

The N(²D) + CH₂CHCN (Vinyl Cyanide)
Reaction: A Combined Crossed Molecular
Beam and Theoretical Study and Implications
for the Atmosphere of Titan

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Table S1: List of all possible exothermic combinations of products identified for the $N(^2D) + CH_2CHCN$ reaction, determined at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory.

$N(^2D) + CH_2CHCN$	\rightarrow	$^1c-C_3H_2N_2 + H$	- 0.04 kJ/mol
	\rightarrow	$^1c-C(N)N + CH_2CH$	- 2 kJ/mol
	\rightarrow	$^3NCCN + CH_3$	- 5 kJ/mol
	\rightarrow	$H_2CN + ^1CCNH$	- 7 kJ/mol
	\rightarrow	$H_2CN + ^3CCNH$	- 11 kJ/mol
	\rightarrow	$^3NCHCCNH + H$	- 12 kJ/mol
	\rightarrow	$^3c-CH(NH)CH + CN$	- 17 kJ/mol
	\rightarrow	$^1c-CH(N)CCHN + H$	- 23 kJ/mol
	\rightarrow	$^1c-CH_2CC(N)N + H$	- 30 kJ/mol
	\rightarrow	$^1c-CH_2NC(N)C + H$	- 47 kJ/mol
	\rightarrow	$^1c-CH_2(NCN)C + H$	- 48 kJ/mol
	\rightarrow	$HCNH + ^1HCCN$	- 54 kJ/mol
	\rightarrow	$^1CHNCCNH + H$	- 61 kJ/mol
	\rightarrow	$^1c-CH(N)CCNH + H$	- 68 kJ/mol
	\rightarrow	$^1c-CH(NCN)CH + H$	- 70 kJ/mol
	\rightarrow	$^3CH_2NCCN + H$	- 70 kJ/mol
	\rightarrow	$^1CCNN + CH_3$	- 72 kJ/mol
	\rightarrow	$^3CHNCHCN + H$	- 87 kJ/mol
	\rightarrow	$^1NHCHCCN-i + H$	- 90 kJ/mol
	\rightarrow	$^3CHNHCCN + H$	- 91 kJ/mol
	\rightarrow	$c-CH(NH)C + ^1HNC$	- 93 kJ/mol
	\rightarrow	$^1c-CH(NH)CCN + H$	- 98 kJ/mol
	\rightarrow	$HCNH + ^3HCCN$	- 104 kJ/mol
	\rightarrow	$^1CH_2CCNN + H$	- 105 kJ/mol
	\rightarrow	$^1CH_2NH + C_2N$	- 106 kJ/mol
	\rightarrow	$^1HCCN + H_2CN$	- 108 kJ/mol
	\rightarrow	$^1c-C(NH)CHCN + H$	- 116 kJ/mol

→	$\text{H}_2\text{CN} + \text{CCNH}$	- 119 kJ/mol
→	$c\text{-CH(NH)C} + {}^1\text{HCN}$	- 150 kJ/mol
<hr/>		
→	${}^1c\text{-CH}_2(\text{N})\text{CH} + \text{CN}$	- 153 kJ/mol
→	${}^3\text{NCHCHCN} + \text{H}$	- 154 kJ/mol
→	${}^3\text{HCCN} + \text{H}_2\text{CN}$	- 157 kJ/mol
→	${}^3\text{CHNCHCN} + \text{H}$	- 161 kJ/mol
→	${}^1\text{CH}_2\text{NCCN} + \text{H}$	- 194 kJ/mol
→	${}^1\text{CHNCHCN} + \text{H}$	-200 kJ/mol
→	$c\text{-CH}_2(\text{N})\text{C} + {}^1\text{HNC}$	- 210 kJ/mol
→	${}^1\text{NHCCCNH} + \text{H}$	- 218 kJ/mol
→	${}^1c\text{-CH}_2(\text{N})\text{CCN} + \text{H}$	- 223 kJ/mol
→	${}^1c\text{-CH(N)CHCN} + \text{H}$	- 236 kJ/mol
→	$c\text{-CH}_2(\text{N})\text{C} + {}^1\text{HCN}$	- 267 kJ/mol
→	${}^1\text{NHCCHCN} + \text{H}$	- 318(.8) kJ/mol
→	${}^1\text{HNCCHCN} + \text{H}$	- 319(.2) kJ/mol
→	$\text{CH}_3\text{CC} + \text{N}_2$	- 344 kJ/mol
→	${}^3\text{CNCHCN} + \text{H}_2$	- 365 kJ/mol
→	$\text{CH}_2\text{NC} + {}^1\text{HCN}$	- 382 kJ/mol
→	${}^1\text{NCCN} + \text{CH}_3$	- 420 kJ/mol
→	$\text{CH}_2\text{CCH} + \text{N}_2$	- 516 kJ/mol
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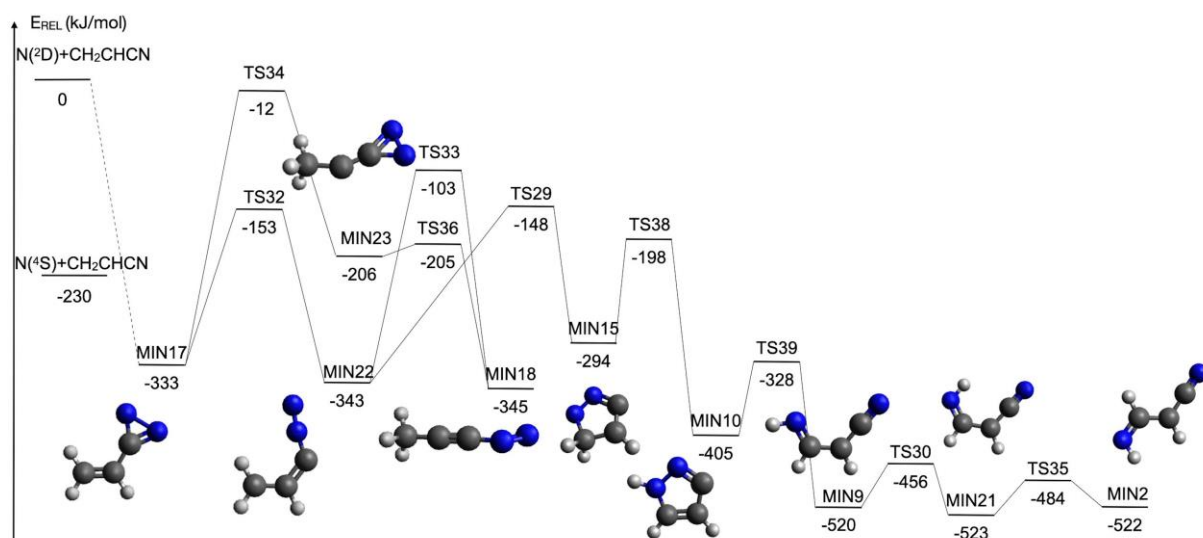
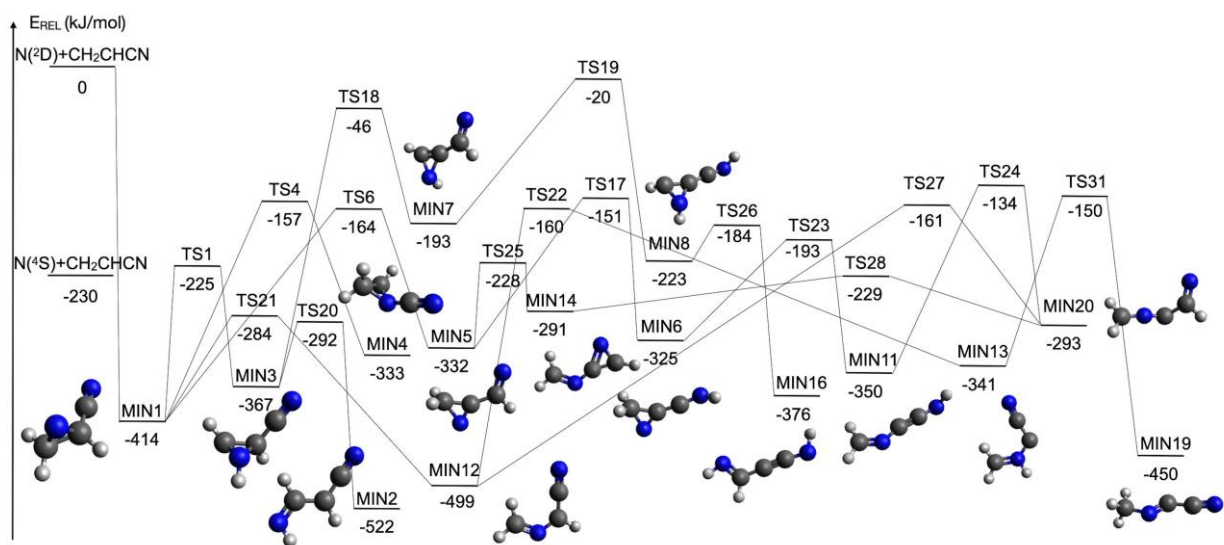
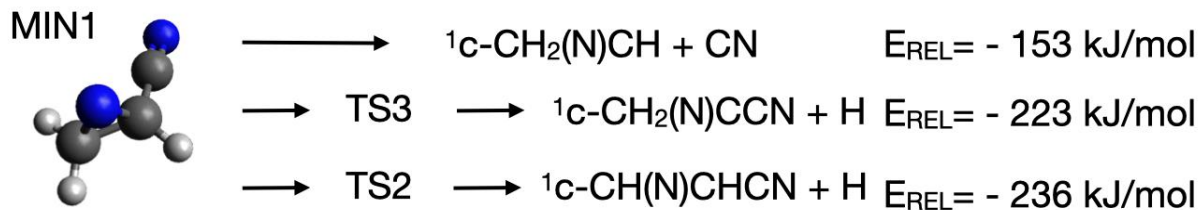
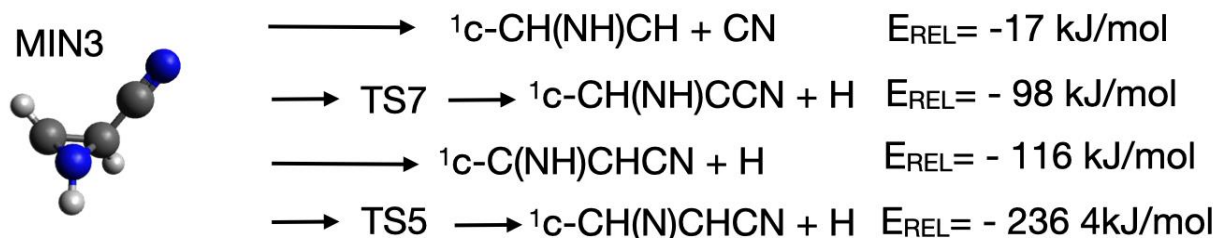


Figure S1: Schematic representation of the Potential Energy Surface including all possible isomerization processes for the $N(^2D) + CH_2CHCN$ reaction identified at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory. (Top): considering only $N(^2D)$ addition to the double bond. (Bottom): considering the attack of the $N(^2D)$ atom to the triple bond of CN and to the lone pair of the nitrogen atom.

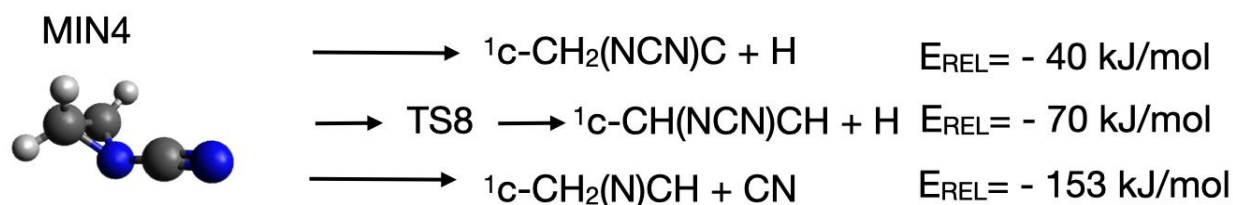
List of all possible products starting from the various minima identified in the Potential Energy Surface, with relative energies reported at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory.



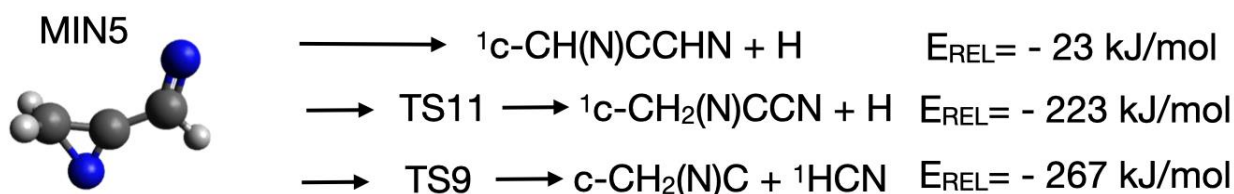
$E_{\text{REL}} = -414 \text{ kJ/mol}$



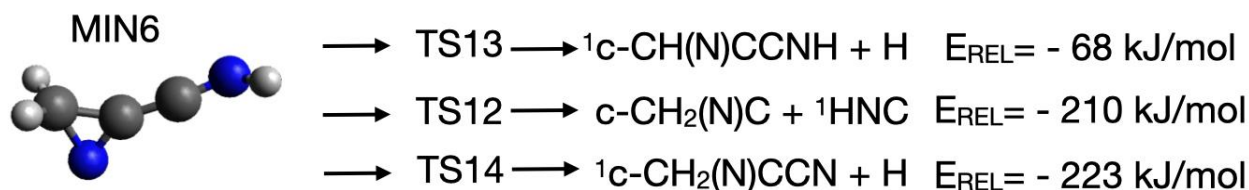
$E_{\text{REL}} = -367 \text{ kJ/mol}$



$E_{\text{REL}} = -333 \text{ kJ/mol}$

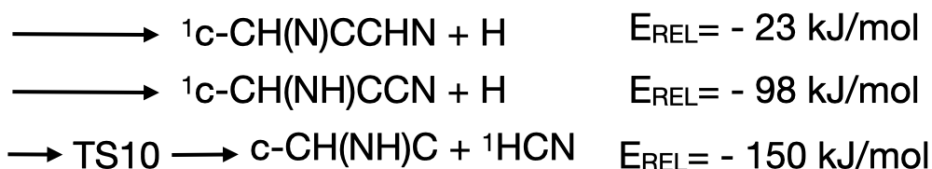
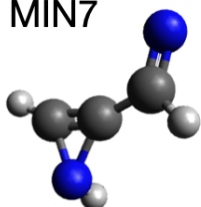


$E_{\text{REL}} = -333 \text{ kJ/mol}$



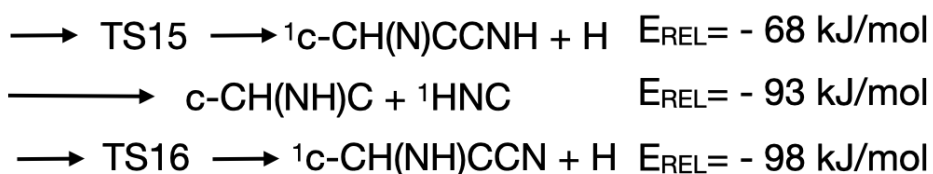
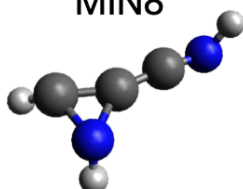
$E_{\text{REL}} = -325 \text{ kJ/mol}$

MIN7



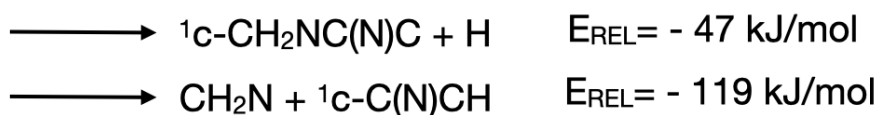
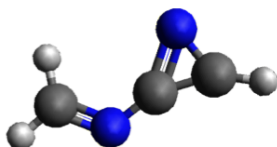
$E_{\text{REL}} = - 193 \text{ kJ/mol}$

MIN8



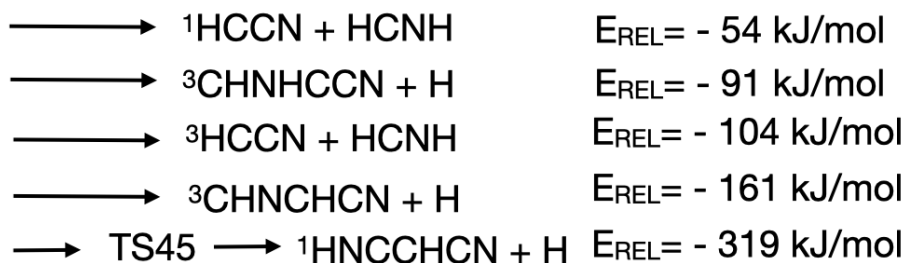
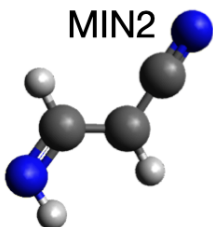
$E_{\text{REL}} = - 223 \text{ kJ/mol}$

MIN14



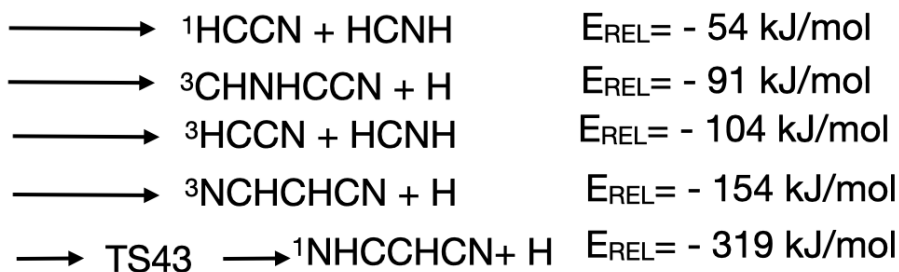
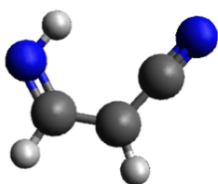
$E_{\text{REL}} = - 291 \text{ kJ/mol}$

MIN2

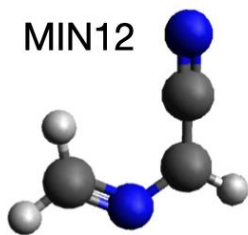


$E_{\text{REL}} = - 522 \text{ kJ/mol}$

MIN21

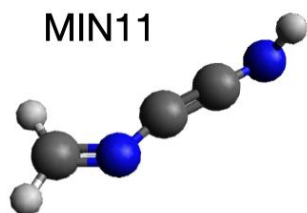
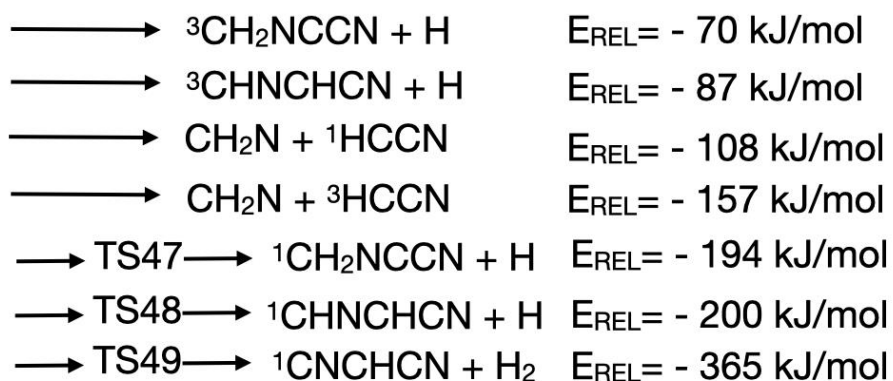


$E_{\text{REL}} = - 523 \text{ kJ/mol}$



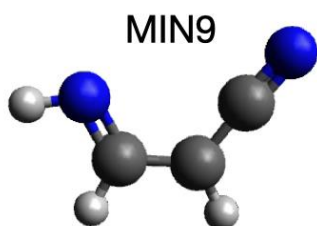
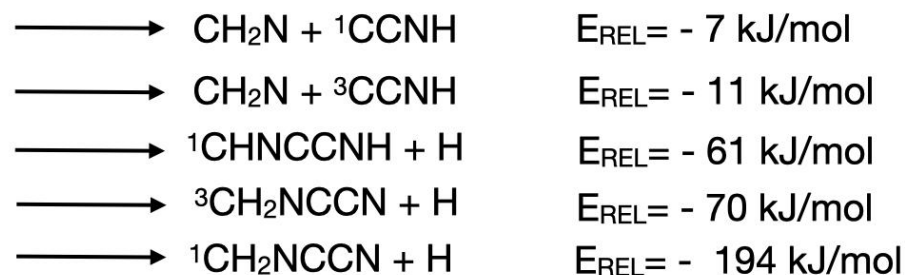
MIN12

$E_{REL} = -499$ kJ/mol



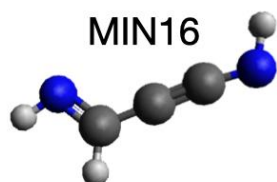
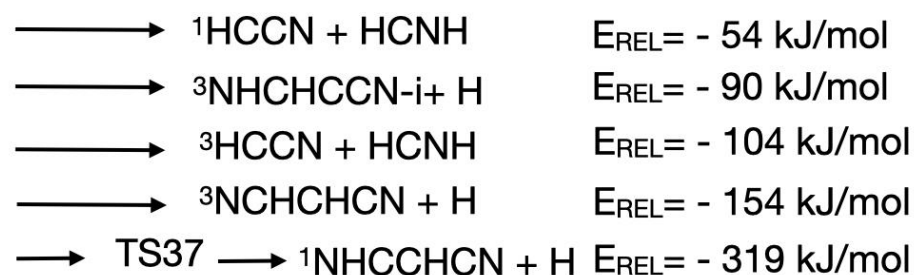
MIN11

$E_{REL} = -350$ kJ/mol



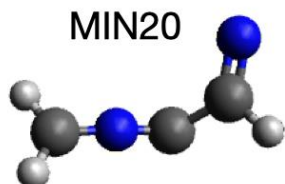
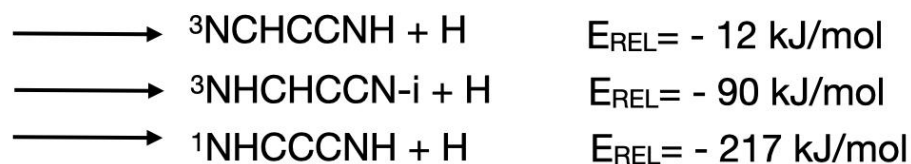
MIN9

$E_{REL} = -520$ kJ/mol



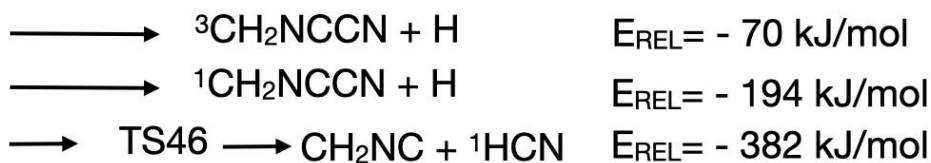
MIN16

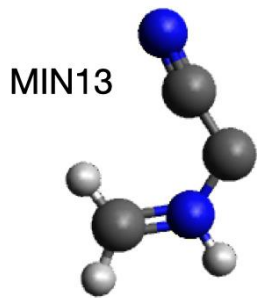
$E_{REL} = -376$ kJ/mol



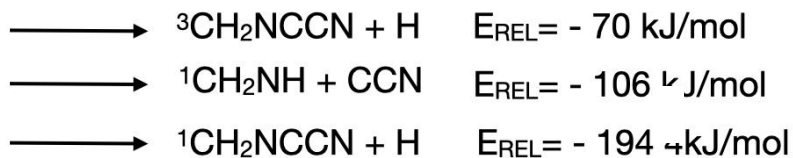
MIN20

$E_{REL} = -293$ kJ/mol



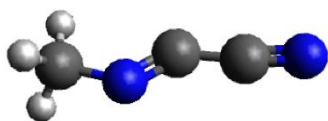


MIN13

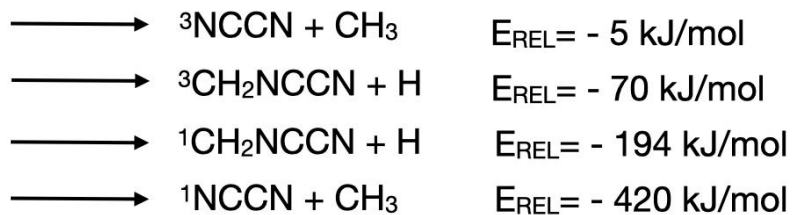


$E_{\text{REL}} = -341 \text{ kJ/mol}$

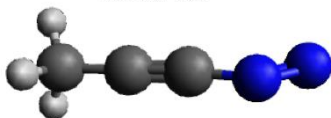
MIN19



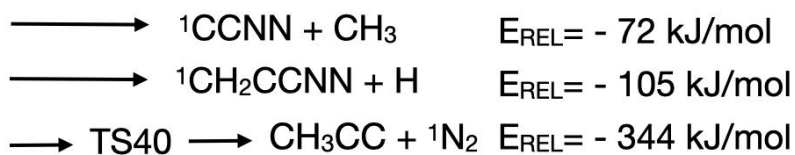
$E_{\text{REL}} = -450 \text{ kJ/mol}$



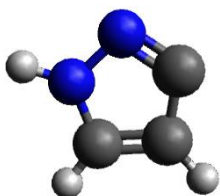
MIN18



$E_{\text{REL}} = -354 \text{ kJ/mol}$



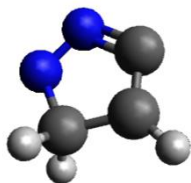
MIN10



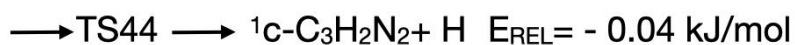
$E_{\text{REL}} = -405 \text{ kJ/mol}$



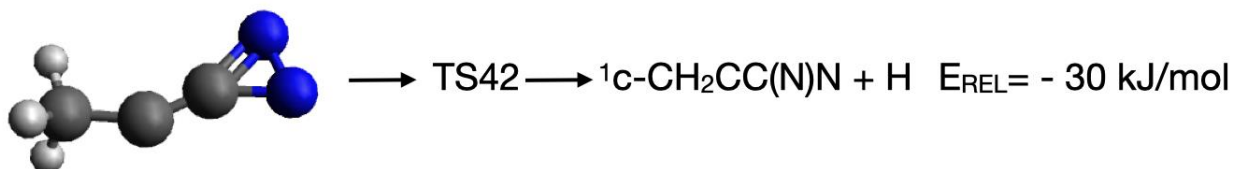
MIN15



$E_{\text{REL}} = -294 \text{ kJ/mol}$

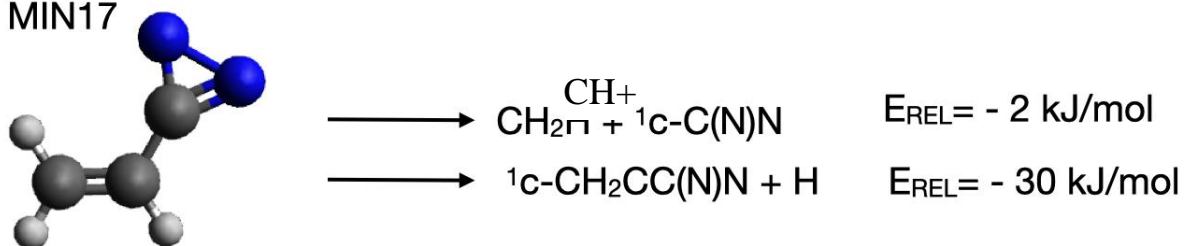


MIN23



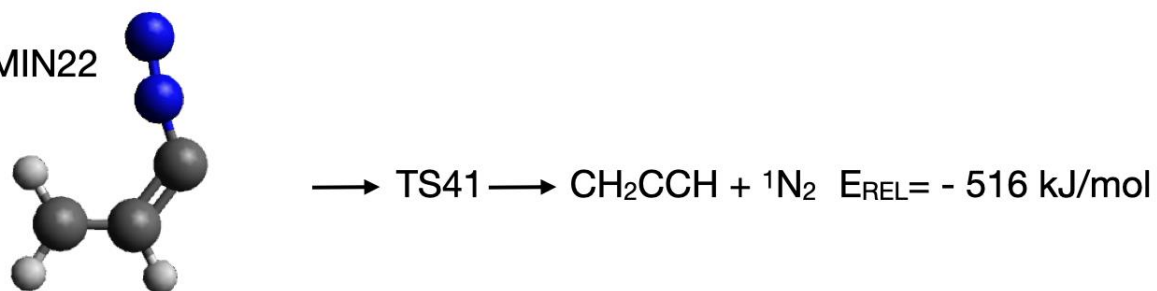
$E_{\text{REL}} = -206 \text{ kJ/mol}$

MIN17



$E_{\text{REL}} = -335 \text{ kJ/mol}$

MIN22



$E_{\text{REL}} = -343 \text{ kJ/mol}$

Table S2: Reaction Enthalpies and Barrier Heights, reported in kJ/mol, evaluated at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level of theory for the reaction $N(^2D) + CH_2CHCN$.

process	ΔH^0_0	Barrier height	process	ΔH^0_0	Barrier height
$N(^2D)+CH_2CHCN \rightarrow MIN1$	-414		$MIN1 \rightarrow ^1c-CH_2(N)CCN+H$	191	215
$MIN1 \rightarrow MIN3$	47	189	$MIN1 \rightarrow ^1c-CH(N)CHCN+H$	178	193
$MIN1 \rightarrow MIN4$	81	260	$MIN3 \rightarrow ^1c-CH(NH)CH+CN$	350	
$MIN1 \rightarrow MIN12$	-85	130	$MIN3 \rightarrow ^1c-CH(NH)CCN+H$	269	275
$MIN1 \rightarrow MIN5$	82	250	$MIN3 \rightarrow ^1c-C(NH)CHCN+H$	251	
$MIN3 \rightarrow MIN2$	-155	75	$MIN3 \rightarrow ^1c-CH(N)CHCN+H$	131	148
$MIN3 \rightarrow MIN7$	174	321	$MIN4 \rightarrow ^1c-CH_2(NCN)C+H$	293	
$MIN7 \rightarrow MIN8$	-30	173	$MIN4 \rightarrow ^1c-CH(NCN)CH+H$	263	272
$MIN5 \rightarrow MIN14$	41	104	$MIN4 \rightarrow ^1c-CH_2(N)CH+CN$	180	
$MIN5 \rightarrow MIN6$	7	181	$MIN5 \rightarrow ^1c-CH(N)CCHN+H$	309	
$MIN12 \rightarrow MIN13$	158	339	$MIN5 \rightarrow ^1c-CH_2(N)CCN+H$	109	128
$MIN12 \rightarrow MIN20$	206	338	$MIN5 \rightarrow c-CH_2(N)C+^1HCN$	65	110
$MIN14 \rightarrow MIN20$	-2	62	$MIN6 \rightarrow ^1c-CH(N)CCNH+H$	257	271
$MIN8 \rightarrow MIN16$	-153	39	$MIN6 \rightarrow ^1c-CH_2(N)C+^1HNC$	115	147
$MIN6 \rightarrow MIN11$	-25	132	$MIN6 \rightarrow ^1c-CH_2(N)CCN+H$	102	128
$MIN11 \rightarrow MIN20$	57	216	$MIN7 \rightarrow ^1c-CH(N)CCHN+H$	170	
$MIN13 \rightarrow MIN19$	-109	191	$MIN7 \rightarrow ^1c-CH(NH)CCN+H$	95	
$MIN2 \rightarrow MIN21$	-1	38	$MIN7 \rightarrow c-CH(NH)C+^1HCN$	43	131
$MIN21 \rightarrow MIN9$	3	67	$MIN8 \rightarrow ^1c-CH(N)CCNH+H$	135	167
$MIN9 \rightarrow MIN10$	115	192	$MIN8 \rightarrow c-CH(NH)C+^1HCN$	130	
$MIN10 \rightarrow MIN15$	111	207	$MIN8 \rightarrow ^1c-CH(NH)CCN+H$	125	152
$MIN15 \rightarrow MIN22$	-49	146	$MIN14 \rightarrow ^1c-CH_2NC(N)C+H$	244	
$MIN22 \rightarrow MIN17$	10	190	$MIN14 \rightarrow H_2CN+^1c-C(N)CH$	172	
$MIN17 \rightarrow MIN23$	127	321	$MIN2 \rightarrow HCNH+^1HCCN$	468	
$MIN23 \rightarrow MIN18$	-139	1	$MIN2 \rightarrow ^3CHNHCCN+H$	431	
$MIN22 \rightarrow MIN18$	-2	240	$MIN2 \rightarrow HCNH+^3HCCN$	418	
$MIN2 \rightarrow ^1HNCCHCN+H$	203	226	$MIN2 \rightarrow ^3CHNCHCN+H$	361	
$MIN21 \rightarrow HCNH+^1HCCN$	469				

process	ΔH^0_0	Barrier height	process	ΔH^0_0	Barrier height
MIN1 \rightarrow 1c -CH ₂ (N)CH+CN	261		MIN21 \rightarrow 3 CHNHCCN+H	432	
MIN21 \rightarrow HCNH+ 3 HCCN	419		MIN16 \rightarrow 3 NCHCCNH+H	364	
MIN21 \rightarrow 3 NCHCHCN+H	369		MIN16 \rightarrow 3 NHCHCCN-i+H	286	
MIN21 \rightarrow 1 NHCCHCN+H	204	239	MIN16 \rightarrow 1 NHCCCNH+H	159	
MIN12 \rightarrow 3 CH ₂ NCCN+H	429		MIN20 \rightarrow 3 CH ₂ NCCN+H	223	
MIN12 \rightarrow 3 CHNCHCN+H	412		MIN20 \rightarrow 1 CH ₂ NCCN+H	99	
MIN12 \rightarrow CH ₂ N+ 1 HCCN	391		MIN20 \rightarrow CH ₂ NC+ 1 HCN	-89	20
MIN12 \rightarrow CH ₂ N+ 3 HCCN	342		MIN13 \rightarrow 3 CH ₂ NCCN+H	271	
MIN12 \rightarrow 1 CH ₂ NCCN+H	305	304	MIN13 \rightarrow 1 CH ₂ NH+CCN	235	
MIN12 \rightarrow 1 CHNCHCN+H	299	299	MIN13 \rightarrow 1 CH ₂ NCCN+H	147	
MIN12 \rightarrow 1 CNCHCN+H ₂	134	349	MIN19 \rightarrow 3 NCCN+CH ₃	445	
MIN11 \rightarrow 1 CH ₂ N+ 1 CCNH	343		MIN19 \rightarrow 3 CH ₂ NCCN+H	380	
MIN11 \rightarrow 1 CH ₂ N+ 3 CCNH	339		MIN19 \rightarrow 1 CH ₂ NCCN+H	256	
MIN11 \rightarrow 1 CHNCCNH+H	289		MIN19 \rightarrow 1 NCCN+CH ₃	30	
MIN11 \rightarrow 3 CH ₂ NCCN+H	280		MIN18 \rightarrow 1 CCNN+CH ₃	282	
MIN11 \rightarrow 1 CH ₂ NCCN+H	156		MIN18 \rightarrow 1 CH ₂ CCNN+H	249	
MIN9 \rightarrow 1 HCCN+HCNH	466		MIN18 \rightarrow CH ₃ CC+N ₂	10	53
MIN9 \rightarrow 3 NHCHCCN-i+H	430		MIN10 \rightarrow 1c -C ₃ H ₂ N ₂ +H	404	
MIN9 \rightarrow 3 HCCN+HCNH	416		MIN15 \rightarrow 1c -C ₃ H ₂ N ₂ +H	293	312
MIN9 \rightarrow 3 NCHCHCN+H	366		MIN23 \rightarrow 1c -CH ₂ CC(N)N+H	176	183
MIN9 \rightarrow 3 NHCCHCN+H	201	224	MIN17 \rightarrow CH ₂ CH+ 1c -C(N)N	333	
MIN17 \rightarrow 1c -CH ₂ CC(N)N+H	305		MIN22 \rightarrow CH ₂ CCH+N ₂	-173	47

In the following pages are reported the structures of all the stationary points identified at the B3LYP/aug-cc-pVTZ level of theory for the N(²D) + CH₂CHCN reaction. In details, the geometries are reported in the form of the z-matrix where the first column indicates the bond distances (in Å), the second column reports the bond angles and the third column reports the dihedral angles (both expressed in degrees °).



C						
C	1	1.48413				
C	2	1.43796	1	121.51173		
N	2	2.58852	1	121.46200	3	359.63806
N	1	1.44099	2	60.63778	3	255.31827
H	1	1.08512	2	118.39739	3	149.13959
H	1	1.08514	2	119.58098	3	359.80186
H	2	1.08454	1	118.56514	3	207.49882

MIN1



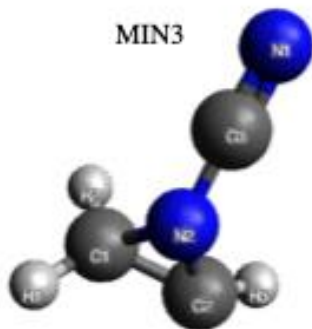
C						
C	1	1.42041				
C	2	1.39590	1	122.60438		
N	2	2.55624	1	122.66544	3	359.99851
N	1	1.29497	2	125.69643	3	179.97771
H	5	1.02254	1	111.14508	2	0.00888
H	1	1.08781	2	117.14578	3	359.97537
H	2	1.08330	1	119.84721	3	180.00045

MIN2



C						
C	1	1.47050				
C	2	1.44290	1	123.08557		
N	2	2.59317	1	123.14645	3	358.81764
N	1	1.38732	2	62.95597	3	259.30795
H	1	1.08061	2	133.23342	3	15.82347
H	2	1.08423	1	117.10265	3	208.37355
H	5	1.01588	1	118.01344	2	255.80009

MIN3



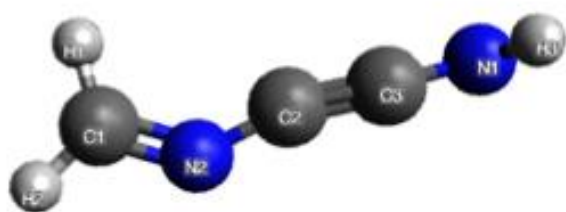
C						
C	1	1.46027				
C	2	2.43280	1	75.64853		
N	3	1.15590	2	154.55843	1	232.01177
N	3	1.33829	2	28.12325	1	58.07189
H	1	1.08143	2	120.62603	3	235.71972
H	1	1.08475	2	119.16431	3	79.20453
H	2	1.08048	1	130.93427	3	270.95231

MIN4



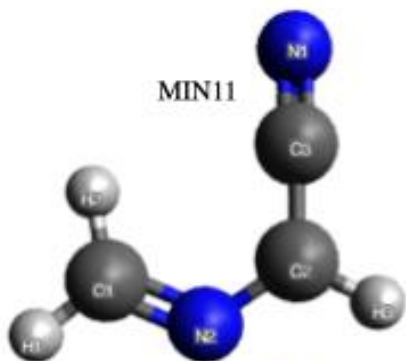
C						
C	1	1.44353				
C	2	1.46116	1	152.60936		
N	3	1.24853	2	123.58389	1	0.11612
N	2	1.25202	1	69.73476	3	180.18661
H	1	1.08268	2	120.42708	3	80.24268
H	1	1.08266	2	120.46259	3	279.43136
H	3	1.09744	2	116.00579	1	180.09011

MIN5



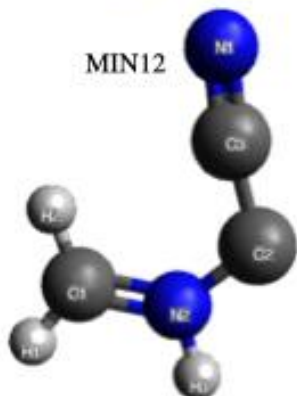
C					
C	1	2.36208			
C	2	1.25507	1	173.30954	
N	3	1.24944	2	171.70926	1
N	1	1.27356	2	22.77085	3
H	1	1.08842	2	99.60938	3
H	1	1.08233	2	141.33908	3
H	4	1.01528	3	117.58679	2

MIN11



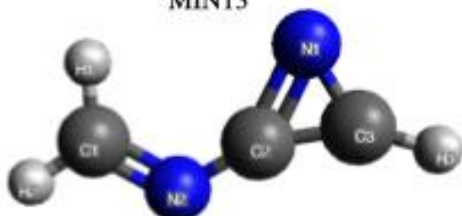
C					
C	1	2.30439			
C	2	1.41411	1	95.80372	
N	2	2.57182	1	95.37976	3
N	1	1.30006	2	29.86353	3
H	1	1.08253	2	147.92001	3
H	1	1.09094	2	93.59184	3
H	2	1.08104	1	146.58686	3

MIN12



C					
C	1	2.45376			
C	2	1.40554	1	89.93147	
N	3	1.16284	2	172.21330	1
N	2	1.34553	1	24.56896	3
H	1	1.07759	2	143.11272	3
H	1	1.07765	2	94.19155	3
H	5	1.01346	2	113.99596	1

MIN13



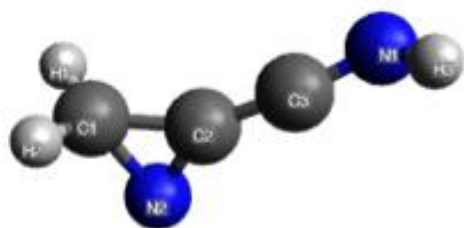
C					
C	1	2.27078			
C	2	1.35188	1	170.47510	
N	3	1.30452	2	67.72048	1
N	2	1.28411	1	30.43000	3
H	1	1.08621	2	93.20937	3
H	1	1.07967	2	147.02558	3
H	3	1.08312	2	155.27275	1

MIN14



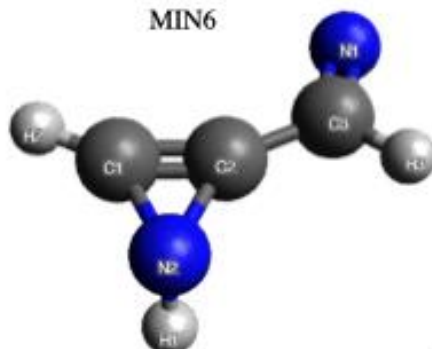
C					
C	1	1.48967			
H	1	1.09391	2	114.39297	
H	1	1.09388	2	114.30550	3
C	2	1.32990	1	102.67130	3
H	2	1.07530	1	127.55533	3
N	5	1.40607	2	114.43586	1
N	7	1.26059	5	108.43173	2

MIN15



MIN6

C						
C	1	1.46101				
C	2	1.32285	1	150.25975		
N	3	1.21436	2	169.46774	1	275.34060
N	2	1.32157	1	64.56729	3	174.43277
H	1	1.08532	2	119.09587	3	81.85062
H	1	1.08537	2	119.61357	3	288.51215
H	4	1.01870	3	120.71285	2	170.28279



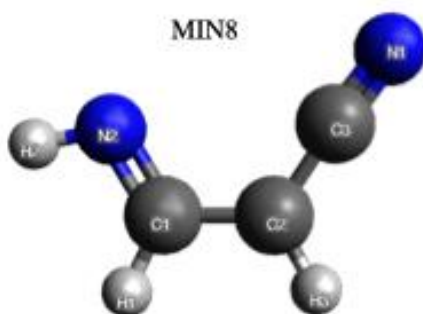
MIN7

C						
C	1	1.27712				
C	2	1.43863	1	157.39000		
N	3	1.25594	2	124.53457	1	343.43125
N	1	1.49596	2	66.10627	3	193.05591
H	5	1.02325	1	108.14793	2	260.98705
H	1	1.07247	2	155.42927	3	2.58430
H	3	1.09709	2	116.45091	1	163.66273



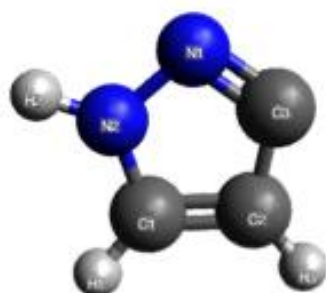
MIN8

C						
C	1	1.39163				
C	2	1.29225	1	158.99765		
N	3	1.22698	2	172.34883	1	269.36726
N	1	1.43095	2	63.35740	3	183.77630
H	5	1.02318	1	113.52443	2	257.86099
H	4	1.02031	3	116.11568	2	179.88952
H	1	1.08069	2	134.69101	3	63.31972



MIN9

C						
C	1	1.41955				
H	1	1.09147	2	115.45191		
H	1	1.91287	2	151.37042	3	179.98219
C	2	1.39875	1	123.59584	3	180.05733
H	2	1.08151	1	119.49415	3	0.06201
N	2	2.55664	1	124.85079	3	180.05924
N	4	1.01867	1	39.16777	2	0.01038



MIN10

C						
C	1	1.38148				
H	1	1.07710	2	131.12999		
H	1	2.12997	2	128.87948	3	179.85213
C	2	1.40673	1	102.34859	3	180.13433
H	2	1.07326	1	128.17504	3	359.98703
N	5	1.29232	2	114.92393	1	359.99341
N	4	1.00445	1	29.91918	2	0.05418



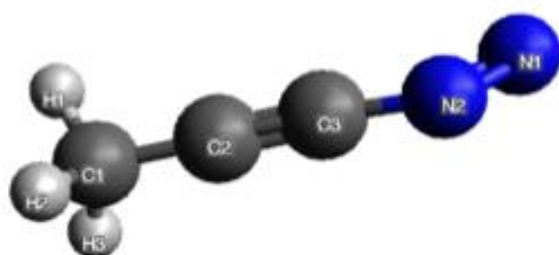
C						
C	1	1.39984				
C	2	1.24724	1	179.97438		
N	3	1.25427	2	174.08611	1	91.66048
N	1	1.29294	2	121.52440	3	88.34434
H	5	1.02075	1	109.98720	2	180.00454
H	4	1.01977	3	114.07047	2	179.88126
H	1	1.09314	2	116.40335	3	268.34743

MIN16



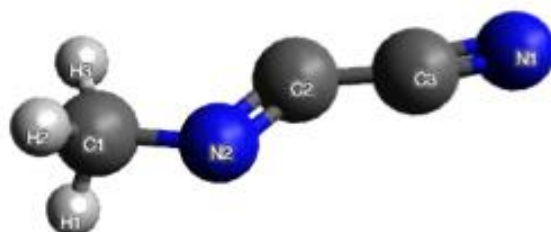
C						
C	1	1.33130				
H	1	1.08194	2	121.11034		
H	1	1.08079	2	121.37253	3	180.05970
C	2	1.44224	1	120.97488	3	0.18433
H	2	1.08201	1	122.33089	3	180.00492
N	5	1.29807	2	143.56535	1	179.49120
N	5	1.31521	2	143.65959	1	359.58295

MIN17



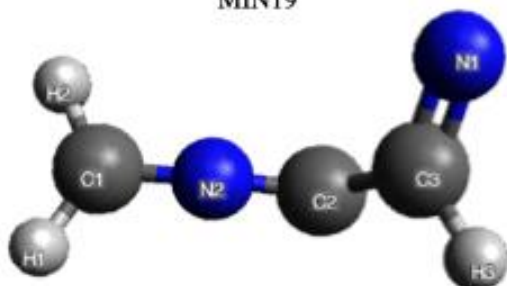
C						
C	1	1.45118				
H	1	1.09110	2	110.87838		
H	1	1.09092	2	111.38676	3	239.14591
C	3	3.19882	1	51.18506	2	0.96206
H	1	1.09156	2	110.24976	3	119.16370
N	5	2.31047	2	168.06293	1	3.77317
N	7	1.18148	5	26.07366	2	180.67675

MIN18



C						
C	1	2.40862				
H	1	1.08944	2	119.12424		
H	1	1.08945	2	119.20949	3	135.18202
C	2	1.38366	1	166.32438	3	292.53123
H	1	1.09028	2	88.85592	3	247.60004
N	5	1.16092	2	170.49350	1	179.82667
N	2	1.22236	1	28.14013	3	292.34580

MIN19



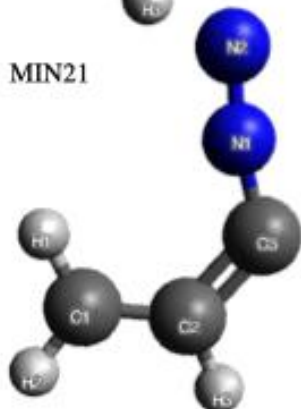
C						
C	1	2.48000				
C	2	1.46976	1	130.41495		
N	3	1.24905	2	124.38819	1	287.50481
N	3	2.40700	1	8.02101	2	359.03458
H	1	1.08051	2	119.71390	3	266.46191
H	1	1.08054	2	119.17330	3	89.75058
H	3	1.09732	2	114.79461	1	113.34406

MIN20



MIN21

C						
C	1	1.42257				
C	2	1.39913	1	122.70734		
N	2	2.55814	1	122.43735	3	359.99999
N	1	1.29476	2	127.46027	3	359.99982
H	5	1.02324	1	111.37344	2	0.00024
H	1	1.08775	2	115.63582	3	180.00095
H	2	1.08173	1	119.89615	3	179.99900



MIN22

C						
C	1	1.35702				
H	1	1.08223	2	121.80386		
H	1	1.08130	2	120.96847	3	180.03475
C	2	1.41697	1	126.02936	3	359.98788
H	2	1.08291	1	118.53757	3	179.99378
N	5	1.27769	2	123.78169	1	359.92965
N	7	1.14462	5	170.18439	2	180.56692



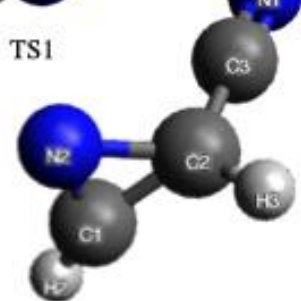
MIN23

C						
C	1	1.46096				
H	1	1.09658	2	111.13729		
H	1	1.09142	2	111.26348	3	240.01327
C	2	1.26262	1	150.45844	3	0.06913
H	1	1.09143	2	111.25629	3	119.97895
N	5	1.46942	2	156.24391	1	359.96484
N	7	1.23808	5	62.66843	2	180.02067



TS1

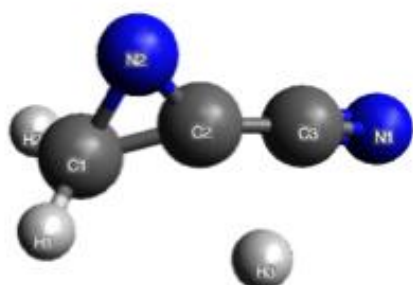
C						
C	1	1.46276				
C	2	1.43954	1	118.68865		
N	2	2.58968	1	119.15000	3	358.98415
N	1	1.45268	2	62.17248	3	259.63693
H	5	1.23186	1	56.60096	2	242.85982
H	1	1.08170	2	135.04126	3	16.15986
H	2	1.08283	1	121.07643	3	208.60482



TS2

C						
C	1	1.46022				
C	2	1.43765	1	121.53232		
N	2	2.58880	1	121.73489	3	359.46185
N	1	1.25345	2	68.88325	3	259.50736
H	1	2.04931	2	99.55583	3	153.05607
H	1	1.07926	2	149.03658	3	60.99933
H	2	1.08162	1	120.02737	3	201.02992





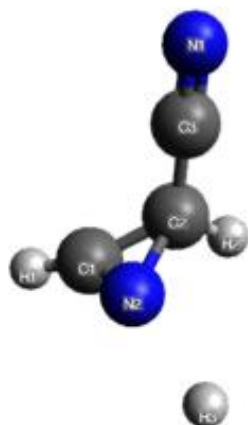
C						
C	1	1.45752				
C	2	1.41012	1	149.72448		
N	2	2.56159	1	148.41478	3	0.39612
N	2	1.26824	1	67.52599	3	155.53253
H	1	1.08194	2	119.22810	3	102.06481
H	1	1.08285	2	120.44464	3	303.74511
H	2	1.99977	1	97.71502	3	260.01139

TS3



C						
C	1	1.44385				
C	2	2.54805	1	101.04628		
N	3	1.16121	2	146.99599	1	287.00614
N	2	1.26407	1	68.78264	3	74.11216
H	1	1.08370	2	120.52447	3	188.07353
H	1	1.08238	2	120.21575	3	27.85906
H	2	1.07941	1	152.19705	3	248.97503

TS4



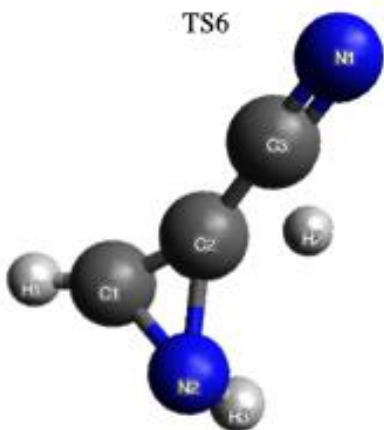
C						
C	1	1.45381				
C	2	1.43836	1	121.63602		
N	2	2.58924	1	121.89536	3	359.45388
N	1	1.25146	2	69.37188	3	258.84856
H	1	1.07885	2	149.52670	3	80.90902
H	2	1.08330	1	120.26102	3	200.16799
H	5	1.89639	1	121.56928	2	263.67664

TS5



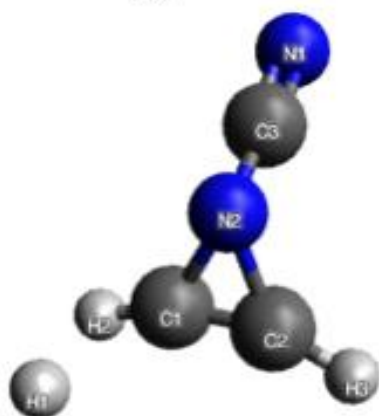
C						
C	1	1.45264				
C	2	1.40279	1	149.98658		
N	3	1.18206	2	172.37115	1	68.84424
N	2	1.29753	1	66.49941	3	173.16826
H	1	1.08410	2	119.99255	3	85.06949
H	1	1.08436	2	119.35918	3	289.42649
H	3	1.38151	2	64.85830	1	265.96302

TS6



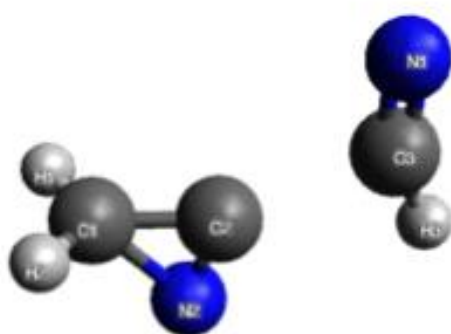
C						
C	1	1.28536				
C	2	1.38317	1	155.85949		
N	2	2.53846	1	156.38711	3	359.97513
N	1	1.45576	2	68.54067	3	212.74490
H	1	1.07442	2	152.66578	3	25.56146
H	2	2.32202	1	101.20654	3	242.10598
H	5	1.02314	1	109.56105	2	262.46439

TS7



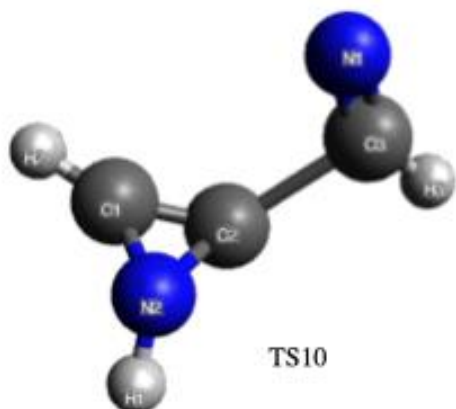
C						
C	1	1.27315				
C	2	2.41900	1	75.58593		
N	3	1.15530	2	150.20026	1	241.68894
N	3	1.36000	2	34.73613	1	66.72238
H	1	2.25479	2	107.93891	3	237.63250
H	1	1.07051	2	157.89697	3	132.54889
H	2	1.07138	1	158.35075	3	206.63855

TS8



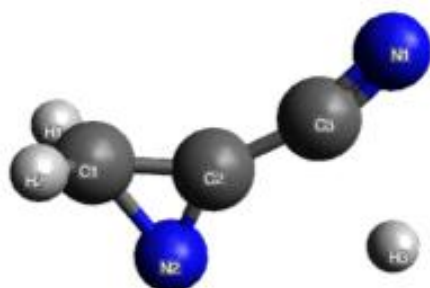
C						
C	1	1.46125				
C	2	2.14731	1	155.54178		
N	3	1.16659	2	114.68134	1	359.99929
N	2	1.22158	1	74.17787	3	179.98862
H	1	1.08031	2	120.32575	3	83.31084
H	1	1.08031	2	120.32580	3	276.71198
H	3	1.07204	2	91.05857	1	179.99860

TS9



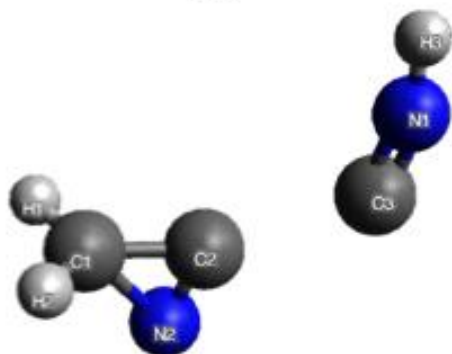
TS10

C						
C	1	1.34081				
C	2	1.94771	1	129.85062		
N	3	1.17623	2	107.31773	1	12.74259
N	1	1.37792	2	66.71955	3	252.34082
H	5	1.01872	1	124.76136	2	256.38308
H	1	1.07411	2	154.57844	3	61.71001
H	3	1.07261	2	104.29773	1	192.02353



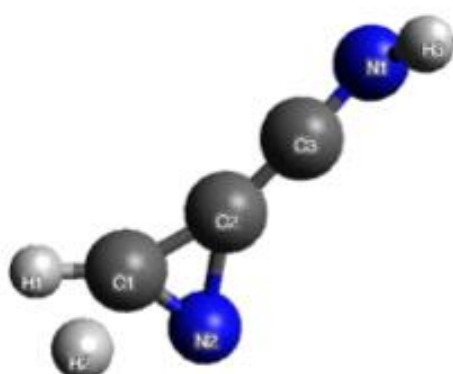
TS11

C						
C	1	1.44979				
C	2	1.41576	1	149.64418		
N	3	1.16247	2	161.98045	1	0.00000
N	2	1.25127	1	69.10094	3	180.00000
H	1	1.08242	2	120.01512	3	79.81988
H	1	1.08242	2	120.01509	3	280.18011
H	3	1.93581	2	93.84601	1	179.99997



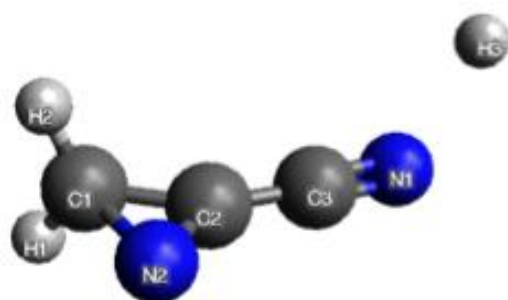
TS12

C						
C	1	1.48573				
C	2	2.21634	1	159.13062		
N	3	1.17133	2	121.85600	1	359.86579
N	2	1.22132	1	71.41010	3	179.95141
H	1	1.08103	2	120.26250	3	82.05618
H	1	1.08103	2	120.26349	3	278.03659
H	4	0.99790	3	165.04315	2	359.99535



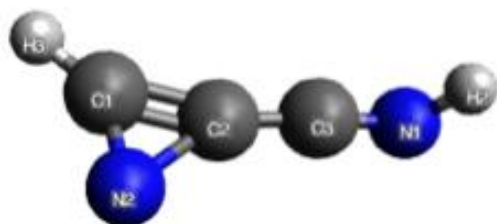
TS13

C						
C	1	1.40276				
C	2	1.28113	1	163.18373		
N	3	1.23334	2	171.24238	1	257.22697
N	1	1.26955	2	68.46899	3	193.61019
H	1	1.07948	2	150.32853	3	29.42746
H	1	2.17130	2	108.69187	3	290.61866
H	4	1.02076	3	114.74527	2	178.90679



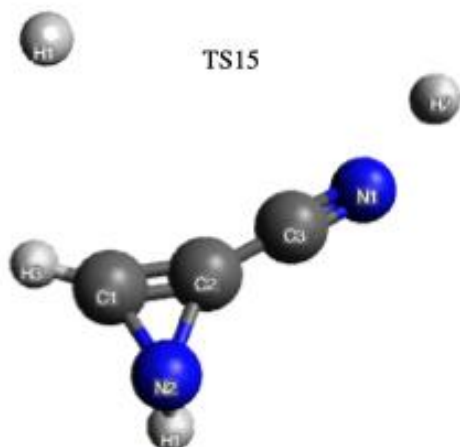
TS14

C						
C	1	1.45073				
C	2	1.39786	1	150.34979		
N	2	2.55545	1	149.05574	3	0.82544
N	2	1.25818	1	68.51310	3	180.89182
H	1	1.08261	2	119.91891	3	78.62016
H	1	1.08259	2	119.86236	3	279.75427
H	4	1.88315	3	118.73902	2	72.44304



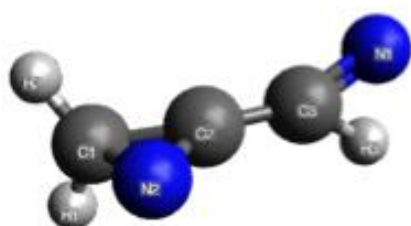
TS15

C						
C	1	1.39090				
C	2	1.28095	1	164.47150		
N	3	1.23275	2	171.62251	1	259.92390
N	1	1.26633	2	70.43894	3	191.35383
H	5	2.05016	1	117.83646	2	254.12354
H	4	1.02058	3	114.97487	2	179.37175
H	1	1.08083	2	149.87003	3	13.70150



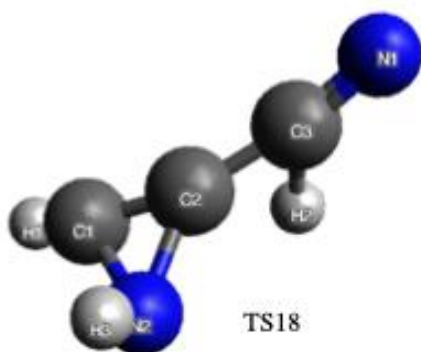
TS16

C						
C	1	1.28199				
C	2	1.37209	1	158.48733		
N	2	2.53442	1	159.01291	3	359.73893
N	1	1.47123	2	67.90895	3	186.81920
H	5	1.02424	1	108.65195	2	261.54389
H	4	1.88837	3	117.17319	2	255.61987
H	1	1.07361	2	153.32515	3	0.97955



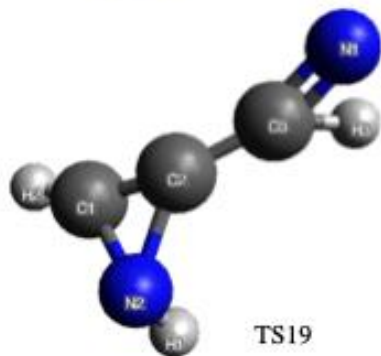
TS17

C						
C	1	1.45658				
C	2	1.39776	1	148.25793		
N	3	1.24406	2	154.42513	1	104.07383
N	2	1.27528	1	67.12012	3	198.45855
H	1	1.08412	2	120.47607	3	61.33968
H	1	1.08372	2	119.08077	3	264.63823
H	3	1.22233	2	142.02245	1	291.24233



TS18

C						
C	1	1.32676				
C	2	1.39661	1	158.68614		
N	3	1.18827	2	167.47670	1	93.82943
N	1	1.46939	2	64.12674	3	167.63602
H	1	1.07285	2	149.73092	3	29.60414
H	3	1.30933	2	68.51834	1	274.07496
H	5	1.02243	1	111.00492	2	99.35570



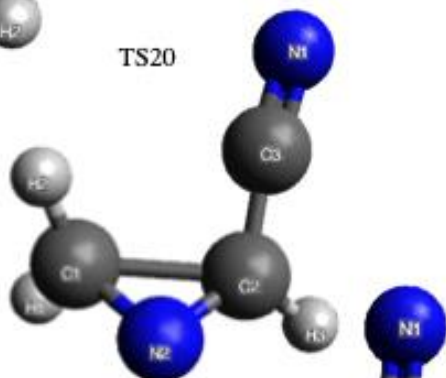
TS19

C						
C	1	1.30300				
C	2	1.37667	1	154.70432		
N	3	1.24947	2	154.67105	1	108.09371
N	1	1.46070	2	67.88197	3	139.37126
H	5	1.02865	1	108.70467	2	259.31164
H	1	1.07294	2	151.91087	3	336.11630
H	3	1.22070	2	141.13333	1	294.31889



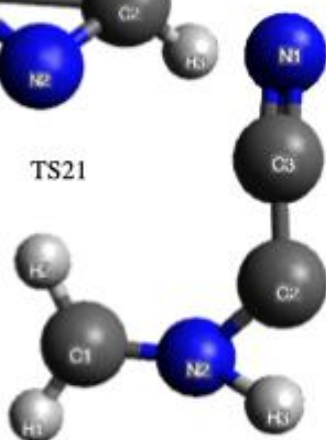
TS20

C						
C	1	1.45547				
C	2	1.40968	1	121.99748		
N	2	2.56606	1	121.74988	3	0.55518
N	1	1.33505	2	86.12000	3	260.36917
H	5	1.01928	1	115.34924	2	66.36000
H	1	1.08084	2	130.53889	3	126.77270
H	2	1.08038	1	120.05297	3	177.20408



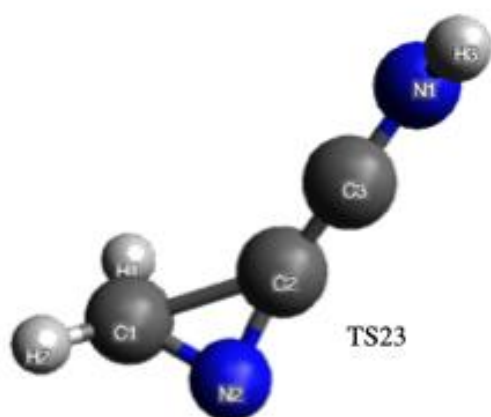
TS21

C						
C	1	1.90526				
C	2	1.43727	1	95.71208		
N	3	1.15533	2	174.50178	1	170.60227
N	2	1.34918	1	46.61021	3	138.83072
H	1	1.08300	2	114.64181	3	115.76314
H	1	1.08767	2	112.78191	3	335.36618
H	2	1.09095	1	140.62180	3	221.42865

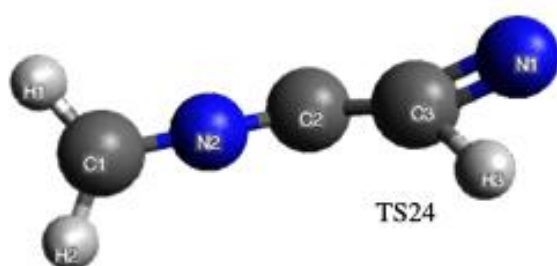


TS22

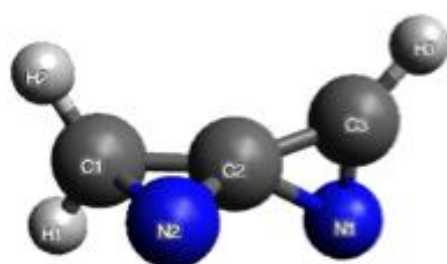
C						
C	1	2.43963				
C	2	1.39473	1	104.85923		
N	3	1.16281	2	174.10044	1	181.32540
N	1	1.31021	2	24.82317	3	158.10323
H	1	1.07904	2	143.10147	3	170.83803
H	1	1.08522	2	95.70608	3	344.07512
H	5	1.20645	1	143.91192	2	101.38188



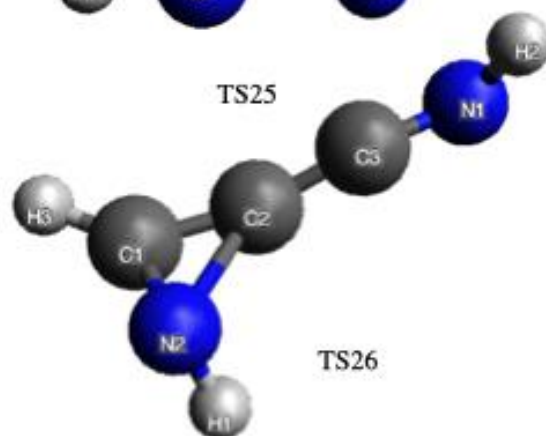
C					
C	1	1.84895			
C	2	1.27267	1	144.69776	
N	3	1.24142	2	167.06794	1
N	2	1.32754	1	47.14302	3
H	1	1.08480	2	93.11190	3
H	1	1.08996	2	137.58665	3
H	4	1.01470	3	119.11289	2



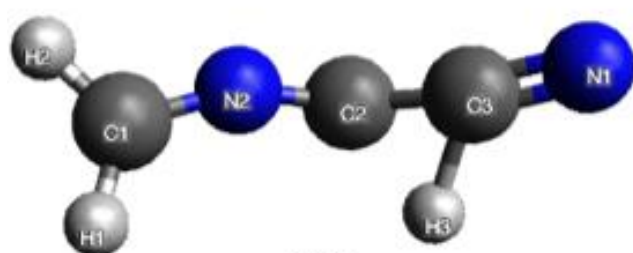
C					
C	1	2.48833			
C	2	1.35842	1	142.07863	
N	3	1.25799	2	156.51208	1
N	3	2.42123	1	5.51098	2
H	1	1.08350	2	119.34866	3
H	1	1.08390	2	120.67692	3
H	3	1.20446	2	138.10287	1



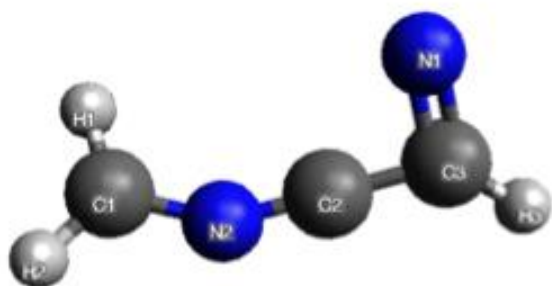
C					
C	1	1.44423			
C	2	1.43748	1	151.57235	
N	3	1.24464	2	77.02147	1
N	2	1.33297	1	66.41235	3
H	1	1.08448	2	120.41796	3
H	1	1.08518	2	120.74992	3
H	3	1.08581	2	144.09187	1



C					
C	1	1.33717			
C	2	1.29521	1	163.97417	
N	3	1.23026	2	164.58603	1
N	1	1.38040	2	84.16921	3
H	5	1.01711	1	111.54274	2
H	4	1.01798	3	118.51204	2
H	1	1.07977	2	139.46696	3



C					
C	1	2.47375			
C	2	1.37226	1	133.91971	
N	3	1.20568	2	166.64930	1
N	2	1.25351	1	10.46144	3
H	1	1.08735	2	111.06302	3
H	1	1.08329	2	129.58539	3
H	3	1.33028	2	65.87033	1



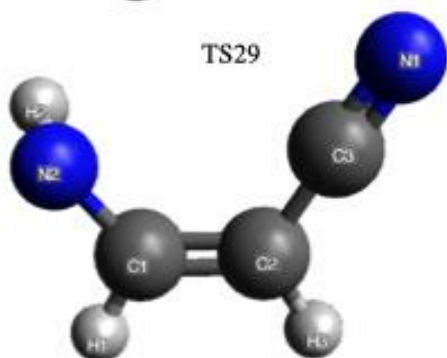
TS28

C						
C	1	2.43962				
C	2	1.37496	1	164.65890		
N	3	1.27319	2	90.11722	1	30.64017
N	2	1.21191	1	14.88483	3	183.74737
H	1	1.08302	2	106.77224	3	9.81281
H	1	1.07878	2	132.22597	3	192.24423
H	3	1.09330	2	134.89548	1	215.92282



TS29

C						
C	1	1.41068				
H	1	1.08736	2	119.47961		
H	1	1.08395	2	119.66619	3	212.30124
C	2	1.37492	1	115.76960	3	304.75880
H	2	1.08123	1	121.98380	3	128.82835
N	5	1.31623	2	110.96198	1	348.88146
N	7	1.18935	5	129.14424	2	357.98211



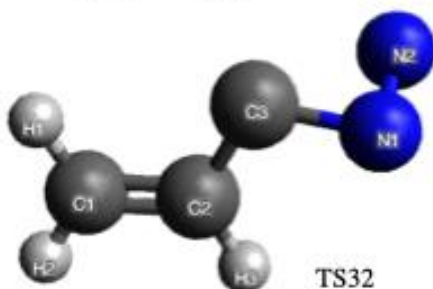
TS30

C						
C	1	1.34283				
H	1	1.09120	2	118.57216		
H	1	2.00656	2	124.19343	3	208.24513
C	2	1.41917	1	123.21496	3	180.65307
H	2	1.07988	1	119.42194	3	0.79130
N	2	2.57264	1	123.61637	3	180.40641
N	4	1.02436	1	39.25050	2	253.33191



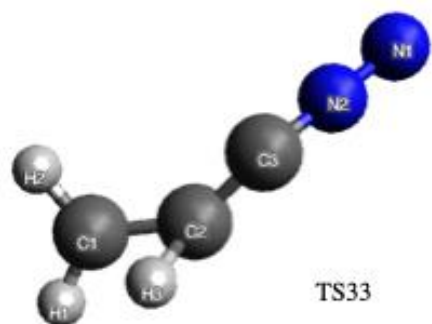
TS31

C						
C	1	2.44341				
H	1	1.07890	2	135.07751		
H	1	1.43349	2	64.96479	3	72.80257
C	2	1.37716	1	147.08661	3	278.79085
H	1	1.08436	2	98.82989	3	206.31635
N	5	1.16378	2	172.73713	1	219.64545
N	4	1.20226	1	62.53729	2	340.14257



TS32

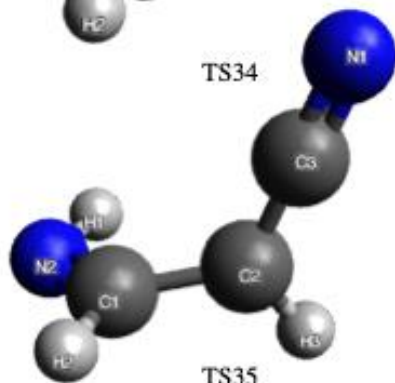
C						
C	1	1.34340				
H	1	1.08158	2	120.14207		
H	1	1.08208	2	121.75567	3	181.18934
C	2	1.43936	1	118.25113	3	4.35331
H	2	1.08849	1	120.18484	3	179.92967
N	5	1.44465	2	109.99959	1	173.98350
N	7	1.18956	5	89.40658	2	115.55562



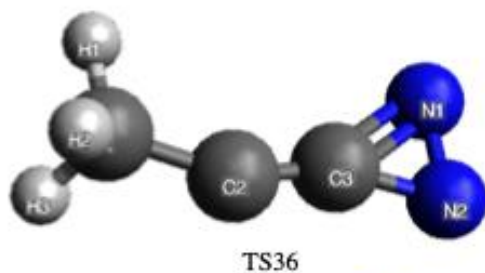
C						
C	1	1.38428				
H	1	1.08220	2	119.50724		
H	1	1.09011	2	123.34932	3	184.99898
C	2	1.32073	1	139.40174	3	185.14492
H	2	1.25570	1	63.39739	3	291.46121
N	5	2.40206	2	147.55099	1	244.60641
N	2	2.44953	1	143.89641	3	158.84284



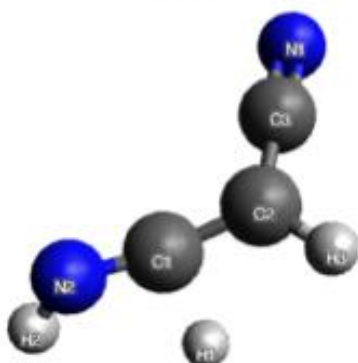
C						
C	1	1.42854				
H	1	1.08502	2	121.95262		
H	2	1.28369	1	59.13994	3	106.26151
C	2	1.29162	1	145.93799	3	336.06896
H	1	1.08078	2	118.62080	3	167.97960
N	5	1.44335	2	155.38748	1	323.44020
N	7	1.25294	5	61.95042	2	185.23931



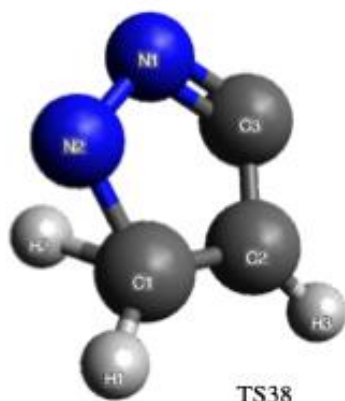
C						
C	1	1.48795				
C	2	1.37967	1	122.25549		
N	2	2.54528	1	122.04985	3	359.95716
N	1	1.26448	2	125.34692	3	91.39238
H	5	1.02208	1	111.87746	2	358.65095
H	1	1.09178	2	116.57792	3	270.26839
H	2	1.08314	1	119.17416	3	178.66512



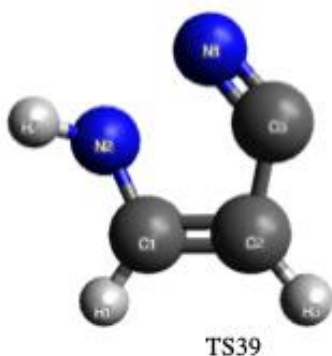
C						
C	1	1.45716				
H	1	1.09573	2	111.24704		
H	1	1.09141	2	111.13621	3	239.92627
C	2	1.24826	1	156.13001	3	0.03658
H	1	1.09141	2	111.13656	3	120.07232
N	5	1.56818	2	152.34007	1	0.00270
N	7	1.23334	5	58.46008	2	179.99929



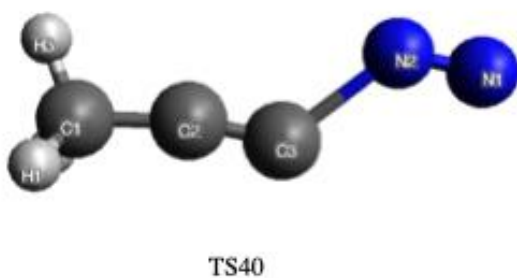
C						
C	1	1.34083				
H	1	1.94348	2	91.59020		
H	1	1.92656	2	169.93413	3	343.22737
C	2	1.41000	1	121.86816	3	99.02638
H	2	1.08162	1	118.59585	3	285.56284
N	2	2.56458	1	122.51921	3	99.14236
N	4	1.01521	1	33.07617	2	187.19601



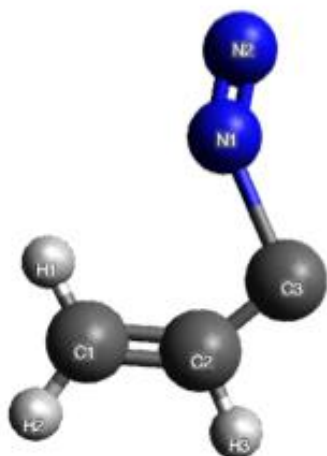
C						
C	1	1.40380				
H	1	1.07990	2	130.42058		
H	1	1.26701	2	112.81397	3	223.98888
C	2	1.38088	1	101.73654	3	196.41329
H	2	1.07421	1	128.65997	3	16.35933
N	5	1.31100	2	115.55170	1	358.44179
N	4	1.31937	1	68.56146	2	261.98088



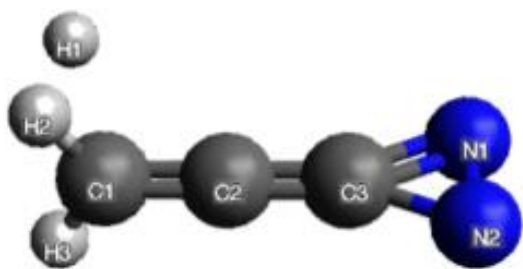
C						
C	1	1.35984				
H	1	1.08303	2	126.05470		
H	1	2.05344	2	128.21388	3	157.74062
C	2	1.42849	1	103.75392	3	184.42844
H	2	1.07372	1	128.32754	3	4.82093
N	5	1.20365	2	127.69943	1	359.23589
N	4	1.01798	1	36.08000	2	66.81549



C						
C	1	1.45247				
H	1	1.09106	2	111.18715		
H	1	1.09092	2	111.23677	3	238.87522
C	2	1.22685	1	168.95885	3	56.81343
H	1	1.09301	2	110.22542	3	119.36682
N	5	2.71997	2	149.14153	1	180.10778
N	7	1.10640	5	31.48954	2	0.15527

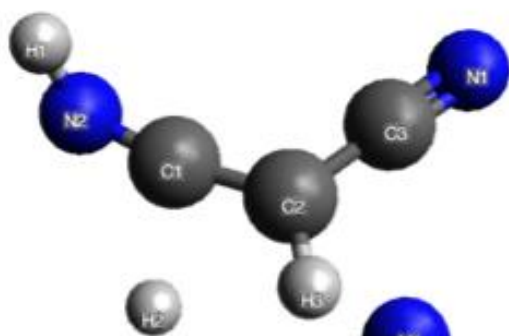


C						
C	1	1.38236				
H	1	1.08028	2	120.76898		
H	1	1.07898	2	121.09228	3	180.00000
C	2	1.36104	1	136.42409	3	0.00000
H	2	1.09598	1	118.17284	3	180.00000
N	5	1.91814	2	105.84406	1	0.00000
N	7	1.09636	5	146.70057	2	180.00000



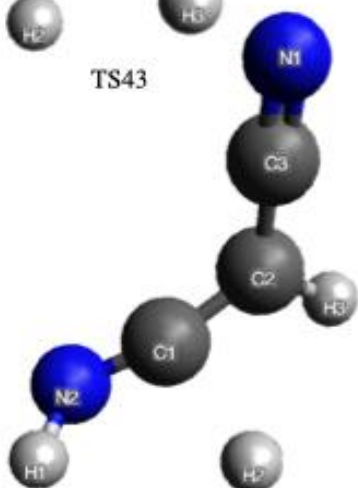
TS42

C					
C	1	1.31125			
H	1	2.36776	2	105.39080	
H	1	1.08308	2	121.39427	3
C	3	3.92659	1	39.44688	2
H	1	1.08308	2	121.39430	3
N	5	1.42313	2	154.15214	1
N	7	1.24170	5	64.09649	2
					180.00000



TS43

C					
C	1	1.34050			
C	2	1.41212	1	120.94722	
N	2	2.56687	1	121.54433	3
N	1	1.21259	2	168.93651	3
H	5	1.01769	1	118.47376	2
H	1	1.88183	2	90.14706	3
H	2	1.07982	1	119.72042	3
					183.80550



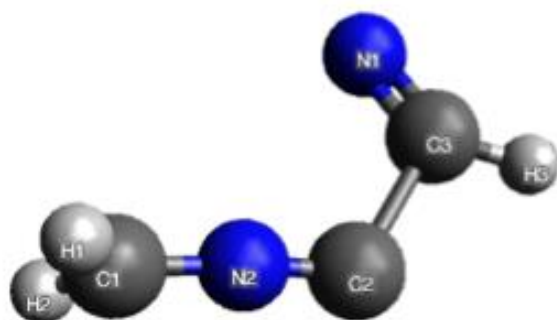
TS45

C					
C	1	1.34083			
C	2	1.41000	1	121.86837	
N	2	2.56457	1	122.51960	3
N	1	1.21015	2	162.69606	3
H	5	1.01521	1	119.67721	2
H	1	1.94350	2	91.58954	3
H	2	1.08162	1	118.59587	3
					173.46428



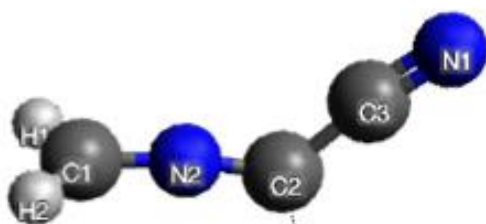
TS44

C					
C	1	1.39745			
H	1	3.86064	2	179.97438	
H	1	1.07929	2	128.64791	3
C	2	1.46762	1	101.78561	3
H	2	1.07645	1	130.22417	3
N	5	1.24227	2	114.97825	1
N	1	1.32624	2	111.85875	3
					352.34426



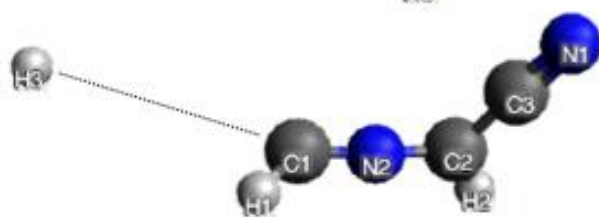
TS46

C					
C	1	2.49264			
C	2	1.82020	1	124.17355	
N	3	1.18981	2	114.11341	1
N	3	2.66457	1	10.40854	2
H	1	1.07971	2	119.50227	3
H	1	1.07976	2	118.97530	3
H	3	1.07782	2	105.38979	1



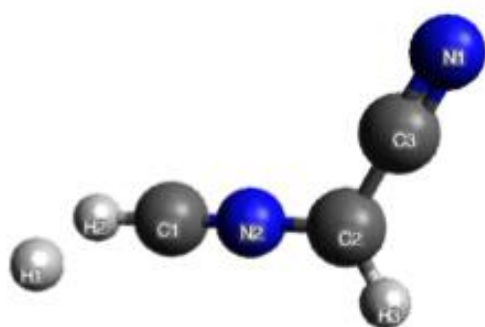
TS47

C					
C	1	2.47853			
C	2	1.39396	1	132.09059	
N	3	1.15792	2	172.72636	1
N	3	2.35394	1	7.23860	2
H	1	1.08137	2	119.50115	3
H	1	1.08137	2	119.50113	3
H	2	4.73075	1	110.49064	3



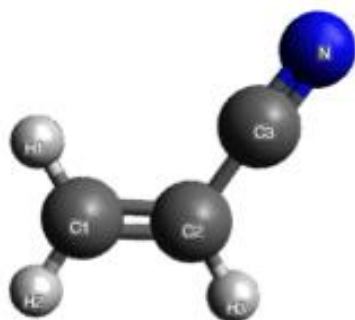
TS48

C					
C	1	2.48309			
C	2	1.41155	1	121.19787	
N	2	2.56644	1	122.03185	3
N	3	2.35523	1	10.43597	2
H	1	1.08464	2	129.91015	3
H	2	1.07987	1	118.44945	3
H	6	4.51344	1	85.50914	2



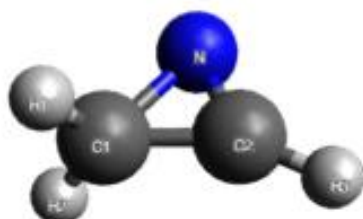
TS49

C					
C	1	2.47873			
C	2	1.40191	1	120.37993	
N	2	2.55943	1	120.97400	3
N	3	2.35655	1	10.03183	2
H	1	2.37232	2	106.37280	3
H	1	1.06263	2	171.95290	3
H	2	1.07755	1	117.58245	3



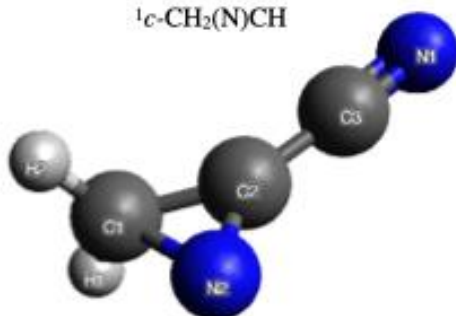
C_3H_7N

C					
C	1	1.33116			
H	1	1.08074	2	121.75956	
H	1	1.08038	2	120.57518	3
C	2	1.42622	1	123.13455	3
H	2	1.08274	1	121.21305	3
N	2	2.57849	1	123.75543	3



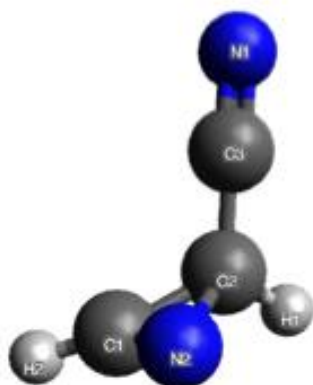
${}^1c\text{-CH}_2(\text{N})\text{CH}$

C					
C	1	1.44757			
N	2	1.24616	1	69.65658	
H	1	1.08314	2	120.63235	3
H	1	1.08313	2	120.61501	3
H	2	1.08061	1	151.43544	3



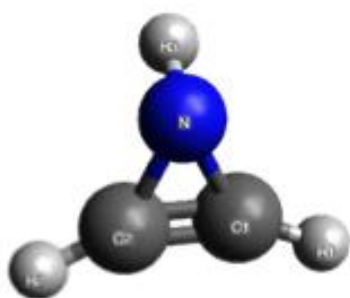
${}^1c\text{-CH}_2(\text{N})\text{CCN}$

C					
C	1	1.44979			
C	2	1.40599	1	150.39673	
N	2	2.55738	1	149.05293	3
N	2	1.25433	1	68.90462	3
H	1	1.08243	2	119.93940	3
H	1	1.08236	2	120.00372	3



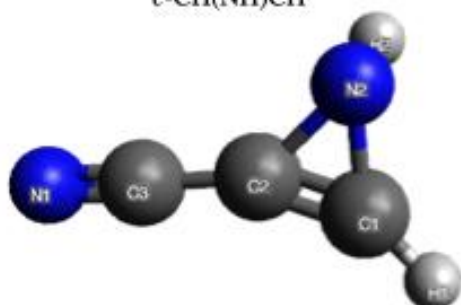
${}^1c\text{-CH}(\text{N})\text{CHCN}$

C					
C	1	1.45579			
C	2	1.43726	1	121.32962	
N	2	2.58848	1	121.57853	3
N	1	1.24229	2	69.87321	3
H	2	1.08195	1	120.50129	3
H	1	1.08005	2	149.20540	3



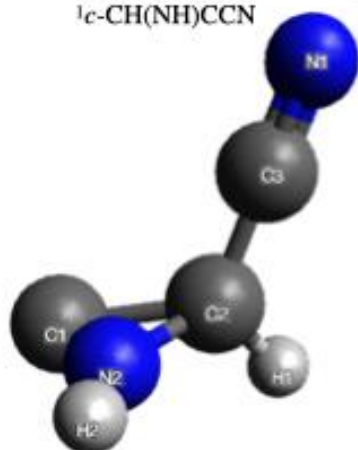
$^1c\text{-CH(NH)CH}$

C						
C	1	1.26892				
N	2	1.51635	1	65.26729		
H	1	1.07113	2	156.29394	3	168.99135
H	2	1.07114	1	156.29124	3	190.94153
H	3	1.02345	2	107.78894	1	98.43148



$^1c\text{-CH(NH)CCN}$

C						
C	1	1.27748				
C	2	1.38034	1	158.14962		
N	2	2.53595	1	158.77554	3	359.07492
N	1	1.47473	2	68.00948	3	189.22702
H	1	1.07388	2	153.37110	3	3.00824
H	5	1.02396	1	108.46518	2	261.73341



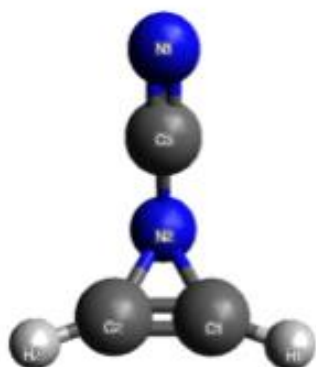
$^1c\text{-C(NH)CHCN}$

C						
C	1	1.61315				
C	2	1.43329	1	119.71668		
N	2	2.58520	1	119.97382	3	359.69485
N	1	1.27313	2	57.84089	3	255.59851
H	2	1.08077	1	118.07308	3	208.40222
H	5	1.01231	1	144.15590	2	176.88069



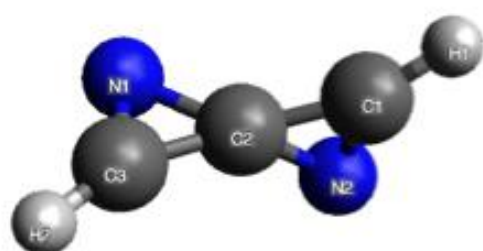
$^1c\text{-CH}_2(\text{NCN})\text{C}$

C						
C	1	1.55299				
C	2	2.52120	1	76.93947		
N	3	1.15348	2	165.28649	1	179.99707
N	2	1.30617	1	59.87601	3	359.99718
H	1	1.08252	2	118.84789	3	257.39776
H	1	1.08249	2	118.88616	3	102.60235



$^1c\text{-CH(NCN)CH}$

C						
C	1	1.26626				
C	2	2.42896	1	74.91384		
N	3	1.15538	2	150.06958	1	241.95124
N	3	1.35964	2	34.81413	1	67.13365
H	1	1.07119	2	158.90927	3	154.05621
H	2	1.07121	1	158.87595	3	205.85137



$^1c\text{-CH(N)CCHN}$

C						
C	1	1.40977				
C	2	1.40973	1	156.41573		
N	3	1.27159	2	67.02909	1	133.10070
N	1	1.27167	2	67.03154	3	133.31860
H	1	1.08360	2	155.75104	3	311.63757
H	3	1.08355	2	155.64791	1	311.14521



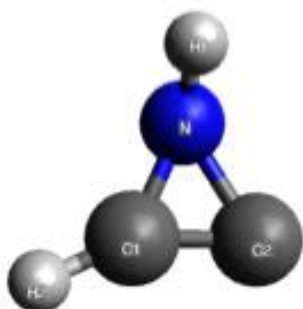
$c\text{-CH}_2(\text{N})\text{C}$

C						
C	1	1.49406				
N	2	1.21141	1	73.94261		
H	1	1.07956	2	119.98477	3	263.58621
H	1	1.07956	2	119.98477	3	96.41379



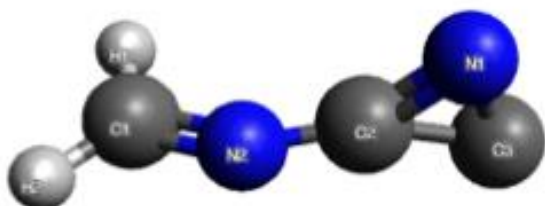
$^1c\text{-CH(N)CCNH}$

C						
C	1	1.39593				
C	2	1.27926	1	164.53064		
N	3	1.23446	2	171.39859	1	257.31372
N	1	1.25832	2	70.47377	3	193.78538
H	1	1.08162	2	149.91244	3	14.14489
H	4	1.02061	3	114.62383	2	179.35090



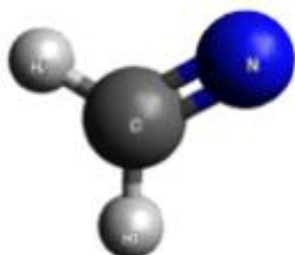
c-CH(NH)C

C					
C	1	1.35584			
N	1	1.36149	2	66.65354	
H	3	1.01774	1	130.23113	2 247.92021
H	1	1.07428	2	155.01873	3 182.68779



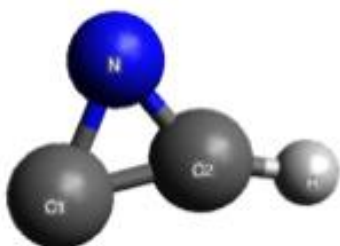
¹c-CH₂NC(N)C

C					
C	1	2.43211			
C	2	1.44644	1	157.18401	
N	3	1.32526	2	57.84292	1 153.58133
N	2	1.25621	1	15.31859	3 241.97085
H	1	1.08626	2	106.38601	3 295.23277
H	1	1.08292	2	134.42274	3 114.28664



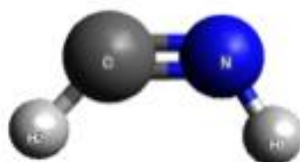
H₂CN

C					
N	1	1.23794			
H	1	1.09755	2	121.50867	
H	1	1.09731	2	121.56479	3 179.99825



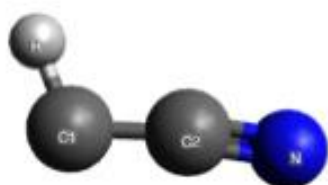
¹c-C(N)CH

C					
C	1	1.39644			
N	2	1.29057	1	62.81549	
H	2	1.07879	1	158.97676	3 179.98521



HCNH

C					
N	1	1.21760			
H	2	1.02522	1	122.72699	
H	1	1.09688	2	133.98864	3 0.00000



¹HCCN

C					
C	1	1.36792			
N	2	1.17415	1	172.29129	
H	1	1.09503	2	112.11024	3 180.02822



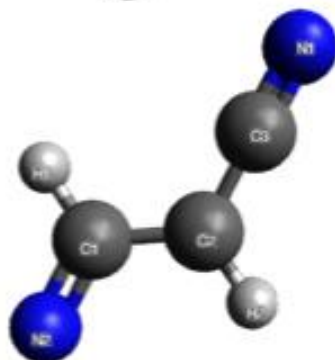
³HCCN

C					
C	1	1.29425			
N	2	1.19838	1	176.18673	
H	1	1.06573	2	157.71586	3 180.03147



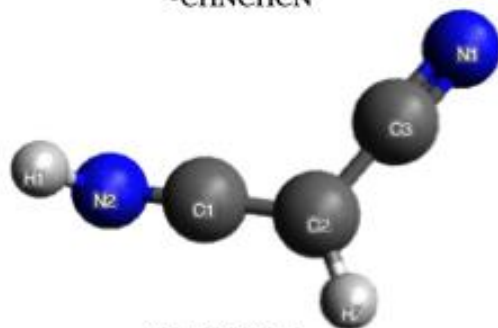
³CHNHCCN

C					
C	1	2.39168			
C	2	1.35405	1	103.99304	
N	3	1.17287	2	172.46910	1 180.02512
N	1	1.31772	2	28.03981	3 179.97611
H	1	1.09683	2	83.46943	3 359.96548
H	5	1.01182	1	118.79414	2 180.00277



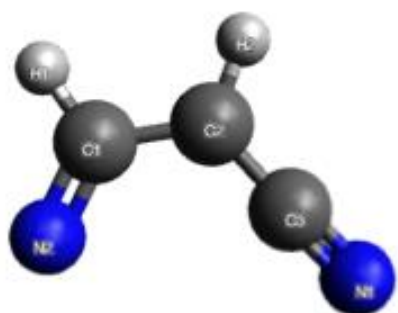
³CHNCHCN

C					
C	1	1.41820			
C	2	1.39589	1	122.13182	
N	2	2.55565	1	122.26147	3 0.00002
N	1	1.27850	2	123.08707	3 179.99999
H	1	1.09487	2	118.56283	3 0.00007
H	2	1.08128	1	119.44159	3 179.99993



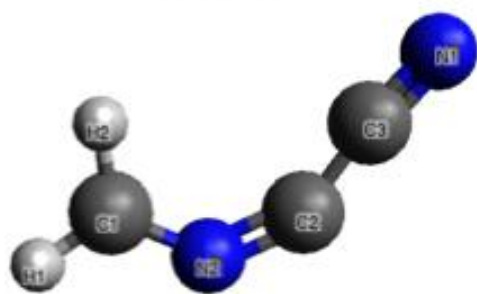
¹HNCCHCN

C					
C	1	1.32092			
C	2	1.41538	1	122.18906	
N	2	2.56874	1	122.92746	3 0.07214
N	1	1.20617	2	173.73335	3 99.66556
H	5	1.01642	1	120.18978	2 171.50080
H	2	1.08196	1	118.71690	3 178.82558



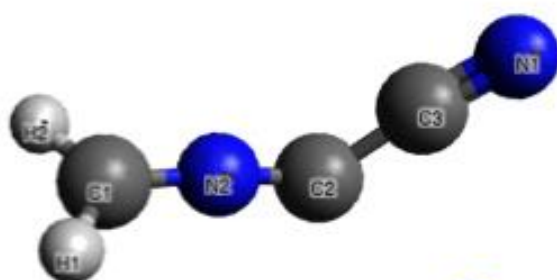
³NCHCHCN

C						
C	1	1.41846				
C	2	1.39911	1	123.69764		
N	2	2.55704	1	124.56582	3	359.99993
N	1	1.27901	2	125.50992	3	359.99993
H	1	1.09499	2	116.86370	3	179.99993
H	2	1.08114	1	119.04772	3	180.00007



³CH₂NCCN

C						
C	1	2.33501				
C	2	1.34561	1	124.26384		
N	3	1.17442	2	172.23196	1	180.00085
N	2	1.26859	1	25.55225	3	180.00011
H	1	1.08091	2	143.19965	3	180.00213
H	1	1.08824	2	97.00451	3	359.99857



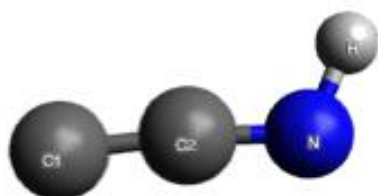
¹CH₂NCCN

C						
C	1	2.47862				
C	2	1.39367	1	132.21286		
N	3	1.15795	2	172.71374	1	180.03762
N	3	2.35472	1	7.20773	2	359.94081
H	1	1.08134	2	119.50762	3	268.46003
H	1	1.08141	2	119.47863	3	91.58547



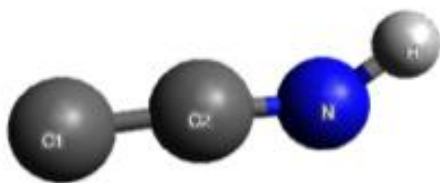
¹CHNCHCN

C						
C	1	2.48305				
C	2	1.41159	1	121.21878		
N	2	2.56648	1	122.04340	3	0.00305
N	3	2.35551	1	10.43332	2	349.07557
H	1	1.08454	2	129.91575	3	267.99654
H	2	1.07988	1	118.46282	3	183.94401



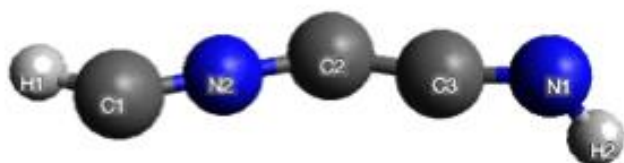
¹CCNH

C						
C	1	1.31353				
N	2	1.23870	1	174.05770		
H	3	1.02583	2	113.96205	1	180.49088



C						
C	1	1.33491				
N	2	1.20865	1	174.54877		
H	3	1.00571	2	137.79861	1	179.99498

³CCNH



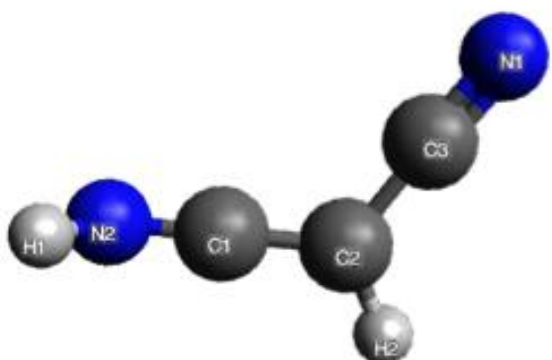
C						
C	1	2.44359				
C	2	1.27076	1	151.67337		
N	3	1.22768	2	171.58546	1	234.70230
N	3	2.45637	2	13.78431	1	0.58631
H	1	1.07240	2	141.40903	3	186.20970
H	4	1.01336	3	119.71047	2	209.90372

¹CHNCCNH



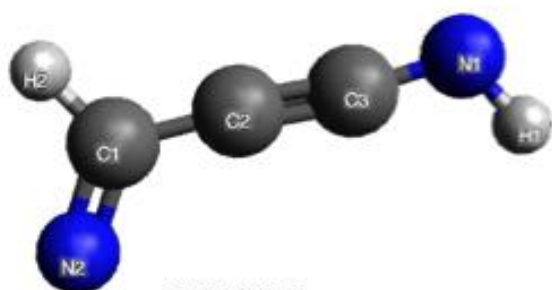
C						
C	1	1.41846				
C	2	1.39911	1	123.69764		
N	2	2.55704	1	124.56582	3	359.99993
N	1	1.27901	2	125.50992	3	359.99993
H	1	1.09499	2	116.86370	3	179.99993
H	2	1.08114	1	119.04772	3	180.00007

³NCHCHCN



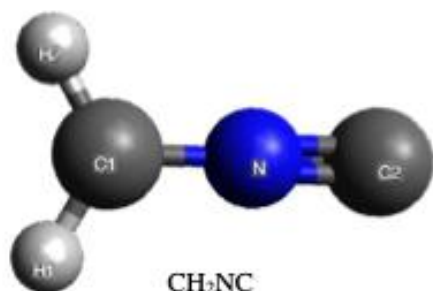
C						
C	1	1.32092				
C	2	1.41538	1	122.18906		
N	2	2.56874	1	122.92746	3	0.07214
N	1	1.20617	2	173.73335	3	99.66556
H	5	1.01642	1	120.18978	2	171.50080
H	2	1.08196	1	118.71690	3	178.82558

¹NHCCHCN



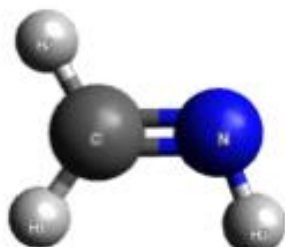
C						
C	1	1.39345				
C	2	1.25020	1	175.61171		
N	3	1.24956	2	172.71029	1	179.24532
N	1	1.27951	2	122.64380	3	0.81057
H	4	1.01910	3	114.78123	2	179.99321
H	1	1.09687	2	119.49238	3	180.69071

³NCHCCNH



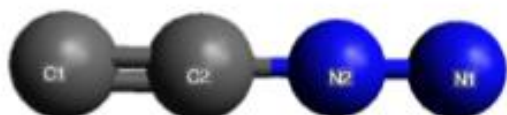
CH₂NC

C						
C	1	2.51428				
N	2	1.18182	1	0.09347		
H	1	1.07856	2	118.77897	3	179.69967
H	1	1.07856	2	119.12869	3	359.69884



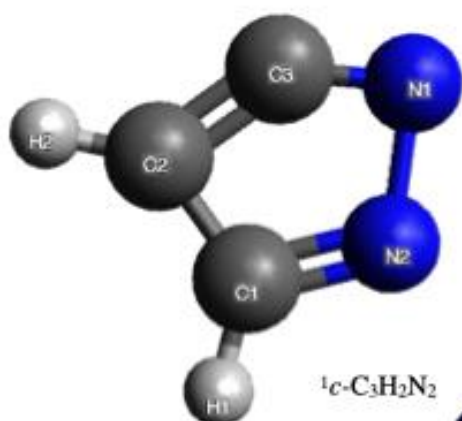
¹CH₂NH

C						
N	1	1.26390				
H	1	1.09345	2	124.67646		
H	1	1.08904	2	118.96024	3	179.97395
H	2	1.02046	1	111.40702	3	359.97675



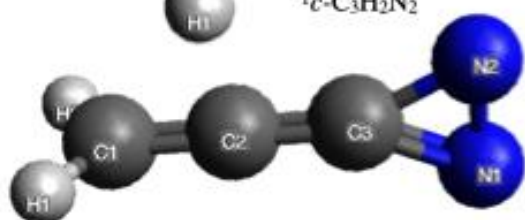
CCNN

C						
C	1	1.26282				
N	2	2.38880	1	179.97438		
N	3	1.12287	2	0.02562	1	0.00000



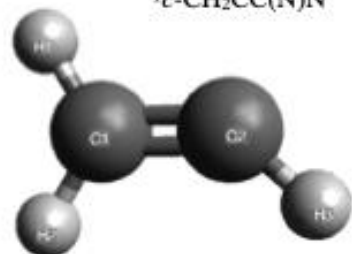
¹c-C₃H₂N₂

C						
C	1	1.39497				
H	1	1.07908	2	130.25993		
C	2	1.37079	1	90.18834	3	179.98758
H	2	1.06974	1	136.97624	3	0.00634
N	4	1.23482	2	138.09125	1	0.00726
N	1	1.36238	2	111.73532	3	179.99314



¹c-CH₂CC(N)N

C						
C	1	1.30671				
H	1	1.08359	2	121.45368		
H	1	1.08367	2	121.44907	3	179.92772
C	3	3.27726	1	42.17991	2	359.95324
N	5	1.42140	2	154.04608	1	26.82282
N	6	1.24275	5	64.08693	2	180.07446



CH₂CH

C						
C	1	1.30127				
H	1	1.08577	2	122.28669		
H	1	1.09129	2	121.83822	3	180.06320
H	2	1.07749	1	138.78445	3	180.08060