

### Supporting Information Available

Manuscript : 1,3-Dipolar Additions Involving Allenes :  
A Density Functional Study of Concerted  
and Stepwise Mechanisms.

Authors : K.Kavitha and P.Venuvanalingam

Address : Department of Chemistry, Bharathidasan  
University, Tiruchirappalli - 24.

**Cartesian co-ordinates of all the structures with their  
computed total energies:**

#### ALLENE-NITRONE

##### CONCERTED TS1

1	C	-1.6943	0.5070	-0.2798
2	N	-1.3685	-0.6656	0.2526
3	O	-0.3036	-1.2692	-0.1502
4	C	1.1202	0.3317	0.0338
5	C	0.3382	1.4339	0.1332
6	C	2.2205	-0.3812	-0.0386
7	H	-1.6399	-0.8317	1.2282
8	H	-2.5113	1.0531	0.1820
9	H	-1.5192	0.6199	-1.3404
10	H	0.0912	1.8472	1.1092
11	H	0.2774	2.1342	-0.6969
12	H	3.1956	0.0957	0.0627
13	H	2.2067	-1.4542	-0.2024

Total Energy = -286.4289 Hartrees

##### ANTI TS1

1	C	-0.3681	-0.2355	0.5515
2	C	-1.6670	-0.1927	0.1663
3	C	-2.8932	-0.0517	-0.2447
4	C	0.6594	0.9220	-0.1863
5	N	1.9239	0.3599	0.0137
6	H	-0.2334	-0.1998	1.6410
7	H	0.3582	-1.0592	0.1257
8	H	-3.5428	-0.9098	-0.4299
9	H	-3.3412	0.9291	-0.4225
10	H	0.5400	1.9135	0.2557
11	H	0.3728	0.8876	-1.2364
12	O	1.9589	-0.9091	-0.3371
13	H	2.3200	0.5400	0.9460

Total Energy = -286.4335 Hartrees

**ANTI INT1**

1	N	.0000	.0000	.0000
2	C	1.4645	.0000	.0000
3	C	2.0864	1.4021	.0000
4	C	3.5049	1.3372	.0627
5	C	4.7714	1.2403	-.1906
6	O	-.6218	-.0838	-1.0422
7	H	-.4173	.4991	.7791
8	H	1.7921	-.5567	.9211
9	H	1.8153	-.5630	-.9091
10	H	1.7136	1.9887	.8893
11	H	1.7613	1.9620	-.9242
12	H	5.1717	1.0196	-1.1938
13	H	5.5303	1.3769	.5955

Total Energy = -286.4742 Hartrees

**ROT TS 1**

1	C	.0000	.0000	.0000
2	C	1.2951	.0000	.0000
3	C	2.6762	.3382	.0000
4	C	2.9030	1.8375	-.2652
5	N	3.8817	2.4695	.6216
6	O	3.5569	3.3903	1.3465
7	H	-.6054	.9210	.0185
8	H	-.5759	-.9384	-.0130
9	H	3.2025	-.2561	-.7996
10	H	3.1216	.0275	.9886
11	H	4.6453	1.8659	.9091
12	H	1.9315	2.4007	-.1781
13	H	3.2909	1.9685	-1.3140

Total Energy = -286.4353 Hartrees

**GAUCHE INT1**

1	C	.0000	.0000	.0000
2	C	1.5314	.0000	.0000
3	C	2.0926	1.3080	.0000
4	C	2.4017	2.5149	.3599
5	N	-.6111	.1695	1.3215
6	H	-.3583	-.9933	-.3908
7	H	-.3700	.8128	-.6874
8	H	1.9237	-.5907	.8756
9	H	1.8679	-.5291	-.9384
10	H	2.0243	2.9766	1.2876
11	H	3.0628	3.1460	-.2522
12	O	-.2771	1.0585	2.0802
13	H	-1.5628	-.1798	1.3735

Total Energy = -286.4768 Hartrees

## GAUCHE TS1

1	C	-0.51487	-0.60179	2.27931
2	C	0.36454	-0.01923	3.12819
3	C	1.60198	-0.74883	3.41677
4	C	1.20925	-2.17869	3.93429
5	N	0.00000	-2.69833	3.35726
6	H	-0.21394	-1.29901	1.49085
7	H	-1.56819	-0.29344	2.24293
8	H	2.24132	-0.21981	4.16871
9	H	2.22203	-0.88673	2.49227
10	O	-1.15625	-2.21645	3.89235
11	H	1.13125	-2.08240	5.05452
12	H	2.10262	-2.83250	3.72421
13	H	0.00000	-3.40768	2.56959

Total Energy = -286.4549 Hartrees

## ALLYLIC TS 1

1	C	-2.20250	1.40882	-2.06218
2	C	-2.63346	0.44804	-1.78061
3	O	-2.40598	-1.31114	-2.71230
4	N	-0.99868	-1.40981	-2.55303
5	C	0.00000	-1.08861	-2.07699
6	C	-3.63744	0.04877	-0.64749
7	H	-2.43996	2.32220	-1.50739
8	H	-1.50840	1.50351	-2.90300
9	H	-4.06140	-0.92142	-0.37066
10	H	-3.94476	0.91227	-0.04851
11	H	-0.83467	-2.19186	-3.24952
12	H	0.94349	-1.39378	-2.52953
13	H	0.00000	-0.47901	-1.17339

Total Energy = -286.4406 Hartrees

## ALLYLIC INT1

1	C	.0000	.0000	.0000
2	C	1.3858	.0000	.0000
3	C	2.1147	1.3169	.0000
4	N	2.6462	1.7120	-1.3081
5	O	3.8167	1.5298	-1.5829
6	C	2.1357	-1.1679	.0128
7	H	-.5731	-.9335	.0092
8	H	-.5751	.9300	-.0016
9	H	1.4188	2.1413	.3249
10	H	2.9755	1.2654	.7257
11	H	1.9607	1.7107	-2.0566
12	H	3.2293	-1.1480	.0002
13	H	1.6536	-2.1509	.0391

Total Energy= -286.4384 Hartrees

ALLYLIC TS 2

1	C	-2.1269	.1680	.4718
2	C	-.7653	.1680	.4718
3	O	-.1575	1.4530	.4718
4	N	1.1404	1.4963	.1058
5	C	1.5022	.4680	-.7739
6	C	.0934	-.9667	.4065
7	H	-2.6866	-.7719	.5028
8	H	-2.7012	1.1004	.4786
9	H	1.7181	1.4633	.9454
10	H	.8910	.3327	-1.6740
11	H	2.5336	.1004	-.7555
12	H	.9623	-1.0649	1.0637
13	H	-.2369	-1.8585	-.1317

Total Energy = -286.4289 Hartrees

REGIO 1 PRODUCT

1	C	-0.01000	-2.37750	-0.00000
2	N	-0.01000	-3.66621	0.27392
3	O	-1.19279	-4.07419	0.68342
4	C	-2.16417	-2.95273	0.71014
5	C	-1.34795	-1.77690	0.23746
6	C	-1.72763	-0.51611	0.07319
7	H	0.86699	-1.83214	-0.35525
8	H	-2.51582	-2.86367	1.76447
9	H	-2.99229	-3.23471	0.01887
10	H	-1.03665	0.26062	-0.28058
11	H	-2.75177	-0.17932	0.28109
12	H	0.72651	-1.87186	0.62449
13	H	0.00000	-4.70305	0.49431

Total Energy = -286.5125 Hartrees

CONCERTED TS2

1	C	-.2051	-.9417	-.9789
2	N	1.1560	-.9417	-.9789
3	O	1.7334	.1647	-.9789
4	C	.7148	1.2388	.4375
5	C	-.4228	.5178	.5654
6	C	-1.5881	.2506	1.0917
7	H	1.6091	-1.6901	-.4592
8	H	-.7287	-1.8694	-.7022
9	H	-.7218	-.2446	-1.6608
10	H	.7712	2.0984	-.2462
11	H	1.5653	1.0940	1.1192
12	H	-2.2038	-.6081	.7938
13	H	-2.0335	.8850	1.8736

Total Energy = -286.4272 Hartrees

**ANTI TS2**

1	C	-1.7214	-2.3970	.0000
2	N	-.3938	-2.3970	.0000
3	O	.3638	-1.3633	.0000
4	C	.1284	.2058	.0003
5	C	1.3986	.7540	.0313
6	C	2.6879	.9041	.0610
7	H	-2.2853	-3.3387	.0011
8	H	-2.2577	-1.4379	-.0008
9	H	.0660	-3.3071	.0011
10	H	-.4857	.3852	.9118
11	H	-.4428	.3903	-.9376
12	H	3.1518	1.9011	.0761
13	H	3.3950	.0604	.0731

Total Energy = -286.3903 Hartrees

**ANTI INT2**

1	O	.0000	.0000	.0000
2	C	1.4538	.0000	.0000
3	C	1.8748	1.3679	.0000
4	C	1.8901	2.6619	.0638
5	N	-.6468	-1.1839	.0502
6	C	-.0206	-2.3427	-.3306
7	H	1.8332	-.5316	.9163
8	H	1.8259	-.5180	-.9287
9	H	.9882	3.2653	.2601
10	H	2.8200	3.2347	-.0730
11	H	-1.5337	-1.0426	-.4332
12	H	-.6521	-3.1951	-.5985
13	H	1.0481	-2.4927	-.1682

Total Energy = -286.4226 Hartrees

**ROT TS2**

1	C	2.39140	1.12005	2.65754
2	C	2.57642	2.26471	3.23645
3	C	2.33638	3.56617	3.79474
4	O	1.10630	4.22836	3.35023
5	N	0.00000	3.77183	3.79117
6	H	1.40173	0.74598	2.34697
7	H	3.23393	0.44355	2.45005
8	H	3.15972	4.26272	3.44719
9	H	2.39723	3.49782	4.92392
10	C	-1.16538	4.25206	3.32734
11	H	-1.29486	4.97711	2.50865
12	H	-2.06484	3.83331	3.80476
13	H	0.00000	3.01659	4.52063

Total Energy = -286.4190 Hartrees

**GAUCHE INT2**

1	O	-1.31238	-1.72279	-0.91329
2	C	-0.21376	-2.78919	-0.94501
3	C	0.87273	-2.45037	-1.79972
4	C	1.89121	-1.82986	-2.30899
5	N	-1.05373	-0.60593	0.00009
6	H	0.16195	-2.99647	0.09681
7	H	-0.68104	-3.74242	-1.32812
8	H	2.28898	-0.89058	-1.88976
9	H	2.41364	-2.21460	-3.19728
10	C	0.00000	0.00000	0.00000
11	H	-1.89517	-0.11457	0.28468
12	H	0.94349	-0.54582	-0.00006
13	H	0.00000	1.09000	-0.00010

Total Energy = -286.4385 Hartrees

**GAUCHE TS2**

1	C	-1.86514	-2.90583	1.08707
2	C	-1.11267	-3.67440	0.26462
3	C	-0.01000	-3.09546	-0.04329
4	N	-0.01000	-1.81290	-0.72524
5	O	-0.92793	-0.98331	-0.03014
6	H	-1.43782	-2.26383	1.86398
7	H	-2.95928	-2.99507	1.11483
8	H	0.10682	-3.59468	0.99169
9	C	-2.15216	-1.23610	-0.57128
10	H	-3.01857	-0.65418	-0.25693
11	H	-2.26406	-2.02112	-1.31915
12	H	0.93728	-3.57160	0.20979
13	H	0.00000	-0.85048	-1.23696

Total Energy = -286.4222 Hartrees

**ALLYLIC TS3**

1	C	1.00384	-2.58846	-1.38814
2	C	1.39590	-2.13122	-0.47967
3	C	1.40749	-0.18590	0.00002
4	N	0.00000	0.00000	0.00000
5	O	-1.08210	-0.39524	0.00003
6	C	2.16359	-2.73640	0.74334
7	H	1.10051	-3.66364	-1.57009
8	H	0.48954	-1.99853	-2.15312
9	H	1.84961	-0.19160	0.91472
10	H	2.55001	-2.26802	1.65380
11	H	2.32122	-3.81461	0.63620
12	H	1.98254	-0.31465	-0.91696
13	H	0.00000	1.06000	-0.00010

Total Energy = -286.4364 Hartrees

ALLYLIC INT 2

1	C	-1.9778	-.8522	.0000
2	C	-.5838	-.8522	.0000
3	C	.2040	-1.9912	.0000
4	O	-.0584	.4605	-.0601
5	N	1.2329	.6109	.3189
6	C	1.3883	1.1975	1.5619
7	H	-2.5468	.0811	.0092
8	H	-2.5268	-1.7966	-.0286
9	H	.5992	1.1149	2.3121
10	H	-.2694	-2.9779	.0148
11	H	1.6983	1.1254	-.4249
12	H	2.3570	1.6477	1.7913
13	H	1.2964	-1.9598	-.0016

Total Energy = -286.5020 Hartrees

ALLYLIC TS4

1	C	.1898	-1.3749	-.3111
2	N	1.6642	-1.3749	-.3111
3	O	2.1382	-.2179	-.3111
4	C	.7072	.8278	.6883
5	C	-.3154	-.1833	.4827
6	C	-1.5770	-.1073	.9079
7	H	2.0332	-1.9883	.4157
8	H	-.1948	-2.3433	.1036
9	H	-.1566	-1.2713	-1.3767
10	H	.7635	1.6828	.0092
11	H	1.2276	.8847	1.6478
12	H	-2.3085	-.9038	.7212
13	H	-1.9572	.7592	1.4638

Total Energy = -286.4700 Hartrees

REGIO 2 PRODUCT

1	C	.0000	.0000	.0000
2	N	1.4824	.0000	.0000
3	O	1.9102	1.2870	.0000
4	C	.8311	2.2320	.2674
5	C	-.4286	1.4227	.2567
6	C	-1.6691	1.8613	.4266
7	H	1.7916	-.4188	.8788
8	H	-.4239	-.7079	.7591
9	H	-.3314	-.3311	-1.0219
10	H	.8772	2.9905	-.5525
11	H	1.0358	2.7068	1.2591
12	H	-2.5372	1.1898	.4003
13	H	-1.8987	2.9207	.6004

Total Energy = -286.5158 Hartrees

ALLENE - DIAZOMETHANE

CONCERTED TS1

1	C	-1.8343	0.4669	-0.0000
2	N	-1.3390	-0.7797	0.0000
3	N	-0.3619	-1.4027	0.0000
4	C	1.1194	0.3354	-0.0000
5	C	0.2897	1.3999	0.0000
6	C	2.2478	-0.3412	-0.0000
7	H	-2.3490	0.7369	0.9200
8	H	-2.3489	0.7369	-0.9200
9	H	0.0899	1.9452	0.9195
10	H	0.0899	1.9452	-0.9195
11	H	3.2093	0.1746	0.0000
12	H	2.2804	-1.4274	-0.0000

Total Energy = -265.3679 Hartrees

ANTI TS 1

1	C	-0.36810	-0.23550	0.55150
2	C	-1.66700	0.06287	0.30414
3	C	-2.89320	0.44980	0.10644
4	C	0.65940	1.10966	0.82484
5	N	1.92390	0.56638	0.57824
6	H	-0.23340	-0.96665	1.36002
7	H	0.35820	-0.53223	-0.32699
8	H	-3.54280	-0.03881	-0.62287
9	H	-3.34120	1.27884	0.65986
10	H	0.54000	1.51584	1.83154
11	H	0.37280	1.81437	0.04556
12	N	1.95890	-0.10277	-0.55563

Total Energy = -265.3799 Hartrees

ANTI INT1

1	N	.0000	.0000	.0000
2	C	1.4588	.0000	.0000
3	C	2.1093	1.3867	.0000
4	C	3.5257	1.2949	.0528
5	C	4.7983	1.1423	-.1280
6	N	-.8597	.4927	-.5863
7	H	1.7626	-.5539	.9321
8	H	1.8087	-.5893	-.8936
9	H	1.7523	1.9733	.8965
10	H	1.7952	1.9626	-.9175
11	H	5.2321	.7579	-1.0656
12	H	5.5295	1.3940	.6563

Total Energy = -265.4267 Hartrees



**ROT TS 1**

1	C	.0000	.0000	.0000
2	C	1.2950	.0000	.0000
3	C	2.6789	.3246	.0000
4	C	2.9329	1.7763	-.4411
5	N	3.6972	2.6248	.4591
6	H	-.6061	.9205	-.0036
7	H	-.5773	-.9377	.0072
8	H	3.2136	-.3641	-.7156
9	H	3.1032	.1181	1.0234
10	H	1.9540	2.3107	-.6022
11	H	3.4972	1.7776	-1.4157
12	N	4.1984	2.5825	1.4943

Total Energy = -265.3850 Hartrees

**GAUCHE INT1**

1	N	.0000	.0000	.0000
2	C	1.4542	.0000	.0000
3	C	2.1467	1.3645	.0000
4	C	1.9199	2.1113	1.1862
5	C	1.5057	2.8618	2.1558
6	N	-.8682	.7566	-.0009
7	H	1.7661	-.5682	-.9207
8	H	1.7656	-.5861	.9099
9	H	3.2562	1.1801	-.1031
10	H	1.8259	1.9634	-.9002
11	H	.4917	3.2933	2.1920
12	H	2.1503	3.1058	3.0149

Total Energy = -265.4278 Hartrees

**GAUCHE TS1**

1	C	0.00000	0.00000	0.00000
2	C	1.35400	0.00000	0.00000
3	C	2.02471	-1.25223	-0.35907
4	C	1.47890	-2.38028	0.58758
5	N	0.10817	-2.20202	0.98077
6	H	-0.59885	-0.66053	-0.63516
7	H	-0.57426	0.76786	0.53526
8	H	3.13898	-1.17542	-0.27829
9	H	1.78849	-1.55672	-1.41247
10	N	-0.10000	-1.30000	1.98000
11	H	2.17198	-2.38887	1.47630
12	H	1.64612	-3.34726	0.03378

Total Energy = -265.4006 Hartrees

**ALLYLIC TS1**

1	C	-1.89933	-2.73357	-0.09217
2	C	-2.19249	-2.00325	-0.77260
3	N	-2.47889	0.00107	-0.31142
4	N	-1.12003	0.26958	0.00002
5	C	0.00000	0.00000	0.00000
6	C	-2.78348	-1.96865	-2.22366
7	H	-1.86414	-3.77559	-0.42597
8	H	-1.56065	-2.52598	0.92760
9	H	-3.12833	-1.16363	-2.87992
10	H	-2.79954	-2.98340	-2.63462
11	H	1.05741	-0.26480	-0.00002
12	H	-0.00000	1.09000	0.00010

Total Energy = -265.3615 Hartrees

**ALLYLIC INT1**

1	C	0.00000	0.00000	0.00000
2	C	1.38580	0.00000	0.00000
3	C	2.11470	1.28812	0.27380
4	N	2.64620	1.94656	-0.92357
5	N	3.81670	1.82547	-1.23025
6	C	2.13570	-1.14504	-0.23030
7	H	-0.57310	-0.91501	-0.18509
8	H	-0.57510	0.91001	0.19179
9	H	1.41880	2.02696	0.76300
10	H	2.97550	1.08687	0.97293
11	H	3.22930	-1.12296	-0.23849
12	H	1.65360	-2.11203	-0.40895

Total Energy = -265.3905 Hartrees

**ALLYLIC TS2**

1	C	2.46564	-1.28467	0.29993
2	C	1.21777	-1.58573	0.68193
3	C	-0.00000	-1.09000	0.00000
4	N	-1.13093	-1.43171	0.47005
5	N	-1.16163	-2.11509	1.46289
6	C	0.93266	-2.43215	1.80067
7	H	3.33860	-1.68208	0.84243
8	H	2.65876	-0.63172	-0.56601
9	H	0.05425	-0.45072	-0.89599
10	H	0.91331	-3.52356	1.66614
11	H	0.96235	-2.01703	2.81874
12	H	0.00000	0.00000	0.00000

Total Energy = -265.3806 Hartrees

S10

**REGIO 1 PRODUCT**

1	C	0.1331	-1.1931	0.0003
2	C	-0.7937	0.0004	0.0005
3	C	0.1338	1.1933	0.0003
4	N	1.5109	0.6205	-0.0004
5	N	1.5107	-0.6212	-0.0003
6	C	-2.1250	0.0001	-0.0003
7	H	0.0385	-1.8386	-0.8820
8	H	0.0388	-1.8389	0.8825
9	H	0.0404	1.8388	0.8827
10	H	0.0392	1.8396	-0.8814
11	H	-2.6994	0.9231	-0.0009
12	H	-2.6984	-0.9234	-0.0007

Total Energy = -265.4629 Hartrees

**CONCERTED TS 2**

1	C	0.48608	-1.31564	0.0001
2	N	1.53591	-0.48193	-0.0001
3	N	1.88306	0.61964	-0.0001
4	C	-0.39551	1.46466	0.0001
5	C	-1.06429	0.29008	0.0000
6	C	-2.18869	-0.40478	-0.00013
7	H	0.38078	-1.88598	0.92074
8	H	0.38066	-1.8866	-0.92004
9	H	-0.17117	1.9932	-0.9226
10	H	-0.17126	1.99319	0.92284
11	H	-2.22665	-1.49084	-0.00013
12	H	-3.1507	0.10713	-0.00024

Total Energy = -265.3681 Hartrees

**ANTI TS2**

1	C	-1.3019	-2.3539	.0000
2	N	.0405	-2.3539	.0000
3	N	1.0707	-1.8154	.0000
4	C	1.2999	.0305	.1070
5	C	1.2867	.3592	1.4218
6	C	1.2564	.4995	2.7108
7	H	-1.8095	-2.7906	-.8672
8	H	-1.8323	-2.1766	.9428
9	H	2.2826	.0460	-.4109
10	H	.4510	.3877	-.5140
11	H	1.0842	-.3405	3.4013
12	H	1.4065	1.4772	3.1933

Total Energy = -265.3539 Hartrees

**ANTI INT2**

1	C	.0000	.0000	.0000
2	N	1.3582	.0000	.0000
3	N	2.1323	.9731	.0000
4	C	1.7019	2.3803	-.0017
5	C	2.8020	3.3024	.0180
6	C	4.0227	3.7390	.0392
7	H	-.6401	.8953	.0015
8	H	-.4788	-.9890	-.0007
9	H	1.0792	2.5988	-.9237
10	H	1.0487	2.5967	.8995
11	H	4.9011	3.0725	.0556
12	H	4.2482	4.8160	.0419

Total Energy = -265.3854 Hartrees

**ROT TS2**

1	C	.0000	.0000	.0000
2	C	1.2960	.0000	.0000
3	C	2.6606	.4483	.0000
4	N	2.8713	1.8344	-.4284
5	N	2.5071	2.7591	.3710
6	H	-.6104	.9152	.0752
7	H	-.5699	-.9387	-.0679
8	H	3.2381	-.1611	-.7609
9	H	3.1133	.2455	1.0185
10	C	2.5577	4.0456	-.0114
11	H	2.8139	4.4204	-1.0147
12	H	2.2727	4.7736	.7639

Total Energy = -265.3703 Hartrees

**GAUCHE INT 2**

1	C	.0000	.0000	.0000
2	N	1.3546	.0000	.0000
3	N	2.1580	.9443	.0000
4	C	1.8904	2.3761	.0616
5	C	.5461	2.8515	.1995
6	C	-.4881	3.6320	.2489
7	H	-.6487	.8871	-.0759
8	H	-.4707	-.9916	.0661
9	H	2.5021	2.7493	.9408
10	H	2.3542	2.8065	-.8801
11	H	-.4429	4.7119	.0328
12	H	-1.4865	3.2528	.5162

Total Energy = -265.3911 Hartrees

**GAUCHE TS 2**

1	C	-0.72026	0.03544	2.25840
2	C	-1.55733	0.93686	1.69263
3	C	-2.50000	0.36022	1.04092
4	N	-2.20000	-0.52862	-0.06812
5	N	-1.18084	-1.40833	0.38065
6	H	-1.05911	-0.92120	2.66872
7	H	0.32988	0.27920	2.46738
8	H	-1.60000	1.00000	0.34000
9	H	-2.78000	0.38224	2.16126
10	C	0.00000	-0.77028	0.14831
11	H	0.94349	-1.28322	0.33494
12	H	0.00000	0.25394	-0.22458

Total Energy = -265.3749 Hartrees

**ALLYLIC TS3**

1	C	0.89316	1.23886	2.35153
2	C	0.11219	0.62739	1.89955
3	C	0.00000	0.00000	0.00000
4	N	1.19631	-0.76449	0.00005
5	N	2.07302	-1.28866	0.53276
6	C	-1.23807	0.07505	2.46795
7	H	0.82393	1.57002	3.39268
8	H	1.78325	1.54135	1.79123
9	H	-0.86333	-0.53558	0.00004
10	H	-2.01448	-0.54239	2.00580
11	H	-1.39892	0.37581	3.50841
12	H	0.00000	1.09000	-0.00010

Total Energy = -265.3851 Hartrees

**ALLYLIC INT2**

1	C	.0000	.0000	.0000
2	C	1.3869	.0000	.0000
3	C	2.1146	1.3175	.0000
4	N	1.8817	2.1872	1.1446
5	N	1.3267	2.1654	2.1539
6	C	2.1316	-1.1683	-.0385
7	H	-.5679	-.9358	-.0151
8	H	-.5751	.9308	.0242
9	H	1.8069	1.9098	-.9093
10	H	3.2290	1.1554	-.0448
11	H	3.2259	-1.1572	-.0342
12	H	1.6467	-2.1494	-.0731

Total Energy = -265.4535 Hartrees

**ALLYLIC TS 4**

1	C	.3696	-1.4801	-.2638
2	N	1.8469	-1.4801	-.2638
3	N	2.4712	-.4842	-.2638
4	C	.9076	.9363	-.2607
5	C	-.1565	-.0592	-.2542
6	C	-1.4623	.2088	-.2388
7	H	.0264	-2.0439	.6457
8	H	.0269	-2.0306	-1.1816
9	H	1.1329	1.4588	-1.1988
10	H	1.1409	1.4634	.6729
11	H	-2.2236	-.5816	-.2344
12	H	-1.8499	1.2357	-.2306

Total Energy = -265.3861 Hartrees

**REGIO 2 PRODUCT**

1	C	.0000	.0000	.0000
2	N	1.4935	.0000	.0000
3	N	1.9741	1.1203	.0000
4	C	.9448	2.2025	.0000
5	C	-.3808	1.4673	.0000
6	C	-1.5978	1.9894	-.0001
7	H	-.3682	-.5358	.9125
8	H	-.3682	-.5358	-.9125
9	H	1.0794	2.8387	-.9124
10	H	1.0793	2.8386	.9126
11	H	-2.5033	1.3682	.0000
12	H	-1.7717	3.0735	-.0001

Total Energy = -265.4650 Hartrees

**ALLENE - NITRILE OXIDE  
CONCERTED TS1**

1	C	-1.7356	0.5695	-0.0000
2	N	-1.4658	-0.6090	-0.0000
3	O	-0.5166	-1.3806	0.0000
4	C	1.1454	0.3736	0.0000
5	C	0.3197	1.4327	0.0000
6	C	2.1815	-0.4265	-0.0000
7	H	-2.6214	1.1790	-0.0000
8	H	0.1331	1.9763	0.9240
9	H	0.1331	1.9763	-0.9240
10	H	3.1903	-0.0119	-0.0000
11	H	2.0932	-1.5077	-0.0000

Total Energy = -285.2052 Hartrees

**ANTI TS1**

1	C	-0.4521	-0.5193	0.6911
2	C	-1.6522	-0.2820	0.1089
3	C	-2.7344	0.1137	-0.4923
4	C	0.7078	0.8547	0.3264
5	N	1.7872	0.4502	-0.1264
6	H	-0.4458	-0.5324	1.7840
7	H	0.2024	-1.2791	0.2347
8	H	-3.6083	-0.5312	-0.5937
9	H	-2.8203	1.1104	-0.9324
10	H	0.3939	1.8629	0.5394
11	O	2.3191	-0.5981	-0.4939

Total Energy = -285.2086 Hartrees

**ANTI INT1**

1	N	.0000	.0000	.0000
2	C	1.3716	.0000	.0000
3	C	2.2227	1.2192	.0000
4	C	3.6150	.9215	.0363
5	C	4.8549	.7083	-.2683
6	O	-.7107	.7799	-.5069
7	H	1.8305	-.9829	.1942
8	H	1.9639	1.8634	.8941
9	H	1.9780	1.8349	-.9184
10	H	5.2381	.7309	-1.3018
11	H	5.6097	.4923	.5042

Total Energy = -285.2519 Hartrees

**ROT TS1**

1	C	0.00000	0.00000	0.00000
2	C	1.29500	0.00000	0.00000
3	C	2.67890	-0.24866	0.20865
4	C	2.93290	-1.07719	1.47969
5	N	3.69720	-2.30582	1.33550
6	H	-0.60610	-0.70283	0.59444
7	H	-0.57730	0.71369	-0.60826
8	H	3.21360	0.73890	0.31414
9	H	3.10320	-0.74830	-0.70806
10	H	3.49720	-0.45173	2.22711
11	O	4.19840	-2.93883	0.51530

Total Energy = -285.2124 Hartrees

## GAUCHE INT 1

1	C	.0000	.0000	.0000
2	C	1.2960	.0000	.0000
3	C	2.6898	.2825	.0000
4	C	3.1535	.9760	-1.2451
5	N	3.1008	2.2608	-1.4738
6	O	2.7731	3.2689	-.9797
7	H	-.6038	.9122	-.1331
8	H	-.5761	-.9294	.1275
9	H	2.9583	.8830	.9177
10	H	3.2526	-.6957	.0562
11	H	3.5819	.3643	-2.0561

Total Energy = -285.2584 Hartrees

## GAUCHE TS 1

1	C	0.00000	0.00000	0.00000
2	C	1.35400	0.00000	0.00000
3	C	2.02471	-1.19007	-0.52985
4	C	1.47890	-2.43889	0.25059
5	N	0.10817	-2.31709	0.66476
6	H	-0.59885	-0.56570	-0.72091
7	H	-0.57426	0.68589	0.63692
8	H	3.13898	-1.12525	-0.43917
9	H	1.78849	-1.34499	-1.61538
10	O	-0.10000	-1.56291	1.77981
11	H	1.64612	-3.31939	-0.43240

Total Energy = -285.2365 Hartrees

## ALLYLIC TS1

1	C	3.09205	-2.29691	-0.09497
2	C	2.45000	-1.55000	0.24000
3	O	0.56877	-1.16136	-0.54863
4	N	-0.01000	-2.39378	-0.14642
5	C	-0.01000	-3.37075	0.46405
6	C	2.55336	-0.28689	1.16191
7	H	4.09660	-2.35536	0.33622
8	H	2.81188	-3.07546	-0.81127
9	H	1.85081	0.50462	1.44044
10	H	3.54333	-0.25680	1.62873
11	H	0.00000	-4.29513	1.04167

Total Energy= -285.2081 Hartrees



**ALLYLIC INT 1**

1	C	.0000	.0000	.0000
2	C	1.3984	.0000	.0000
3	C	2.0601	1.2907	.0000
4	N	3.3612	1.5215	-.0137
5	O	4.3868	.9645	-.0294
6	C	2.1207	-1.1930	-.0026
7	H	-.5601	-.9398	-.0017
8	H	-.5757	.9297	.0018
9	H	1.4398	2.2058	.0131
10	H	3.2151	-1.2146	-.0107
11	H	1.6051	-2.1586	-.0030

Total Energy = -285.2157 Hartrees

**ALLYLIC TS2**

1	C	.0000	.0000	.0000
2	C	1.3393	.0000	.0000
3	C	2.1680	1.2276	.0000
4	N	3.4326	1.0967	-.0191
5	O	3.8980	-.0145	-.0673
6	C	2.1143	-1.2036	.0044
7	H	-.5693	-.9435	.0015
8	H	-.5737	.9404	-.0019
9	H	1.7182	2.2333	.0257
10	H	2.3393	-1.7023	.9585
11	H	2.2837	-1.7453	-.9377

Total Energy = -285.2495 Hartrees

**REGIO 1 PRODUCT**

1	C	.0000	.0000	.0000
2	N	1.3175	.0000	.0000
3	O	1.8017	1.2242	.0000
4	C	.7103	2.2296	.0000
5	C	-.5381	1.3848	.0000
6	C	-1.8055	1.7778	-.0001
7	H	-.6073	-.9077	.0000
8	H	.8424	2.8401	-.9236
9	H	.8424	2.8402	.9235
10	H	-2.6388	1.0626	.0000
11	H	-2.0917	2.8378	-.0001

Total Energy = -285.3133 Hartrees

**CONCERTED TS2**

1	C	-.1246	-1.1165	-1.1712
2	N	1.1182	-1.1165	-1.1712
3	O	1.9267	-.2338	-1.1712
4	C	.5239	1.5013	-1.1365
5	C	-.6674	.8827	-1.1190
6	C	-1.9735	.8313	-1.0826
7	H	-.9837	-1.7626	-1.1738
8	H	1.0144	1.7843	-2.0795
9	H	1.0557	1.7591	-.2086
10	H	-2.5512	-.1021	-1.0829
11	H	-2.5816	1.7488	-1.0486

Total Energy = -285.1959 Hartrees

**ANTI TS 2**

1	C	-1.9404	-2.8582	.0000
2	N	-.7101	-2.8582	.0000
3	O	.2248	-2.0663	.0000
4	C	.0080	-.3139	-.0216
5	C	1.3002	.1155	.0290
6	C	2.5724	.3551	.0797
7	H	-2.8159	-3.4726	.0006
8	H	-.6146	-.2014	.8871
9	H	-.5348	-.2189	-.9819
10	H	3.3255	-.4481	.1187
11	H	2.9748	1.3795	.0868

Total Energy = -285.1771 Hartrees

**ANTI INT 2**

1	C	.0000	.0000	.0000
2	N	1.2436	.0000	.0000
3	O	2.0431	1.0205	.0000
4	C	1.4968	2.3909	.0059
5	C	2.6058	3.2825	-.0304
6	C	3.8072	3.7661	-.0618
7	H	-.8996	-.5767	.0001
8	H	.8387	2.5168	-.8972
9	H	.8904	2.5261	.9431
10	H	4.7111	3.1345	-.0692
11	H	3.9910	4.8513	-.0833

Total Energy = -285.1921 Hartrees

**ROT TS 2**

1	C	0.00000	0.00000	0.00000
2	C	1.29500	0.00000	0.00000
3	C	2.67890	-0.24866	0.20865
4	C	2.93290	-1.07719	1.47969
5	N	3.69720	-2.30582	1.33550
6	H	-0.60610	-0.70283	0.59444
7	H	-0.57730	0.71369	-0.60826
8	H	3.21360	0.73890	0.31414
9	H	3.10320	-0.74830	-0.70806
10	H	3.49720	-0.45173	2.22711
11	O	4.19840	-2.93883	0.51530

Total Energy = -285.1883 Hartrees

**GAUCHE INT 2**

1	C	0.00000	0.00000	0.00000
2	N	1.35460	0.00000	0.00000
3	O	2.15800	0.90772	0.26028
4	C	1.89040	2.26708	0.71416
5	C	0.54610	2.68605	0.97775
6	C	-0.48810	3.42270	1.24037
7	H	-0.64870	0.87366	0.17156
8	H	2.50210	2.38348	1.66216
9	H	2.35420	2.94037	-0.07243
10	H	-0.44290	4.52033	1.33031
11	H	-1.48650	2.98451	1.39280

Total Energy = -285.2167 Hartrees

**GAUCHE TS 2**

1	C	-0.72026	0.03544	2.25840
2	C	-1.55733	-0.14728	3.30686
3	C	-2.50000	0.72288	3.31441
4	N	-2.20000	2.14181	3.39597
5	O	-1.18084	2.39695	2.44193
6	H	-1.05911	0.37063	1.27292
7	H	0.32988	-0.28297	2.29971
8	H	-2.78000	-0.12443	2.58112
9	C	0.00000	2.14268	3.07156
10	H	0.94349	2.34721	2.56549
11	H	0.00000	1.73445	4.08222

Total Energy = -285.2025 Hartrees

ALLYLIC TS3

1	C	0.00000	0.00000	0.00000
2	C	1.09000	0.00000	0.00000
3	C	2.31000	-1.36959	0.80643
4	N	1.88170	-2.46854	0.01620
5	O	1.32670	-2.92313	-0.88518
6	C	2.13160	1.04962	-0.51449
7	H	-0.56790	0.83335	-0.42600
8	H	-0.57510	-0.83321	0.41561
9	H	3.22900	-0.99913	0.58198
10	H	3.22590	1.03781	-0.51308
11	H	1.64670	1.93212	-0.94454

Total Energy = -285.2123 Hartrees

ALLYLIC INT2

1	C	.0000	.0000	.0000
2	C	1.3984	.0000	.0000
3	C	2.0601	1.2907	.0000
4	N	3.3612	1.5215	-.0137
5	O	4.3868	.9645	-.0294
6	C	2.1207	-1.1930	-.0026
7	H	-.5601	-.9398	-.0017
8	H	-.5757	.9297	.0018
9	H	1.4398	2.2058	.0131
10	H	3.2151	-1.2146	-.0107
11	H	1.6051	-2.1586	-.0030

Total Energy = -285.2915 Hartrees

ALLYLIC TS 4

1	C	.3486	-1.7273	-.2187
2	N	1.6871	-1.7273	-.2187
3	O	2.2933	-.6779	-.2187
4	C	.6482	.6740	-.2107
5	C	-.3097	-.4172	-.2200
6	C	-1.6539	-.2772	-.2332
7	H	-.2003	-2.6749	-.2188
8	H	.9366	1.1563	-1.1490
9	H	.9477	1.1307	.7371
10	H	-2.3250	-1.1443	-.2425
11	H	-2.1347	.7079	-.2354

Total Energy = -285.2605 Hartrees

REGIO 2 PRODUCT

1	C	.0000	.0000	.0000
2	N	1.3175	.0000	.0000
3	O	1.8017	1.2242	.0000
4	C	.7103	2.2296	.0000
5	C	-.5381	1.3848	.0000
6	C	-1.8055	1.7778	-.0001
7	H	-.6073	-.9077	.0000
8	H	.8424	2.8401	-.9236
9	H	.8424	2.8402	.9235
10	H	-2.6388	1.0626	.0000
11	H	-2.0917	2.8378	-.0001

Total Energy = -285.3200 Hartrees

**Mailing address:**

Dr.P.VENUVANALINGAM  
DEPARTMENT OF CHEMISTRY  
BHARATHIDASAN UNIVERSITY  
TIRUCHIRAPPALLI – 620 024  
INDIA

**Phone :** ++91 431 660353 (office)  
++91 431 771600 (home)

**Fax:** ++91 431 660245  
++91 431 660320  
++91 431 412750

**E-mail :** [venuvanalingam@yahoo.com](mailto:venuvanalingam@yahoo.com)

