Electronic Supporting Information for the paper

Unsaturated Dinitriles Formation Routes in Extraterrestrial Environments: A Combined Experimental and Theoretical Investigation of the Reaction Between Cyano Radicals and Cyanoethene (C_2H_3CN)

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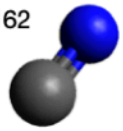
The following data report the cartesian coordinates for all the stationary points identified in the Potential Energy Surface, including minima, transition states, reactants and possible products, evaluated at the B3LYP/aug-cc-pVTZ level of theory. Together with the xyz cartesian coordinates of all the stationary points, the geometries are reported including the values of bond distances (in Å, in black) and angles (in °, in red).

S1: Structures of the stationary points identified in the PES for the $C_2H_3CN + CN$ reaction

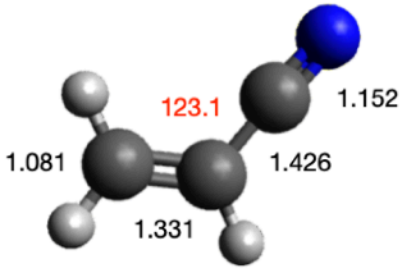
CN

C	0.00000	0.00000	-0.62586
N	0.00000	0.00000	0.53645



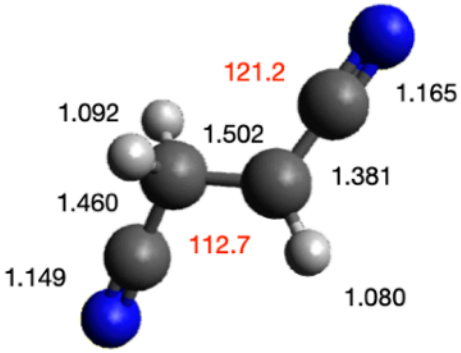
C_2H_3CN

C	1.60314	-0.35429	0.00000
C	0.58301	0.50089	0.00000
H	1.44874	-1.42395	0.00000
H	2.62185	0.00549	0.00000
C	-0.78167	0.08647	0.00000
H	0.74791	1.57100	0.00000
N	-1.89220	-0.22157	0.00000



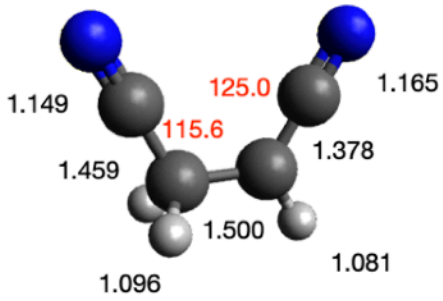
MIN1

C	0.51396	0.63520	-0.17035
C	-0.52891	-0.44270	-0.25952
C	-1.85661	-0.17625	0.00962
N	-2.97298	0.06042	0.24264
C	1.85529	0.10326	0.05404
N	2.90853	-0.32369	0.22219
H	0.27009	1.34107	0.62625
H	0.53067	1.21983	-1.09890
H	-0.25201	-1.43517	-0.58393



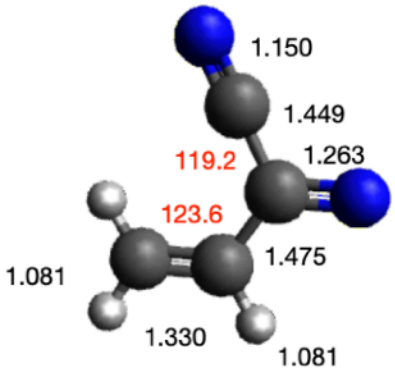
MIN2

C	0.77326	1.08412	0.00013
C	-0.72608	1.03799	-0.00015
C	-1.48134	-0.11422	0.00000
N	-2.14120	-1.07485	0.00007
H	-1.24830	1.98481	-0.00040
C	1.44295	-0.21162	-0.00002
H	1.11828	1.65111	0.87211
H	1.11859	1.65145	-0.87150
N	1.99243	-1.22015	-0.00007



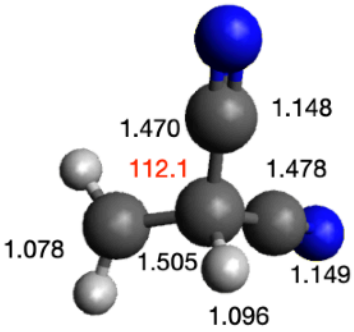
MIN3

C	1.70854	-1.03644	-0.00012
C	1.32380	0.23635	0.00017
H	0.99757	-1.85196	-0.00044
H	2.75785	-1.29460	-0.00003
C	-0.08830	0.66107	0.00000
H	2.03757	1.04877	0.00052
N	-0.43785	1.87484	-0.00013
C	-1.12968	-0.34702	-0.00002
N	-1.94489	-1.15855	0.00009



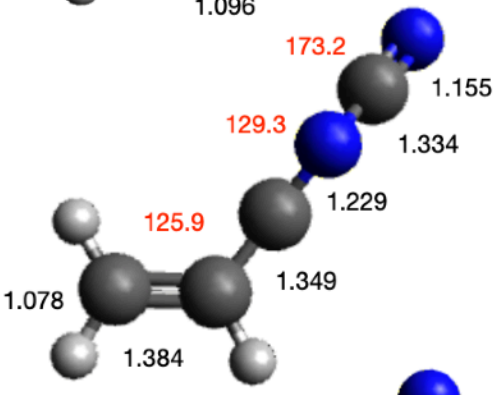
MIN4

C	-0.04904	1.74215	-0.21179
C	-0.00089	0.37959	0.42596
C	1.22974	-0.34779	0.08432
N	2.20948	-0.88604	-0.17769
C	-1.19514	-0.41182	0.06463.
N	-2.15481	-0.97902	-0.21369
H	0.45800	1.91850	-1.14610
H	-0.72890	2.47601	0.19036
H	-0.01985	0.48806	1.51660



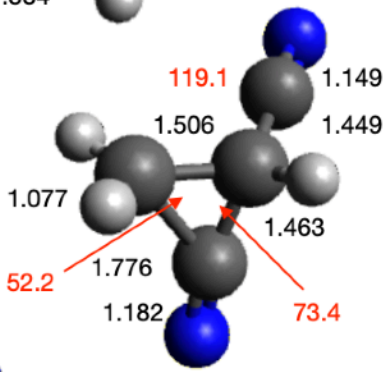
MIN5

C	-2.68891	0.54470	-0.01939
C	-1.72812	-0.43720	-0.18574
H	-2.43516	1.52932	0.34215
H	-3.71827	0.33555	-0.26163
C	-0.40052	-0.28398	0.00151
H	-2.01367	-1.41083	-0.57404
N	0.70532	-0.26876	0.53672.
C	1.89075	0.05463	0.01797
N	2.97009	0.30833	-0.30709



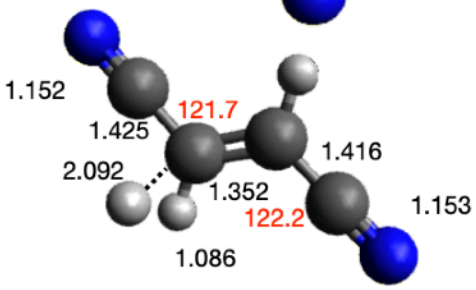
TS1

C	0.66007	-1.32553	-0.30408
C	-0.10184	-0.34801	0.55104
C	-1.39243	0.12837	0.09715
N	-2.42073	0.49082	-0.26613
C	1.09340	0.35294	0.08054
N	1.96976	1.10841	-0.16299
H	0.39271	-1.43921	-1.34127
H	1.29748	-2.04705	0.17897
H	-0.08868	-0.55502	1.61826



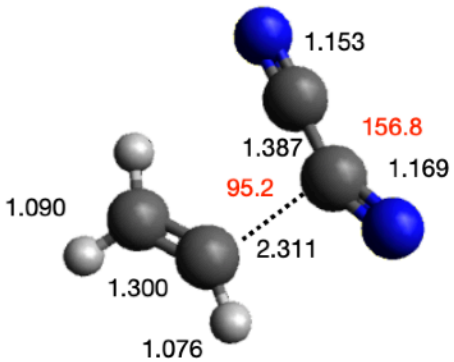
TS2

C	-0.47390	0.41878	0.15338
C	0.50694	-0.45624	-0.16250
C	1.87891	-0.14099	-0.00923
N	3.00210	0.09451	0.10670
C	-1.85087	0.05849	0.08176
N	-2.96720	-0.22285	0.04591
H	-0.63882	1.68451	-1.50442
H	-0.24385	1.36421	0.62556
H	0.27176	-1.43052	-0.56980



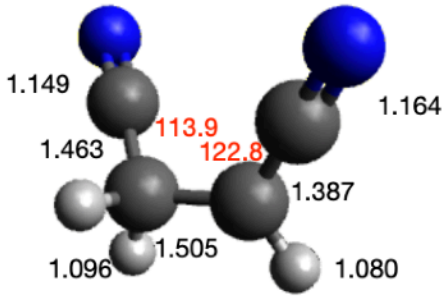
TS3

C	2.13291	-0.32606	0.00000
C	1.38681	0.73849	0.00000
H	1.72692	-1.33225	-0.00000
H	3.21935	-0.24117	0.00000
C	-0.92081	0.60574	0.00000
H	1.50012	1.80892	0.00000
N	-1.34564	1.69520	0.00000
C	-0.96690	-0.78025	0.00000
N	-0.97413	-1.93278	0.00000



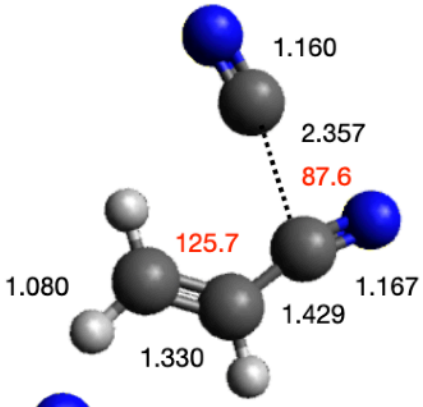
TS4

C	0.70486	1.00889	0.28384
C	-0.67956	0.93731	-0.30279
C	-1.54413	-0.11161	-0.05665
N	-2.28092	-0.98845	0.15287
C	1.51658	-0.18266	0.03361
N	2.16293	-1.11144	-0.16520
H	0.64711	1.15546	1.36853
H	1.22805	1.87437	-0.12208
H	-1.03576	1.75786	-0.90821



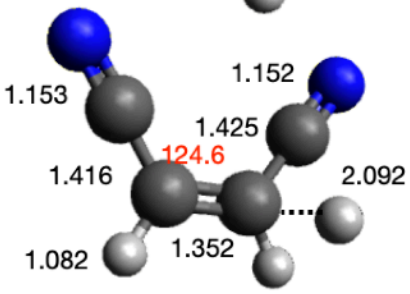
TS5

C	1.25351	-1.48294	0.00012
C	1.56890	-0.19079	-0.00016
H	0.22853	-1.82397	0.00054
H	2.03603	-2.22762	-0.00007
C	0.63865	0.89462	0.00001
H	2.60179	0.13673	-0.00057
N	0.13244	1.94666	0.00000
C	-1.52668	-0.03606	0.00049
N	-2.48566	-0.68868	-0.00038



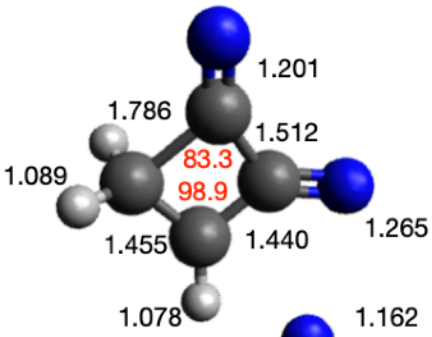
TS6

C	-0.67218	0.98688	-0.10089
C	0.67942	1.01094	-0.13623
C	1.50716	-0.13012	-0.00770
N	2.21751	-1.03326	0.09240
H	1.18674	1.96004	-0.24471
C	-1.44743	-0.20765	-0.05131
H	-1.22069	1.90160	-0.27754
H	-1.16033	1.48389	1.87131
N	-2.10431	-1.15329	-0.03130



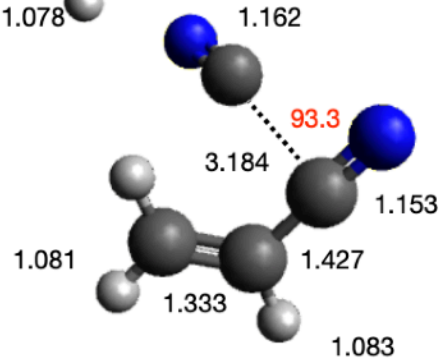
TS7

C	-0.89895	-1.23377	-0.06103
C	0.54980	-1.26389	0.06591
C	0.81567	0.14464	-0.07600
N	1.84435	0.87773	-0.01565
H	1.20460	-2.03822	0.43226
C	-0.64435	0.53349	-0.02839
N	-1.45897	1.40624	0.09970
H	-1.52560	-1.77357	0.64596
H	-1.30968	-1.25880	-1.06948



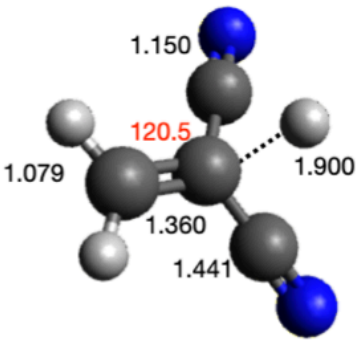
TS8

C	0.77696	1.64089	-0.33228
C	1.36121	0.67853	0.38149
C	1.28480	-0.70288	0.03225
N	1.22275	-1.82619	-0.22063
C	-1.87519	-0.33256	0.15041
N	-2.97759	0.01051	0.01920
H	0.22062	1.42561	-1.23334
H	0.85113	2.67388	-0.02490
H	1.92539	0.90633	1.27705



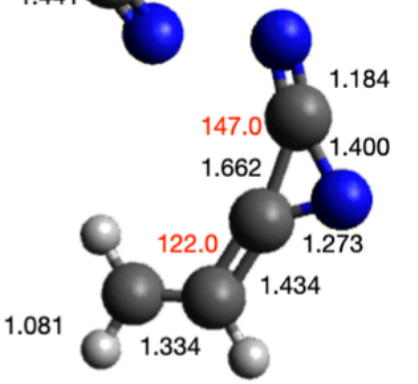
TS9

C	0.00002	1.73992	-0.10645
C	0.00001	0.39346	0.08233
C	1.22604	-0.35808	-0.00812
N	2.21133	-0.94416	-0.10030
C	-1.22602	-0.35808	-0.00812
N	-2.21130	-0.94416	-0.10036
H	0.92975	2.28508	-0.15948
H	-0.92970	2.28510	-0.15945
H	-0.00049	0.14479	1.96570



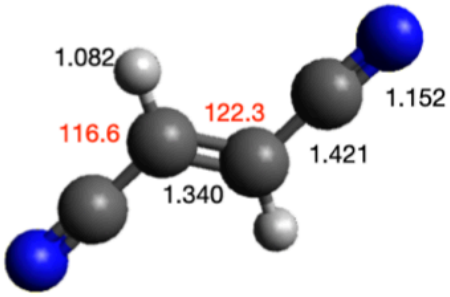
TS10

C	2.29210	-0.72923	0.00000
C	1.55043	0.37967	-0.00001
H	1.83302	-1.70823	0.00002
H	3.37157	-0.67949	-0.00001
C	0.11687	0.33601	0.00000
H	1.99686	1.37124	-0.00003
N	-0.84728	1.16665	0.00001
C	-1.49321	-0.07495	0.00000
N	-2.29537	-0.94558	-0.00001



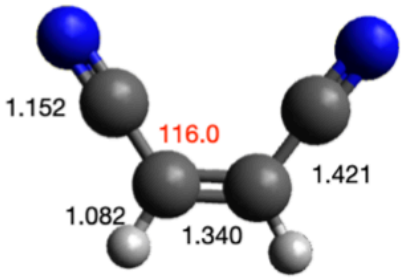
E-NC-CH=CH-CN

C	-0.48638	0.46058	-0.00038
C	0.48638	-0.46058	-0.00038
C	1.86375	-0.11174	0.00008
N	2.98774	0.14250	0.00034
C	-1.86375	0.11174	0.00008
N	-2.98775	-0.14250	0.00034
H	-0.25467	1.51772	-0.00060
H	0.25467	-1.51772	-0.00060



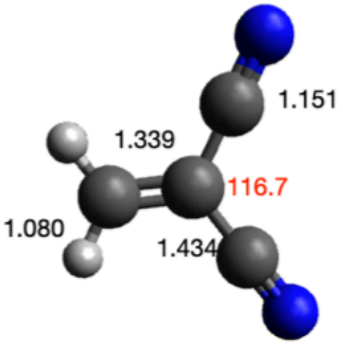
Z-NC-CH=CH-CN

C	0.67014	1.03479	0.00167
C	-0.66998	1.03475	-0.00168
C	-1.47665	-0.13457	-0.00130
N	-2.17125	-1.05395	0.00152
C	1.47683	-0.13450	0.00115
N	2.17096	-1.05422	-0.00143
H	-1.20131	1.97713	-0.00390
H	1.20139	1.97725	0.00418



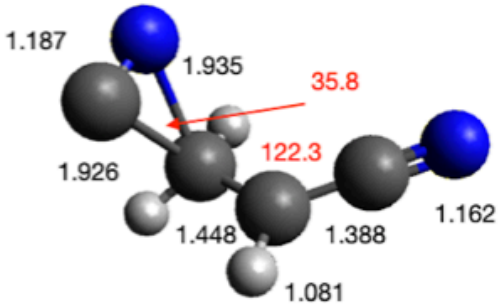
$CH_2C(CN)_2$

C	-0.00227	1.74281	-0.00013
C	0.00010	0.40416	0.00028
C	-1.21981	-0.34986	0.00004
N	-2.20166	-0.95007	-0.00010
C	1.22199	-0.34655	0.00010
N	2.20257	-0.94867	-0.00012
H	-0.93159	2.29238	-0.00005
H	0.92520	2.29549	-0.00016



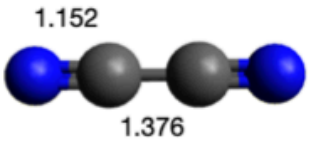
TS-iso

C	0.71075	0.59437	-0.60697
C	-0.44830	0.77891	0.24185
H	1.32055	1.47412	-0.75798
H	0.53630	0.05404	-1.52705
H	-0.41026	1.49892	1.04709
C	-1.59777	0.01274	0.10348
N	-2.57041	-0.61160	-0.01896
N	1.78107	-0.94502	-0.13040
C	2.01511	-0.07448	0.64223



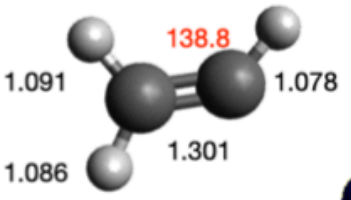
NCCN

C	0.00000	0.00000	0.68786
N	0.00000	0.00000	1.84006
C	0.00000	0.00000	-0.68786
N	0.00000	0.00000	-1.84006



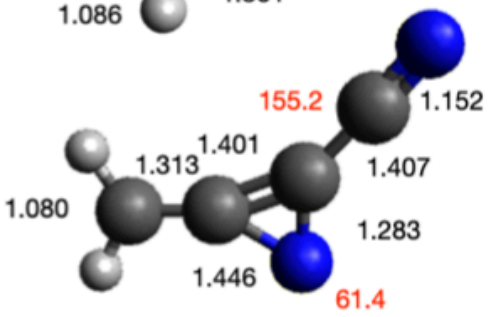
CH_2CH

C	0.58557	0.02928	0.00007
C	-0.70447	-0.14161	-0.00004
H	1.03472	1.02353	-0.00016
H	1.28054	-0.80503	-0.00011
H	-1.60186	0.45547	0.00007



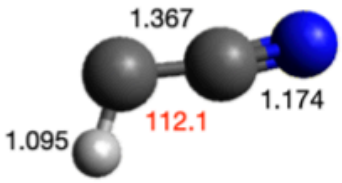
$CH_2C(N)CCN$

C	2.28621	-0.68738	-0.00001
C	1.14857	-0.03103	0.00002
H	2.29687	-1.76648	-0.00000
H	3.22587	-0.15497	-0.00005
C	-0.22862	0.22394	0.00001
N	0.51526	1.26893	-0.00001
C	-1.58944	-0.12326	0.00001
N	-2.68999	-0.46495	-0.00001



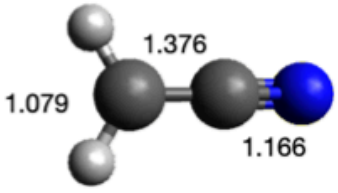
HCCN

C	-0.06935	-1.27358	0.00000
C	0.00000	0.09212	0.00000
N	0.21709	1.24600	0.00000
H	-1.10348	-1.63326	0.00000



CH_2CN

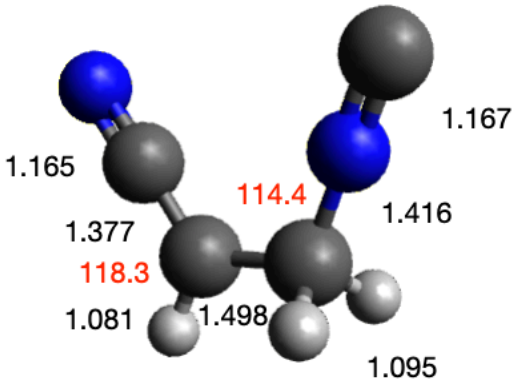
C	0.00024	-1.18907	0.00000
C	0.00000	0.18727	0.00000
N	-0.00027	1.35325	0.00000
H	0.00025	-1.73099	0.93324
H	0.00025	-1.73099	-0.93324



S2: Structures of the stationary points identified in the PES for the $C_2H_3CN + NC$ reaction

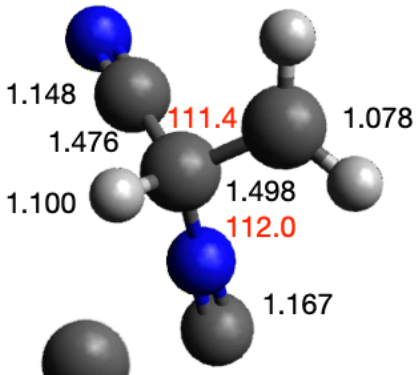
MIN6

C	-0.85682	1.01071	0.00019
C	0.64033	1.04832	-0.00020
C	1.45362	-0.06261	-0.00012
N	2.16170	-0.98822	0.00016
N	-1.40992	-0.29241	0.00000
C	-1.88765	-1.35678	-0.00014
H	-1.23229	1.55080	0.87599
H	-1.23273	1.55126	-0.87512
H	1.10572	2.02452	-0.00046



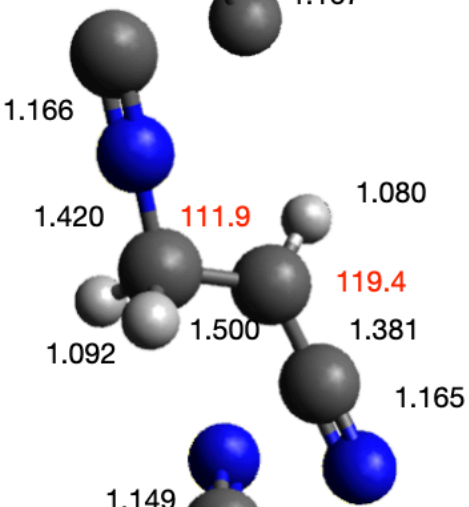
MIN7

C	0.11524	1.72171	-0.20897
C	0.05743	0.35747	0.40759
H	-0.78622	2.30884	-0.27340
H	1.07355	2.13727	-0.47302
C	-1.19602	-0.33959	0.05800
N	-2.19592	-0.84434	-0.19412
N	1.18974	-0.43738	0.05386
C	2.13880	-1.05932	-0.21933
H	0.06335	0.44427	1.50456



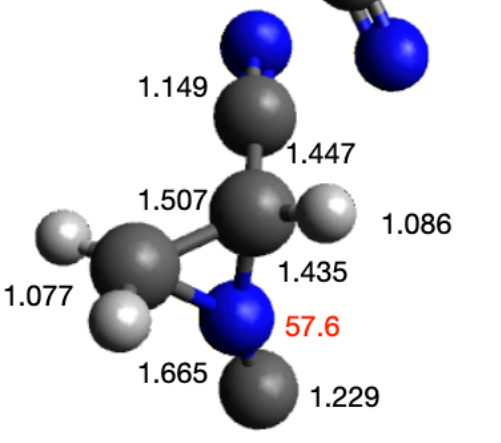
MIN8

C	-0.54935	0.61503	0.12608
C	0.48930	-0.46591	0.17410
C	1.82679	-0.17550	-0.00771
N	2.95098	0.08409	-0.16594
N	-1.85658	0.08759	-0.04250
C	-2.93084	-0.34601	-0.17706
H	-0.33845	1.31352	-0.68663
H	-0.53013	1.19866	1.05354
H	0.19242	-1.47964	0.39974



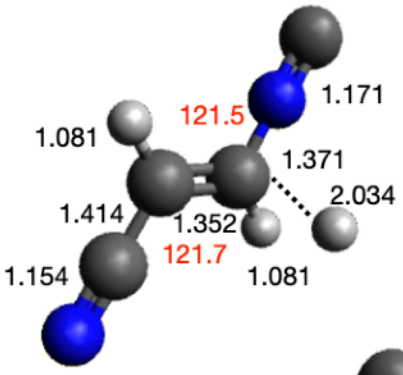
TS12

C	-0.76796	1.26030	-0.29956
C	0.05870	0.33529	0.55644
C	1.36469	-0.08963	0.09952
N	2.40678	-0.41384	-0.26133
N	-1.08783	-0.34203	0.02136
C	-1.87696	-1.26643	-0.15910
H	-0.47360	1.42373	-1.32241
H	-1.44779	1.93825	0.18854
H	0.01791	0.49193	1.62986



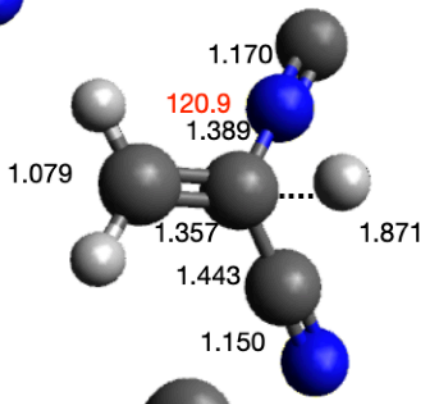
TS13

C	-0.51734	0.40269	-0.13548
C	0.46786	-0.47751	0.15305
C	1.83276	-0.13995	0.00449
N	2.95228	0.11461	-0.10898
N	-1.83943	0.04378	-0.07338
C	-2.98064	-0.21976	-0.04924
H	-0.31529	1.35589	-0.60326
H	-0.52284	1.60355	1.50664
H	0.23244	-1.46092	0.53625



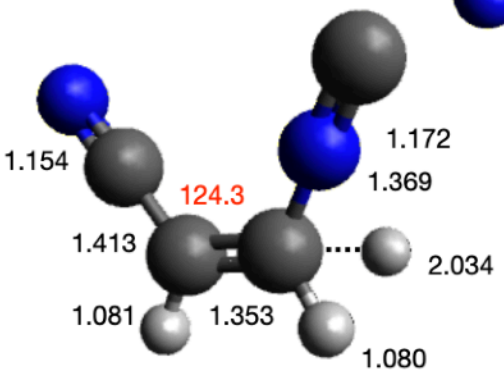
TS14

C	0.13674	1.72165	-0.11892
C	0.06230	0.38240	0.08513
H	-0.76446	2.31278	-0.15086
H	1.09586	2.21050	-0.18741
C	-1.19809	-0.31391	-0.00620
N	-2.20968	-0.85265	-0.10074
N	1.19338	-0.41777	-0.00910
C	2.13678	-1.10400	-0.10027
H	-0.04380	0.25278	1.94870



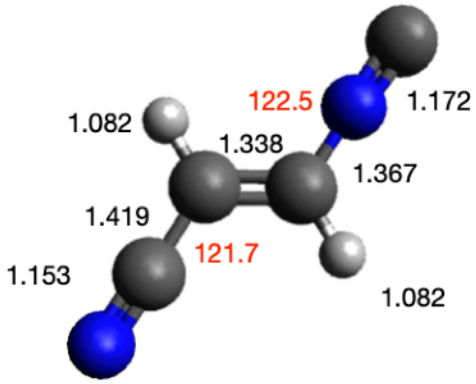
TS15

C	0.74840	0.91610	-0.09745
C	-0.60065	1.01080	-0.13625
C	-1.48042	-0.08741	-0.00919
N	-2.22738	-0.96125	0.08787
N	1.41764	-0.27764	-0.04720
C	2.03415	-1.27390	-0.01724
H	1.36360	1.78217	-0.29360
H	1.14110	1.50618	1.80881
H	-1.04533	1.99047	-0.23921



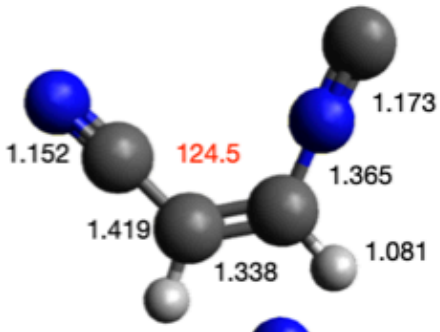
E-NC-CH=CH-NC

C	-0.52624	0.43323	-0.00006
C	0.45068	-0.48066	-0.00006
C	1.82000	-0.10828	-0.00004
N	2.93973	0.16505	0.00008
N	-1.84984	0.09213	0.00001
C	-2.99957	-0.13721	0.00006
H	-0.32123	1.49527	-0.00009
H	0.22274	-1.53805	-0.00003



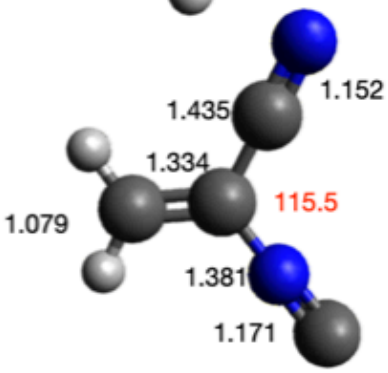
Z-NC-CH=CH-NC

C	0.74422	0.96647	0.00071
C	-0.59250	1.03399	-0.00061
C	-1.45344	-0.09337	-0.00093
N	-2.18540	-0.98342	0.00086
N	1.45325	-0.20021	0.00134
C	2.10936	-1.17213	-0.00147
H	1.34120	1.86789	0.00127
H	-1.06196	2.00768	-0.00285



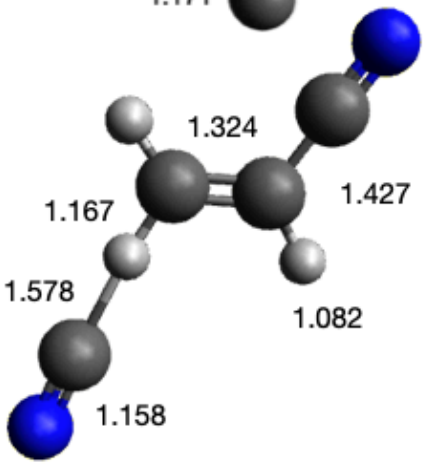
CH_2CCNNC

C	-0.13020	1.72720	0.00000
C	-0.06264	0.39449	0.00000
H	0.77392	2.31532	0.00000
H	-1.08483	2.23055	0.00000
C	1.19099	-0.30466	0.00000
N	2.20149	-0.85492	0.00000
N	-1.18966	-0.40397	0.00000
C	-2.12680	-1.10597	0.00000



TS-Abs

C	0.01584	0.69996	-0.00000
C	0.84068	-0.33535	-0.00002
H	0.27806	1.74940	0.00002
H	-1.12786	0.49196	-0.00002
C	2.25839	-0.17525	0.00000
H	0.47012	-1.35330	-0.00004
N	3.40539	-0.06715	0.00002
C	-2.64857	0.07190	-0.00003
N	-3.75088	-0.28365	0.00003



TS-Mig

C	0.45343	0.43810	-0.07283
C	-0.55301	-0.50154	0.01560
C	-1.90776	-0.12789	-0.00052
N	-3.02669	0.16540	-0.02342
C	1.85042	0.12868	0.01801
N	2.98349	-0.18463	-0.09185
H	0.22622	1.48301	-0.23939
H	1.33942	0.57973	1.16398
H	-0.32179	-1.55219	0.12067