190	-347.3809290
7		NO_2	-459.6930830	-459.6131700	-459.6450440

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	CH_3	-294.5411197	-294.4338450	-294.4631480
2		NH_2	-310.5723749	-310.4761930	-310.5056070
3		OH	-330.4408012	-330.3573100	-330.3863320
4		F	-354.4665812	-354.3949440	-354.4237330
5		$C(O)CH_3$	-407.8684619	-407.7519630	-407.7853620
6		CN	-347.4644642	-347.3864800	-347.4167390
7		NO_2	-459.7316444	-459.6496270	-459.6827810

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9729971	-347.8215770	-347.8566710
2		NH_2	-364.0167708	-363.8761240	-363.9109880
3		OH	-383.8759720	-383.7476320	-383.7822370
4		F	-407.8916602	-407.7759080	-407.8102410
5		$C(O)CH_3$	-461.3052410	-461.1441310	-461.1828530
6		CN	-400.8978147	-400.7756230	-400.8116230
7		NO_2	-513.1607605	-513.0344990	-513.0722100

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9039227	-347.7545100	-347.7888810
2		NH_2	-363.9599183	-363.8206350	-363.8542120
3		OH	-383.8171419	-383.6902890	-383.7235670
4		F	-407.8311977	-407.7168870	-407.7501140
5		$C(O)CH_3$	-461.2372908	-461.0782280	-461.1160850
6		CN	-400.8285636	-400.7080250	-400.7426630
7		NO_2	-513.0966329	-512.9720500	-513.0085060

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	CH_3	-347.9455097	-347.7932200	-347.8268450
2		NH_2	-363.9755424	-363.8344210	-363.8682130
3		OH	-383.8439441	-383.7155730	-383.7492860
4		F	-407.8684619	-407.7519630	-407.7853620
5		$C(O)CH_3$	-461.2755984	-461.1143820	-461.1520150
6		CN	-400.8675451	-400.7446510	-400.7792940
7		NO_2	-513.1342062	-513.0074310	-513.0451330

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.5662949	-287.4537740	-287.4860120
2		NH_2	-303.6102384	-303.5084520	-303.5403920
3		OH	-323.4674960	-323.3783230	-323.4100330
4		F	-347.4841328	-347.4072710	-347.4387660
5		$C(O)CH_3$	-400.8978147	-400.7756220	-400.8116190
6		CN	-340.4893639	-340.4060240	-340.4390450
7		NO_2	-452.7519440	-452.6645250	-452.6992980

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.4994660	-287.3885760	-287.4199810
2		NH_2	-303.5544130	-303.4536110	-303.4840500
3		OH	-323.4114140	-323.3230830	-323.3533500
4		F	-347.4265293	-347.3507200	-347.3809310
5		$C(O)CH_3$	-400.8285636	-400.7080250	-400.7426630
6		CN	-340.4229949	-340.3410480	-340.3727990
7		NO_2	-452.6873695	-452.6013690	-452.6348790

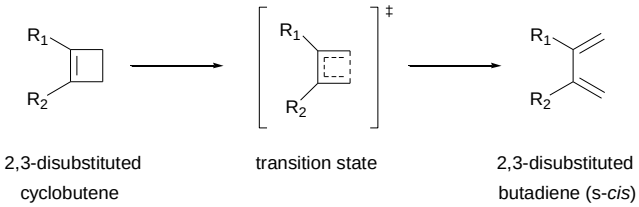
Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CH_3	-287.5417025	-287.4279430	-287.4586180
2		NH_2	-303.5725979	-303.4701430	-303.5011570
3		OH	-323.4402195	-323.3503150	-323.3807500
4		F	-347.4644643	-347.3864800	-347.4167380
5		$C(O)CH_3$	-400.8675451	-400.7446510	-400.7792940
6		CN	-340.4617415	-340.3774200	-340.4091110
7		NO_2	-452.7277645	-452.6394720	-452.6715590

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.8309939	-399.7143060	-399.7483230
2		NH_2	-415.8772863	-415.7715590	-415.8056750
3		OH	-435.7329974	-435.6395940	-435.6732060
4		F	-459.7481698	-459.6671550	-459.7004320
5		$C(O)CH_3$	-513.1607606	-513.0345000	-513.0722140
6		CN	-452.7519441	-452.6645270	-452.6993070
7		NO_2	-565.0139371	-564.9225100	-564.9590890

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.7673586	-399.6523190	-399.6852420
2		NH_2	-415.8246861	-415.7196480	-415.7516050
3		OH	-435.6799311	-435.5874170	-435.6192770
4		F	-459.6930828	-459.6131710	-459.6450360
5		$C(O)CH_3$	-513.0966329	-512.9720500	-513.0085050
6		CN	-452.6873696	-452.6013680	-452.6348860
7		NO_2	-564.9508585	-564.8608640	-564.8961680

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	CH_3	-399.8094490	-399.6915880	-399.7245730
2		NH_2	-415.8405217	-415.7339230	-415.7674980
3		OH	-435.7086370	-435.6146090	-435.6473980
4		F	-459.7316444	-459.6496270	-459.6827790
5		$C(O)CH_3$	-513.1342062	-513.0074310	-513.0451330
6		CN	-452.7277645	-452.6394720	-452.6715590
7		NO_2	-564.9949230	-564.9026000	-564.9391110

5.3.4 2,3-Disubstituted butadienes



Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6324811	-234.4908510	-234.5215960
2		NH_2	-250.6730504	-250.5423770	-250.5729040
3		OH	-270.5355160	-270.4178910	-270.4486510
4		F	-294.5593409	-294.4537810	-294.4841550
5		$C(O)CH_3$	-347.9615921	-347.8108730	-347.8458040
6		CN	-287.5594499	-287.4472230	-287.4790090
7		NO_2	-399.8218081	-399.7056410	-399.7391170

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.5667970	-234.4273560	-234.4584050
2		NH_2	-250.6092191	-250.4802510	-250.5100350
3		OH	-270.4717888	-270.3554080	-270.3851640
4		F	-294.4922832	-294.3881240	-294.4178680
5		$C(O)CH_3$	-347.9037153	-347.7542740	-347.7880140
6		CN	-287.4980905	-287.3874060	-287.4189590
7		NO_2	-399.7641197	-399.6493760	-399.6819660

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CH_3	CH_3	-234.6266161	-234.4840560	-234.5143240
2		NH_2	-250.6653470	-250.5335070	-250.5634920
3		OH	-270.5287670	-270.4096870	-270.4397420
4		F	-294.5496988	-294.4423250	-294.4719200
5		$C(O)CH_3$	-347.9615173	-347.8091900	-347.8429120
6		CN	-287.5574633	-287.4437020	-287.4747840
7		NO_2	-399.8211254	-399.7034350	-399.7362070

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	NH_2	-266.7159621	-266.5959680	-266.6258150
2		OH	-286.5803862	-286.4728210	-286.5025260
3		F	-310.5982570	-310.5037430	-310.5336550
4		$C(O)CH_3$	-364.0043637	-363.8643720	-363.8985520
5		CN	-303.5984368	-303.4973090	-303.5287410
6		NO_2	-415.8613986	-415.7559520	-415.7890600

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	NH_2	-266.6491713	-266.5310040	-266.5603050
2		OH	-286.5122680	-286.4064510	-286.4355960
3		F	-310.5321891	-310.4386060	-310.4676200
4		$C(O)CH_3$	-363.9503898	-363.8116440	-363.8446370
5		CN	-303.5441730	-303.4440130	-303.4745130
6		NO_2	-415.8143210	-415.7100060	-415.7416350

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NH_2	NH_2	-266.6921892	-266.5742370	-266.6036470
2		OH	-286.5611928	-286.4545070	-286.4836030
3		F	-310.5837994	-310.4883450	-310.5174530
4		$C(O)CH_3$	-364.0089290	-363.8674200	-363.9005370
5		CN	-303.6032762	-303.5008010	-303.5312280
6		NO_2	-415.8750826	-415.7679220	-415.7998470

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	OH	-306.4434338	-306.3491510	-306.3790000
2		F	-330.4589063	-330.3771040	-330.4069720
3		$C(O)CH_3$	-383.8681277	-383.7408370	-383.7747700
4		CN	-323.4608971	-323.3723960	-323.4037250
5		NO_2	-435.7224868	-435.6301800	-435.6630510

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	OH	-306.3739625	-306.2809410	-306.3099870
2		F	-330.3911852	-330.3103410	-330.3392620
3		$C(O)CH_3$	-383.8115153	-383.6853290	-383.7183890
4		CN	-323.4017002	-323.3140710	-323.3443890
5		NO_2	-435.6648658	-435.5733570	-435.6051880

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	OH	OH	-306.4240683	-306.3293530	-306.3593220
2		F	-330.4451608	-330.3615190	-330.3909540
3		$C(O)CH_3$	-383.8685617	-383.7394640	-383.7729930
4		CN	-323.4598842	-323.3692280	-323.3996660
5		NO_2	-435.7217429	-435.6270210	-435.6589210

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	F	-354.4782489	-354.4087740	-354.4386040
2		$C(O)CH_3$	-407.8882098	-407.7732300	-407.8070550
3		CN	-347.4792500	-347.4030790	-347.4343790
4		NO_2	-459.7407515	-459.6606860	-459.6934860

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	F	-354.4091651	-354.3404530	-354.3692220
2		$C(O)CH_3$	-407.8285477	-407.7147640	-407.7477800
3		CN	-347.4173700	-347.3420700	-347.3723100
4		NO_2	-459.6796934	-459.6004880	-459.6322470

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	F	F	-354.4637186	-354.3916920	-354.4204770
2		$C(O)CH_3$	-407.8843297	-407.7675120	-407.8010950
3		CN	-347.4749201	-347.3964040	-347.4266650
4		NO_2	-459.7341134	-459.6517080	-459.6835980

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	$C(O)CH_3$	-461.2924416	-461.1322950	-461.1703030
2		CN	-400.8868009	-400.7651840	-400.8005350
3		NO_2	-513.1510919	-513.0256560	-513.0626720

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	$C(O)CH_3$	-461.2355083	-461.0764250	-461.1134380
2		CN	-400.8298668	-400.7095510	-400.7439490
3		NO_2	-513.0920487	-512.9678000	-513.0036660

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	$C(O)CH_3$	$C(O)CH_3$	-461.2854982	-461.1234040	-461.1607210
2		CN	-400.8860555	-400.7629460	-400.7977250
3		NO_2	-513.1445384	-513.0174940	-513.0544030

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CN	-340.4778516	-340.3950240	-340.4277570
2		NO_2	-452.7405833	-452.6538350	-452.6880980

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CN	-340.4183856	-340.3367060	-340.3684390
2		NO_2	-452.6804783	-452.5949170	-452.6281670

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	CN	CN	-340.4758236	-340.3911410	-340.4229180
2		NO_2	-452.7352720	-452.6467870	-452.6802320

Entry	R_1	R_2	Butadiene [Product], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	NO_2	-565.0054468	-564.9147420	-564.9501290

Entry	R_1	R_2	Transition State, (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	NO_2	-564.9383045	-564.8489710	-564.8837910

Entry	R_1	R_2	Cyclobutene [Starting Material], (Hartree)		
			Total Electronic Energy	Sum of Electronic and Zero-Point Energies	Gibbs Free Energy
1	NO_2	NO_2	-564.9863494	-564.8944090	-564.9289600

6 Cartesian coordinates for

6.1 Butadiene

Butadiene (Product)

C	0.72804900	0.55279600	-0.10498400
C	-0.72814800	0.55286500	0.10497700
C	-1.54954600	-0.49279200	-0.07769000
H	-1.16000500	1.50560300	0.41439300
H	-2.61571700	-0.41398300	0.11653800
H	-1.18661800	-1.45212900	-0.43973600
C	1.54959300	-0.49274200	0.07767500
H	1.16000300	1.50554500	-0.41433600
H	2.61572900	-0.41366700	-0.11659200
H	1.18692200	-1.45213400	0.43986000

Transition state

C	-0.68376900	0.73503100	0.08458700
C	0.68376800	0.73503100	-0.08459000
C	1.06556100	-0.62765600	0.11906700
H	1.34123200	1.54429300	-0.40024700
H	1.87767300	-1.10389600	-0.44161300
H	0.87805200	-1.08464700	1.08402500
C	-1.06556100	-0.62765600	-0.11906700
H	-1.34123200	1.54429000	0.40025600
H	-1.87767300	-1.10389500	0.44161400
H	-0.87805200	-1.08464900	-1.08402400

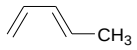
Cyclobutene (Starting material)

C	-0.81532000	-0.67167500	0.00001200
C	-0.81532800	0.67166600	-0.00010500
C	0.70046700	0.78701500	-0.00002400
H	-1.60358900	1.42096600	-0.00021700
H	1.14639500	1.24731900	-0.89082800

H	1.14628600	1.24746300	0.89076000
C	0.70047600	-0.78700800	0.00010400
H	-1.60357200	-1.42098500	0.00003300
H	1.14630900	-1.24730700	0.89095800
H	1.14640200	-1.24744800	-0.89063000

6.2 Monosubstituted butadienes

6.2.1 1-Substituted butadienes (outward rotation of substituents)



Butadiene (Product)

C	0.72804900	0.55279600	-0.10498400
C	-0.72814800	0.55286500	0.10497700
C	-1.54954600	-0.49279200	-0.07769000
H	-1.16000500	1.50560300	0.41439300
H	-2.61571700	-0.41398300	0.11653800
H	-1.18661800	-1.45212900	-0.43973600
C	1.54959300	-0.49274200	0.07767500
H	1.16000300	1.50554500	-0.41433600
H	2.61572900	-0.41366700	-0.11659200
H	1.18692200	-1.45213400	0.43986000

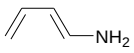
Transition state

C	-0.68376900	0.73503100	0.08458700
C	0.68376800	0.73503100	-0.08459000
C	1.06556100	-0.62765600	0.11906700
H	1.34123200	1.54429300	-0.40024700
H	1.87767300	-1.10389600	-0.44161300
H	0.87805200	-1.08464700	1.08402500
C	-1.06556100	-0.62765600	-0.11906700
H	-1.34123200	1.54429000	0.40025600
H	-1.87767300	-1.10389500	0.44161400
H	-0.87805200	-1.08464900	-1.08402400

Cyclobutene (Starting material)

C	-0.81532000	-0.67167500	0.00001200
C	-0.81532800	0.67166600	-0.00010500
C	0.70046700	0.78701500	-0.00002400

H	-1.60358900	1.42096600	-0.00021700
H	1.14639500	1.24731900	-0.89082800
H	1.14628600	1.24746300	0.89076000
C	0.70047600	-0.78700800	0.00010400
H	-1.60357200	-1.42098500	0.00003300
H	1.14630900	-1.24730700	0.89095800
H	1.14640200	-1.24744800	-0.89063000



Butadiene (Product)

C	0.01757000	0.69099400	-0.04223300
C	-1.42814300	0.51659600	0.09042300
C	-2.13545200	-0.61260100	-0.10355000
H	-1.97751300	1.41583300	0.37479200
H	-3.20712000	-0.64137700	0.07260000
H	-1.67278200	-1.53433900	-0.45012500
C	0.92724600	-0.29357800	0.13056700
H	0.37129500	1.69544300	-0.28009200
H	0.60602100	-1.28512400	0.44440800
N	2.29150000	-0.20301100	-0.11729600
H	2.89283900	-0.76876500	0.46904200
H	2.65943400	0.73093900	-0.26079300

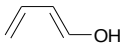
Transition state

C	-0.26385000	1.02515600	-0.00781000
C	-1.48151100	0.39612500	-0.05760100
C	-1.17972200	-1.00700100	-0.11392200
H	-2.46991300	0.84585700	0.04553800
H	-1.80847000	-1.75316100	0.38407400
H	-0.68591300	-1.39008900	-1.00199000
C	0.64555600	-0.02450000	0.39023500
H	0.02258300	2.04646600	-0.25791300
H	0.56523900	-0.41338300	1.39897200
N	1.92681100	-0.12095100	-0.13393800

H	2.03014300	0.01187100	-1.13221400
H	2.53581700	-0.83958200	0.23568600

Cyclobutene (Starting material)

C	0.56452500	-1.04396700	0.07911700
C	1.48906200	-0.12728400	-0.24369300
C	0.58168300	1.06068600	0.02496100
H	2.52503200	-0.19354000	-0.56843000
H	0.27976200	1.62886700	-0.86213200
H	0.90124300	1.75493100	0.81345700
C	-0.48841200	-0.01226400	0.45302500
H	0.55298600	-2.13158300	0.09544500
H	-0.69229200	0.02091500	1.53782700
N	-1.70112800	-0.02380400	-0.36667000
H	-2.20663900	-0.90046300	-0.24609000
H	-2.33333700	0.72447100	-0.08384800



Butadiene (Product)

C	0.03517800	0.68617200	-0.07719900
C	-1.40836200	0.51146100	0.10189500
C	-2.11356900	-0.61446200	-0.10442900
H	-1.94782100	1.40215300	0.42770700
H	-3.18009100	-0.65538100	0.09885100
H	-1.65464800	-1.52113700	-0.49296700
C	0.94114800	-0.27911100	0.14172100
H	0.39730500	1.66865900	-0.37655000
H	0.66418700	-1.26319800	0.51690500
O	2.27541500	-0.07988700	-0.10042300
H	2.79137500	-0.81636100	0.25751100

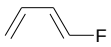
Transition state

C	0.03517800	0.68617200	-0.07719900
C	-1.40836200	0.51146100	0.10189500

C	-2.11356900	-0.61446200	-0.10442900
H	-1.94782100	1.40215300	0.42770700
H	-3.18009100	-0.65538100	0.09885100
H	-1.65464800	-1.52113700	-0.49296700
C	0.94114800	-0.27911100	0.14172100
H	0.39730500	1.66865900	-0.37655000
H	0.66418700	-1.26319800	0.51690500
O	2.27541500	-0.07988700	-0.10042300
H	2.79137500	-0.81636100	0.25751100

Cyclobutene (Starting material)

C	0.55204700	-1.04112500	0.06693700
C	1.48039000	-0.11192500	-0.21105600
C	0.55291200	1.07099800	0.01545700
H	2.53412700	-0.16752600	-0.47317200
H	0.26143800	1.61261900	-0.89133200
H	0.84214300	1.79132300	0.79325000
C	-0.50750800	-0.02468200	0.42808700
H	0.54069800	-2.12748900	0.07565000
H	-0.75387900	0.00322200	1.50047100
O	-1.69389900	-0.12421800	-0.34741900
H	-2.34038200	0.52199800	-0.02206200



Butadiene (Product)

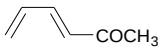
C	0.06680000	0.65657500	-0.09685200
C	-1.38143800	0.52292500	0.10883500
C	-2.10898900	-0.58322000	-0.11127900
H	-1.88930100	1.42202800	0.45937900
H	-3.17477900	-0.60577100	0.09818000
H	-1.66983400	-1.49045500	-0.51996300
C	0.94312200	-0.31375300	0.16739100
H	0.45186200	1.61104400	-0.45238500
H	0.72626600	-1.28858500	0.59090900
F	2.27097900	-0.14926900	-0.06496500

Transition state

C	-0.16319500	1.00958400	-0.05965900
C	-1.42685200	0.45043300	-0.01871800
C	-1.22637600	-0.95494000	-0.12449800
H	-2.37092500	0.94692300	0.20225000
H	-1.86938800	-1.67572000	0.39042800
H	-0.74440700	-1.35132400	-1.01064100
C	0.64906400	-0.07441100	0.35290600
H	0.17873500	1.99837300	-0.35567400
H	0.61730200	-0.49289300	1.35091600
F	1.91031500	-0.22326100	-0.16416200

Cyclobutene (Starting material)

C	0.53252000	-1.04949300	0.05025100
C	1.45762300	-0.11070300	-0.21125500
C	0.52323300	1.06756100	0.02816000
H	2.51429600	-0.15653000	-0.46237300
H	0.21890500	1.61195400	-0.87170300
H	0.80634600	1.78542100	0.80855300
C	-0.51078600	-0.03065000	0.43781300
H	0.52726700	-2.13528100	0.05342300
H	-0.81627900	-0.02007400	1.48942300
F	-1.69623000	-0.03841900	-0.31634800



Butadiene (Product)

C	0.82819200	0.63081700	-0.06357200
C	2.28841300	0.52427000	-0.13457900
C	3.01788400	-0.55727800	0.18699300
H	2.80923300	1.42697900	-0.45353600
H	4.10051200	-0.54974900	0.09900000
H	2.56418700	-1.47148200	0.56191200
C	-0.04818800	-0.39519200	-0.11736900

H	0.44164700	1.64593200	0.02204600
H	0.29581600	-1.41862300	-0.25323500
C	-1.51983600	-0.26747300	-0.01644100
O	-2.21570200	-1.27776800	-0.05721100
C	-2.15582500	1.10562000	0.13724600
H	-1.80806200	1.60134900	1.05178200
H	-1.90135000	1.75627000	-0.70840300
H	-3.24021100	0.98687800	0.18445600

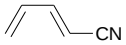
Transition state

C	-1.17675300	-0.88506300	-0.42543000
C	-2.30862800	-0.19768200	-0.07501700
C	-1.83494300	1.01156600	0.53422300
H	-3.35204200	-0.43961200	-0.27175900
H	-2.33428400	1.97653800	0.39729000
H	-1.24760300	0.94518300	1.44288800
C	-0.14053400	0.11824400	-0.44844000
H	-1.03054500	-1.94726000	-0.60385500
H	-0.23722600	0.92895200	-1.16611500
C	1.24157100	-0.16075600	0.02365000
O	1.51221600	-1.22172900	0.57826300
C	2.29362000	0.90913400	-0.20770800
H	2.50347800	1.00165800	-1.28201000
H	1.93849200	1.88928500	0.13477000
H	3.21600300	0.64643400	0.31501300

Cyclobutene (Starting material)

C	1.27327900	0.46501600	-0.91375500
C	2.09921800	0.31579600	0.13349100
C	1.23205400	-0.72077700	0.82172100
H	3.05557400	0.75712700	0.40277100
H	0.80346400	-0.43073900	1.78917000
H	1.65578600	-1.72730200	0.91651700
C	0.25802700	-0.56099700	-0.42379600
H	1.30381400	1.07307800	-1.81467200
H	0.18487700	-1.47342600	-1.02540800
C	-1.15848400	-0.12211800	-0.07904900

O	-2.09145500	-0.90039600	-0.19876000
C	-1.37136100	1.29527100	0.41930700
H	-0.58764300	1.60566000	1.11924400
H	-1.32560600	1.98759200	-0.43217500
H	-2.35502100	1.37803600	0.88712400



Butadiene (Product)

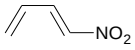
C	-0.37143400	0.65611600	-0.04288400
C	-1.82568100	0.53029900	0.06779600
C	-2.53309500	-0.59705700	-0.11396500
H	-2.35923600	1.45448600	0.28719200
H	-3.61378300	-0.60472200	-0.00607400
H	-2.06417600	-1.53692100	-0.39589300
C	0.51899900	-0.33771200	0.17136500
H	0.01078600	1.64271800	-0.30033200
H	0.19741900	-1.32741400	0.48776800
C	1.92507300	-0.15456800	0.01872500
N	3.07797400	-0.03008800	-0.09698300

Transition state

C	0.66239600	-1.02192700	-0.04576600
C	1.85172600	-0.34884500	-0.14918800
C	1.49628300	1.03950100	-0.13533000
H	2.86546900	-0.74523400	-0.14570300
H	2.10271900	1.79795900	0.36946400
H	0.87344500	1.43134200	-0.93114700
C	-0.24735100	-0.03842300	0.49344800
H	0.40283000	-2.03883300	-0.33079600
H	-0.05430600	0.35576900	1.48517000
C	-1.61908100	0.05300000	0.08659700
N	-2.72199900	0.15702200	-0.27793600

Cyclobutene (Starting material)

C	0.89671100	-1.05075500	0.06086000
C	1.75570900	-0.13696700	-0.41165400
C	0.91944400	1.05880700	0.00394500
H	2.71813500	-0.20709000	-0.91034300
H	0.49883400	1.65585700	-0.81179900
H	1.35661000	1.72925600	0.75299900
C	-0.08365000	-0.01053300	0.60537800
H	0.86607900	-2.13555800	0.08660800
H	-0.14403400	0.02575300	1.70006100
C	-1.43881000	-0.01362100	0.05676600
N	-2.51315000	-0.02140100	-0.38704300



Butadiene (Product)

C	0.78138300	0.64820800	-0.05469100
C	2.23041200	0.47473200	-0.15210000
C	2.91101500	-0.63134800	0.19149700
H	2.78204100	1.34594600	-0.50237900
H	3.99128000	-0.67794600	0.08975700
H	2.42090100	-1.50887000	0.60625200
C	-0.12001600	-0.34233400	-0.13211400
H	0.40072000	1.65997700	0.06823800
H	0.08053000	-1.39013000	-0.31028400
N	-1.54197100	-0.07415200	0.00509600
O	-1.92775900	1.08384000	0.18431300
O	-2.28454600	-1.05952300	-0.07216500

Transition state

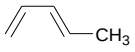
C	0.99653700	0.93510000	-0.36072300
C	2.19057600	0.32293700	-0.06274300
C	1.83974300	-0.94438400	0.49713400
H	3.20103900	0.64932900	-0.30073900
H	2.42120400	-1.85142700	0.30696700
H	1.25033200	-0.97838300	1.40579400

C	0.09510600	-0.16998100	-0.44271500
H	0.75025000	1.98223600	-0.50655800
H	0.16554400	-0.93438900	-1.20507200
N	-1.29941900	-0.02302100	-0.01311200
O	-2.06354100	-0.96549500	-0.24367300
O	-1.61448600	1.01946400	0.56938300

Cyclobutene (Starting material)

C	2.08336200	0.13312300	-0.24537700
C	1.26017100	0.83002100	0.55331600
C	0.21190500	-0.25140100	0.57651500
H	1.30979700	1.79236800	1.05082500
H	0.01676100	-0.76666700	1.51855000
C	1.12749500	-1.03302400	-0.43696400
H	3.08659000	0.31103500	-0.62174700
H	1.45404400	-2.01966900	-0.08987600
H	0.69457100	-1.12836800	-1.43877800
N	-1.15283200	0.08611000	0.01643200
O	-1.28282700	1.13602900	-0.60730300
O	-2.04086500	-0.74400200	0.20493600

6.2.2 1-Substituted butadienes (intward rotation of substituents)



Butadiene (Product)

C	1.31971300	0.39238900	0.19431500
C	0.05129700	1.08213000	-0.07608200
H	0.14458100	2.15874900	-0.22446500
H	2.06585500	0.99553900	0.71516900
C	-1.19478800	0.56862300	-0.11502600
C	1.66606200	-0.85621300	-0.16237600
H	-2.00453400	1.26561500	-0.33307700
H	1.00904100	-1.50115100	-0.73887700
H	2.64379200	-1.25834900	0.09037000
C	-1.61625000	-0.85080200	0.14030500
H	-1.78477800	-1.39597400	-0.80016200
H	-0.86560900	-1.40523100	0.71282100
H	-2.56455100	-0.87595900	0.69140200

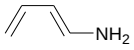
Transition state

C	-1.33798900	0.11996900	-0.41793800
C	-0.45991800	1.10075400	-0.00893000
H	-0.62635800	2.17644600	0.06523300
H	-2.12280100	0.16982200	-1.17344400
C	0.68333000	0.40298200	0.50358900
C	-0.95503800	-1.04350200	0.31223200
H	1.16403500	0.80293100	1.40970600
H	-0.97163300	-1.00931400	1.39566800
H	-1.03538100	-2.05535900	-0.09973600
C	1.68735700	-0.33739400	-0.36312100
H	1.23908400	-0.69056800	-1.29584700
H	2.51702800	0.34224300	-0.61780400
H	2.12957200	-1.19305000	0.16123400

Cyclobutene (Starting material)

C	1.50250800	-0.12474500	-0.27247300

C	0.59347000	-1.04484000	0.08779100
H	0.59311500	-2.13304500	0.10465800
H	2.52128800	-0.18559700	-0.64852100
C	-0.46390600	-0.01964800	0.48167500
C	0.60381600	1.05801900	0.04580100
H	-0.65881400	0.00727600	1.56359600
H	0.94798500	1.72688500	0.84567800
H	0.29980900	1.66976200	-0.81368200
C	-1.78811300	-0.03169300	-0.28011100
H	-1.61776400	-0.03088200	-1.36423000
H	-2.37704200	-0.92478400	-0.03427600
H	-2.39522700	0.84783000	-0.02932600



Butadiene (Product)

C	-1.28512000	0.44943300	-0.12964300
C	0.01676400	1.07742700	0.05427700
H	0.02217600	2.16138600	0.13565000
H	-2.05806000	1.11953000	-0.51063000
C	1.23355700	0.47667600	0.07299400
C	-1.65316800	-0.82697000	0.11573400
H	2.12247300	1.08910400	0.20547000
H	-0.99665200	-1.55665500	0.58189200
H	-2.66957100	-1.15584200	-0.08265100
N	1.50154300	-0.87880200	-0.02810700
H	2.42521800	-1.11885300	-0.36606300
H	0.77141700	-1.44645700	-0.44709100

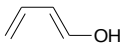
Transition state

C	-1.33448200	0.17553000	-0.39559300
C	-0.39616900	1.10373800	-0.01356100
H	-0.50177300	2.18566300	0.09355500
H	-2.15765800	0.28742500	-1.10303100
C	0.73290100	0.33496400	0.46330500
C	-0.98030200	-1.01898500	0.30849500

H	1.25885700	0.70215100	1.35445800
H	-0.99211200	-1.00005000	1.39269800
H	-1.09795100	-2.02047800	-0.11775700
N	1.65292900	-0.43871300	-0.30527300
H	2.52229100	0.07223100	-0.45825700
H	1.26615300	-0.72743400	-1.20063400

Cyclobutene (Starting material)

C	-1.49080000	0.13250300	-0.23968600
C	-0.56352800	1.05647300	0.06052000
H	-0.55784700	2.14506900	0.05942800
H	-2.53072700	0.19106100	-0.55233600
C	0.49471800	0.01810700	0.45119300
C	-0.58352000	-1.05415200	0.04693300
H	0.71104200	0.00399900	1.52672000
H	-0.89876100	-1.73971800	0.84459000
H	-0.29123800	-1.64891200	-0.82684400
N	1.76867400	-0.07896900	-0.25118300
H	1.63573100	0.03044500	-1.25610200
H	2.40985600	0.65325200	0.04906600



Butadiene (Product)

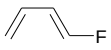
C	-1.29875500	0.46005200	0.00003800
C	0.03116800	1.06352500	-0.00003400
H	0.07010000	2.15010800	-0.00011500
H	-2.11575500	1.18207700	0.00026800
C	1.23291300	0.45684000	0.00000800
C	-1.62082400	-0.84834700	-0.00005400
H	2.15618800	1.03270800	-0.00009200
H	-0.87197700	-1.63224800	-0.00014000
H	-2.66382300	-1.15434400	0.00008700
O	1.37984500	-0.90427500	-0.00000400
H	2.31948700	-1.13651400	0.00027600

Transition state

C	-1.28085800	0.22387900	-0.39714200
C	-0.32096600	1.10405700	0.05526400
H	-0.38176900	2.18209300	0.20361400
H	-2.05139900	0.39019300	-1.15238600
C	0.76612100	0.27270300	0.47704900
C	-1.03310500	-1.00885900	0.27450000
H	1.34504100	0.49514100	1.38548100
H	-1.05405700	-1.02096900	1.35809500
H	-1.21892300	-1.98126700	-0.19172200
O	1.56165900	-0.32258800	-0.49633900
H	2.08067200	-1.03516200	-0.09039500

Cyclobutene (Starting material)

C	1.46732000	-0.13104000	-0.22758900
C	0.53385700	-1.05090700	0.07112600
H	0.52280300	-2.13803600	0.09508000
H	2.51697700	-0.19985000	-0.50315800
C	-0.51258800	-0.01201400	0.44579100
C	0.56155500	1.06514100	0.02326300
H	-0.75882300	0.02329900	1.51180800
H	0.87444100	1.77086300	0.80435500
H	0.27222000	1.63542500	-0.86754100
O	-1.76484600	-0.02072900	-0.21848500
H	-1.60971200	-0.15294600	-1.16821800



Butadiene (Product)

C	-1.25708300	0.50403500	-0.00001500
C	0.10234600	1.04735600	0.00009800
H	0.19443800	2.13129600	0.00013600
H	-2.04008600	1.26156600	-0.00050000
C	1.27297000	0.40053700	-0.00001300
C	-1.63091700	-0.78828500	0.00007900
H	2.25267500	0.86524900	-0.00000600

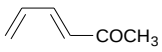
H	-0.91760700	-1.60525300	0.00055200
H	-2.68494000	-1.05219700	-0.00040600
F	1.36351400	-0.95361300	-0.00007500

Transition state

C	-1.24799800	0.22350100	-0.39503500
C	-0.28875300	1.12234100	0.03554700
H	-0.33863500	2.20455800	0.14916300
H	-1.99976300	0.34902600	-1.17504300
C	0.77674400	0.28735500	0.46837000
C	-0.98748200	-0.98148200	0.31580800
H	1.46713700	0.53596400	1.27822000
H	-1.00421600	-0.96166600	1.39863100
H	-1.14780900	-1.97033800	-0.12243200
F	1.50091300	-0.45198100	-0.45296500

Cyclobutene (Starting material)

C	1.45773800	-0.11066900	-0.21110500
C	0.53260500	-1.04949600	0.05013800
H	0.52732100	-2.13529300	0.05301600
H	2.51456400	-0.15642500	-0.46153900
C	-0.51080400	-0.03068400	0.43756000
C	0.52326500	1.06754700	0.02806200
H	-0.81599600	-0.02009100	1.48933600
H	0.80609300	1.78564300	0.80834100
H	0.21907400	1.61171100	-0.87200400
F	-1.69643100	-0.03841500	-0.31611900



Butadiene (Product)

C	2.15678700	0.32222500	-0.00008100
C	0.99860800	1.21201900	0.00005100
H	1.29509500	2.26205000	0.00003400
H	3.10339100	0.86307200	-0.00018700

C	-0.35266700	1.03896100	0.00010200
C	2.21412100	-1.02492300	-0.00003000
H	-0.93843200	1.95748700	0.00016300
H	1.32167800	-1.63807700	0.00004500
H	3.18397300	-1.51740200	-0.00021200
C	-1.17504200	-0.18879200	0.00003400
C	-2.67969200	0.04083700	-0.00013000
O	-0.72203100	-1.33120100	0.00013400
H	-2.98161100	0.61980200	-0.88281100
H	-3.19877900	-0.91972600	0.00014700
H	-2.98176000	0.62044300	0.88207500

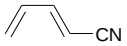
Transition state

C	-1.95224100	-0.30898100	-0.14236100
C	-1.41328000	0.92326800	-0.41335600
H	-1.85005500	1.76310500	-0.95084300
H	-2.70724300	-0.86335500	-0.69676400
C	-0.11746600	0.90279900	0.19722900
C	-1.23060800	-0.80519400	0.98854100
H	0.26416200	1.79147600	0.71617400
H	-1.25189800	-0.24326200	1.91521300
H	-0.98628800	-1.86455700	1.10734900
C	0.98588300	-0.01000600	-0.25094600
C	2.28230500	0.11996600	0.54108800
H	2.88559400	-0.78038000	0.40223900
H	2.85507700	0.97664300	0.16061800
H	2.10107700	0.29112500	1.60850400
O	0.92025100	-0.75023800	-1.22295700

Cyclobutene (Starting material)

C	-2.17956300	0.00600100	-0.27454900
C	-1.42998200	0.79603200	0.50790100
H	-1.56962900	1.78079800	0.94281200
H	-3.17406100	0.10055700	-0.70268200
C	-0.26516500	-0.17368700	0.57381200
C	-1.13912000	-1.09375700	-0.38476900
H	-0.10531400	-0.64519400	1.55429300

H	-1.40326400	-2.07299500	0.03312800
H	-0.71200300	-1.23744600	-1.38526200
C	1.07385200	0.25761600	0.00124600
C	2.20964900	-0.74531100	0.11837500
H	1.87312300	-1.76295800	-0.11413200
H	3.03182800	-0.46091800	-0.54254500
H	2.57702200	-0.75677600	1.15381200
O	1.23303400	1.34669600	-0.52393900



Butadiene (Product)

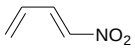
C	-1.66599200	0.01385500	-0.00003500
C	-0.71972800	1.12836100	0.00000400
H	-1.18263800	2.11355000	0.00002000
H	-2.71096200	0.32052600	-0.00008400
C	0.63590000	1.13522800	0.00001500
C	-1.39715600	-1.30526500	0.00002800
H	1.16116600	2.08693200	0.00003300
H	-0.39024800	-1.70863500	0.00007600
H	-2.21055600	-2.02561200	0.00001500
C	1.47617000	-0.01452700	0.00000800
N	2.19401000	-0.93323900	-0.00002600

Transition state

C	1.51799500	0.21360300	-0.53381900
C	0.98001900	-1.00348400	-0.21076300
H	1.34685000	-2.00577100	-0.42369300
H	2.15693800	0.48057400	-1.37379800
C	-0.19184900	-0.70566200	0.58098200
C	0.97176300	1.13277400	0.41847400
H	-0.44524400	-1.32909100	1.44589400
H	1.17304100	0.98025300	1.47228200
H	0.67951100	2.15287000	0.15649000
C	-1.35614000	-0.09132900	0.01386100
N	-2.34883200	0.34939300	-0.41279800

Cyclobutene (Starting material)

C	1.75551000	-0.13698000	-0.41182200
C	0.89674200	-1.05073600	0.06117000
H	0.86627200	-2.13557000	0.08629400
H	2.71759100	-0.20716900	-0.91112100
C	-0.08361600	-0.01047900	0.60581400
C	0.91925400	1.05882000	0.00394000
H	-0.14461500	0.02592100	1.70051900
H	1.35653100	1.72970400	0.75253400
H	0.49818600	1.65553000	-0.81183900
C	-1.43843000	-0.01346200	0.05637100
N	-2.51296000	-0.02162800	-0.38703200



Butadiene (Product)

C	-2.03424500	0.35301000	-0.03476800
C	-0.84140100	1.19386300	0.01225800
H	-1.09528900	2.25414800	0.02812300
H	-2.94552500	0.94491200	-0.10990200
C	0.50248500	1.04050100	0.03045200
C	-2.18024500	-0.98614200	0.01566600
H	1.16039700	1.89909800	0.05593400
H	-1.34559900	-1.66725500	0.09869000
H	-3.18160000	-1.40769500	-0.02520200
N	1.27909200	-0.17501200	0.00052400
O	0.71483000	-1.27488500	0.00526700
O	2.50697000	-0.02580500	-0.02938600

Transition state

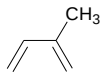
C	-1.82291200	-0.28155700	-0.24880000
C	-1.24412000	0.94233100	-0.49190700
H	-1.60017000	1.77910100	-1.08887800
H	-2.49820700	-0.85465300	-0.88127300
C	-0.02810500	0.91054700	0.24541800

C	-1.25084000	-0.74950900	0.97041700
H	0.43639400	1.77271500	0.71966200
H	-1.34641900	-0.14791800	1.86606500
H	-1.03691100	-1.80640900	1.14767000
N	1.07828500	-0.02042000	-0.11146200
O	0.94233400	-0.87195700	-0.98783600
O	2.12931300	0.18061100	0.50861400

Cyclobutene (Starting material)

C	-2.08333900	0.13319900	-0.24530100
C	-1.26013500	0.82985400	0.55358700
H	-1.30973300	1.79208800	1.05132200
H	-3.08654000	0.31125800	-0.62166900
C	-0.21187700	-0.25160300	0.57649300
C	-1.12751400	-1.03295000	-0.43714800
H	-0.01661800	-0.76702800	1.51841400
H	-1.45411300	-2.01965500	-0.09028900
H	-0.69459200	-1.12806500	-1.43898200
N	1.15281500	0.08611400	0.01639200
O	1.28259300	1.13597300	-0.60747600
O	2.04104200	-0.74377200	0.20506000

6.2.3 2-Substituted butadieness



Butadiene (Product)

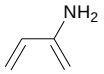
C	0.45563400	0.10963500	-0.05950500
C	-0.85428100	-0.55138900	-0.24956900
C	-2.03691800	-0.10078400	0.19382900
H	-0.82661800	-1.50876800	-0.77411300
H	-2.95700500	-0.64589300	0.00032700
H	-2.12140600	0.81710600	0.77111900
C	0.59750400	1.44594400	-0.08999300
H	-0.24296700	2.10542000	-0.28900600
C	1.63376300	-0.81689500	0.14468400
H	2.57060100	-0.26088500	0.25042100
H	1.49807700	-1.43739100	1.04068500
H	1.74068800	-1.50599500	-0.70460300
H	1.56441900	1.91734500	0.06848700

Transition state

C	0.44559900	-0.01579300	-0.09780300
C	-0.59697600	-0.92028900	-0.17369700
C	-1.75451200	-0.19342800	0.23512200
H	-0.58634800	-1.94386400	-0.54909100
H	-2.74340900	-0.36464800	-0.20534800
H	-1.79060900	0.23145000	1.23166500
C	-0.20775000	1.25843200	-0.14859900
H	-0.78836000	1.52149800	-1.02530900
C	1.91670000	-0.24307400	0.11692500
H	2.52049800	0.14946700	-0.71124700
H	2.25478000	0.27189200	1.02807800
H	2.14465300	-1.30781800	0.23401700
H	0.17042600	2.12693500	0.40554500

Cyclobutene (Starting material)

C	-0.48214800	0.05784700	-0.00045700
C	0.42693900	1.05075300	-0.00024500
C	1.62872200	0.12195900	0.00051400
H	0.34161000	2.13589200	-0.00130300
H	2.26742000	0.16155400	0.89235000
H	2.27029500	0.16173200	-0.88920000
C	0.57352600	-1.04237100	-0.00033400
H	0.59314300	-1.68289300	-0.89221400
C	-1.97294200	-0.01528400	0.00032000
H	-2.34283300	-0.55586400	0.88284500
H	-2.42249200	0.98431200	-0.00010700
H	-2.34413100	-0.55693000	-0.88101800
H	0.59241200	-1.68522600	0.88986100



Butadiene (Product)

C	0.48371500	0.06733800	-0.05570700
C	-0.85968200	-0.51358000	-0.27032600
C	-2.00526000	-0.00874700	0.20691100
H	-0.88148600	-1.43582300	-0.85282000
H	-2.96059400	-0.47867100	-0.01096000
H	-2.02298400	0.88409800	0.82712100
C	0.72180100	1.39554800	-0.07398500
H	-0.06497800	2.09713000	-0.32440100
H	1.71412700	1.80101000	0.10857600
N	1.50073300	-0.89779900	0.06454000
H	2.40727400	-0.52453300	0.32444600
H	1.26006900	-1.70197700	0.63490400

Transition state

C	0.46682600	-0.03723900	-0.09012800
C	-0.59008400	-0.92689100	-0.18175300
C	-1.71546600	-0.15216500	0.23321200

H	-0.60574800	-1.93506100	-0.59120000
H	-2.69848700	-0.26906400	-0.23978900
H	-1.77114600	0.24710100	1.23971400
C	-0.13881600	1.26371300	-0.12123800
H	-0.66566800	1.56721600	-1.01900100
H	0.28620700	2.10119700	0.44863400
N	1.82707400	-0.29598800	0.04814100
H	2.43516000	0.51145400	0.09848600
H	2.09540900	-1.03543100	0.68561900

Cyclobutene (Starting material)

C	0.50675800	0.07086400	-0.00456100
C	-0.40872300	1.06479600	-0.01442300
C	-1.58970800	0.10627900	-0.00449200
H	-0.34376900	2.14919600	-0.00636800
H	-2.23644600	0.11695100	-0.89208700
H	-2.22628400	0.12648800	0.89043900
C	-0.51739000	-1.04473200	0.00567000
H	-0.52105200	-1.67190000	0.90644400
H	-0.52723800	-1.69551000	-0.87920300
N	1.88754600	-0.02569900	0.08364700
H	2.29415700	-0.84599800	-0.35151700
H	2.40219000	0.81741800	-0.14640600

Butadiene (Product)

C	-0.48330600	0.03770500	0.03499200
C	0.86113900	-0.54920100	0.17008100
C	2.01530200	0.05892900	-0.13254700
H	0.86855900	-1.57600600	0.53247800
H	2.96671900	-0.44330900	0.01670200
H	2.05087100	1.06518500	-0.54269300
C	-0.78566600	1.34706100	0.07519600
H	-0.01525100	2.08843000	0.24867800
H	-1.80400300	1.70694400	-0.04966300

O	-1.42505900	-0.95579200	-0.11685500
H	-2.31123400	-0.56187300	-0.15699500

Transition state

C	0.47673600	-0.01849200	-0.09021700
C	-0.55207400	-0.93571600	-0.17276100
C	-1.68897800	-0.16993400	0.22730100
H	-0.55137400	-1.94383900	-0.58279600
H	-2.66282500	-0.28349600	-0.26285600
H	-1.74978500	0.23909000	1.22881100
C	-0.11226100	1.27739900	-0.12817300
H	-0.66917400	1.56816200	-1.01093600
H	0.32067200	2.11109300	0.43388100
O	1.82224600	-0.19011000	0.09517100
H	1.99398200	-1.08967700	0.41563200

Cyclobutene (Starting material)

C	-0.51527600	0.08716800	-0.00000400
C	0.39891400	1.07049100	-0.00011100
C	1.56030100	0.08500500	-0.00002900
H	0.34763600	2.15351400	-0.00021400
H	2.19870100	0.09024800	0.89244900
H	2.19867900	0.09007300	-0.89252500
C	0.47428800	-1.05702300	0.00009800
H	0.47528600	-1.69368200	-0.89446500
H	0.47530700	-1.69350300	0.89478900
O	-1.87479700	0.09449200	0.00002000
H	-2.20658700	-0.81642900	0.00007900

Butadiene (Product)

C	-0.47990600	0.03955600	0.03519500
C	0.86449700	-0.52760200	0.16534700
C	2.00694800	0.11051000	-0.12355900

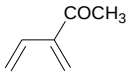
H	0.88937100	-1.55741700	0.51764200
H	2.96831100	-0.37189000	0.02542700
H	2.02149500	1.12284300	-0.51973800
C	-0.88375500	1.31085300	0.07074700
H	-0.16896200	2.10822100	0.23659400
H	-1.92960500	1.56751200	-0.05488900
F	-1.42525800	-0.94101800	-0.12126800

Transition state

C	0.46823900	-0.04546000	-0.07876400
C	-0.56388500	-0.94260100	-0.14404300
C	-1.67984500	-0.12285900	0.21013200
H	-0.57873600	-1.96140200	-0.52024400
H	-2.64294000	-0.20037100	-0.30544500
H	-1.74062200	0.31068300	1.20094300
C	-0.04575300	1.27335300	-0.13919300
H	-0.58968500	1.58343900	-1.02360600
H	0.40821000	2.08927600	0.43036100
F	1.78569300	-0.31069100	0.12546700

Cyclobutene (Starting material)

C	-0.51363200	0.05222100	-0.00000100
C	0.34062300	1.07804400	-0.00010700
C	1.53361400	0.12423400	-0.00003200
H	0.24761600	2.15759600	-0.00021100
H	2.16675600	0.15962500	0.89392600
H	2.16672800	0.15944700	-0.89401700
C	0.49197900	-1.06168300	0.00010300
H	0.50941200	-1.69562300	-0.89398700
H	0.50943300	-1.69544000	0.89432300
F	-1.85727100	-0.02694400	0.00002100



Butadiene (Product)

C	-0.27553800	0.33371700	-0.10308400
C	-1.46160500	-0.54539700	-0.16747100
C	-2.69108200	-0.21733200	0.25279100
H	-1.27604500	-1.54281600	-0.55780800
H	-3.51804500	-0.91611100	0.16182700
H	-2.91386200	0.74250700	0.71454900
C	-0.34416700	1.67775700	-0.18071000
H	-1.29247600	2.18680800	-0.32980000
H	0.53478000	2.30999800	-0.11294000
C	1.05499500	-0.36710900	0.00418000
O	1.10960100	-1.58800800	-0.05735400
C	2.32584700	0.44816100	0.18039600
H	2.50468600	1.09287900	-0.68851200
H	2.26790000	1.09300600	1.06507500
H	3.16555300	-0.24097800	0.28982300

Transition state

C	-0.27961700	0.11017900	-0.18661200
C	-1.16546700	-0.96388800	-0.17072000
C	-2.37883900	-0.42021500	0.32516000
H	-1.03643400	-1.96923400	-0.56959700
H	-3.36349900	-0.76240700	-0.00710900
H	-2.38162200	0.05209600	1.30198700
C	-1.13840400	1.25648100	-0.20914600
H	-1.80442400	1.39229300	-1.05303700
H	-0.90231400	2.17015900	0.34168200
C	1.18602500	0.15356600	-0.00329300
C	1.93768600	-1.16614000	0.02727000
H	1.59380500	-1.84398700	-0.76343000
H	3.00739100	-0.97688100	-0.08752700
H	1.76835600	-1.67151700	0.98686000
O	1.76880400	1.22369800	0.14427800

Cyclobutene (Starting material)

C	0.25456700	-0.00037500	0.00014400
C	1.05907800	-1.08757200	0.00014300
C	2.33925800	-0.27737500	-0.00004300
H	0.87174900	-2.15927600	0.00023300
H	2.96980200	-0.39245700	-0.89044800
H	2.97000000	-0.39236400	0.89023400
C	1.40830100	0.99018400	0.00000100
H	1.48343800	1.62411200	0.89003000
H	1.48326700	1.62404200	-0.89009300
C	-1.20553900	0.20911500	0.00028700
C	-2.10278200	-1.01629400	0.00004300
H	-3.14855400	-0.70153100	-0.00033000
H	-1.90878300	-1.63745500	-0.88318000
H	-1.90938300	-1.63734800	0.88347300
O	-1.66610500	1.34577300	-0.00042100

Butadiene (Product)

C	0.09232300	0.30734200	-0.08293600
C	-0.99720100	-0.68357600	-0.24499200
C	-2.24611700	-0.52339700	0.21082200
H	-0.72432300	-1.60495200	-0.75668100
H	-3.00452500	-1.28125400	0.03771400
H	-2.54774000	0.35295700	0.77948200
C	-0.07476900	1.64491000	-0.06667100
H	-1.05749100	2.08276900	-0.21140700
H	0.76191300	2.32051400	0.07749200
C	1.42297200	-0.23548900	0.04108300
N	2.48413200	-0.70411000	0.13279500

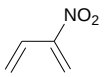
Transition state

C	0.11196800	0.04488400	-0.13787800
C	-0.86190800	-0.94339100	-0.18599600

C	-2.03479800	-0.29859300	0.28867300
H	-0.79566800	-1.94350000	-0.60878200
H	-3.03231000	-0.53276300	-0.09361700
H	-2.03107500	0.13107900	1.28455800
C	-0.62850200	1.27282000	-0.14741700
H	-1.24823300	1.49261200	-1.00804600
C	1.52438500	-0.08337100	0.01707900
H	-0.31424600	2.14856800	0.42648300
N	2.67923800	-0.17858500	0.14180500

Cyclobutene (Starting material)

C	-0.14574800	0.05743400	-0.00000600
C	0.76628800	1.05237200	-0.00010600
C	1.95346100	0.11150000	-0.00004400
H	0.67921800	2.13515000	-0.00020600
H	2.59113600	0.15748600	0.89078600
H	2.59109400	0.15731000	-0.89091400
C	0.89926500	-1.05465200	0.00009800
H	0.90587500	-1.68884500	-0.89286400
C	-1.56665500	0.02741900	0.00001500
H	0.90590300	-1.68865700	0.89319500
N	-2.73041400	-0.03384000	0.00003700



Butadiene (Product)

C	-0.21488700	0.37718100	-0.10833400
C	-1.34198000	-0.55679000	-0.22467100
C	-2.57123400	-0.29653500	0.24010500
H	-1.13208300	-1.50415000	-0.71113700
H	-3.38150800	-1.00457700	0.09407200
H	-2.80707800	0.61276200	0.78803200
C	-0.25364200	1.71437700	-0.13449300
H	-1.19825200	2.22623200	-0.28319700
H	0.64683000	2.30520500	-0.01850300

N	1.12988200	-0.26123600	0.02941100
O	2.11500400	0.46255200	0.15973100
O	1.16666800	-1.49208000	0.00142200

Transition state

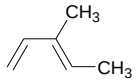
C	-0.22398900	0.05896000	-0.15585200
C	-1.17024000	-0.94338500	-0.12588300
C	-2.33603100	-0.25119900	0.29859900
H	-1.10193000	-1.96500100	-0.48724000
H	-3.33296900	-0.48309400	-0.08513300
H	-2.33088900	0.24846000	1.26142900
C	-0.91861500	1.29828900	-0.22820700
H	-1.54122300	1.49069700	-1.09395200
H	-0.59012900	2.18354800	0.31805200
N	1.20747800	-0.07225500	0.01364500
O	1.85919600	0.96797600	0.15641700
O	1.68305900	-1.21107800	0.00100600

Cyclobutene (Starting material)

C	-0.19792000	-0.04330900	-0.00006500
C	-1.05496500	-1.07479500	-0.00017100
C	-2.25653200	-0.14403300	0.00016700
H	-0.93670500	-2.15245200	-0.00045700
H	-2.88885600	-0.20524500	0.89302800
H	-2.89015100	-0.20538700	-0.89172100
C	-1.22970100	1.05346800	-0.00011000
H	-1.24996600	1.68537800	-0.89322100
H	-1.24993700	1.68606700	0.89251800
N	1.24345600	0.00221200	0.00003300
O	1.85557900	-1.06929600	0.00007600
O	1.76268800	1.12281700	0.00001200

6.3 Disubstituted butadienes

6.3.1 1,2-Disubstituted butadienes



Butadiene (Product)

C	0.05757100	0.32661700	-0.07845400
C	1.51948000	0.16471800	-0.24813400
C	2.26930700	-0.84691300	0.21475800
H	2.02190700	0.97677800	-0.77889300
H	3.33859600	-0.88896600	0.02425800
H	1.84343900	-1.65703900	0.80252200
C	-0.76745700	-0.73840300	-0.14928300
H	-0.30992900	-1.70246700	-0.37344200
C	-2.25878500	-0.77904600	0.02990400
H	-2.74886100	-1.18882300	-0.86447200
H	-2.52816700	-1.44391600	0.86318500
H	-2.69923000	0.20052100	0.23481000
C	-0.39263800	1.75429100	0.14530200
H	-1.47950400	1.86385000	0.16417200
H	0.00271300	2.14548600	1.09285700
H	-0.00583200	2.40699800	-0.64954800

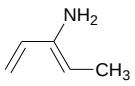
Transition state

C	0.17058000	0.61131700	-0.14307700
C	1.51773600	0.32200900	-0.05398000
C	1.58696700	-1.07379100	0.23593600
H	2.36560100	0.97850800	-0.25374700
H	2.38295000	-1.71741200	-0.15586200
H	1.14032900	-1.44748500	1.15100100
C	-0.43949000	-0.66611500	-0.39866300
H	-0.13849200	-1.17150300	-1.31087800
C	-1.79344100	-1.07582600	0.12779400
H	-2.59847800	-0.61742400	-0.47002800
H	-1.93052500	-2.16134000	0.06408400

H	-1.94690300	-0.77104100	1.17000500
C	-0.55145800	1.90719900	0.10758200
H	-1.32346900	2.10891500	-0.64606700
H	-1.05045200	1.90407700	1.08793600
H	0.15407400	2.74594600	0.10999300

Cyclobutene (Starting material)

C	0.74999500	0.13772100	0.04212000
C	0.39479700	1.39262700	-0.28777400
C	-1.06759700	1.21271400	0.07870000
H	0.95183700	2.24503200	-0.67275300
H	-1.78148200	1.27267000	-0.75372300
H	-1.44235100	1.83248000	0.90427400
C	-0.66338000	-0.25645700	0.47639400
H	-0.74693000	-0.43186200	1.55970400
C	-1.34877400	-1.39142600	-0.28332800
H	-0.87246000	-2.35785900	-0.07261200
H	-2.40589700	-1.47365600	0.00075800
H	-1.30100200	-1.22249500	-1.36697100
C	2.02213000	-0.64359500	0.02744800
H	1.93344800	-1.53965200	-0.60272400
H	2.85599600	-0.04282900	-0.35375900
H	2.28581700	-0.99132800	1.03644900



Butadiene (Product)

C	0.05711100	0.31129500	-0.07281500
C	1.52221700	0.22047600	-0.23585000
C	2.29884800	-0.77770900	0.20798900
H	1.99434200	1.05741800	-0.75646000
H	3.36810800	-0.78666700	0.01411300
H	1.89141400	-1.61050800	0.77548400
C	-0.76135200	-0.76180500	-0.16646100
H	-0.31616000	-1.71562900	-0.43052200
C	-2.25096600	-0.69950800	0.04095400

H	-2.77859400	-0.23325900	-0.80820200
H	-2.67419200	-1.70259400	0.15863100
H	-2.51321800	-0.12171700	0.93884800
N	-0.43043700	1.59861300	0.22034400
H	0.21040900	2.36044300	0.03673100
H	-1.36418900	1.80572500	-0.11392900

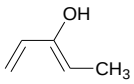
Transition state

C	0.23275000	0.60180800	-0.14120200
C	1.54949200	0.18834600	-0.05680800
C	1.45083400	-1.20897600	0.22184000
H	2.45939800	0.75277400	-0.25855600
H	2.15797200	-1.93345600	-0.20049700
H	0.98489400	-1.55040300	1.14022400
C	-0.52942300	-0.59160000	-0.39919900
H	-0.30761400	-1.10534900	-1.32951600
C	-1.91563900	-0.83163600	0.14899300
H	-2.69571700	-0.41487500	-0.50926000
H	-2.11753600	-1.90725800	0.22427100
H	-2.04570000	-0.38251000	1.14000000
N	-0.34427300	1.83635700	0.17081500
H	0.30962100	2.56961300	0.41814000
H	-1.06349000	2.16931300	-0.46224900

Cyclobutene (Starting material)

C	0.77751800	0.05356100	0.03784200
C	0.56484000	1.34556600	-0.29250200
C	-0.90820800	1.29926100	0.08273700
H	1.20361500	2.14500300	-0.65769100
H	-1.62520400	1.43496900	-0.73903600
H	-1.22040100	1.93273700	0.92473500
C	-0.65599600	-0.20678700	0.47058200
H	-0.74908100	-0.37936600	1.55282400
C	-1.45247600	-1.26254300	-0.29606500
H	-1.08615700	-2.27746400	-0.08894800
H	-2.51200200	-1.23428300	-0.01186600
H	-1.38653200	-1.09348400	-1.37846700

N	1.86794200	-0.80038100	0.11596800
H	1.65962000	-1.78359600	-0.01758300
H	2.68647400	-0.51619600	-0.41130200



Butadiene (Product)

C	-0.06744400	0.32470800	0.05211100
C	-1.53222500	0.24858400	0.17818700
C	-2.29971900	-0.79727900	-0.15756200
H	-1.99665300	1.15399700	0.56707400
H	-3.37455500	-0.77376800	-0.00206800
H	-1.88761000	-1.70090600	-0.59993800
C	0.77882700	-0.72128500	0.12775900
H	0.33859900	-1.69058300	0.34332700
C	2.27483000	-0.67545600	-0.02441100
H	2.79100900	-0.76522200	0.94279300
H	2.62591400	-1.50716600	-0.64830800
H	2.63755500	0.24402600	-0.50358900
O	0.33021300	1.63444300	-0.12883200
H	1.29842100	1.68844600	-0.12513900

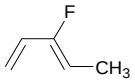
Transition state

C	0.25432600	0.58316400	-0.14068000
C	1.55567600	0.13904500	-0.04486100
C	1.39388900	-1.25386900	0.23110500
H	2.48316400	0.66373100	-0.26834200
H	2.04995200	-2.01085300	-0.21408900
H	0.91911700	-1.57655700	1.15092900
C	-0.57148500	-0.55515800	-0.39335900
H	-0.36378800	-1.10130100	-1.30794000
C	-1.97258900	-0.70227400	0.14276200
H	-2.70201600	-0.21195300	-0.52034400
H	-2.25541300	-1.76014000	0.20135600
H	-2.08214300	-0.25609000	1.13727700
O	-0.29410700	1.82498800	0.06524800

H	0.34508500	2.38781500	0.52937000

Cyclobutene (Starting material)

C	0.78817100	-0.02075300	0.03641600
C	0.72127200	1.28008100	-0.28648000
C	-0.75196300	1.36870300	0.08949400
H	1.43375500	2.00569300	-0.66305800
H	-1.44741100	1.56798900	-0.73651200
H	-1.00102600	2.03113500	0.92896000
C	-0.65838400	-0.15780400	0.47528800
H	-0.77177200	-0.31938600	1.55783400
C	-1.55481000	-1.12638000	-0.29662000
H	-1.29033200	-2.17384800	-0.09676300
H	-2.60559900	-0.99614700	-0.00976500
H	-1.47165300	-0.95935500	-1.37752700
O	1.80104400	-0.92861600	-0.00216100
H	1.47996500	-1.79023600	0.30552500



Butadiene (Product)

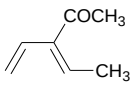
C	-0.06656900	0.28347200	0.04932000
C	-1.52586800	0.25956900	0.16202100
C	-2.32040200	-0.77768500	-0.13908400
H	-1.96464300	1.19099500	0.51716300
H	-3.39467500	-0.71770500	0.00790800
H	-1.93125400	-1.70987200	-0.54107200
C	0.81162200	-0.72364100	0.11688100
H	0.39618200	-1.71201700	0.29892800
C	2.30003500	-0.60532300	-0.02446000
H	2.80900000	-0.97868200	0.87436700
H	2.66030200	-1.21134000	-0.86716600
H	2.61037400	0.42928200	-0.19034000
F	0.40242300	1.56566600	-0.12087200

Transition state

C	0.25849700	0.58098000	-0.12707000
C	1.56131500	0.18279200	-0.01167800
C	1.41310500	-1.22221500	0.21107700
H	2.47633500	0.73812700	-0.19852900
H	2.07260900	-1.95722500	-0.26258100
H	0.93252100	-1.57708300	1.11535100
C	-0.56885600	-0.54116000	-0.40499500
H	-0.35872200	-1.07746100	-1.32510500
C	-1.96223300	-0.70860200	0.14272800
H	-2.70119100	-0.23111000	-0.51857500
H	-2.22880600	-1.77031000	0.20266000
H	-2.07170000	-0.26506700	1.13801500
F	-0.25911200	1.82104000	0.10982100

Cyclobutene (Starting material)

C	0.76587600	-0.10085300	0.04576700
C	0.85656800	1.18629100	-0.29344900
C	-0.60677600	1.41846900	0.07883900
H	1.64162800	1.83038800	-0.67174500
H	-1.26807600	1.67961800	-0.75589900
H	-0.78106200	2.11137900	0.91072300
C	-0.67571200	-0.11059200	0.47945900
H	-0.80378800	-0.25051000	1.56153000
C	-1.65456100	-0.99474500	-0.29062300
H	-1.47043600	-2.05602200	-0.08537900
H	-2.68872900	-0.77094600	-0.00207700
H	-1.55818700	-0.83828400	-1.37196600
F	1.64625300	-1.12189400	0.03276100



Butadiene (Product)

C	0.32752700	0.08573700	0.10877200
C	1.71221100	-0.42217700	0.27461800

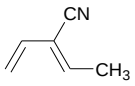
C	2.82013300	0.17007900	-0.19171700
H	1.80175500	-1.37391200	0.79286000
H	3.80247700	-0.25536000	-0.00512900
H	2.78881900	1.07959800	-0.78828500
C	0.08864300	1.42095500	0.12972500
H	0.96044800	2.04033600	0.34068700
C	-1.16430900	2.21940300	-0.09834900
H	-1.63174700	2.49649000	0.85867500
H	-0.90599300	3.16088400	-0.59761100
H	-1.91671500	1.71481200	-0.70482400
C	-0.69954800	-1.00495100	-0.03542500
C	-2.19157700	-0.73000500	0.05923200
H	-2.44009400	-0.01405700	0.84837500
H	-2.56736500	-0.32868000	-0.89051100
H	-2.69711100	-1.68023800	0.24736400
O	-0.31911900	-2.15926600	-0.19784200

Transition state

C	-0.04606000	-0.30018200	-0.20803200
C	-0.49519500	-1.61106400	-0.09065000
C	-1.86061200	-1.50061600	0.27989900
H	0.01747800	-2.53481900	-0.35831000
H	-2.61997900	-2.22090800	-0.03827200
H	-2.11606900	-0.96496600	1.18856000
C	-1.26311600	0.45162000	-0.40903700
H	-1.81878800	0.20496900	-1.30891000
C	-1.56873900	1.80139600	0.17414200
H	-1.08201900	2.57928200	-0.43220300
H	-2.64750000	1.99575600	0.16262200
H	-1.19149500	1.91267900	1.19512700
C	1.30667700	0.25521500	-0.02851300
C	2.45889500	-0.72865400	0.10677200
H	2.37655300	-1.55348600	-0.61090900
H	3.40275900	-0.19968700	-0.04442900
H	2.45818800	-1.16815900	1.11262600
O	1.50372200	1.46788200	0.02332600

Cyclobutene (Starting material)

C	0.04236200	-0.30724300	-0.11125900
C	-0.46076500	-1.54652500	0.08327700
C	-1.89444600	-1.12729500	-0.16498900
H	-0.01113600	-2.50965500	0.31608900
H	-2.56445300	-1.21393600	0.70021300
H	-2.38242600	-1.59125800	-1.03189000
C	-1.31850500	0.32198100	-0.40266400
H	-1.41929600	0.64455000	-1.44702400
C	-1.80699700	1.42358600	0.53457500
H	-1.20737900	2.33144800	0.40933300
H	-2.85564300	1.67285000	0.32784100
H	-1.73330700	1.10984700	1.58397000
C	1.39794700	0.27344100	-0.09127000
C	2.55495300	-0.62319100	0.31431300
H	2.55235100	-1.55823500	-0.25853500
H	3.49796900	-0.09569000	0.15370900
H	2.46966800	-0.89060400	1.37552900
O	1.57079400	1.45152000	-0.38764100



Butadiene (Product)

C	0.13990900	0.08693900	-0.10249000
C	1.58109300	0.40514000	-0.23681900
C	2.58362300	-0.35123500	0.22915400
H	1.80915100	1.34251200	-0.74208700
H	3.61899000	-0.06584800	0.06726800
H	2.40877700	-1.26424700	0.79346500
C	-0.37143100	-1.16601500	-0.12617000
H	0.33435300	-1.97939500	-0.28863500
C	-1.80787400	-1.54990800	0.03395800
H	-2.15528200	-2.11170700	-0.84370800
H	-1.92962200	-2.21696700	0.89878000
H	-2.46005300	-0.68329300	0.17317100
C	-0.73815200	1.22068600	0.03335500

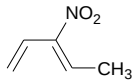
N	-1.42133100	2.15790200	0.13654600

Transition state

C	0.18688300	-0.40880400	-0.18110500
C	-0.68321400	-1.48098500	-0.04958000
C	-1.92830600	-0.88540100	0.28508100
H	-0.50274800	-2.52908400	-0.28062600
H	-2.88551300	-1.29439100	-0.05026400
H	-1.99634700	-0.28626300	1.18712000
C	-0.67334500	0.72489500	-0.41394000
H	-1.27010300	0.67925300	-1.31882800
C	-0.42985800	2.10206300	0.13717000
H	0.34704300	2.61035400	-0.45561500
H	-1.33428800	2.71664000	0.07554400
H	-0.08672100	2.08122600	1.17685800
C	1.60019900	-0.36009700	0.00103700
N	2.75636100	-0.30396600	0.14197600

Cyclobutene (Starting material)

C	-0.39196900	-0.37271300	0.04417700
C	0.28620900	-1.49117100	-0.28468200
C	1.63756300	-0.91251500	0.07715200
H	-0.02701100	-2.46055100	-0.66221800
H	2.33178600	-0.78521800	-0.76272100
H	2.16669600	-1.41443300	0.89674100
C	0.85973400	0.39906600	0.47789800
H	0.88281800	0.58144300	1.56005600
C	1.19841100	1.67642200	-0.28373000
H	0.46957200	2.46703100	-0.06926200
H	2.19009900	2.04612300	0.00482300
H	1.19938600	1.50274700	-1.36680000
C	-1.76522600	-0.00832300	0.01930500
N	-2.88024000	0.33118100	0.01409400



Butadiene (Product)

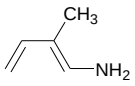
C	0.26099800	-0.15937900	-0.12695700
C	1.70483500	0.07607400	-0.29174200
C	2.66376000	-0.72945500	0.18309800
H	1.97954100	0.97518400	-0.83680400
H	3.71121200	-0.52398800	-0.01681300
H	2.44368200	-1.60244400	0.79311700
C	-0.33490500	-1.36977400	-0.10170400
H	0.35321000	-2.19692300	-0.26662500
C	-1.76701700	-1.75103900	0.11856700
H	-2.34330700	-1.62588800	-0.80811300
H	-1.82905500	-2.80301400	0.41418700
H	-2.25865900	-1.12800500	0.86975200
N	-0.53730300	1.07354000	0.01391900
O	-1.76084500	1.01150200	-0.13469900
O	0.07815400	2.11246500	0.26798600

Transition state

C	-0.03068800	-0.34553800	-0.17985700
C	-0.60411500	-1.59267600	-0.05948800
C	-1.95647200	-1.28956000	0.24912900
H	-0.18238600	-2.56269500	-0.30710400
H	-2.79253500	-1.88673800	-0.12375600
H	-2.17827300	-0.72299000	1.14736900
C	-1.09832500	0.58504600	-0.41554300
H	-1.65905500	0.41706300	-1.33019000
C	-1.23599400	1.95702300	0.17670600
H	-0.70944600	2.68810300	-0.45309900
H	-2.29128500	2.25217400	0.20761900
H	-0.81064500	2.02698400	1.18160500
N	1.36095900	-0.01017500	0.00116300
O	2.16189300	-0.94220800	0.12620800
O	1.66941500	1.18890200	0.00425700

Cyclobutene (Starting material)

C	-0.08640600	-0.34873500	0.08122100
C	0.44347700	-1.56070300	-0.13561600
C	1.84619800	-1.06191700	0.16451800
H	0.02903500	-2.52570000	-0.40538500
H	2.53834700	-1.09349600	-0.68518200
H	2.32760600	-1.52154000	1.03577600
C	1.20514400	0.36112000	0.42446400
H	1.26194900	0.65677200	1.47908700
C	1.66178600	1.50536400	-0.47629300
H	1.01880400	2.38170500	-0.34498600
H	2.69076600	1.79564700	-0.23241900
H	1.62999100	1.21395800	-1.53339600
N	-1.45066900	0.11641100	0.02747900
O	-2.32365000	-0.68356000	-0.31890700
O	-1.64672700	1.29693500	0.33695600



Butadiene (Product)

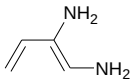
C	0.03464600	0.33007700	-0.07444400
C	1.49581700	0.26661700	-0.19813700
C	2.30837900	-0.72917800	0.20164400
H	1.95850700	1.14250500	-0.65970700
H	3.37734800	-0.69295600	0.00971600
H	1.93626100	-1.60260700	0.73291300
C	-0.71848700	-0.79352200	-0.14469800
H	-0.25213800	-1.74655500	-0.38109400
N	-2.10569100	-0.84800600	-0.03201400
H	-2.50501700	-1.76665700	0.10306700
H	-2.55035500	-0.14520900	0.54530000
C	-0.60609400	1.68875100	0.11352200
H	-1.56876300	1.76375700	-0.40941100
H	-0.78310300	1.92537900	1.17442800
H	0.04153400	2.48191100	-0.27843600

Transition state

C	-0.05896200	0.62895000	-0.12475300
C	1.30673800	0.75995000	-0.02520800
C	1.81298100	-0.55902600	0.21733700
H	1.89743100	1.65986100	-0.20682000
H	2.77120100	-0.89504400	-0.19456400
H	1.55153300	-1.05426800	1.14802400
C	-0.22591600	-0.78329900	-0.39363300
H	0.13361200	-1.16654400	-1.34156400
N	-1.30596300	-1.50381100	0.10740500
H	-1.54257300	-1.36223400	1.08234700
H	-1.38762100	-2.47244800	-0.17456300
C	-1.15902900	1.63470000	0.07976300
H	-1.55776400	1.61957700	1.10511300
H	-0.77541800	2.64795800	-0.09224300
H	-2.00353400	1.46217500	-0.59860900

Cyclobutene (Starting material)

C	0.73041400	0.17495300	0.04128100
C	0.29802800	1.41362100	-0.24963500
C	-1.16077300	1.11918300	0.05053000
H	0.80618800	2.31817800	-0.57925500
H	-1.82691700	1.11125900	-0.82031600
H	-1.62697600	1.69677700	0.85999700
C	-0.65772000	-0.31416100	0.44693100
H	-0.74461900	-0.49568900	1.53390000
N	-1.20575100	-1.40050000	-0.36842400
H	-0.70103800	-2.26935900	-0.19612900
H	-2.17984000	-1.57450600	-0.12201900
C	2.04543000	-0.52955500	0.02055900
H	2.02560300	-1.38524500	-0.66905200
H	2.85127500	0.14049600	-0.30027600
H	2.30430400	-0.92265600	1.01412300



Butadiene (Product)

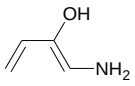
C	0.03492500	0.31180400	-0.06903700
C	1.49100500	0.26730100	-0.21494100
C	2.30672700	-0.71810100	0.20279000
H	1.93823200	1.13604000	-0.70580200
H	3.37319900	-0.69058300	-0.00317300
H	1.93275100	-1.57673900	0.75550900
C	-0.75414600	-0.78562200	-0.16058500
H	-0.33801100	-1.74189200	-0.45780000
N	-2.14418900	-0.73106600	-0.01754900
H	-2.58931500	-1.61960900	0.17715000
H	-2.45493900	-0.00274500	0.62157700
N	-0.59283600	1.56948300	0.19372700
H	0.06839300	2.31863700	0.36753600
H	-1.24220000	1.85568600	-0.53760800

Transition state

C	0.11763100	0.62213900	-0.14770500
C	1.47458400	0.40764100	-0.05715400
C	1.59511000	-0.99313400	0.22902500
H	2.27975000	1.11593800	-0.25475100
H	2.40974900	-1.59521000	-0.19111100
H	1.22582800	-1.37816900	1.17597900
C	-0.44764700	-0.68527400	-0.38370500
H	-0.21327400	-1.17488300	-1.32087000
N	-1.71132800	-1.01858900	0.11094100
H	-1.90319000	-0.73023800	1.06461300
H	-2.03933100	-1.95609600	-0.08390000
N	-0.66477400	1.74695200	0.16153700
H	-0.12878900	2.58962400	0.33661700
H	-1.43609700	1.92226600	-0.47668300

Cyclobutene (Starting material)

C	0.77097900	0.08568100	0.03517400
C	0.49235700	1.37734500	-0.23452800
C	-0.99404300	1.22029000	0.04690500
H	1.09289400	2.23327800	-0.52963900
H	-1.65053200	1.29274900	-0.83007900
H	-1.41958300	1.81981100	0.86374200
C	-0.65250300	-0.25991400	0.43745600
H	-0.74931300	-0.42685100	1.52394500
N	-1.32375700	-1.28861900	-0.36483000
H	-1.13394900	-2.21954300	0.00461200
H	-2.33418500	-1.16309600	-0.32050200
N	1.90016200	-0.71910200	0.09780700
H	1.74202600	-1.68208900	-0.18186700
H	2.71706600	-0.34062700	-0.37109300



Butadiene (Product)

C	0.04932500	0.30455500	-0.05796600
C	1.51076900	0.30421600	-0.19009400
C	2.32557000	-0.69644900	0.17229500
H	1.92689600	1.21909400	-0.61009600
H	3.39768400	-0.63229300	0.00919300
H	1.95380700	-1.60080100	0.64747200
C	-0.75822200	-0.77502100	-0.14545700
H	-0.35838700	-1.76016100	-0.37296300
N	-2.17018200	-0.56425200	0.02916500
H	-2.72176000	-1.01466300	-0.69783300
H	-2.50980800	-0.90658000	0.92751800
O	-0.47646700	1.55011900	0.13617500
H	-1.45007600	1.42040700	0.13049100

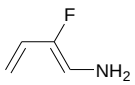
Transition state

C	-0.17531600	0.60539800	0.15428000

C	-1.50253300	0.28341000	0.03444400
C	-1.46075800	-1.12834900	-0.23271800
H	-2.37424500	0.90531000	0.23549200
H	-2.18806100	-1.81520300	0.21490600
H	-1.04830700	-1.48360200	-1.17206300
C	0.52740600	-0.62716200	0.38658600
H	0.33532000	-1.16371700	1.30751700
N	1.75267300	-0.90845000	-0.19753400
H	2.12538800	-0.21501700	-0.83392700
H	2.45876200	-1.37162200	0.36004500
O	0.51726700	1.78621500	-0.03433000
H	-0.04849400	2.41350000	-0.51014000

Cyclobutene (Starting material)

C	0.77138300	0.04515900	0.03759000
C	0.60268700	1.34729100	-0.24745500
C	-0.89342000	1.30116500	0.05143800
H	1.27058500	2.14910500	-0.54201300
H	-1.55652500	1.42591400	-0.81477500
H	-1.25594300	1.93922900	0.86968700
C	-0.66101500	-0.21823200	0.44013500
H	-0.78772000	-0.39062200	1.51739000
N	-1.30362700	-1.32086300	-0.26080500
H	-2.25763100	-1.47098000	0.06099600
H	-1.33635000	-1.14983700	-1.26511400
O	1.82944300	-0.80046200	0.02054300
H	1.49561900	-1.70536100	0.14487200



Butadiene (Product)

C	-0.04671000	0.28197400	0.05331100
C	-1.49370700	0.29550700	0.15213400
C	-2.32613200	-0.72024100	-0.13815100
H	-1.90682900	1.23963800	0.50664000
H	-3.39462900	-0.62911200	0.03116700

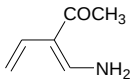
H	-1.97271700	-1.66374300	-0.54703500
C	0.81248300	-0.75208700	0.11218000
H	0.41872000	-1.74845600	0.28283300
N	2.18029100	-0.66470500	-0.10717900
H	2.55938800	0.27546600	-0.09457300
H	2.75255600	-1.32197700	0.40801600
F	0.51176400	1.54113400	-0.10151500

Transition state

C	-0.19844200	0.60247600	0.13694700
C	-1.51186900	0.27672100	-0.00528100
C	-1.43448800	-1.14508500	-0.20774100
H	-2.39016200	0.89724500	0.15530500
H	-2.14354000	-1.82830400	0.27114500
H	-1.00805900	-1.52616600	-1.12978600
C	0.54890300	-0.59178400	0.40112400
H	0.37857800	-1.11221600	1.33610000
N	1.76698800	-0.85892300	-0.18992500
H	2.10788800	-0.22343800	-0.89919400
H	2.48692800	-1.32868500	0.34194900
F	0.41942500	1.80889500	-0.07737100

Cyclobutene (Starting material)

C	0.75580100	-0.03706700	0.04224900
C	0.73365000	1.25911500	-0.26557000
C	-0.75781500	1.34456000	0.05343400
H	1.46812600	1.98377200	-0.59711800
H	-1.40892300	1.51316800	-0.81022300
H	-1.03433600	2.01755900	0.87411000
C	-0.68291800	-0.18179600	0.45148200
H	-0.81419500	-0.33243700	1.53651600
N	-1.48391200	-1.07839200	-0.37668600
H	-1.13491100	-2.03340200	-0.31287100
H	-2.45221800	-1.09182800	-0.06022900
F	1.71905900	-0.97966300	0.03522700



Butadiene (Product)

C	-0.31608100	0.03045000	-0.08127700
C	-1.65869300	-0.57841600	-0.19012200
C	-2.81952500	-0.04798300	0.22621800
H	-1.66647300	-1.57046600	-0.63572100
H	-3.75958600	-0.56752000	0.06249100
H	-2.87971000	0.90216900	0.75466900
C	-0.21606300	1.39844700	-0.13352000
H	-1.13693100	1.94485400	-0.32319000
N	0.85747000	2.22952900	-0.01584400
H	0.71235600	3.22681700	-0.04283400
H	1.76127800	1.91551800	0.30035400
C	0.80909000	-0.92547200	0.01167100
C	2.25230000	-0.43755000	0.09136700
H	2.50791500	0.21626600	-0.75229800
H	2.43556400	0.10729800	1.02882100
H	2.90960000	-1.30961000	0.07422900
O	0.60094100	-2.13861100	0.01229600

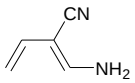
Transition state

C	0.04965900	-0.30692400	0.18650000
C	0.57526300	-1.57121700	-0.00256900
C	1.95811300	-1.31051800	-0.28440200
H	0.10280800	-2.53918700	0.16467900
H	2.75053000	-1.98553300	0.05620100
H	2.19862800	-0.80800200	-1.21728800
C	1.26636500	0.47262100	0.42526100
H	1.75437200	0.32616800	1.38348800
N	1.48842200	1.70458100	-0.15202000
H	0.70515300	2.09325100	-0.66588000
H	2.01143200	2.38945100	0.37850600
C	-1.30914600	0.21440100	0.01922300
C	-2.45919500	-0.78010900	0.01448400
H	-2.58326700	-1.18970400	-0.99655000

H	-2.28598900	-1.62005400	0.69594500
H	-3.38165900	-0.26102300	0.28718900
O	-1.52216500	1.41913000	-0.14664100

Cyclobutene (Starting material)

C	-0.02474800	-0.32242700	0.11229600
C	0.51863200	-1.54214700	-0.08767900
C	1.94389300	-1.06633600	0.10230500
H	0.09767400	-2.52306600	-0.29943800
H	2.55660700	-1.08362600	-0.80627200
H	2.50275200	-1.52264400	0.92950000
C	1.31354700	0.34886500	0.38669000
H	1.42683000	0.64700900	1.44229200
N	1.67577000	1.39102500	-0.56795700
H	0.99610800	2.14892700	-0.51494600
H	2.58758800	1.78629300	-0.34140100
C	-1.38179000	0.24700700	0.08356300
C	-2.54408300	-0.67071500	-0.24463200
H	-2.54157800	-1.55684600	0.40158800
H	-3.48426400	-0.12815900	-0.12247900
H	-2.46352100	-1.02255800	-1.28119500
O	-1.54516200	1.44400200	0.30659900



Butadiene (Product)

C	-0.12947200	-0.13428000	-0.08481600
C	-1.53108700	-0.57447500	-0.18627700
C	-2.61310000	0.12268600	0.19558900
H	-1.67152500	-1.56558400	-0.61578500
H	-3.61248100	-0.26847300	0.03046100
H	-2.54342900	1.08992300	0.68840300
C	0.25406800	1.18018100	-0.11459800
H	-0.50128800	1.94354500	-0.27818900
N	1.51581800	1.65316400	0.07129100
H	2.28998300	1.00215600	0.13650100

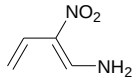
H	1.74569300	2.59077000	-0.22277300
C	0.89637200	-1.12133000	0.02394200
N	1.77451900	-1.88588200	0.10847300

Transition state

C	-0.22834500	-0.38050400	0.14691200
C	0.60818100	-1.46837800	-0.00160400
C	1.89685000	-0.89440300	-0.23612800
H	0.36771600	-2.51566300	0.17576900
H	2.80967300	-1.36131400	0.14477500
H	2.04961800	-0.34145000	-1.15864500
C	0.70569000	0.70728300	0.41544700
H	1.19155400	0.71302200	1.38417300
N	0.54204900	1.95443100	-0.13282100
H	0.17493400	2.03994900	-1.07149400
H	1.13772900	2.71423300	0.16537100
C	-1.63991500	-0.26356100	0.00754000
N	-2.79719000	-0.16177400	-0.10045700

Cyclobutene (Starting material)

C	-0.37379000	-0.37381400	0.03832800
C	0.34024500	-1.47710000	-0.25944800
C	1.67609800	-0.84017200	0.05834400
H	0.05589500	-2.47162200	-0.59191600
H	2.32456400	-0.67559500	-0.80913400
H	2.25319700	-1.30519800	0.86703700
C	0.85209900	0.44113400	0.45345400
H	0.87550800	0.63319600	1.53889800
N	1.11692100	1.61192700	-0.37179400
H	0.37445700	2.30286800	-0.27043400
H	1.98583600	2.06227300	-0.08734600
C	-1.75447400	-0.04330100	0.01680300
N	-2.87556700	0.27572800	0.01579600



Butadiene (Product)

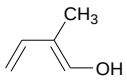
C	-0.26586500	0.08458700	-0.08190200
C	-1.67368900	-0.30865600	-0.19584500
C	-2.72299200	0.42132600	0.21318300
H	-1.84485400	-1.27869200	-0.65398100
H	-3.73777300	0.07729400	0.03813700
H	-2.61600100	1.36696400	0.74083200
C	0.14828900	1.39853600	-0.12198100
H	-0.63253800	2.13721800	-0.27781100
N	1.38549300	1.89840200	0.00512200
H	2.15929400	1.25013700	0.11823900
H	1.55443200	2.88524200	-0.12012100
N	0.69417300	-0.96998500	0.02362000
O	1.90996000	-0.67316300	0.12716600
O	0.29570500	-2.14081700	0.00693100

Transition state

C	0.02263400	-0.34350600	0.14560700
C	0.63955800	-1.55439200	-0.03062600
C	1.99795400	-1.14518200	-0.24845500
H	0.23966500	-2.55151800	0.13213800
H	2.83615800	-1.72342200	0.15126900
H	2.23292500	-0.62202200	-1.17060600
C	1.11525600	0.57980000	0.42573600
H	1.58271700	0.48667800	1.40054900
N	1.24251800	1.81704000	-0.15596400
H	0.48496600	2.12406100	-0.75404800
H	1.67869700	2.55628100	0.37881400
N	-1.36765500	-0.01730900	0.00403600
O	-1.66988200	1.18189700	-0.12642400
O	-2.18406600	-0.94296000	0.02290100

Cyclobutene (Starting material)

C	-0.06585400	-0.35887800	0.08119700
C	0.50996900	-1.54752800	-0.13990300
C	1.89893000	-0.98604500	0.11001500
H	0.13009100	-2.53213700	-0.38982800
H	2.53693100	-0.94913100	-0.77913000
H	2.44806400	-1.43192900	0.94758500
C	1.19766500	0.39810900	0.40901700
H	1.26509900	0.67497600	1.47336300
N	1.52916900	1.46865100	-0.51943500
H	0.82010900	2.19926500	-0.47219300
H	2.42146700	1.89433100	-0.27339500
N	-1.43473800	0.08055100	0.02959900
O	-1.63402700	1.28101200	0.25787300
O	-2.30685300	-0.74772900	-0.23781100



Butadiene (Product)

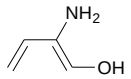
C	0.01122500	0.32820500	-0.07810900
C	1.47159300	0.24825500	-0.24537500
C	2.28255500	-0.71787500	0.21738400
H	1.92195400	1.08116800	-0.79044500
H	3.34865200	-0.70703700	0.00642800
H	1.91188000	-1.53907600	0.82695200
C	-0.73530200	-0.78846200	-0.14383500
H	-0.29878200	-1.75952000	-0.36771600
O	-2.09276700	-0.77479700	0.07743500
H	-2.47868600	-1.61548700	-0.20676900
C	-0.59943900	1.69271800	0.13783800
H	-1.68917500	1.66260800	0.05817800
H	-0.34137700	2.09059600	1.12903000
H	-0.21612800	2.40808000	-0.60255300

Transition state

C	0.14772700	-0.60078400	-0.12444400
C	-1.19941300	-0.90127200	-0.06940800
C	-1.86242900	0.32608300	0.23321400
H	-1.67761800	-1.84741200	-0.32637600
H	-2.85227100	0.56657400	-0.17068600
H	-1.64593000	0.82088500	1.17424800
C	0.12869700	0.81105300	-0.36221400
H	-0.26689100	1.19467200	-1.29662400
O	1.09862400	1.60043800	0.21361300
H	1.15942200	2.45376300	-0.24388100
C	1.36182500	-1.45662700	0.09939400
H	1.72895300	-1.37399300	1.13150300
H	1.11639800	-2.51126400	-0.07411800
H	2.19050600	-1.17744200	-0.56221500

Cyclobutene (Starting material)

C	0.71314900	0.19713500	0.04077200
C	0.22374000	1.42280100	-0.22085400
C	-1.22786700	1.05306900	0.03538000
H	0.69613900	2.36421700	-0.49412400
H	-1.86525000	1.01293500	-0.85554500
H	-1.75211100	1.59958100	0.83198800
C	-0.64593300	-0.35695000	0.42588500
H	-0.74761600	-0.58255000	1.49933500
O	-1.04318100	-1.48132600	-0.35088600
H	-1.89889700	-1.80468000	-0.02785300
C	2.05361300	-0.45475000	0.01977500
H	2.05448400	-1.31544900	-0.66150400
H	2.83276900	0.24388700	-0.30524100
H	2.32572000	-0.83516600	1.01428700



Butadiene (Product)

C	0.01772400	0.32279500	-0.07862000
C	1.47335200	0.24827200	-0.26187700
C	2.27866700	-0.70703900	0.22937100
H	1.90466700	1.06201800	-0.84746200
H	3.34192500	-0.71516300	0.00490600
H	1.90303600	-1.50359600	0.86717200
C	-0.76220800	-0.77502800	-0.14279800
H	-0.37156000	-1.75721300	-0.38583000
O	-2.12070100	-0.67050500	0.11294400
H	-2.59490900	-1.39056200	-0.32658300
N	-0.52899700	1.61750800	0.04875900
H	-1.52317000	1.60495200	0.25351000
H	-0.03661600	2.20705000	0.71297000

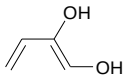
Transition state

C	-0.05960700	0.62191300	0.12125900
C	-1.43575300	0.47584500	0.09896800
C	-1.64663600	-0.89606300	-0.23628300
H	-2.19059200	1.20350500	0.39491600
H	-2.47975200	-1.46670300	0.19173400
H	-1.31265000	-1.27606800	-1.19646200
C	0.41549600	-0.71324500	0.33777100
H	0.18048300	-1.20087500	1.27727200
O	1.62989000	-1.08499700	-0.21085400
H	1.95826900	-1.88727800	0.22295200
N	0.75219500	1.71330400	-0.17251400
H	0.27527300	2.60108000	-0.26726100
H	1.62348300	1.78248000	0.34099500

Cyclobutene (Starting material)

C	0.74006900	0.15761100	0.04086300
C	0.33431600	1.42039300	-0.21647800

C	-1.13761800	1.11234000	0.02514200
H	0.85504800	2.33992000	-0.46710200
H	-1.77571800	1.10647800	-0.86713500
H	-1.64511700	1.66705900	0.82794900
C	-0.63634400	-0.32517300	0.41955400
H	-0.74966700	-0.54240600	1.49250500
O	-1.07222400	-1.43952300	-0.35529200
H	-1.94312800	-1.72611100	-0.03844600
N	1.92759900	-0.54897000	0.10927300
H	1.83108200	-1.53809800	-0.09532500
H	2.70955700	-0.13889600	-0.38950000



Butadiene (Product)

C	0.01192900	0.32670100	-0.06786800
C	1.45969800	0.20916300	-0.26419100
C	2.24277800	-0.76885800	0.22045500
H	1.91205400	1.00587000	-0.85959500
H	3.30206000	-0.81068600	-0.01788400
H	1.84916100	-1.55396900	0.86148800
C	-0.82756900	-0.72247200	-0.14164000
H	-0.45236900	-1.70834500	-0.39692500
O	-2.17209600	-0.59165500	0.09182900
H	-2.63001900	-1.39339600	-0.19768600
O	-0.50876300	1.59690300	0.10471500
H	0.14497200	2.15133200	0.55770700

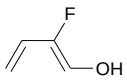
Transition state

C	-0.13680900	0.60884300	0.12218400
C	-1.47698700	0.29337300	0.07261300
C	-1.48981500	-1.10221700	-0.23080900
H	-2.32496700	0.91496400	0.35731600
H	-2.22919300	-1.77570300	0.21632200
H	-1.08927200	-1.45536300	-1.17458300
C	0.54179500	-0.62580700	0.35230100

H	0.36641700	-1.15988600	1.27952500
O	1.76432400	-0.84374600	-0.22984600
H	2.25200800	-1.52912100	0.25251900
O	0.53767600	1.78803000	-0.05475800
H	-0.02009600	2.40568000	-0.55200100

Cyclobutene (Starting material)

C	0.75282700	0.02359000	0.03966300
C	0.55633000	1.32800500	-0.22477900
C	-0.94239000	1.24114100	0.04279000
H	1.20803700	2.15517300	-0.48936300
H	-1.58739700	1.33648500	-0.83796800
H	-1.33419700	1.86740400	0.85612900
C	-0.67249900	-0.26705400	0.42143100
H	-0.81091100	-0.47673700	1.49236500
O	-1.29108900	-1.26861300	-0.36939800
H	-2.17324100	-1.45321800	-0.01138700
O	1.78316000	-0.85233000	0.06401000
H	2.59553000	-0.41565500	-0.24130300



Butadiene (Product)

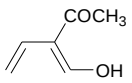
C	-0.02468600	0.30917600	0.05393600
C	-1.47474700	0.27024100	0.19183700
C	-2.27554900	-0.74636200	-0.16597300
H	-1.90741900	1.16942200	0.62990900
H	-3.34323000	-0.71023300	0.02871400
H	-1.89660400	-1.63698300	-0.66135300
C	0.83125700	-0.72094300	0.12797400
H	0.45848400	-1.71910700	0.33585000
O	2.17341600	-0.56169800	-0.06919800
H	2.63854700	-1.37329100	0.17916400
F	0.48058300	1.56567800	-0.13392800

Transition state

C	-0.15110500	0.60538500	0.10710800
C	-1.48437500	0.30991200	0.03883600
C	-1.48245700	-1.09730100	-0.21034200
H	-2.33138300	0.94472700	0.28692700
H	-2.21102100	-1.76256500	0.26374600
H	-1.07167700	-1.47559900	-1.13926000
C	0.55263900	-0.60238400	0.36555200
H	0.38421600	-1.13125100	1.29727900
O	1.76447800	-0.81598000	-0.23001700
H	2.26990300	-1.48738000	0.25426100
F	0.47065900	1.79402600	-0.10330400

Cyclobutene (Starting material)

C	0.75190000	-0.02201100	0.03161800
C	0.66621800	1.28364200	-0.23166200
C	-0.83548900	1.29390400	0.04620400
H	1.37739600	2.05731200	-0.49609100
H	-1.47173900	1.43558700	-0.83328000
H	-1.17150700	1.94665900	0.86207400
C	-0.68095800	-0.23530800	0.42390700
H	-0.83096700	-0.43161000	1.49522800
O	-1.36967900	-1.18503600	-0.36678900
H	-2.24592700	-1.34413000	0.01686300
F	1.76557200	-0.90054400	0.02990200



Butadiene (Product)

C	-0.32179000	0.05171300	-0.09942500
C	-1.66804300	-0.54820400	-0.21664000
C	-2.80193800	-0.04101300	0.28872900
H	-1.69788700	-1.50078300	-0.74031500
H	-3.75574300	-0.53590100	0.12782800
H	-2.82076400	0.86361900	0.89391200

C	-0.20491100	1.40010800	-0.15660800
H	-1.08734200	2.01190000	-0.33383100
O	0.95942900	2.08822300	-0.00816900
H	0.80626600	3.03084400	-0.16991300
C	0.81875100	-0.91156500	0.00726800
C	2.23990500	-0.41504600	0.18619300
H	2.54585300	0.21263900	-0.65821400
H	2.33116400	0.20585800	1.08439900
H	2.89986100	-1.28193500	0.26343000
O	0.59141400	-2.11599900	-0.05738000

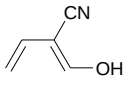
Transition state

C	0.12774800	-0.34124000	0.12030500
C	0.99756100	-1.42152900	0.08513700
C	2.27300600	-0.86972900	-0.21064400
H	0.78263400	-2.44612000	0.38168400
H	3.19908900	-1.30252000	0.17936900
H	2.40240900	-0.32492000	-1.14053300
C	1.04072100	0.74618000	0.36643700
H	1.55164500	0.81089200	1.32208100
O	0.87799000	1.94097500	-0.27855600
H	1.39262700	2.63976100	0.15706100
C	-1.34369100	-0.34522900	-0.01140900
C	-2.09285300	0.97422800	0.03305700
H	-1.85678300	1.57188200	-0.85553600
H	-3.16650800	0.77523400	0.06397200
H	-1.79927100	1.57212900	0.90435200
O	-1.94308900	-1.41002900	-0.13516200

Cyclobutene (Starting material)

C	0.00611800	-0.40732000	0.07193400
C	0.76189100	-1.51778200	-0.05621000
C	2.08202500	-0.79761300	0.12754400
H	0.50771400	-2.56354200	-0.20349800
H	2.69131300	-0.72202800	-0.78035700
H	2.71465000	-1.12719400	0.96272500
C	1.19987500	0.48683200	0.36777900

H	1.24529700	0.84792200	1.40613400
O	1.34570200	1.56777900	-0.54140200
H	2.10169500	2.11333100	-0.27228000
C	-1.45608200	-0.17634000	-0.00927500
C	-1.94544800	1.23476200	0.23860800
H	-1.43237100	1.93719500	-0.42920000
H	-3.02610500	1.28542600	0.08861300
H	-1.70505600	1.54239300	1.26570600
O	-2.21912900	-1.09887100	-0.26861200



Butadiene (Product)

C	-0.08567900	-0.10665100	-0.10009300
C	-1.48551900	-0.55797800	-0.24736500
C	-2.56150000	0.07543600	0.24064300
H	-1.61801900	-1.48896100	-0.79677000
H	-3.56274000	-0.29887400	0.04831800
H	-2.48246900	0.96974300	0.85459200
C	0.25653300	1.20332700	-0.12625500
H	-0.49680400	1.96579200	-0.30904600
O	1.52750900	1.62112500	0.06620900
H	1.60236700	2.57354600	-0.09439000
C	0.92837500	-1.10941300	0.03660500
N	1.71776300	-1.95979600	0.13520200

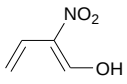
Transition state

C	-0.21861100	-0.35592300	0.14116300
C	0.63889700	-1.44190600	0.04934900
C	1.90823200	-0.88042100	-0.25569000
H	0.42519400	-2.47604200	0.31322800
H	2.83943300	-1.31987500	0.11195700
H	2.01866700	-0.31741300	-1.17691500
C	0.68601200	0.73695000	0.38283500
H	1.21855700	0.77753100	1.32710400
O	0.47469900	1.93004200	-0.23176400

H	0.94302000	2.64701800	0.22606000
C	-1.63193400	-0.27137700	-0.00853300
N	-2.79114900	-0.21078500	-0.11458100

Cyclobutene (Starting material)

C	-0.37075100	-0.35022800	0.03263200
C	0.33655800	-1.47052100	-0.22002000
C	1.68383100	-0.82973100	0.04416200
H	0.04030500	-2.48275900	-0.47916400
H	2.30142200	-0.67744800	-0.84739400
H	2.29330800	-1.27665500	0.84019100
C	0.85755400	0.46188900	0.42212500
H	0.89578100	0.70080200	1.49355600
O	1.05246400	1.61569600	-0.36628400
H	1.69009400	2.20287700	0.06808300
C	-1.75315800	-0.02380100	0.01413700
N	-2.88069000	0.26885300	0.01382600



Butadiene (Product)

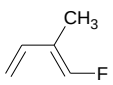
C	-0.23857300	0.10201300	-0.10882600
C	-1.64390700	-0.30299700	-0.25608200
C	-2.68329600	0.35587700	0.27522300
H	-1.81480400	-1.20311900	-0.83998300
H	-3.70253500	0.03493600	0.08153100
H	-2.55787200	1.21689100	0.92828900
C	0.14085500	1.40373500	-0.15073800
H	-0.64061800	2.13595300	-0.34246300
O	1.38127700	1.88292700	0.02240200
H	1.38251800	2.84332300	-0.11542700
N	0.73243200	-0.97707000	0.03164100
O	1.92408800	-0.69310500	0.16626000
O	0.28911200	-2.13235400	-0.00002400

Transition state

C	0.03847800	-0.29116700	0.12781100
C	0.69367300	-1.50093200	0.09255000
C	2.04322000	-1.14431700	-0.17438400
H	0.31064700	-2.47194800	0.39532400
H	2.88151000	-1.69664900	0.25679900
H	2.27504800	-0.63038700	-1.10131900
C	1.06848400	0.68139400	0.36318800
H	1.57628000	0.68622300	1.32260800
O	1.10546100	1.83287400	-0.34065500
H	1.65181800	2.49975300	0.10634500
N	-1.37299100	-0.04101500	-0.00613700
O	-2.09675700	-1.02249600	-0.21361100
O	-1.77714000	1.11840200	0.13029200

Cyclobutene (Starting material)

C	-0.06048200	-0.35617500	0.08052000
C	0.55434600	-1.52963800	-0.12080500
C	1.93079200	-0.91709600	0.09785300
H	0.20716900	-2.53430800	-0.33611400
H	2.54456000	-0.85318000	-0.80619900
H	2.52240100	-1.33659200	0.91918500
C	1.18992800	0.43315500	0.39917400
H	1.26128200	0.74965500	1.44842900
O	1.55765200	1.47191600	-0.48008400
H	0.91705300	2.19638300	-0.38173500
N	-1.43572400	0.05749400	0.02673200
O	-2.29938200	-0.78524100	-0.21733500
O	-1.64450700	1.26258800	0.22602600



Butadiene (Product)

C	-0.01351200	0.30814200	-0.08067200
C	1.44986900	0.27000800	-0.27391700

C	2.28976400	-0.64213700	0.23752900
H	1.86184700	1.08332500	-0.87478900
H	3.35448600	-0.60965300	0.02238900
H	1.94480300	-1.43845600	0.89301200
C	-0.71201100	-0.82986700	-0.15410500
H	-0.31546300	-1.81148300	-0.38630200
F	-2.05932300	-0.86609800	0.04361000
C	-0.65894300	1.65201300	0.15557800
H	-1.74860400	1.57975000	0.18845500
H	-0.31173500	2.08878700	1.10098900
H	-0.38243200	2.35366500	-0.64272400

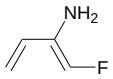
Transition state

C	0.19298900	-0.56793000	-0.11307200
C	-1.13661800	-0.96142800	-0.08044300
C	-1.88639000	0.20112400	0.24644300
H	-1.54886600	-1.92159300	-0.39089500
H	-2.88697600	0.38078200	-0.16057100
H	-1.69768800	0.71020700	1.18457800
C	0.05581700	0.82301200	-0.35916300
H	-0.34271400	1.22702400	-1.28106500
F	0.99426600	1.69581400	0.14580800
C	1.46452400	-1.33422300	0.10822000
H	1.81658600	-1.22975500	1.14320700
H	1.29746600	-2.40253700	-0.07160300
H	2.27186200	-0.98979000	-0.54783100

Cyclobutene (Starting material)

C	0.70118300	0.21686900	0.03582600
C	0.14015600	1.41500800	-0.21564800
C	-1.29026100	0.96095200	0.03869100
H	0.55667700	2.38647400	-0.47324400
H	-1.92057500	0.87219900	-0.85263500
H	-1.85279100	1.47412100	0.82949900
C	-0.62586100	-0.39207000	0.43594400
H	-0.73181300	-0.68021200	1.48820600
F	-1.04159500	-1.50631000	-0.31785700

C	2.07650900	-0.35782100	0.01279300
H	2.13002700	-1.21081000	-0.67617300
H	2.81426400	0.38701000	-0.30520900
H	2.36821600	-0.72962300	1.00463000



Butadiene (Product)

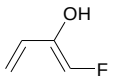
C	-0.00734300	0.30936800	-0.07944500
C	1.45149200	0.26340900	-0.28432800
C	2.27671500	-0.64924400	0.24766100
H	1.85454500	1.05543800	-0.91691400
H	3.33948100	-0.64461200	0.02124900
H	1.91839400	-1.42252100	0.92268100
C	-0.74610200	-0.81028900	-0.15124200
H	-0.40300800	-1.79780000	-0.42431400
F	-2.10043100	-0.74779000	0.05884300
N	-0.57542100	1.58430200	0.06877500
H	-1.56348800	1.57080100	0.29823900
H	-0.06267100	2.19922200	0.69217800

Transition state

C	0.03872900	0.60846100	0.10731800
C	-1.34797000	0.66884100	0.09619200
C	-1.76340100	-0.64712300	-0.25231800
H	-1.98101100	1.48095400	0.44766000
H	-2.66787500	-1.08875300	0.18142000
H	-1.49010700	-1.07689200	-1.20899200
C	0.27682700	-0.77700900	0.33480000
H	0.02943500	-1.25681000	1.27339000
F	1.45670600	-1.32734600	-0.15182200
N	0.99863200	1.60108700	-0.03464400
H	0.82616800	2.28728700	-0.75909800
H	1.95751200	1.27370000	-0.04143000

Cyclobutene (Starting material)

C	0.72678800	0.18976800	0.03246900
C	0.22387300	1.42092400	-0.21293200
C	-1.22267900	1.00306700	0.03101000
H	0.67322800	2.38230500	-0.44288700
H	-1.85945600	0.93892800	-0.85872500
H	-1.77304700	1.51661200	0.83107500
C	-0.61106500	-0.37240300	0.42922600
H	-0.72330300	-0.65501900	1.48148300
F	-1.05046600	-1.48176100	-0.32315300
N	1.96555600	-0.41903400	0.09989800
H	1.96013100	-1.41528000	-0.08943500
H	2.71624700	0.05340600	-0.39105600



Butadiene (Product)

C	0.01285600	0.30993300	0.07396500
C	-1.43901200	0.22725700	0.29153800
C	-2.24580900	-0.70158300	-0.24200300
H	-1.85916100	0.99877800	0.94038000
H	-3.30582700	-0.72829400	-0.00488800
H	-1.87175500	-1.45969300	-0.92544700
C	0.81181400	-0.76336700	0.15614300
H	0.48325000	-1.75664800	0.43102900
F	2.14579500	-0.67348800	-0.06068200
O	0.56381900	1.55360100	-0.13331700
H	-0.10830500	2.14499400	-0.50627400

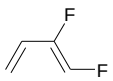
Transition state

C	0.01285600	0.30993300	0.07396500
C	-1.43901200	0.22725700	0.29153800
C	-2.24580900	-0.70158300	-0.24200300
H	-1.85916100	0.99877800	0.94038000
H	-3.30582700	-0.72829400	-0.00488800

H	-1.87175500	-1.45969300	-0.92544700
C	0.81181400	-0.76336700	0.15614300
H	0.48325000	-1.75664800	0.43102900
F	2.14579500	-0.67348800	-0.06068200
O	0.56381900	1.55360100	-0.13331700
H	-0.10830500	2.14499400	-0.50627400

Cyclobutene (Starting material)

C	0.74512800	0.07642600	0.03585400
C	0.42070300	1.35790000	-0.21957600
C	-1.06541200	1.12494300	0.04659900
H	0.98767700	2.24870500	-0.47170300
H	-1.71522900	1.14642400	-0.83455600
H	-1.52298200	1.71033800	0.85417200
C	-0.64489100	-0.32891300	0.43350900
H	-0.78857800	-0.60527700	1.48305700
F	-1.23430600	-1.34194000	-0.33374000
O	1.84932100	-0.70125900	0.05556500
H	2.62013200	-0.19479500	-0.25014900



Butadiene (Product)

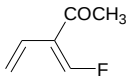
C	-0.00207400	0.29516100	0.06072300
C	-1.45396300	0.29326100	0.22273000
C	-2.27378000	-0.68370800	-0.19053900
H	-1.85721000	1.17442000	0.72055100
H	-3.34028800	-0.63887300	0.00893500
H	-1.91116100	-1.54908800	-0.73951800
C	0.81359100	-0.76025800	0.14805900
H	0.48696300	-1.76489000	0.38290400
F	2.14384700	-0.64611400	-0.04389900
F	0.53604800	1.52519100	-0.15818000

Transition state

C	-0.05868200	0.60328000	0.09262700
C	-1.42436200	0.47630200	0.04927100
C	-1.61038500	-0.90898400	-0.22144800
H	-2.17849500	1.19912700	0.34915000
H	-2.41210300	-1.48114000	0.25462700
H	-1.24640300	-1.33368400	-1.14863000
C	0.46217200	-0.68057100	0.36251500
H	0.27126400	-1.21081200	1.28663600
F	1.66778200	-1.04486300	-0.15896500
F	0.70480400	1.69890100	-0.11209800

Cyclobutene (Starting material)

C	0.74694300	0.04251200	0.02670900
C	0.50897700	1.33137300	-0.23053800
C	-0.98593700	1.16985000	0.05371800
H	1.12458500	2.18482100	-0.48920700
H	-1.63909900	1.22991000	-0.82194100
H	-1.39489100	1.77964800	0.86776600
C	-0.65012400	-0.31097100	0.43757300
H	-0.80414400	-0.57859300	1.48744700
F	-1.29469500	-1.28426400	-0.33004000
F	1.84962800	-0.71711000	0.02239100



Butadiene (Product)

C	-0.33004700	0.06903500	-0.11016500
C	-1.67250700	-0.54156000	-0.22935600
C	-2.79131400	-0.05919400	0.32780800
H	-1.70634200	-1.46979300	-0.79445800
H	-3.74772500	-0.55174300	0.17622900
H	-2.79222600	0.82173700	0.96653500
C	-0.22841800	1.40762900	-0.17882000
H	-1.05994200	2.08059100	-0.35824800

F	0.93115800	2.08862300	-0.04677800
C	0.82999800	-0.88414500	0.00607900
C	2.23674700	-0.37121600	0.23386100
O	0.61222100	-2.08456600	-0.09119500
H	2.28979000	0.25903500	1.12857200
H	2.90211400	-1.23016600	0.34406700
H	2.56939100	0.24597100	-0.60858000

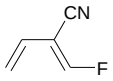
Transition state

C	-0.08291200	-0.23430400	-0.16497600
C	-0.68629100	-1.49163900	-0.13339700
C	-2.03007800	-1.27523400	0.24999000
H	-0.28094900	-2.43255300	-0.50393600
H	-2.84996500	-1.90146800	-0.11120800
H	-2.23877700	-0.76304600	1.18317000
C	-1.22054300	0.60523200	-0.35828800
H	-1.81194500	0.58424200	-1.26555300
F	-1.32854200	1.80833200	0.24617700
C	1.33227700	0.17565900	-0.02649200
C	2.35299000	-0.93670900	0.14887400
H	2.21525000	-1.72970800	-0.59676400
H	3.35816200	-0.51922900	0.05888300
H	2.24218500	-1.39771800	1.13867500
O	1.66628200	1.35330700	-0.05164000

Cyclobutene (Starting material)

C	-0.01640900	0.26995300	-0.09462600
C	0.56393900	1.48879800	-0.02655200
C	1.98240800	0.96636100	-0.16315100
H	0.16740500	2.49959600	0.03512400
H	2.59072700	1.03429000	0.74502600
H	2.56490900	1.33300100	-1.01740600
C	1.30593000	-0.43274900	-0.33164200
H	1.42839500	-0.91208300	-1.30696800
F	1.67965500	-1.36807000	0.63613400
C	-1.40587700	-0.23598200	-0.09273000
C	-2.50179500	0.71083500	0.35779800

H	-2.41673900	1.68618800	-0.13634100
H	-3.47738300	0.27038000	0.14030100
H	-2.41948400	0.88464300	1.43862300
O	-1.64048800	-1.38583500	-0.43976800



Butadiene (Product)

C	-0.07998100	-0.08506000	-0.11291200
C	-1.46749900	-0.57592000	-0.28059800
C	-2.54727400	-0.00611000	0.26915000
H	-1.57598100	-1.47040600	-0.89160600
H	-3.54208900	-0.39620800	0.07496000
H	-2.47595700	0.84896600	0.93706200
C	0.21471000	1.22718600	-0.13620700
H	-0.50306500	2.01962900	-0.31488800
F	1.46110800	1.68328100	0.05172200
C	0.96496800	-1.05627000	0.03903300
N	1.77679600	-1.88206600	0.15116800

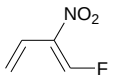
Transition state

C	-0.19258300	-0.34455500	0.14199100
C	0.71658000	-1.39698300	0.07159600
C	1.95080600	-0.80272600	-0.28215600
H	0.56038400	-2.42417300	0.39431400
H	2.90713700	-1.19004400	0.07784000
H	2.01789100	-0.23150600	-1.20162500
C	0.66628900	0.76782600	0.37747500
H	1.23101900	0.88110800	1.29413800
F	0.38322800	1.97827500	-0.16184200
C	-1.60779600	-0.32443000	-0.00972800
N	-2.76646500	-0.31923600	-0.12902100

Cyclobutene (Starting material)

C	-0.36874600	-0.33774500	0.02880000

C	0.36390600	-1.44362400	-0.22050200
C	1.69917800	-0.77481800	0.04899500
H	0.09104900	-2.46335300	-0.47565100
H	2.31468600	-0.60052500	-0.83959800
H	2.31970100	-1.20736300	0.84270800
C	0.84838700	0.47686500	0.43699400
H	0.88816300	0.77405700	1.48914800
F	1.09857100	1.61602700	-0.32283800
C	-1.75610100	-0.03621600	0.01153400
N	-2.88864100	0.23516800	0.00771600



Butadiene (Product)

C	-0.26772800	0.09963200	-0.10065300
C	-1.63057200	-0.44292500	-0.19620600
C	-2.69673200	0.13035300	0.37775100
H	-1.73378100	-1.36183300	-0.76627700
H	-3.69072200	-0.28549500	0.24225600
H	-2.61522300	1.01418800	1.00615600
C	-0.00089800	1.40952100	-0.23722900
H	-0.77921100	2.13138100	-0.46108500
F	1.20713300	1.96265600	-0.15891300
N	0.82371000	-0.87758100	0.06197900
O	1.86187700	-0.51134300	0.60561500
O	0.60866700	-2.01347800	-0.36644800

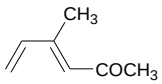
Transition state

C	-0.26772800	0.09963200	-0.10065300
C	-1.63057200	-0.44292500	-0.19620600
C	-2.69673200	0.13035300	0.37775100
H	-1.73378100	-1.36183300	-0.76627700
H	-3.69072200	-0.28549500	0.24225600

H	-2.61522300	1.01418800	1.00615600
C	-0.00089800	1.40952100	-0.23722900
H	-0.77921100	2.13138100	-0.46108500
F	1.20713300	1.96265600	-0.15891300
N	0.82371000	-0.87758100	0.06197900
O	1.86187700	-0.51134300	0.60561500
O	0.60866700	-2.01347800	-0.36644800

Cyclobutene (Starting material)

C	0.05925800	0.30811300	0.05730300
C	-0.54765500	1.49836000	-0.05294000
C	-1.93034100	0.89812500	0.15860500
H	-0.18517900	2.51216900	-0.18159300
H	-2.57075600	0.89669800	-0.72877800
H	-2.49268900	1.27513100	1.02029900
C	-1.19155000	-0.46955500	0.36652500
H	-1.25963600	-0.90822800	1.36514400
F	-1.53774500	-1.45452800	-0.55024200
N	1.45052600	-0.07316000	0.01999800
O	2.26535800	0.78081800	-0.33587300
O	1.71664300	-1.22871400	0.35589200



Butadiene (Product)

C	0.83940000	0.40371000	-0.13050500
C	2.25746900	-0.01517500	-0.20478800
C	2.78048700	-1.12755400	0.33298200
H	2.92832800	0.68304000	-0.70764900
H	3.83835200	-1.35415700	0.23189800
H	2.17884200	-1.83447700	0.89893100
C	-0.13462900	-0.54194500	-0.17287000
H	0.17809000	-1.57153700	-0.33136800
C	-1.60990200	-0.46658600	-0.03764000
O	-2.24658200	-1.51135100	-0.16121100
C	-2.35767800	0.82174900	0.26689000

H	-1.92390100	1.35797200	1.11768700
H	-2.34009700	1.49542600	-0.59911800
H	-3.39736700	0.56811800	0.48610500
C	0.65743200	1.90089600	-0.02513200
H	-0.35042400	2.24285500	-0.25213000
H	0.91840900	2.24719800	0.98488200
H	1.34695200	2.40579800	-0.71318400

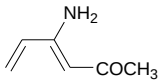
Transition state

C	-1.17596200	0.34318400	0.21272800
C	-2.06451200	-0.67832500	-0.02807200
C	-1.27537300	-1.80355700	-0.42559400
H	-3.14367100	-0.68773400	0.12415700
H	-1.52596500	-2.82918800	-0.13358300
H	-0.66460400	-1.73850900	-1.31876500
C	0.08065000	-0.35333100	0.42189900
H	0.13213000	-1.04856800	1.25592200
C	1.39234400	0.14554300	-0.05801300
O	1.48012400	1.14733900	-0.76479900
C	2.62634100	-0.64328600	0.34898700
H	2.80376100	-0.52870000	1.42710100
H	2.49197600	-1.71528500	0.15841800
H	3.49884000	-0.27696700	-0.19667000
C	-1.41610200	1.82480800	0.22139500
H	-0.86763500	2.32815500	1.02492600
H	-1.08401900	2.27404100	-0.72200000
H	-2.48611700	2.03384200	0.33890000

Cyclobutene (Starting material)

C	-1.25951200	-0.24482400	-0.11774700
C	-1.70340400	0.89803400	0.43536400
C	-0.50844600	1.72407600	0.00509700
H	-2.60882300	1.15634200	0.98066800
H	0.11932200	2.13601800	0.80542700
H	-0.70277200	2.51821700	-0.72561100
C	0.02764500	0.38793300	-0.65750700
H	0.09591300	0.44376900	-1.74996800

C	1.36967200	-0.10563300	-0.13867200
O	2.33394100	-0.18246400	-0.88423500
C	1.47632300	-0.50619300	1.32275400
H	0.87178600	0.13138900	1.97612600
H	1.10087200	-1.53186100	1.44074000
H	2.52376200	-0.48635100	1.63299400
C	-1.78637900	-1.63480800	-0.25106300
H	-1.09969900	-2.37196000	0.18745200
H	-2.75804800	-1.73892800	0.24465600
H	-1.90923500	-1.90843300	-1.30795400



Butadiene (Product)

C	0.82462100	0.40923400	-0.10386600
C	2.25713900	0.04423300	-0.20744900
C	2.81462500	-1.06815400	0.28744300
H	2.88824500	0.77640500	-0.71326400
H	3.87623400	-1.26212600	0.16281200
H	2.23700100	-1.81164800	0.83014300
C	-0.14582500	-0.55771800	-0.15084700
H	0.19505400	-1.57244600	-0.32555000
C	-1.60096500	-0.46899800	-0.02758900
O	-2.27996800	-1.49617800	-0.09333500
C	-2.30985200	0.86645400	0.18282500
H	-1.97508300	1.35556300	1.10821900
H	-2.13410400	1.54925900	-0.65932000
H	-3.38351400	0.68125000	0.26028800
N	0.62790500	1.77536300	-0.04133400
H	-0.28792500	2.13719900	0.17728800
H	1.39004500	2.33812400	0.31230400

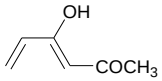
Transition state

C	-1.18100900	0.40370700	0.17219100
C	-2.11309500	-0.59007100	-0.05362400
C	-1.31145200	-1.74178900	-0.35376500

H	-3.19175900	-0.56924000	0.08201800
H	-1.57785100	-2.73835100	0.02087800
H	-0.70952500	-1.77716300	-1.25609800
C	0.04593300	-0.33632900	0.44724000
H	0.05463900	-0.96684300	1.33232200
C	1.37605800	0.14091400	0.01697700
O	1.54293900	1.27199900	-0.44977800
C	2.53744100	-0.83095800	0.12859300
H	2.48897700	-1.41506300	1.05499100
H	2.49884000	-1.54396200	-0.70616400
H	3.48343000	-0.28632700	0.07593400
N	-1.29797500	1.77471500	0.16904600
H	-2.01645500	2.16199600	-0.43014000
H	-0.41123300	2.26310800	0.09550200

Cyclobutene (Starting material)

C	-1.24402000	-0.31218200	-0.14912000
C	-1.77021600	0.78805700	0.43037700
C	-0.61600100	1.68009700	0.01129400
H	-2.67865100	0.98342500	0.99245200
H	-0.00221800	2.10817000	0.81512900
H	-0.84064500	2.47338500	-0.71232500
C	0.00401900	0.38577600	-0.66474300
H	0.08899400	0.46064200	-1.75507700
C	1.35633000	-0.05564300	-0.11987400
O	2.33816200	-0.07038300	-0.84641700
C	1.43682000	-0.48346300	1.33238200
H	0.87855800	0.19298200	1.98879700
H	0.97674300	-1.47479100	1.43879000
H	2.48262700	-0.53711000	1.64300700
N	-1.55265300	-1.66052600	-0.22981400
H	-1.23355100	-2.12980200	-1.07053500
H	-2.51017500	-1.90601100	-0.00210400



Butadiene (Product)

C	0.82456200	0.40468800	-0.05292000
C	2.27401200	0.14953600	-0.10317000
C	2.88598100	-1.01628200	0.14514100
H	2.86626200	1.02966400	-0.34599400
H	3.96662900	-1.09797000	0.07670900
H	2.34627300	-1.91546700	0.42958100
C	-0.12902900	-0.56815900	-0.08717400
H	0.22342800	-1.58932900	-0.18524100
C	-1.59159600	-0.47954400	-0.01598300
O	-2.26369900	-1.50919700	-0.05181700
C	-2.30689400	0.86516000	0.10222700
H	-2.00879600	1.40446200	1.01263000
H	-2.11587400	1.50144100	-0.77438300
H	-3.38278200	0.68374000	0.15438700
O	0.60231200	1.74717400	0.01218100
H	-0.34626400	1.94725500	0.02067300

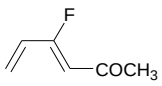
Transition state

C	1.14468300	0.41413700	-0.24249200
C	2.13006400	-0.50329300	0.03502500
C	1.40534700	-1.66778800	0.43745700
H	3.20242100	-0.43765800	-0.13870400
H	1.72116100	-2.67169900	0.13415800
H	0.77562300	-1.64887100	1.31880800
C	-0.07829400	-0.32764000	-0.44152400
H	-0.10293800	-1.00788100	-1.28783400
C	-1.39144800	0.09077800	0.10593600
O	-1.47944800	0.90147400	1.02341400
C	-2.62450300	-0.57907700	-0.47942500
H	-2.77436600	-0.24644800	-1.51553400
H	-2.50597400	-1.66978600	-0.50640400
H	-3.50549200	-0.31895500	0.11166500
O	1.19188400	1.76433900	-0.36101800

H	1.97498500	2.11209100	0.09480800

Cyclobutene (Starting material)

C	-1.23682000	-0.36584700	-0.13271900
C	-1.81478800	0.71165900	0.42007900
C	-0.69557000	1.63402000	-0.03577700
H	-2.73183000	0.88067000	0.97304100
H	-0.10116200	2.11389200	0.75171800
H	-0.96044000	2.38870600	-0.78546500
C	-0.01501300	0.35214300	-0.67869000
H	0.06356100	0.39925200	-1.77101000
C	1.35401700	-0.02261800	-0.12348100
O	2.32366800	-0.07471900	-0.86361600
C	1.46687100	-0.35074300	1.35338900
H	0.83904100	0.29764800	1.97286200
H	1.11869300	-1.37925800	1.52031800
H	2.51157900	-0.28196700	1.66497300
O	-1.58292300	-1.67779900	-0.17810500
H	-1.01759700	-2.15048300	-0.80947600



Butadiene (Product)

C	0.81370900	0.34433000	-0.05405100
C	2.26636500	0.18278000	-0.10233300
C	2.93700200	-0.95311900	0.13979600
H	2.80897000	1.09425100	-0.34513900
H	4.01984400	-0.98215700	0.06775600
H	2.43990000	-1.87799900	0.42022900
C	-0.14261300	-0.60289400	-0.08656500
H	0.18901600	-1.63236500	-0.17946500
C	-1.61543900	-0.45808100	-0.01315300
O	-2.29788800	-1.47824900	-0.04314000
C	-2.26423700	0.90751700	0.09649800
H	-1.91734300	1.43564900	0.99196900
H	-2.00207200	1.53557300	-0.76258200

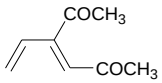
H	-3.34746100	0.77608700	0.14096500
F	0.46928100	1.66152900	0.01447000

Transition state

C	-1.13041700	-0.42433200	-0.22833900
C	-2.16081900	0.42521700	0.04520700
C	-1.48393900	1.62396100	0.43628600
H	-3.22623300	0.29906100	-0.12523200
H	-1.82633800	2.61101100	0.11057700
H	-0.85934300	1.63323100	1.32107800
C	0.06989800	0.33743200	-0.42973600
H	0.07492600	1.03500800	-1.26222800
C	1.39562500	-0.07086300	0.10299200
O	1.49444300	-0.93194800	0.96987700
C	2.61131800	0.65337300	-0.44775800
H	2.76064200	0.38615100	-1.50265300
H	2.47262700	1.74133600	-0.40878800
H	3.50017000	0.37435100	0.12221100
F	-1.18466500	-1.76592200	-0.32065400

Cyclobutene (Starting material)

C	-1.23737100	-0.30863200	-0.19218400
C	-1.81988500	0.65694400	0.52046500
C	-0.65968400	1.60712500	0.24456900
H	-2.74788900	0.75708000	1.07053400
H	-0.07386000	1.91207700	1.11940500
H	-0.89277800	2.49015900	-0.35951600
C	0.00097800	0.43632900	-0.60919700
H	0.07532000	0.67329700	-1.67535100
C	1.37275300	-0.02365000	-0.12403500
O	2.36859700	0.25830100	-0.76790800
C	1.44764200	-0.81592300	1.16519800
H	0.82642400	-0.37067900	1.95117500
H	1.05974100	-1.82876000	0.99158000
H	2.48576900	-0.88349900	1.49744700
F	-1.58978800	-1.56991600	-0.49787800



Butadiene (Product)

C	-0.66999800	-0.28192100	-0.18589300
C	-2.00354900	-0.90236000	-0.33316000
C	-2.38326500	-2.06428400	0.21934400
H	-2.72120200	-0.33387000	-0.92555800
H	-3.37909700	-2.46397500	0.04976800
H	-1.72209200	-2.64273700	0.85990700
C	0.46303700	-1.01883600	-0.14621200
H	0.37079700	-2.09866700	-0.24666800
C	1.88027300	-0.59636000	0.01049800
O	2.72015200	-1.47261200	0.19157300
C	2.29826900	0.85922600	-0.08519600
H	1.97010500	1.30384500	-1.03090500
H	1.86350800	1.45745500	0.72481400
H	3.38655100	0.91158500	-0.01074400
C	-0.74043800	1.23507700	-0.12647900
C	-0.95120000	1.85893900	1.23718900
H	-0.22263000	1.48535500	1.96561200
H	-0.89590500	2.94779000	1.16346000
H	-1.94323700	1.57035400	1.61056100
O	-0.72834900	1.88835800	-1.15417200

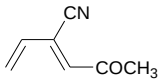
Transition state

C	-0.69842500	0.51722500	-0.14472700
C	-0.99148200	1.86099800	-0.00844100
C	0.25338400	2.51925200	0.17614000
H	-1.95197600	2.34982400	-0.15796000
H	0.46325200	3.51331500	-0.22663500
H	0.89531200	2.22799100	0.99965100
C	0.69576800	0.51182800	-0.55623200
H	0.95221700	0.98948200	-1.49714800
C	1.78294600	-0.38448700	-0.06619300
O	2.81431100	-0.49761600	-0.72126200
C	1.64357700	-1.05197300	1.29115800

H	2.05990400	-0.37721500	2.05220100
H	0.60612800	-1.25238000	1.57327700
H	2.22802200	-1.97545800	1.30970800
C	-1.67200700	-0.59915200	-0.02529300
C	-1.31436400	-1.95656800	-0.60206500
H	-0.25341600	-2.20382800	-0.49942600
H	-1.92846700	-2.72795200	-0.13117100
H	-1.53682000	-1.94824800	-1.67786900
O	-2.78062700	-0.38966800	0.45492300

Cyclobutene (Starting material)

C	-0.69308500	0.57116600	-0.14309300
C	-0.53800400	1.88740400	0.10905700
C	0.88212900	1.93794900	-0.40555100
H	-1.20525700	2.64436300	0.51106000
H	1.65489700	2.19688200	0.32861500
H	1.04294800	2.54493800	-1.30421800
C	0.71900200	0.39135600	-0.71398600
H	0.76899100	0.15824900	-1.78267500
C	1.70267000	-0.52262600	0.00550200
O	2.49547800	-1.19543800	-0.63340600
C	1.66652700	-0.57772400	1.52254000
H	1.43978900	0.39388100	1.97352800
H	0.87258200	-1.26720000	1.83998000
H	2.61997600	-0.95751500	1.89689400
C	-1.85601100	-0.33661300	0.01885000
C	-1.73377100	-1.73515400	-0.55201500
H	-0.89027700	-2.27245100	-0.09910200
H	-2.65723400	-2.28954600	-0.37237300
H	-1.53422300	-1.69158500	-1.63074600
O	-2.87159500	0.05111700	0.58230800



Butadiene (Product)

C	0.81660900	0.12564400	-0.10897600

C	2.24994500	-0.23915400	-0.19689700
C	2.77752300	-1.38687700	0.25100300
H	2.89937100	0.51678100	-0.63418000
H	3.83861300	-1.58888700	0.13948600
H	2.18317400	-2.14624500	0.75269100
C	-0.18482400	-0.79108500	-0.14706800
H	0.09703700	-1.83130500	-0.28803600
C	-1.66110800	-0.62590300	-0.02244100
O	-2.33287800	-1.65212900	-0.03431500
C	-2.31271100	0.73241400	0.11251700
H	-1.96618900	1.25274900	1.01275500
H	-2.07182700	1.37817400	-0.73954800
H	-3.39398300	0.59075500	0.16854900
C	0.58694500	1.54262900	-0.00065600
N	0.49179200	2.69985800	0.07684400

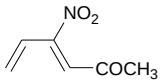
Transition state

C	-1.04754500	0.16755200	-0.18192900
C	-1.63599300	1.39945800	0.02442100
C	-0.56724200	2.26861300	0.38232700
H	-2.66812500	1.69315100	-0.15448500
H	-0.53879600	3.31871600	0.07985100
H	0.03360400	2.03429100	1.25381000
C	0.34467900	0.47283400	-0.43874800
H	0.55838300	1.07552000	-1.31628600
C	1.46554600	-0.34851000	0.09812700
O	1.25732000	-1.17753100	0.97483900
C	2.84811500	-0.10083100	-0.47177400
H	2.88554400	-0.42942100	-1.51916600
H	3.09098300	0.96934200	-0.46205700
H	3.59281200	-0.65423600	0.10401100
C	-1.66358800	-1.11898000	-0.16262100
N	-2.21097000	-2.14684700	-0.18331600

Cyclobutene (Starting material)

C	-1.05256900	0.37803800	-0.07862300
C	-1.04058600	1.59237100	0.50837400

C	0.38111800	1.90259800	0.09790700
H	-1.78651800	2.15261200	1.06459500
H	1.10139300	2.00523600	0.91844200
H	0.51246800	2.74553700	-0.58951100
C	0.37526500	0.48660900	-0.61757100
H	0.44554900	0.56151400	-1.70701000
C	1.45931600	-0.47689700	-0.13814500
O	2.46481200	-0.62297000	-0.81097900
C	1.25718800	-1.19973800	1.17662200
H	0.89725300	-0.52120100	1.95939700
H	0.48991300	-1.97620700	1.05481400
H	2.19294100	-1.66966000	1.48649700
C	-2.03226000	-0.64441700	-0.20054600
N	-2.80804700	-1.50649200	-0.31249900



Butadiene (Product)

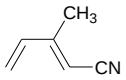
C	0.77452300	-0.18171500	-0.11923300
C	2.16756800	-0.64477900	-0.19108700
C	2.59517800	-1.80491200	0.32369300
H	2.86612200	0.02091400	-0.68882000
H	3.62875000	-2.11646700	0.20684800
H	1.94282900	-2.47162600	0.88308800
C	-0.32636500	-0.94872800	-0.17966100
H	-0.16761100	-2.01353200	-0.34140600
C	-1.78711100	-0.55001000	-0.17128700
O	-2.38550000	-0.58885600	-1.23001200
C	-2.46005800	-0.30960000	1.15866900
H	-2.55013500	-1.26886400	1.68815000
H	-1.87667400	0.36823900	1.78787000
H	-3.46061300	0.09743600	0.99200900
N	0.60606300	1.28926600	-0.01222200
O	1.62574000	1.97611500	0.01674300
O	-0.54118100	1.73742900	0.04217600

Transition state

C	-0.76492000	0.41902500	-0.17244300
C	-1.28817600	1.65829300	0.10353700
C	-0.14380700	2.45132600	0.38573700
H	-2.30650300	2.01041500	-0.03484300
H	-0.05415800	3.49059500	0.06301600
H	0.51798500	2.16899800	1.19649600
C	0.61749100	0.59772500	-0.52294700
H	0.83273800	1.21103500	-1.39243900
C	1.80675600	-0.20180700	-0.08389400
O	2.86341100	-0.02262900	-0.67694800
C	1.70845000	-1.14198800	1.09817700
H	1.02509100	-0.76877100	1.86956900
H	1.32049800	-2.10912000	0.75964300
H	2.70501400	-1.28873500	1.52147300
N	-1.47960500	-0.84026300	-0.14831600
O	-2.66638900	-0.81346700	0.18769600
O	-0.85929700	-1.85490600	-0.48496100

Cyclobutene (Starting material)

C	-0.73435200	0.49690600	-0.10685300
C	-0.74686000	1.74398300	0.38383300
C	0.69594300	1.97840800	-0.02101000
H	-1.49803300	2.35510900	0.87125800
H	1.39504000	2.12961500	0.80932500
H	0.85831900	2.75969700	-0.77080200
C	0.68405400	0.50463800	-0.62223600
H	0.77826300	0.49253500	-1.71184000
C	1.74743500	-0.42981500	-0.04341500
O	2.78885000	-0.58561500	-0.65489600
C	1.47871400	-1.10306900	1.28415800
H	1.08567100	-0.39496700	2.02429200
H	0.71627000	-1.88092100	1.14585900
H	2.39632600	-1.56255000	1.65749900
N	-1.75984500	-0.51819300	-0.16036500
O	-2.86926700	-0.24131200	0.29936600
O	-1.43990200	-1.60025700	-0.66320600



Butadiene (Product)

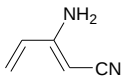
C	0.38993000	0.34856000	-0.08072700
C	1.84223600	0.12659400	-0.20463000
C	2.51054200	-0.95940500	0.21235400
H	2.40537800	0.95357500	-0.63872200
H	3.58602700	-1.04016800	0.08218800
H	2.01478700	-1.78796700	0.71255100
C	-0.48251600	-0.68561600	-0.17371600
H	-0.12655800	-1.69029200	-0.38592500
C	-1.89391500	-0.54808200	-0.02891400
N	-3.05129600	-0.46257200	0.08267100
C	-0.04768300	1.77541100	0.12757500
H	-1.13459500	1.87394300	0.17881600
H	0.38336200	2.17754200	1.05370600
H	0.31910900	2.40659800	-0.69295700

Transition state

C	-0.67221600	0.54229800	0.11226700
C	-1.79522800	-0.23099000	-0.06772400
C	-1.32602100	-1.57012300	-0.24673800
H	-2.84006200	0.06954700	-0.00020000
H	-1.85837000	-2.43706400	0.15793300
H	-0.68048800	-1.80339000	-1.08548700
C	0.32915900	-0.42880100	0.51118300
H	0.18604500	-0.96973800	1.44013100
C	1.69929100	-0.33400400	0.09957300
N	2.80211300	-0.28273400	-0.27801100
C	-0.44812600	2.01061800	-0.09245700
H	0.31183400	2.17822500	-0.86802000
H	-1.36931600	2.50652000	-0.41416600
H	-0.08558700	2.50105200	0.81926600

Cyclobutene (Starting material)

C	0.95153600	-0.25283000	0.02181700
C	1.35011200	0.94983400	-0.42501500
C	0.11007900	1.69372900	0.03028600
H	2.25033400	1.28759400	-0.93205400
H	-0.53217800	2.09142700	-0.76283300
H	0.24801900	2.46308400	0.79930000
C	-0.36195600	0.29750100	0.60187600
H	-0.41485900	0.27417400	1.69808200
C	-1.60355300	-0.24797400	0.05717400
N	-2.57876500	-0.69642400	-0.38995500
C	1.49008100	-1.64152900	0.02259700
H	0.80541400	-2.32869300	-0.49216000
H	2.46251300	-1.68548000	-0.47963000
H	1.61432200	-2.01951500	1.04656600



Butadiene (Product)

C	0.37312900	0.34615900	-0.08673700
C	1.83556600	0.18169400	-0.20105400
C	2.52540200	-0.88080900	0.23375500
H	2.36530000	1.01592300	-0.66129300
H	3.60238400	-0.93828400	0.10454800
H	2.04363500	-1.71541300	0.73634700
C	-0.48660700	-0.71463400	-0.19431500
H	-0.11111400	-1.69691600	-0.45282400
C	-1.88345500	-0.55077800	-0.03096000
N	-3.02852700	-0.36775500	0.11425100
N	-0.05816600	1.64416000	0.05858600
H	-1.04258300	1.80095000	0.24261800
H	0.56501600	2.30910900	0.49662200

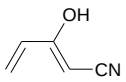
Transition state

C	-0.65986600	0.57356900	0.10507000

C	-1.81568600	-0.15469700	-0.08632200
C	-1.35070200	-1.50082900	-0.23950900
H	-2.85010800	0.17038800	-0.00824700
H	-1.89402400	-2.34489400	0.20117700
H	-0.73114700	-1.78389900	-1.08344300
C	0.31602700	-0.42611800	0.51474200
H	0.17464900	-0.90404200	1.47843300
C	1.68438700	-0.34495100	0.09245300
N	2.78235600	-0.30398300	-0.30229600
N	-0.41018900	1.92131100	-0.02398600
H	-0.88771700	2.42354200	-0.76104300
H	0.53821100	2.23575800	0.13848600

Cyclobutene (Starting material)

C	-0.92648500	0.35598900	0.01571200
C	-1.46460000	-0.80050600	-0.42381700
C	-0.29297900	-1.65274700	0.03152600
H	-2.40288000	-1.05546500	-0.90520600
H	0.30944000	-2.11817600	-0.75679200
H	-0.48803800	-2.39301200	0.81761400
C	0.32008300	-0.30635400	0.59351100
H	0.37098400	-0.27941600	1.68942500
C	1.60659100	0.12157300	0.04603500
N	2.61664100	0.48790000	-0.39855200
N	-1.28508800	1.68585200	0.11030600
H	-0.51537500	2.34637100	0.08322500
H	-2.05066300	1.97570100	-0.48834100



Butadiene (Product)

C	0.37809400	0.34208100	-0.08381100
C	1.83014800	0.14909400	-0.22198100
C	2.51039000	-0.91108900	0.23498500
H	2.36590200	0.95565700	-0.72601900
H	3.58250100	-0.99591200	0.08313200

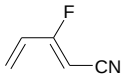
H	2.02216000	-1.71693100	0.77675000
C	-0.53145100	-0.65751100	-0.19822600
H	-0.19278000	-1.65346300	-0.45939000
C	-1.92827700	-0.46557400	-0.02764000
N	-3.08046100	-0.34850400	0.10631000
O	-0.05665400	1.61425300	0.12527600
H	0.68525800	2.19413900	0.35919100

Transition state

C	-0.66550200	0.55751700	0.10788300
C	-1.80652600	-0.18253300	-0.09010700
C	-1.31374900	-1.51826100	-0.23666600
H	-2.84720400	0.12154300	-0.00514500
H	-1.82750500	-2.37145600	0.21837800
H	-0.67492800	-1.78278900	-1.07100200
C	0.35297800	-0.37879800	0.51754000
H	0.21726500	-0.89551700	1.46135600
C	1.71478600	-0.26759000	0.09003300
N	2.81495000	-0.23807000	-0.29585400
O	-0.39777800	1.87875900	-0.03574300
H	-1.08196800	2.30262400	-0.57877500

Cyclobutene (Starting material)

C	0.92729700	-0.36049200	0.02638500
C	1.45881100	0.78662700	-0.42805400
C	0.27262300	1.61926400	0.03706700
H	2.38503000	1.05020900	-0.92712000
H	-0.33883400	2.07171400	-0.75052300
H	0.47084300	2.36258800	0.81789600
C	-0.32784800	0.26517000	0.60294600
H	-0.38099100	0.23621100	1.69809800
C	-1.61104300	-0.15982100	0.04682600
N	-2.63190400	-0.48737800	-0.40134000
O	1.23646400	-1.67183300	0.07994000
H	2.07652800	-1.83890200	-0.37950800



Butadiene (Product)

C	0.38612200	0.31788700	-0.04831800
C	1.84129500	0.23075200	-0.12018900
C	2.56702700	-0.86859400	0.13085500
H	2.33271000	1.16446100	-0.38547700
H	3.64847900	-0.85181400	0.03829400
H	2.11766600	-1.80748600	0.44410800
C	-0.52294600	-0.67517500	-0.12565100
H	-0.17960400	-1.69138500	-0.28803700
C	-1.92374400	-0.46654300	-0.01815800
N	-3.07840500	-0.33554400	0.06356900
F	-0.05077200	1.58945300	0.09276500

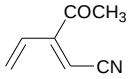
Transition state

C	-0.65687900	0.55958900	0.09135600
C	-1.81867900	-0.12258400	-0.11262400
C	-1.36583500	-1.47753500	-0.21973500
H	-2.84448200	0.22796600	-0.05113500
H	-1.89819800	-2.30236100	0.26308700
H	-0.72799000	-1.77569000	-1.04295000
C	0.34869700	-0.36978900	0.52034300
H	0.20104200	-0.88418900	1.46386400
C	1.71064900	-0.28914600	0.08882700
N	2.81303700	-0.27217500	-0.28980400
F	-0.41437200	1.87069900	-0.09036100

Cyclobutene (Starting material)

C	0.91797200	-0.38484900	0.01725500
C	1.49704300	0.72748900	-0.43381200
C	0.33355600	1.59075000	0.04159400
H	2.43105300	0.95647500	-0.93164400
H	-0.25942700	2.06418400	-0.74639700
H	0.56331500	2.32093000	0.82470500

C	-0.31884700	0.25685500	0.60630500
H	-0.36790500	0.22889200	1.70122800
C	-1.61693200	-0.12010800	0.05053400
N	-2.64896300	-0.41351700	-0.39474900
F	1.25543900	-1.67741000	0.02489900



Butadiene (Product)

C	0.50851800	-0.14057200	-0.07972800
C	1.97279800	-0.29384900	-0.11188200
C	2.64766500	-1.35277000	0.36040500
H	2.51156900	0.56129200	-0.51100600
H	3.73174000	-1.39116900	0.30495900
H	2.15520000	-2.19839300	0.83602500
C	-0.30785600	-1.22233200	-0.18103100
H	0.14233600	-2.20000000	-0.34150400
C	-1.73089700	-1.24570000	-0.14975000
N	-2.89233300	-1.34187400	-0.13400300
C	0.01958700	1.29744200	-0.02626900
C	-1.32804000	1.63871000	0.56817800
H	-2.12999900	1.41573300	-0.14535000
H	-1.53711600	1.06510100	1.47699100
H	-1.34304900	2.70915300	0.78553200
O	0.75312400	2.16822900	-0.46839400

Transition state

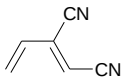
0 1

C	-0.29652900	0.42549900	-0.21127100
C	-0.41730300	1.79228700	-0.03269200
C	0.89495300	2.26307200	0.24994800
H	-1.28845500	2.42352300	-0.19984500
H	1.26366400	3.23078100	-0.10019600
H	1.42726700	1.86449000	1.10651700
C	1.10821000	0.25312500	-0.52051000
H	1.48883400	0.71654400	-1.42418200

C	1.93415900	-0.80025800	-0.01521500
N	2.67491800	-1.58147800	0.43203900
C	-1.29370800	-0.66304500	-0.06630200
C	-2.71402700	-0.27145600	0.29613800
H	-3.08445600	0.53221700	-0.35238300
H	-3.36283400	-1.14492100	0.20391200
H	-2.75295600	0.09798900	1.32870100
O	-0.96375300	-1.83070200	-0.22342100

Cyclobutene (Starting material)

C	0.30637500	0.44152900	0.10778800
C	0.03996900	1.72251300	-0.22001600
C	-1.42012800	1.65314900	0.16906500
H	0.65021100	2.53762200	-0.59933700
H	-2.13736400	1.76029100	-0.65136100
H	-1.72797900	2.29611700	1.00165400
C	-1.12043500	0.15477700	0.58672500
H	-1.20036800	-0.02763400	1.66399500
C	-1.87750600	-0.86503700	-0.13521000
N	-2.49683300	-1.64918600	-0.72821300
C	1.50102200	-0.42860200	0.12506900
C	2.76151300	0.08207200	-0.54387900
H	2.98191100	1.11552400	-0.25157700
H	3.60109400	-0.56458600	-0.27961900
H	2.63139300	0.06993100	-1.63391800
O	1.44176000	-1.52567100	0.66380000



Butadiene (Product)

C	0.43025400	0.12114700	-0.10296700
C	1.90008300	0.02868400	-0.19981200
C	2.63011200	-1.01138900	0.22728600
H	2.39563200	0.89890600	-0.62479500
H	3.70954400	-1.01608000	0.11054900
H	2.18778700	-1.87230400	0.72238500

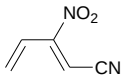
C	-0.39626100	-0.95723900	-0.15106800
H	0.02719400	-1.94474800	-0.31286800
C	-1.81092500	-0.89698300	-0.02014100
N	-2.97151500	-0.89615200	0.08019000
C	-0.10635300	1.44886100	0.02597400
N	-0.48586000	2.54411500	0.12396700

Transition state

C	0.69059100	0.14118300	0.14267100
C	1.16847800	1.41957800	-0.06715300
C	0.00866600	2.21560400	-0.28940900
H	2.18874200	1.78148800	0.03584500
H	-0.07381100	3.24454500	0.06946700
H	-0.64562800	1.97687700	-1.12053500
C	-0.69270400	0.34580400	0.52485700
H	-0.88594000	0.88773600	1.44365900
C	-1.76237500	-0.50215000	0.09786700
N	-2.65248700	-1.15055400	-0.28415900
C	1.35664500	-1.10986300	-0.00638900
N	1.90975000	-2.12824300	-0.12199800

Cyclobutene (Starting material)

C	0.69144400	0.37997400	0.01354700
C	0.40887600	1.62156200	-0.42606800
C	-1.02837600	1.59829300	0.04405300
H	1.00508100	2.37826900	-0.92591100
H	-1.78508600	1.61467200	-0.74680900
H	-1.29695100	2.32797400	0.81599100
C	-0.70880500	0.15259100	0.60427700
H	-0.72014700	0.09846700	1.69874100
C	-1.50024700	-0.94511900	0.05485900
N	-2.13721600	-1.80885700	-0.38975400
C	1.84778900	-0.44319700	0.00416000
N	2.78478900	-1.13457200	0.01675700



Butadiene (Product)

C	0.45823800	-0.17076900	-0.08075000
C	1.89695600	-0.42837300	-0.14463700
C	2.47079800	-1.56151300	0.28702000
H	2.50182400	0.37938900	-0.54372000
H	3.54327800	-1.70532800	0.19892600
H	1.90654400	-2.36482400	0.75480600
C	-0.50970400	-1.10698100	-0.18835100
H	-0.18688500	-2.12589900	-0.38849000
C	-1.91941700	-0.93865700	-0.11136100
N	-3.08371300	-0.94429400	-0.08315400
N	0.07323700	1.26025500	0.05548000
O	0.88695200	2.09141900	-0.34660700
O	-1.02103400	1.51391800	0.54669100

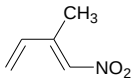
Transition state

C	0.40539100	0.39339900	0.15833600
C	0.72479000	1.71252700	-0.03290200
C	-0.53959100	2.33689500	-0.23310800
H	1.68542600	2.20234300	0.09380800
H	-0.77605800	3.32367200	0.17125700
H	-1.16143400	2.02533400	-1.06485000
C	-0.98287700	0.34670700	0.53271900
H	-1.26894100	0.83606100	1.45782800
C	-1.93472300	-0.60168700	0.04639800
N	-2.77066700	-1.29762300	-0.37129100
N	1.27883000	-0.75429700	0.00119400
O	2.46576200	-0.52274100	-0.23997500
O	0.77497700	-1.87113600	0.12797300

Cyclobutene (Starting material)

C	0.37709400	0.44197900	0.06366000
C	0.17550500	1.71990200	-0.27807800

C	-1.27473100	1.68499700	0.16691500
H	0.81057400	2.49426600	-0.69183000
H	-2.01297700	1.80037700	-0.63223200
H	-1.52932900	2.34594500	1.00200300
C	-1.01649900	0.17747200	0.59902400
H	-1.06079600	0.01731800	1.68148600
C	-1.83047300	-0.82703300	-0.08149500
N	-2.49913700	-1.60188400	-0.63003700
N	1.54340500	-0.40626400	0.01845400
O	1.42852700	-1.52672300	0.51907600
O	2.55863300	0.05362600	-0.50638900



Butadiene (Product)

C	0.77103700	0.40255300	-0.11538200
C	2.17419100	-0.04039000	-0.24121700
C	2.69248600	-1.15924300	0.28743300
H	2.83229300	0.64665900	-0.77322500
H	3.74217500	-1.40532200	0.15457900
H	2.09939900	-1.84537500	0.88702400
C	-0.19363300	-0.54442900	-0.16417300
H	0.00724900	-1.59007800	-0.35072100
N	-1.60765900	-0.30778900	-0.00204000
O	-2.02091200	0.83672000	0.22368100
O	-2.33674800	-1.30343200	-0.10174600
C	0.55079200	1.88739700	0.04043500
H	-0.19628800	2.26507000	-0.66289300
H	0.16849700	2.11564000	1.04186100
H	1.49233200	2.42630100	-0.10039600

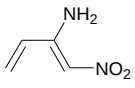
Transition state

C	1.03353200	0.43348000	-0.18159600
C	2.03824600	-0.49140800	0.02160800
C	1.39814500	-1.70477300	0.40790600
H	3.10116500	-0.38102100	-0.18832600

H	1.76808100	-2.68558100	0.09343400
H	0.77963000	-1.73077100	1.29730800
C	-0.09056200	-0.43018500	-0.42320000
H	-0.14678700	-1.08132200	-1.28522400
N	-1.44534500	-0.06757600	-0.00263800
O	-2.37167200	-0.77394500	-0.41552100
O	-1.58015600	0.89324500	0.76482700
C	1.09833600	1.93153600	-0.18521800
H	0.40874500	2.37455100	-0.91022700
H	0.83637100	2.33388900	0.80007700
H	2.11865000	2.25698500	-0.42002400

Cyclobutene (Starting material)

C	1.65868300	0.99444500	0.34181100
C	1.24359000	-0.19389900	-0.13195200
C	-0.09079200	0.36470100	-0.58509500
H	-0.29899400	0.39445100	-1.65594600
C	0.35840200	1.72462100	0.05800500
H	2.59760100	1.33376300	0.77169100
H	0.38907600	2.56664200	-0.64307500
H	-0.22550300	2.00843400	0.94052100
N	-1.33433800	-0.22388300	0.04612700
O	-1.23257200	-0.71504800	1.16843100
O	-2.37796600	-0.14698100	-0.60071700
C	1.81211100	-1.56537500	-0.25339700
H	2.83700100	-1.59952100	0.13107400
H	1.20908600	-2.28607100	0.31388800
H	1.82445000	-1.90123400	-1.29898300



Butadiene (Product)

C	0.76392700	0.41624600	-0.09314700
C	2.18637000	0.02785200	-0.21383700
C	2.71697100	-1.10997000	0.25024700
H	2.82829400	0.76129800	-0.70188500

H	3.77427200	-1.32278100	0.12213300
H	2.12536000	-1.85331500	0.77765800
C	-0.21337900	-0.55358700	-0.15909400
H	0.01684000	-1.58866200	-0.35340500
N	-1.59022300	-0.30221400	-0.00818500
O	-1.99136800	0.87762900	0.16347300
O	-2.36232500	-1.27151400	-0.05326700
N	0.52229900	1.73886600	0.03534300
H	1.27941600	2.38175800	0.21552800
H	-0.44249800	2.03297600	0.16320600

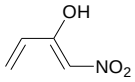
Transition state

C	1.04016100	0.48755800	-0.15636000
C	2.07585900	-0.41200000	0.03916400
C	1.41989200	-1.63605300	0.37493000
H	3.13246300	-0.28709700	-0.18242900
H	1.78881900	-2.59860900	0.00243200
H	0.82907100	-1.72657900	1.27985800
C	-0.06709000	-0.41188000	-0.42209600
H	-0.09415800	-1.01529000	-1.32004900
N	-1.43019700	-0.08838500	-0.02154000
O	-2.29477100	-0.94557200	-0.22327500
O	-1.64714000	1.00374000	0.53314600
N	1.03254600	1.85753500	-0.19357600
H	1.73439600	2.32809400	0.36359800
H	0.11531800	2.28433600	-0.13039900

Cyclobutene (Starting material)

C	1.70388700	-0.96935000	-0.37241200
C	1.23669700	0.24070300	0.01171500
C	-0.03262600	-0.34148200	0.58531600
H	-0.16051900	-0.25250800	1.67023100
C	0.45621500	-1.72731900	0.06979300
H	2.64649500	-1.30948300	-0.78836300
H	0.57736000	-2.47510500	0.86365400
H	-0.16884000	-2.15049800	-0.72253800
N	-1.32392800	0.20144900	0.01232400

O	-1.38496600	1.42600100	-0.12981900
O	-2.22926000	-0.58345100	-0.24169400
N	1.67250500	1.54464500	0.08242600
H	0.92849900	2.23269800	0.02391800
H	2.46573500	1.77652900	-0.50450600



Butadiene (Product)

C	0.76064900	0.40394200	-0.10476800
C	2.17108800	-0.00529700	-0.25376000
C	2.71133700	-1.10465300	0.28731000
H	2.79498900	0.67493200	-0.83668400
H	3.75888200	-1.34608800	0.13228000
H	2.13174200	-1.78703900	0.90334300
C	-0.23622600	-0.51324700	-0.18380100
H	-0.02692300	-1.54914500	-0.40000500
N	-1.63579800	-0.25568200	-0.00580000
O	-2.03245100	0.89746600	0.18383100
O	-2.37410300	-1.25270300	-0.05789300
O	0.52911200	1.72086100	0.06986400
H	1.37034700	2.18764800	0.20537800

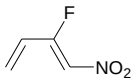
Transition state

C	1.00560400	0.48947600	-0.20170700
C	2.08590900	-0.33611700	0.02763800
C	1.50235700	-1.57976100	0.40501000
H	3.13542400	-0.15996800	-0.19668800
H	1.92553900	-2.53156200	0.06972200
H	0.87678200	-1.65635200	1.28569100
C	-0.09213400	-0.40197300	-0.44289600
H	-0.12744100	-1.02728000	-1.32435800
N	-1.44159000	-0.08854400	0.01823400
O	-2.37630500	-0.66520900	-0.55124700
O	-1.56530100	0.67086700	0.98464200
O	0.89718300	1.83192200	-0.29234400

H	1.62579800	2.26457900	0.18131300

Cyclobutene (Starting material)

C	1.77341700	0.80305100	0.31290200
C	1.20970500	-0.33245300	-0.13441500
C	-0.05571200	0.31325600	-0.61332100
H	-0.26789000	0.30193100	-1.68241800
C	0.54728900	1.64226500	-0.02766000
H	2.73516700	1.05877100	0.74435700
H	0.67606100	2.43076200	-0.77779400
H	-0.01510300	2.03257700	0.82697400
N	-1.33551200	-0.13048200	0.06589000
O	-1.28227400	-0.41129900	1.25963300
O	-2.35120600	-0.15215400	-0.62647500
O	1.51019400	-1.64061500	-0.25499300
H	2.35844900	-1.83484000	0.17730100



Butadiene (Product)

C	0.76675900	0.38388400	-0.07383600
C	2.19752700	0.09159000	-0.16669300
C	2.77493200	-1.06239100	0.19631500
H	2.79880100	0.91831100	-0.53975300
H	3.84547500	-1.20480100	0.08567300
H	2.21227000	-1.88804800	0.62407900
C	-0.22351600	-0.52884200	-0.13914400
H	-0.00903000	-1.57401000	-0.30336600
N	-1.63347700	-0.26283700	-0.00323100
O	-2.03068100	0.89375500	0.14413300
O	-2.36424700	-1.26216800	-0.04909200
F	0.51689300	1.69225300	0.05508800

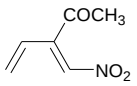
Transition state

C	0.99227700	0.49521700	-0.18760000

C	2.10385100	-0.26610500	0.04508600
C	1.56295400	-1.53530900	0.40698100
H	3.14392800	-0.03709200	-0.16774800
H	2.00834900	-2.46892600	0.05261000
H	0.93943600	-1.63645300	1.28624600
C	-0.08565700	-0.40525700	-0.43707100
H	-0.10176400	-1.05723200	-1.29967700
N	-1.44141300	-0.10872700	0.01753800
O	-2.35631300	-0.76251900	-0.49409200
O	-1.57997500	0.73355200	0.90885000
F	0.90552200	1.82902800	-0.25295900

Cyclobutene (Starting material)

C	1.79492400	0.76003200	0.33512600
C	1.20736300	-0.34342500	-0.12940900
C	-0.05192100	0.30315700	-0.61216300
H	-0.25969300	0.31108700	-1.68202500
C	0.57676900	1.61539500	-0.00733700
H	2.75965700	0.99124500	0.76947800
H	0.72735300	2.40670000	-0.74887200
H	0.02112600	2.00438200	0.85119200
N	-1.34028500	-0.12282900	0.06152300
O	-1.28501400	-0.45204800	1.24229900
O	-2.35955800	-0.07936900	-0.62305000
F	1.56970300	-1.62369300	-0.23241500



Butadiene (Product)

C	0.62664600	-0.28808000	-0.13976200
C	1.94359600	-0.93964300	-0.23689500
C	2.27913100	-2.08874400	0.36894700
H	2.68264900	-0.39667300	-0.82438200
H	3.27360900	-2.50970600	0.25266000
H	1.58802800	-2.62927100	1.01113000
C	-0.50507400	-1.01448000	-0.14087400

H	-0.54545300	-2.09022600	-0.24963500
N	-1.82302700	-0.42683200	-0.03722100
O	-1.92708400	0.80494800	0.00860800
O	-2.77244100	-1.21447000	-0.00357300
C	0.68978200	1.23902900	-0.15101100
C	0.60543300	1.96749400	1.16655000
H	1.52177900	1.76349600	1.73854700
H	0.53152800	3.04213000	0.98320300
H	-0.24645000	1.62753700	1.76133300
O	0.96432700	1.77540800	-1.20679100

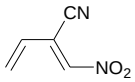
Transition state

C	-0.62644600	0.52613000	-0.13506400
C	-0.88442400	1.88398200	-0.05592000
C	0.35606400	2.51410900	0.21873500
H	-1.81525800	2.39274600	-0.29395700
H	0.61425700	3.50074900	-0.17423000
H	0.93016200	2.21024400	1.08674000
C	0.77057000	0.51104900	-0.46834500
H	1.15889700	0.90431800	-1.39809800
N	1.69080500	-0.48982400	0.07468900
O	2.77516100	-0.62875700	-0.49996700
O	1.34430700	-1.09751200	1.09400900
C	-1.64878000	-0.56300800	-0.05063900
C	-1.26681600	-1.99281800	-0.35901100
H	-0.61051000	-2.06182300	-1.23429500
H	-0.72141000	-2.41838300	0.49095300
H	-2.17563100	-2.57404800	-0.52986300
O	-2.79661200	-0.24894400	0.23488200

Cyclobutene (Starting material)

C	0.47536700	1.89260600	0.18157500
C	0.66100800	0.59096900	-0.11796700
C	-0.76447600	0.40573900	-0.60074000
H	-0.93118400	0.20264200	-1.65937800
C	-1.00005500	1.89595100	-0.15912700
H	1.14900400	2.67032200	0.52731500

H	-1.32901100	2.56489200	-0.96210000
H	-1.67513400	2.00143300	0.69745600
N	-1.63612500	-0.58194700	0.14175500
O	-1.29472200	-0.91807100	1.27349500
O	-2.65340200	-0.95915000	-0.43600600
C	1.85833600	-0.28757600	-0.05512200
C	1.68598800	-1.73837600	-0.44583600
H	1.24378500	-1.82687900	-1.44696500
H	2.65400100	-2.24318900	-0.42728800
H	1.00172500	-2.23282000	0.25590400
O	2.92845900	0.17489100	0.31327000



Butadiene (Product)

C	0.74067900	0.09951900	-0.11632800
C	2.13905200	-0.37151300	-0.22564200
C	2.58926100	-1.53599800	0.26166000
H	2.82600400	0.32133700	-0.70634300
H	3.63007600	-1.82026600	0.13985100
H	1.95379900	-2.22401600	0.81339700
C	-0.29638100	-0.76457800	-0.15773900
H	-0.17531000	-1.82624800	-0.31955800
N	-1.68798200	-0.38902700	-0.00348900
O	-1.97815200	0.79832100	0.13924700
O	-2.49335600	-1.32596400	-0.03155100
C	0.60067500	1.52475200	0.00765100
N	0.67338000	2.68291900	0.08827100

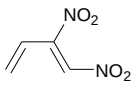
Transition state

C	-0.95246100	0.18544300	-0.15436500
C	-1.51031300	1.43951900	0.03579400
C	-0.43100400	2.29360000	0.37969700
H	-2.53016100	1.75291100	-0.17431400
H	-0.38913900	3.33824800	0.06280300
H	0.18578700	2.05678500	1.23913300

C	0.41610500	0.49511600	-0.45095500
H	0.70348500	1.04228500	-1.33825700
N	1.51167900	-0.36434900	0.00328000
O	2.62989800	-0.12499900	-0.46084300
O	1.24944000	-1.23585600	0.83458600
C	-1.59263000	-1.08820900	-0.12775600
N	-2.16637300	-2.10082400	-0.12810800

Cyclobutene (Starting material)

C	0.95198700	1.65187300	0.34577500
C	1.01308700	0.37388700	-0.07938900
C	-0.40876700	0.37558300	-0.60360600
H	-0.55382000	0.26517000	-1.67800900
C	-0.50207900	1.83870400	-0.03592700
H	1.68644600	2.32031600	0.78361700
H	-0.72222000	2.60442600	-0.78730500
H	-1.19437100	1.94374300	0.80606900
N	-1.37913300	-0.58302800	0.05151200
O	-1.15386000	-0.92390200	1.20826500
O	-2.35142300	-0.91736800	-0.62054600
C	2.03051300	-0.61606300	-0.12092700
N	2.85310200	-1.43802900	-0.17460900



Butadiene (Product)

C	0.49425400	0.11407000	0.02485900
C	0.50163100	1.53220600	0.37614400
C	-0.30328400	2.48392000	-0.12155500
H	1.28524800	1.80862400	1.07532600
H	-0.19135900	3.50827000	0.22236100
H	-1.06004300	2.28648700	-0.86965100
C	-0.48125000	-0.79031200	-0.16076400
N	1.88006200	-0.50098800	-0.04757000
N	-1.90202400	-0.52206800	-0.00962300
H	-0.26850600	-1.83797900	-0.32451200

O	1.97937300	-1.68447200	-0.35670400
O	2.82197000	0.24391200	0.20095100
O	-2.39444000	0.46701100	-0.55050700
O	-2.51686800	-1.35686500	0.65434900

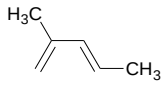
Transition state

C	-0.69825000	0.39272100	-0.17649700
C	-1.23040800	1.65455200	-0.06031700
C	-0.11888500	2.48786200	0.22065000
H	-2.23810900	1.98081900	-0.30071900
H	-0.03371700	3.50213700	-0.17439400
H	0.51026000	2.26917900	1.07569400
C	0.67684000	0.56118300	-0.49284400
H	1.01328000	1.02538800	-1.40946800
N	1.71606100	-0.29412100	0.09012500
O	2.75508300	-0.42192200	-0.56029200
O	1.49643200	-0.77038400	1.20422800
N	-1.41351500	-0.87253800	-0.09542400
O	-0.80735500	-1.88800200	-0.43240700
O	-2.58732500	-0.81829300	0.27597500

Cyclobutene (Starting material)

C	0.66478300	1.77897000	0.18369500
C	0.69844000	0.47810000	-0.13068900
C	-0.71040000	0.38703600	-0.62931600
H	-0.87654200	0.16162900	-1.68157600
C	-0.79917100	1.90462600	-0.20634200
H	1.40172900	2.48346800	0.55117100
H	-1.02357600	2.58814600	-1.03129700
H	-1.48219900	2.09087200	0.62832300
N	-1.64741600	-0.50474100	0.15439900
O	-1.40360000	-0.67741200	1.34452100
O	-2.61142700	-0.95391000	-0.45674000
N	1.74353300	-0.51489400	-0.09168900
O	1.45803900	-1.62661900	-0.54113300
O	2.83022100	-0.17694200	0.37714300

6.3.2 1,3-Disubstituted butadienes



Butadiene (Product)

C	-0.30243400	-0.35975300	-0.23406900
C	1.09605400	0.08694000	-0.05847900
C	1.45603800	1.38227700	-0.09186700
H	2.48767700	1.68823100	0.06443300
H	0.73587200	2.17194200	-0.28891600
C	-1.39800100	0.27926000	0.20773500
H	-1.27404400	1.20608000	0.76989100
C	-2.80974900	-0.18925000	0.00147300
H	-3.32662300	-0.33080700	0.96080900
H	-3.39357600	0.55235700	-0.56204400
H	-2.84533500	-1.13628000	-0.54887400
H	-0.43269400	-1.31840700	-0.74268400
C	2.11337100	-1.01556900	0.13914500
H	1.88866300	-1.60460100	1.03863900
H	2.10002200	-1.71524100	-0.70823600
H	3.12835900	-0.61670200	0.23335300

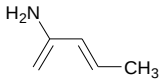
Transition state

C	-0.09057800	-0.84282300	-0.07313100
C	1.02040700	-0.02273200	-0.08818700
C	0.47164400	1.30045700	-0.12382700
H	0.95994400	2.14394400	0.38068700
H	-0.13872000	1.59649800	-0.96991200
C	-1.16858400	-0.02009800	0.38402800
H	-0.18505600	-1.87214400	-0.42361000
H	-1.07097300	0.40681000	1.37756800
C	-2.58860500	-0.12267800	-0.11596300
H	-3.14506100	-0.88375800	0.45477800
H	-3.12440100	0.82450100	0.01947100
H	-2.63754300	-0.39530900	-1.17590800
C	2.47904800	-0.36930700	0.03474700

H	2.91882400	0.13170900	0.90970800
H	2.62696900	-1.44728300	0.16089500
H	3.05602600	-0.04188600	-0.83967500

Cyclobutene (Starting material)

C	-0.05411600	-1.00327100	-0.27635800
C	-0.97988900	-0.05952000	-0.02568900
C	0.00832900	1.09118600	-0.17460800
H	0.19955000	1.67329100	0.73743700
H	-0.18982800	1.79039100	-0.99880100
C	1.08808600	-0.01601800	-0.47521200
H	-0.09442800	-2.09063000	-0.32621500
H	1.45138200	0.03105500	-1.51232900
C	2.27598100	-0.09824300	0.48242300
H	2.86121200	-1.01053200	0.30834700
H	2.94909200	0.75960700	0.35366200
H	1.93692000	-0.11247500	1.52628200
C	-2.44169900	-0.06113200	0.27634100
H	-3.00284000	0.50293600	-0.48210500
H	-2.84328000	-1.08050800	0.30903600
H	-2.64792700	0.41884800	1.24330600



Butadiene (Product)

C	-0.29218200	-0.36892500	-0.25611900
C	1.11286500	0.04533500	-0.05721700
C	1.51850800	1.33290900	-0.07831500
H	2.55424200	1.60857700	0.10585500
H	0.82868000	2.12955500	-0.33056500
C	-1.36386900	0.27447200	0.23195400
H	-1.20577400	1.16162100	0.84642700
C	-2.79016000	-0.13158900	-0.00237400
H	-3.31409700	-0.30784400	0.94718000
H	-3.34435700	0.66224100	-0.52273400
H	-2.85840700	-1.04327800	-0.60634500

H	-0.43461600	-1.28393800	-0.83475200
N	2.00547900	-1.03735800	0.05985300
H	2.95309400	-0.77648000	0.31073900
H	1.67191100	-1.80216100	0.63764800

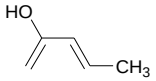
Transition state

C	-0.07768300	-0.87317500	-0.07736200
C	1.03072500	-0.04599500	-0.08435400
C	0.50629700	1.28960300	-0.08963800
H	1.02753400	2.10520600	0.42996300
H	-0.06489700	1.61580800	-0.95231600
C	-1.13171800	-0.02858400	0.39948900
H	-0.18346200	-1.88556500	-0.46525000
H	-1.05286800	0.36847900	1.40744100
C	-2.54498800	-0.08196000	-0.12903400
H	-3.13283400	-0.83253400	0.42374100
H	-3.05535500	0.87899600	0.00781700
H	-2.57981000	-0.34219100	-1.19257400
N	2.38024500	-0.38750200	-0.04457700
H	3.03587300	0.38363800	-0.04073300
H	2.64831300	-1.13866300	0.57934300

Cyclobutene (Starting material)

C	0.07345400	-1.02975900	0.26515300
C	0.99730800	-0.07614600	0.01626300
C	0.03472900	1.08029600	0.18006600
H	-0.15546000	1.66558400	-0.72927700
H	0.24621600	1.77051000	1.00874500
C	-1.05117200	-0.02335800	0.48090400
H	0.09817400	-2.11611100	0.29441400
H	-1.41318100	0.02968500	1.51893000
C	-2.24507000	-0.07012400	-0.47284900
H	-2.84164700	-0.97685400	-0.30810100
H	-2.90654300	0.79499100	-0.32849700
H	-1.91005900	-0.07671400	-1.51810700
N	2.33191800	-0.04034200	-0.35629500
H	2.84013500	0.79180200	-0.08032500

H	2.86343400	-0.88595700	-0.18093700



Butadiene (Product)

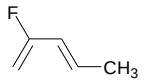
C	-0.28134500	-0.35941200	-0.26978900
C	1.12313000	0.03431600	-0.05609000
C	1.59693400	1.28931200	-0.08687200
H	2.64462000	1.49342100	0.10846200
H	0.94536000	2.11691100	-0.33950600
C	-1.34492700	0.28159600	0.24010300
H	-1.17102600	1.14536200	0.88281100
C	-2.77667800	-0.09278400	-0.00732000
H	-2.86099700	-0.98387300	-0.63901400
H	-3.30294700	-0.28760500	0.93697000
H	-3.31540400	0.72700600	-0.50254400
H	-0.43789100	-1.24834200	-0.88673100
O	2.00913500	-1.00994000	0.13801100
H	1.52251400	-1.80153500	0.41527400

Transition state

C	-0.07093900	-0.89174700	-0.03654800
C	1.02903900	-0.06913800	-0.06674600
C	0.55321800	1.27839200	-0.09329500
H	1.08877400	2.08160000	0.42814000
H	-0.02216600	1.61158800	-0.95011900
C	-1.12018300	-0.01949300	0.40183600
H	-0.17569900	-1.91627100	-0.38682900
H	-1.04140400	0.40407500	1.39824100
C	-2.52082800	-0.05435500	-0.15492200
H	-3.10245100	-0.84737200	0.34271000
H	-3.04865000	0.88826000	0.02982600
H	-2.53488400	-0.25663800	-1.23139900
O	2.33777700	-0.45989600	0.04329400
H	2.91242500	0.25197100	-0.27887400

Cyclobutene (Starting material)

C	0.08663200	-1.04648300	0.23713900
C	1.00018600	-0.09176600	0.00304100
C	0.06581500	1.08128400	0.19175900
H	-0.13220000	1.68774400	-0.70233000
H	0.28888300	1.74802600	1.03580400
C	-1.02343100	-0.02634300	0.47845400
H	0.11037400	-2.13084100	0.26221500
H	-1.36743200	0.01242100	1.52223300
C	-2.22660900	-0.04797700	-0.46292900
H	-2.82789900	-0.95262500	-0.30649200
H	-2.87881200	0.81968100	-0.29679800
H	-1.90310800	-0.04020300	-1.51168400
O	2.32878500	-0.13944100	-0.28299600
H	2.66435400	0.75904000	-0.42375900



Butadiene (Product)

C	-0.28921800	-0.40306300	-0.17191300
C	1.10438800	0.02326600	-0.04107700
C	1.64345400	1.24389200	-0.08305500
H	2.70890900	1.38796200	0.05727000
H	1.02166000	2.11191300	-0.26792000
C	-1.35810000	0.33645700	0.16460100
H	-1.20042800	1.32311000	0.60193000
C	-2.78386700	-0.09518600	-0.00888500
H	-3.31819400	-0.08311800	0.95082000
H	-3.32331900	0.59090500	-0.67666000
H	-2.85342300	-1.10416900	-0.42919000
H	-0.42550300	-1.41131700	-0.56199800
F	1.94337200	-1.04972000	0.12974700

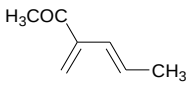
Transition state

C	-0.05099600	-0.90198100	-0.02394800
C	1.01871200	-0.05267600	-0.07687200

C	0.57010000	1.29003800	-0.10247900
H	1.12081800	2.08463000	0.40864800
H	-0.03675400	1.62289400	-0.93701200
C	-1.10110400	-0.02747700	0.41300600
H	-0.14766100	-1.92563700	-0.37714100
H	-1.01227500	0.39956200	1.40639200
C	-2.49573300	-0.05439600	-0.15494000
H	-3.03667700	-0.93236000	0.23413000
H	-3.06873300	0.83220400	0.13668300
H	-2.49652700	-0.12853800	-1.24806400
F	2.33688100	-0.38597900	0.00530700

Cyclobutene (Starting material)

C	0.11960900	-1.03746600	0.25446300
C	0.99271700	-0.06154800	0.00028100
C	0.06685500	1.10552000	0.17016300
H	-0.13969600	1.69135400	-0.73335500
H	0.29200500	1.78496300	1.00081800
C	-1.00273100	-0.01910400	0.48229700
H	0.16175100	-2.11999500	0.29549100
H	-1.33525000	0.02520200	1.52815800
C	-2.20629000	-0.08282300	-0.45506000
H	-2.79274200	-0.99302600	-0.27790700
H	-2.87026300	0.77787600	-0.30452900
H	-1.88586000	-0.08982900	-1.50442500
F	2.30545500	-0.05600200	-0.30190200



Butadiene (Product)

C	-0.96741000	-0.22167200	-0.20589600
C	0.34353900	0.44943600	-0.11216800
C	0.50834100	1.78724900	-0.16706600
H	1.48066400	2.25791100	-0.06837000
H	-0.33426000	2.45499400	-0.32445700
C	-2.13797800	0.30114300	0.19260200

H	-2.15305600	1.29200000	0.65074900
C	-3.46582300	-0.38927300	0.07750000
H	-3.94036000	-0.50070900	1.06227500
H	-4.16175400	0.19475100	-0.54125600
H	-3.36595700	-1.38430700	-0.36924800
H	-0.94063000	-1.23737600	-0.59474900
C	1.53768900	-0.46404700	0.00554600
C	2.92537000	0.12586600	0.20299700
H	3.63721400	-0.69540000	0.30719100
H	3.21736400	0.74486400	-0.65378800
H	2.96783900	0.75781300	1.09784800
O	1.39132200	-1.67709400	-0.06591100

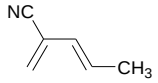
Transition state

C	-0.73933800	-0.75397500	-0.12556500
C	0.27099200	0.20124900	-0.16792600
C	-0.43873800	1.44559300	-0.18393100
H	-0.07825900	2.32629300	0.35314400
H	-1.08948300	1.66121000	-1.02369300
C	-1.87672800	-0.05993400	0.37817800
H	-0.74515200	-1.77096300	-0.51891800
H	-1.76450500	0.39806100	1.35756700
C	-3.30231800	-0.32162100	-0.03744900
H	-3.77582500	-1.04950300	0.63945500
H	-3.90033800	0.59560300	0.02172800
H	-3.37275500	-0.70852800	-1.05935100
C	1.73312000	0.05660100	-0.01262600
C	2.30949600	-1.34926100	0.01951000
H	1.85169600	-1.99109600	-0.74285300
H	3.38975400	-1.30196000	-0.13632500
H	2.11335100	-1.81114900	0.99579200
O	2.45407600	1.04251600	0.11153800

Cyclobutene (Starting material)

C	0.63512500	-0.96601700	-0.31846200
C	-0.22746700	0.05795900	-0.13353400
C	0.84793600	1.12793000	-0.22458700

H	1.01840400	1.69702600	0.69644600
H	0.74930700	1.83026400	-1.05992700
C	1.85316900	-0.06643100	-0.45137600
H	0.51905300	-2.04766300	-0.36089900
H	2.27245800	-0.06951100	-1.46768000
C	2.97514100	-0.24011200	0.57212700
H	3.49830000	-1.19402900	0.42927900
H	3.71410200	0.56525000	0.47793200
H	2.58066400	-0.22113700	1.59563000
C	-1.68501500	0.16142500	0.07000200
C	-2.49323900	-1.12414500	0.10916000
H	-2.12759900	-1.78892800	0.90161600
H	-3.54446200	-0.88778000	0.28846000
H	-2.39916900	-1.66665600	-0.83993400
O	-2.21437000	1.25993900	0.19988700



Butadiene (Product)

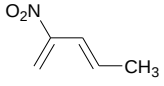
C	-0.52796400	-0.29338200	-0.25425200
C	0.77537400	0.38661100	-0.08649600
C	0.96472200	1.72190000	-0.06254600
H	1.94771400	2.15331800	0.09507200
H	0.13299600	2.40351800	-0.21140300
C	-1.69683900	0.17279400	0.21231900
H	-1.70329200	1.09910300	0.78860000
C	-3.02366900	-0.49955300	0.01954500
H	-3.48920300	-0.73330000	0.98654500
H	-3.72236600	0.15924900	-0.51437800
H	-2.92858100	-1.42954200	-0.55075900
H	-0.50012400	-1.25043900	-0.77427700
C	1.92164300	-0.48066400	0.04212000
N	2.82617900	-1.20687800	0.13663700

Transition state

C	-0.35583800	-0.81789400	-0.10574300
C	0.69718800	0.08378300	-0.11571100
C	0.06574300	1.37155000	-0.13037700
H	0.47685200	2.22867800	0.40941300
H	-0.55210000	1.62833400	-0.98267600
C	-1.46432100	-0.06385600	0.38044500
H	-0.38969500	-1.83084700	-0.50379100
H	-1.35256600	0.36759700	1.37139700
C	-2.88792300	-0.23937600	-0.07892700
H	-3.40290000	-0.98301700	0.54872400
H	-3.44851100	0.69726900	0.02190600
H	-2.95242100	-0.56832500	-1.12102000
C	2.09779100	-0.16776500	-0.00419200
N	3.24364400	-0.36262000	0.08329700

Cyclobutene (Starting material)

C	0.26725100	-0.99426100	-0.31923000
C	-0.65787500	-0.03651200	-0.10432700
C	0.34258800	1.11146600	-0.18771100
H	0.48533100	1.66984800	0.74433200
H	0.18324400	1.81682700	-1.01101600
C	1.41907500	-0.01111000	-0.44919000
H	0.21007500	-2.07809800	-0.37984000
H	1.82186800	0.03515100	-1.47057100
C	2.56290500	-0.12565900	0.55764000
H	3.14508400	-1.03984600	0.38895000
H	3.24585300	0.72797500	0.46824700
H	2.18222400	-0.15248000	1.58593000
C	-2.06287400	-0.05857600	0.11055000
N	-3.21430000	-0.04163800	0.28965300



Butadiene (Product)

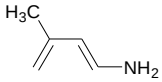
C	-0.87709900	-0.20169100	-0.26246200
C	0.40990800	0.48634900	-0.12234800
C	0.64662500	1.80392200	-0.13260200
H	1.64491400	2.19752000	0.01489000
H	-0.16899200	2.49926100	-0.29867600
C	-2.03168200	0.28109900	0.22413100
H	-2.01864200	1.20704400	0.80121500
C	-3.36938600	-0.37379200	0.05113400
H	-3.82370700	-0.59834900	1.02560200
H	-4.06688400	0.29314900	-0.47425400
H	-3.29405600	-1.30642700	-0.51743100
H	-0.86196800	-1.15674200	-0.77997600
N	1.59700000	-0.41190500	0.03360300
O	2.70618300	0.09637200	0.18731800
O	1.38633300	-1.62480300	-0.00653100

Transition state

C	-0.71527100	-0.80911400	-0.05712900
C	0.30347100	0.11394800	-0.12936600
C	-0.28958600	1.40541600	-0.18844400
H	0.12903000	2.26325600	0.33957400
H	-0.91167400	1.64646500	-1.04290300
C	-1.81892000	-0.02160900	0.38812200
H	-0.74078500	-1.83682800	-0.40949800
H	-1.70466600	0.46115700	1.35496800
C	-3.23888900	-0.19631000	-0.07933900
H	-3.74554600	-0.95512100	0.53713200
H	-3.80746000	0.73337100	0.03396700
H	-3.29780500	-0.51467000	-1.12486100
N	1.72468600	-0.13860600	-0.00236400
O	2.10091600	-1.31464500	-0.01303700
O	2.46924300	0.84197300	0.10367500

Cyclobutene (Starting material)

C	0.61128100	-1.00638100	-0.30950800
C	-0.27036600	-0.01325400	-0.13044400
C	0.70724000	1.12552100	-0.23509400
H	0.85175300	1.70879200	0.68016800
H	0.56063400	1.80584100	-1.08007500
C	1.77040000	-0.02588100	-0.45648400
H	0.53324900	-2.08795900	-0.33891000
H	2.17694200	-0.01504200	-1.47655700
C	2.90192300	-0.12774900	0.56518600
H	3.47404200	-1.05307000	0.42731500
H	3.59450400	0.71569700	0.45917600
H	2.51051100	-0.12122400	1.58961700
N	-1.69804100	-0.02921900	0.07875100
O	-2.25463300	1.06757900	0.19206100
O	-2.26264400	-1.12533400	0.13119800



Butadiene (Product)

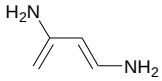
C	-0.31440700	-0.40948400	-0.21598100
C	1.06157300	0.08937000	-0.06112800
C	1.39729600	1.39396800	-0.10627400
H	2.42009800	1.72062200	0.06309600
H	0.66735500	2.17086100	-0.31948100
C	-1.42526600	0.25468300	0.16760400
H	-0.42491800	-1.41356800	-0.63101700
H	-1.34177100	1.22008400	0.66192000
N	-2.73107600	-0.21740700	0.08159400
H	-3.46113600	0.48253500	0.07524100
H	-2.90002400	-0.95956300	-0.58748200
C	2.11536300	-0.97855500	0.14561100
H	2.11067500	-1.69559100	-0.68741800
H	3.11964300	-0.54847100	0.21491900
H	1.92025500	-1.55495400	1.06007100

Transition state

C	-0.10006100	-0.86513900	-0.03553200
C	0.98075200	-0.01558800	-0.08868900
C	0.40633900	1.30312600	-0.12233300
H	0.90081200	2.14971400	0.36989100
H	-0.17664100	1.59423100	-0.99093000
C	-1.19454000	-0.03244000	0.39436600
H	-0.18072400	-1.92005800	-0.30013900
H	-1.18139800	0.36667100	1.40218100
N	-2.47399300	-0.18490800	-0.11748300
H	-2.56081300	-0.33900100	-1.11415300
H	-3.21119300	0.39368100	0.26393000
C	2.44492600	-0.34104900	0.02137000
H	2.88889900	0.19156200	0.87511400
H	2.61416500	-1.41311900	0.17174600
H	3.00034000	-0.02278300	-0.87035300

Cyclobutene (Starting material)

C	0.03317600	-1.00216300	0.24493400
C	0.96346400	-0.05853000	0.01698600
C	-0.02553000	1.09421000	0.13762700
H	-0.22616500	1.63799400	-0.79319900
H	0.16283400	1.81287400	0.94746900
C	-1.09975400	-0.01144200	0.44370400
H	0.06510300	-2.08940500	0.29180500
H	-1.46006000	0.03829200	1.48636000
N	-2.18444400	-0.09076100	-0.53840300
H	-2.65139200	-0.99486000	-0.48200100
H	-2.89180400	0.61970100	-0.35198600
C	2.43255500	-0.06100900	-0.24227800
H	2.97006200	0.50873400	0.52884200
H	2.83657200	-1.07967800	-0.25884200
H	2.66249400	0.41527300	-1.20546400



Butadiene (Product)

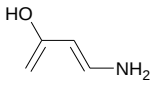
C	-0.30143300	-0.42901400	-0.23374400
C	1.08010800	0.04546900	-0.05770800
C	1.44033200	1.34832600	-0.12588700
H	2.45558000	1.67050800	0.09227300
H	0.72456000	2.10946900	-0.41119100
C	-1.38448500	0.24371000	0.20649500
H	-0.43933700	-1.38333800	-0.74762500
H	-1.25622100	1.16171900	0.77569500
N	-2.71126800	-0.07578600	-0.05473300
N	2.00918100	-0.96689400	0.24787400
H	1.72326100	-1.90841900	0.01115500
H	2.96455500	-0.77994300	-0.03214600
H	-3.38045100	0.17656800	0.66187800
H	-2.88447300	-0.99876000	-0.43696000

Transition state

C	-0.08575200	-0.88560300	-0.04195400
C	0.99403100	-0.02871900	-0.08654200
C	0.44909000	1.30284400	-0.09351800
H	0.96878600	2.11437300	0.42950200
H	-0.09922200	1.62377800	-0.97416700
C	-1.16274100	-0.03821100	0.40276600
H	-0.17192300	-1.93673200	-0.31547500
H	-1.16859800	0.34868500	1.41645700
N	-2.43332200	-0.15434800	-0.13598500
H	-2.50173800	-0.31570800	-1.13301200
H	-3.16594700	0.43921800	0.23091200
N	2.34504500	-0.31781400	0.07962200
H	2.99445000	0.22815600	-0.47259200
H	2.59436200	-1.29849900	0.12840700

Cyclobutene (Starting material)

C	-0.08575200	-0.88560300	-0.04195400
C	0.99403100	-0.02871900	-0.08654200
C	0.44909000	1.30284400	-0.09351800
H	0.96878600	2.11437300	0.42950200
H	-0.09922200	1.62377800	-0.97416700
C	-1.16274100	-0.03821100	0.40276600
H	-0.17192300	-1.93673200	-0.31547500
H	-1.16859800	0.34868500	1.41645700
N	-2.43332200	-0.15434800	-0.13598500
H	-2.50173800	-0.31570800	-1.13301200
H	-3.16594700	0.43921800	0.23091200
N	2.34504500	-0.31781400	0.07962200
H	2.99445000	0.22815600	-0.47259200
H	2.59436200	-1.29849900	0.12840700



Butadiene (Product)

C	0.29439600	-0.39998000	0.29431600
C	-1.08855200	0.03679300	0.07030800
C	-1.53911700	1.30257000	0.11122800
H	-2.56907000	1.53395300	-0.14013300
H	-0.88986400	2.10954400	0.42908500
C	1.36374600	0.24394100	-0.22241000
H	0.44014500	-1.29333200	0.90547400
H	1.21075100	1.10040200	-0.87501300
N	2.69051800	-0.11804800	-0.06628100
H	3.38633000	0.59260100	-0.24487100
H	2.92217700	-0.71853100	0.71542900
O	-1.99934000	-0.97988400	-0.16897100
H	-1.52221500	-1.75917900	-0.49488500

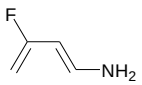
Transition state

C	-0.08007000	-0.91282200	0.00330000

C	0.98902800	-0.06295000	-0.07069900
C	0.48403800	1.28091000	-0.09034200
H	1.01294500	2.08146700	0.44103600
H	-0.05149300	1.61738800	-0.97324400
C	-1.14782500	-0.02947500	0.41123100
H	-0.16855100	-1.96938400	-0.23701100
H	-1.16483100	0.37061500	1.41923400
N	-2.40103800	-0.11336800	-0.15990700
H	-2.45706000	-0.32727200	-1.14752400
H	-3.13179100	0.50111500	0.17402200
O	2.30502900	-0.43057600	0.02423700
H	2.85678500	0.31027600	-0.27200800

Cyclobutene (Starting material)

C	0.05931400	-1.03541500	0.23129700
C	0.98080100	-0.08925900	-0.00581100
C	0.05359400	1.09342200	0.14842000
H	-0.15691900	1.66216800	-0.76442600
H	0.27708600	1.77865300	0.97777300
C	-1.03740200	-0.00690900	0.44947200
H	0.07259500	-2.11888000	0.28176700
H	-1.39252100	0.05137400	1.49236400
N	-2.12870300	-0.04061700	-0.52650500
H	-2.53004900	-0.97468200	-0.58282400
H	-2.87996700	0.59512700	-0.26102700
O	2.31507900	-0.15184600	-0.24393300
H	2.65222100	0.73429500	-0.44689900



Butadiene (Product)

C	0.30101600	-0.43925800	0.20360400
C	-1.06813600	0.02565700	0.05558600
C	-1.58650600	1.25804100	0.11007000
H	-2.63750900	1.42926700	-0.09367800
H	-0.96292100	2.10670000	0.36586200

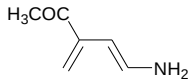
C	1.37776100	0.29098400	-0.16320200
H	0.42645900	-1.44267200	0.60754800
H	1.24228100	1.25963600	-0.63873100
N	2.69678800	-0.10400200	-0.06299800
H	3.40650800	0.61359500	-0.10113800
H	2.91732200	-0.86531000	0.56657400
F	-1.93494000	-1.02063800	-0.16686700

Transition state

C	-0.05197400	-0.92299700	0.01440700
C	0.97888900	-0.04068800	-0.08269400
C	0.48456600	1.29302700	-0.09768400
H	1.01808800	2.08923500	0.42872500
H	-0.07008900	1.62711300	-0.96938000
C	-1.12508000	-0.03980800	0.41804900
H	-0.12439200	-1.97905800	-0.23068000
H	-1.13763300	0.35349100	1.42819800
N	-2.37431200	-0.12158900	-0.15827500
H	-2.42843700	-0.33908100	-1.14522400
H	-3.10293500	0.49878100	0.16956100
F	2.30524200	-0.34850700	-0.00952700

Cyclobutene (Starting material)

C	0.09720200	-1.03416600	0.23482900
C	0.97338100	-0.05928700	-0.00839400
C	0.04858000	1.11056200	0.13736100
H	-0.16948600	1.66355900	-0.78180100
H	0.26681600	1.80436700	0.95799600
C	-1.01709600	-0.01354000	0.45295800
H	0.13234000	-2.11632800	0.28140700
H	-1.35628400	0.03582000	1.50086400
N	-2.10561100	-0.07640300	-0.51898500
H	-2.56994800	-0.98217200	-0.48316300
H	-2.81143700	0.63203000	-0.32213100
F	2.29276400	-0.05820800	-0.26897800



Butadiene (Product)

C	-0.97136200	-0.27469500	-0.18363600
C	0.30837500	0.43262500	-0.10980400
C	0.45507400	1.77664000	-0.17367600
H	1.41725900	2.26199100	-0.05443700
H	-0.39177700	2.43290900	-0.35485200
C	-2.15767100	0.26089900	0.17636700
H	-0.92507300	-1.31034100	-0.51202500
H	-2.21135700	1.26355500	0.59764500
N	-3.39922500	-0.33427200	0.00932200
H	-3.39544300	-1.32014600	-0.22777300
H	-4.10928600	-0.09971200	0.69175400
C	1.52574100	-0.45148700	0.01201100
C	2.90228100	0.17194700	0.18817800
H	3.63313500	-0.63223400	0.29486600
H	3.17136100	0.78734800	-0.67837200
H	2.93941200	0.81529600	1.07506400
O	1.41146400	-1.66929200	-0.04422100

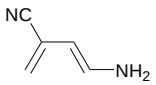
Transition state

C	-0.73457200	-0.78565700	-0.08011100
C	0.23603900	0.19937100	-0.15723400
C	-0.50617700	1.43009300	-0.17586200
H	-0.14745700	2.31982700	0.34677900
H	-1.12373100	1.64091200	-1.04302700
C	-1.89428800	-0.07948100	0.39088300
H	-0.71865800	-1.82903300	-0.39452200
H	-1.86176600	0.32782900	1.39583000
N	-3.17416900	-0.37880100	-0.04652400
H	-3.30349800	-0.54085600	-1.03722400
H	-3.94648300	0.11707500	0.37917800
C	1.70556600	0.07423400	-0.01720800
C	2.30180800	-1.32391700	0.01604100
H	3.38289000	-1.26068500	-0.12806500

H	2.10038500	-1.79396700	0.98720900
H	1.86135400	-1.96797800	-0.75469900
O	2.41573600	1.06882800	0.08939500

Cyclobutene (Starting material)

C	-0.64552000	-0.96929200	0.28992000
C	0.21405800	0.05548900	0.11037700
C	-0.86405800	1.12492700	0.15880400
H	-1.04452500	1.63380400	-0.79342400
H	-0.77613900	1.86528100	0.96164400
C	-1.85914500	-0.06435300	0.42231900
H	-0.53368700	-2.05022200	0.34113100
H	-2.25725300	-0.04594100	1.45210900
N	-2.88346000	-0.24200500	-0.60535300
H	-3.37887500	-1.12313000	-0.47479100
H	-3.57833200	0.50158800	-0.54669100
C	1.67793200	0.16304900	-0.05520500
C	2.48521300	-1.12141600	-0.11372800
H	2.19343300	-1.71436900	-0.98992500
H	3.54865400	-0.88079400	-0.17877100
H	2.30189500	-1.73957000	0.77364700
O	2.20727000	1.26462000	-0.14779600



Butadiene (Product)

C	0.53028800	-0.35340600	0.22518100
C	-0.73565500	0.37734500	0.08696700
C	-0.90454800	1.71977600	0.07773300
H	-1.87926800	2.16554000	-0.08768300
H	-0.06719800	2.39196000	0.23857400
C	1.72712800	0.13992500	-0.16723000
H	0.47081000	-1.36179400	0.63044400
H	1.78635700	1.10993100	-0.65585500
N	2.93656500	-0.51500200	-0.08386300
H	3.78158000	0.03017400	-0.17339900

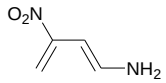
H	3.01465100	-1.30453300	0.54439800
C	-1.91176000	-0.45215200	-0.04528500
N	-2.84223000	-1.14502800	-0.13909000

Transition state

C	-0.35992800	-0.84753200	-0.05165300
C	0.65810600	0.08066900	-0.10483500
C	-0.00131200	1.36188800	-0.12902100
H	0.41258100	2.22632500	0.39607900
H	-0.57474500	1.61262600	-1.01535400
C	-1.49030100	-0.07152800	0.39156600
H	-0.37713100	-1.89258100	-0.35505000
H	-1.46664700	0.32057700	1.40250700
N	-2.76242900	-0.28576000	-0.09352500
H	-2.87559100	-0.47048500	-1.08179000
H	-3.53265800	0.22093000	0.32176600
C	2.06574400	-0.15168500	-0.01010500
N	3.21676200	-0.32113500	0.05868600

Cyclobutene (Starting material)

C	-0.28216100	-1.00121300	0.26422600
C	0.64165900	-0.03854100	0.07940100
C	-0.35965700	1.10827200	0.15292100
H	-0.51951100	1.63279800	-0.79405500
H	-0.20486100	1.82918000	0.96349200
C	-1.42770500	-0.01590500	0.42191600
H	-0.23096500	-2.08574000	0.30312500
H	-1.80691200	0.02247700	1.45771400
N	-2.47286000	-0.11296500	-0.59267600
H	-2.97762500	-0.99429600	-0.51022400
H	-3.15640800	0.63425800	-0.47718900
C	2.05256100	-0.05546900	-0.09876700
N	3.20830300	-0.03296800	-0.24461700



Butadiene (Product)

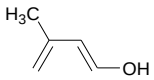
C	-0.88033500	-0.26428800	-0.24911700
C	0.36933000	0.46888100	-0.13509400
C	0.57555500	1.79545200	-0.16541000
H	1.55607900	2.21722900	0.01564600
H	-0.24800600	2.46772900	-0.37975200
C	-2.05139500	0.23499200	0.20884400
H	-0.84479000	-1.24858300	-0.70553100
H	-2.07358800	1.17919100	0.74972000
N	-3.29687400	-0.32304600	0.01278800
N	1.58853500	-0.39015700	0.04145100
H	-4.00897900	-0.12640700	0.70351300
H	-3.33211000	-1.26962200	-0.34700200
O	1.42663000	-1.61032500	-0.01040200
O	2.67722400	0.15565800	0.21395100

Transition state

C	-0.70814400	-0.84211200	-0.00258200
C	0.26678600	0.11056400	-0.12140600
C	-0.37209600	1.38714000	-0.18123500
H	0.03302900	2.25241300	0.34511100
H	-0.93930700	1.62553000	-1.07566200
C	-1.83534400	-0.03466300	0.40048900
H	-0.71106900	-1.89794900	-0.25765400
H	-1.81427900	0.39308900	1.39715700
N	-3.10328600	-0.24924700	-0.09116900
H	-3.20595700	-0.49751600	-1.06659400
H	-3.86641400	0.30324800	0.27629500
N	1.70085700	-0.11877100	-0.00803300
O	2.43032000	0.87253000	0.08454200
O	2.09640400	-1.28856300	-0.02152000

Cyclobutene (Starting material)

C	-0.62269900	-1.01264400	0.26334300
C	0.25458100	-0.01536100	0.10526400
C	-0.72396300	1.12263600	0.19400900
H	-0.88390300	1.66978500	-0.73935100
H	-0.58260500	1.82153100	1.02438800
C	-1.77824500	-0.02981300	0.42869600
H	-0.54894400	-2.09418600	0.28002500
H	-2.16409900	-0.01940900	1.46186600
N	-2.80378900	-0.12056800	-0.60237600
H	-3.32625000	-0.99158900	-0.52342700
H	-3.47311700	0.64248500	-0.51333500
N	1.68925500	-0.02646800	-0.07015100
O	2.25600600	-1.12091000	-0.11650300
O	2.24432000	1.07237600	-0.16229100



Butadiene (Product)

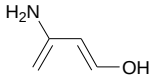
C	-0.32832700	-0.40494600	-0.25939800
C	1.04564200	0.09155600	-0.06718900
C	1.36680700	1.39875800	-0.09989900
H	2.38231000	1.73659100	0.09139000
H	0.63278300	2.16527600	-0.33407600
C	-1.42404000	0.21919900	0.19548500
H	-0.45853800	-1.35917000	-0.76984400
H	-1.37106000	1.13632200	0.78000000
O	-2.68330100	-0.26207500	-0.05834500
H	-3.33546200	0.22490700	0.46521600
C	2.09503400	-0.97481700	0.16147100
H	1.87557000	-1.55863000	1.06541400
H	2.11479500	-1.68529200	-0.67655000
H	3.09531600	-0.54190200	0.26239200

Transition state

C	-0.12470000	-0.85930400	-0.10002000
C	0.96858100	-0.01483100	-0.09904100
C	0.40745600	1.30271100	-0.13476600
H	0.89526400	2.14475400	0.37166200
H	-0.18692700	1.59577600	-0.99346000
C	-1.19284100	-0.03443800	0.35754400
H	-0.21924100	-1.89650000	-0.41778900
H	-1.18950900	0.35736900	1.36935400
O	-2.44043700	-0.17581800	-0.19774500
H	-3.11612700	0.21684700	0.37780400
C	2.42532300	-0.34968900	0.06453000
H	3.01252800	-0.03834900	-0.80886800
H	2.84330500	0.18217500	0.93150100
H	2.58129800	-1.42222400	0.22227200

Cyclobutene (Starting material)

C	0.02015600	-1.00949200	0.20097300
C	0.94994800	-0.05600300	0.00639400
C	-0.04527700	1.09460300	0.11603900
H	-0.24866300	1.62441500	-0.82217900
H	0.13477800	1.82805000	0.91557700
C	-1.10633900	-0.03010200	0.41909400
H	0.04790900	-2.09603800	0.23025400
H	-1.48975300	0.00403800	1.45036600
O	-2.18579300	-0.17788500	-0.49763700
H	-2.88448800	0.45448600	-0.26639100
C	2.42656700	-0.04721100	-0.20180800
H	2.93222800	0.51245800	0.59770300
H	2.83690300	-1.06300300	-0.22103900
H	2.68709600	0.44790700	-1.14734600



Butadiene (Product)

C	-0.31625000	-0.41429000	-0.28024700
C	1.06585900	0.05035900	-0.06384300
C	1.42535400	1.35311900	-0.11205700
H	2.43903400	1.67345500	0.11578100
H	0.71218800	2.11623700	-0.39826600
C	-1.38755300	0.21876800	0.21491800
H	-0.47118000	-1.32676500	-0.85652300
H	-1.29690100	1.09881100	0.84870900
O	-2.66144900	-0.20110000	-0.06426800
H	-3.29696500	0.28747600	0.47795700
N	1.97700200	-0.97099400	0.25160000
H	1.69664500	-1.90788500	-0.00858600
H	2.94530200	-0.78331400	0.02124600

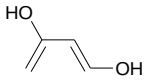
Transition state

C	-0.11001900	-0.87721100	-0.10009800
C	0.98350300	-0.02768300	-0.09445400
C	0.45313800	1.30391700	-0.10617600
H	0.97014800	2.11291900	0.42355600
H	-0.10499000	1.62305800	-0.97979200
C	-1.16162200	-0.03727500	0.36375700
H	-0.21088200	-1.90886400	-0.43054600
H	-1.18021400	0.35061800	1.37787700
O	-2.40069400	-0.14816800	-0.21735700
H	-3.07623800	0.26344400	0.34532400
N	2.32216800	-0.33248000	0.12079300
H	3.00132900	0.21629800	-0.39090200
H	2.56122600	-1.31526400	0.16961500

Cyclobutene (Starting material)

C	0.03681600	-1.03283300	0.18358700
C	0.96672000	-0.06864800	-0.00710800

C	-0.00214900	1.08636800	0.14258600
H	-0.20945100	1.65133200	-0.77398200
H	0.19985700	1.78188000	0.96957600
C	-1.06981700	-0.04205300	0.41899600
H	0.05746800	-2.11756400	0.21708500
H	-1.47117500	-0.01006300	1.44388600
O	-2.14866900	-0.14464700	-0.51126100
H	-2.86162200	0.45183800	-0.23180400
N	2.33876600	-0.01962100	-0.13513500
H	2.71184200	0.77045300	-0.64745000
H	2.80166100	-0.89035900	-0.36964200



Butadiene (Product)

C	0.30963200	-0.39666900	0.31216300
C	-1.07249500	0.03807200	0.06771000
C	-1.51317300	1.30669500	0.09196200
H	-2.54334100	1.54114900	-0.15563500
H	-0.85808400	2.11237700	0.40014800
C	1.36860800	0.22602000	-0.22568600
H	0.47285800	-1.26300200	0.95356000
H	1.25553400	1.06793700	-0.90632600
O	2.64809200	-0.15463900	0.06590500
H	3.27570500	0.33402500	-0.48572500
O	-1.98000200	-0.97780000	-0.17107700
H	-1.50282700	-1.77768500	-0.44154200

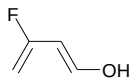
Transition state

C	-0.10483100	-0.90562000	-0.06019600
C	0.97938300	-0.06176200	-0.07961000
C	0.48873900	1.28069200	-0.10561100
H	1.01681900	2.08140200	0.42651800
H	-0.06279300	1.61237400	-0.97887000
C	-1.14637800	-0.03148800	0.37119600
H	-0.20862600	-1.94307100	-0.36324800

H	-1.17051500	0.37071200	1.37925300
O	-2.36985900	-0.11215000	-0.23668800
H	-3.04542500	0.33804900	0.29598400
O	2.28339400	-0.44262400	0.07239800
H	2.86077600	0.28779000	-0.19998400

Cyclobutene (Starting material)

C	0.04937400	-1.04496500	0.18542200
C	0.96825900	-0.08520600	-0.01296900
C	0.02904400	1.09031600	0.14171700
H	-0.18270900	1.65721200	-0.77235600
H	0.23991900	1.78137200	0.97051500
C	-1.04523300	-0.03591000	0.42422800
H	0.06269400	-2.12809400	0.20991200
H	-1.43594300	-0.00158900	1.45212300
O	-2.12218100	-0.12956300	-0.50259800
H	-2.82537400	0.48268300	-0.23292200
O	2.30829400	-0.13204300	-0.20433400
H	2.64385000	0.75585200	-0.40219900



Butadiene (Product)

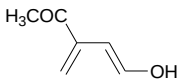
C	-0.31674400	-0.43649700	-0.24083600
C	1.05301100	0.02573200	-0.06002400
C	1.55935600	1.26169000	-0.10260200
H	2.60679900	1.44207300	0.11240800
H	0.93168200	2.10369500	-0.36930000
C	-1.37907100	0.26258400	0.18556200
H	-0.46243700	-1.39918900	-0.72519400
H	-1.27576800	1.19532200	0.73748000
O	-2.65309500	-0.15760100	-0.06221300
H	-3.28787000	0.39460100	0.41673300
F	1.91256000	-1.01741700	0.18144200

Transition state

C	-0.07909900	-0.91820700	-0.05076900
C	0.96952800	-0.04259300	-0.09150100
C	0.49358300	1.29142600	-0.11272300
H	1.02683100	2.08563400	0.41681400
H	-0.08060200	1.62174500	-0.97153700
C	-1.12498100	-0.04365500	0.37860700
H	-0.16943400	-1.95468700	-0.35939200
H	-1.14174100	0.35345900	1.38835100
O	-2.34193300	-0.11714000	-0.23530900
H	-3.01774500	0.34608000	0.28591700
F	2.28488500	-0.35966000	0.04229300

Cyclobutene (Starting material)

C	0.08299400	-1.03801200	0.20216400
C	0.95986100	-0.05539200	-0.01538700
C	0.02810200	1.11227100	0.12310900
H	-0.19087600	1.65912000	-0.79969200
H	0.23925300	1.81489500	0.93900600
C	-1.02693700	-0.03151200	0.42867700
H	0.11379200	-2.11983500	0.23609900
H	-1.40362600	0.00463100	1.46070700
O	-2.09875400	-0.16842200	-0.49106000
H	-2.79371100	0.47075400	-0.26650500
F	2.28456400	-0.04514700	-0.23028000



Butadiene (Product)

C	-0.98336000	-0.27810500	-0.23444700
C	0.29678100	0.43303300	-0.12799500
C	0.42888100	1.77653500	-0.18485400
H	1.38459100	2.27161900	-0.05154700
H	-0.42234800	2.42330800	-0.37911400
C	-2.14827700	0.22515900	0.19771700

H	-0.96170600	-1.28599000	-0.63844200
H	-2.22297500	1.18859900	0.70103900
O	-3.32545800	-0.45096700	0.02678800
H	-4.03078000	-0.02713700	0.53657600
C	1.51484500	-0.44752100	0.01085400
C	2.88400600	0.18157600	0.21647800
H	2.90076600	0.82214600	1.10600400
H	3.61650100	-0.61937500	0.33464300
H	3.16707400	0.80079100	-0.64304600
O	1.40191100	-1.66378500	-0.05586600

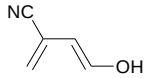
Transition state

C	-0.75421000	-0.78390800	-0.13808500
C	0.22582200	0.20072300	-0.18595700
C	-0.50433300	1.43167700	-0.21571000
H	-0.14635400	2.32319300	0.30438400
H	-1.14622700	1.62829800	-1.06726400
C	-1.88559200	-0.08265700	0.36319400
H	-0.75408700	-1.81439400	-0.48763700
H	-1.85420500	0.33286500	1.36572500
O	-3.13514500	-0.37714500	-0.11051000
H	-3.81893200	-0.04774500	0.49441000
C	1.69173800	0.07313400	-0.00262100
C	2.28584200	-1.32487600	0.01664400
H	1.88885200	-1.93873500	-0.80115000
H	3.37305800	-1.25851700	-0.06550600
H	2.02956400	-1.83008100	0.95665900
O	2.39423600	1.06721400	0.14495900

Cyclobutene (Starting material)

C	-0.65720900	-0.97154400	0.24398000
C	0.20270000	0.05638900	0.07651200
C	-0.87411200	1.12971400	0.11050900
H	-1.06557200	1.61056100	-0.85384400
H	-0.78168000	1.89403700	0.89102700
C	-1.85917700	-0.06899100	0.39933600
H	-0.55545800	-2.05272300	0.28740600

H	-2.25929900	-0.05179500	1.42464600
O	-2.89147000	-0.33153300	-0.53658300
H	-3.63251500	0.27231100	-0.36954300
C	1.67211800	0.16544400	-0.04727800
C	2.48024500	-1.11815500	-0.09351000
H	2.17675500	-1.73171400	-0.95112500
H	3.54236700	-0.87755700	-0.17665000
H	2.31016200	-1.71612900	0.81038400
O	2.20120100	1.26851600	-0.11336700



Butadiene (Product)

C	-0.54816700	-0.34094200	-0.29755300
C	0.72033400	0.38081000	-0.10529700
C	0.86858600	1.72275700	-0.06793400
H	1.83109300	2.18100100	0.13371600
H	0.02537100	2.38159800	-0.25075000
C	-1.71183900	0.08984600	0.21287000
H	-0.52615900	-1.27749900	-0.84927600
H	-1.77735500	0.97399300	0.84530900
O	-2.88149300	-0.56358100	-0.03808000
H	-3.59110700	-0.21245300	0.51935400
C	1.89282700	-0.44778900	0.05063400
N	2.82280700	-1.13801200	0.16428200

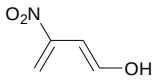
Transition state

C	-0.38360700	-0.84067300	-0.13333700
C	0.64546900	0.08614600	-0.13388600
C	-0.00113000	1.36637000	-0.14013300
H	0.41067900	2.22176200	0.40115300
H	-0.60557300	1.62312200	-1.00256200
C	-1.48394100	-0.08345200	0.36258000
H	-0.41793400	-1.86185900	-0.50367600
H	-1.45488200	0.29526700	1.37955400
O	-2.72844300	-0.28373100	-0.15681400

H	-3.41340800	0.05584200	0.44151100
C	2.04795600	-0.15258600	0.00444000
N	3.19431100	-0.33130300	0.11150700

Cyclobutene (Starting material)

C	-0.29544100	-1.00599800	0.21364800
C	0.62993100	-0.03863500	0.05302300
C	-0.36973900	1.11209400	0.11386100
H	-0.53731700	1.61421100	-0.84365600
H	-0.21343500	1.85399000	0.90601200
C	-1.43056500	-0.02425900	0.39621600
H	-0.25469700	-2.09043000	0.23636300
H	-1.81543100	0.00678600	1.42618300
O	-2.48370500	-0.19323300	-0.53224800
H	-3.21965600	0.39290200	-0.29537900
C	2.04532300	-0.05218400	-0.08133000
N	3.20473200	-0.02538600	-0.19200700



Butadiene (Product)

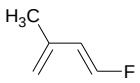
C	-0.89318000	-0.25302200	-0.30132400
C	0.36033400	0.47497600	-0.14519000
C	0.56150300	1.80012300	-0.15222300
H	1.54078600	2.22068400	0.04047000
H	-0.26188700	2.47358700	-0.36346300
C	-2.04100400	0.20133600	0.22555700
H	-0.88668300	-1.19389400	-0.84119400
H	-2.08400400	1.09261800	0.85027800
O	-3.22304800	-0.43571000	-0.00013600
H	-3.91880900	-0.06847000	0.56437200
N	1.57141800	-0.39002800	0.04101300
O	2.66103400	0.15147700	0.21965300
O	1.39760800	-1.60761900	-0.00682700

Transition state

C	-0.73064900	-0.83930400	-0.07748200
C	0.25811100	0.11213200	-0.15389200
C	-0.36162200	1.39101600	-0.21214500
H	0.04882600	2.25355500	0.31433500
H	-0.96544700	1.62333600	-1.08261300
C	-1.82774100	-0.04417700	0.37134800
H	-0.75298500	-1.87809400	-0.38970400
H	-1.79702400	0.38935900	1.36636900
O	-3.06695000	-0.25128000	-0.14998800
H	-3.75151100	0.15403900	0.40672600
N	1.68638100	-0.12186200	0.00417200
O	2.07713900	-1.29210800	-0.00864200
O	2.41292100	0.86749300	0.13221900

Cyclobutene (Starting material)

C	-0.63554800	-1.01105200	0.22601400
C	0.24363000	-0.01316700	0.07095000
C	-0.73257900	1.13026300	0.13861700
H	-0.90330300	1.64748300	-0.80971200
H	-0.58466400	1.85676300	0.94459700
C	-1.78015900	-0.03083400	0.40291600
H	-0.57281300	-2.09253200	0.24473500
H	-2.17119300	-0.01334200	1.43044700
O	-2.81530400	-0.21297200	-0.53950500
H	-3.53589100	0.40892300	-0.35050600
N	1.68410200	-0.02542900	-0.05849100
O	2.24879700	-1.12046600	-0.09861500
O	2.24239200	1.07336900	-0.12201800



Butadiene (Product)

C	-0.35479500	-0.36790100	-0.28662500
C	1.03307700	0.09122600	-0.07336800

C	1.37252500	1.39180800	-0.09902900
H	2.39353400	1.71253400	0.09205200
H	0.64904900	2.16932900	-0.32858900
C	-1.42139500	0.23757000	0.23472700
H	-0.51353500	-1.27677800	-0.86658500
H	-1.42326700	1.10474700	0.88642500
F	-2.68038700	-0.21416200	-0.00598000
C	2.05154300	-1.00216800	0.16040600
H	1.80864100	-1.58322300	1.05984900
H	2.06322000	-1.70929200	-0.68042700
H	3.06011600	-0.59307600	0.27442400

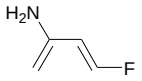
Transition state

C	-0.16078900	-0.84088400	-0.14419000
C	0.95339500	-0.01443300	-0.11803800
C	0.42590000	1.31065900	-0.14429300
H	0.92700500	2.13628900	0.37424800
H	-0.18559400	1.62406300	-0.98215800
C	-1.18227000	-0.00749200	0.36040700
H	-0.27752200	-1.86880200	-0.48143900
H	-1.20544000	0.37990200	1.37087100
F	-2.46709300	-0.14154600	-0.10318700
C	2.39771900	-0.38105500	0.08264100
H	3.01451800	-0.07033100	-0.76986600
H	2.80056600	0.13017300	0.96850500
H	2.52657000	-1.45815200	0.22935600

Cyclobutene (Starting material)

C	0.00311500	-1.02179500	0.17807100
C	0.93152100	-0.06103400	0.00246900
C	-0.06882400	1.08733200	0.12580600
H	-0.28433600	1.62117500	-0.80641600
H	0.10605100	1.81677500	0.92828800
C	-1.10696800	-0.03698800	0.42545300
H	0.03357300	-2.10778400	0.19949700
H	-1.54840000	-0.02338000	1.42766300
F	-2.19050700	-0.08717300	-0.47375500

C	2.40892100	-0.04199400	-0.19142000
H	2.90260200	0.50673800	0.62266500
H	2.82503300	-1.05472700	-0.22503100
H	2.67345700	0.47263700	-1.12515300



Butadiene (Product)

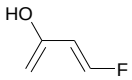
C	-0.34521300	-0.37543700	-0.30608500
C	1.04946300	0.04771400	-0.06909800
C	1.43656100	1.34094900	-0.08260800
H	2.46161800	1.63019700	0.13582100
H	0.74764200	2.12610200	-0.37019500
C	-1.38684100	0.23883800	0.25271600
H	-0.51769400	-1.24014200	-0.94490800
H	-1.35215900	1.07261000	0.94562000
F	-2.66006200	-0.15015100	-0.00971600
N	1.94184300	-1.02743000	0.07990000
H	1.59977600	-1.79500200	0.64839000
H	2.88464400	-0.76278100	0.34386400

Transition state

C	-0.15215400	-0.86062900	-0.13743200
C	0.96873600	-0.03703800	-0.11115900
C	0.47491800	1.30425400	-0.11194800
H	1.01567100	2.10006600	0.41501500
H	-0.09749400	1.64514300	-0.96672600
C	-1.14970300	-0.00590900	0.37430300
H	-0.28319600	-1.87902900	-0.49365700
H	-1.20089600	0.38044400	1.38452500
F	-2.42807500	-0.10219400	-0.12303300
N	2.29493300	-0.40593600	0.00938600
H	2.98275100	0.33351500	0.05846400
H	2.52052200	-1.22290000	0.56138700

Cyclobutene (Starting material)

C	0.01874100	-1.04489200	0.16666800
C	0.94821200	-0.07325400	-0.01062900
C	-0.02709900	1.07752800	0.15892300
H	-0.24742600	1.65256100	-0.74740100
H	0.17149900	1.76384200	0.99280000
C	-1.06973000	-0.05172700	0.42936100
H	0.04355700	-2.12892300	0.19839500
H	-1.53886300	-0.04162600	1.41891200
F	-2.14893700	-0.05542100	-0.49031700
N	2.31352300	-0.01668400	-0.13622600
H	2.70057600	0.79995700	-0.59189800
H	2.79568400	-0.87616900	-0.37031500



Butadiene (Product)

C	0.33677500	-0.36010100	0.32465000
C	-1.05930000	0.03493400	0.06908900
C	-1.52208100	1.29361600	0.08837000
H	-2.56041300	1.50564700	-0.14461600
H	-0.87658600	2.11438100	0.37590200
C	1.36777500	0.24788400	-0.26208100
H	0.52704300	-1.18746800	1.00813200
H	1.31449900	1.05162800	-0.98853300
F	2.64545800	-0.10512200	0.01546900
O	-1.93800800	-1.00519500	-0.15899400
H	-1.44860500	-1.79452300	-0.43831400

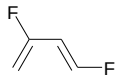
Transition state

C	-0.14360500	-0.88528900	-0.09993500
C	0.96665400	-0.06372600	-0.09541000
C	0.51272900	1.28595900	-0.11863900
H	1.05907300	2.07262200	0.41452200
H	-0.05716700	1.63307200	-0.97229900

C	-1.13654800	-0.00060900	0.37366000
H	-0.27239300	-1.91379900	-0.42175500
H	-1.18588900	0.41161700	1.37345600
F	-2.40055300	-0.06855500	-0.14774800
O	2.25057300	-0.47979600	0.09119100
H	2.86138600	0.23383900	-0.15178300

Cyclobutene (Starting material)

C	-0.81532200	-0.67167200	0.00001200
C	-0.81532600	0.67166900	-0.00010500
C	0.70047000	0.78701300	-0.00002400
H	1.14629000	1.24745900	0.89076000
H	1.14639900	1.24731500	-0.89082800
C	0.70047300	-0.78701000	0.00010400
H	-1.60357700	-1.42097900	0.00003300
H	1.09317364	-1.21074619	-0.90052570
F	1.19581255	-1.32144560	1.13655344
O	-1.86414998	1.64371233	-0.00025266
H	-1.48361185	2.52506964	-0.00038655



Butadiene (Product)

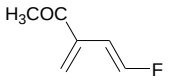
C	-0.34306300	-0.40669800	-0.25157800
C	1.04149600	0.02237800	-0.06143900
C	1.56536400	1.24864800	-0.10121300
H	2.61867600	1.41021500	0.09970200
H	0.94674500	2.10226700	-0.35149700
C	-1.37905000	0.29175100	0.21319100
H	-0.51481700	-1.34528500	-0.77324300
H	-1.33507200	1.20343600	0.79966000
F	-2.65078100	-0.10366600	-0.01583500
F	1.87033500	-1.04156800	0.17490300

Transition state

C	-0.12009000	-0.90071600	-0.09191000
C	0.95699400	-0.04797800	-0.10688100
C	0.52086200	1.29438800	-0.12518400
H	1.07337700	2.07223600	0.40762700
H	-0.07337100	1.64265000	-0.96144000
C	-1.11593200	-0.01434700	0.38032800
H	-0.23682200	-1.92792400	-0.42054100
H	-1.15533300	0.39385200	1.38205800
F	-2.37220100	-0.06673500	-0.14783100
F	2.25455100	-0.39647500	0.06496100

Cyclobutene (Starting material)

C	0.06667200	-1.04850000	0.18442000
C	0.94247100	-0.05888300	-0.01749000
C	0.00244100	1.10483700	0.13581100
H	-0.22866300	1.65925900	-0.77874700
H	0.20792200	1.80103600	0.95712400
C	-1.02861400	-0.03814200	0.43431600
H	0.10217600	-2.12989500	0.21589200
H	-1.47022300	-0.02288400	1.43476200
F	-2.09872600	-0.07888500	-0.47288900
F	2.26438800	-0.03926900	-0.22170800



Butadiene (Product)

C	-1.00143500	-0.25068200	-0.25288800
C	0.29127400	0.44606200	-0.13368900
C	0.42636600	1.78680200	-0.18688200
H	1.38593600	2.27641700	-0.05950400
H	-0.42386800	2.43687700	-0.37375900
C	-2.14156700	0.24148600	0.22948000
H	-1.00187700	-1.23655900	-0.70873600
H	-2.27380700	1.16545700	0.78336700

F	-3.31447500	-0.42205300	0.08302700
C	1.49478300	-0.45248900	0.00715300
C	2.86990100	0.15655400	0.22164800
H	3.59186400	-0.65403800	0.33795200
H	3.16432100	0.77740500	-0.63295900
H	2.89067600	0.79120200	1.11535100
O	1.35763700	-1.66558500	-0.06473600

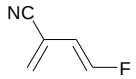
Transition state

C	-0.78158200	-0.76896900	-0.17662900
C	0.21365400	0.20779800	-0.21015100
C	-0.48995800	1.44807100	-0.23166300
H	-0.11517400	2.32928200	0.29306300
H	-1.15839800	1.65569700	-1.05879000
C	-1.87122700	-0.06103900	0.36953400
H	-0.79816500	-1.79403100	-0.53918700
H	-1.86659600	0.35310400	1.37056800
F	-3.14889200	-0.35670600	-0.00929800
C	1.67807300	0.06410400	-0.00011700
C	2.25769800	-1.33809800	0.01546000
H	3.34771400	-1.28126000	-0.02189700
H	1.95763500	-1.86065400	0.93271200
H	1.88857500	-1.92985700	-0.83142300
O	2.38056200	1.05335900	0.16750300

Cyclobutene (Starting material)

C	-0.66803600	-0.98701100	0.22758200
C	0.18807300	0.04619100	0.06782300
C	-0.89354800	1.11853100	0.10548800
H	-1.09833000	1.59356100	-0.85826900
H	-0.80513100	1.88658200	0.88125100
C	-1.85711800	-0.07394300	0.40437300
H	-0.56345100	-2.06725100	0.27340200
H	-2.31108100	-0.07048400	1.40113000
F	-2.90081200	-0.24781900	-0.51303100
C	1.66023200	0.16687200	-0.04421500
C	2.47828800	-1.10869300	-0.09452900

H	2.17125800	-1.73002700	-0.94522000
H	3.53734700	-0.85937300	-0.18905700
H	2.32294700	-1.70276800	0.81477700
O	2.17580000	1.27605600	-0.09498400



Butadiene (Product)

C	0.57282400	-0.31175000	0.31609300
C	-0.70975900	0.39080800	0.10823100
C	-0.86085200	1.73000800	0.06572100
H	-1.82630300	2.18435200	-0.13112900
H	-0.01782900	2.39111900	0.24069500
C	1.70896200	0.09642900	-0.24952500
H	0.57650300	-1.21139600	0.92668700
H	1.82939600	0.92808900	-0.93614800
F	2.87616200	-0.54149600	-0.01620700
C	-1.86823700	-0.45474300	-0.04690500
N	-2.78640800	-1.16045900	-0.15942000

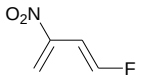
Transition state

C	-0.41331900	-0.82239000	-0.18076700
C	0.63066500	0.09636600	-0.15885200
C	0.00844900	1.38208200	-0.14546700
H	0.43232100	2.22293500	0.40817500
H	-0.62424200	1.65632000	-0.98073500
C	-1.47171600	-0.06744900	0.36883000
H	-0.46415800	-1.83263800	-0.57662800
H	-1.46662900	0.30471000	1.38625100
F	-2.74784400	-0.26535700	-0.05595600
C	2.02654900	-0.16150700	0.00632100
N	3.16707600	-0.36081900	0.13230700

Cyclobutene (Starting material)

C	-0.30988300	-1.02020900	0.19240200

C	0.61164300	-0.04540800	0.04889300
C	-0.39425400	1.10299100	0.12693500
H	-0.57267300	1.61407800	-0.82329100
H	-0.24377900	1.83753000	0.92542700
C	-1.43226100	-0.03240000	0.40352900
H	-0.26519600	-2.10410900	0.20712800
H	-1.87759800	-0.02295900	1.40353300
F	-2.48553400	-0.10475500	-0.51052200
C	2.02780900	-0.04889700	-0.07816200
N	3.18724800	-0.01688600	-0.18281100



Butadiene (Product)

C	0.91209900	-0.22496800	0.31038500
C	-0.35654100	0.48586900	0.14496500
C	-0.56696400	1.80721000	0.15037600
H	-1.55417700	2.21666100	-0.02726500
H	0.25330700	2.48945200	0.34517700
C	2.03468700	0.21790300	-0.25685300
H	0.92887700	-1.14075600	0.89204900
H	2.13541400	1.07138400	-0.91984500
F	3.21312600	-0.40659000	-0.05507600
N	-1.54969600	-0.39861800	-0.03737700
O	-1.34980100	-1.61211000	0.01425500
O	-2.64687000	0.12421100	-0.21750800

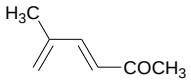
Transition state

C	-0.75847700	-0.82326000	-0.11340100
C	0.24748800	0.11911500	-0.17852200
C	-0.34369700	1.40574800	-0.23660900
H	0.08387100	2.26111500	0.28712200
H	-0.97759500	1.64441000	-1.08254000
C	-1.81370100	-0.02028600	0.37639100
H	-0.79885900	-1.85667900	-0.43996700
H	-1.80636600	0.42658900	1.36351700

F	-3.08510100	-0.21895400	-0.05059900
N	1.67076800	-0.13226900	0.00740500
O	2.04497400	-1.30659000	-0.01395300
O	2.40250200	0.84823100	0.16248600

Cyclobutene (Starting material)

C	-0.64631000	-1.02248400	0.21752600
C	0.22913700	-0.02019300	0.06586800
C	-0.75388900	1.12199300	0.13240500
H	-0.93635500	1.63277900	-0.81671300
H	-0.61179200	1.85428300	0.93282100
C	-1.77931600	-0.03235700	0.40780500
H	-0.57976400	-2.10325700	0.24380900
H	-2.23052100	-0.02151400	1.40466900
F	-2.81552400	-0.12997600	-0.51809300
N	1.67207700	-0.02407000	-0.05537600
O	2.23904000	-1.11657400	-0.10519700
O	2.22294400	1.07835200	-0.10177000



Butadiene (Product)

C	0.48011800	0.28529000	0.10281300
C	1.90849800	-0.07681600	0.05126200
C	2.34500800	-1.31344300	0.35163700
H	3.40147700	-1.56503100	0.30756500
H	1.66733700	-2.10132100	0.66822100
C	-0.55919500	-0.53704400	-0.14995500
H	0.27527800	1.32932400	0.34345800
H	-0.39350100	-1.56999700	-0.44902900
C	-1.98871200	-0.15785100	-0.06707400
O	-2.84970400	-1.00165600	-0.29722200
C	-2.37857900	1.26571300	0.30101300
H	-1.99835900	1.53494000	1.29398800
H	-1.96720800	1.98634200	-0.41646200
H	-3.46777600	1.34260900	0.30148700

C	2.85693100	1.04059700	-0.32401500
H	2.63420900	1.42913800	-1.32662000
H	2.76386400	1.88465300	0.37308900
H	3.89789900	0.70392400	-0.31201100

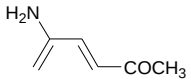
Transition state

C	-0.71166400	-0.75965500	-0.33047300
C	-1.79545400	-0.00097600	0.04153900
C	-1.21820200	1.18695900	0.60989600
H	-1.67680600	2.17460200	0.47984300
H	-0.59427900	1.10380000	1.49222400
C	0.38880600	0.16373700	-0.41835800
H	-0.64401600	-1.83340800	-0.49094600
H	0.32368200	0.97366100	-1.14027300
C	1.76336600	-0.20439800	0.01041800
O	1.97853000	-1.26686100	0.58697000
C	2.88239000	0.77603300	-0.29414600
H	3.05618000	0.82119100	-1.37789300
H	2.61512700	1.78984400	0.02971000
H	3.80264000	0.45969000	0.20203200
C	-3.26644000	-0.24048100	-0.15892000
H	-3.80870700	-0.28362000	0.79379800
H	-3.71256200	0.57672300	-0.74388100
H	-3.44631800	-1.17491600	-0.70010500

Cyclobutene (Starting material)

C	-0.74934500	0.07155600	1.07346300
C	-1.63461400	-0.05218500	0.06807000
C	-0.67978600	-0.84838200	-0.80942000
H	-0.37608700	-0.37139800	-1.75059300
H	-0.96755900	-1.88515400	-1.02322000
C	0.35692000	-0.71530900	0.38325700
H	-0.79468300	0.54067600	2.05431400
H	0.60868200	-1.67922000	0.83901000
C	1.66349700	-0.02237500	0.02620100
O	2.71300300	-0.64676500	0.01431500
C	1.62573000	1.45750800	-0.31196000

H	0.74732500	1.72143700	-0.91107000
H	1.55914700	2.03715500	0.61853000
H	2.54259000	1.73914400	-0.83500200
C	-3.04366100	0.37752100	-0.16398400
H	-3.12342800	1.00646600	-1.06149500
H	-3.69800100	-0.49012600	-0.32661500
H	-3.43445900	0.94513700	0.68785400



Butadiene (Product)

C	0.48831100	0.31712400	0.09928600
C	1.91905900	-0.03363000	0.04086300
C	2.38596500	-1.25400400	0.38188300
H	3.44492400	-1.49360800	0.32958600
H	1.72251800	-2.01619000	0.77232000
C	-0.53170500	-0.52105500	-0.17151500
H	0.28071100	1.35163800	0.37299400
H	-0.34228600	-1.54276000	-0.49332200
C	-1.96941500	-0.17346900	-0.07200100
O	-2.81270000	-1.02669400	-0.32917900
C	-2.38530600	1.22799200	0.34660000
H	-2.00982500	1.46670700	1.34909900
H	-1.98623100	1.98206900	-0.34293300
H	-3.47566900	1.28562100	0.34854800
N	2.75375000	1.05165000	-0.28430500
H	2.42119600	1.63528700	-1.04510200
H	3.72855300	0.80548300	-0.41831900

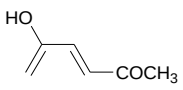
Transition state

C	-0.72374700	-0.79461300	-0.34492900
C	-1.79934100	-0.01944000	0.03147400
C	-1.22858800	1.18270900	0.58402200
H	-1.71224600	2.15762600	0.44060600
H	-0.64284800	1.10717200	1.49312000
C	0.35693700	0.15051500	-0.44033400

H	-0.65153600	-1.87041700	-0.47548000
H	0.31184300	0.94453900	-1.18169200
C	1.73288300	-0.19749200	0.01829800
O	1.94973700	-1.23781200	0.63081200
C	2.84724300	0.78217400	-0.30576400
H	3.01880200	0.81032300	-1.39043400
H	2.57393200	1.79985400	0.00077500
H	3.76976200	0.48003300	0.19501300
N	-3.15852400	-0.26818300	-0.09804300
H	-3.79179500	0.43864600	0.25178800
H	-3.47646600	-0.71112100	-0.95048800

Cyclobutene (Starting material)

C	-0.76325800	0.08094000	1.09782800
C	-1.64212900	-0.03675600	0.07768400
C	-0.70969300	-0.83841600	-0.80162000
H	-0.40495900	-0.35825300	-1.74022900
H	-1.01026500	-1.87176500	-1.01455000
C	0.32651300	-0.71775500	0.39308600
H	-0.79518000	0.55514500	2.07426700
H	0.58328400	-1.68746400	0.83502900
C	1.63256000	-0.02891200	0.02142900
O	2.68464700	-0.65009800	0.02657200
C	1.59486900	1.44588400	-0.34040900
H	0.68732500	1.71781000	-0.88967400
H	1.59389200	2.03889300	0.58386800
H	2.48576200	1.70493700	-0.91769400
N	-2.90613800	0.43319000	-0.21836000
H	-3.44823400	-0.12454600	-0.86738500
H	-3.45900900	0.76378400	0.56432600



Butadiene (Product)

C	0.49774500	0.32405000	0.09221400
C	1.92524200	-0.02187800	0.03537400

C	2.44442400	-1.21011800	0.38390200
H	3.51281400	-1.38700900	0.32011800
H	1.81068300	-1.99883000	0.77018600
C	-0.51866700	-0.52155800	-0.17059800
H	0.28107800	1.35790700	0.36630500
H	-0.32208100	-1.54386900	-0.48619000
C	-1.95999900	-0.18508400	-0.06656500
O	-2.79409700	-1.04976500	-0.31157200
C	-2.38606100	1.21602800	0.34061900
H	-2.01280800	1.46541800	1.34143200
H	-1.99375500	1.96768700	-0.35553400
H	-3.47675200	1.26547800	0.34267500
O	2.77920700	0.99954800	-0.33076700
H	2.30385000	1.66631500	-0.84995500

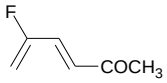
Transition state

C	-0.73215300	-0.79347800	-0.39789700
C	-1.79311900	-0.02859600	0.00871900
C	-1.25849600	1.16976400	0.58943700
H	-1.75675800	2.13749000	0.45594800
H	-0.65726200	1.09330200	1.48797600
C	0.34765000	0.15612900	-0.45363100
H	-0.66688900	-1.86345400	-0.56455300
H	0.30032200	0.96954800	-1.17254100
C	1.71665300	-0.19356800	0.02611700
O	1.91604900	-1.23370700	0.64374200
C	2.83809300	0.78067700	-0.28391600
H	3.01882900	0.81319500	-1.36688600
H	2.56728300	1.79834600	0.02502800
H	3.75444000	0.47149500	0.22360100
O	-3.11792700	-0.28805100	-0.20078000
H	-3.65672100	0.20856600	0.43476200

Cyclobutene (Starting material)

C	-0.77973800	0.13142900	1.09672100
C	-1.64293600	-0.01052700	0.07822600
C	-0.73265700	-0.84015300	-0.79568800

H	-0.41629400	-0.38515400	-1.74335400
H	-1.04262900	-1.87555700	-0.98215000
C	0.29807900	-0.69756400	0.40375200
H	-0.81830100	0.61609200	2.06569200
H	0.53214000	-1.66217600	0.86746700
C	1.61765500	-0.03877900	0.02202800
O	2.65196400	-0.68761500	0.02195400
C	1.61117900	1.43407600	-0.34534200
H	0.72246300	1.71519500	-0.92069500
H	1.59093800	2.03235200	0.57524000
H	2.51986400	1.67827900	-0.90054700
O	-2.91165100	0.42396300	-0.11504900
H	-3.24016800	0.11929900	-0.97507400



Butadiene (Product)

C	0.48973700	0.31319100	0.02473000
C	1.91075900	-0.02229000	0.01174800
C	2.51874500	-1.20663300	0.12068000
H	3.59991900	-1.28008200	0.09220300
H	1.94113600	-2.11475300	0.24589700
C	-0.53138600	-0.56283300	-0.05671600
H	0.29029700	1.37958400	0.10254000
H	-0.35572700	-1.63146000	-0.15955700
C	-1.96814900	-0.19463500	-0.01908700
O	-2.81093600	-1.08270200	-0.08616900
C	-2.37548500	1.26398800	0.10069300
H	-1.99589000	1.70417400	1.03101500
H	-1.97616300	1.85609800	-0.73178900
H	-3.46545400	1.32581400	0.09458000
F	2.68711600	1.09750100	-0.11975900

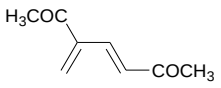
Transition state

C	-0.74603600	-0.79703200	-0.40797400
C	-1.77782200	-0.01746700	0.02050300

C	-1.27357900	1.17987000	0.60042900
H	-1.78874900	2.13542700	0.47032700
H	-0.64494600	1.11211000	1.48015200
C	0.33448800	0.15351400	-0.46462100
H	-0.68766400	-1.86827900	-0.56572200
H	0.27848200	0.96705000	-1.18199900
C	1.70099500	-0.19450500	0.02348000
O	1.89157300	-1.23620700	0.64023700
C	2.82384600	0.77818100	-0.28045100
H	3.00670900	0.81524200	-1.36286700
H	2.55452600	1.79490800	0.03280300
H	3.73834800	0.46482200	0.22757700
F	-3.10673800	-0.23855500	-0.13004000

Cyclobutene (Starting material)

C	-0.80084000	0.12952000	1.08707800
C	-1.63121400	-0.01633500	0.05272600
C	-0.73931000	-0.83932900	-0.82604400
H	-0.41899200	-0.37804000	-1.76713200
H	-1.05780100	-1.86942800	-1.01738900
C	0.27970200	-0.70137300	0.38892700
H	-0.84984100	0.60980200	2.05702800
H	0.49993600	-1.66618000	0.85661300
C	1.60463000	-0.03876600	0.03082100
O	2.63650400	-0.68921300	0.05050500
C	1.60199700	1.43277600	-0.33903900
H	0.73490300	1.70647800	-0.95011800
H	1.54449900	2.03430200	0.57797100
H	2.52860100	1.68089600	-0.86156100
F	-2.88479200	0.39965700	-0.18514100



Butadiene (Product)

C	0.20684000	-0.03705500	0.13415700
C	-1.15921800	0.51558300	0.11777600

C	-1.43704000	1.82399500	0.28905500
H	-2.45143500	2.20719500	0.26581600
H	-0.65315900	2.55299100	0.47395900
C	1.33716000	0.65217400	-0.11553900
H	0.25524800	-1.10296900	0.33912300
H	1.31646400	1.70780300	-0.38081200
C	2.70571100	0.07992800	-0.07617500
O	3.66505000	0.81234400	-0.29648000
C	2.90296000	-1.39390500	0.23431200
H	2.51585600	-1.64095200	1.23039300
H	2.37155100	-2.02443900	-0.48864400
H	3.97012700	-1.62179100	0.19712500
C	-2.26517000	-0.49741900	-0.05637600
C	-3.70414800	-0.02824600	-0.17683800
H	-3.82683900	0.67746500	-1.00676000
H	-4.33874000	-0.89997700	-0.34735300
H	-4.03185100	0.47723300	0.73963700
O	-1.99627500	-1.69020600	-0.09410900

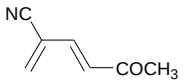
Transition state

C	-0.01519200	0.69580200	0.08075600
C	-1.03982200	-0.19878900	-0.16836700
C	-0.37432400	-1.43443400	-0.47559100
H	-0.75407100	-2.39927200	-0.13229900
H	0.27009000	-1.47650700	-1.34576800
C	1.11719600	-0.12380400	0.39105300
H	0.00381800	1.77900300	-0.00971600
H	1.03394200	-0.80331900	1.23628000
C	2.50034800	0.24734500	-0.01701700
O	2.69411000	1.22200300	-0.73578700
C	3.63941400	-0.61467400	0.49172700
H	3.72961300	-0.51439100	1.58180300
H	3.44998300	-1.67519200	0.28260000
H	4.57758600	-0.30820600	0.02423700
C	-2.50545300	-0.06093600	0.00454200
C	-3.05791300	1.31964800	0.30570100
H	-2.63713500	2.07311800	-0.37122800
H	-4.14570800	1.30310800	0.20934300

H	-2.79442000	1.61718900	1.32876200
O	-3.23401300	-1.04406300	-0.07431700

Cyclobutene (Starting material)

C	0.03967900	0.60803800	-0.88498400
C	0.90044600	-0.18765100	-0.21383600
C	-0.12509100	-1.27650300	0.04164000
H	-0.37971600	-1.45510300	1.09184800
H	0.06874300	-2.23936600	-0.44135600
C	-1.13449300	-0.34866000	-0.76047500
H	0.13232500	1.57786700	-1.36888000
H	-1.46848400	-0.79254400	-1.70431100
C	-2.37803400	0.08419100	0.01077600
O	-3.47567600	-0.33853100	-0.31011500
C	-2.20409800	1.03870100	1.17693700
H	-1.32851000	0.78796000	1.78619800
H	-2.04396700	2.05464800	0.79093200
H	-3.10616000	1.03648400	1.79283800
C	2.32865800	-0.10424200	0.15524100
C	3.11420700	1.11277100	-0.29614800
H	4.11918300	1.07608000	0.12993800
H	3.18770900	1.13130800	-1.39113700
H	2.61680600	2.04027500	0.01256200
O	2.84497900	-1.00865300	0.80092400



Butadiene (Product)

C	-0.24565100	-0.13221000	0.13305400
C	-1.61979900	0.41015700	0.10038200
C	-1.94915100	1.70588400	0.28218700
H	-2.98078700	2.03815700	0.23561000
H	-1.19000900	2.45171300	0.49533700
C	0.86833700	0.57083300	-0.14455200
H	-0.17045500	-1.18700700	0.38833300
H	0.81735400	1.61263800	-0.45431500

C	2.25365800	0.03513000	-0.07703200
O	3.18915800	0.78739500	-0.32206800
C	2.48874200	-1.41881000	0.29090400
H	2.10454700	-1.63786600	1.29477200
H	1.98073100	-2.09127000	-0.41112100
H	3.56173000	-1.61872300	0.26725500
C	-2.66701300	-0.55750500	-0.11785600
N	-3.48730100	-1.36395300	-0.29169300

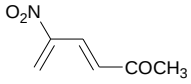
Transition state

C	-0.43580300	-0.73955000	-0.25909300
C	-1.49117200	0.07200100	0.10781600
C	-0.88106700	1.26006800	0.64147400
H	-1.29874600	2.25580200	0.47306500
H	-0.25890000	1.16637100	1.52310700
C	0.66891100	0.16124900	-0.39522500
H	-0.39455200	-1.82121200	-0.34660900
H	0.58232700	0.96183600	-1.12590800
C	2.05631800	-0.22924100	-0.00687400
O	2.25583800	-1.29154300	0.56970000
C	3.18008300	0.72398400	-0.35841000
H	3.30041400	0.77642300	-1.44895000
H	2.95286500	1.74042100	-0.01254900
H	4.11500800	0.38134300	0.08975800
C	-2.89274200	-0.12384900	-0.07963300
N	-4.03889900	-0.26808600	-0.22997800

Cyclobutene (Starting material)

C	-0.44542700	-0.00162800	1.10882700
C	-1.33968100	-0.18670300	0.11648300
C	-0.36480400	-0.93561000	-0.78210600
H	-0.11813200	-0.44178300	-1.72828900
H	-0.60801700	-1.98484500	-0.97667400
C	0.68105700	-0.72563100	0.39198700
H	-0.50754900	0.47345100	2.08376100
H	0.99389900	-1.66603600	0.85752500
C	1.94519700	0.04074500	0.00188500

O	3.01038700	-0.54594100	-0.07252700
C	1.82496700	1.52266000	-0.29290000
H	0.93643600	1.75143300	-0.89243800
H	1.71946500	2.07268800	0.65212500
H	2.72516700	1.87133500	-0.80356400
C	-2.70719700	0.16148100	-0.05282900
N	-3.82700600	0.43420000	-0.22290200



Butadiene (Product)

C	0.13622500	-0.04747600	0.14579500
C	-1.20971000	0.52831200	0.12523200
C	-1.56029400	1.80949800	0.29370200
H	-2.59832400	2.11615400	0.25030200
H	-0.80354900	2.56185200	0.48793600
C	1.25629900	0.64530100	-0.13545000
H	0.18958800	-1.10142900	0.39620100
H	1.22057200	1.68865400	-0.44279000
C	2.63422400	0.08932500	-0.07368700
O	3.57886400	0.82982200	-0.31961800
C	2.84800900	-1.36890200	0.28785600
H	2.47170600	-1.58299200	1.29579300
H	2.31861500	-2.03060500	-0.40840000
H	3.91696500	-1.58760700	0.25127300
N	-2.31773900	-0.45735500	-0.08156300
O	-3.46878400	-0.03565900	-0.15107100
O	-2.00006900	-1.64402500	-0.16931800

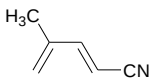
Transition state

C	0.03759300	-0.75979500	0.18537700
C	1.05648200	0.10745200	-0.11508000
C	0.48168800	1.35515400	-0.50016000
H	0.90791900	2.31127500	-0.19445700
H	-0.14845800	1.38183300	-1.38125400
C	-1.06472700	0.12530000	0.41714100

H	0.00919200	-1.84319600	0.14954100
H	-0.97560100	0.84413200	1.22805100
C	-2.45096600	-0.20949700	-0.02819000
O	-2.64365900	-1.18893400	-0.73697600
C	-3.57532500	0.69244700	0.43561700
H	-3.68982000	0.62146300	1.52564700
H	-3.35291000	1.74217000	0.20509900
H	-4.51128800	0.39947700	-0.04429600
N	2.48183400	-0.11005600	0.04555700
O	2.86009600	-1.25130600	0.31430900
O	3.21851900	0.87109800	-0.09926500

Cyclobutene (Starting material)

C	0.07179800	0.54596700	-0.98489700
C	0.92958400	-0.14436500	-0.22190400
C	-0.01858900	-1.23503600	0.19012100
H	-0.26025700	-1.28627900	1.25629700
H	0.21275900	-2.23901400	-0.17658200
C	-1.05908400	-0.43948800	-0.71540100
H	0.14958600	1.44650000	-1.58371500
H	-1.38053400	-1.01067500	-1.59186800
C	-2.31228600	0.04315300	0.01777700
O	-3.38469700	-0.48571900	-0.21128900
C	-2.16856000	1.16885500	1.02181100
H	-1.28019200	1.04651600	1.65200900
H	-2.04897600	2.12009300	0.48545900
H	-3.06539700	1.22609000	1.64226300
N	2.32199300	0.07284200	0.09263700
O	2.87164300	1.06644600	-0.38808700
O	2.85829000	-0.76168300	0.82720500



Butadiene (Product)

C	0.01431500	-0.31588700	-0.18807800
C	1.43259700	0.05682200	-0.05381200

C	1.84244600	1.33651600	-0.11806300
H	2.89192900	1.59864500	-0.01333800
H	1.15157500	2.15455800	-0.30272100
C	-1.03349600	0.42322900	0.23496100
H	-0.19056900	-1.28562900	-0.64188100
H	-0.88579500	1.36918200	0.75093000
C	-2.38737500	0.01082700	0.05242800
N	-3.50077800	-0.30585000	-0.08164300
C	2.39871800	-1.09390300	0.12045600
H	2.32978600	-1.79348300	-0.72354500
H	3.43209800	-0.74099400	0.18545400
H	2.17319100	-1.66695600	1.02923400

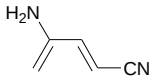
Transition state

C	0.21285300	-0.83775300	0.00296700
C	1.32525500	-0.03524500	-0.09863100
C	0.79730600	1.30042700	-0.12992400
H	1.31368300	2.13884600	0.35131300
H	0.13809000	1.59433800	-0.93827900
C	-0.82340500	0.02782900	0.50546500
H	0.08731400	-1.88630200	-0.26016800
H	-0.70357300	0.47992600	1.48379100
C	-2.18645800	-0.06791900	0.07179800
N	-3.28620200	-0.11751200	-0.31385500
C	2.78392600	-0.39631700	-0.06670700
H	3.28362300	0.10567300	0.77392400
H	2.92508100	-1.47460600	0.05702000
H	3.30233300	-0.08142200	-0.98042800

Cyclobutene (Starting material)

C	0.35832000	-0.97341800	0.40518100
C	1.26185800	-0.06811800	-0.00704000
C	0.32186500	1.11732200	0.16566300
H	0.02512900	1.62934700	-0.75646600
H	0.61045700	1.86547300	0.91428800
C	-0.73122000	0.05912400	0.68690600
H	0.36050400	-2.05352000	0.52109500

H	-0.98279100	0.18579100	1.74738500
C	-1.97178700	-0.05009200	-0.08044800
N	-2.95384400	-0.14403700	-0.69562400
C	2.67813200	-0.12348600	-0.46758200
H	3.32637600	0.48131700	0.18119300
H	3.05792300	-1.15082800	-0.47083200
H	2.77630400	0.28268700	-1.48337700



Butadiene (Product)

C	0.02603800	-0.33866200	-0.20405800
C	1.44684400	0.01711000	-0.04931900
C	1.88517500	1.29376100	-0.10567000
H	2.93647600	1.54021000	0.01736000
H	1.20953300	2.10707500	-0.34202700
C	-1.00218600	0.40145500	0.25840700
H	-0.18180400	-1.27800000	-0.71506600
H	-0.82882000	1.31739200	0.81833800
C	-2.36580600	0.03290700	0.05411900
N	-3.48698900	-0.24833600	-0.09191200
N	2.29886100	-1.09520900	0.03987900
H	1.97153000	-1.84877700	0.63502400
H	3.26957800	-0.87250500	0.22972500

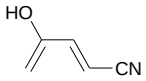
Transition state

C	0.22592200	-0.86338800	-0.00973100
C	1.33666700	-0.04829000	-0.10076700
C	0.83149400	1.29879500	-0.09496900
H	1.38003000	2.10249000	0.40835600
H	0.20214700	1.62281400	-0.91538000
C	-0.78948600	0.00952300	0.51753700
H	0.09404100	-1.90296800	-0.29958200
H	-0.68207200	0.43981200	1.50730900
C	-2.15122300	-0.05752300	0.06667800
N	-3.24822500	-0.08151700	-0.32850100

N	2.68367300	-0.36178800	-0.01753100
H	3.31720900	0.14847200	-0.61955700
H	2.92025300	-1.34218900	0.06858500

Cyclobutene (Starting material)

C	0.37784600	-1.02212000	0.33649700
C	1.27528000	-0.08215700	-0.03323200
C	0.35743800	1.09300300	0.22541200
H	0.05292000	1.66998700	-0.65500700
H	0.66855700	1.77904300	1.02219400
C	-0.69342800	0.00581000	0.68880700
H	0.37818200	-2.10414200	0.40493400
H	-0.94240200	0.08518300	1.75517300
C	-1.94217900	-0.03677800	-0.07785500
N	-2.92927700	-0.07801200	-0.69090200
N	2.60051900	-0.05930800	-0.40571000
H	2.89322400	0.72330700	-0.97792000
H	3.00108700	-0.93868300	-0.71087000



Butadiene (Product)

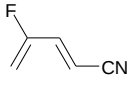
C	0.03535900	-0.34037500	-0.20150500
C	1.45430800	0.00529300	-0.04677200
C	1.95008600	1.25134900	-0.11680800
H	3.01319300	1.43074400	0.00294600
H	1.30546600	2.09286000	-0.33939700
C	-0.98763300	0.40699300	0.26228400
H	-0.18376000	-1.27386200	-0.72092300
H	-0.80559400	1.31937900	0.82534700
C	-2.35382500	0.05278400	0.05221000
N	-3.47626900	-0.21951400	-0.09953900
O	2.32035200	-1.05675100	0.09910700
H	1.85198800	-1.83477700	0.43949000

Transition state

C	0.23825000	-0.89493700	0.02442300
C	1.33173100	-0.07439400	-0.08864000
C	0.85328300	1.27731300	-0.08901500
H	1.41347200	2.07782100	0.40746200
H	0.21436300	1.60991500	-0.89866300
C	-0.77179500	-0.00301300	0.53360000
H	0.11110300	-1.93606000	-0.25450000
H	-0.66493200	0.43290300	1.52068500
C	-2.12682800	-0.04309300	0.06244500
N	-3.21734900	-0.04309200	-0.35021800
O	2.63770900	-0.46123000	-0.06709200
H	3.19792300	0.23564600	-0.44360100

Cyclobutene (Starting material)

C	0.39601100	-1.04044200	0.31372300
C	1.27762800	-0.09447400	-0.04567500
C	0.38103600	1.09197200	0.22841000
H	0.06774600	1.67459400	-0.64507400
H	0.69588000	1.77087000	1.03034500
C	-0.66453000	-0.00474200	0.68747700
H	0.39403100	-2.12228100	0.35550700
H	-0.89857900	0.05769900	1.75757300
C	-1.91964300	-0.02828000	-0.06752800
N	-2.91528100	-0.05285100	-0.66696700
O	2.55529400	-0.16013600	-0.47868500
H	2.88252200	0.72596600	-0.69853800



Butadiene (Product)

C	0.02812600	-0.36786200	-0.09675800
C	1.44024400	-0.00582400	-0.02752200
C	2.01845600	1.19669000	-0.08547500
H	3.09584600	1.29791500	-0.01973300

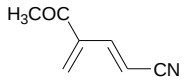
H	1.42245400	2.09249500	-0.21439600
C	-0.99902400	0.47147200	0.14945100
H	-0.17230300	-1.40363800	-0.36034600
H	-0.83291800	1.50048800	0.45954000
C	-2.36086000	0.06704400	0.02723200
N	-3.48202400	-0.23597200	-0.06281700
F	2.23327000	-1.11162100	0.08589900

Transition state

C	0.25770300	-0.90662100	0.03500000
C	1.32033400	-0.06135900	-0.09708600
C	0.86925500	1.28718900	-0.10004600
H	1.44421100	2.07879300	0.38697700
H	0.20369500	1.61945000	-0.88768000
C	-0.75386700	-0.01317100	0.54258300
H	0.13896800	-1.94714600	-0.24802300
H	-0.63747300	0.42535400	1.52705200
C	-2.10581000	-0.04375800	0.06637500
N	-3.19479900	-0.04026400	-0.34972400
F	2.63205700	-0.38536400	-0.11235700

Cyclobutene (Starting material)

C	0.41934000	-1.02108300	0.34680200
C	1.26917600	-0.07253400	-0.05004000
C	0.39070500	1.12310000	0.17391800
H	0.07276400	1.66372000	-0.72262200
H	0.71320300	1.83241600	0.94341800
C	-0.64336100	0.03240000	0.68564000
H	0.42643500	-2.10018000	0.42877000
H	-0.86080200	0.12855100	1.75552200
C	-1.90205900	-0.03969600	-0.05674500
N	-2.90130900	-0.10340100	-0.64643100
F	2.52830700	-0.10375800	-0.49750200



Butadiene (Product)

C	-0.67252800	-0.11366500	-0.16908000
C	0.67512800	0.47375100	-0.09423000
C	0.91203500	1.79926700	-0.16131200
H	1.91373900	2.20999100	-0.09650500
H	0.10895200	2.51695700	-0.30499700
C	-1.80803800	0.51640700	0.19443600
H	-0.71870900	-1.14231800	-0.51544500
H	-1.79818000	1.52136000	0.61159700
C	-3.09466300	-0.09047200	0.07761000
N	-4.15932600	-0.55574200	-0.00657600
C	1.80762400	-0.52140600	0.00539500
C	3.23121600	-0.02399900	0.17546700
H	3.88923600	-0.88906200	0.27694000
H	3.54910300	0.56564000	-0.69294400
H	3.32951900	0.61199600	1.06305800
O	1.56712300	-1.71795800	-0.05817300

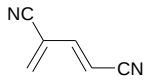
Transition state

C	-0.47430600	-0.71130300	-0.02711000
C	0.55737600	0.20257800	-0.13759900
C	-0.09529600	1.48121400	-0.17624400
H	0.31386800	2.35593500	0.33341000
H	-0.77114100	1.69963000	-0.99457500
C	-1.57296400	0.05849000	0.48192600
H	-0.51878400	-1.75835100	-0.31813300
H	-1.46070100	0.54637000	1.44500300
C	-2.93171700	-0.16954700	0.08971000
N	-4.03169100	-0.33139400	-0.26097100
C	2.02767400	0.01500500	-0.03938400
C	2.56386200	-1.40298400	-0.01581800
H	3.64973900	-1.38180900	-0.12981400
H	2.31357000	-1.88564600	0.93759600
H	2.12002500	-2.00942200	-0.81499500

O	2.76593600	0.98904200	0.03942800

Cyclobutene (Starting material)

C	-0.37003900	-0.89786700	0.50826400
C	0.50106100	0.07569900	0.17487500
C	-0.52043100	1.19612500	0.25251100
H	-0.76164200	1.67803000	-0.69903000
H	-0.34247800	1.96250800	1.01322300
C	-1.54058000	0.06496000	0.68906700
H	-0.30931400	-1.97540800	0.62986700
H	-1.87523600	0.16675700	1.72892600
C	-2.70552000	-0.14317300	-0.16841000
N	-3.62558300	-0.31695000	-0.85684100
C	1.94699600	0.11980900	-0.14034500
C	2.70866800	-1.18950700	-0.18683800
H	2.30614200	-1.83700400	-0.97617300
H	3.76385300	-0.99038700	-0.38559000
H	2.60999300	-1.73187000	0.76162300
O	2.48335400	1.19871800	-0.35621300



Butadiene (Product)

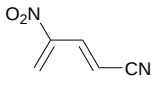
C	-0.22499600	-0.20295000	-0.19845500
C	1.12868600	0.37123700	-0.07574500
C	1.41023800	1.69070000	-0.08864400
H	2.42779400	2.05160900	0.01733900
H	0.62723600	2.42983900	-0.22619800
C	-1.34696700	0.40857400	0.23079200
H	-0.29442300	-1.19007700	-0.64952000
H	-1.31080000	1.36605100	0.74562000
C	-2.64378500	-0.16148500	0.05896700
N	-3.71513300	-0.60030700	-0.06681500
C	2.20538900	-0.58168700	0.03313900
N	3.05496100	-1.37165800	0.11716300

Transition state

C	-0.06197500	-0.79831900	-0.01432600
C	1.00377200	0.07525800	-0.10334300
C	0.41234900	1.38537700	-0.13701100
H	0.86379800	2.24082500	0.37073000
H	-0.24332500	1.63496100	-0.96226700
C	-1.12749900	0.01823000	0.49199900
H	-0.13354400	-1.83884600	-0.31867700
H	-1.00666000	0.48195800	1.46577800
C	-2.49004600	-0.13728400	0.07587000
N	-3.59168100	-0.23398300	-0.29175400
C	2.40251600	-0.20379500	-0.05143900
N	3.54668400	-0.41683200	-0.01197000

Cyclobutene (Starting material)

C	0.03508100	-0.93093300	0.51754900
C	0.94708200	-0.02492600	0.11713300
C	-0.01443100	1.15622600	0.15387200
H	-0.25105100	1.59436800	-0.81969100
H	0.22311600	1.94871200	0.87041800
C	-1.07672400	0.10267500	0.67069300
H	0.05533000	-2.00170900	0.69032300
H	-1.37841000	0.27661600	1.71094300
C	-2.27252600	-0.07946500	-0.14983400
N	-3.21975700	-0.22879100	-0.80569100
C	2.32752900	-0.10418600	-0.21194900
N	3.45903500	-0.13325600	-0.48527700



Butadiene (Product)

C	-0.59072400	-0.11171900	-0.19545400
C	0.73747100	0.49404800	-0.09746300
C	1.04893900	1.79528100	-0.13802400
H	2.07705300	2.12559800	-0.04909700

H	0.27437800	2.54176600	-0.27771800
C	-1.71347400	0.50297800	0.22807600
H	-0.64548700	-1.10629300	-0.62505600
H	-1.68349200	1.47042000	0.72471200
C	-3.00849200	-0.07519500	0.06976900
N	-4.07911800	-0.51792300	-0.04704700
N	1.86639900	-0.47892900	0.02651000
O	1.57299800	-1.67390700	-0.00017800
O	3.00503400	-0.03683000	0.14636500

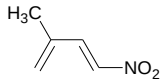
Transition state

C	-0.44202400	-0.78655700	0.03917700
C	0.58370100	0.11219500	-0.10011100
C	0.02287700	1.42204400	-0.16985200
H	0.47833000	2.27629200	0.33195700
H	-0.63570100	1.66011800	-0.99689600
C	-1.51008500	0.05242300	0.50607200
H	-0.49652900	-1.83662600	-0.22765400
H	-1.39312800	0.55759400	1.45960200
C	-2.86615400	-0.10338500	0.07429100
N	-3.96280100	-0.20268700	-0.30685200
N	2.00891600	-0.16370200	-0.03788100
O	2.76426000	0.80962600	0.02549800
O	2.36003100	-1.34374700	-0.05691500

Cyclobutene (Starting material)

C	-0.33399300	-0.97712500	0.45015200
C	0.53990200	-0.00588800	0.16407100
C	-0.39919100	1.16038300	0.30665500
H	-0.62975700	1.69910300	-0.61588200
H	-0.17646900	1.87060800	1.10781700
C	-1.45432100	0.03767600	0.69457900
H	-0.29465400	-2.05800800	0.50812500
H	-1.76595800	0.09586300	1.74394200
C	-2.63461800	-0.07112500	-0.15916200
N	-3.57006700	-0.16097400	-0.84182600
N	1.94845400	-0.05115300	-0.15683000

O	2.50259900	1.03424800	-0.34593700
O	2.48633200	-1.15752300	-0.21546000



Butadiene (Product)

C	0.43876600	-0.31812800	-0.13721000
C	1.84695000	0.09875100	-0.04751200
C	2.23107300	1.36011900	-0.31537100
H	3.27514300	1.65522400	-0.25418100
H	1.52519200	2.12338000	-0.63083800
C	-0.61331000	0.45558700	0.16416700
H	0.23345700	-1.34331300	-0.44190600
H	-0.58550800	1.46939300	0.53988700
N	-1.97411300	-0.03747800	0.01979200
O	-2.16463300	-1.19127500	-0.37307800
O	-2.86951300	0.76226200	0.31391400
C	2.83015300	-0.99082900	0.31720300
H	2.60419300	-1.41417800	1.30433000
H	2.78171600	-1.81750000	-0.40405600
H	3.85598100	-0.61156200	0.33387900

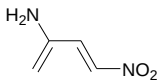
Transition state

C	-0.58489400	-0.76586500	-0.24564100
C	-1.70845200	-0.02993800	0.06978600
C	-1.19915000	1.21411100	0.56566900
H	-1.70990100	2.16421200	0.37428500
H	-0.55914300	1.22329300	1.43972100
C	0.42460500	0.22433000	-0.41775500
H	-0.45712100	-1.83886300	-0.35746300
H	0.40587400	0.97389800	-1.19732100
N	1.81207000	-0.06160600	-0.03946600
O	2.66695600	0.77400400	-0.35202000
O	2.03684900	-1.10510300	0.58301100
C	-3.15974700	-0.34263400	-0.16306200
H	-3.72695800	-0.35206600	0.77533200

H	-3.61689100	0.42203000	-0.80651100
H	-3.28496700	-1.31249400	-0.65370000

Cyclobutene (Starting material)

C	-1.60856400	0.02053100	0.07116800
C	-0.72081800	-0.49224000	0.94270500
C	0.37772300	0.46012500	0.55618100
H	-0.75746900	-1.27845300	1.69049800
H	0.73493700	1.18072500	1.29275500
C	-0.61784500	1.01577900	-0.52326600
H	-0.85386700	2.08152900	-0.41704200
H	-0.31168200	0.81307000	-1.55581300
N	1.63467100	-0.14207500	-0.04513500
O	1.53483600	-1.20763400	-0.64771000
O	2.67513400	0.50151700	0.08770700
C	-3.04238000	-0.22293900	-0.24651700
H	-3.16291500	-0.51137000	-1.29942800
H	-3.46243400	-1.01744100	0.37911000
H	-3.63772900	0.68787700	-0.09573200



Butadiene (Product)

C	0.44793600	-0.34756800	-0.13316700
C	1.85857600	0.05736700	-0.03372400
C	2.26894200	1.31621000	-0.30553700
H	3.31597800	1.59904200	-0.23851000
H	1.57462900	2.06541200	-0.66608800
C	-0.58737200	0.44247200	0.17878500
H	0.23942100	-1.36382200	-0.46244300
H	-0.53757800	1.45111200	0.56548000
N	-1.95690000	-0.02030400	0.01735500
O	-2.16704200	-1.16817800	-0.38285100
O	-2.83749800	0.79651800	0.30861800
N	2.73066100	-1.00528900	0.24178100
H	2.40616200	-1.67446000	0.93126100

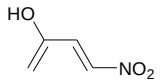
H	3.69289400	-0.73574400	0.41207900

Transition state

C	-0.59187900	-0.78767600	-0.24830100
C	-1.71889100	-0.04375700	0.06279500
C	-1.23547200	1.22360300	0.53327100
H	-1.78118400	2.14749600	0.31458700
H	-0.62789100	1.25293500	1.42940300
C	0.39540800	0.21731600	-0.43334300
H	-0.45589300	-1.86077500	-0.34070200
H	0.39573200	0.95962200	-1.22030100
N	1.78676700	-0.05530900	-0.03020300
O	2.64095500	0.77280700	-0.36266100
O	2.01109100	-1.07826500	0.62392000
N	-3.04887900	-0.30514000	-0.20005300
H	-3.73422800	0.00709100	0.47508500
H	-3.27312300	-1.19647800	-0.62288400

Cyclobutene (Starting material)

C	-1.61222300	-0.07595600	-0.06764600
C	-0.69794800	-0.62798200	-0.90112300
C	0.35037100	-0.71284600	0.17122800
H	-0.69289300	-0.94713700	-1.93704200
H	0.74229200	-1.68761500	0.46574300
C	-0.68746600	-0.04337600	1.13273200
H	-0.97808600	-0.67290600	1.98238900
H	-0.39876800	0.95239600	1.48455300
N	1.60495100	0.13749300	-0.05470300
N	-2.94000600	0.25116200	-0.12491600
H	-3.27454800	0.94074400	0.53605100
H	-3.36298100	0.33062700	-1.04183300
O	1.46050700	1.32970500	-0.31096700
O	2.68873800	-0.43917200	0.03050700



Butadiene (Product)

C	-0.45454700	-0.34903700	0.12136800
C	-1.86365800	0.04569100	0.02754400
C	-2.33166600	1.27432400	0.30514300
H	-3.39242900	1.48934100	0.23376400
H	-1.66728900	2.05750700	0.64859800
C	0.57761200	0.45156900	-0.17543500
H	-0.23257300	-1.36650900	0.44207300
H	0.52386300	1.46541100	-0.54814300
N	1.94837700	-0.00848200	-0.01296000
O	2.15751200	-1.16215800	0.37085100
O	2.82673500	0.81558900	-0.28620700
O	-2.75185500	-0.95563200	-0.29107000
H	-2.29580000	-1.70405100	-0.70587800

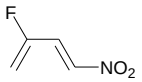
Transition state

C	-0.60068000	-0.80371700	-0.30438500
C	-1.71030900	-0.06467800	0.04013900
C	-1.24972400	1.19451000	0.53879400
H	-1.80483700	2.11829600	0.34156300
H	-0.63238000	1.21906200	1.42844700
C	0.38142000	0.21400100	-0.45110200
H	-0.47056500	-1.87346900	-0.42089900
H	0.38129500	0.97332500	-1.22139700
N	1.76857500	-0.04733100	-0.02404500
O	2.61769300	0.79354300	-0.33419700
O	1.98834800	-1.07250500	0.62631700
O	-3.00324100	-0.40582200	-0.19793300
H	-3.60017400	0.13168400	0.34643100

Cyclobutene (Starting material)

C	-1.60970800	-0.07345000	-0.07805600
C	-0.70967300	-0.68560300	-0.86758700

C	0.32842200	-0.69208600	0.22458900
H	-0.70173200	-1.07324600	-1.87829200
H	0.70176700	-1.64832000	0.59254600
C	-0.70761100	0.05639600	1.13174800
H	-1.00298300	-0.50487900	2.02675100
H	-0.41257600	1.07491400	1.40369800
N	1.58738300	0.12744200	-0.05687500
O	1.45102000	1.29972200	-0.39425200
O	2.66410400	-0.45312000	0.06976300
O	-2.89894500	0.26206100	-0.26421900
H	-3.23416800	0.75859300	0.49892200



Butadiene (Product)

C	-1.60035800	0.00221700	0.06489700
C	-0.74912400	-0.29000700	1.05195600
C	0.31274200	0.58388400	0.42280700
H	-0.77090800	-0.87592200	1.96135100
H	0.66371100	1.45327400	0.97815100
C	-0.69121300	0.87295700	-0.75523800
H	-0.97462900	1.92541500	-0.85995200
H	-0.38195600	0.46341400	-1.72132100
N	1.57356700	-0.13374000	-0.03646500
O	1.44486000	-1.21078600	-0.60993700
O	2.64197600	0.42979900	0.19135600
F	-2.87535200	-0.31071200	-0.16231700

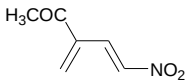
Transition state

C	-0.61534300	-0.81334100	-0.31708300
C	-1.69479800	-0.05607100	0.05150900
C	-1.26093800	1.20061600	0.54754900
H	-1.82974900	2.11240900	0.35018300
H	-0.61773200	1.23576100	1.41803600
C	0.36855600	0.20505800	-0.46375700
H	-0.49442200	-1.88457200	-0.42601200

H	0.35767200	0.96425800	-1.23378200
N	1.75144000	-0.04752000	-0.02560300
O	2.59602700	0.79995600	-0.32634900
O	1.96900500	-1.07549200	0.62083600
F	-2.99788500	-0.34538800	-0.13271200

Cyclobutene (Starting material)

C	-1.60035800	0.00221700	0.06489700
C	-0.74912400	-0.29000700	1.05195600
C	0.31274200	0.58388400	0.42280700
H	-0.77090800	-0.87592200	1.96135100
H	0.66371100	1.45327400	0.97815100
C	-0.69121300	0.87295700	-0.75523800
H	-0.97462900	1.92541500	-0.85995200
H	-0.38195600	0.46341400	-1.72132100
N	1.57356700	-0.13374000	-0.03646500
O	1.44486000	-1.21078600	-0.60993700
O	2.64197600	0.42979900	0.19135600
F	-2.87535200	-0.31071200	-0.16231700



Butadiene (Product)

C	-0.23799500	-0.09892400	-0.18657800
C	1.10505400	0.50089500	-0.13585000
C	1.33216000	1.81789200	-0.31165800
H	2.33107900	2.23882600	-0.27224800
H	0.52589000	2.51426800	-0.52453900
C	-1.36251400	0.54499900	0.14623000
H	-0.30078400	-1.14256000	-0.48174800
H	-1.44998900	1.55459200	0.52540800
N	-2.66253900	-0.10572400	0.04333000
O	-2.72918800	-1.26741400	-0.35934500
O	-3.63195200	0.58408600	0.37885600
C	2.23825800	-0.47805100	0.06657800
C	3.65830800	0.03801800	0.20164700

H	4.31742200	-0.81083900	0.39261700
H	3.98296300	0.54208700	-0.71678400
H	3.74623300	0.75718300	1.02452200
O	1.99680800	-1.67448000	0.11389700

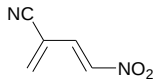
Transition state

C	0.07866800	0.66862300	0.03356500
C	-0.96896100	-0.21070800	-0.18903400
C	-0.34727100	-1.47429700	-0.44987700
H	-0.76812600	-2.41143600	-0.08050300
H	0.31907000	-1.56935000	-1.29882100
C	1.14199200	-0.19492900	0.40879800
H	0.13636900	1.74776000	-0.07118700
H	1.11389800	-0.81984600	1.29220500
N	2.52695900	0.13325000	0.06076100
O	3.41041100	-0.59315200	0.52318800
O	2.71619700	1.10089100	-0.68310700
C	-2.43433700	-0.02654600	0.00184100
C	-2.94699800	1.37882600	0.24016100
H	-2.63433200	1.73388200	1.23050300
H	-2.54112600	2.07895700	-0.50053100
H	-4.03773700	1.38007300	0.18869100
O	-3.17851900	-0.99756500	-0.02238100

Cyclobutene (Starting material)

C	0.87593200	-0.12563500	0.18581200
C	0.02312800	0.79837900	0.67614500
C	-1.13407500	-0.16362100	0.72310700
H	0.10643800	1.83886400	0.97191100
H	-1.53106600	-0.44094100	1.70124300
C	-0.17199300	-1.22140200	0.06571700
H	-0.01333300	-2.12976200	0.65409000
H	-0.44260700	-1.49414200	-0.95888400
N	-2.33777300	0.17849100	-0.12397500
O	-2.23387000	1.10244900	-0.92753800
O	-3.33561700	-0.51969400	0.03604200
C	2.32482600	-0.15457200	-0.12382900

C	3.11531600	1.12643000	0.04331000
H	3.04085800	1.49724700	1.07326200
H	4.16325100	0.94319000	-0.20314400
H	2.71704100	1.90937000	-0.61439000
O	2.83511400	-1.19909700	-0.50573300



Butadiene (Product)

C	-0.20425600	-0.17633300	0.18117100
C	-1.55482100	0.41139700	0.10683300
C	-1.83168800	1.72113200	0.27430100
H	-2.84796500	2.09476500	0.20694200
H	-1.04769500	2.43566100	0.50453200
C	0.90959800	0.47374700	-0.17282500
H	-0.11658600	-1.20353800	0.52655900
H	0.97910800	1.46908100	-0.59091600
N	2.21832700	-0.15643200	-0.03356300
O	2.28962700	-1.30472200	0.40434800
O	3.18037000	0.53565000	-0.37795500
C	-2.63090800	-0.51914500	-0.12625600
N	-3.48324000	-1.28759400	-0.31466600

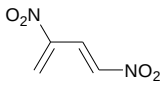
Transition state

C	-0.32809100	-0.73721500	-0.17172100
C	-1.40839700	0.07275800	0.13727700
C	-0.84428300	1.31594200	0.57542200
H	-1.30261800	2.27779700	0.33522500
H	-0.19829700	1.31728400	1.44459900
C	0.70221200	0.21013300	-0.40892100
H	-0.24405100	-1.81846300	-0.19658600
H	0.66719000	0.93721000	-1.21008000
N	2.09408700	-0.10521900	-0.06340300
O	2.95238200	0.71091600	-0.40448900
O	2.30426200	-1.15112300	0.55597000
C	-2.80001000	-0.17583900	-0.06398800

N	-3.93751000	-0.36718700	-0.22137100

Cyclobutene (Starting material)

C	-1.31354200	0.05869200	0.13990700
C	-0.42610200	-0.67433300	0.84169300
C	0.68272200	0.32604100	0.65096700
H	-0.47793600	-1.61324100	1.38036400
H	1.05178200	0.85351300	1.53230000
C	-0.31356800	1.14492500	-0.24720700
H	-0.52537700	2.15963200	0.10260900
H	-0.04378200	1.16638700	-1.30739700
N	1.91311500	-0.15103600	-0.08724200
O	1.87971000	-1.26463100	-0.60315400
O	2.85520300	0.63504600	-0.13511500
C	-2.70011800	-0.08009200	-0.13882200
N	-3.83602200	-0.16053700	-0.38146600



Butadiene (Product)

C	0.16849800	-0.09681100	0.19689800
C	-1.15515600	0.52195900	0.13632300
C	-1.46232600	1.81487200	0.29344400
H	-2.49010900	2.15307800	0.23300300
H	-0.68665500	2.54399400	0.50187000
C	1.28495200	0.54312600	-0.16706900
H	0.23809200	-1.12248800	0.54450500
H	1.36229700	1.53530400	-0.59175900
N	2.58950700	-0.09691100	-0.03018300
O	2.65447900	-1.23796600	0.42567500
O	3.55374000	0.58212900	-0.39451100
N	-2.28292500	-0.43446900	-0.09037700
O	-1.98492400	-1.62291400	-0.19701700
O	-3.42148300	0.01761400	-0.15930600

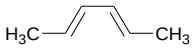
Transition state

C	0.05543000	-0.73819700	-0.12869200
C	-0.98620200	0.11668200	0.14405100
C	-0.45290200	1.39440600	0.47187800
H	-0.91820000	2.32032000	0.13303000
H	0.19898500	1.48205000	1.33278300
C	1.08631300	0.19118100	-0.43173000
H	0.12296800	-1.81799400	-0.07067500
H	1.05128500	0.86050400	-1.28181100
N	2.47575200	-0.08765000	-0.04631300
O	3.33346800	0.70045600	-0.44777600
O	2.68079500	-1.07729700	0.66012600
N	-2.40638000	-0.14844600	-0.03359500
O	-2.74189300	-1.31475400	-0.23437200
O	-3.16693000	0.81951400	0.03614600

Cyclobutene (Starting material)

C	-0.90311300	0.05040900	0.19172200
C	-0.05083300	-0.85798700	0.68129100
C	1.06415300	0.16236000	0.72589700
H	-0.11573800	-1.89927900	0.96926500
H	1.44466000	0.45014800	1.70661600
C	0.06845300	1.19513800	0.06813600
H	-0.13280500	2.08825800	0.66529200
H	0.32949700	1.48021500	-0.95497100
N	2.27378700	-0.13463900	-0.12842900
O	2.17233500	-1.01816600	-0.97502100
O	3.26559000	0.55936600	0.07303600
N	-2.31694300	-0.02091600	-0.10513000
O	-2.88617100	-1.09501000	0.08733600
O	-2.83868900	1.01256400	-0.52954800

6.3.3 1,4-Disubstituted butadienes



Butadiene (Product)

C	0.73157500	0.71381500	-0.06997400
C	-0.73156300	0.71381500	0.07003600
C	-1.55315200	-0.32738800	-0.15058700
H	-1.17729800	1.66787300	0.36033900
H	-1.12701300	-1.26934300	-0.50001500
C	1.55316000	-0.32737900	0.15072400
H	1.12699700	-1.26932800	0.50012700
C	3.04350800	-0.30117300	-0.03263500
H	3.39222300	0.68500100	-0.35976900
H	3.56528200	-0.55638300	0.90040200
H	3.36459500	-1.03868600	-0.78211700
H	1.17731000	1.66780200	-0.36049000
C	-3.04351500	-0.30116800	0.03251500
H	-3.39236800	0.68514500	0.35911100
H	-3.56517500	-0.55691900	-0.90043500
H	-3.36462600	-1.03829900	0.78237300

Transition state

C	-0.68327900	1.21952300	-0.08092100
C	0.68325500	1.21953200	0.08091200
C	1.02350700	-0.14502100	0.35840700
H	1.39277400	2.03440800	-0.07179600
H	0.59944800	-0.57152800	1.26283100
C	-1.02348600	-0.14504900	-0.35838400
H	-1.39280700	2.03439100	0.07178300
H	-0.59940100	-0.57154700	-1.26280000
C	-2.28535300	-0.81950800	0.12409700
H	-3.14666600	-0.51896800	-0.49491600
H	-2.20735800	-1.91057100	0.05069200
H	-2.52173800	-0.56324500	1.16321400
C	2.28536400	-0.81948500	-0.12410400
H	3.14648800	-0.52002100	0.49568600

H	2.20685900	-1.91060100	-0.05189300
H	2.52235100	-0.56227100	-1.16284300

Cyclobutene (Starting material)

C	0.57501400	1.32311700	0.34583900
C	-0.57497200	1.32315700	-0.34581900
C	-0.67370700	-0.19562300	-0.41584300
H	-1.22291300	2.11156400	-0.72436400
H	-0.51911100	-0.59160000	-1.43046400
C	0.67367500	-0.19566600	0.41582600
H	1.22300200	2.11148200	0.72439800
H	0.51903500	-0.59167400	1.43043000
C	1.89277200	-0.86328800	-0.21932100
H	2.80291700	-0.65409800	0.35756500
H	1.76977100	-1.95325600	-0.26246100
H	2.05355700	-0.49780500	-1.24143100
C	-1.89278600	-0.86327100	0.21931600
H	-2.80297300	-0.65403600	-0.35748300
H	-1.76976800	-1.95324500	0.26234500
H	-2.05349200	-0.49788500	1.24147200

Butadiene (Product)

C	-0.75883700	0.73727400	0.06326100
C	0.70034600	0.71362300	-0.06344700
C	1.52409500	-0.32626800	0.16777600
H	1.15480900	1.65887700	-0.37043700
H	1.10489800	-1.26370100	0.53830000
C	-1.57356700	-0.32288900	-0.12540200
H	-1.16376800	-1.28100000	-0.43806600
H	-1.21038300	1.70403900	0.29380700
C	3.01250400	-0.30291600	-0.04003100
H	3.35535400	0.68567400	-0.36757700
H	3.55204400	-0.56155300	0.88232100
H	3.32540900	-1.03337500	-0.80049200

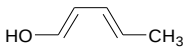
N	-2.96577400	-0.30809800	-0.05350800
H	-3.40877900	-1.19578300	0.14495800
H	-3.37640100	0.45057200	0.47879700

Transition state

C	-0.61250000	1.21744200	-0.09368200
C	0.74474800	1.19650200	0.10800100
C	1.03452100	-0.19196600	0.36703800
H	1.48525800	1.99260800	0.02628300
H	0.67300900	-0.62436300	1.29360300
C	-0.98360100	-0.14557600	-0.36139400
H	-1.29745100	2.05665600	0.04625100
H	-0.59499100	-0.57057600	-1.28381400
C	-2.27924200	-0.76264900	0.11679800
H	-3.14324200	-0.36729500	-0.44376400
H	-2.28043300	-1.85059600	-0.02239100
H	-2.46490400	-0.56047600	1.17911500
N	2.19830000	-0.79767500	-0.10217700
H	2.45014200	-0.61449900	-1.06585000
H	2.36095900	-1.76024800	0.16524100

Cyclobutene (Starting material)

C	-0.50609900	1.34317300	-0.32254000
C	0.67100900	1.28328400	0.31678100
C	0.68414300	-0.23441000	0.38817600
H	1.37492800	2.03200400	0.67394700
H	0.52554400	-0.61814000	1.41183100
C	-0.67638900	-0.16740600	-0.41469800
H	-1.13675400	2.16672500	-0.65243100
H	-0.53133300	-0.55092300	-1.43291500
C	-1.91499900	-0.79296400	0.22482100
H	-2.82144800	-0.52702300	-0.33402800
H	-1.84490300	-1.88857600	0.23924900
H	-2.04734600	-0.44666700	1.25771100
N	1.79032900	-0.89010100	-0.31252800
H	1.71979900	-1.90391700	-0.23069800
H	2.68322000	-0.62284500	0.09978900



Butadiene (Product)

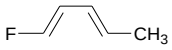
C	-0.77626200	0.74200400	0.07333800
C	0.68109900	0.72013000	-0.08264800
C	1.49999500	-0.31382300	0.18369800
H	1.12897100	1.64991400	-0.44068900
H	1.07776600	-1.22527800	0.61051900
C	-1.57673300	-0.31075200	-0.15063700
H	-1.19916200	-1.26305800	-0.52029400
H	-1.24266400	1.68174200	0.36726000
C	2.98499000	-0.31345600	-0.04463600
H	3.33184800	0.65186300	-0.43107800
H	3.53240500	-0.52606500	0.88438800
H	3.27959800	-1.08915100	-0.76613500
O	-2.92756600	-0.25047100	0.08988900
H	-3.36677500	-1.02082100	-0.29776400

Transition state

C	-0.58322300	1.22059900	-0.06208900
C	0.78584400	1.17388900	0.07882200
C	1.03729700	-0.20864900	0.33042200
H	1.54173400	1.94856600	-0.03759200
H	0.69289300	-0.65699900	1.25726300
C	-0.98397400	-0.12196000	-0.36075500
H	-1.25153600	2.05826500	0.14453400
H	-0.60069500	-0.53802900	-1.28828300
C	-2.27655000	-0.74019600	0.12149000
H	-3.12741900	-0.41039500	-0.49676400
H	-2.24359200	-1.83444400	0.05435300
H	-2.50227000	-0.47218100	1.16048900
O	2.15536800	-0.80218800	-0.21305500
H	2.37157700	-1.61937500	0.26310300

Cyclobutene (Starting material)

C	-0.44917800	1.36060700	-0.29142400
C	0.74763000	1.25081400	0.30600400
C	0.69465600	-0.25746900	0.37195500
H	1.49355600	1.96071000	0.65274300
H	0.55646200	-0.65688600	1.38905800
C	-0.67574000	-0.14155900	-0.41648500
H	-1.06994200	2.21097200	-0.56606400
H	-0.54515900	-0.50575200	-1.44374000
C	-1.92936700	-0.74534900	0.21446700
H	-2.83161800	-0.43603800	-0.32841400
H	-1.89491800	-1.84261900	0.19783400
H	-2.04324500	-0.42438700	1.25784800
O	1.78636300	-0.90570800	-0.26775300
H	1.71595600	-1.86260100	-0.12435400



Butadiene (Product)

C	-0.79840400	0.70677800	0.09118000
C	0.65964800	0.71523100	-0.08566800
C	1.49108000	-0.30567100	0.18467600
H	1.08429700	1.65064100	-0.45489700
H	1.07954800	-1.21925400	0.61680000
C	-1.57454900	-0.34599600	-0.17068500
H	-1.26152500	-1.30142600	-0.57802600
H	-1.28109700	1.62276400	0.42958900
C	2.97495800	-0.28754200	-0.04327000
H	3.31017900	0.67562600	-0.44401400
H	3.52224900	-0.48056400	0.88962700
H	3.27625300	-1.07201700	-0.75165300
F	-2.91625500	-0.30806200	0.04835300

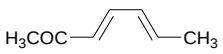
Transition state

C	-0.54486600	1.21744000	-0.05785300

C	0.82982900	1.13498100	0.05494400
C	1.01923000	-0.24111100	0.32732800
H	1.60610800	1.88701900	-0.06723700
H	0.69880400	-0.70995500	1.24982700
C	-0.99114700	-0.10307300	-0.36734700
H	-1.18840000	2.06110800	0.19358900
H	-0.61433900	-0.53638300	-1.28871800
C	-2.28860100	-0.69722500	0.12399800
H	-3.09729200	-0.52979600	-0.60421600
H	-2.19912600	-1.78365400	0.24676600
H	-2.60230300	-0.27282900	1.08394800
F	2.13887500	-0.88684300	-0.14448600

Cyclobutene (Starting material)

C	-0.35924200	1.37191900	-0.29305700
C	0.83488300	1.20416300	0.29864300
C	0.67576800	-0.29206700	0.38435700
H	1.61524500	1.87460100	0.64605200
H	0.56583200	-0.71604700	1.38892000
C	-0.66613700	-0.11994200	-0.40931600
H	-0.94077800	2.25100500	-0.56217600
H	-0.54546900	-0.49903200	-1.43154700
C	-1.95096500	-0.65912600	0.21629600
H	-2.83059700	-0.31789800	-0.34326600
H	-1.95860000	-1.75584900	0.21313900
H	-2.06286400	-0.31926900	1.25352400
F	1.66126500	-1.06079900	-0.26068800



Butadiene (Product)

C	0.15395700	0.72101700	-0.06685000
C	1.61506900	0.72195100	-0.13597100
C	2.42371200	-0.32031400	0.13609300
H	2.07296000	1.67379300	-0.40828600

H	1.98127500	-1.26313400	0.45995700
C	-0.65907900	-0.35834000	-0.11412100
H	-0.25593800	-1.36076200	-0.24385200
C	-2.13277100	-0.31855900	-0.01104500
H	-0.30156000	1.70746400	0.01568900
C	3.91922500	-0.29026700	0.04653600
H	4.37756500	-0.53542200	1.01461500
H	4.28240100	-1.04178900	-0.66856700
H	4.28864100	0.69067100	-0.27134600
C	-2.85051700	1.01564100	0.13607900
H	-2.63112200	1.67933300	-0.70928900
H	-3.92610700	0.83209200	0.17773500
H	-2.53877100	1.53318000	1.05159600
O	-2.77086600	-1.36777500	-0.04532300

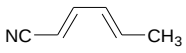
Transition state

C	1.56292600	1.23702400	-0.06236700
C	0.25399900	1.40517800	-0.42497700
C	-0.26396000	0.06185900	-0.55220500
H	-0.30235300	2.33122300	-0.56265400
H	0.17754800	-0.59100000	-1.30006200
C	1.64278900	-0.11226800	0.43476200
H	2.41157000	1.90578900	-0.20676900
H	1.05794400	-0.33860000	1.32111200
C	2.79055900	-1.04948300	0.18215500
H	3.56540200	-0.91449700	0.95423800
H	2.46328300	-2.09360000	0.24517600
H	3.25487000	-0.88770700	-0.79603700
C	-1.60573300	-0.39361100	-0.11633100
C	-2.50510400	0.59748000	0.60582100
H	-3.48568300	0.14557300	0.77041500
H	-2.06824600	0.87734000	1.57323100
H	-2.61982200	1.52346600	0.02781300
O	-1.96342100	-1.55438300	-0.30345200

Cyclobutene (Starting material)

C	1.49720500	1.25532500	0.12885100

C	0.51627300	1.37708200	-0.77792800
C	0.01072500	-0.04994700	-0.61568300
H	0.18867000	2.18742600	-1.42491000
H	0.18716100	-0.70885300	-1.47312500
C	1.15886700	-0.18410100	0.48624100
H	2.27386100	1.92646400	0.48940900
H	0.74935000	-0.29669400	1.50036300
C	2.21073200	-1.26173200	0.23475500
H	3.04011900	-1.16584000	0.94706800
H	1.78077200	-2.26365300	0.35099400
H	2.62433000	-1.18021500	-0.77767800
C	-1.39881300	-0.31562300	-0.11012800
C	-2.06213800	0.73546700	0.76039300
H	-2.39404100	1.57139300	0.12961000
H	-2.93237200	0.30539300	1.26143800
H	-1.36592000	1.15446900	1.49568800
O	-1.96862900	-1.35858900	-0.39223300



Butadiene (Product)

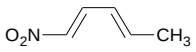
C	-0.35945900	0.73859500	0.03359200
C	1.09837400	0.72963400	-0.05812800
C	1.89544600	-0.34243300	0.11242300
H	1.56192500	1.69763400	-0.25028000
H	1.44445400	-1.30257700	0.36761000
C	-1.17801500	-0.32168300	-0.15848400
H	-0.78871600	-1.29597400	-0.44495000
C	-2.59341400	-0.23155300	-0.01637100
H	-0.81863500	1.69944300	0.26179800
C	3.38975400	-0.32515500	0.00375900
H	3.85663300	-0.65430300	0.94215500
H	3.73197500	-1.02059400	-0.77534600
H	3.76874000	0.67327200	-0.23880700
N	-3.75321300	-0.18304800	0.09101100

Transition state

C	-1.14500400	1.16983700	-0.17927900
C	0.17962700	1.40258000	0.07066700
C	0.69916500	0.11312500	0.46699400
H	0.75901100	2.31738300	-0.03433900
H	0.32197900	-0.33448100	1.38049300
C	-1.25498000	-0.25271400	-0.37112100
H	-1.98153600	1.86730400	-0.14904300
H	-0.70932500	-0.66891000	-1.21225900
C	-2.40442800	-1.08983900	0.11691300
H	-3.22345700	-1.06592100	-0.62022500
H	-2.11025400	-2.14006800	0.22365700
H	-2.80318700	-0.73792400	1.07390200
C	2.00101900	-0.34767800	0.08796900
N	3.04205500	-0.74417800	-0.25929100

Cyclobutene (Starting material)

C	-1.13005200	1.17161700	-0.44730900
C	-0.08082400	1.51268400	0.31228400
C	0.37711100	0.07080900	0.52812100
H	0.33344900	2.44900100	0.67333900
H	0.24505000	-0.29558000	1.55393700
C	-0.84210600	-0.32252400	-0.41806500
H	-1.92341400	1.74256800	-0.92274300
H	-0.48841900	-0.71209700	-1.38078900
C	-1.89118700	-1.25579700	0.17933700
H	-2.76691800	-1.31969800	-0.47798200
H	-1.49117200	-2.26931100	0.30321400
H	-2.23158900	-0.89631700	1.15818800
C	1.71467800	-0.29097600	0.06329200
N	2.77675500	-0.57335000	-0.31616000



Butadiene (Product)

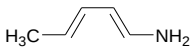
C	0.10709900	0.75869100	-0.05395000
C	1.56249700	0.72206800	-0.13712700
C	2.34360900	-0.34313400	0.13086600
H	2.03908800	1.66366100	-0.40868900
H	1.87819100	-1.27303600	0.46035100
C	-0.71578500	-0.30236200	-0.11465200
H	-0.43598900	-1.33559900	-0.26816400
H	-0.36125000	1.73531000	0.04868700
C	3.83765400	-0.35231400	0.03860600
H	4.28842700	-0.60650500	1.00766800
H	4.17713400	-1.11823600	-0.67253800
H	4.23290600	0.61632900	-0.28427300
N	-2.15095400	-0.14245200	0.00902100
O	-2.81745700	-1.18314200	-0.05711100
O	-2.62907700	0.98533600	0.16603000

Transition state

C	1.51780300	1.20388300	-0.07792900
C	0.18816300	1.40682800	-0.34215500
C	-0.31846300	0.07402700	-0.46664500
H	-0.37976200	2.32694900	-0.44277300
H	-0.03107700	-0.58819500	-1.27282900
C	1.61950700	-0.14268900	0.41379200
H	2.36395300	1.85487600	-0.29368800
H	1.07833600	-0.36726000	1.32775500
C	2.74564800	-1.08380600	0.09663200
H	3.21278000	-0.86997400	-0.86962900
H	3.51900100	-1.01911000	0.87816700
H	2.39412000	-2.12226200	0.09440300
N	-1.66484500	-0.25218700	-0.00896900
O	-2.27340400	0.59972400	0.64978400
O	-2.10401900	-1.37462100	-0.28738300

Cyclobutene (Starting material)

C	-1.49749700	1.21889300	-0.24102900
C	-0.45221100	1.50860800	0.54825100
C	0.04870900	0.08965400	0.57194400
H	-0.08757900	2.40572700	1.03663000
H	0.00321800	-0.46184400	1.51292600
C	-1.11910800	-0.24393800	-0.44251700
H	-2.33895700	1.79964300	-0.61003300
H	-0.72139500	-0.44522000	-1.44567300
C	-2.10641300	-1.33233400	-0.03319700
H	-2.96097200	-1.34986800	-0.72065600
H	-1.63340700	-2.32064400	-0.05990600
H	-2.49229000	-1.16005000	0.97880900
N	1.42848000	-0.17665800	0.01717600
O	1.88816800	-1.30225300	0.21016800
O	1.98572400	0.71769900	-0.61429700



Butadiene (Product)

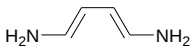
C	-0.75886200	0.73702600	0.06324600
C	0.70037000	0.71345000	-0.06343200
C	1.52423000	-0.32633300	0.16763600
H	1.15458300	1.65885300	-0.37033700
H	1.10513200	-1.26393200	0.53788400
C	-1.57373000	-0.32296400	-0.12542100
H	-1.21014100	1.70390600	0.29391400
H	-1.16407400	-1.28117900	-0.43794000
N	-2.96593400	-0.30789900	-0.05356700
H	-3.40878200	-1.19546300	0.14571700
H	-3.37617500	0.45094300	0.47874900
C	3.01263100	-0.30274100	-0.03999200
H	3.35531600	0.68584300	-0.36766200
H	3.55196100	-0.56097300	0.88256600
H	3.32589000	-1.03332500	-0.80014600

Transition state

C	0.74474700	1.19651000	0.10799200
C	-0.61250300	1.21743900	-0.09368400
C	-0.98359900	-0.14558000	-0.36139000
H	-1.29746000	2.05664800	0.04624400
H	-0.59497700	-0.57058900	-1.28380100
C	1.03453100	-0.19195000	0.36704800
H	1.48524800	1.99262400	0.02626300
H	0.67302200	-0.62432900	1.29362500
N	2.19829700	-0.79768700	-0.10217700
H	2.45014300	-0.61451700	-1.06585200
H	2.36092700	-1.76026800	0.16522700
C	-2.27924300	-0.76265100	0.11679800
H	-3.14323700	-0.36731900	-0.44379100
H	-2.28042200	-1.85060100	-0.02236400
H	-2.46492400	-0.56045100	1.17910600

Cyclobutene (Starting material)

C	0.67108700	1.28325300	0.31672200
C	-0.50606800	1.34321400	-0.32246200
C	-0.67647700	-0.16736100	-0.41467900
H	-1.13665000	2.16679600	-0.65241600
H	-0.53132800	-0.55073800	-1.43293900
C	0.68419200	-0.23443200	0.38817200
H	1.37510800	2.03189100	0.67387100
H	0.52555000	-0.61805600	1.41187400
N	1.79028700	-0.89014400	-0.31248800
H	2.68324100	-0.62309500	0.09974000
H	1.71955600	-1.90392800	-0.23098000
C	-1.91502600	-0.79294200	0.22480500
H	-1.84484300	-1.88852200	0.23929200
H	-2.04740300	-0.44662200	1.25765700
H	-2.82148800	-0.52711700	-0.33402900



Butadiene (Product)

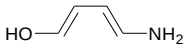
C	-0.72591400	0.74478200	0.09238500
C	0.73026700	0.74580600	-0.05810100
C	1.53810300	-0.30484900	0.19631100
H	1.18580600	1.67491000	-0.41043100
H	1.13171900	-1.21962100	0.62553100
C	-1.53428500	-0.30197500	-0.17842100
H	-1.18283400	1.67683400	0.43348700
H	-1.12625300	-1.21192500	-0.61326500
N	-2.92940100	-0.31681200	-0.04832800
H	-3.33963500	-1.23146300	0.09359400
H	-3.31214700	0.36273100	0.59980900
N	2.90051100	-0.39323000	-0.12420100
H	3.32635300	0.48598600	-0.40116200
H	3.47019800	-0.86973600	0.56710200

Transition state

C	0.67777600	1.20036100	0.12904100
C	-0.67458300	1.21031600	-0.10870000
C	-0.97938300	-0.17615000	-0.36395900
H	-1.39394700	2.02471400	-0.01399600
H	-0.63799600	-0.60071000	-1.30283800
C	0.97661100	-0.19056400	0.36887300
H	1.40367600	2.01103800	0.03390800
H	0.64468700	-0.63428100	1.30225400
N	2.10207800	-0.83617700	-0.17868400
H	2.65401700	-0.28477700	-0.82598400
H	2.67803700	-1.38305100	0.45181800
N	-2.18967200	-0.74762800	0.08081000
H	-2.32979300	-1.71949400	-0.17006500
H	-2.40805200	-0.59057400	1.05849900

Cyclobutene (Starting material)

C	0.61331200	1.31588300	0.27704500
C	-0.59415600	1.32430700	-0.30762800
C	-0.68826900	-0.20111800	-0.38524600
H	-1.26818800	2.11745500	-0.62681300
H	-0.55184300	-0.58880000	-1.40069300
C	0.68381800	-0.20012100	0.38744600
H	1.31369100	2.09454800	0.56995300
H	0.54022700	-0.56150400	1.42048800
N	1.79527200	-0.84920800	-0.30864800
H	2.68232000	-0.61311500	0.13458800
H	1.69904300	-1.86287900	-0.25468900
N	-1.77491500	-0.94284900	0.24344300
H	-2.60390200	-0.95518200	-0.34733100
H	-2.04207200	-0.51983400	1.13123600



Butadiene (Product)

C	-0.74366800	0.75242100	0.09219400
C	0.71064100	0.75515500	-0.06427400
C	1.51166700	-0.30227700	0.18710900
H	1.16594200	1.68518900	-0.41152800
H	1.09801300	-1.21321100	0.61685700
C	-1.53662000	-0.29315900	-0.18991700
H	-1.21938500	1.66093500	0.46211000
H	-1.15879600	-1.21018100	-0.64059000
O	-2.88153200	-0.27803800	0.11229100
H	-3.33592500	-0.97189800	-0.38668400
N	2.87179200	-0.39616700	-0.12183700
H	3.31369600	0.47780100	-0.38826900
H	3.43404600	-0.90400700	0.55196800

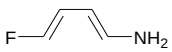
Transition state

C	-0.64732000	1.20405200	-0.10170300

C	0.71592900	1.18728400	0.08514500
C	0.98482200	-0.19527500	0.33323100
H	1.45043500	1.98229300	-0.03564600
H	0.66538400	-0.63661100	1.27365300
C	-0.98017400	-0.17064400	-0.36972300
H	-1.35717700	2.02001900	0.04604800
H	-0.65091900	-0.60650100	-1.30667400
N	-2.10138100	-0.80704900	0.17926800
H	-2.64450200	-0.27162900	0.84613900
H	-2.67273900	-1.37473500	-0.43544500
O	2.14034300	-0.75494900	-0.19906600
H	2.35689400	-1.57641200	0.26787700

Cyclobutene (Starting material)

C	-0.53121700	1.34299700	-0.27868000
C	0.69298400	1.27875400	0.26990800
C	0.69334100	-0.23015900	0.37142300
H	1.43632000	2.01626000	0.55859300
H	0.56862600	-0.61003600	1.39670900
C	-0.69116900	-0.17553100	-0.38918100
H	-1.19159800	2.16720300	-0.54105500
H	-0.57261800	-0.54853900	-1.41207900
N	-1.80002700	-0.88784800	0.23122000
H	-2.06719800	-0.45997900	1.11646200
H	-2.62417300	-0.89352900	-0.36579300
O	1.79250300	-0.86623300	-0.26228700
H	1.72716400	-1.82295000	-0.11390300



Butadiene (Product)

C	-0.68615100	0.74432700	0.08045600
C	0.76681500	0.70959100	-0.09719200
C	1.54296100	-0.33443000	0.20471300
H	1.25690600	1.60020800	-0.49082000
H	1.23795800	-1.26467000	0.67189400

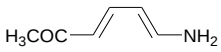
C	-1.50957500	-0.29750500	-0.16649700
H	-1.11660900	1.69285200	0.40488500
H	-1.11176500	-1.22106400	-0.58180500
N	-2.89406900	-0.29348900	-0.03371500
H	-3.33923400	-1.19626700	0.06189300
H	-3.28900600	0.40203100	0.58811900
F	2.88177000	-0.32117400	-0.06078200

Transition state

C	-0.60768100	1.19944100	-0.08627300
C	0.76006800	1.13758800	0.06768700
C	0.98597000	-0.23889600	0.33068400
H	1.51215900	1.91538300	-0.05258300
H	0.70876400	-0.69941800	1.27303500
C	-1.01037200	-0.15006600	-0.37307700
H	-1.28609200	2.03293600	0.09423900
H	-0.69047100	-0.58836400	-1.31118400
N	-2.20526700	-0.67669200	0.10441800
H	-2.43910300	-0.49385000	1.07228100
H	-2.45303600	-1.61252300	-0.18952600
F	2.14630400	-0.83396900	-0.13903500

Cyclobutene (Starting material)

C	0.45939000	1.33646200	0.27338000
C	-0.76054600	1.23587800	-0.27740800
C	-0.68227900	-0.26373000	-0.38824500
H	-1.52022400	1.95055800	-0.57918100
H	-0.58537100	-0.67898800	-1.39532200
C	0.67836000	-0.16581200	0.38658000
H	1.09882500	2.17763000	0.53054600
H	0.55276700	-0.53908500	1.41488900
N	1.84385200	-0.70238500	-0.31077200
H	2.69879900	-0.25480900	0.01486700
H	1.94470400	-1.70140400	-0.13775600
F	-1.69622400	-0.98822100	0.26239100



Butadiene (Product)

C	-1.62941100	0.75423900	-0.06146200
C	-0.18256900	0.71747700	-0.03928200
C	0.63623800	-0.36719300	-0.07215500
H	0.28665100	1.69959100	0.00793700
H	0.23760500	-1.37658900	-0.15579700
C	-2.44147100	-0.32779400	0.07226300
H	-2.08985300	1.73455000	-0.18244500
H	-2.02011000	-1.31653500	0.23765300
N	-3.80980200	-0.32166000	-0.02779100
H	-4.33043000	-1.08511000	0.38008300
H	-4.29396700	0.56730900	-0.03176100
C	2.10192300	-0.31994100	-0.00814100
O	2.75497300	-1.36458700	-0.02904400
C	2.82005700	1.02253400	0.08364300
H	2.53842200	1.56230700	0.99623900
H	3.89681300	0.84063900	0.09598000
H	2.57509600	1.66622000	-0.77019600

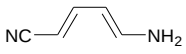
Transition state

C	-1.73277600	-1.08476100	-0.08758200
C	-0.46958900	-1.40218800	-0.46613200
C	0.25237400	-0.13636200	-0.51021700
H	-0.04131500	-2.38735900	-0.63918900
H	-0.01366400	0.55903900	-1.30420800
C	-1.61784300	0.27044300	0.44017600
H	-2.66007100	-1.65420900	-0.14001600
H	-1.11416900	0.40736000	1.39098000
N	-2.54793900	1.23688400	0.16397900
H	-2.99032200	1.24637900	-0.74598700
H	-2.48513600	2.13869700	0.61732400
C	1.60452400	-0.00597700	0.04053800
C	2.39024100	1.25797900	-0.28686400
H	3.15588900	1.42834900	0.47467000

H	2.89274400	1.13317700	-1.25599300
H	1.74028700	2.13771500	-0.36651300
O	2.09871800	-0.88276700	0.75519600

Cyclobutene (Starting material)

C	0.55445000	1.39892000	-0.71149800
C	1.56191300	1.20492200	0.15070200
C	1.17038200	-0.22777800	0.46914600
H	2.37712300	1.82708300	0.51207900
H	0.75931000	-0.34775900	1.48690000
C	0.01792700	-0.02146200	-0.61137000
H	0.22931200	2.25307000	-1.30094500
H	0.20725700	-0.64704400	-1.48943300
C	-1.39239800	-0.30235200	-0.11436200
O	-1.91496700	-1.38412100	-0.33553200
C	-2.10330200	0.77412600	0.68208300
H	-1.45876600	1.16588200	1.47858900
H	-2.34121100	1.62333200	0.02743000
H	-3.02786800	0.37579600	1.10576200
N	2.14239100	-1.25282900	0.10502400
H	1.75177600	-2.18362100	0.24779300
H	2.97222400	-1.18222300	0.69270300



Butadiene (Product)

C	1.11938600	0.75430000	-0.02198900
C	-0.32542400	0.73314700	0.02104700
C	-1.14984800	-0.33769100	-0.13401700
H	-0.79926800	1.69849000	0.19366600
H	-0.76767100	-1.32848700	-0.36859400
C	1.91847400	-0.34052100	0.07993900
H	1.58670100	1.73335500	-0.12055800
H	1.48661400	-1.32443400	0.25009600
N	3.28343100	-0.35458000	-0.05207600
C	-2.56268100	-0.23074000	-0.01361200

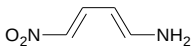
N	-3.72463300	-0.16794700	0.07788600
H	3.80350600	-1.12004600	0.35328800
H	3.77909200	0.52784100	-0.07676400

Transition state

C	-1.19716900	1.12843700	-0.22490400
C	0.09720000	1.39335700	0.09275600
C	0.65566700	0.10553500	0.48513000
H	0.63692600	2.33581300	0.01905900
H	0.32203000	-0.31758100	1.42859000
C	-1.24015700	-0.31901600	-0.38307500
H	-2.05451400	1.79333100	-0.31779700
H	-0.75146100	-0.75349300	-1.24803100
N	-2.27569500	-1.07204800	0.10182300
H	-2.71296400	-0.80419200	0.97407300
H	-2.31377200	-2.06093600	-0.10670600
C	1.96684300	-0.30614300	0.09686600
N	3.01561800	-0.67166100	-0.26608400

Cyclobutene (Starting material)

C	-1.19532600	1.11119900	-0.42578300
C	-0.13199700	1.50037600	0.28798900
C	0.37583300	0.08142200	0.53123200
H	0.26922800	2.46049800	0.59779000
H	0.23785000	-0.27671100	1.55719600
C	-0.84736000	-0.36600700	-0.39085200
H	-2.02311900	1.64237000	-0.88815400
H	-0.48858700	-0.74885900	-1.35854000
N	-1.81030900	-1.23323600	0.27101900
H	-2.75027300	-1.07682800	-0.08638600
H	-1.58779400	-2.21683900	0.12957900
C	1.71978900	-0.25046700	0.06420000
N	2.78417400	-0.51573200	-0.32133300



Butadiene (Product)

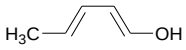
C	1.57609700	0.75149900	-0.02943200
C	0.13813400	0.74495500	-0.01630600
C	-0.69829400	-0.32032100	-0.03318500
H	-0.34661100	1.71837700	0.00804000
H	-0.42701300	-1.36587300	-0.07962100
C	2.36741400	-0.35777100	0.03504000
H	2.05471800	1.72745600	-0.08763400
H	1.92692800	-1.34833500	0.11965500
N	3.72692100	-0.36663500	-0.02116800
H	4.24781400	0.50012300	-0.01257700
H	4.24476900	-1.20435900	0.19626300
N	-2.12083200	-0.13995300	0.00246300
O	-2.59994500	1.00245900	0.05118300
O	-2.80547200	-1.17639000	-0.01991900

Transition state

C	1.56169900	1.16032900	-0.04603600
C	0.26943900	1.37714900	-0.40237300
C	-0.29176600	0.04680800	-0.50266200
H	-0.25322400	2.31669000	-0.56063100
H	-0.05091300	-0.60855600	-1.33078000
C	1.58596700	-0.21527100	0.43950300
H	2.43314600	1.80894500	-0.11484600
H	1.09327800	-0.43585500	1.38017000
N	2.58456400	-1.08346600	0.12105700
H	3.04862000	-1.00807000	-0.77492000
H	2.61764200	-1.99809100	0.55140300
N	-1.61987600	-0.21258200	-0.01573000
O	-2.15323000	0.64656500	0.70683500
O	-2.14594500	-1.29866700	-0.30912100

Cyclobutene (Starting material)

C	-1.53037900	1.17028500	-0.28915000
C	-0.46736600	1.52373300	0.44795600
C	0.04409700	0.11429400	0.56224000
H	-0.09701700	2.45885300	0.85277400
H	-0.01710800	-0.38395100	1.53102200
C	-1.13125200	-0.29216900	-0.41367300
H	-2.39059700	1.71183200	-0.67348200
H	-0.74014800	-0.54776400	-1.41129700
N	-2.06178700	-1.26781500	0.13092200
H	-2.98492800	-1.16008400	-0.28475700
H	-1.74943100	-2.21889200	-0.05715400
N	1.42409100	-0.17830800	0.02697100
O	2.07804500	0.74782900	-0.44624100
O	1.79101800	-1.35207900	0.08291700



Butadiene (Product)

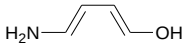
C	-0.77624600	0.74210400	0.07351500
C	0.68114800	0.72021800	-0.08265700
C	1.49991600	-0.31373300	0.18424800
H	1.12907900	1.64971700	-0.44130000
H	1.07759500	-1.22475900	0.61179700
C	-1.57660500	-0.31066500	-0.15078800
H	-1.24277400	1.68170000	0.36764800
H	-1.19907500	-1.26284700	-0.52076900
O	-2.92752200	-0.25056500	0.08972200
H	-3.36646300	-1.02135200	-0.29741600
C	2.98492100	-0.31360500	-0.04484300
H	3.33129400	0.65148300	-0.43227200
H	3.53282400	-0.52562800	0.88388900
H	3.27889300	-1.08970300	-0.76620500

Transition state

C	0.78584000	1.17388600	0.07882500
C	-0.58322700	1.22059300	-0.06208900
C	-0.98397200	-0.12196600	-0.36076700
H	-1.25154300	2.05825700	0.14453200
H	-0.60069500	-0.53802400	-1.28829900
C	1.03729900	-0.20865400	0.33041600
H	1.54172500	1.94857000	-0.03757600
H	0.69289600	-0.65699700	1.25726100
O	2.15536200	-0.80217900	-0.21305100
H	2.37160000	-1.61936600	0.26309200
C	-2.27654100	-0.74019800	0.12149500
H	-3.12747900	-0.41002000	-0.49646300
H	-2.24376600	-1.83442400	0.05394300
H	-2.50202600	-0.47253200	1.16063600

Cyclobutene (Starting material)

C	0.74764100	1.25079800	0.30601500
C	-0.44915500	1.36061400	-0.29139900
C	-0.67576800	-0.14157900	-0.41643600
H	-1.06983900	2.21095400	-0.56629500
H	-0.54502300	-0.50574600	-1.44368100
C	0.69467200	-0.25748500	0.37205300
H	1.49363900	1.96060200	0.65279200
H	0.55661700	-0.65699400	1.38913200
O	1.78629500	-0.90569900	-0.26787500
H	1.71623600	-1.86254400	-0.12407000
C	-1.92938400	-0.74530100	0.21442300
H	-1.89502100	-1.84256900	0.19783900
H	-2.04335800	-0.42436900	1.25779900
H	-2.83164800	-0.43602500	-0.32844800



Butadiene (Product)

C	-0.74366800	0.75242100	0.09219400
C	0.71064100	0.75515500	-0.06427400

C	1.51166700	-0.30227700	0.18710900
H	1.16594200	1.68518900	-0.41152800
H	1.09801300	-1.21321100	0.61685700
C	-1.53662000	-0.29315900	-0.18991700
H	-1.21938500	1.66093500	0.46211000
H	-1.15879600	-1.21018100	-0.64059000
O	-2.88153200	-0.27803800	0.11229100
H	-3.33592500	-0.97189800	-0.38668400
N	2.87179200	-0.39616700	-0.12183700
H	3.31369600	0.47780100	-0.38826900
H	3.43404600	-0.90400700	0.55196800

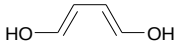
Transition state

C	-0.64732000	1.20405200	-0.10170300
C	0.71592900	1.18728400	0.08514500
C	0.98482200	-0.19527500	0.33323100
H	1.45043500	1.98229300	-0.03564600
H	0.66538400	-0.63661100	1.27365300
C	-0.98017400	-0.17064400	-0.36972300
H	-1.35717700	2.02001900	0.04604800
H	-0.65091900	-0.60650100	-1.30667400
N	-2.10138100	-0.80704900	0.17926800
H	-2.64450200	-0.27162900	0.84613900
H	-2.67273900	-1.37473500	-0.43544500
O	2.14034300	-0.75494900	-0.19906600
H	2.35689400	-1.57641200	0.26787700

Cyclobutene (Starting material)

C	0.69276400	1.27877100	0.27000500
C	-0.53133300	1.34282500	-0.27882900
C	-0.69111900	-0.17563200	-0.38926600
H	-1.19175400	2.16692800	-0.54146600
H	-0.57283700	-0.54894400	-1.41211300
C	0.69339100	-0.23016600	0.37144300
H	1.43579300	2.01644700	0.55902300
H	0.56860100	-0.61022700	1.39663300
O	1.79267400	-0.86596800	-0.26233400

H	1.72790100	-1.82265400	-0.11354800
N	-1.79997100	-0.88781800	0.23138000
H	-2.62393100	-0.89443400	-0.36587600
H	-2.06758400	-0.45943800	1.11624400



Butadiene (Product)

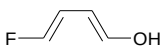
C	0.71643700	0.74507100	-0.09459800
C	-0.73750300	0.72177500	0.08782400
C	-1.52183700	-0.33206300	-0.19763100
H	-1.20374700	1.63428100	0.46763200
H	-1.14843200	-1.24101300	-0.65854000
C	1.52665000	-0.28435400	0.19355500
H	1.16868400	1.65612800	-0.48577700
H	1.16395300	-1.20099200	0.65702800
O	2.86762000	-0.24871200	-0.10835000
H	3.32804800	-0.96403200	0.35322700
O	-2.87055300	-0.42261200	0.01759400
H	-3.18752800	0.38364900	0.45758000

Transition state

C	-0.68694000	1.18079100	-0.06025100
C	0.68702100	1.18076200	0.06023600
C	1.00140000	-0.18223400	0.33425100
H	1.40396700	1.98029900	-0.11854600
H	0.69611400	-0.62005500	1.27988300
C	-1.00145400	-0.18216100	-0.33432000
H	-1.40384300	1.98035300	0.11860600
H	-0.69605500	-0.62019100	-1.27981400
O	-2.14849700	-0.72986500	0.21419300
H	-2.42127200	-1.51255200	-0.28911400
O	2.14853100	-0.72983800	-0.21407800
H	2.42066300	-1.51317300	0.28856600

Cyclobutene (Starting material)

C	-0.68694000	1.18079100	-0.06025100
C	0.68702100	1.18076200	0.06023600
C	1.00140000	-0.18223400	0.33425100
H	1.40396700	1.98029900	-0.11854600
H	0.69611400	-0.62005500	1.27988300
C	-1.00145400	-0.18216100	-0.33432000
H	-1.40384300	1.98035300	0.11860600
H	-0.69605500	-0.62019100	-1.27981400
O	-2.14849700	-0.72986500	0.21419300
H	-2.42127200	-1.51255200	-0.28911400
O	2.14853100	-0.72983800	-0.21407800
H	2.42066300	-1.51317300	0.28856600



Butadiene (Product)

C	-0.70362300	0.74663100	0.09016500
C	0.74777900	0.71505800	-0.10590700
C	1.51881800	-0.32990500	0.20302200
H	1.23272700	1.60094200	-0.51453900
H	1.20885900	-1.24977600	0.68726100
C	-1.51296900	-0.28908400	-0.17862400
H	-1.14978300	1.66863000	0.45989800
H	-1.14735100	-1.21263700	-0.62529200
O	-2.85292300	-0.24225900	0.10497500
H	-3.30838500	-0.98412000	-0.31820300
F	2.85414300	-0.32679600	-0.06453900

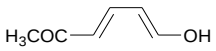
Transition state

C	-0.64660400	1.17812000	-0.05940500
C	0.73190600	1.14076900	0.03840700
C	0.98952600	-0.21804400	0.33429500
H	1.46907100	1.92005700	-0.14264700
H	0.70911300	-0.67666300	1.27525100
C	-1.01465400	-0.16726100	-0.34012800

H	-1.33771200	1.99086800	0.15454500
H	-0.70905100	-0.62621100	-1.27440600
O	-2.16192500	-0.67922700	0.21493600
H	-2.45190500	-1.46868300	-0.26850200
F	2.13942700	-0.81189500	-0.14475000

Cyclobutene (Starting material)

C	-0.52583200	1.31846400	-0.26536800
C	0.71385300	1.25446500	0.24943500
C	0.68176200	-0.24421700	0.39039300
H	1.47024700	1.99040400	0.50283300
H	0.60406800	-0.64289100	1.40612800
C	-0.69324800	-0.18225500	-0.37050500
H	-1.20270300	2.13093000	-0.51255800
H	-0.59913000	-0.57463400	-1.39170000
O	-1.84333000	-0.69344400	0.27758100
H	-1.95903200	-1.62678600	0.04015600
F	1.70821900	-0.95646800	-0.25436000



Butadiene (Product)

C	0.20019200	0.70630900	-0.06129500
C	1.65445100	0.71397300	-0.10936100
C	2.44419000	-0.35733100	0.11515400
H	2.12950500	1.67427400	-0.31445900
H	2.05985000	-1.33637200	0.38241300
C	-0.62431800	-0.36775200	-0.10392000
H	-0.25132100	1.69505700	0.00904600
H	-0.23492500	-1.37736200	-0.21966400
C	-2.09460500	-0.30862500	-0.01161100
O	-2.74887300	-1.34904400	-0.04320500
C	-2.79745900	1.03617400	0.12097900
H	-2.49352400	1.55281900	1.03968200
H	-2.55982800	1.69490000	-0.72337000
H	-3.87557400	0.86518500	0.14837800

O	3.79788600	-0.37624100	0.06472300
H	4.13900700	0.49728800	-0.19384600

Transition state

C	-0.47655800	-1.38695800	-0.43647900
C	-1.76430100	-1.04333900	-0.14298800
C	-1.64409900	0.28212900	0.40256800
H	-2.70050400	-1.57978900	-0.28133300
H	-1.14900800	0.42617400	1.35794100
C	0.25182100	-0.13765400	-0.49341600
H	-0.04200600	-2.37882900	-0.53632100
H	-0.01784100	0.55977500	-1.28297800
C	1.61771900	-0.01173500	0.05131600
O	2.09802300	-0.88545500	0.77329400
C	2.41054000	1.23634600	-0.30497400
H	2.75673800	1.16936500	-1.34547900
H	1.79241900	2.13969300	-0.23006500
H	3.28089100	1.32609000	0.34940700
O	-2.56790000	1.22680100	0.07851700
H	-2.53240600	1.97401600	0.69816700

Cyclobutene (Starting material)

C	0.58641700	1.41087900	-0.65475500
C	1.61419000	1.15925900	0.16968800
C	1.18447600	-0.25923600	0.46008300
H	2.45677600	1.73902600	0.53540300
H	0.79145800	-0.41247900	1.47652300
C	0.01964400	-0.00102900	-0.61147700
H	0.25732200	2.30332800	-1.18111400
H	0.20891400	-0.59859800	-1.50881200
C	-1.39048600	-0.28954000	-0.12568700
O	-1.88452800	-1.39176700	-0.31176900
C	-2.12938800	0.79655600	0.63043200
H	-1.51444900	1.18915600	1.45035000
H	-2.33624100	1.64362500	-0.03729700
H	-3.07081100	0.40529800	1.02213700
O	2.14774800	-1.23990900	0.14572400

H	1.79215300	-2.11727800	0.36147100

Butadiene (Product)

C	-1.13957700	0.75048200	0.05428100
C	0.30990300	0.74326400	-0.03133500
C	1.13120400	-0.31396100	0.18548400
H	0.77229400	1.69570500	-0.28614200
H	0.74834600	-1.27748500	0.51401300
C	-1.91851800	-0.33616900	-0.10728400
H	-1.62928300	1.70759600	0.21991200
H	-1.51420900	-1.31533400	-0.35919200
O	-3.26967200	-0.25978700	0.02567800
H	-3.68547200	-1.09569700	-0.23207000
C	2.54299700	-0.23034400	0.01752600
N	3.70137800	-0.18801700	-0.11056800

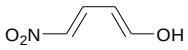
Transition state

C	-1.23442800	1.09977100	-0.18547000
C	0.08036600	1.38089800	0.05652400
C	0.65675900	0.12204000	0.47969300
H	0.61946700	2.31367800	-0.09485900
H	0.31688900	-0.29982500	1.42030600
C	-1.25542300	-0.32916200	-0.34379800
H	-2.10775000	1.74701800	-0.21332100
H	-0.76684900	-0.78217500	-1.20073000
O	-2.27550500	-1.04558900	0.19349800
H	-2.31293100	-1.93894500	-0.18635700
C	1.97132400	-0.28967800	0.09214600
N	3.02051900	-0.65403700	-0.26679800

Cyclobutene (Starting material)

C	-1.26588800	1.06441900	-0.41164800
C	-0.18870700	1.49987400	0.25539500
C	0.36717400	0.10429300	0.53043500

H	0.20106800	2.47856200	0.51668300
H	0.23826900	-0.23103600	1.56533600
C	-0.85825600	-0.38950300	-0.37538300
H	-2.12906700	1.55081500	-0.85487500
H	-0.51662900	-0.78634300	-1.34044000
O	-1.79542400	-1.24800800	0.23127800
H	-1.53848800	-2.17139200	0.07908100
C	1.71761300	-0.20980000	0.07077400
N	2.78237400	-0.46746400	-0.31906400



Butadiene (Product)

C	1.59481500	0.74008900	-0.11571000
C	0.14870800	0.75488800	-0.05357300
C	-0.67988000	-0.30765100	-0.10627400
H	-0.32562100	1.72980800	0.03408900
H	-0.40702000	-1.34420600	-0.24933500
C	2.36398000	-0.34638900	0.10357600
H	2.09612000	1.68299100	-0.31962800
H	1.95022800	-1.31539200	0.37800600
O	3.71341400	-0.27683500	0.00568000
H	4.12140300	-1.11685400	0.26369000
N	-2.10912400	-0.13994800	0.00859400
O	-2.78336600	-1.17783200	-0.05296200
O	-2.58467000	0.99187500	0.15539400

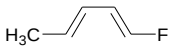
Transition state

C	1.59675500	1.12105400	-0.08698500
C	0.27960200	1.36400200	-0.36068900
C	-0.29080900	0.05329600	-0.48830100
H	-0.24771600	2.31000000	-0.44175200
H	-0.04307000	-0.60571600	-1.31057400
C	1.61513300	-0.22974800	0.40342700
H	2.47832500	1.73845700	-0.23977800
H	1.12561700	-0.47180500	1.34153000

O	2.61488300	-1.05961600	0.03127800
H	2.64301900	-1.85178000	0.59363400
N	-1.63604100	-0.20530200	-0.01102600
O	-2.15297000	-1.28981000	-0.31122700
O	-2.17540900	0.65771800	0.69612400

Cyclobutene (Starting material)

C	-1.60180600	1.10707200	-0.24640500
C	-0.53205000	1.49403700	0.46601900
C	0.03724900	0.10581400	0.56988200
H	-0.18066800	2.44216700	0.85653600
H	-0.01004900	-0.40547100	1.53221700
C	-1.13745800	-0.32248900	-0.41274900
H	-2.49592500	1.60776500	-0.60417500
H	-0.76037800	-0.56029800	-1.41682100
O	-2.03906200	-1.29812700	0.04427800
H	-1.71560300	-2.18014700	-0.20025700
N	1.42250500	-0.13502700	0.03047100
O	2.00121800	0.79315600	-0.52930400
O	1.86402800	-1.27820900	0.15486700



Butadiene (Product)

C	-0.79839200	0.70680400	0.09119700
C	0.65963600	0.71537100	-0.08561500
C	1.49099100	-0.30555400	0.18492300
H	1.08428700	1.65068600	-0.45507700
H	1.07931600	-1.21903500	0.61709600
C	-1.57437100	-0.34609200	-0.17065100
H	-1.28134800	1.62269300	0.42948700
H	-1.26151100	-1.30153000	-0.57807200
F	-2.91620700	-0.30808300	0.04827200
C	2.97491200	-0.28765000	-0.04337300
H	3.31009900	0.67540000	-0.44445300
H	3.52238200	-0.48047900	0.88940500

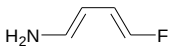
H	3.27598300	-1.07226600	-0.75172300

Transition state

C	0.82982900	1.13499700	0.05492400
C	-0.54486900	1.21743800	-0.05786400
C	-0.99112400	-0.10309200	-0.36731700
H	-1.18841400	2.06108400	0.19362100
H	-0.61430800	-0.53641500	-1.28867800
C	1.01923900	-0.24109400	0.32732800
H	1.60610400	1.88703800	-0.06724800
H	0.69879900	-0.70994600	1.24981800
F	2.13888800	-0.88685600	-0.14447800
C	-2.28863200	-0.69721800	0.12397900
H	-3.09723000	-0.53006400	-0.60437600
H	-2.19910100	-1.78360600	0.24707100
H	-2.60249000	-0.27257200	1.08378600

Cyclobutene (Starting material)

C	0.83483900	1.20429200	0.29847900
C	-0.35943100	1.37184400	-0.29298600
C	-0.66617400	-0.11997800	-0.40928600
H	-0.94131800	2.25087100	-0.56158100
H	-0.54539000	-0.49892800	-1.43155300
C	0.67597900	-0.29202000	0.38417800
H	1.61513500	1.87486200	0.64575900
H	0.56578000	-0.71565100	1.38885500
F	1.66138800	-1.06077700	-0.26054000
C	-1.95093200	-0.65926100	0.21627300
H	-1.95890600	-1.75605200	0.21279400
H	-2.06280200	-0.31970400	1.25369500
H	-2.83068500	-0.31767000	-0.34305800



Butadiene (Product)

C	-0.68615100	0.74432700	0.08045600
C	0.76681500	0.70959100	-0.09719200
C	1.54296100	-0.33443000	0.20471300
H	1.25690600	1.60020800	-0.49082000
H	1.23795800	-1.26467000	0.67189400
C	-1.50957500	-0.29750500	-0.16649700
H	-1.11660900	1.69285200	0.40488500
H	-1.11176500	-1.22106400	-0.58180500
N	-2.89406900	-0.29348900	-0.03371500
H	-3.33923400	-1.19626700	0.06189300
H	-3.28900600	0.40203100	0.58811900
F	2.88177000	-0.32117400	-0.06078200

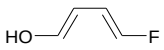
Transition state

C	0.76033800	1.13749000	0.06777700
C	-0.60745600	1.19961900	-0.08617400
C	-1.01034900	-0.14978400	-0.37309600
H	-1.28579300	2.03307100	0.09480500
H	-0.69032400	-0.58803500	-1.31116900
C	0.98575100	-0.23906600	0.33062900
H	1.51269400	1.91489900	-0.05334700
H	0.70877300	-0.69904700	1.27332300
F	2.14610300	-0.83411400	-0.13902000
N	-2.20554500	-0.67660000	0.10425800
H	-2.45234500	-1.61276700	-0.18945500
H	-2.43882100	-0.49444800	1.07239600

Cyclobutene (Starting material)

C	-0.76046000	1.23578000	-0.27771300
C	0.45926700	1.33645800	0.27355200
C	0.67827800	-0.16585300	0.38665000
H	1.09848400	2.17767200	0.53108100

H	0.55273200	-0.53926800	1.41484800
C	-0.68209600	-0.26379200	-0.38839600
H	-1.52011100	1.95039400	-0.57972300
H	-0.58549900	-0.67945200	-1.39532400
F	-1.69619700	-0.98810500	0.26259000
N	1.84390000	-0.70217100	-0.31083300
H	1.94413000	-1.70140400	-0.13881300
H	2.69880600	-0.25535800	0.01589200



Butadiene (Product)

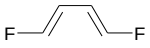
C	-0.70362300	0.74663100	0.09016500
C	0.74777900	0.71505800	-0.10590700
C	1.51881800	-0.32990500	0.20302200
H	1.23272700	1.60094200	-0.51453900
H	1.20885900	-1.24977600	0.68726100
C	-1.51296900	-0.28908400	-0.17862400
H	-1.14978300	1.66863000	0.45989800
H	-1.14735100	-1.21263700	-0.62529200
O	-2.85292300	-0.24225900	0.10497500
H	-3.30838500	-0.98412000	-0.31820300
F	2.85414300	-0.32679600	-0.06453900

Transition state

C	0.73217300	1.14078400	0.03824100
C	-0.64637000	1.17811000	-0.05925900
C	-1.01451900	-0.16730100	-0.33980900
H	-1.33749900	1.99093100	0.15435100
H	-0.70878800	-0.62633000	-1.27401500
C	0.98964900	-0.21798600	0.33439400
H	1.46926300	1.91992500	-0.14373800
H	0.70950300	-0.67591700	1.27578300
F	2.13924700	-0.81217000	-0.14476400
O	-2.16231400	-0.67907700	0.21477200
H	-2.45278100	-1.46810700	-0.26908400

Cyclobutene (Starting material)

C	0.71399300	1.25438000	0.24949600
C	-0.52567000	1.31855200	-0.26534500
C	-0.69323900	-0.18214900	-0.37044100
H	-1.20236600	2.13113900	-0.51263100
H	-0.59900800	-0.57438500	-1.39163900
C	0.68172200	-0.24431700	0.39047700
H	1.47056500	1.99020800	0.50266800
H	0.60411700	-0.64303800	1.40619600
F	1.70799200	-0.95658900	-0.25444200
O	-1.84338300	-0.69334000	0.27751500
H	-1.95900400	-1.62669400	0.04014000



Butadiene (Product)

C	0.72594500	0.70997900	-0.10621600
C	-0.72595100	0.70996900	0.10630900
C	-1.51186700	-0.32441800	-0.19715600
H	-1.18787800	1.60783100	0.51357700
H	-1.21104800	-1.25202000	-0.67293200
C	1.51193300	-0.32430200	0.19746800
H	1.18782000	1.60772100	-0.51381400
H	1.21113100	-1.25182300	0.67335000
F	2.84362600	-0.29663400	-0.06000900
F	-2.84366900	-0.29659600	0.05971900

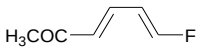
Transition state

C	-0.69224100	1.13966000	-0.03663000
C	0.69200800	1.13966300	0.03644200
C	1.00056600	-0.20369100	0.33965000
H	1.40489900	1.93113200	-0.18184800
H	0.72064900	-0.68332100	1.26924100
C	-1.00064100	-0.20371900	-0.33966900
H	-1.40520000	1.93078100	0.18270300
H	-0.72030000	-0.68339800	-1.26910500
F	-2.15215100	-0.76267000	0.14710600

F	2.15235100	-0.76251600	-0.14707900

Cyclobutene (Starting material)

C	-0.61924700	1.27865100	-0.26208900
C	0.61882500	1.27877200	0.26215500
C	0.67646500	-0.22412500	0.38655300
H	1.33554500	2.05211300	0.51919200
H	0.61126900	-0.64245900	1.39466200
C	-0.67636000	-0.22420500	-0.38646400
H	-1.33611000	2.05185200	-0.51926400
H	-0.61060000	-0.64198800	-1.39460000
F	-1.74333000	-0.85985200	0.26047200
F	1.74353000	-0.85949000	-0.26057500



Butadiene (Product)

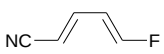
C	1.66677200	0.69961900	-0.18475400
C	0.20864500	0.71734500	-0.09421400
C	-0.61151800	-0.35452200	-0.15560000
H	-0.23014500	1.70761500	0.02014300
H	-0.21885800	-1.35453800	-0.32942000
C	2.42944300	-0.33559800	0.18170900
H	2.16752200	1.59974200	-0.53557800
H	2.09549600	-1.27311600	0.61362500
F	3.77425400	-0.28821700	0.06006300
C	-2.08466800	-0.30802400	-0.01532700
C	-2.78866700	1.02604500	0.17984600
H	-2.57563400	1.71233400	-0.64892700
H	-3.86497500	0.85013900	0.23206300
H	-2.45953400	1.51350100	1.10579800
O	-2.72527500	-1.35386500	-0.05852800

Transition state

C	1.67339000	1.10881300	-0.11225000
C	0.35939200	1.32817700	-0.44617200
C	-0.22900000	0.01915300	-0.55737300
H	-0.16030100	2.28117800	-0.52600700
H	0.16568500	-0.66144700	-1.30582400
C	1.63493900	-0.20760600	0.42851800
H	2.56175700	1.72213100	-0.24154500
H	1.14105300	-0.45564300	1.36015600
F	2.66845800	-1.06263100	0.21119500
C	-1.60156400	-0.34641800	-0.11326400
C	-2.43005100	0.69844200	0.61644400
H	-3.41852100	0.28929000	0.83550800
H	-1.94328400	0.99537000	1.55437500
H	-2.53912100	1.60721900	0.01016500
O	-2.03325300	-1.47722400	-0.31037500

Cyclobutene (Starting material)

C	0.63970700	1.28023900	-0.80003400
C	1.66527300	1.09808100	0.04629400
C	1.17347800	-0.25481500	0.49192000
H	2.51959200	1.69504900	0.35019500
H	0.83134300	-0.33880700	1.52897900
C	0.02986700	-0.10413600	-0.59013800
H	0.32248900	2.11498600	-1.41977900
H	0.18834200	-0.80518600	-1.41479000
C	-1.41042900	-0.24709100	-0.10823900
O	-2.08107300	-1.20571200	-0.45118700
C	-1.96911200	0.82980400	0.80311300
H	-1.27364400	1.07631200	1.61455800
H	-2.12284600	1.75414500	0.22999600
H	-2.92620200	0.50420100	1.21603500
F	2.03742300	-1.32972100	0.27186600



Butadiene (Product)

C	-1.16144100	0.71735600	0.07691500
C	0.29246500	0.73829400	-0.04331400
C	1.12020500	-0.30071800	0.20960000
H	0.73288000	1.68539400	-0.35046800
H	0.74418500	-1.24881000	0.58742500
C	-1.91195200	-0.36772800	-0.14023900
H	-1.66655600	1.65144100	0.31322600
H	-1.56741300	-1.34541200	-0.46132600
F	-3.25309800	-0.32809000	0.00045500
C	2.53148500	-0.21688000	0.02207700
N	3.68717300	-0.17310600	-0.12045400

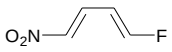
Transition state

C	-1.26011600	1.06184300	-0.15753900
C	0.06517400	1.35536800	0.04733600
C	0.65858200	0.11655500	0.47944100
H	0.60047400	2.27996000	-0.15577100
H	0.31996600	-0.32004200	1.41277000
C	-1.24642500	-0.34988000	-0.33719900
H	-2.14090400	1.69849300	-0.16140600
H	-0.78344500	-0.83665800	-1.18709800
F	-2.27237000	-1.10390600	0.13350700
C	1.98087700	-0.27696600	0.09035000
N	3.03809700	-0.61830300	-0.26348300

Cyclobutene (Starting material)

C	-1.29949400	1.03047500	-0.40724000
C	-0.23048800	1.47128500	0.27127500
C	0.34826300	0.07642700	0.52196800
H	0.14889500	2.45076200	0.54454600
H	0.22203300	-0.28340300	1.54878300
C	-0.84450000	-0.40610000	-0.39352500
H	-2.16442800	1.50867200	-0.85441200
H	-0.53980400	-0.83867900	-1.35052500

F	-1.69884500	-1.32072400	0.22067000
C	1.70958500	-0.19743500	0.06365900
N	2.78895800	-0.39982200	-0.31589200



Butadiene (Product)

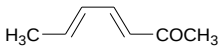
C	1.61452400	0.69539400	-0.18232700
C	0.16301100	0.75134400	-0.07542700
C	-0.66833000	-0.30040100	-0.15289600
H	-0.28771900	1.73167600	0.06265000
H	-0.40219600	-1.32935500	-0.35410800
C	2.35055400	-0.36438000	0.17228200
H	2.13206000	1.58767400	-0.52662200
H	1.99205800	-1.29357100	0.60369400
F	3.69042800	-0.35171200	0.04692500
N	-2.10132800	-0.13005700	0.01107600
O	-2.77775900	-1.16115800	-0.07279100
O	-2.55940500	0.99711300	0.21588300

Transition state

C	1.62424800	1.07165200	-0.12613200
C	0.29490800	1.33205500	-0.36233700
C	-0.28838400	0.03610300	-0.48105100
H	-0.23015700	2.28144700	-0.40075000
H	-0.04628100	-0.64634500	-1.28494700
C	1.61174400	-0.24679200	0.40409100
H	2.51212100	1.66625100	-0.32324200
H	1.15119400	-0.50818400	1.34911500
F	2.61957900	-1.10074400	0.11717400
N	-1.65190800	-0.19608300	-0.00526200
O	-2.17529100	0.68556500	0.68561700
O	-2.18156300	-1.26956600	-0.30628300

Cyclobutene (Starting material)

C	1.67524300	1.02764500	0.09601900
C	0.60666100	1.36928500	-0.64069300
C	-0.03051400	0.00223800	-0.56501100
H	0.27749400	2.27889400	-1.13136600
H	-0.03282800	-0.61836200	-1.46059700
C	1.12521900	-0.33193000	0.44318100
H	2.59141000	1.53031700	0.38688800
H	0.79652600	-0.47944200	1.47578300
F	1.90070300	-1.43142200	0.08663500
N	-1.42519500	-0.07290200	0.01506900
O	-1.70598600	0.72757000	0.90546100
O	-2.17179100	-0.94278600	-0.42507200



Butadiene (Product)

C	0.15394000	0.72089200	-0.06667400
C	1.61507300	0.72194700	-0.13555100
C	2.42379500	-0.32053500	0.13545400
H	2.07292800	1.67411400	-0.40676700
H	1.98148000	-1.26381200	0.45814300
C	-0.65912400	-0.35845200	-0.11368100
H	-0.30160900	1.70735600	0.01550300
H	-0.25605500	-1.36097100	-0.24288200
C	-2.13281600	-0.31852500	-0.01097400
O	-2.77097800	-1.36772100	-0.04519300
C	-2.85051400	1.01574600	0.13565500
H	-2.53887400	1.53356000	1.05105000
H	-2.63098100	1.67915100	-0.70989100
H	-3.92610400	0.83222500	0.17723500
C	3.91933300	-0.29010000	0.04644800
H	4.28865200	0.69120600	-0.27037800
H	4.37730400	-0.53595900	1.01455400
H	4.28296700	-1.04093400	-0.66909000

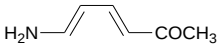
Transition state

C	1.56292600	1.23702400	-0.06236700
C	0.25399900	1.40517800	-0.42497700
C	-0.26396000	0.06185900	-0.55220500
H	-0.30235300	2.33122300	-0.56265400
H	0.17754800	-0.59100000	-1.30006200
C	1.64278900	-0.11226800	0.43476200
H	2.41157000	1.90578900	-0.20676900
H	1.05794400	-0.33860000	1.32111200
C	2.79055900	-1.04948300	0.18215500
H	3.56540200	-0.91449700	0.95423800
H	2.46328300	-2.09360000	0.24517600
H	3.25487000	-0.88770700	-0.79603700
C	-1.60573300	-0.39361100	-0.11633100
C	-2.50510400	0.59748000	0.60582100
H	-3.48568300	0.14557300	0.77041500
H	-2.06824600	0.87734000	1.57323100
H	-2.61982200	1.52346600	0.02781300
O	-1.96342100	-1.55438300	-0.30345200

Cyclobutene (Starting material)

C	0.51565900	1.37633600	-0.77838600
C	1.49688600	1.25562100	0.12817000
C	1.15946800	-0.18375300	0.48648900
H	2.27335700	1.92733800	0.48807500
H	0.75046500	-0.29611900	1.50082200
C	0.01084400	-0.05096600	-0.61521600
H	0.18704000	2.18607900	-1.42559000
H	0.18741200	-0.71030000	-1.47230800
C	-1.39889000	-0.31592600	-0.10986600
O	-1.96957100	-1.35840200	-0.39205100
C	-2.06194400	0.73571900	0.76041100
H	-1.36574000	1.15469500	1.49573600
H	-2.39362800	1.57169100	0.12957300
H	-2.93227000	0.30585100	1.26147800
C	2.21162700	-1.26106900	0.23479100
H	1.78182900	-2.26308500	0.35098400

H	2.62506400	-1.17942700	-0.77769500
H	3.04114000	-1.16527100	0.94697800



Butadiene (Product)

C	-0.18256700	0.71734800	-0.03913300
C	-1.62940800	0.75413800	-0.06122800
C	-2.44157700	-0.32786800	0.07205500
H	-2.08980500	1.73451700	-0.18184900
H	-2.02034700	-1.31674800	0.23693300
C	0.63629700	-0.36728000	-0.07189700
H	0.28663500	1.69947800	0.00789800
H	0.23775600	-1.37673900	-0.15525000
C	2.10198700	-0.31991600	-0.00811300
O	2.75510300	-1.36452300	-0.02896200
C	2.82005100	1.02261800	0.08336400
H	2.57503400	1.66610400	-0.77060800
H	2.53840800	1.56257900	0.99584900
H	3.89681800	0.84078300	0.09570600
N	-3.80992800	-0.32151000	-0.02796600
H	-4.29392000	0.56756200	-0.03126400
H	-4.33060000	-1.08502100	0.37975200

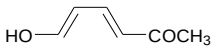
Transition state

C	-0.46959900	-1.40221400	-0.46613700
C	-1.73276500	-1.08478300	-0.08754600
C	-1.61785300	0.27044900	0.44016500
H	-2.66004000	-1.65427400	-0.13988500
H	-1.11406000	0.40740800	1.39090200
C	0.25236900	-0.13639100	-0.51027700
H	-0.04132400	-2.38739200	-0.63915200
H	-0.01367400	0.55900900	-1.30426100
C	1.60451000	-0.00597500	0.04052900
O	2.09868300	-0.88276200	0.75520600
C	2.39022900	1.25798500	-0.28684300

H	2.89334700	1.13285900	-1.25561700
H	1.74020600	2.13759800	-0.36724300
H	3.15542300	1.42874100	0.47506100
N	-2.54790200	1.23693400	0.16398100
H	-2.48500300	2.13876700	0.61728000
H	-2.99036800	1.24641400	-0.74594900

Cyclobutene (Starting material)

C	0.55445000	1.39892000	-0.71149800
C	1.56191300	1.20492200	0.15070200
C	1.17038200	-0.22777800	0.46914600
H	2.37712300	1.82708300	0.51207900
H	0.75931000	-0.34775900	1.48690000
C	0.01792700	-0.02146200	-0.61137000
H	0.22931200	2.25307000	-1.30094500
H	0.20725700	-0.64704400	-1.48943300
C	-1.39239800	-0.30235200	-0.11436200
O	-1.91496700	-1.38412100	-0.33553200
C	-2.10330200	0.77412600	0.68208300
H	-1.45876600	1.16588200	1.47858900
H	-2.34121100	1.62333200	0.02743000
H	-3.02786800	0.37579600	1.10576200
N	2.14239100	-1.25282900	0.10502400
H	1.75177600	-2.18362100	0.24779300
H	2.97222400	-1.18222300	0.69270300



Butadiene (Product)

C	0.20019200	0.70630900	-0.06129500
C	1.65445100	0.71397300	-0.10936100
C	2.44419000	-0.35733100	0.11515400
H	2.12950500	1.67427400	-0.31445900
H	2.05985000	-1.33637200	0.38241300
C	-0.62431800	-0.36775200	-0.10392000
H	-0.25132100	1.69505700	0.00904600

H	-0.23492500	-1.37736200	-0.21966400
C	-2.09460500	-0.30862500	-0.01161100
O	-2.74887300	-1.34904400	-0.04320500
C	-2.79745900	1.03617400	0.12097900
H	-2.49352400	1.55281900	1.03968200
H	-2.55982800	1.69490000	-0.72337000
H	-3.87557400	0.86518500	0.14837800
O	3.79788600	-0.37624100	0.06472300
H	4.13900700	0.49728800	-0.19384600

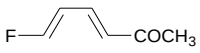
Transition state

C	-0.47655800	-1.38695800	-0.43647900
C	-1.76430100	-1.04333900	-0.14298800
C	-1.64409900	0.28212900	0.40256800
H	-2.70050400	-1.57978900	-0.28133300
H	-1.14900800	0.42617400	1.35794100
C	0.25182100	-0.13765400	-0.49341600
H	-0.04200600	-2.37882900	-0.53632100
H	-0.01784100	0.55977500	-1.28297800
C	1.61771900	-0.01173500	0.05131600
O	2.09802300	-0.88545500	0.77329400
C	2.41054000	1.23634600	-0.30497400
H	2.75673800	1.16936500	-1.34547900
H	1.79241900	2.13969300	-0.23006500
H	3.28089100	1.32609000	0.34940700
O	-2.56790000	1.22680100	0.07851700
H	-2.53240600	1.97401600	0.69816700

Cyclobutene (Starting material)

C	0.58641700	1.41087900	-0.65475500
C	1.61419000	1.15925900	0.16968800
C	1.18447600	-0.25923600	0.46008300
H	2.45677600	1.73902600	0.53540300
H	0.79145800	-0.41247900	1.47652300
C	0.01964400	-0.00102900	-0.61147700
H	0.25732200	2.30332800	-1.18111400
H	0.20891400	-0.59859800	-1.50881200

C	-1.39048600	-0.28954000	-0.12568700
O	-1.88452800	-1.39176700	-0.31176900
C	-2.12938800	0.79655600	0.63043200
H	-1.51444900	1.18915600	1.45035000
H	-2.33624100	1.64362500	-0.03729700
H	-3.07081100	0.40529800	1.02213700
O	2.14774800	-1.23990900	0.14572400
H	1.79215300	-2.11727800	0.36147100



Butadiene (Product)

C	0.20860700	0.71728800	-0.09452500
C	1.66673600	0.69953000	-0.18505000
C	2.42939000	-0.33551100	0.18193900
H	2.16749500	1.59948800	-0.53629900
H	2.09538200	-1.27278900	0.61432900
C	-0.61151600	-0.35460300	-0.15581000
H	-0.23020100	1.70755600	0.01983000
H	-0.21883300	-1.35462000	-0.32956900
C	-2.08467100	-0.30803900	-0.01533100
O	-2.72539500	-1.35379200	-0.05863100
C	-2.78841000	1.02611400	0.18018900
H	-2.45906200	1.51337900	1.10616800
H	-2.57537200	1.71248400	-0.64852200
H	-3.86475000	0.85042900	0.23253600
F	3.77418700	-0.28825200	0.06023400

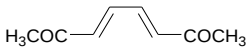
Transition state

C	1.67339000	1.10881300	-0.11225000
C	0.35939200	1.32817700	-0.44617200
C	-0.22900000	0.01915300	-0.55737300
H	-0.16030100	2.28117800	-0.52600700
H	0.16568500	-0.66144700	-1.30582400
C	1.63493900	-0.20760600	0.42851800
H	2.56175700	1.72213100	-0.24154500

H	1.14105300	-0.45564300	1.36015600
F	2.66845800	-1.06263100	0.21119500
C	-1.60156400	-0.34641800	-0.11326400
C	-2.43005100	0.69844200	0.61644400
H	-3.41852100	0.28929000	0.83550800
H	-1.94328400	0.99537000	1.55437500
H	-2.53912100	1.60721900	0.01016500
O	-2.03325300	-1.47722400	-0.31037500

Cyclobutene (Starting material)

C	0.63970700	1.28023900	-0.80003400
C	1.66527300	1.09808100	0.04629400
C	1.17347800	-0.25481500	0.49192000
H	2.51959200	1.69504900	0.35019500
H	0.83134300	-0.33880700	1.52897900
C	0.02986700	-0.10413600	-0.59013800
H	0.32248900	2.11498600	-1.41977900
H	0.18834200	-0.80518600	-1.41479000
C	-1.41042900	-0.24709100	-0.10823900
O	-2.08107300	-1.20571200	-0.45118700
C	-1.96911200	0.82980400	0.80311300
H	-1.27364400	1.07631200	1.61455800
H	-2.12284600	1.75414500	0.22999600
H	-2.92620200	0.50420100	1.21603500
F	2.03742300	-1.32972100	0.27186600



Butadiene (Product)

C	0.73037100	-0.73815200	0.02929300
C	-0.73037600	-0.73817600	-0.02941900
C	-1.53352100	0.33644500	0.12906100
H	-1.18624300	-1.71315900	-0.19536200
H	-1.12241700	1.32094600	0.34233900
C	1.53349800	0.33653600	-0.12884700
H	1.18625700	-1.71318000	0.19492000

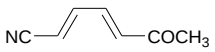
H	1.12235400	1.32107400	-0.34184100
C	3.01545400	0.31220400	-0.05052200
O	3.63595200	1.35908000	-0.19935300
C	3.74254900	-0.99605300	0.21269200
H	3.44278300	-1.42714300	1.17578500
H	3.51844400	-1.73635900	-0.56513800
H	4.81721000	-0.80406000	0.22550800
C	-3.01545400	0.31219700	0.05056100
C	-3.74255800	-0.99604300	-0.21265500
H	-3.51903400	-1.73605900	0.56565000
H	-4.81719800	-0.80393900	-0.22611700
H	-3.44229900	-1.42755200	-1.17537700
O	-3.63590600	1.35913000	0.19918300

Transition state

C	-0.66548000	-1.74111300	0.14825500
C	0.66540900	-1.74110700	-0.14824600
C	0.97905500	-0.36214400	-0.45211300
H	1.38423100	-2.55598300	-0.13212400
H	0.49735200	0.08625100	-1.31722900
C	-0.97910700	-0.36217500	0.45221300
H	-1.38432000	-2.55597100	0.13199500
H	-0.49748000	0.08613100	1.31741000
C	-2.25341900	0.27493000	0.01438500
O	-3.01211400	-0.31798200	-0.74485400
C	-2.56781700	1.66113500	0.54307500
H	-2.75500900	1.61663700	1.62450300
H	-1.71843700	2.33984000	0.39413500
H	-3.45228000	2.06088700	0.04249400
C	2.25339500	0.27493500	-0.01438500
C	2.56789800	1.66112900	-0.54303300
H	3.45158400	2.06135400	-0.04145600
H	2.75659900	1.61629700	-1.62419000
H	1.71807900	2.33957900	-0.39549300
O	3.01212500	-0.31808800	0.74473500

Cyclobutene (Starting material)

C	-0.57924700	1.78166600	-0.55950800
C	0.40812000	1.88656500	0.34076500
C	0.58385600	0.39115000	0.50599400
H	0.93391700	2.72196900	0.79183600
H	0.25774600	-0.01450800	1.47480900
C	-0.55767500	0.26206400	-0.61528600
H	-1.17430100	2.50718500	-1.10784900
H	-0.16972800	-0.15889700	-1.55003200
C	-1.75668400	-0.57377600	-0.18733700
O	-1.82572700	-1.74751300	-0.51714500
C	-2.82255700	0.08009400	0.66777400
H	-2.37974900	0.64841600	1.49446500
H	-3.38788300	0.80069600	0.06152200
H	-3.50712700	-0.67866100	1.05293400
C	1.91330200	-0.24213800	0.11695100
C	2.01544700	-1.74544700	0.28418300
H	1.11977800	-2.25074500	-0.09652200
H	2.90718200	-2.11840700	-0.22479500
H	2.09069700	-1.98756600	1.35341000
O	2.83598900	0.43369400	-0.30422900



Butadiene (Product)

C	-0.18812900	0.74540100	-0.05157200
C	1.27017400	0.74890000	-0.11968600
C	2.07300500	-0.30427400	0.15558200
H	1.73668400	1.69280600	-0.39520400
H	1.66912300	-1.25870500	0.48530200
C	-0.98287900	-0.34511100	-0.10649500
H	-0.64713700	1.72931300	0.02704800
H	-0.56652700	-1.34207800	-0.23692800
C	-2.46562200	-0.32862100	-0.01540300
O	-3.07134600	-1.39341200	-0.04999500
C	-3.20455500	0.99123600	0.11985500

H	-2.90241800	1.52086700	1.03173900
H	-2.99395900	1.65078500	-0.73099200
H	-4.27695200	0.79113900	0.16129300
C	3.49274600	-0.22772200	0.05293900
N	4.65478800	-0.18795400	-0.02194500

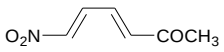
Transition state

C	1.11268600	1.52988600	-0.05451300
C	-0.19377200	1.50127300	-0.44571800
C	-0.51897200	0.09553700	-0.55691200
H	-0.87588100	2.33365300	-0.60497100
H	0.00879800	-0.50198200	-1.29434400
C	1.35782600	0.20016100	0.46648900
H	1.85588100	2.31850600	-0.14461700
H	0.82824900	-0.11801700	1.35797700
C	2.58142600	-0.50340800	0.23027400
N	3.56736200	-1.08290900	0.00264900
C	-1.79721400	-0.53490700	-0.10950100
C	-2.83215500	0.33631600	0.57765700
H	-3.71722100	-0.26157700	0.80416700
H	-2.42842800	0.75799900	1.50702400
H	-3.11842100	1.18285700	-0.06016400
O	-1.97293300	-1.73502800	-0.27878400

Cyclobutene (Starting material)

C	0.95406700	1.65215800	0.09279200
C	-0.03162700	1.52801500	-0.80503000
C	-0.20968300	0.02862600	-0.61762200
H	-0.53626400	2.23062800	-1.46192800
H	0.11116700	-0.59048200	-1.46055000
C	0.93328000	0.17896500	0.49295300
H	1.57694700	2.47018900	0.44066900
H	0.57911400	-0.01492200	1.51303000
C	2.15121000	-0.59398600	0.26229100
N	3.13179300	-1.18984800	0.07841100
C	-1.53796200	-0.52763600	-0.10261400
C	-2.37604300	0.34363000	0.81269300

H	-3.15173700	-0.26139000	1.28680300
H	-1.76906800	0.84598300	1.57483200
H	-2.85557300	1.13509100	0.22105000
O	-1.89707400	-1.64310000	-0.43444600



Butadiene (Product)

C	0.68623900	-0.76135500	0.02217100
C	-0.77116900	-0.78335600	-0.06205400
C	-1.57287900	0.27160700	0.14772400
H	-1.24800200	-1.73465800	-0.28751100
H	-1.27481100	1.27174200	0.43248900
C	1.46778900	0.32633100	-0.14615900
H	1.15131800	-1.72772900	0.20743500
H	1.03973600	1.29736800	-0.38715600
C	2.95271300	0.33696000	-0.04838900
O	3.54239000	1.39979100	-0.19783500
C	3.70507300	-0.95024200	0.23513800
H	3.40492100	-1.37712200	1.20005200
H	3.50436400	-1.70334500	-0.53676000
H	4.77505600	-0.73496700	0.25669100
N	-3.01824100	0.14605900	0.02218600
O	-3.66432800	1.17786900	0.22916400
O	-3.50699800	-0.94683100	-0.27272100

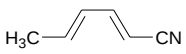
Transition state

C	0.52734100	1.68842700	0.20817400
C	-0.81080900	1.61986500	-0.07563300
C	-0.99204500	0.24998300	-0.44835800
H	-1.58284500	2.38234900	-0.04576600
H	-0.55171000	-0.18477200	-1.33604000
C	0.92984200	0.33136100	0.47053100
H	1.19915200	2.54093400	0.16783200
H	0.46892800	-0.18630900	1.30719300

C	2.25351100	-0.20267900	0.01540700
O	2.98221600	0.49557100	-0.67743100
C	2.62907800	-1.60385400	0.44343200
H	2.75342100	-1.64434500	1.53398800
H	1.83171000	-2.31329600	0.18734000
H	3.56162700	-1.90516300	-0.03785200
N	-2.22738000	-0.46194300	-0.10081800
O	-2.35703400	-1.60748600	-0.54296000
O	-3.03894900	0.11761400	0.62635500

Cyclobutene (Starting material)

C	-0.40706300	1.72531400	-0.55067100
C	0.59838400	1.75971800	0.33509000
C	0.61418100	0.26706200	0.52957800
H	1.19451700	2.54547800	0.78641800
H	0.33733400	-0.13791500	1.50388300
C	-0.50710500	0.20394900	-0.59222300
H	-0.96844200	2.49067400	-1.07879400
H	-0.14191300	-0.25398100	-1.51694600
C	-1.81941800	-0.48463900	-0.20925200
O	-2.18295300	-1.47373100	-0.81862300
C	-2.64742300	0.11612700	0.90980700
H	-2.03152100	0.44928400	1.75254000
H	-3.17389000	1.00333900	0.53233400
H	-3.38771600	-0.61145300	1.24908400
N	1.88093100	-0.46584700	0.13876900
O	2.04808600	-1.57689100	0.63585400
O	2.63684000	0.08191100	-0.65896500



Butadiene (Product)

C	-0.35945400	0.73852100	0.03350600
C	1.09839100	0.72955500	-0.05808900
C	1.89548800	-0.34249800	0.11228000
H	1.56197500	1.69760900	-0.24992600

H	1.44450000	-1.30271800	0.36718300
C	-1.17805800	-0.32176200	-0.15833800
H	-0.81862000	1.69940900	0.26157000
H	-0.78886100	-1.29616000	-0.44454900
C	-2.59342700	-0.23132700	-0.01633400
N	-3.75326800	-0.18307000	0.09094700
C	3.38978900	-0.32506300	0.00377800
H	3.85657700	-0.65436100	0.94219600
H	3.73221200	-1.02031300	-0.77541000
H	3.76872300	0.67346900	-0.23850500

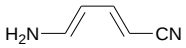
Transition state

C	0.17964800	1.40256900	0.07065700
C	-1.14498900	1.16984100	-0.17927000
C	-1.25498700	-0.25270800	-0.37111300
H	-1.98151000	1.86732100	-0.14904200
H	-0.70932800	-0.66891400	-1.21224400
C	0.69916900	0.11311000	0.46699400
H	0.75904500	2.31736400	-0.03434600
H	0.32198500	-0.33446700	1.38050800
C	2.00101200	-0.34769200	0.08797500
N	3.04205000	-0.74417600	-0.25929500
C	-2.40445000	-1.08982000	0.11690600
H	-3.22341300	-1.06600700	-0.62029500
H	-2.11024400	-2.14003100	0.22376300
H	-2.80329500	-0.73783500	1.07383600

Cyclobutene (Starting material)

C	-0.08109600	1.51269300	0.31201800
C	-1.13051200	1.17138500	-0.44716300
C	-0.84220600	-0.32266300	-0.41810700
H	-1.92404600	1.74211500	-0.92264500
H	-0.48845100	-0.71187600	-1.38093600
C	0.37723100	0.07096200	0.52799900
H	0.33298800	2.44886200	0.67361800
H	0.24494900	-0.29517400	1.55377600
C	1.71498100	-0.29060500	0.06340600

N	2.77690700	-0.57326900	-0.31616500
C	-1.89086700	-1.25593600	0.17939700
H	-2.76689300	-1.32005100	-0.47750600
H	-1.49095700	-2.26945000	0.30324700
H	-2.23112300	-0.89656100	1.15829600



Butadiene (Product)

C	0.32540500	0.73329900	0.02126500
C	-1.11935700	0.75423300	-0.02213500
C	-1.91834400	-0.34059100	0.08079300
H	-1.58684200	1.73312900	-0.12157300
H	-1.48644900	-1.32409100	0.25316200
C	1.14983400	-0.33728400	-0.13541200
H	0.79914500	1.69837600	0.19565200
H	0.76772500	-1.32754200	-0.37232100
C	2.56255000	-0.23069600	-0.01383600
N	3.72441800	-0.16828600	0.07867900
N	-3.28329300	-0.35495300	-0.05245200
H	-3.77849200	0.52767900	-0.07861200
H	-3.80348400	-1.11865400	0.35604100

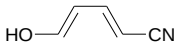
Transition state

C	0.09710700	1.39352200	0.09298800
C	-1.19711600	1.12859200	-0.22501900
C	-1.23996700	-0.31896800	-0.38318800
H	-2.05437000	1.79354000	-0.31840900
H	-0.75116000	-0.75326900	-1.24818000
C	0.65548800	0.10557400	0.48521900
H	0.63688600	2.33595200	0.01932400
H	0.32181500	-0.31762400	1.42862100
C	1.96650100	-0.30614300	0.09684300
N	3.01526300	-0.67167800	-0.26613200
N	-2.27497600	-1.07244500	0.10198600
H	-2.31322300	-2.06132300	-0.10648700

H	-2.71403600	-0.80388300	0.97310100

Cyclobutene (Starting material)

C	-1.19532600	1.11119900	-0.42578300
C	-0.13199700	1.50037600	0.28798900
C	0.37583300	0.08142200	0.53123200
H	0.26922800	2.46049800	0.59779000
H	0.23785000	-0.27671100	1.55719600
C	-0.84736000	-0.36600700	-0.39085200
H	-2.02311900	1.64237000	-0.88815400
H	-0.48858700	-0.74885900	-1.35854000
N	-1.81030900	-1.23323600	0.27101900
H	-2.75027300	-1.07682800	-0.08638600
H	-1.58779400	-2.21683900	0.12957900
C	1.71978900	-0.25046700	0.06420000
N	2.78417400	-0.51573200	-0.32133300



Butadiene (Product)

C	-1.13957700	0.75048200	0.05428100
C	0.30990300	0.74326400	-0.03133500
C	1.13120400	-0.31396100	0.18548400
H	0.77229400	1.69570500	-0.28614200
H	0.74834600	-1.27748500	0.51401300
C	-1.91851800	-0.33616900	-0.10728400
H	-1.62928300	1.70759600	0.21991200
H	-1.51420900	-1.31533400	-0.35919200
O	-3.26967200	-0.25978700	0.02567800
H	-3.68547200	-1.09569700	-0.23207000
C	2.54299700	-0.23034400	0.01752600
N	3.70137800	-0.18801700	-0.11056800

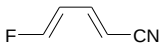
Transition state

C	-0.66649362	0.75560403	0.05495068
C	0.70104338	0.75560403	-0.11422632
C	1.08283638	-0.60708297	0.08943068

H	1.35850738	1.56486603	-0.42988332
H	0.89532738	-1.06407397	1.05438868
C	-1.04828562	-0.60708297	-0.14870332
H	-1.32395662	1.56486303	0.37061968
H	-0.87189425	-1.07657139	-1.09388410
C	-1.71339275	-1.39914679	0.99229073
N	-2.20859146	-1.98887290	1.84181584
O	2.14266603	-1.22858995	-0.64227294
H	2.98746820	-0.93340289	-0.29474757

Cyclobutene (Starting material)

C	-0.18867000	1.49989000	0.25542500
C	-1.26579500	1.06442800	-0.41171100
C	-0.85820900	-0.38949100	-0.37536000
H	-2.12890900	1.55087300	-0.85501500
H	-0.51648800	-0.78627900	-1.34037500
C	0.36715400	0.10426800	0.53055100
H	0.20113100	2.47859600	0.51660300
H	0.23823300	-0.23102800	1.56546300
C	1.71756500	-0.20986400	0.07083800
N	2.78227900	-0.46748300	-0.31914900
O	-1.79545800	-1.24797600	0.23123500
H	-1.53852500	-2.17135700	0.07902600



Butadiene (Product)

C	0.29244100	0.73839500	-0.04334800
C	-1.16145500	0.71729300	0.07700500
C	-1.91191600	-0.36784500	-0.14009000
H	-1.66667400	1.65133400	0.31329000
H	-1.56739900	-1.34547700	-0.46136400
C	1.12022100	-0.30049600	0.20977100
H	0.73278600	1.68542700	-0.35080900
H	0.74435900	-1.24857500	0.58778100
C	2.53150400	-0.21673700	0.02208000
N	3.68718400	-0.17333600	-0.12058600

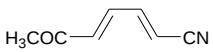
F	-3.25312600	-0.32811300	0.00029900

Transition state

C	0.06506500	1.35558800	0.04709200
C	-1.26020900	1.06170200	-0.15788500
C	-1.24630500	-0.35003400	-0.33689800
H	-2.14129200	1.69795200	-0.16071400
H	-0.78291900	-0.83712300	-1.18640700
C	0.65873800	0.11718300	0.47970800
H	0.60011700	2.28028800	-0.15617300
H	0.32035000	-0.31928200	1.41315900
C	1.98090600	-0.27677100	0.09004400
N	3.03806900	-0.61874700	-0.26333500
F	-2.27243500	-1.10406800	0.13345700

Cyclobutene (Starting material)

C	-0.23065500	1.47139400	0.27113400
C	-1.29965500	1.03040800	-0.40728500
C	-0.84439000	-0.40614600	-0.39333700
H	-2.16464000	1.50843400	-0.85454100
H	-0.53954700	-0.83883800	-1.35037300
C	0.34829100	0.07665900	0.52214000
H	0.14858100	2.45100100	0.54412900
H	0.22184200	-0.28290100	1.54893600
C	1.70954900	-0.19708800	0.06379900
N	2.78874100	-0.39995200	-0.31604800
F	-1.69847300	-1.32104400	0.22060900



Butadiene (Product)

C	1.27017200	0.74889300	-0.11955400
C	-0.18815500	0.74543900	-0.05128500
C	-0.98288400	-0.34506600	-0.10651900
H	-0.64709700	1.72935700	0.02761800
H	-0.56650400	-1.34195200	-0.23744900

C	2.07297700	-0.30427000	0.15578600
H	1.73668900	1.69274000	-0.39526300
H	1.66914500	-1.25865600	0.48567700
C	3.49271900	-0.22773900	0.05285600
N	4.65475200	-0.18798100	-0.02218700
C	-2.46566600	-0.32864800	-0.01539600
C	-3.20449300	0.99124000	0.11963300
H	-2.99473700	1.65004100	-0.73201500
H	-4.27684900	0.79122600	0.16232900
H	-2.90133400	1.52173700	1.03069500
O	-3.07132500	-1.39346400	-0.04992500

Transition state

C	1.11268600	1.52988600	-0.05451300
C	-0.19377200	1.50127300	-0.44571800
C	-0.51897200	0.09553700	-0.55691200
H	-0.87588100	2.33365300	-0.60497100
H	0.00879800	-0.50198200	-1.29434400
C	1.35782600	0.20016100	0.46648900
H	1.85588100	2.31850600	-0.14461700
H	0.82824900	-0.11801700	1.35797700
C	2.58142600	-0.50340800	0.23027400
N	3.56736200	-1.08290900	0.00264900
C	-1.79721400	-0.53490700	-0.10950100
C	-2.83215500	0.33631600	0.57765700
H	-3.71722100	-0.26157700	0.80416700
H	-2.42842800	0.75799900	1.50702400
H	-3.11842100	1.18285700	-0.06016400
O	-1.97293300	-1.73502800	-0.27878400

Cyclobutene (Starting material)

C	0.95406700	1.65215800	0.09279200
C	-0.03162700	1.52801500	-0.80503000
C	-0.20968300	0.02862600	-0.61762200
H	-0.53626400	2.23062800	-1.46192800
H	0.11116700	-0.59048200	-1.46055000
C	0.93328000	0.17896500	0.49295300

H	1.57694700	2.47018900	0.44066900
H	0.57911400	-0.01492200	1.51303000
C	2.15121000	-0.59398600	0.26229100
N	3.13179300	-1.18984800	0.07841100
C	-1.53796200	-0.52763600	-0.10261400
C	-2.37604300	0.34363000	0.81269300
H	-3.15173700	-0.26139000	1.28680300
H	-1.76906800	0.84598300	1.57483200
H	-2.85557300	1.13509100	0.22105000
O	-1.89707400	-1.64310000	-0.43444600

Butadiene (Product)

C	0.72762800	0.75790600	-0.04307800
C	-0.72765200	0.75788600	0.04309100
C	-1.52339700	-0.31920500	-0.14535800
H	-1.19529200	1.71806600	0.25104400
H	-1.11487700	-1.28980100	-0.41797100
C	1.52340400	-0.31915300	0.14539600
H	1.19523500	1.71809500	-0.25108400
H	1.11489300	-1.28976400	0.41799900
C	2.94251800	-0.25146800	0.02747500
N	4.10356800	-0.22169200	-0.06239300
C	-2.94250800	-0.25145900	-0.02749800
N	-4.10355700	-0.22168500	0.06237000

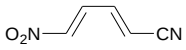
Transition state

C	0.66005600	1.45039200	0.17020300
C	-0.66011800	1.45029800	-0.17033100
C	-0.95557800	0.06654900	-0.48228000
H	-1.37943900	2.26519100	-0.17393000
H	-0.46515000	-0.38921500	-1.33596900
C	0.95563200	0.06672200	0.48242000
H	1.37928400	2.26536500	0.17380300
H	0.46525800	-0.38891700	1.33620400
C	2.18222800	-0.56323000	0.09999500

N	3.16296700	-1.08554700	-0.25342200
C	-2.18218200	-0.56325000	-0.09995800
N	-3.16299200	-1.08549600	0.25336600

Cyclobutene (Starting material)

C	-0.52489000	1.55674700	-0.41408400
C	0.52526800	1.55671100	0.41416900
C	0.60215500	0.03559500	0.52457000
H	1.13557000	2.32728100	0.87277200
H	0.30638700	-0.36426600	1.50084100
C	-0.60222600	0.03588600	-0.52439400
H	-1.13488300	2.32747000	-0.87287600
H	-0.30646800	-0.36400300	-1.50057000
C	-1.83310800	-0.61537300	-0.08106500
N	-2.81597300	-1.11776600	0.28105900
C	1.83275700	-0.61586000	0.08085700
N	2.81592400	-1.11776600	-0.28112800



Butadiene (Product)

C	1.21742000	0.75777000	-0.14787600
C	-0.23722300	0.78615900	-0.04858900
C	-1.03286200	-0.29032300	-0.12993000
H	-0.71335000	1.75666300	0.07131400
H	-0.73055700	-1.31313600	-0.31207100
C	1.99754200	-0.29365600	0.18820900
H	1.69310700	1.67382100	-0.49141600
H	1.57551700	-1.20876100	0.59776000
C	3.41749900	-0.26324700	0.05997100
N	4.57822600	-0.26306400	-0.03530600
N	-2.47866400	-0.16252800	0.00267400
O	-2.97114600	0.95332700	0.17637100
O	-3.11584300	-1.21703500	-0.07235500

Transition state

C	1.06532400	1.50638800	-0.06811900
C	-0.26850300	1.49236700	-0.37275500
C	-0.56577900	0.09500900	-0.46892500
H	-0.97026800	2.30914000	-0.50697600
H	-0.16123100	-0.54530700	-1.24207300
C	1.33442900	0.19322000	0.46947600
H	1.81067200	2.27774300	-0.24306400
H	0.84285300	-0.10646300	1.38884000
C	2.54610200	-0.51731300	0.18819400
N	3.51520200	-1.10804700	-0.07627300
N	-1.86467500	-0.41679700	-0.01298100
O	-2.60702900	0.36791400	0.58474600
O	-2.11111400	-1.60281800	-0.24214200

Cyclobutene (Starting material)

C	-0.86015400	1.66926600	-0.31364900
C	0.20193600	1.66005900	0.50313100
C	0.28576200	0.15899600	0.55314600
H	0.79216100	2.42521800	0.99289600
H	0.05727500	-0.34559200	1.49365700
C	-0.89227500	0.15102900	-0.50266300
H	-1.50715500	2.44046300	-0.71796200
H	-0.56443300	-0.18887600	-1.49186700
C	-2.11153600	-0.55957800	-0.12148700
N	-3.09378300	-1.09659200	0.18779400
N	1.55501600	-0.48718900	0.03622800
O	2.45536200	0.24897600	-0.35576100
O	1.57602700	-1.71439800	0.03629400

Butadiene (Product)

C	0.10711300	0.75828000	-0.05404000
C	1.56252200	0.72197600	-0.13721500
C	2.34372800	-0.34323400	0.13042200
H	2.03889700	1.66379200	-0.40835900
H	1.87831800	-1.27328600	0.45951200
C	-0.71576600	-0.30271800	-0.11447600
H	-0.36144000	1.73484200	0.04840300
H	-0.43655900	-1.33619500	-0.26733000
N	-2.15117700	-0.14224700	0.00905300
O	-2.62881100	0.98549900	0.16606100
O	-2.81774900	-1.18289300	-0.05713300
C	3.83782000	-0.35210500	0.03879600
H	4.23304800	0.61682500	-0.28321400
H	4.28821200	-0.60680500	1.00792600
H	4.17775100	-1.11748400	-0.67264900

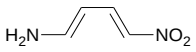
Transition state

C	0.18816300	1.40683700	-0.34215000
C	1.51779900	1.20388900	-0.07790100
C	1.61949000	-0.14269600	0.41378500
H	2.36395200	1.85489000	-0.29362100
H	1.07828900	-0.36729000	1.32772400
C	-0.31847000	0.07404400	-0.46668100
H	-0.37979000	2.32694900	-0.44270100
H	-0.03106700	-0.58818000	-1.27285700
N	-1.66484000	-0.25219200	-0.00898000
O	-2.10397200	-1.37465200	-0.28734300
O	-2.27342300	0.59973100	0.64975300
C	2.74564300	-1.08380000	0.09662700
H	3.51907000	-1.01894200	0.87807800
H	2.39417100	-2.12227400	0.09458100
H	3.21267700	-0.87008200	-0.86970500

Cyclobutene (Starting material)

C	1.49760500	1.21855500	-0.24083900
C	0.45275600	1.50873200	0.54882500
C	-0.04903200	0.09011800	0.57291400

H	0.08877400	2.40624500	1.03696500
H	-0.00332300	-0.46173900	1.51364700
C	1.11856900	-0.24399200	-0.44223900
H	2.33919700	1.79891600	-0.61020600
H	0.72004900	-0.44480100	-1.44516700
N	-1.42813800	-0.17602200	0.01748100
O	-1.98483600	0.71706800	-0.61643400
O	-1.88815000	-1.30151400	0.21140400
C	2.10550000	-1.33304000	-0.03400800
H	1.63173400	-2.32093400	-0.06000500
H	2.95905400	-1.35119500	-0.72267600
H	2.49298200	-1.16100300	0.97738900



Butadiene (Product)

C	0.13813900	0.74501600	-0.01649800
C	1.57608000	0.75159200	-0.02989200
C	2.36735300	-0.35769800	0.03534400
H	2.05470800	1.72750400	-0.08872600
H	1.92675700	-1.34813600	0.12081300
C	-0.69827800	-0.32028200	-0.03354900
H	-0.34664300	1.71841700	0.00817700
H	-0.42694500	-1.36580200	-0.08047600
N	-2.12078200	-0.13997900	0.00250200
O	-2.59989700	1.00241500	0.05174200
O	-2.80542500	-1.17642200	-0.02013300
N	3.72680300	-0.36671500	-0.02055000
H	4.24801300	0.49984700	-0.01422700
H	4.24478700	-1.20468700	0.19548400

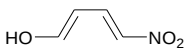
Transition state

C	0.26956300	1.37714200	-0.40257300
C	1.56179300	1.16023200	-0.04617400
C	1.58585600	-0.21533800	0.43947000
H	2.43331200	1.80874100	-0.11509800

H	1.09325200	-0.43566500	1.38025600
C	-0.29177000	0.04683600	-0.50272800
H	-0.25299900	2.31670800	-0.56102200
H	-0.05095200	-0.60867400	-1.33074400
N	-1.61983300	-0.21248500	-0.01567500
O	-2.14622900	-1.29828000	-0.30954000
O	-2.15283500	0.64638500	0.70742000
N	2.58437500	-1.08358000	0.12122600
H	2.61716200	-1.99820900	0.55158900
H	3.04829800	-1.00852600	-0.77485300

Cyclobutene (Starting material)

C	-0.71085609	-0.68140823	-0.00412077
C	-0.71086009	0.66193277	-0.00423777
C	0.80493591	0.77727677	-0.00415677
H	-1.49911809	1.41123577	-0.00434977
H	1.25086491	1.23757877	-0.89496077
C	0.80493891	-0.79674623	-0.00402877
H	-1.49911109	-1.43071523	-0.00409977
H	1.19754136	-1.22033593	0.89671263
N	1.40213119	1.39406421	1.18908714
O	1.07104310	2.71245606	1.23179099
O	2.54628161	1.28742930	1.14382342
N	1.34444352	-1.37888846	-1.24134247
H	2.22570787	-1.81096623	-1.04981715
H	0.70667122	-2.06412235	-1.59305402



Butadiene (Product)

C	1.59481500	0.74008900	-0.11571000
C	0.14870800	0.75488800	-0.05357300
C	-0.67988000	-0.30765100	-0.10627400
H	-0.32562100	1.72980800	0.03408900
H	-0.40702000	-1.34420600	-0.24933500
C	2.36398000	-0.34638900	0.10357600

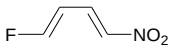
H	2.09612000	1.68299100	-0.31962800
H	1.95022800	-1.31539200	0.37800600
O	3.71341400	-0.27683500	0.00568000
H	4.12140300	-1.11685400	0.26369000
N	-2.10912400	-0.13994800	0.00859400
O	-2.78336600	-1.17783200	-0.05296200
O	-2.58467000	0.99187500	0.15539400

Transition state

C	0.28004700	1.36397700	-0.36117200
C	1.59712800	1.12086600	-0.08732200
C	1.61508100	-0.22983600	0.40347500
H	2.47877000	1.73817100	-0.24010800
H	1.12559400	-0.47126500	1.34176300
C	-0.29077200	0.05340700	-0.48840800
H	-0.24703200	2.31009200	-0.44253800
H	-0.04299800	-0.60609400	-1.31028200
N	-1.63606300	-0.20511100	-0.01079400
O	-2.15364800	-1.28895400	-0.31219900
O	-2.17475800	0.65737900	0.69729500
O	2.61421300	-1.06014600	0.03150000
H	2.64273900	-1.85182300	0.59452200

Cyclobutene (Starting material)

C	1.60181700	1.10704300	-0.24635600
C	0.53204400	1.49402800	0.46599400
C	-0.03737400	0.10583200	0.56983700
H	0.18072200	2.44211200	0.85667300
H	0.01006100	-0.40552300	1.53212000
C	1.13754100	-0.32250000	-0.41282500
H	2.49593500	1.60773100	-0.60414100
H	0.76043400	-0.56037600	-1.41687400
N	-1.42248200	-0.13499900	0.03042000
O	-2.00129700	0.79317800	-0.52924900
O	-1.86401200	-1.27828300	0.15487100
O	2.03913300	-1.29804900	0.04427300
H	1.71546600	-2.18013500	-0.19977900



Butadiene (Product)

C	0.16305100	0.75126400	-0.07503100
C	1.61457600	0.69572200	-0.18200400
C	2.35057400	-0.36422700	0.17219000
H	2.13183200	1.58823700	-0.52609000
H	1.99156100	-1.29349700	0.60303500
C	-0.66812600	-0.30055100	-0.15278000
H	-0.28781900	1.73149100	0.06328700
H	-0.40224400	-1.32949300	-0.35433200
N	-2.10139000	-0.12997100	0.01118100
O	-2.55949800	0.99706000	0.21528000
O	-2.77761700	-1.16119200	-0.07261300
F	3.69031900	-0.35190400	0.04669400

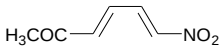
Transition state

C	0.29473500	1.33223500	-0.36250100
C	1.62394100	1.07156300	-0.12584700
C	1.61135900	-0.24700000	0.40401600
H	2.51188600	1.66630400	-0.32228900
H	1.15031100	-0.50872600	1.34869400
C	-0.28854600	0.03636400	-0.48197900
H	-0.23039900	2.28160200	-0.40065800
H	-0.04659100	-0.64565300	-1.28625000
N	-1.65163800	-0.19608300	-0.00549100
O	-2.18154700	-1.26967400	-0.30601300
O	-2.17437400	0.68557800	0.68618400
F	2.61940800	-1.10079400	0.11727100

Cyclobutene (Starting material)

C	-0.71085609	-0.68140823	-0.00412077
C	-0.71086009	0.66193277	-0.00423777
C	0.80493591	0.77727677	-0.00415677

H	-1.49911809	1.41123577	-0.00434977
H	1.25086491	1.23757877	-0.89496077
C	0.80493891	-0.79674623	-0.00402877
H	-1.49911109	-1.43071523	-0.00409977
H	1.19754136	-1.22033593	0.89671263
N	1.40213119	1.39406421	1.18908714
O	1.07104310	2.71245606	1.23179099
O	2.54628161	1.28742930	1.14382342
F	1.30040233	-1.33136665	-1.14033727



Butadiene (Product)

C	-0.77115900	-0.78335300	-0.06210800
C	0.68623600	-0.76128200	0.02216200
C	1.46779400	0.32640200	-0.14617900
H	1.15135300	-1.72762500	0.20747900
H	1.03977400	1.29743300	-0.38725100
C	-1.57287800	0.27160600	0.14769500
H	-1.24800800	-1.73463600	-0.28758300
H	-1.27478400	1.27173600	0.43245600
N	-3.01826000	0.14608500	0.02219900
O	-3.50700300	-0.94684400	-0.27268500
O	-3.66436400	1.17783000	0.22917000
C	2.95272900	0.33697100	-0.04834500
C	3.70502200	-0.95029900	0.23514600
H	3.50471000	-1.70312000	-0.53712200
H	4.77498700	-0.73496700	0.25725600
H	3.40449600	-1.37752500	1.19978400
O	3.54247100	1.39974300	-0.19781500

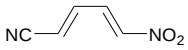
Transition state

C	-0.81084300	1.61992700	-0.07562700
C	0.52729500	1.68849300	0.20820600
C	0.92976600	0.33139000	0.47049300
H	1.19910700	2.54100100	0.16791900

H	0.46885000	-0.18626500	1.30716800
C	-0.99203800	0.25005300	-0.44842100
H	-1.58290400	2.38238300	-0.04569600
H	-0.55169700	-0.18464800	-1.33612400
N	-2.22729500	-0.46196000	-0.10083100
O	-2.35692100	-1.60748100	-0.54309300
O	-3.03883100	0.11745300	0.62650300
C	2.25343000	-0.20269600	0.01538900
C	2.62905300	-1.60381600	0.44354300
H	3.56147200	-1.90522200	-0.03793300
H	2.75369200	-1.64411800	1.53407100
H	1.83160800	-2.31329000	0.18778300
O	2.98212200	0.49549900	-0.67751900

Cyclobutene (Starting material)

C	-0.40706300	1.72531400	-0.55067100
C	0.59838400	1.75971800	0.33509000
C	0.61418100	0.26706200	0.52957800
H	1.19451700	2.54547800	0.78641800
H	0.33733400	-0.13791500	1.50388300
C	-0.50710500	0.20394900	-0.59222300
H	-0.96844200	2.49067400	-1.07879400
H	-0.14191300	-0.25398100	-1.51694600
C	-1.81941800	-0.48463900	-0.20925200
O	-2.18295300	-1.47373100	-0.81862300
C	-2.64742300	0.11612700	0.90980700
H	-2.03152100	0.44928400	1.75254000
H	-3.17389000	1.00333900	0.53233400
H	-3.38771600	-0.61145300	1.24908400
N	1.88093100	-0.46584700	0.13876900
O	2.04808600	-1.57689100	0.63585400
O	2.63684000	0.08191100	-0.65896500



Butadiene (Product)

C	-0.23714600	0.78511100	-0.04817000
C	1.21748000	0.75745300	-0.14675300
C	1.99805500	-0.29442900	0.18679600
H	1.69272900	1.67464600	-0.48780800
H	1.57640900	-1.21106000	0.59335700
C	-1.03310700	-0.29116900	-0.12880400
H	-0.71372100	1.75553500	0.07077600
H	-0.73190600	-1.31453300	-0.30957700
N	-2.47908700	-0.16219000	0.00273500
O	-2.97097000	0.95412500	0.17500200
O	-3.11677200	-1.21643900	-0.07191600
C	3.41807700	-0.26297700	0.05953300
N	4.57884100	-0.26209700	-0.03517000

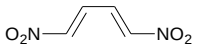
Transition state

C	-0.26844200	1.49227600	-0.37276300
C	1.06540600	1.50620900	-0.06820900
C	1.33434400	0.19302100	0.46942200
H	1.81074900	2.27759300	-0.24303200
H	0.84283200	-0.10646100	1.38887700
C	-0.56573200	0.09492500	-0.46891500
H	-0.97020900	2.30907600	-0.50680900
H	-0.16123900	-0.54544500	-1.24204600
N	-1.86472300	-0.41678000	-0.01294900
O	-2.11127500	-1.60265700	-0.24216000
O	-2.60691500	0.36804400	0.58474600
C	2.54609300	-0.51726700	0.18832300
N	3.51520400	-1.10791100	-0.07631200

Cyclobutene (Starting material)

C	-0.86015400	1.66926600	-0.31364900
C	0.20193600	1.66005900	0.50313100
C	0.28576200	0.15899600	0.55314600
H	0.79216100	2.42521800	0.99289600
H	0.05727500	-0.34559200	1.49365700
C	-0.89227500	0.15102900	-0.50266300
H	-1.50715500	2.44046300	-0.71796200

H	-0.56443300	-0.18887600	-1.49186700
C	-2.11153600	-0.55957800	-0.12148700
N	-3.09378300	-1.09659200	0.18779400
N	1.55501600	-0.48718900	0.03622800
O	2.45536200	0.24897600	-0.35576100
O	1.57602700	-1.71439800	0.03629400



Butadiene (Product)

C	-0.72720400	-0.80028000	-0.06183700
C	0.72728800	-0.80040300	0.06149500
C	1.50835300	0.26114400	-0.17824700
H	1.20919500	-1.73689200	0.33323200
H	1.19427900	1.23951800	-0.51775400
C	-1.50829000	0.26115500	0.17837900
H	-1.20914000	-1.73659600	-0.33410200
H	-1.19430200	1.23936700	0.51840200
N	-2.95744900	0.17310600	0.01829500
O	-3.45869600	-0.89665600	-0.32844400
O	-3.58080300	1.21177400	0.24963200
N	2.95744100	0.17317100	-0.01821500
O	3.45844300	-0.89658200	0.32878300
O	3.58094900	1.21158600	-0.24985600

Transition state

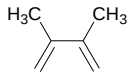
C	-0.67437100	1.57296100	-0.13096500
C	0.67443100	1.57295100	0.13087200
C	0.94637800	0.21220400	0.46055500
H	1.40283000	2.37518400	0.07502000
H	0.54026700	-0.28531600	1.33165800
C	-0.94639500	0.21221500	-0.46059100
H	-1.40274500	2.37521900	-0.07512800
H	-0.54025300	-0.28539500	-1.33162800
N	-2.23684200	-0.39324100	-0.08320700

O	-2.47387900	-1.51765800	-0.52445400
O	-2.97341300	0.26170200	0.65804400
N	2.23681900	-0.39328900	0.08320900
O	2.47376100	-1.51776400	0.52435000
O	2.97350600	0.26172300	-0.65783400

Cyclobutene (Starting material)

C	-0.63949400	1.74480700	0.18812200
C	0.47101100	1.70100800	-0.56304700
C	0.58052200	0.18628600	-0.51510400
H	1.09523400	2.43907300	-1.05485300
H	0.42654500	-0.36011800	-1.44525000
C	-0.62934400	0.25969900	0.45929700
H	-1.31069100	2.52928100	0.51573200
H	-0.40956600	-0.06601800	1.47860600
N	1.87581400	-0.34559100	0.07012200
O	2.70254400	-0.75643000	-0.73726800
O	2.02612600	-0.28682600	1.28717100
N	-1.84039200	-0.53659900	0.02245200
O	-1.65493600	-1.72207600	-0.23465500
O	-2.91694000	0.05062100	-0.00998000

6.3.4 2,3-Disubstituted butadienes



Butadiene (Product)

C	0.74561300	0.12453300	-0.02784400
C	-0.74562400	0.12454300	0.02779500
C	-1.42748900	1.18356300	0.49561000
H	-2.51500500	1.19252600	0.51738800
H	-0.92022000	2.06360400	0.88108700
C	1.42742800	1.18362300	-0.49561500
H	0.92005800	2.06365600	-0.88099100
C	1.45905600	-1.12389900	0.44639000
C	-1.45899300	-1.12395000	-0.44638300
H	2.51494600	1.19263500	-0.51733700
H	2.54471600	-0.98571500	0.43007600
H	1.16100500	-1.38676100	1.47038100
H	1.22174900	-1.98884600	-0.18663700
H	-1.22148000	-1.98887200	0.18661900
H	-2.54466600	-0.98591400	-0.42988800
H	-1.16104600	-1.38678400	-1.47041000

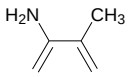
Transition state

C	0.69169100	-0.04134600	-0.05096100
C	-0.69169100	-0.04134500	0.05096200
C	-1.02807000	1.31905500	0.33348000
H	-1.94871800	1.77701200	-0.05106200
H	-0.64914800	1.79351600	1.23135200
C	1.02807300	1.31905500	-0.33347900
H	0.64915200	1.79351300	-1.23135300
C	1.68066200	-1.15295800	0.17403800
C	-1.68066400	-1.15295400	-0.17403900
H	1.94872400	1.77701200	0.05105600
H	1.21717400	-2.02484600	0.64852500
H	2.14900600	-1.48518200	-0.76263400
H	2.49608900	-0.80902400	0.82645700

H	-2.49611300	-0.80900400	-0.82642300
H	-1.21718900	-2.02482600	-0.64856500
H	-2.14897900	-1.48520900	0.76263800

Cyclobutene (Starting material)

C	0.67494000	-0.11815000	0.00010700
C	-0.67493900	-0.11815700	-0.00010800
C	-0.78473300	1.39999100	-0.00026900
H	-1.24690700	1.84802100	0.89008200
H	-1.24576900	1.84732100	-0.89157800
C	0.78475500	1.39999000	0.00026800
H	1.24690200	1.84799200	-0.89010100
H	1.24576000	1.84728800	0.89160300
C	1.73279400	-1.17274600	-0.00013900
C	-1.73280600	-1.17273200	0.00013900
H	-2.38322900	-1.08511200	-0.88191500
H	-1.30066300	-2.18037700	0.00057000
H	-2.38334300	-1.08438400	0.88202800
H	2.38321200	-1.08514300	0.88192100
H	1.30063000	-2.18038100	-0.00057800
H	2.38334200	-1.08440500	-0.88202100



Butadiene (Product)

C	0.72508500	0.14826100	-0.03434100
C	-0.76340500	0.05690300	0.00620900
C	-1.53208000	1.04502100	0.50802000
H	-2.61767500	0.97398700	0.51762200
H	-1.08468100	1.92129300	0.96143300
C	1.33113500	1.24916200	-0.50683900
H	0.76294400	2.08434400	-0.90627700
C	1.50513200	-1.04087200	0.48295400
H	2.41491100	1.34089100	-0.50684500
H	2.58025600	-0.83508300	0.47368300
H	1.20276500	-1.28824400	1.50840500

H	1.32556300	-1.94081300	-0.11801100
N	-1.28800500	-1.17931200	-0.41718800
H	-0.86320000	-1.55580000	-1.25905300
H	-2.30004800	-1.19623600	-0.48666900

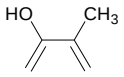
Transition state

C	-0.68940100	-0.15438300	0.03951500
C	0.68177000	0.03946400	-0.04545900
C	0.79687000	1.43920700	-0.31294500
H	1.61831700	2.02905800	0.11651900
H	0.38706300	1.86852800	-1.22022300
C	-1.25556600	1.13405000	0.30270100
H	-1.00629900	1.63669200	1.23017900
C	1.81561500	-0.91969500	0.18451000
H	-2.22933300	1.41530800	-0.11718400
H	2.62439400	-0.42110100	0.73755600
H	1.50136300	-1.79512800	0.76724300
H	2.26051100	-1.28359900	-0.75315600
N	-1.44654100	-1.29352600	-0.23798000
H	-0.92730100	-2.11919200	-0.51061300
H	-2.19865200	-1.50774000	0.40561100

Cyclobutene (Starting material)

C	0.63769100	-0.28502300	-0.00509100
C	-0.68200000	0.01094500	-0.01363000
C	-0.42924300	1.51249300	-0.00508500
H	-0.76625700	2.05532400	0.88991600
H	-0.76387700	2.06834000	-0.89273700
C	1.10113100	1.15396400	0.00598900
H	1.66134400	1.48856300	-0.87813700
H	1.64273400	1.47080400	0.90701900
C	-1.95045100	-0.77724800	-0.00222500
H	-2.60122800	-0.50967400	-0.84771200
H	-1.76014300	-1.85670100	-0.06153400
H	-2.53354800	-0.59925700	0.91398000
N	1.40497800	-1.44417900	0.08790900
H	2.30433800	-1.39529100	-0.37910900

H	0.91901400	-2.30363900	-0.14679200



Butadiene (Product)

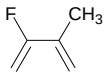
C	0.70460600	0.17747500	-0.02940700
C	-0.77457300	0.02268500	-0.00126700
C	-1.62671900	0.92283100	0.50937800
H	-2.69758100	0.74673600	0.48954700
H	-1.25669300	1.82526300	0.98018500
C	1.26498900	1.31214300	-0.47792600
H	0.66271900	2.12699500	-0.86907300
C	1.53052600	-0.98490600	0.48264900
H	2.34314500	1.45442200	-0.46374800
H	2.59532000	-0.73264400	0.48542000
H	1.23121500	-1.25613200	1.50290600
H	1.40818000	-1.88866900	-0.12949000
O	-1.27854000	-1.17518200	-0.47505800
H	-0.65096200	-1.57588500	-1.09584000

Transition state

C	-0.67573700	-0.22393400	0.04014400
C	0.66651600	0.09029400	-0.06173700
C	0.62681500	1.49657800	-0.32156600
H	1.36482900	2.17393900	0.12812100
H	0.17397900	1.88388800	-1.22666600
C	-1.38740500	0.97673700	0.31163500
H	-1.17294200	1.52228400	1.22295300
C	1.88965500	-0.74700800	0.18458600
H	-2.39448100	1.13619200	-0.08777600
H	2.62502300	-0.17540100	0.76828300
H	1.65500100	-1.65971100	0.74601000
H	2.39454100	-1.04203000	-0.74630200
O	-1.32478100	-1.42147400	-0.13389300
H	-0.76676600	-2.02337500	-0.65186200

Cyclobutene (Starting material)

C	-0.59915000	-0.35708400	0.00000000
C	0.67894800	0.05978700	-0.00012400
C	0.25713000	1.52600500	-0.00013900
H	0.53017900	2.10481000	-0.89300000
H	0.53063200	2.10514200	0.89236100
C	-1.23124400	1.01417300	0.00015600
H	-1.80991300	1.28292800	0.89427500
H	-1.81057100	1.28309300	-0.89347900
C	2.01910800	-0.59323900	0.00010100
H	2.60754000	-0.30440100	0.88304600
H	1.92615900	-1.68490000	-0.00013400
H	2.60814100	-0.30409200	-0.88233600
O	-1.15164200	-1.60596900	-0.00014300
H	-2.11777900	-1.53268400	0.00044400



Butadiene (Product)

C	0.70826300	0.20272800	-0.01410500
C	-0.75649300	0.01713900	0.00059700
C	-1.71360700	0.86528400	0.37917900
H	-2.76001500	0.58572900	0.32161600
H	-1.45658800	1.84554000	0.76181600
C	1.24197600	1.39376900	-0.33058100
H	0.62845600	2.23586400	-0.63742000
C	1.54792700	-1.00203200	0.34402000
H	2.31663300	1.55292600	-0.29845000
H	2.60992800	-0.73998000	0.36249600
H	1.26935500	-1.40091400	1.32772300
H	1.40328700	-1.81175000	-0.38035500
F	-1.13105000	-1.23652700	-0.41467600

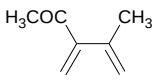
Transition state

C	-0.65198000	-0.24697300	0.03105000

C	0.66935900	0.10592400	-0.06906400
C	0.55829400	1.51661000	-0.29110500
H	1.24454700	2.22276400	0.19222000
H	0.09055600	1.89693300	-1.19109700
C	-1.44932000	0.88816100	0.30673000
H	-1.28007200	1.44862200	1.21851000
C	1.92099600	-0.68621600	0.16534700
H	-2.45237700	0.99426600	-0.11697100
H	2.59361500	-0.14323900	0.84419100
H	1.69973300	-1.66240100	0.60858700
H	2.47707300	-0.85439800	-0.76598500
F	-1.18412900	-1.48528800	-0.18302300

Cyclobutene (Starting material)

C	-0.56561200	0.41256500	0.00000000
C	0.65970300	-0.12312800	-0.00008200
C	0.05869000	-1.53139400	-0.00007100
H	0.26786800	-2.13151000	0.89418000
H	0.26766000	-2.13133900	-0.89449000
C	-1.36566100	-0.85445300	0.00008100
H	-1.97019400	-1.04745400	-0.89392300
H	-1.96976800	-1.04737800	0.89440000
C	2.06494000	0.37023600	0.00005100
H	2.61173200	0.01128800	-0.88277200
H	2.10135600	1.46485900	0.00032100
H	2.61164600	0.01083000	0.88273800
F	-1.00362800	1.69197200	-0.00003600



Butadiene (Product)

C	1.27394100	-0.02026200	-0.01280100
C	-0.06310200	0.64861500	0.00958800
C	-0.18989900	1.98586300	0.02379600
H	-1.17384900	2.44638500	0.03951100
H	0.68014200	2.63670900	0.02243300

C	2.08870700	0.08805300	-1.07256900
H	1.79673400	0.64060200	-1.96181200
C	1.67129900	-0.76913200	1.24137100
C	-1.33065300	-0.18223100	-0.00846100
H	3.07150500	-0.37855900	-1.08217300
H	2.62724000	-1.28698800	1.11248600
H	1.76565500	-0.07290300	2.08548900
H	0.91655200	-1.50991700	1.53519900
C	-1.26065700	-1.57113400	-0.61558900
H	-0.50928500	-2.19429700	-0.11835700
H	-2.24108700	-2.04674300	-0.54434500
H	-0.96046400	-1.50216100	-1.66911200
O	-2.38887000	0.27365500	0.39858400

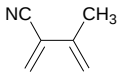
Transition state

C	-0.00343000	-0.44182000	-0.15837000
C	1.19609700	0.26058400	0.03331100
C	2.09597700	-0.73436700	0.50206500
H	3.16633200	-0.70670000	0.26944100
H	1.85120600	-1.30114800	1.39428500
C	0.41090400	-1.79920400	-0.32359400
H	1.06654500	-2.05843100	-1.14636900
C	-1.41381500	-0.03600500	0.00354800
C	1.58926900	1.67408400	-0.29538400
H	-0.16718600	-2.63182200	0.08474500
H	2.66178500	1.72130700	-0.52245500
H	1.03664100	2.07984300	-1.14876800
H	1.42115200	2.34362500	0.55987400
C	-1.73131400	1.43612300	0.20865100
H	-1.39645800	2.02755800	-0.65299400
H	-2.81015800	1.55731000	0.32886200
H	-1.21703300	1.83234600	1.09271700
O	-2.30936900	-0.87753100	-0.01008800

Cyclobutene (Starting material)

C	0.02201700	-0.36304400	0.00003500
C	1.13690700	0.41696800	0.00000100

C	2.08040500	-0.77413400	0.00002700
H	2.71600400	-0.86656300	0.89047600
H	2.71599700	-0.86660400	-0.89042500
C	0.79380400	-1.67151600	0.00002800
H	0.66131700	-2.29596800	-0.89020400
H	0.66128800	-2.29609500	0.89015600
C	-1.43464000	-0.14876900	0.00000700
C	1.45622700	1.87320100	-0.00005900
H	2.06190600	2.13159800	-0.88009700
H	0.56505000	2.50649800	-0.00021300
H	2.06163700	2.13172200	0.88014200
C	-1.98206200	1.26954500	0.00006300
H	-1.63829600	1.82002100	-0.88442700
H	-3.07394800	1.23225900	0.00010400
H	-1.63820400	1.82001800	0.88451800
O	-2.19108800	-1.11629900	-0.00008000



Butadiene (Product)

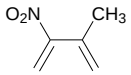
C	0.97410600	-0.14606900	-0.03684100
C	-0.33930900	0.55323500	0.09284600
C	-0.48098200	1.84181300	0.46055300
H	-1.45758400	2.31167700	0.52115000
H	0.38663700	2.44198700	0.71626400
C	2.01625500	0.47620400	-0.60919900
H	1.92910200	1.47125500	-1.03630200
C	1.05507600	-1.55748000	0.49555300
C	-1.52456200	-0.22410600	-0.17604600
H	2.98722000	-0.00676700	-0.68129700
H	2.06127200	-1.96594800	0.36465700
H	0.80216100	-1.59248600	1.56328600
H	0.34671800	-2.21729900	-0.02081100
N	-2.46557600	-0.87200000	-0.39830600

Transition state

C	0.34304300	-0.36808900	0.10121400
C	-0.85723700	0.32258200	-0.06720800
C	-1.78045100	-0.70068400	-0.42220400
H	-2.83369600	-0.66026000	-0.12519700
H	-1.58933000	-1.30774100	-1.30007800
C	-0.03358500	-1.72318100	0.36184200
H	-0.64249600	-1.93817000	1.23112100
C	1.67498900	0.11583500	-0.05861100
C	-1.17958100	1.76293800	0.20076500
H	0.54706300	-2.57072600	-0.01223600
H	-1.98788000	1.84057100	0.94148600
H	-0.31083100	2.30305700	0.58876900
H	-1.52744000	2.27349300	-0.70562500
N	2.76307800	0.51476700	-0.18757500

Cyclobutene (Starting material)

C	0.34026300	-0.31462600	-0.00023500
C	-0.78733000	0.43641700	0.00006900
C	-1.70283300	-0.77724400	0.00043600
H	-2.33446000	-0.88830200	-0.88979700
H	-2.33269100	-0.88825900	0.89195500
C	-0.39665100	-1.64839000	-0.00032200
H	-0.24986200	-2.26660100	0.89201200
H	-0.25068700	-2.26536000	-0.89367800
C	1.72173200	0.01456800	-0.00009900
C	-1.07235100	1.89605900	-0.00017600
H	-1.66392500	2.17729600	0.88183100
H	-0.15013600	2.48610000	-0.00126000
H	-1.66569800	2.17655800	-0.88119500
N	2.86149700	0.26112300	0.00030000



Butadiene (Product)

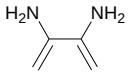
C	1.25004100	0.02872000	-0.00546500
C	-0.12019700	0.59074900	0.10434600
C	-0.43995500	1.85401400	0.39874300
H	-1.47352000	2.17794300	0.44417900
H	0.34383500	2.57549100	0.60178800
C	2.12300900	0.60118500	-0.84733300
H	1.83646400	1.41664100	-1.50552200
C	1.62008500	-1.12144200	0.90402200
H	3.15076500	0.25285100	-0.91182900
H	2.67395900	-1.38619900	0.77591900
H	1.45796900	-0.85444800	1.95666300
H	1.01397300	-2.00771700	0.69041300
N	-1.25091700	-0.35051000	-0.15646100
O	-2.38892900	-0.01168300	0.16498800
O	-0.96668600	-1.41836100	-0.70027000

Transition state

C	0.07313800	-0.38966900	0.12598000
C	-1.18011400	0.18503100	-0.04658700
C	-1.96302900	-0.94142400	-0.42508200
H	-3.00711800	-1.04988100	-0.11556600
H	-1.69439000	-1.50875800	-1.30968100
C	-0.10531600	-1.78096200	0.34146400
H	-0.67847500	-2.10925600	1.20020100
C	-1.68666600	1.56491400	0.23431800
H	0.57078100	-2.52459200	-0.08314900
H	-2.75972900	1.53716600	0.45924600
H	-1.14954400	2.04122200	1.05905700
H	-1.55267600	2.20374900	-0.64839100
N	1.35916800	0.24180200	-0.03849900
O	1.38244300	1.47253500	-0.16393500
O	2.35866900	-0.48623600	-0.04516400

Cyclobutene (Starting material)

C	0.05382000	-0.31742400	-0.00017300
C	-1.12904000	0.33371500	0.00001900
C	-1.89242500	-0.98613200	0.00014800
H	-2.50498500	-1.16267200	-0.89203900
H	-2.50422400	-1.16260100	0.89288600
C	-0.49743200	-1.71640700	-0.00019600
H	-0.28366000	-2.31304300	0.89212800
H	-0.28406400	-2.31270500	-0.89285300
C	-1.59649000	1.74220900	0.00002500
H	-2.22552000	1.93266400	0.88060700
H	-0.75931100	2.44298200	-0.00003200
H	-2.22562300	1.93262200	-0.88048100
N	1.41156900	0.14923400	-0.00000800
O	1.61225300	1.37069300	-0.00010700
O	2.29722200	-0.71290000	0.00021900



Butadiene (Product)

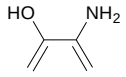
C	-0.74541600	0.09693800	-0.00070700
C	0.74541400	0.09694000	0.00071200
C	1.47108400	1.17802700	-0.34963800
H	2.55737300	1.17024700	-0.30539800
H	0.99055400	2.07519100	-0.71933100
C	-1.47109200	1.17802700	0.34963800
H	-0.99053900	2.07518400	0.71933200
H	-2.55738400	1.17023400	0.30538100
N	-1.31686000	-1.15393500	-0.29272300
H	-2.31848700	-1.13126000	-0.44785600
H	-0.83281600	-1.68643300	-1.00834900
N	1.31686400	-1.15393700	0.29271900
H	0.83284100	-1.68641100	1.00837800
H	2.31849200	-1.13123500	0.44784900

Transition state

C	0.69007900	-0.07451200	-0.03357900
C	-0.69006300	-0.07442100	0.03354600
C	-1.03577800	1.29670900	0.26820800
H	-1.93069500	1.72794400	-0.20456300
H	-0.77711100	1.77144500	1.20867700
C	1.03594800	1.29658700	-0.26820300
H	0.77731700	1.77141100	-1.20863600
H	1.93090900	1.72770900	0.20458400
N	-1.56481100	-1.16145800	-0.09815000
H	-2.54810700	-0.93013800	-0.01700400
H	-1.38330500	-1.77137100	-0.89067800
N	1.56464000	-1.16157700	0.09819200
H	1.38309900	-1.77142200	0.89075900
H	2.54796500	-0.93051400	0.01673400

Cyclobutene (Starting material)

C	0.67581100	-0.15889800	0.00006600
C	-0.67586700	-0.15874100	-0.00006500
C	-0.78657900	1.34593400	-0.00005000
H	-1.23908500	1.80289300	0.89306900
H	-1.23890600	1.80292600	-0.89324300
C	0.78691200	1.34567500	0.00011400
H	1.23966000	1.80269000	-0.89287500
H	1.23946900	1.80264700	0.89322100
N	-1.68577600	-1.11278100	-0.00014400
H	-2.65297000	-0.83518700	-0.00047300
H	-1.49306600	-2.10122700	-0.00026600
N	1.68548000	-1.11312500	0.00019100
H	2.65272000	-0.83569200	-0.00007500
H	1.49258700	-2.10153200	-0.00008000



Butadiene (Product)

C	0.71363500	0.15943000	0.01730300
C	-0.76924300	0.03963500	-0.00280700
C	-1.61941300	1.01228100	0.35794800
H	-2.69208400	0.86532100	0.28986400
H	-1.24547300	1.95597300	0.73487700
C	1.37144000	1.27805300	-0.33469400
H	0.83818100	2.13879200	-0.72039200
H	2.45489400	1.34370900	-0.27283700
N	1.35480300	-1.07185300	0.30740800
H	2.36779700	-1.02062700	0.26543000
H	1.06175000	-1.49104800	1.18789700
O	-1.24562600	-1.18636200	-0.40055300
H	-0.48218700	-1.73463800	-0.65876700

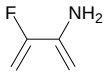
Transition state

C	-0.68556500	-0.16893500	0.04243200
C	0.67713600	0.01432800	-0.03217600
C	0.82118500	1.42069400	-0.26640300
H	1.62954100	1.98635000	0.21806000
H	0.48836600	1.85319800	-1.20384100
C	-1.24859000	1.11886300	0.27399600
H	-1.04826500	1.64049800	1.20279200
H	-2.19550900	1.39881100	-0.20169900
N	1.68503100	-0.95746200	0.10729800
H	2.61544500	-0.63977700	-0.13891200
H	1.69216900	-1.45674700	0.99281300
O	-1.43308400	-1.30471700	-0.13737300
H	-0.89728500	-1.95206700	-0.62841700

Cyclobutene (Starting material)

C	0.64775400	-0.25517000	0.00003600
C	-0.68648300	-0.08138600	-0.00004900

C	-0.57063700	1.42713500	-0.00000700
H	-0.95230100	1.93908500	0.89434100
H	-0.95218000	1.93912900	-0.89438400
C	0.99132900	1.21248500	0.00010000
H	1.49884400	1.60604200	-0.89345200
H	1.49871100	1.60599500	0.89374800
N	-1.80511300	-0.88540500	-0.00010400
H	-2.72998400	-0.48918500	-0.00046900
H	-1.72535400	-1.89008200	-0.00032700
O	1.41889400	-1.39759700	0.00009200
H	2.35513000	-1.15076100	0.00005300



Butadiene (Product)

C	0.74209300	0.13086300	0.00045700
C	-0.73554200	0.05884500	0.00244500
C	-1.62859900	0.99472300	0.31584200
H	-2.69166700	0.79582800	0.23648700
H	-1.30264100	1.96776600	0.66134100
C	1.38580000	1.27931600	-0.29407900
H	0.84017100	2.16705700	-0.58761500
H	2.46889000	1.34877200	-0.24401100
N	1.37713500	-1.05211200	0.39176600
H	2.34921800	-1.12680000	0.11809500
H	0.86045600	-1.90127700	0.19905100
F	-1.19409800	-1.18544900	-0.36374300

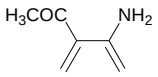
Transition state

C	-0.66272300	-0.18579700	0.01737100
C	0.69106500	0.01966700	-0.05943600
C	0.77722700	1.43904500	-0.24533100
H	1.53930000	2.01957900	0.28766500
H	0.43150800	1.88110600	-1.17203200
C	-1.30838400	1.04703100	0.27057900
H	-1.12208600	1.58533400	1.19296100

H	-2.26759200	1.28156000	-0.20312800
N	1.75906600	-0.82706200	0.22661100
H	2.53610200	-0.79024200	-0.42252700
H	1.50049200	-1.78265700	0.44585400
F	-1.32381100	-1.36943600	-0.17935200

Cyclobutene (Starting material)

C	0.62066800	-0.32530600	0.00004000
C	-0.68388000	-0.00910000	-0.00004500
C	-0.36450700	1.47536500	-0.00000400
H	-0.68107100	2.02444200	0.89590000
H	-0.68093400	2.02446600	-0.89594300
C	1.16252800	1.07035500	0.00011000
H	1.71377500	1.39061800	-0.89383000
H	1.71363300	1.39058700	0.89415000
N	-1.89109300	-0.65840800	-0.00011400
H	-2.75634100	-0.14425600	-0.00043300
H	-1.94415200	-1.66518400	-0.00032000
F	1.27376500	-1.51996600	0.00007400



Butadiene (Product)

C	1.28107000	-0.03484800	0.04792800
C	-0.04434500	0.64984200	0.03492300
C	-0.14263000	1.98905800	0.06290600
H	-1.11709400	2.46855500	0.03691700
H	0.74051200	2.61984500	0.10929400
C	2.19356500	0.14225700	-0.92698100
H	1.96696900	0.75112800	-1.79432500
C	-1.32135400	-0.16652200	-0.04214000
H	3.16519000	-0.34604300	-0.89635800
N	1.44568200	-0.93099700	1.11989600
H	2.38083700	-1.31505800	1.20899800
H	1.10415400	-0.58987100	2.01311900
C	-1.24030800	-1.55891200	-0.63153900

H	-0.56519300	-2.18640200	-0.03978500
H	-2.23954300	-1.99841800	-0.65973100
H	-0.82473700	-1.51536600	-1.64645900
O	-2.38585800	0.31291900	0.31981000

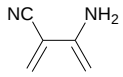
Transition state

C	0.00732300	-0.41920600	-0.19043300
C	1.19363500	0.31316300	0.02082200
C	2.14117800	-0.62127700	0.52462400
H	3.21311400	-0.51458700	0.32253300
H	1.90496500	-1.15647100	1.43732400
C	0.48452700	-1.75615600	-0.34558000
H	1.15769900	-2.00806300	-1.15594100
C	-1.40065800	-0.06677300	0.01163900
H	-0.06499000	-2.60143600	0.07699500
N	1.46232100	1.63110400	-0.27494200
H	2.39438700	1.97710900	-0.08829400
H	1.00644800	2.05745900	-1.07088300
C	-1.76920500	1.39336300	0.22938400
H	-1.02801600	1.92557800	0.83489900
H	-1.83160400	1.90469700	-0.74169600
H	-2.75421500	1.44589900	0.70030500
O	-2.27185500	-0.93832400	0.01332600

Cyclobutene (Starting material)

C	0.02384900	-0.36747100	0.00486400
C	1.10857800	0.47302800	0.00213300
C	2.12385200	-0.64700600	-0.00382600
H	2.76580800	-0.70061800	0.88473800
H	2.75351600	-0.69719500	-0.90074900
C	0.88786500	-1.61944700	0.00235700
H	0.80466600	-2.25150600	-0.88895700
H	0.81093400	-2.25310800	0.89300700
C	-1.41629100	-0.19993700	0.00144900
N	1.32434700	1.81646300	-0.04377300
H	2.24717400	2.17048800	0.16593100
H	0.56195200	2.45880900	0.12526800

C	-1.97040300	1.22306200	-0.00520600
H	-1.61056300	1.78136400	-0.88007400
H	-3.06208700	1.18618700	-0.03218000
H	-1.65881700	1.76727200	0.89745100
O	-2.17846400	-1.16878900	0.00391900



Butadiene (Product)

C	-0.96676900	-0.21668700	0.01262800
C	0.30729700	0.55830500	-0.08269900
C	0.37661500	1.86229700	-0.40922500
H	1.32446300	2.39058700	-0.43038100
H	-0.52127500	2.41599400	-0.66299800
C	-2.06861800	0.33106100	0.56433100
H	-2.04426200	1.32476900	0.99339400
C	1.52438100	-0.16858600	0.17819600
H	-3.00907100	-0.21145100	0.60733600
N	2.48125600	-0.80065700	0.37884800
N	-0.92693000	-1.49201900	-0.55726500
H	-1.64887100	-2.12915300	-0.24292000
H	-0.01869900	-1.94035300	-0.59489800

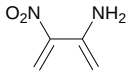
Transition state

C	-0.32869600	-0.37435700	-0.10932700
C	0.84132900	0.38168900	0.05128500
C	1.84631800	-0.55957900	0.42260200
H	2.88976000	-0.42055600	0.12287700
H	1.70280300	-1.13180800	1.33143300
C	0.14155100	-1.70080800	-0.35927600
H	0.75932700	-1.89892000	-1.22599900
C	-1.67290100	0.04701500	0.06735900
H	-0.38075600	-2.57547600	0.03913600
N	-2.77107500	0.41586700	0.21425600
N	1.06365800	1.69821500	-0.26981200
H	1.74058800	2.21748000	0.27289000

H	0.27458800	2.24694200	-0.58730000

Cyclobutene (Starting material)

C	-0.34264300	-0.31533100	0.00004600
C	0.76445600	0.48627100	-0.00008200
C	1.74132900	-0.66784500	-0.00000300
H	2.37315100	-0.74440000	0.89313800
H	2.37309300	-0.74456900	-0.89317100
C	0.47633100	-1.60284200	0.00012500
H	0.37869300	-2.23076400	-0.89293400
H	0.37876100	-2.23060900	0.89329900
C	-1.72471400	-0.03861900	0.00007900
N	-2.87011200	0.19525800	0.00010700
N	0.99163500	1.82021800	-0.00021400
H	1.92948600	2.19045700	-0.00031000
H	0.22760300	2.48175000	-0.00026100



Butadiene (Product)

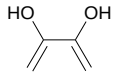
C	-1.26623600	-0.01627900	0.01976800
C	0.09714400	0.55799100	-0.15049300
C	0.36443100	1.80959400	-0.53318200
H	1.38302500	2.17621600	-0.58847700
H	-0.44893800	2.47444900	-0.80023400
C	-2.15526700	0.64688500	0.78687600
H	-1.88030700	1.55420900	1.31038300
H	-3.17576100	0.29103800	0.90279300
N	-1.57407500	-1.14551600	-0.74964900
H	-2.46149100	-1.57071600	-0.50172900
H	-0.83422800	-1.83988300	-0.76485900
N	1.26454800	-0.32395100	0.13825100
O	1.03237700	-1.52303700	0.32297100
O	2.38561700	0.17451200	0.17504000

Transition state

C	-0.05109500	-0.39630700	-0.13906400
C	1.17049000	0.26568200	0.04434900
C	2.07780400	-0.77542900	0.39904400
H	3.12735800	-0.74276100	0.09456500
H	1.86940400	-1.35597900	1.28932600
C	0.22676800	-1.76460600	-0.37883000
H	0.82248700	-2.04683800	-1.23766300
H	-0.39704100	-2.55482600	0.04247800
N	1.48504500	1.55916200	-0.24080700
H	2.27785900	1.97656500	0.22724400
H	0.69929700	2.17773800	-0.41009000
N	-1.34570800	0.16491600	0.04171500
O	-2.31111600	-0.59730800	0.16969500
O	-1.42869900	1.40999700	0.05965400

Cyclobutene (Starting material)

C	-0.03848700	-0.34896000	0.00003900
C	1.08142900	0.43495900	-0.00008400
C	2.00217200	-0.77046800	-0.00001700
H	2.62725100	-0.87200300	0.89419600
H	2.62717200	-0.87216400	-0.89426700
C	0.69635100	-1.66380600	0.00012100
H	0.57344000	-2.28606200	-0.89261400
H	0.57352100	-2.28590500	0.89297600
N	1.30165000	1.75480900	-0.00021200
H	2.23307000	2.14273700	-0.00029300
H	0.50078600	2.37693100	-0.00023000
N	-1.38229800	0.03273200	0.00006700
O	-1.61877500	1.26590100	-0.00005600
O	-2.25866300	-0.84423500	0.00016800



Butadiene (Product)

C	-0.71793000	0.11922700	-0.00925600
C	0.76663500	0.06410500	-0.00040300
C	1.56763600	1.11853800	-0.21292100
H	2.64516100	1.00724700	-0.16376700
H	1.15847500	2.09330700	-0.44536200
C	-1.47803700	1.19946900	0.21874000
H	-1.02875900	2.14993300	0.47664100
H	-2.56242000	1.15901900	0.15455900
O	-1.23507800	-1.13740600	-0.26470900
H	-2.19874000	-1.13187300	-0.15472100
O	1.30587500	-1.16980000	0.25197500
H	0.59008200	-1.82801400	0.25756200

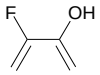
Transition state

C	0.69626600	-0.10368200	-0.04429700
C	-0.67355200	-0.07302300	0.02227400
C	-1.02456400	1.29039900	0.25318700
H	-1.88644100	1.73801200	-0.25878900
H	-0.76624100	1.77149200	1.18975300
C	1.09836400	1.24998400	-0.23454300
H	0.84691100	1.76468000	-1.15397000
H	1.98441700	1.64038600	0.27794700
O	-1.51440100	-1.13781500	-0.22140000
H	-2.35338200	-1.00104600	0.24476600
O	1.57654200	-1.13626700	0.12587600
H	1.09852400	-1.90293300	0.48476500

Cyclobutene (Starting material)

C	0.67071300	-0.19168500	0.00003900
C	-0.67050600	-0.19148500	-0.00007400
C	-0.78857000	1.31567200	0.00001000
H	-1.23462800	1.77113600	0.89496500

H	-1.23447700	1.77125000	-0.89496300
C	0.78849800	1.31655900	0.00014700
H	1.23347300	1.77127600	-0.89550100
H	1.23331500	1.77116000	0.89593200
O	-1.60491200	-1.18677100	-0.00019500
H	-2.49148400	-0.79626100	-0.00031800
O	1.60510900	-1.18664600	0.00007500
H	2.49142000	-0.79559000	0.00011300



Butadiene (Product)

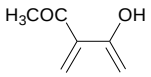
C	0.73507500	0.08864600	0.00425900
C	-0.74196800	0.05319600	0.00490400
C	-1.57717800	1.02418300	0.37120600
H	-2.65052700	0.89045300	0.29178900
H	-1.19380800	1.95753800	0.76444100
C	1.44529400	1.16935700	-0.35723200
H	0.95085900	2.05566900	-0.73435000
H	2.53061300	1.18628600	-0.29528900
F	-1.24424500	-1.13580900	-0.42614800
O	1.26978600	-1.10091600	0.41822100
H	2.23544700	-1.07263100	0.32415800

Transition state

C	-0.67760300	-0.14796600	0.03902100
C	0.68534300	-0.06860100	-0.04480900
C	0.94102300	1.32147200	-0.25332600
H	1.76502400	1.82259100	0.26923500
H	0.63956800	1.79447100	-1.18049100
C	-1.17455700	1.16035500	0.25820600
H	-0.93703800	1.69028700	1.17312700
H	-2.08530700	1.50276400	-0.24390100
F	-1.46577700	-1.23333100	-0.16971000
O	1.59163400	-1.05621700	0.21712900
H	2.43144700	-0.85195700	-0.22217100

Cyclobutene (Starting material)

C	0.65558800	-0.24642200	0.00005000
C	-0.67700800	-0.13382700	-0.00007700
C	-0.62718200	1.38242800	0.00001400
H	-1.02576200	1.87409900	0.89643100
H	-1.02560000	1.87420000	-0.89642000
C	0.94522800	1.22674200	0.00014600
H	1.43560600	1.62790700	-0.89494500
H	1.43544100	1.62782000	0.89536600
F	1.50553200	-1.29186500	0.00008600
O	-1.70044600	-1.02496100	-0.00021100
H	-2.54565900	-0.55107600	-0.00031800



Butadiene (Product)

C	-1.27354800	-0.05869000	-0.04399000
C	0.03319700	0.64646900	-0.07087300
C	0.09684700	1.98301700	-0.18522400
H	1.06046900	2.48395000	-0.17642900
H	-0.79862700	2.58682000	-0.29607800
C	-2.28314900	0.24268600	0.78784000
H	-2.16819700	1.01684200	1.53654100
H	-3.23633400	-0.28048100	0.74886200
O	-1.33127900	-1.05871600	-0.98849300
H	-2.17881900	-1.52777200	-0.91601200
C	1.33014800	-0.12964900	0.06546800
C	1.26862800	-1.57428400	0.51533800
O	2.39974400	0.41704500	-0.15675000
H	0.87290700	-2.19733100	-0.29480000
H	2.27419300	-1.91005300	0.77712000
H	0.59395700	-1.69589500	1.37138100

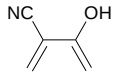
Transition state

C	0.01672600	-0.41900100	-0.17009100

C	1.17319200	0.34036300	0.00793200
C	2.19125400	-0.53387200	0.46758800
H	3.24205700	-0.38771300	0.19426600
H	2.03355100	-1.07951400	1.39088900
C	0.53562800	-1.74445900	-0.29993900
H	1.18834300	-1.99412900	-1.12736600
H	0.03967600	-2.59557500	0.17355300
O	1.33608000	1.64568700	-0.34315700
H	2.15728900	1.98982800	0.04392600
C	-1.40673500	-0.08823800	0.01032000
C	-1.79270900	1.36985000	0.17605800
O	-2.25103200	-0.98172600	0.03475000
H	-1.50487800	1.94474700	-0.71247300
H	-2.87227400	1.44078200	0.32671100
H	-1.26828700	1.82202100	1.02655200

Cyclobutene (Starting material)

C	0.02943200	-0.34718400	0.00017900
C	1.09698600	0.49026300	-0.00003700
C	2.14746700	-0.59296000	-0.00020200
H	2.78265900	-0.63852700	0.89350000
H	2.78198900	-0.63874000	-0.89437400
C	0.92121800	-1.58221700	0.00024300
H	0.85074900	-2.21289800	-0.89206700
H	0.85115900	-2.21238500	0.89295900
O	1.19622000	1.83605900	0.00006900
H	2.12987300	2.10051000	-0.00052500
C	-1.42482500	-0.20305200	0.00001600
C	-1.99827600	1.20374500	0.00007000
O	-2.14985500	-1.19645300	-0.00022700
H	-1.65481100	1.76126700	-0.88015800
H	-3.08950000	1.15117500	-0.00011800
H	-1.65505600	1.76117600	0.88042800



Butadiene (Product)

C	-0.96695700	-0.20338000	0.00480700
C	0.32241200	0.53212700	-0.08554500
C	0.40829200	1.84237900	-0.38105300
H	1.36491100	2.35403600	-0.40330100
H	-0.48215900	2.41817500	-0.61164400
C	-2.07744300	0.30514300	0.56068800
H	-2.06597300	1.27948500	1.03302200
H	-3.01261800	-0.24871000	0.57642100
O	-0.86355900	-1.45346400	-0.54138900
H	-1.67685600	-1.95704600	-0.37555400
C	1.52515600	-0.22305500	0.15891800
N	2.50177400	-0.81964400	0.36646900

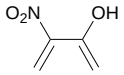
Transition state

C	0.34063700	0.33244400	-0.12323600
C	-0.84277600	-0.38191200	0.03584400
C	-1.83930700	0.55782700	0.41234100
H	-2.88064700	0.44374100	0.09344900
H	-1.70287900	1.12584500	1.32524200
C	-0.11247100	1.67424500	-0.33006000
H	-0.71823200	1.90880000	-1.19610600
H	0.40923100	2.52763800	0.11208800
O	-1.02391600	-1.68881500	-0.26869600
H	-1.84401000	-2.01613300	0.13475900
C	1.68435600	-0.09596500	0.05227200
N	2.79217500	-0.42845800	0.19959600

Cyclobutene (Starting material)

C	-0.35053600	-0.26684200	0.00003900
C	0.77388400	0.48735600	-0.00007800
C	1.73662500	-0.67592400	-0.00000400
H	2.36442600	-0.77175700	0.89428400

H	2.36434800	-0.77194100	-0.89432800
C	0.44360900	-1.57296700	0.00014800
H	0.32650000	-2.19376800	-0.89429600
H	0.32657600	-2.19357600	0.89473500
O	0.96181700	1.81665200	-0.00021700
H	1.90970100	2.02477900	-0.00028500
C	-1.73509900	0.01389100	0.00006400
N	-2.88528500	0.20856500	0.00008900



Butadiene (Product)

C	-1.24688200	-0.01881600	-0.05768200
C	0.09980300	0.59325400	-0.07530200
C	0.37532100	1.88677700	-0.24515100
H	1.39699700	2.24906600	-0.22357100
H	-0.42941800	2.59458700	-0.41039300
C	-2.21628400	0.37626000	0.77894700
H	-2.01822700	1.11903800	1.54186800
H	-3.21483400	-0.05183300	0.73953900
O	-1.36895900	-0.98024600	-1.02347600
H	-2.18266000	-1.49102700	-0.88344100
N	1.23719600	-0.34434900	0.14863200
O	0.97063300	-1.41506700	0.68915500
O	2.36282900	0.01603400	-0.19184100

Transition state

C	0.06064800	0.34163100	-0.16018600
C	-1.17289600	-0.27420500	0.02560100
C	-2.04784300	0.76523000	0.43676500
H	-3.09785900	0.78399100	0.12835900
H	-1.82588000	1.30635300	1.34930000
C	-0.21541900	1.72346800	-0.32340800
H	-0.80616400	2.05719300	-1.16757200
H	0.40222700	2.48725600	0.15227000
O	-1.51036600	-1.53304300	-0.31127400

H	-2.37877600	-1.75578000	0.06238400
N	1.37445700	-0.20158600	0.03354400
O	2.31599700	0.60446100	0.05247400
O	1.48665800	-1.42200100	0.17977700

Cyclobutene (Starting material)

C	-0.05101200	-0.27666700	0.00002600
C	1.10734900	0.42399800	-0.00009300
C	1.97067400	-0.82035600	-0.00001700
H	2.58728400	-0.95977900	0.89558700
H	2.58720700	-0.95994400	-0.89564800
C	0.61461000	-1.62895100	0.00011800
H	0.45247300	-2.23920800	-0.89360500
H	0.45255400	-2.23904900	0.89396400
O	1.40052800	1.72346900	-0.00022700
H	2.36350900	1.85061100	-0.00028500
N	-1.41969800	0.09872800	0.00005500
O	-1.69324100	1.30567200	-0.00003800
O	-2.25164500	-0.82062600	0.00018900

Butadiene (Product)

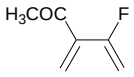
C	-0.73540500	0.07957000	-0.00036400
C	0.73540400	0.07958900	0.00036200
C	1.54414500	1.08128400	-0.34219900
H	2.62039100	0.97881300	-0.25608200
H	1.13615600	2.01048600	-0.72089300
C	-1.54414500	1.08125200	0.34218900
H	-1.13628800	2.01048300	0.72089800
H	-2.62038700	0.97888700	0.25612900
F	-1.25860200	-1.10605700	-0.41129700
F	1.25861700	-1.10603700	0.41129900

Transition state

C	0.67942600	-0.11024600	-0.05353400
C	-0.67948700	-0.11008400	0.05325400
C	-1.06561800	1.23645700	0.26621800
H	-1.93508300	1.65911200	-0.24602800
H	-0.77834700	1.74348200	1.17935300
C	1.06590400	1.23620400	-0.26617000
H	0.77879500	1.74379900	-1.17902000
H	1.93532400	1.65880700	0.24617400
F	1.54038100	-1.12895300	0.17039300
F	-1.54060700	-1.12873500	-0.17029100

Cyclobutene (Starting material)

C	0.66674000	-0.18892400	0.00005100
C	-0.66670200	-0.18884500	-0.00007300
C	-0.79156700	1.31204200	0.00001300
H	-1.23914100	1.75424800	0.89672700
H	-1.23899700	1.75436000	-0.89671700
C	0.79161800	1.31195100	0.00013800
H	1.23939100	1.75431900	-0.89639600
H	1.23924600	1.75422300	0.89679100
F	-1.61126000	-1.13852900	-0.00021300
F	1.61114500	-1.13863700	0.00008200



Butadiene (Product)

C	-1.27151400	-0.06720300	-0.03598000
C	0.01716000	0.65232400	-0.06112900
C	0.05885300	1.99122600	-0.16697600
H	1.01460700	2.50668400	-0.14735500
H	-0.84495000	2.58214400	-0.27988500
C	-2.34614100	0.17563200	0.71287400
H	-2.32825500	0.96819900	1.45142500
H	-3.24818200	-0.41734300	0.60475100

C	1.32509700	-0.10949700	0.07294000
F	-1.31462900	-1.10907500	-0.92851600
C	1.27742300	-1.56798300	0.47530700
H	0.90924200	-2.17494600	-0.36037700
H	2.28315100	-1.89695700	0.74443300
H	0.58962900	-1.72948600	1.31395500
O	2.38639400	0.46204800	-0.11906600

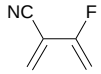
Transition state

C	1.16330700	0.36198600	0.01885600
C	0.03087800	-0.41191200	-0.17135000
C	0.60692700	-1.71669800	-0.28928000
H	0.16225700	-2.58159900	0.20860800
H	1.25998300	-1.94391400	-1.12272900
C	2.22742900	-0.44383600	0.46308700
H	2.10594200	-1.01280400	1.37792600
H	3.26078700	-0.24447200	0.17024300
F	1.32622600	1.66869900	-0.30425600
C	-1.40572500	-0.11971400	0.00860600
C	-1.82302500	1.32768600	0.17810300
H	-2.90813200	1.38080000	0.28961100
H	-1.33974400	1.77295400	1.05659700
H	-1.51128900	1.92078900	-0.69047200
O	-2.22057300	-1.03688900	0.02504900

Cyclobutene (Starting material)

C	0.04716600	-0.33606000	0.00009700
C	1.09309800	0.51212300	0.00000700
C	2.18798800	-0.50788700	-0.00004700
H	2.82157900	-0.52566000	0.89381800
H	2.82136700	-0.52571800	-0.89406200
C	0.99118200	-1.53731400	0.00007700
H	0.93744700	-2.16548900	-0.89412800
H	0.93758200	-2.16543300	0.89432900
C	-1.41876600	-0.23633000	-0.00001300
F	1.18285200	1.84971200	-0.00004500
C	-2.03401300	1.15029300	0.00004600

H	-1.70777300	1.71695900	-0.88097000
H	-3.12297300	1.06552500	-0.00025700
H	-1.70828500	1.71657300	0.88150800
O	-2.10306800	-1.25414000	-0.00010500



Butadiene (Product)

C	-0.96307700	-0.21245000	0.00825600
C	0.30592200	0.54450000	-0.07151600
C	0.36199200	1.86391000	-0.33483700
H	1.30716100	2.39651700	-0.34405500
H	-0.54049400	2.42676400	-0.55045700
C	-2.12552200	0.19672200	0.51307300
H	-2.21320800	1.17333000	0.97353100
H	-2.99749100	-0.44739100	0.48609600
C	1.52095500	-0.19644000	0.15317800
F	-0.85432600	-1.46750000	-0.50482200
N	2.50447800	-0.78845300	0.33848000

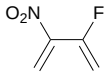
Transition state

C	-0.83512100	-0.39682100	0.04931000
C	0.33003200	0.32855400	-0.12458100
C	-0.17517300	1.65384700	-0.32828400
H	0.29903000	2.52480700	0.13111400
H	-0.78378000	1.86265000	-1.19875000
C	-1.87506400	0.48164200	0.41002600
H	-1.76775100	1.08006000	1.30727400
H	-2.90212200	0.31642800	0.07749200
F	-1.02834300	-1.70020700	-0.22222700
C	1.68623400	-0.06027200	0.05178600
N	2.80346600	-0.36053900	0.19048200

Cyclobutene (Starting material)

C	-0.33586200	-0.26499200	0.00005600

C	0.76889100	0.50235800	-0.00010900
C	1.77946500	-0.60274000	0.00002700
H	2.40833000	-0.67041800	0.89434000
H	2.40833500	-0.67061300	-0.89426700
C	0.51309000	-1.54207600	0.00011400
H	0.41123200	-2.16114100	-0.89618300
H	0.41127800	-2.16101600	0.89650100
C	-1.73013900	-0.02922100	0.00009900
F	0.95351100	1.82063700	-0.00027200
N	-2.88477900	0.12821200	0.00013500



Butadiene (Product)

C	1.24325000	-0.02396200	0.04036000
C	-0.09342300	0.59430500	0.06668200
C	-0.35316500	1.89204900	0.23375800
H	-1.37150900	2.26383000	0.20965000
H	0.45799400	2.59266200	0.39875000
C	2.26334200	0.32012800	-0.74054600
H	2.13875600	1.08167000	-1.50104600
H	3.22658200	-0.16904500	-0.64295900
F	1.39131000	-1.00394500	0.97102800
N	-1.23828600	-0.33714500	-0.14526000
O	-2.36890400	0.06243500	0.12397800
O	-0.96430100	-1.44602400	-0.59752200

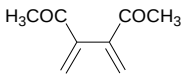
Transition state

C	-1.16225300	-0.30292600	0.03910700
C	0.04598800	0.33582800	-0.15903900
C	-0.29502500	1.70596200	-0.31212900
H	0.26928100	2.49516300	0.18731100
H	-0.88711800	2.01476500	-1.16495300
C	-2.09356500	0.67859400	0.43008700
H	-1.90764200	1.24725500	1.33418300
H	-3.13341900	0.64398900	0.09875200

N	1.38093300	-0.16675500	0.03372600
F	-1.50255500	-1.55782100	-0.27165400
O	1.52400900	-1.38220500	0.18053300
O	2.29405300	0.66742400	0.04013600

Cyclobutene (Starting material)

C	-0.03298800	-0.27111300	0.00000300
C	1.10091500	0.45055800	-0.00008400
C	2.02293500	-0.73447200	-0.00001300
H	2.64345600	-0.84343000	0.89554200
H	2.64340300	-0.84358300	-0.89558600
C	0.69537400	-1.59521300	0.00010100
H	0.55366200	-2.20647000	-0.89535000
H	0.55371200	-2.20631400	0.89566700
F	1.38104700	1.74083100	-0.00020200
N	-1.42257700	0.05869300	0.00000800
O	-1.73132300	1.25431100	-0.00000900
O	-2.21655600	-0.88894700	0.00018900



Butadiene (Product)

C	0.70703100	0.69917400	-0.23889600
C	-0.70826500	0.69957400	0.23578900
C	-1.19654200	1.66989500	1.02644100
H	-2.23837200	1.65396100	1.33405600
H	-0.56978500	2.48437800	1.37918800
C	1.19458600	1.66679900	-1.03328800
H	0.56727300	2.47957000	-1.38899900
C	-1.65918400	-0.38934200	-0.22621400
H	2.23633500	1.65028700	-1.34114600
C	1.65890600	-0.38727200	0.22688700
C	1.26880000	-1.19680400	1.44854400
O	2.72284100	-0.57494300	-0.34306800
H	2.06082200	-1.91372500	1.67394300
H	1.11130300	-0.53448500	2.30913900

H	0.32408500	-1.73269400	1.29474600
O	-2.72542700	-0.57230600	0.34097900
C	-1.26428500	-1.20890700	-1.43963000
H	-0.32933200	-1.75704200	-1.26913900
H	-2.06230900	-1.91708700	-1.67139900
H	-1.08561900	-0.55386700	-2.30146500

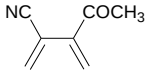
Transition state

C	-0.66091400	0.50291700	0.10885100
C	0.72169000	0.55589100	-0.16552600
C	0.95265300	1.93434900	-0.42973900
H	1.87879700	2.43112600	-0.13420000
H	0.40344500	2.42063700	-1.22874400
C	-0.95242400	1.83035200	0.54098500
H	-0.42722300	2.23852600	1.39794000
C	-1.65121400	-0.56661200	-0.17251000
H	-1.88793300	2.34527800	0.30540900
C	1.85295300	-0.39655500	0.03938100
O	-1.30615500	-1.65455400	-0.62114200
O	2.99228900	0.00403900	-0.18051900
C	1.58846200	-1.79587100	0.54171600
H	2.54235800	-2.29957500	0.71303900
H	1.00562900	-1.77547800	1.47071300
H	0.98907000	-2.34920200	-0.18815600
C	-3.11167700	-0.26960000	0.11921000
H	-3.72151600	-1.11305800	-0.21099700
H	-3.26811600	-0.10427000	1.19236700
H	-3.44075900	0.64091800	-0.39828900

Cyclobutene (Starting material)

C	0.68478700	0.51655300	0.00501500
C	-0.68475700	0.51659600	-0.00502600
C	-0.78172900	2.02961100	-0.02219100
H	-1.28421300	2.47260000	0.84483200
H	-1.22612300	2.44632100	-0.93229600
C	0.78183400	2.02954400	0.02241500
H	1.28436500	2.47263800	-0.84453200

H	1.22627300	2.44611800	0.93256300
C	1.84209300	-0.41655300	-0.00788300
C	-1.84208700	-0.41647100	0.00777500
C	-1.67425400	-1.89774100	0.27455300
O	-2.95467400	0.06239600	-0.18306400
H	-1.07670000	-2.07584600	1.17560700
H	-2.66283800	-2.34613600	0.39566300
H	-1.16429200	-2.38650300	-0.56329000
O	2.95475800	0.06230500	0.18264600
C	1.67407000	-1.89786500	-0.27434100
H	1.07621700	-2.07603900	-1.17517900
H	2.66256200	-2.34640500	-0.39568100
H	1.16432900	-2.38640600	0.56376100



Butadiene (Product)

C	0.38263200	0.70366800	-0.15737800
C	-1.05194900	0.47324200	0.19581200
C	-1.73977200	1.26183900	1.04333800
H	-2.79279200	1.09471800	1.24812800
H	-1.24891900	2.08746400	1.54973000
C	0.77790200	1.88291500	-0.66381400
H	0.07168400	2.68116600	-0.87197700
C	-1.73041900	-0.62577700	-0.44449000
H	1.82718400	2.04999000	-0.88875400
N	-2.25914300	-1.51518700	-0.97746700
C	1.43063700	-0.37144400	0.08288900
C	1.02421400	-1.63914200	0.80320400
O	2.58027100	-0.19252400	-0.28546800
H	1.92113500	-2.21166000	1.04755400
H	0.46130800	-1.41685800	1.71786100
H	0.37276800	-2.25013000	0.16609600

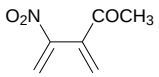
Transition state

C	-1.01108600	0.36982500	0.11442300

C	0.35644900	0.52878900	-0.16118300
C	0.48430100	1.92481200	-0.40657700
H	1.36555200	2.48684500	-0.09276800
H	-0.08839600	2.37108800	-1.21198900
C	-1.44144700	1.66107600	0.53527000
H	-0.96184300	2.11101300	1.39702400
C	-1.86808900	-0.74419200	-0.12695300
H	-2.43186000	2.05541200	0.29745800
N	-2.57598600	-1.64985900	-0.31905600
C	1.50699000	-0.39979300	0.00401200
C	1.22636500	-1.86249300	0.27241500
O	2.64711700	0.04275600	-0.07094500
H	2.17148600	-2.40794000	0.31218400
H	0.69119700	-1.98865900	1.22172900
H	0.58793600	-2.28893900	-0.51113200

Cyclobutene (Starting material)

C	-1.01334600	0.28278800	-0.00001500
C	0.32976600	0.49822000	-0.00004700
C	0.19198500	2.00742300	0.00009600
H	0.58657000	2.50837200	-0.89001000
H	0.58675600	2.50829500	0.89015800
C	-1.35953400	1.76523000	0.00019600
H	-1.88995200	2.11363800	0.89292100
H	-1.89016700	2.11389200	-0.89229900
C	-1.83249600	-0.87615200	-0.00011100
N	-2.53399000	-1.80707700	-0.00027500
C	1.53785600	-0.36022100	-0.00006500
C	1.36187200	-1.86317100	0.00043100
O	2.63941500	0.17502600	-0.00043100
H	0.79509500	-2.18922300	-0.88050300
H	2.34343200	-2.34182900	0.00109200
H	0.79427100	-2.18851700	0.88109600



Butadiene (Product)

C	0.66011100	0.74403500	-0.13516500
C	-0.75986600	0.62564500	0.27184800
C	-1.41272600	1.40306300	1.13958200
H	-2.46788000	1.25681700	1.34176100
H	-0.88467100	2.19438000	1.66087200
C	1.10202800	1.86914800	-0.71882100
H	0.43331800	2.69061300	-0.95861400
H	2.15269300	1.96714500	-0.97586600
C	1.66233200	-0.35894800	0.16980500
C	1.24829900	-1.48528900	1.09352900
O	2.78553000	-0.30337600	-0.30079500
H	2.13764800	-2.04113700	1.39738600
H	0.72267400	-1.10973100	1.97937400
H	0.56830100	-2.16723900	0.56891600
N	-1.53821300	-0.45679700	-0.40307800
O	-0.93576000	-1.11272800	-1.25440300
O	-2.71172800	-0.63129500	-0.08442200

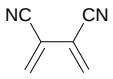
Transition state

C	-0.73918000	0.47542300	0.14748200
C	0.62084900	0.56604800	-0.16530800
C	0.75782800	1.95991800	-0.41848300
H	1.63810200	2.51916900	-0.09746400
H	0.17897800	2.41359600	-1.21590100
C	-1.16025300	1.76140400	0.55314100
H	-0.67944800	2.22357800	1.40833200
H	-2.13328500	2.17041700	0.27972000
C	1.80460700	-0.32480200	0.03505900
C	1.62622700	-1.73395300	0.54496200
O	2.91140200	0.14304000	-0.20530200
H	2.60290600	-2.13616500	0.82282900
H	0.94439100	-1.77144200	1.40181100
H	1.18031100	-2.35638500	-0.23843700

N	-1.67428100	-0.59873000	-0.13478000
O	-1.23228000	-1.64515000	-0.61713700
O	-2.86317800	-0.38487500	0.12262000

Cyclobutene (Starting material)

C	0.75250800	0.42771100	-0.00006900
C	-0.59936600	0.53045200	0.00000400
C	-0.52259600	2.04912200	0.00001600
H	-0.94560600	2.52248000	0.89150400
H	-0.94570200	2.52251500	-0.89140700
C	1.04198900	1.89959800	-0.00004600
H	1.55215300	2.27649200	-0.89205400
H	1.55223900	2.27646200	0.89192100
C	-1.83899200	-0.30272900	0.00003800
C	-1.77581300	-1.80791100	0.00030200
O	-2.90105100	0.30729000	-0.00014200
H	-1.22666200	-2.17364200	0.87488600
H	-2.79402600	-2.20277400	0.00053100
H	-1.22695900	-2.17393500	-0.87434700
N	1.68946700	-0.67423000	-0.00006100
O	1.24924000	-1.82736600	-0.00049300
O	2.88455000	-0.36810400	0.00037600



Butadiene (Product)

C	-0.73374200	0.47311900	0.14268000
C	0.73386200	0.47306900	-0.14272600
C	1.36619300	1.52033500	-0.70300600
H	2.43862700	1.50823400	-0.86788800
H	0.81483900	2.40095400	-1.01728200
C	-1.36599800	1.52039500	0.70304200
H	-0.81460000	2.40096200	1.01738100
C	-1.47652700	-0.70765900	-0.21351900
H	-2.43841500	1.50832500	0.86802100
N	-2.07266800	-1.66036000	-0.51315500

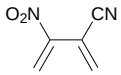
C	1.47649900	-0.70779100	0.21352200
N	2.07235700	-1.66068000	0.51312800

Transition state

C	-0.68848700	0.28330000	0.12654400
C	0.68847500	0.28329700	-0.12657000
C	0.98029100	1.63919800	-0.45549700
H	1.91801800	2.11876800	-0.16768700
H	0.47490300	2.08617100	-1.30371200
C	-0.98024500	1.63920000	0.45551200
H	-0.47487800	2.08600100	1.30382800
C	1.64165600	-0.75909700	0.06024900
H	-1.91797100	2.11879000	0.16774200
N	2.43606800	-1.59793100	0.20813900
C	-1.64166800	-0.75905800	-0.06032000
N	-2.43609800	-1.59789400	-0.20809300

Cyclobutene (Starting material)

C	0.67892100	0.22024800	0.00006400
C	-0.67880500	0.22003900	-0.00003900
C	-0.78517100	1.73791000	0.00002500
H	-1.25165200	2.16659200	0.89299300
H	-1.25148300	2.16668300	-0.89298800
C	0.78437400	1.73831100	0.00017700
H	1.25080400	2.16742600	-0.89262500
H	1.25063500	2.16730900	0.89312300
C	-1.66087500	-0.80258500	-0.00017700
N	-2.50044900	-1.61020400	-0.00029300
C	1.66124200	-0.80213700	0.00008400
N	2.50096000	-1.60961400	0.00010600



Butadiene (Product)

C	-0.99667900	0.50023100	0.16749900
C	0.43996900	0.62205000	-0.19080800
C	1.00842900	1.66267300	-0.80114800
H	2.07477500	1.67738900	-0.99686700
H	0.40502700	2.50588600	-1.11943900
C	-1.61909200	1.41972000	0.92591800
H	-1.06861800	2.25060200	1.35598800
C	-1.73631100	-0.60511600	-0.38478000
H	-2.68118400	1.34951900	1.13761400
N	1.30362200	-0.52536600	0.20745800
N	-2.34290500	-1.47522800	-0.86141900
O	0.77127400	-1.39111600	0.89983900
O	2.47461100	-0.53095800	-0.16229700

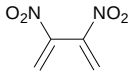
Transition state

C	0.41499700	0.42430000	-0.14168100
C	-0.94982900	0.39276100	0.12394000
C	-1.22368100	1.74872800	0.47255900
H	-2.14417300	2.25199600	0.17074300
H	-0.71740400	2.17650700	1.33030800
C	0.75149400	1.76811300	-0.42407900
H	0.26997900	2.25875900	-1.26271200
C	-1.92357000	-0.62271000	-0.09731900
H	1.68650500	2.21490100	-0.08617800
N	1.38223000	-0.64106500	0.04435800
N	-2.76361500	-1.40993600	-0.26965900
O	2.57466900	-0.32805300	-0.01885200
O	0.94512100	-1.77348600	0.24690600

Cyclobutene (Starting material)

C	0.40547500	0.37857800	0.00003700
C	-0.94301500	0.33746900	-0.00007100

C	-1.03877900	1.86240500	0.00002200
H	-1.50553300	2.28525900	0.89488800
H	-1.50540700	2.28537400	-0.89485500
C	0.53539500	1.87421900	0.00013100
H	0.99952500	2.30426200	-0.89245200
H	0.99940000	2.30415800	0.89283000
C	-1.93251100	-0.67472400	-0.00020700
N	-2.80207600	-1.44904500	-0.00031800
N	1.40051600	-0.66623100	0.00004900
O	1.00438100	-1.83225100	0.00002400
O	2.57856300	-0.29772600	0.00022500



Butadiene (Product)

C	-0.71005800	0.66015000	0.19683600
C	0.71008500	0.66015600	-0.19693700
C	1.32030100	1.59124700	-0.92953700
H	2.38315500	1.52642700	-1.13451100
H	0.75652300	2.42166700	-1.34064100
C	-1.32012300	1.59129300	0.92959500
H	-0.75612100	2.42161400	1.34056600
H	-2.38299700	1.52653700	1.13439300
N	1.51895700	-0.46562900	0.34971200
O	2.67295400	-0.59913500	-0.04285200
O	0.96154400	-1.17564800	1.18524700
N	-1.51886500	-0.46538800	-0.34975600
O	-0.96176200	-1.17573300	-1.18523700
O	-2.67304100	-0.59900800	0.04293700

Transition state

C	-0.67701400	0.47217000	0.14261500
C	0.67696300	0.47225000	-0.14253100
C	0.98013000	1.81961500	-0.44754200
H	1.88962200	2.30530800	-0.09241700
H	0.49971600	2.28256000	-1.30287200

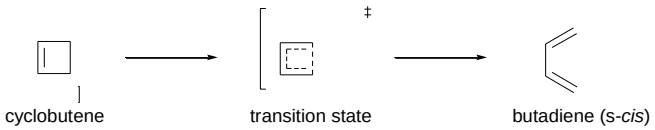
C	-0.98039100	1.81948300	0.44767600
H	-0.50002600	2.28256100	1.30296100
H	-1.88991000	2.30506300	0.09246600
N	-1.68856300	-0.53784000	-0.13193600
O	-1.34319400	-1.56444600	-0.70886900
O	-2.83731200	-0.25746400	0.22628000
N	1.68862900	-0.53771100	0.13191700
O	1.34352000	-1.56423200	0.70916200
O	2.83723600	-0.25732500	-0.22673800

Cyclobutene (Starting material)

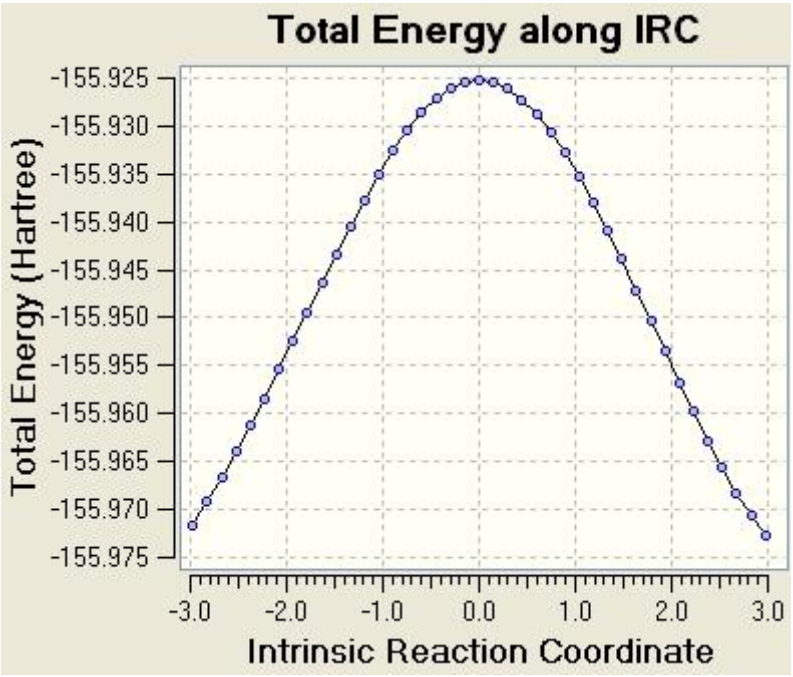
C	0.67425100	0.41789600	0.00007500
C	-0.67409600	0.41782500	-0.00001600
C	-0.78770600	1.91773400	0.00003300
H	-1.25364900	2.34245500	0.89383100
H	-1.25349900	2.34252600	-0.89380900
C	0.78767000	1.91784500	0.00016700
H	1.25350100	2.34273900	-0.89360100
H	1.25335200	2.34264300	0.89405700
N	1.74244500	-0.56508700	0.00009300
O	1.45926700	-1.75756900	-0.00001100
O	2.88142600	-0.08541200	0.00026900
N	-1.74240100	-0.56515900	-0.00013500
O	-1.45947800	-1.75761900	-0.00013700
O	-2.88130600	-0.08520600	-0.00033900

7 Intrinsic reaction coordinates (IRC) for

7.1 Butadiene

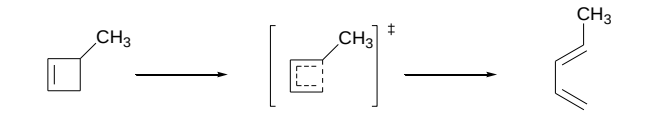


IRC



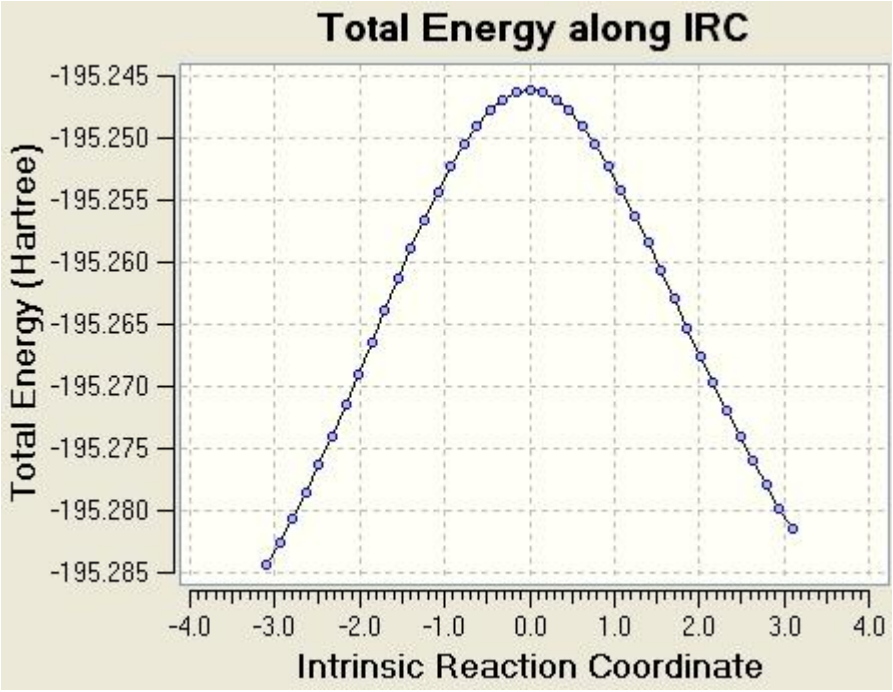
7.2 Monosubstituted Butadiene

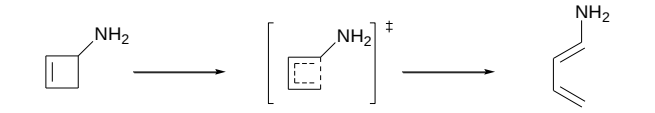
7.2.1 1-Substituted butadienes (outward rotation of substituents)



1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

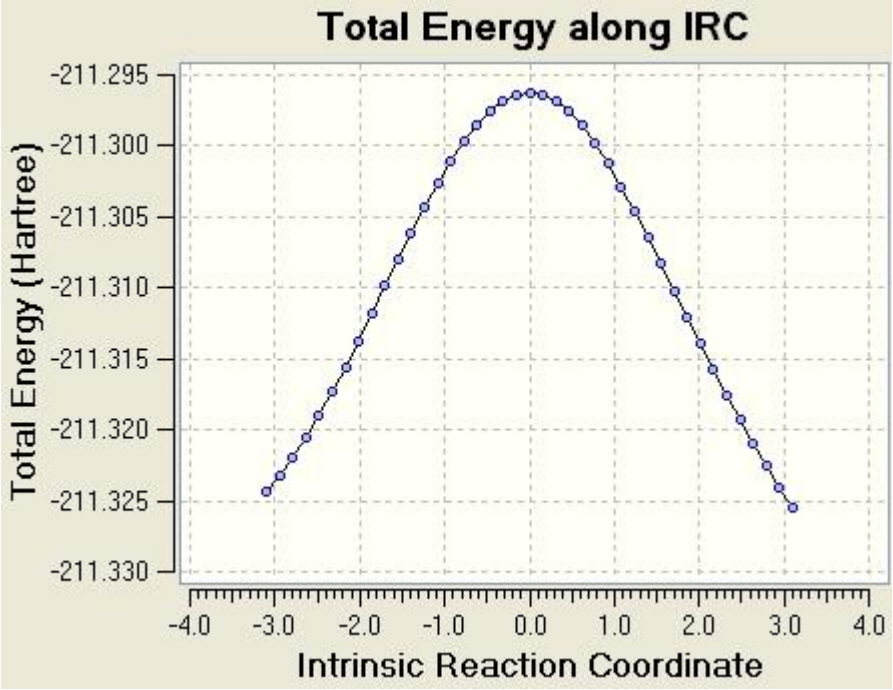
IRC

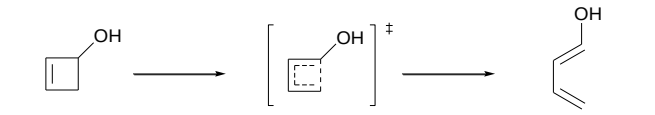




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

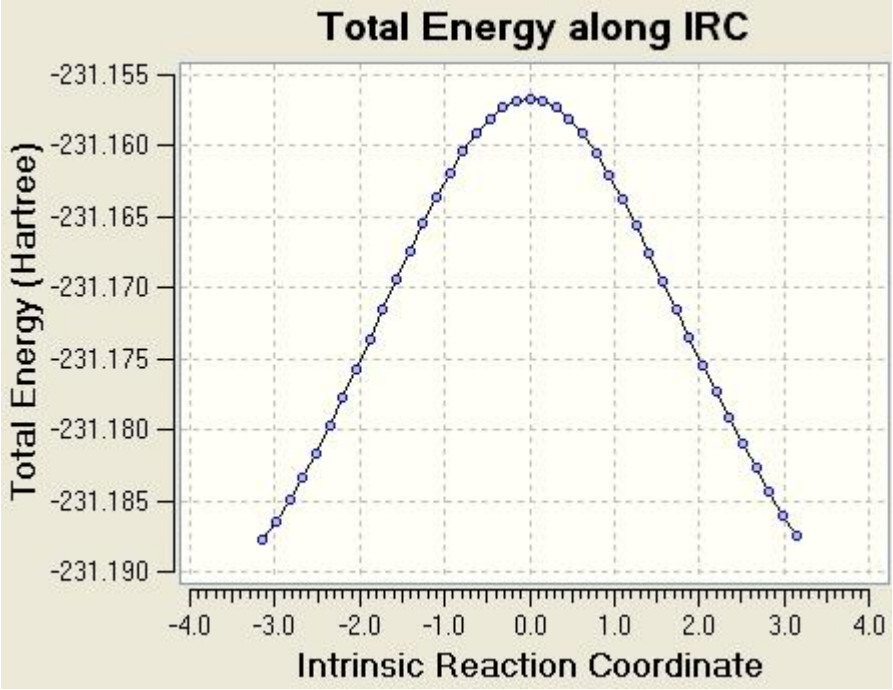
IRC

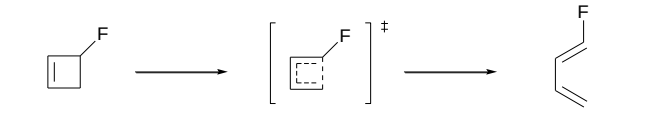




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

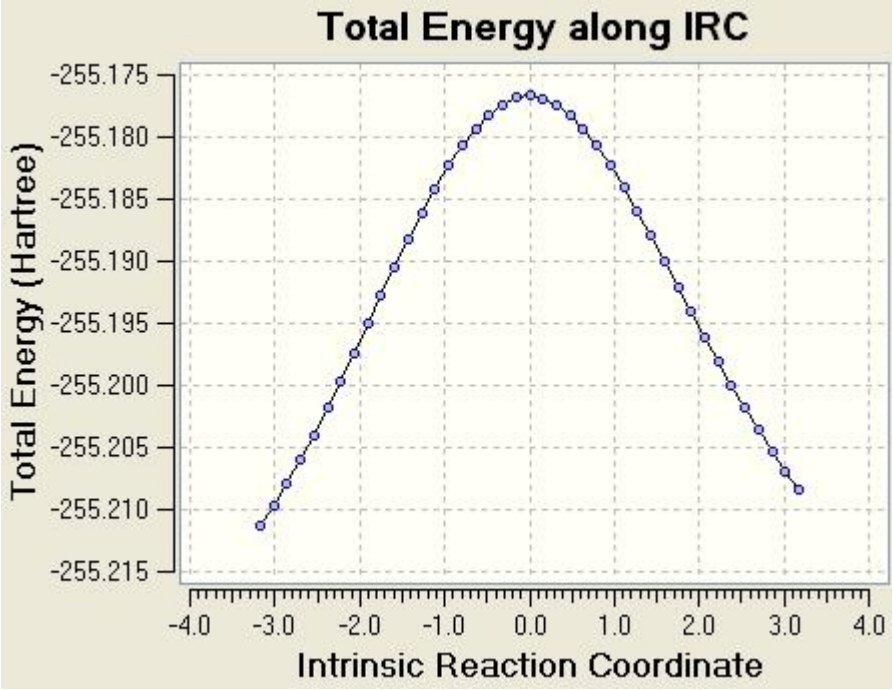
IRC

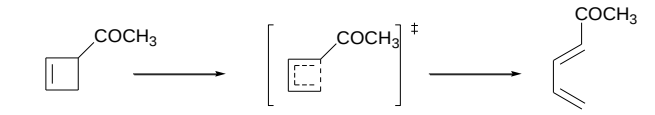




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

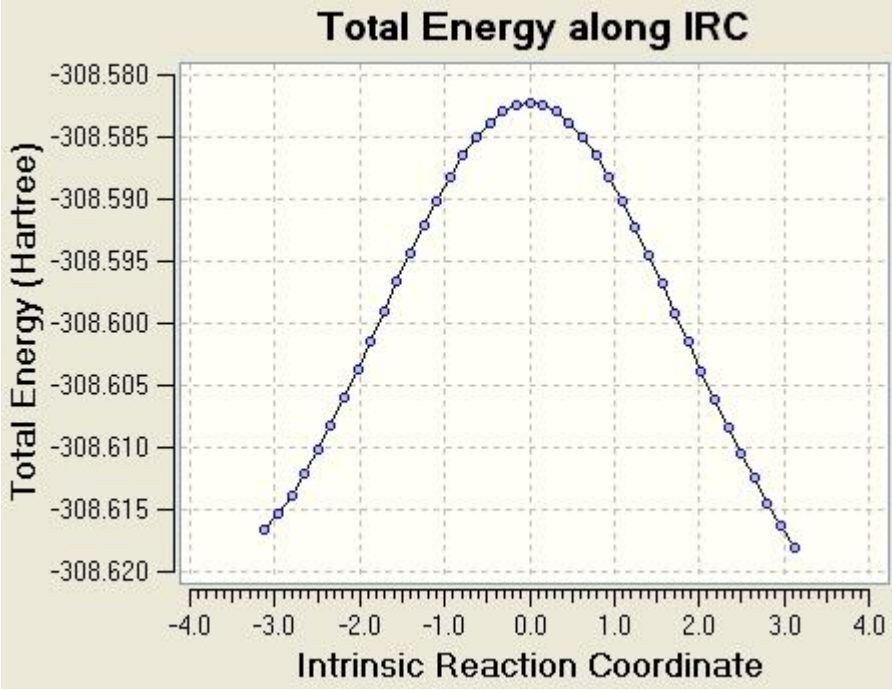
IRC

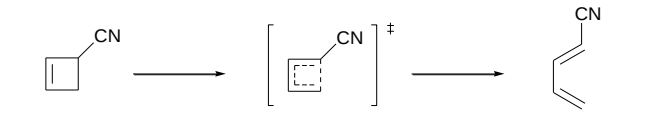




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

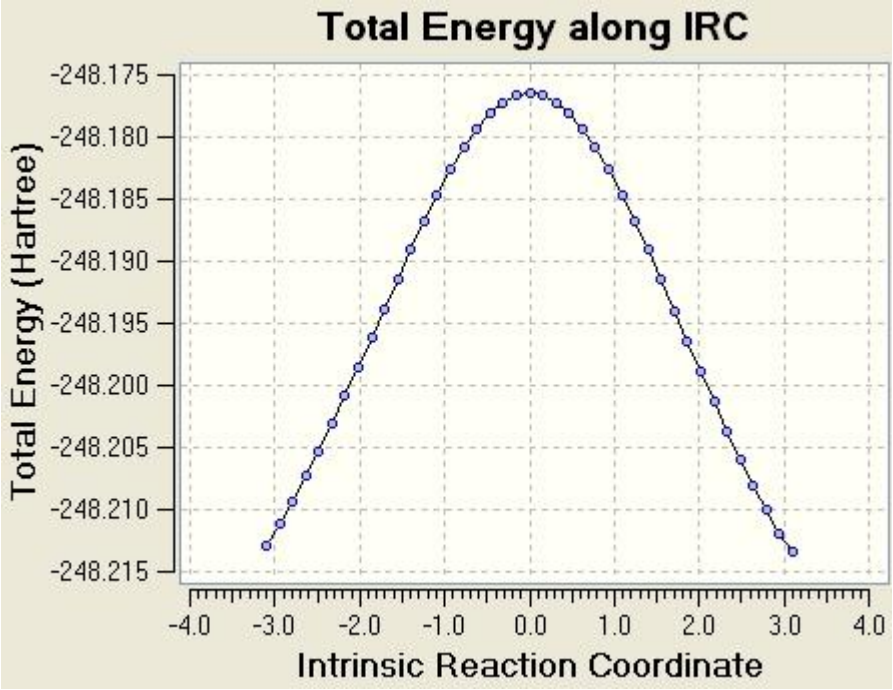
IRC

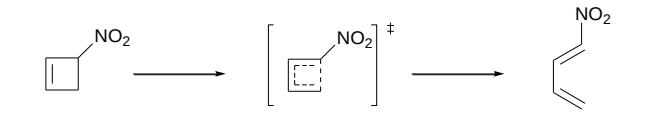




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

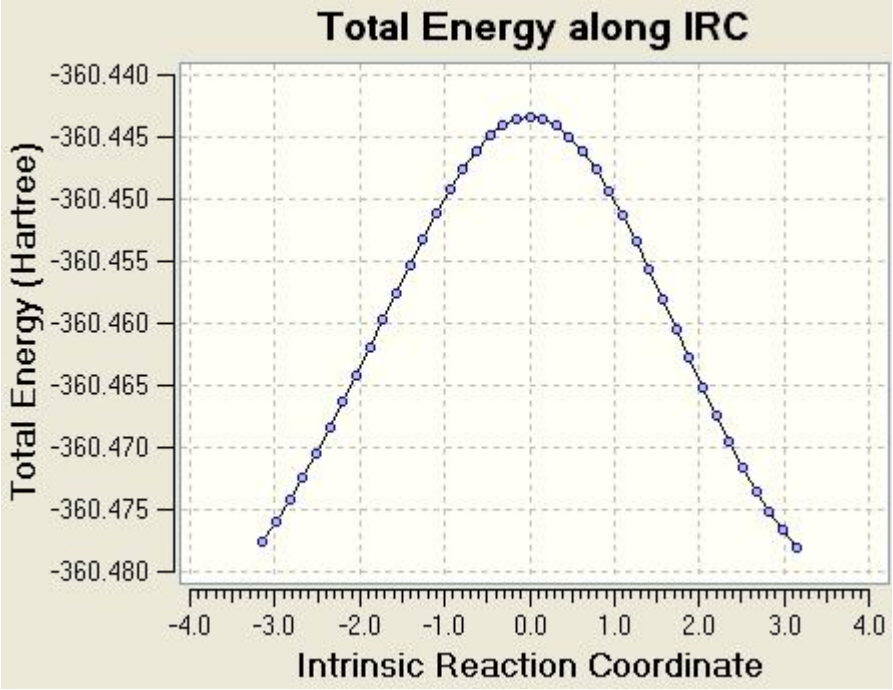
IRC



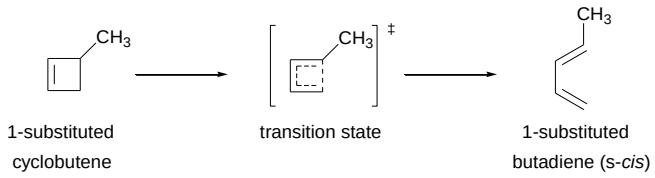


1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

IRC

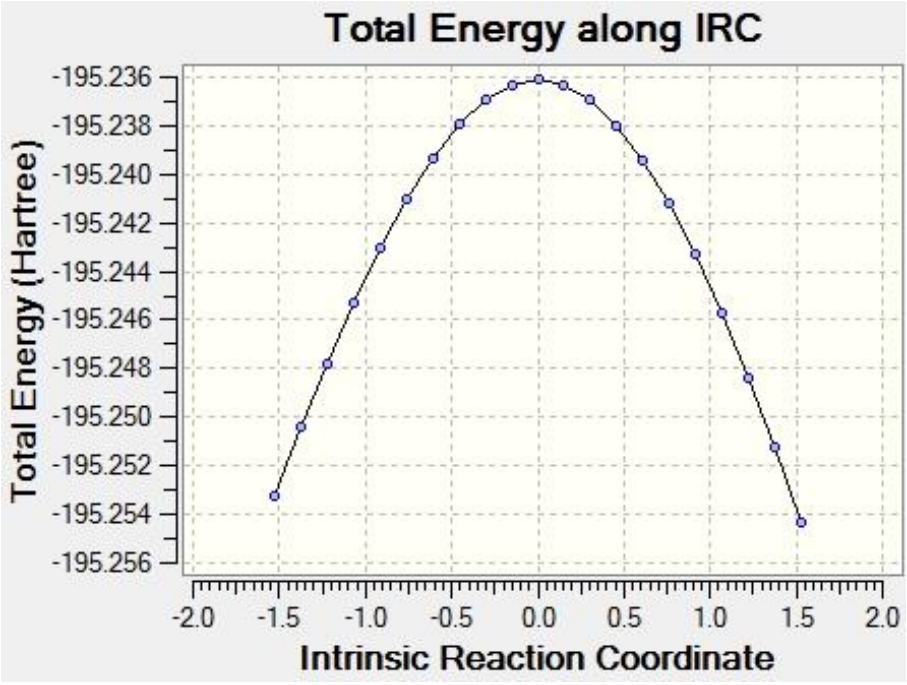


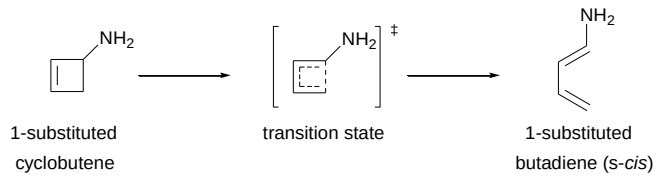
7.2.2 1-Substituted butadienes (intward rotation of substituents)



1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

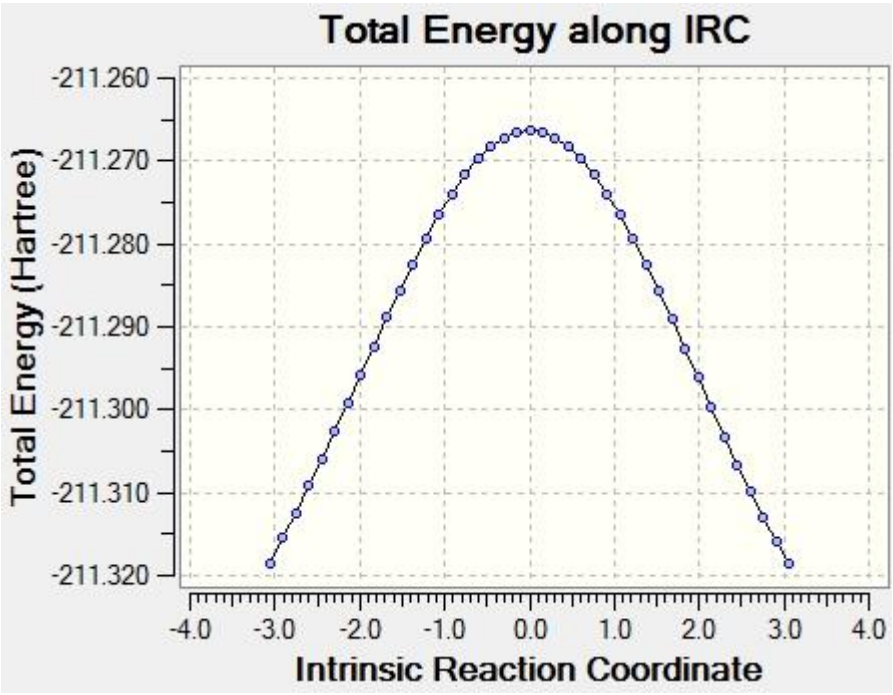
IRC

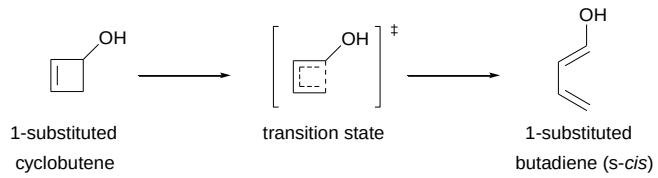




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

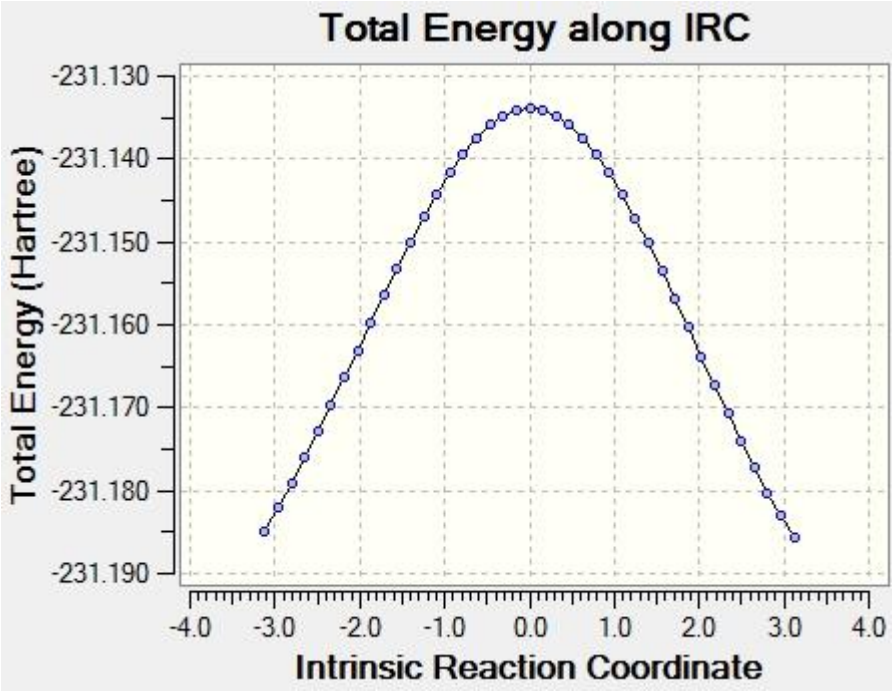
IRC

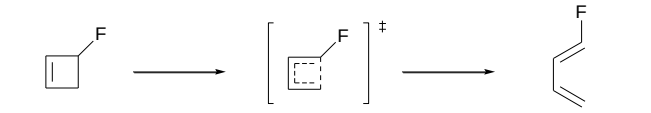




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

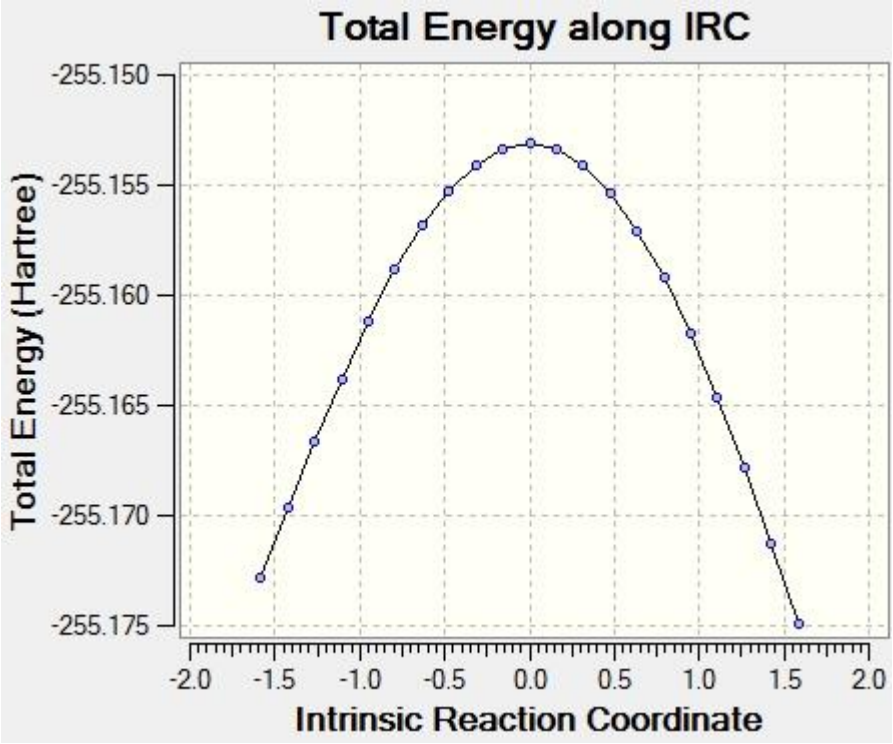
IRC

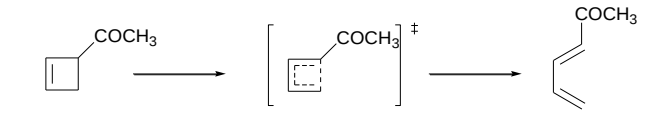




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

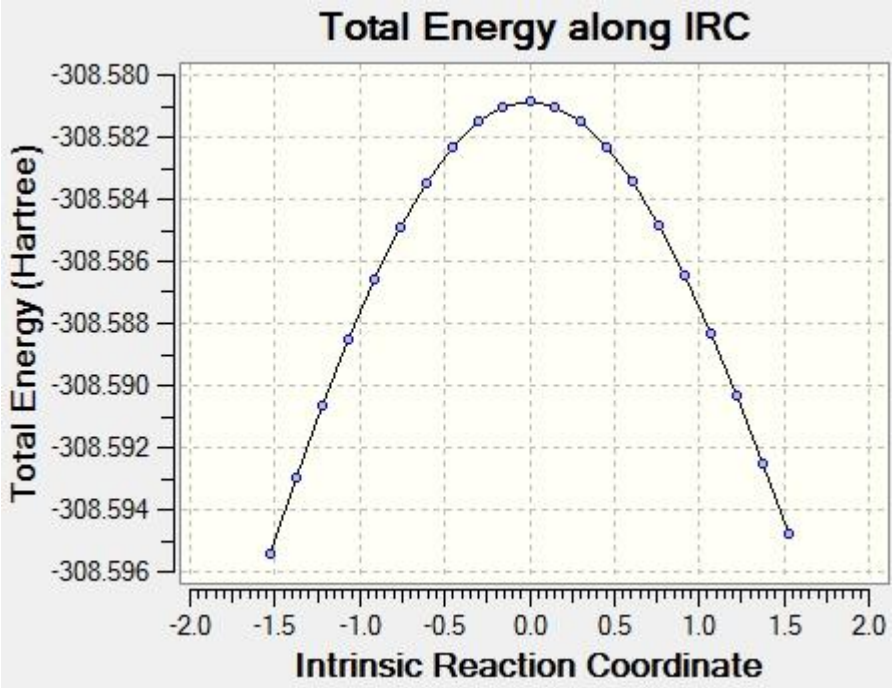
IRC

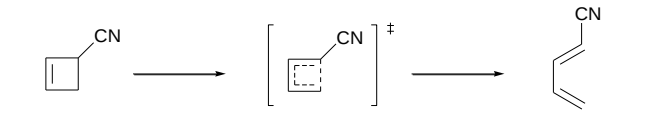




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

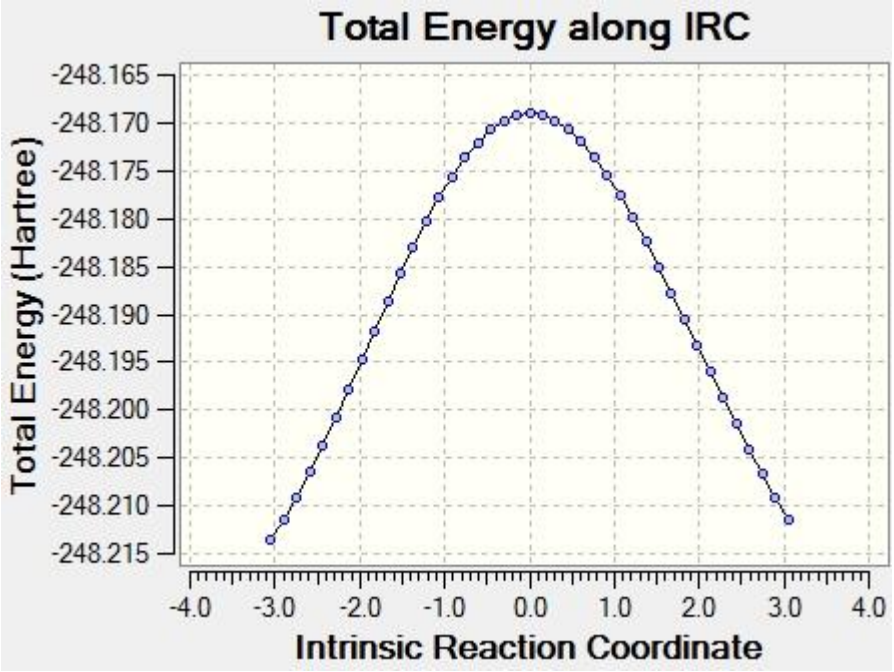
IRC

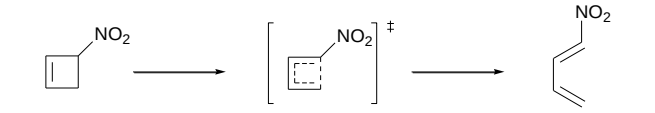




1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

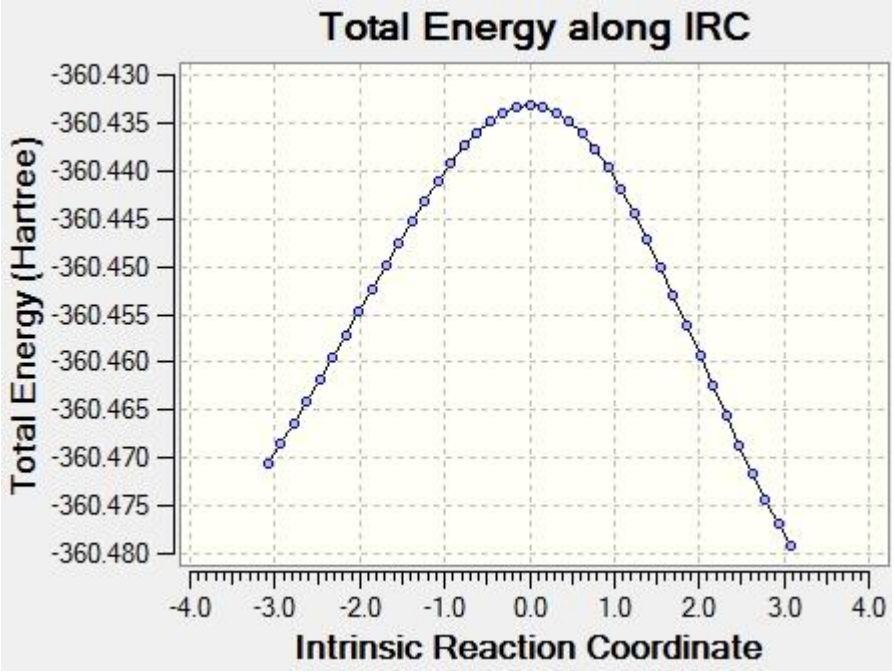
IRC



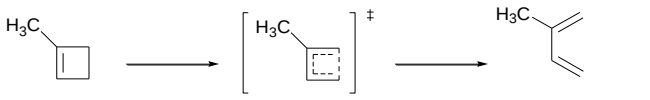


1-substituted cyclobutene | transition state | 1-substituted butadiene (s-*cis*)

IRC

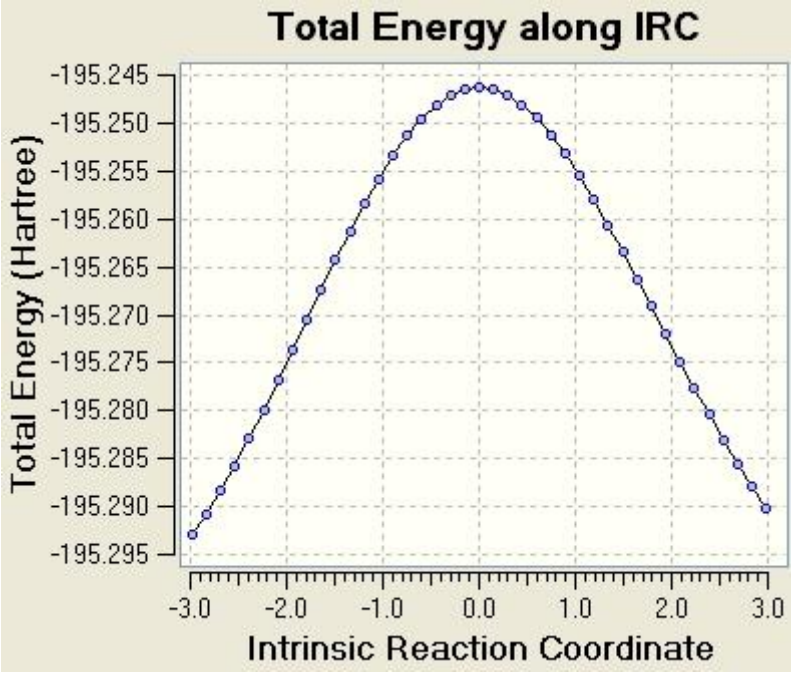


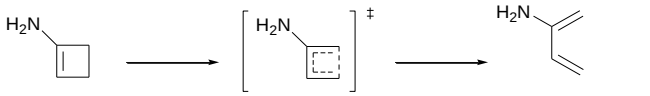
7.2.3 2-Substituted butadienes



2-monosubstituted cyclobutene | transition state | 2-monosubstituted butadiene (s-*cis*)

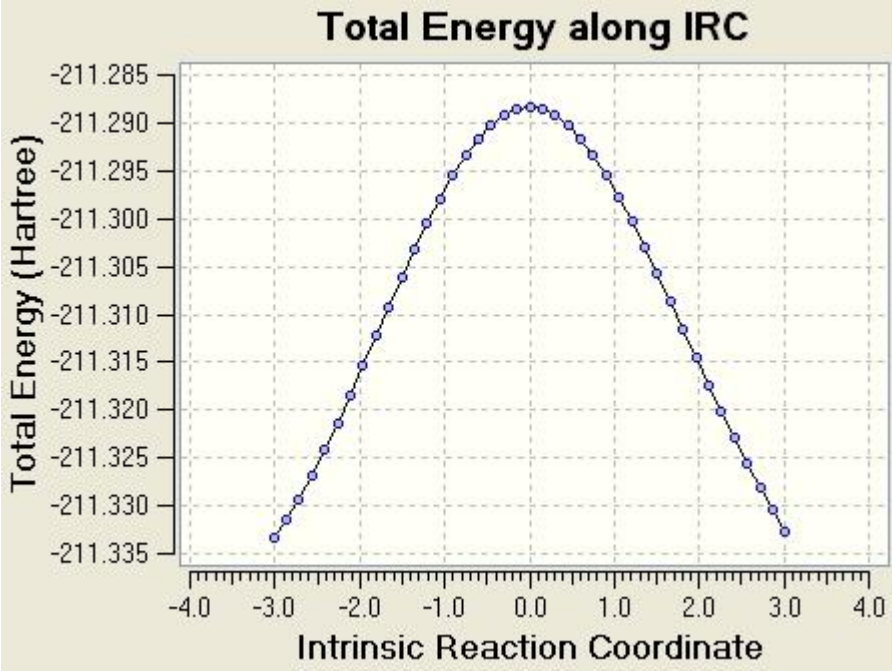
IRC

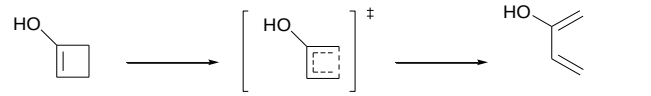




2-monosubstituted cyclobutene | transition state | 2-monosubstituted butadiene (s-*cis*)

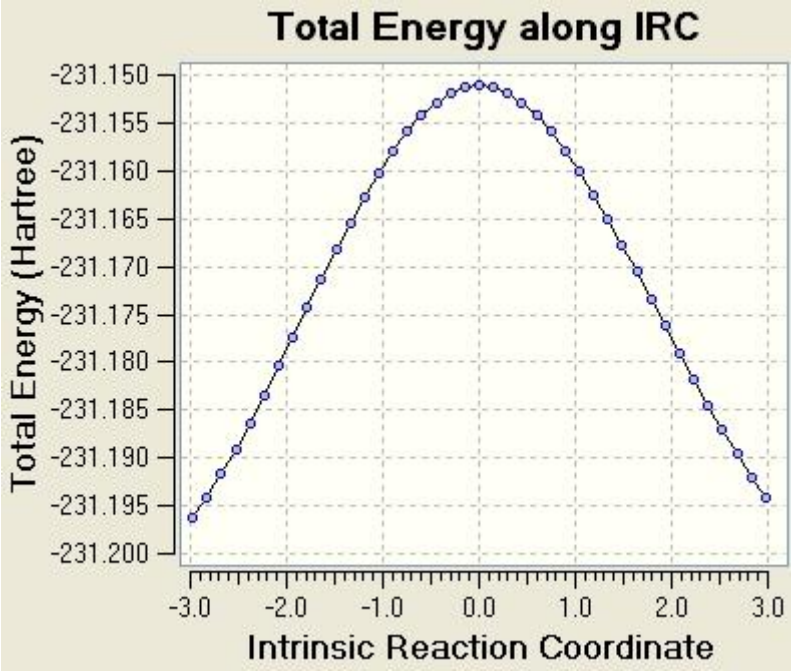
IRC

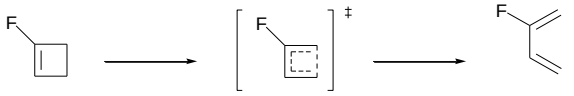




2-monosubstituted cyclobutene | transition state | 2-monosubstituted butadiene (s-*cis*)

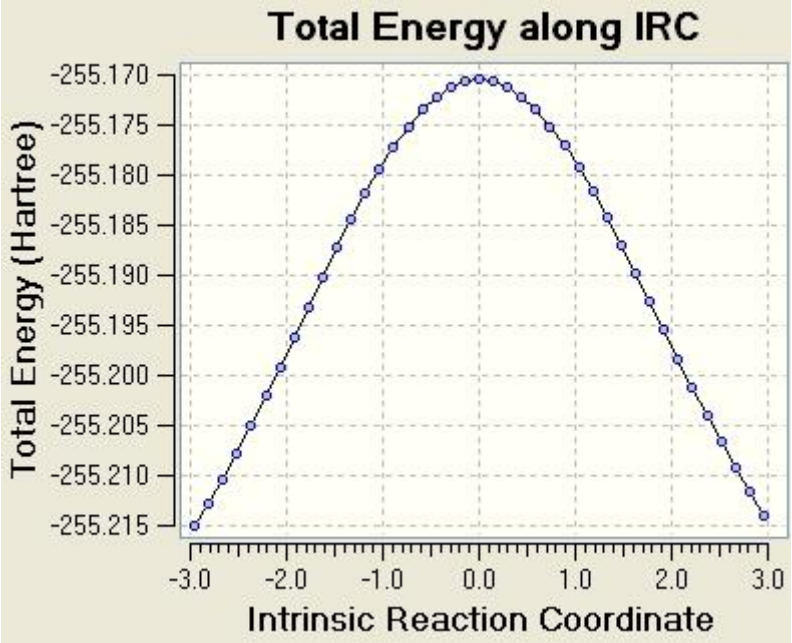
IRC

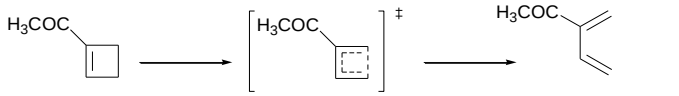




2-monosubstituted cyclobutene | transition state | 2-monosubstituted butadiene (s-*cis*)

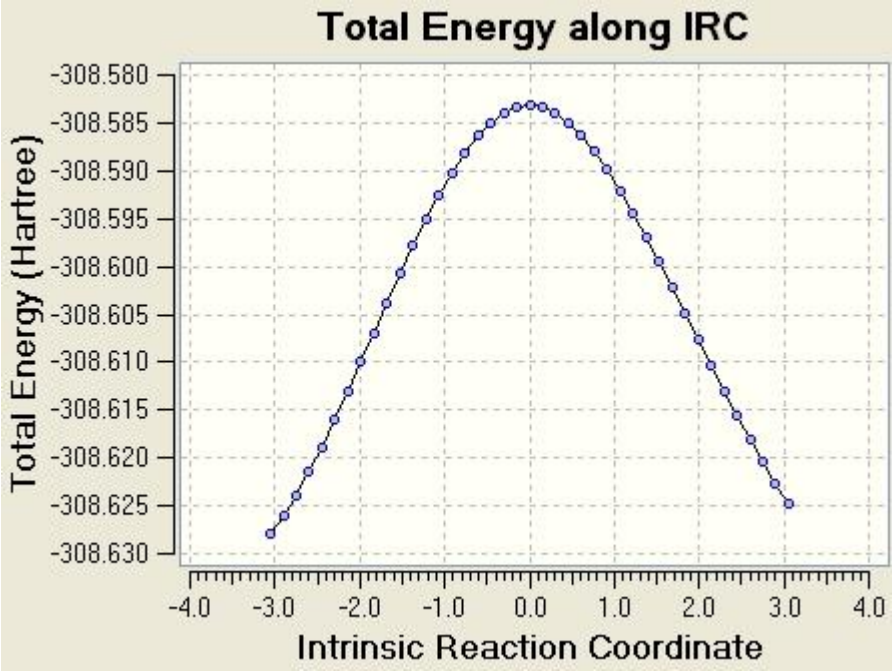
IRC

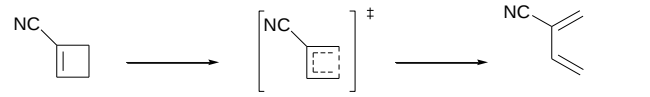




2-monosubstituted cyclobutene | transition state | 2-monosubstituted butadiene (s-*cis*)

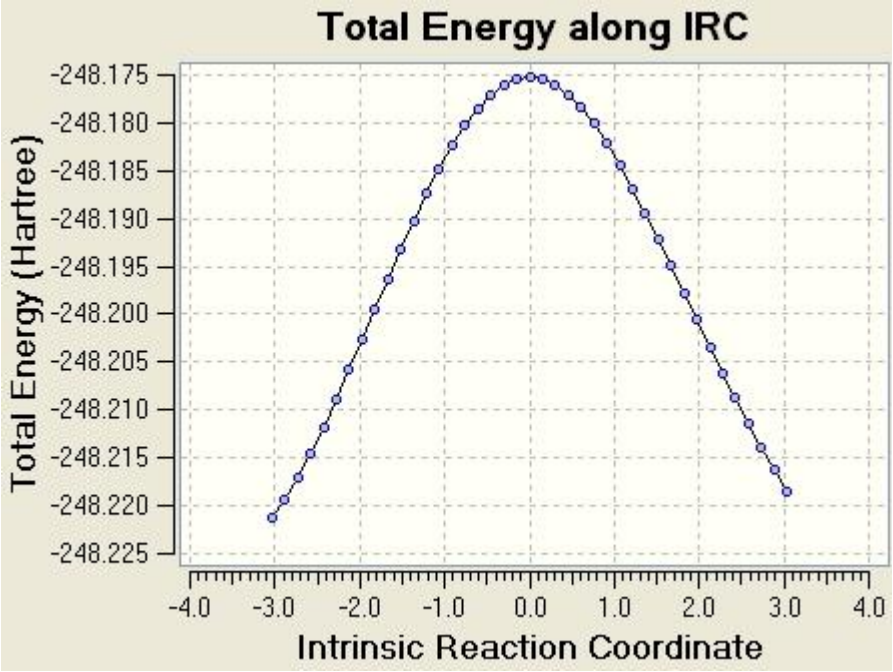
IRC

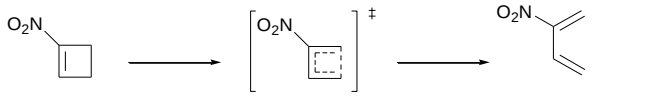




2-monosubstituted cyclobutene | transition state | 2-monosubstituted butadiene (s-*cis*)

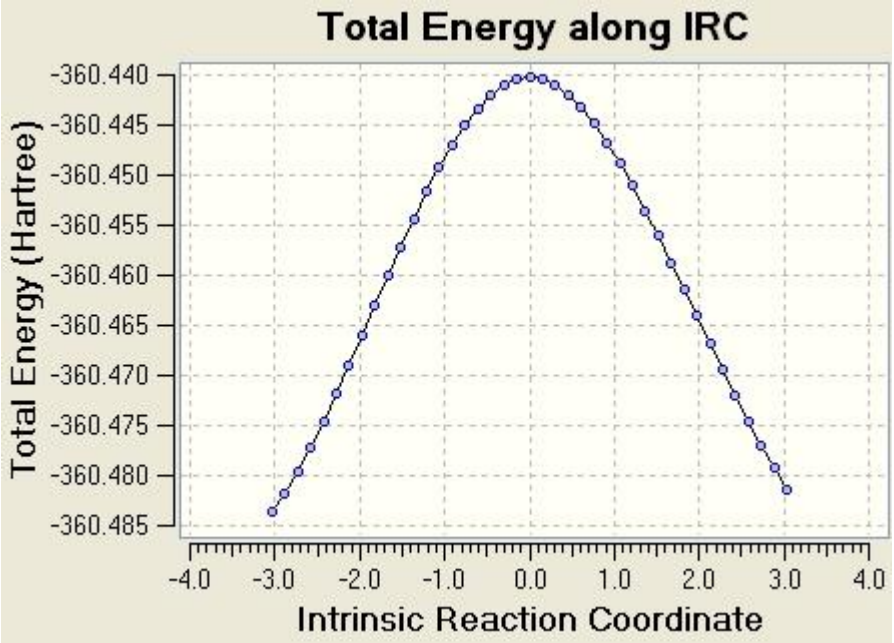
IRC





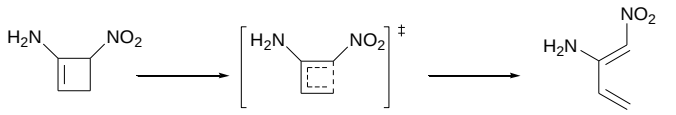
2-monosubstituted cyclobutene | transition state | 2-monosubstituted butadiene (s-*cis*)

IRC



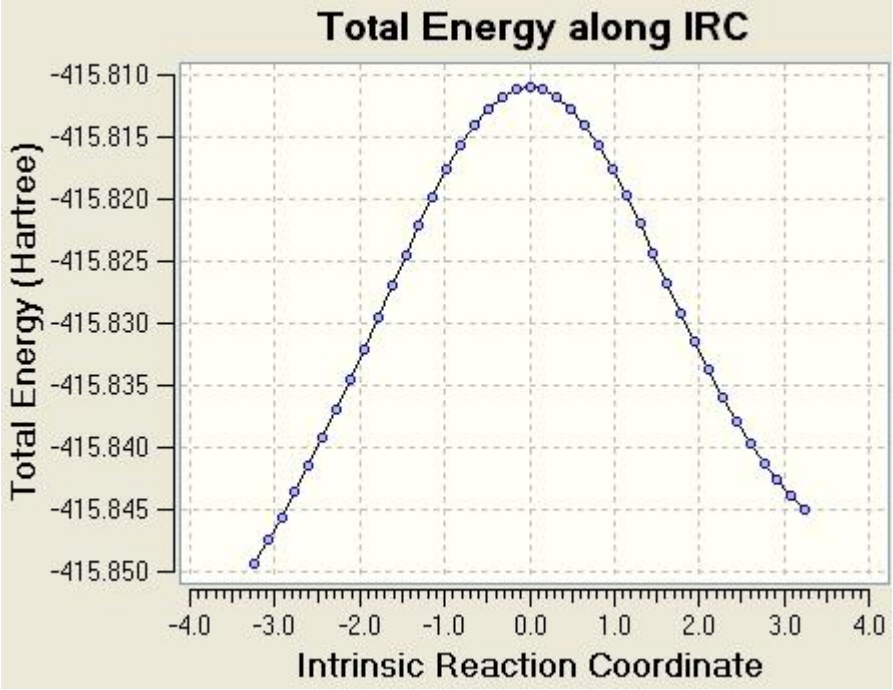
7.3 Representative disubstituted butadienes

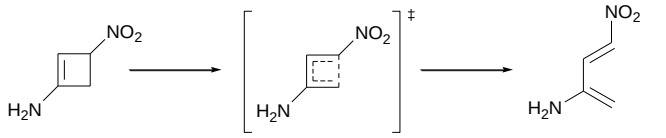
7.3.1 NO_2–NH_2-disubstituted butadienes



1,2-disubstituted cyclobutene | transition state | 1,2-disubstituted butadiene (s-*cis*)

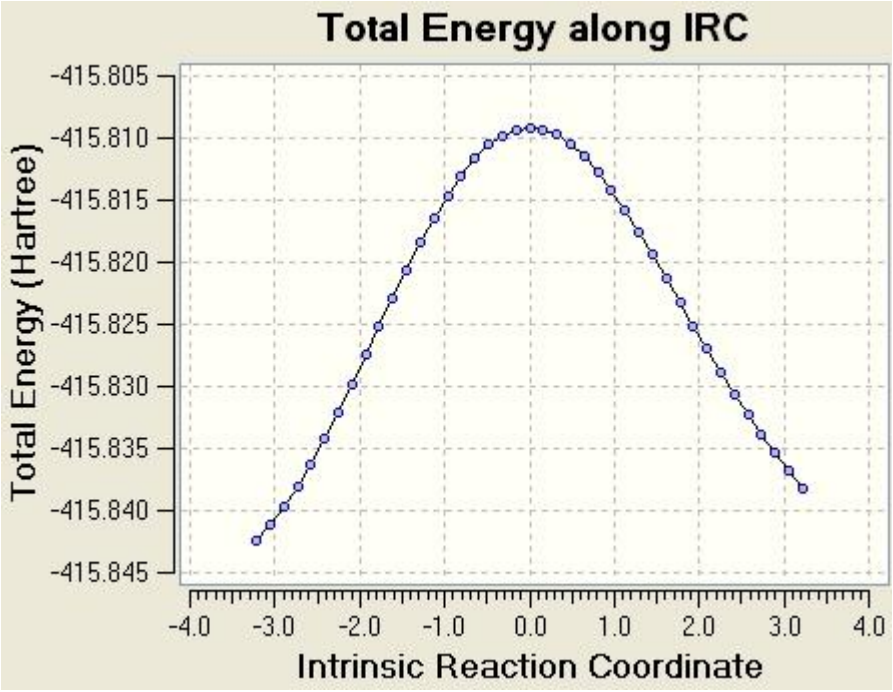
IRC

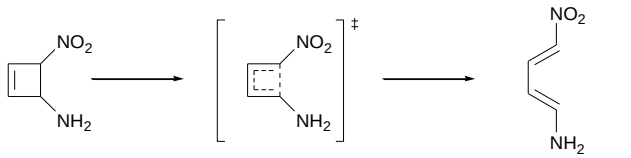




1,3-disubstituted cyclobutene | transition state | 1,3-disubstituted butadiene (s-*cis*)

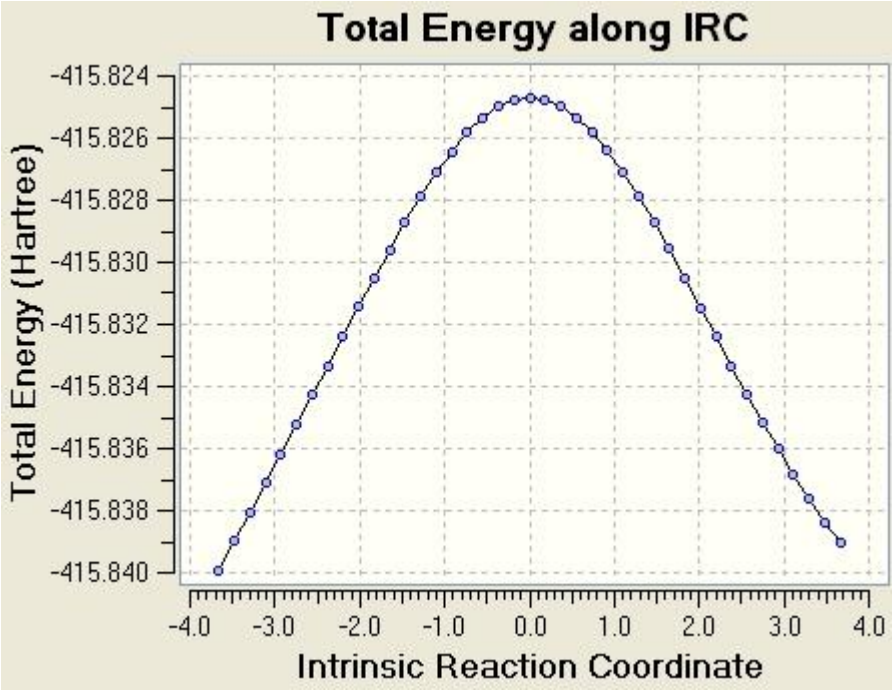
IRC

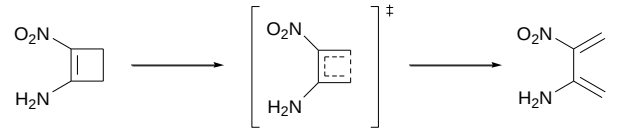




1,4-disubstituted cyclobutene | transition state | 1,4-disubstituted butadiene (s-*cis*)

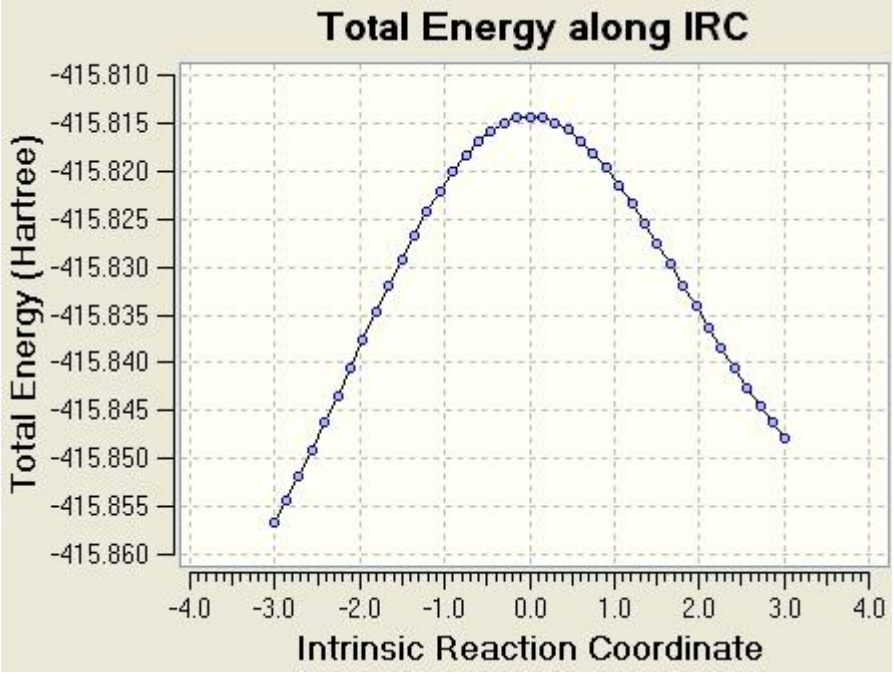
IRC



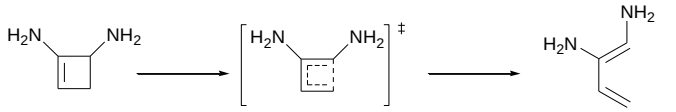


2,3-disubstituted cyclobutene | transition state | 2,3-disubstituted butadiene (s-*cis*)

IRC

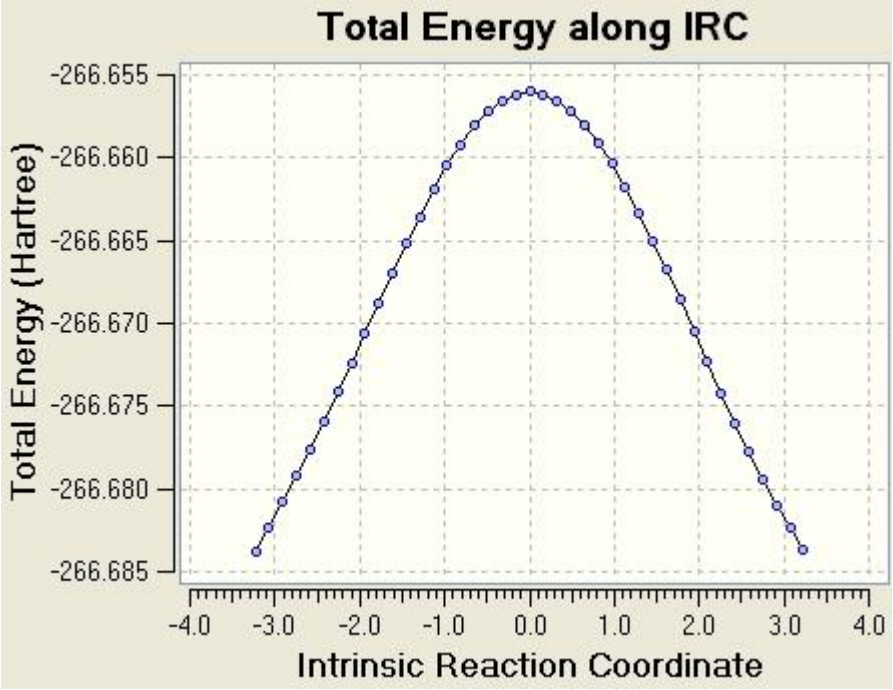


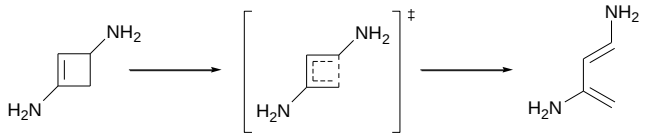
7.3.2 NH_2–NH_2-Disubstituted butadienes



1,2-disubstituted cyclobutene | transition state | 1,2-disubstituted butadiene (s-*cis*)

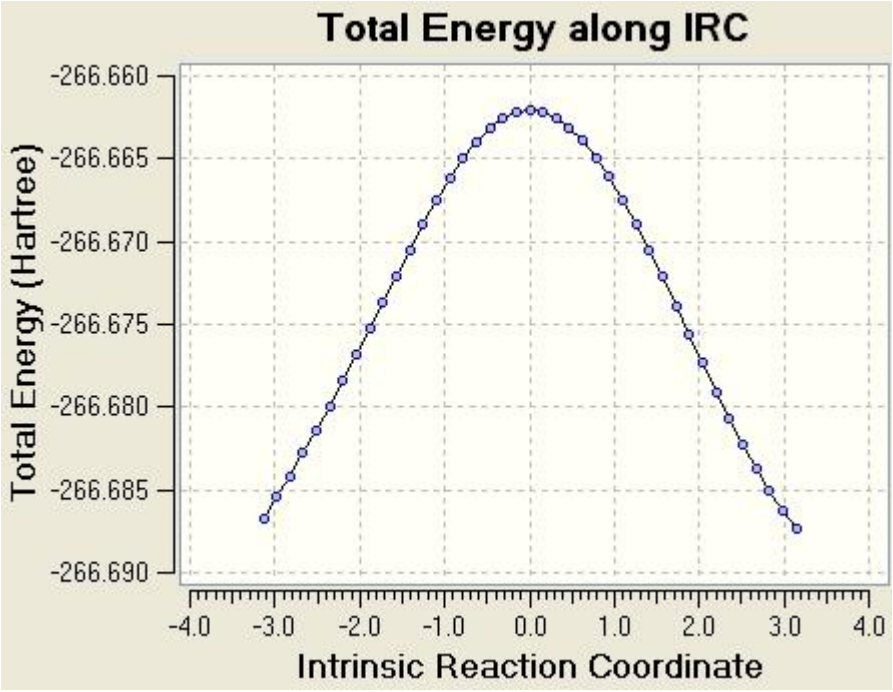
IRC

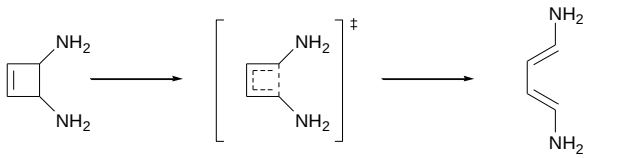




1,3-disubstituted cyclobutene | transition state | 1,3-disubstituted butadiene (s-*cis*)

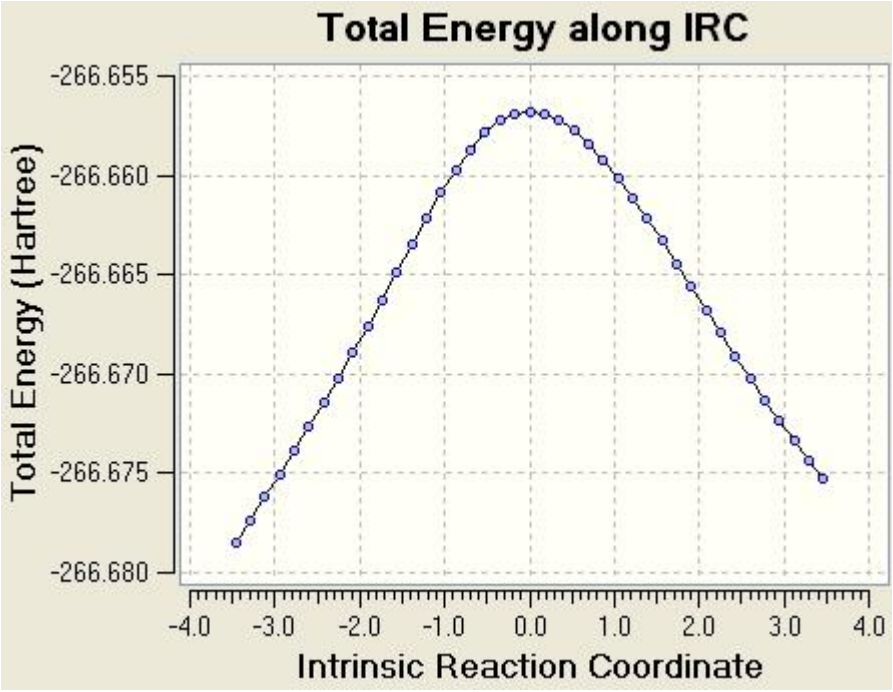
IRC

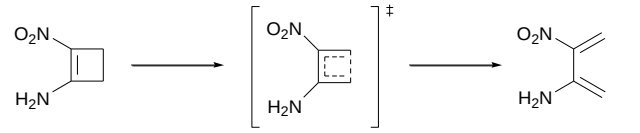




1,4-disubstituted cyclobutene | transition state | 1,4-disubstituted butadiene (s-*cis*)

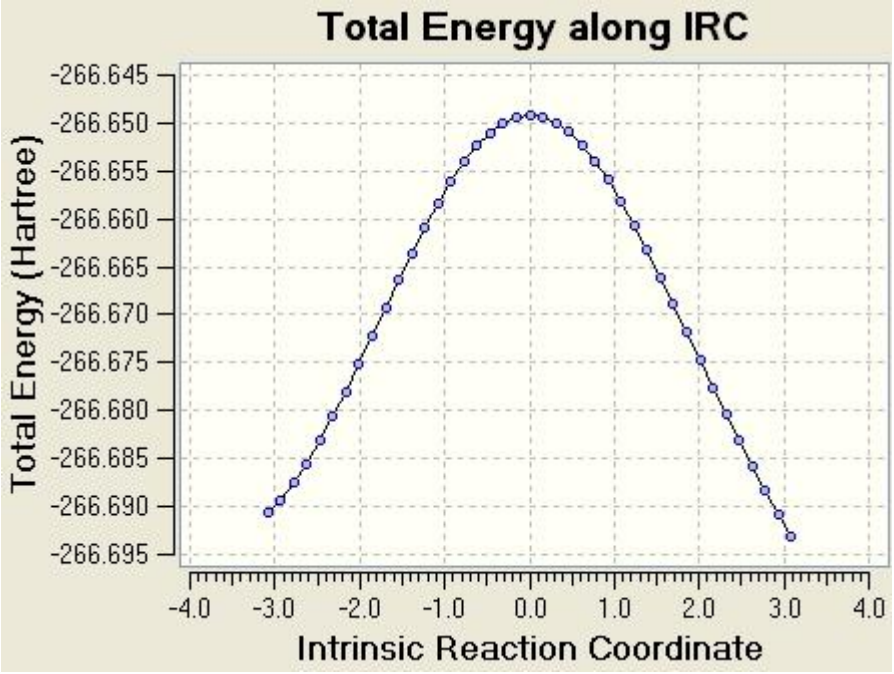
IRC



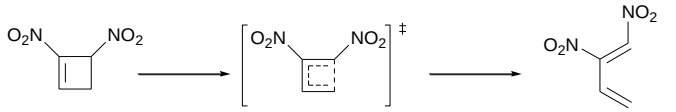


2,3-disubstituted cyclobutene | transition state | 2,3-disubstituted butadiene (s-*cis*)

IRC

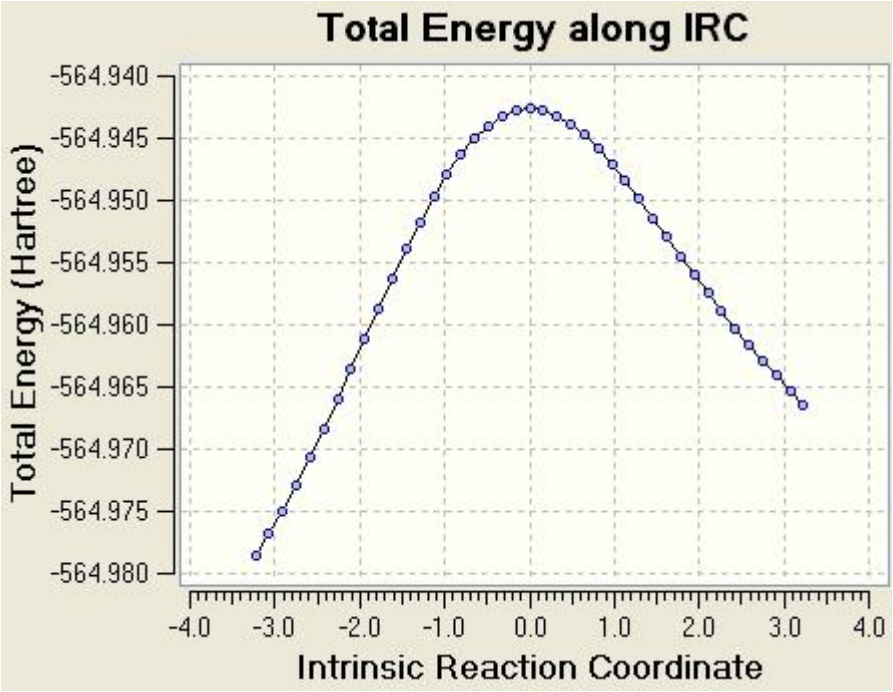


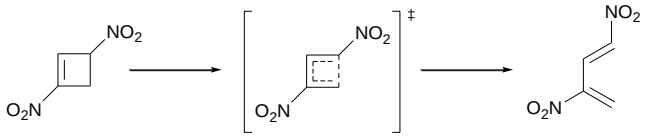
7.3.3 NO_2–NO_2-Disubstituted Butadienes



1,2-disubstituted cyclobutene | transition state | 1,2-disubstituted butadiene (s-*cis*)

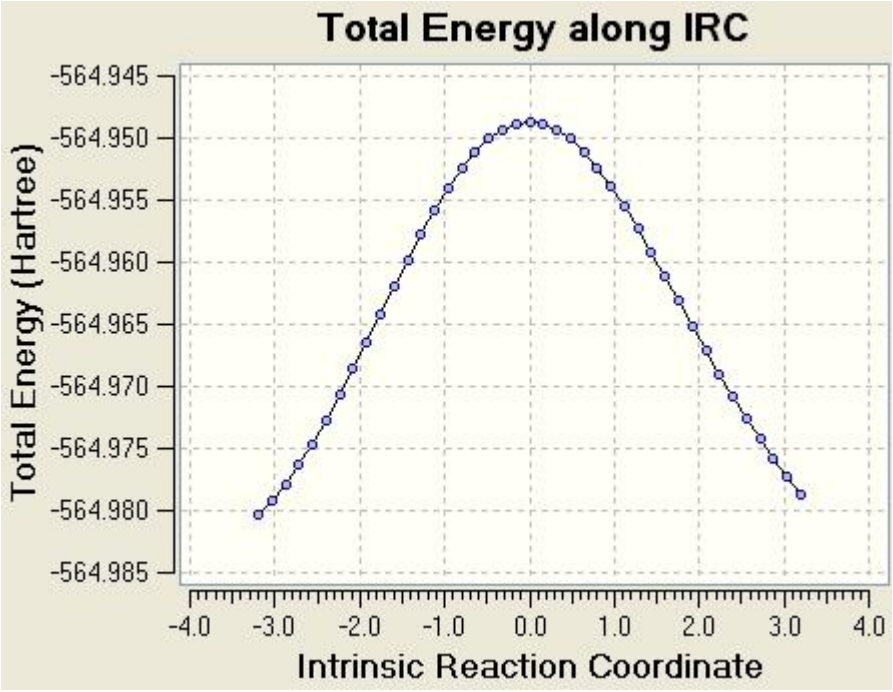
IRC

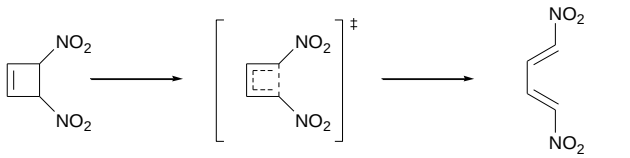




1,3-disubstituted cyclobutene | transition state | 1,3-disubstituted butadiene (s-*cis*)

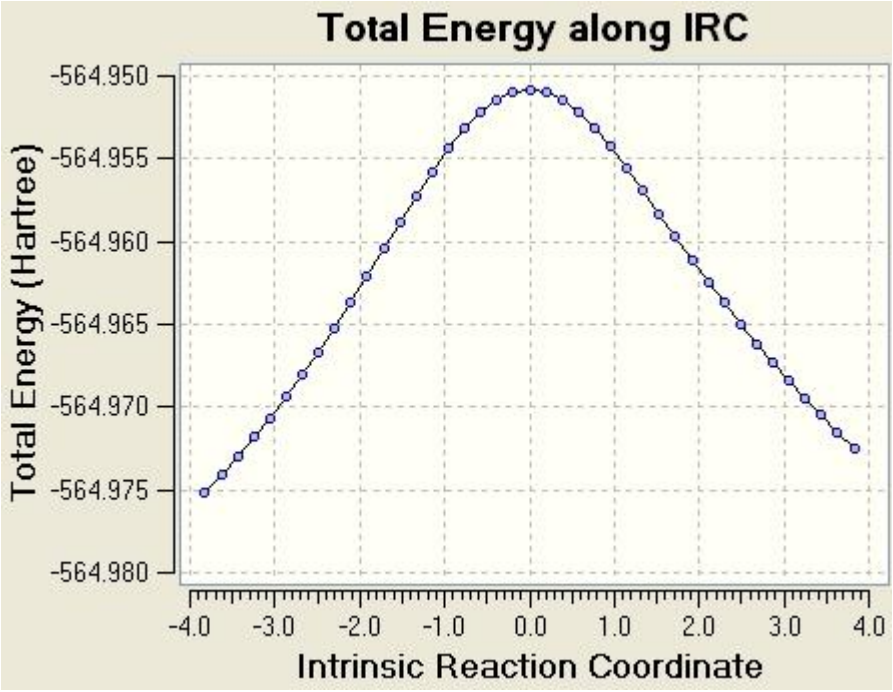
IRC

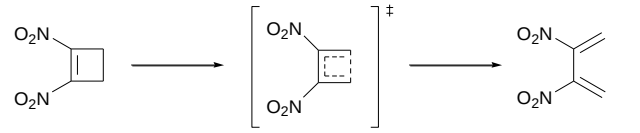




1,4-disubstituted cyclobutene | transition state | 1,4-disubstituted butadiene (s-*cis*)

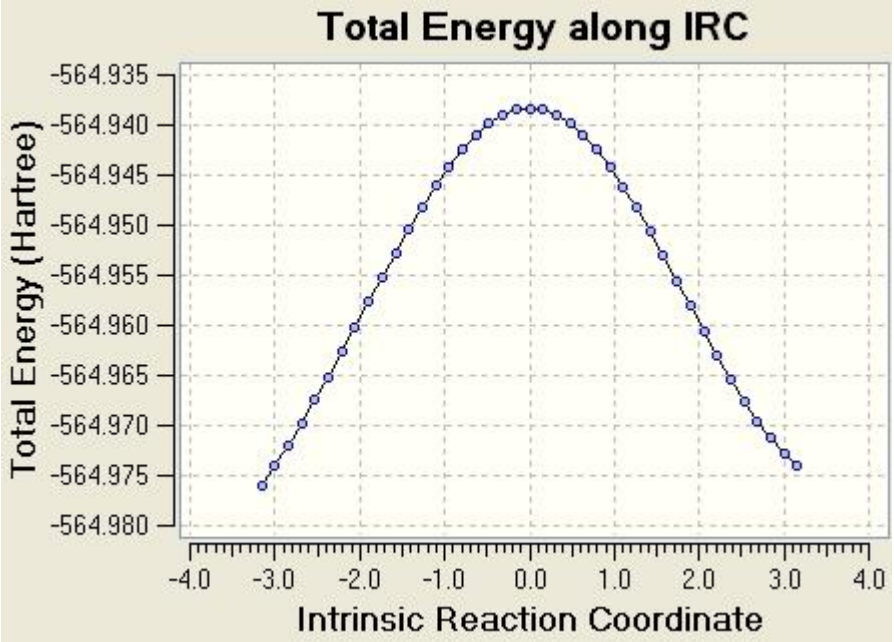
IRC





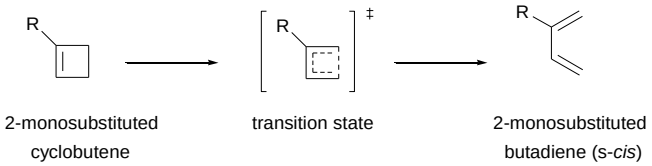
2,3-disubstituted cyclobutene | transition state | 2,3-disubstituted butadiene (s-*cis*)

IRC



8 Reaction exoergonicity values for

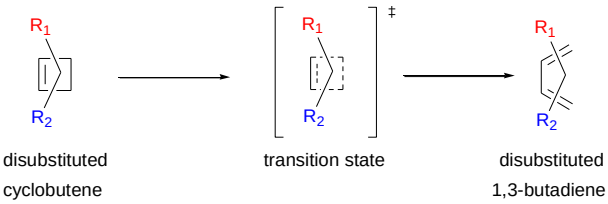
8.1 Monosubstituted cyclobutenes



Entry	R	E_R (Kcal mol^{-1})
1	CH_3	-11.4
2	NH_2	-8.4
3	OH	-8.7
4	F	-10.3
5	$C(O)CH_3$	-11.1
6	CN	-6.5
7	NO_2	-7.3

Note: Reaction exoergonicity values for unsubstituted cyclobutene and 1-monosubstituted cyclobutenes (for both inward and outward rotations of the substituents) are provided in the Table 1 of the manuscript.

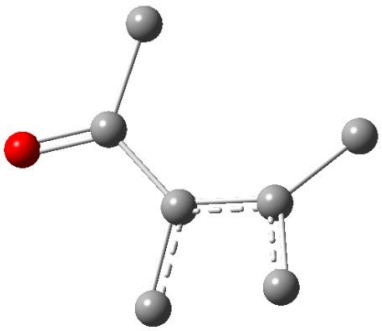
8.2 Disubstituted cyclobutenes



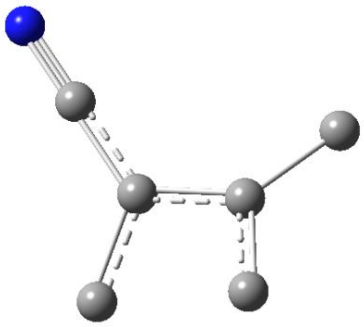
		$R_2 = CH_3$	$R_2 = NH_2$	$R_2 = OH$	$R_2 = F$	$R_2 = C(O)CH_3$	$R_2 = CN$	$R_2 = NO_2$
1,4-disubstituted cyclobutenes	$R_1 = CH_3$	-8.7	-8.8	-11.0	-12.8	-3.9	-10.2	-8.9
	$R_1 = NH_2$	-14.7	-13.6	-12.5	-17.6	-13.9	-20.7	-25.0
	$R_1 = OH$	-10.6	-9.2	-7.9	-10.5	-11.2	-11.8	-8.4
	$R_1 = F$	-6.3	-5.2	-3.8	-5.7	-5.8	-5.7	-4.1
	$R_1 = C(O)CH_3$	-8.4	-12.4	-13.7	-15.0	-5.7	-9.1	-6.9
	$R_1 = CN$	-12.0	-16.4	-13.1	-14.8	-8.2	-9.5	-8.7
	$R_1 = NO_2$	-6.4	-16.5	-6.9	-7.8	-4.3	-3.5	-2.5
		$R_2 = CH_3$	$R_2 = NH_2$	$R_2 = OH$	$R_2 = F$	$R_2 = C(O)CH_3$	$R_2 = CN$	$R_2 = NO_2$
1,3-disubstituted cyclobutenes	$R_1 = CH_3$	-10.5	-10.7	-11.3	-13.5	-9.1	-10.0	-11.6
	$R_1 = NH_2$	-15.4	-14.2	-16.4	-19.4	-15.7	-17.0	-19.2
	$R_1 = OH$	-10.9	-9.2	-11.6	-14.2	-10.3	-11.6	-13.8
	$R_1 = F$	-5.9	-3.8	-5.6	-8.6	-6.4	-6.9	-9.4
	$R_1 = C(O)CH_3$	-12.5	-11.6	-12.1	-15.4	-12.4	-12.0	-13.8
	$R_1 = CN$	-11.0	-9.8	-10.7	-13.9	-11.0	-11.0	-13.3
	$R_1 = NO_2$	-7.6	-5.3	-6.8	-10.2	-8.2	-7.8	-10.4
		$R_2 = CH_3$	$R_2 = NH_2$	$R_2 = OH$	$R_2 = F$	$R_2 = C(O)CH_3$	$R_2 = CN$	$R_2 = NO_2$
trans-3,4-disubstituted cyclobutenes	$R_1 = CH_3$	-15.6	-20.2	-15.8	-11.4	-18.7	-17.2	-14.9
	$R_1 = NH_2$		-22.4	-18.4	-15.8	-26.8	-24.6	-24.0
	$R_1 = OH$			-16.1	-11.2	-20.7	-18.4	-16.2
	$R_1 = F$				-7.6	-15.6	-13.8	-11.1
	$R_1 = C(O)CH_3$					-19.4	-20.3	-17.0
	$R_1 = CN$						-18.8	-17.4
	$R_1 = NO_2$							-12.5
		$R_2 = CH_3$	$R_2 = NH_2$	$R_2 = OH$	$R_2 = F$	$R_2 = C(O)CH_3$	$R_2 = CN$	$R_2 = NO_2$
1,2-disubstituted cyclobutenes	$R_1 = CH_3$	-4.6	-5.9	-5.6	-7.7	-1.8	-2.7	-1.8
	$R_1 = NH_2$		-13.9	-11.9	-10.2	1.2	1.6	6.8
	$R_1 = OH$			-12.3	-10.1	-1.1	-2.5	-2.6
	$R_1 = F$				-11.4	-3.7	-4.8	-6.2
	$R_1 = C(O)CH_3$					-6.0	-1.8	-5.2
	$R_1 = CN$						-3.0	-4.9
	$R_1 = NO_2$							-13.3

Note: For the highlighted examples described in 1,2-disubstituted cyclobutenes section, computed values indicate endoergonicity for these systems. It might be due to an effective conjugation of the lone pair of NH_2 substituents with the π bond of the cyclobutenes, which is clear from the corresponding transition states.

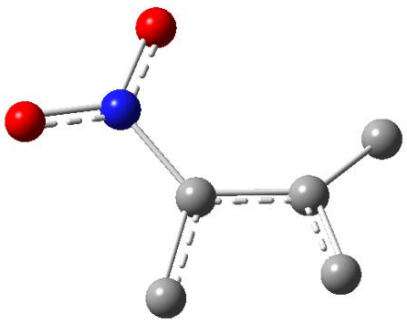
8.3 Optimised transition state structures for representative 1,2-disubstituted compounds



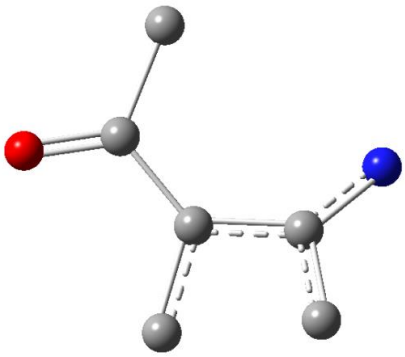
1-CH_3–2-$C(O)CH_3$



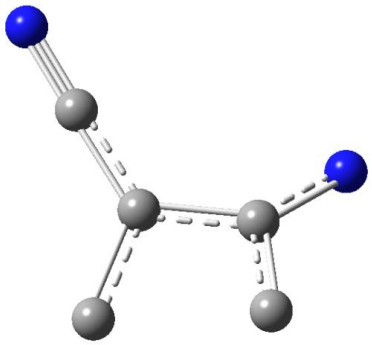
1-CH_3–2-CN



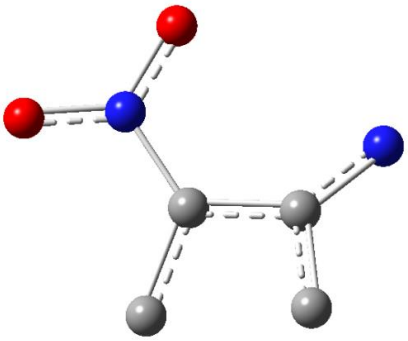
1-CH_3–2-NO_2



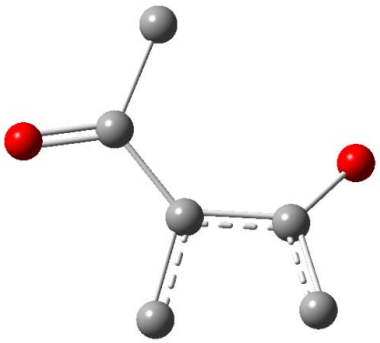
1-NH_2–2-$C(O)CH_3$



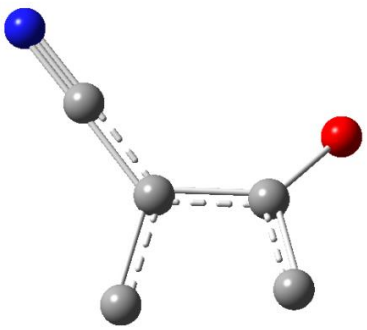
1-NH_2–2-CN



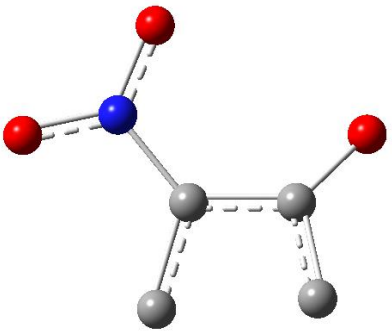
1-NH_2–2-NO_2



1-OH–2-$C(O)CH_3$



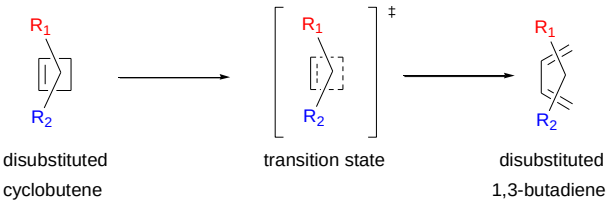
1-OH–2-CN



1-OH–2-NO_2

Note: For clarity, hydrogen atoms are not shown.

9 E_{extra} values for disubstituted cyclobutenes



		R_2 = CH_3	R_2 = NH_2	R_2 = OH	R_2 = F	R_2 = $C(O)CH_3$	R_2 = CN	R_2 = NO_2
1,4-disubstituted cyclobutenes	R_1 = CH_3	0.9	1.3	0.7	0.4	0.1	-0.3	0.3
	R_1 = NH_2	1.2	2.1	5.4	1.5	-0.7	-1.7	-0.9
	R_1 = OH	0.8	3.7	2.7	1.5	-0.9	-0.8	2.1
	R_1 = F	0.2	1.4	2.2	1.4	0.5	0.1	1.2
	R_1 = $C(O)CH_3$	-0.6	-2.6	0.8	1.0	2.4	0.7	1.9
	R_1 = CN	-0.1	-1.5	0.0	-0.4	1.2	0.3	1.2
	R_1 = NO_2	0.4	-1.4	1.2	1.1	1.2	1.7	3.9
		R_2 = CH_3	R_2 = NH_2	R_2 = OH	R_2 = F	R_2 = $C(O)CH_3$	R_2 = CN	R_2 = NO_2
1,3-disubstituted cyclobutenes	R_1 = CH_3	0.1	0.2	-0.2	-0.7	-0.1	-0.2	-0.6
	R_1 = NH_2	0.2	-0.1	-1.1	-1.9	-0.2	-1.5	-1.9
	R_1 = OH	0.2	0.3	-0.7	-1.3	-0.2	-1.0	-1.5
	R_1 = F	0.4	1.4	0.5	-0.3	-0.1	-0.4	-0.8
	R_1 = $C(O)CH_3$	-0.7	0.4	0.4	-0.1	-1.6	-0.7	-0.6
	R_1 = CN	0.3	0.8	0.7	0.4	-0.2	0.0	-0.1
	R_1 = NO_2	0.6	1.7	1.6	1.1	-0.1	0.6	0.5
		R_2 = CH_3	R_2 = NH_2	R_2 = OH	R_2 = F	R_2 = $C(O)CH_3$	R_2 = CN	R_2 = NO_2
trans-3,4-disubstituted cyclobutenes	R_1 = CH_3	0.6	1.8	1.4	0.9	-0.7	-0.4	-1.1
	R_1 = NH_2		8.2	6.7	2.5	-4.8	-3.0	-4.9
	R_1 = OH			3.5	2.2	-2.4	-1.4	-2.2
	R_1 = F				1.3	-0.9	-0.6	-0.6
	R_1 = $C(O)CH_3$					-0.6	-0.2	-1.4
	R_1 = CN						-0.5	-1.5
	R_1 = NO_2							1.2
		R_2 = CH_3	R_2 = NH_2	R_2 = OH	R_2 = F	R_2 = $C(O)CH_3$	R_2 = CN	R_2 = NO_2
1,2-disubstituted cyclobutenes	R_1 = CH_3	-0.4	-0.9	-0.1	-0.5	-0.3	0.2	0.6
	R_1 = NH_2		-6.1	-3.1	-2.0	1.5	1.9	4.2
	R_1 = OH			-2.1	-0.8	0.8	1.1	1.5
	R_1 = F				-1.1	-0.1	0.4	-0.1
	R_1 = $C(O)CH_3$					-4.2	-0.3	-0.8
	R_1 = CN						0.1	0.0
	R_1 = NO_2							-8.6