Electronic Supporting Information (ESI)

Spectroscopic Identification of Fragment Ions of DNA/RNA Building Blocks: The Case of Pyrimidine

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Figure Captions

Figure S1. Typical mass spectrum of the EI ions source for an expansion of Pym seeded in 10 bar N_2 compared to the standard EI spectrum of isolated Pym at 70 eV kinetic energy taken from the NIST data base. Apart from the peaks arising from the N_2 carrier gas and the H_2O impurity (N_n^+, H_2O), the mass spectrum is dominated by the Pym^+ parent ion (m/z 80) and its major $C_3H_3N^+$ and $C_2H_2^+$ fragments (m/z 53 and 28), similar to the NIST spectrum. Our ionization conditions are softer (lower effective electron kinetic energy caused by scattering at neutral carrier gas molecules and/or generation of secondary electrons) leading to less pronounced fragmentation. In addition, the $C_3H_3N^+$-N_2 mass peak occurs with high abundance (m/z 81). The mass peaks at m/z 40 and 68 are tentatively attributed to CN_2^+ or $C_2H_2N^+$ with its N_2 cluster.

Figure S2. Collision-induced dissociation (CID) mass spectrum of mass-selected Pym^+ (a) and its major fragment ion $C_3H_3N^+$ (b), illustrating the exclusive loss of HCN.

Figure S3. HOMO (b_2) of Pym ($^1A_1$, C_{2v}, b_2) and SOMO (b_2) and SOMO-1 (a_1) of Pym^+ ($^2B_2$, C_{2v}) calculated at the B3LYP-D3/aug-cc-pVTZ level.

Figure S4. NBO atomic charge distribution (in e) of Pym, Pym^+, and selected $C_3H_3N^+$ and $C_3H_3N^+$-N_2 isomers calculated at the B3LYP-D3/aug-cc-pVTZ level.

Figure S5. Comparison of experimental IRPD spectrum of $C_3H_3N^+$ with the linear IR absorption spectra of various $C_3H_3N^+$ isomers along with the corresponding optimized structures calculated at the B3LYP-D3/aug-cc-pVTZ level. The IR stick spectra are convoluted with Gaussian line profiles with FWHM=10 cm^{-1}. The relative energies (E_0), free energies (G) in parentheses and bond lengths are in kJ mol^{-1} and Å, respectively.

Figure S6. Comparison of experimental IRPD spectrum of $C_3H_3N^+$-Ar with the linear IR absorption spectra of various $C_3H_3N^+$-Ar isomers along with the corresponding optimized structures calculated at the B3LYP-D3/aug-cc-pVTZ level. The IR stick spectra are convoluted with Gaussian line profiles with FWHM=10 cm^{-1}. Binding energies (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parentheses correspond to relative energies in kJ mol^{-1} (E_0).

Figure S7. Comparison of experimental IRPD $C_3H_3N^+$-N_2 spectrum with the linear IR absorption spectra of various $C_3H_3N^+$-N_2 isomers along with the corresponding optimized structures calculated at the B3LYP-D3/aug-cc-pVTZ level. The IR stick spectra are convoluted with Gaussian line profiles with FWHM=10 cm^{-1}. Binding energies (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parentheses correspond to relative energies in kJ mol^{-1} (E_0).

Figure S8. NBO interaction energies of donor-acceptor orbitals ($E^{(2)}$ in kJ mol^{-1}) involved in the H-bonds of the type XH…L (X=N and C, L=Ar and N_2) and π-bonding of few selected $C_3H_3N^+$-Ar/N_2 isomers calculated at the B3LYP-D3/aug-cc-pVTZ level.

Figure S9. IRPD spectrum of $C_2H_2^+$-Ar measured in the present work with a laser resolution of 1 cm^{-1} compared to a spectrum published previously using a laser with a resolution of 0.02 cm^{-1} (Dopfer et al., *J. Chem. Phys.* **2004**, *121*, 1744).

Figure S10. IRPD spectrum of $C_2H_2^+$-Ar compared to the linear IR absorption spectra of $HCCH^+$ and H_2CC^+ calculated at the B3LYP-D3/aug-cc-pVTZ level. The relative energies (E_0), free energies (G) in parentheses and bond lengths are in kJ mol^{-1} and Å, respectively.

Table S1. Experimental and calculated structural parameters of Pym and Pym^+ at the B3LYP-D3/aug-cc-pVTZ level (in Å and degree).

structural parameters	Pym		Pym^+
	exp[a]	Calc	Calc
r_{N1C2}	1.340 (1.33333(38))	1.3327	1.3222
r_{N3C2}	1.340 (1.33333(38))	1.3327	1.3222
r_{N3C4}	1.340	1.3335	1.3156
r_{N1C6}	1.340	1.3335	1.3156
r_{C4C5}	1.393 (1.38675(45))	1.3878	1.3937
r_{C5C6}	1.393	1.3878	1.3937
r_{C2H7}	1.099 (1.08165(39))	1.0837	1.0795
r_{C4H8}	1.099 (1.08224(30))	1.0841	1.0859
r_{C6H10}	1.099 (1.08224(30))	1.0841	1.0859
r_{C5H9}	1.099 (1.07929(36))	1.0804	1.0797
∠(N1C2N3)	127.6	126.9	113.8
∠(C2N3C4)	115.5	116.1	125.8
∠(N3C4C5)	122.3	122.2	120.1
∠(C4C5C6)	116.8	116.7	114.3
∠(N1C2H7)	116.2 (116.332(24))	116.5	123.1
∠(C5C4H8)	122.4 (121.261(38))	121.2	122.6
∠(C6C5H9)	121.6 (121.665(22))	121.7	122.9

[a] From electron diffraction data (L. Fernholt and C. Romming, C., *Acta Chem. Scand.* **1978,** *32*, 271-273). Numbers in parentheses are from a recent and more reliable microwave study combined with CCSD(T) corrections (Z.N. Heim et al., *J. Chem. Phys.* **2020**, *152*, 104303). The latter values agree much better with our B3LYP-D3 data.

Table S2. Experimental and calculated frequencies (in cm^{-1}) of Pym^+ in its cation ground state. Calculated frequencies are scaled by a factor of 0.98 (<2000 cm^{-1}) and 0.96221 (>2000 cm^{-1}).

mode	symmetry	B3LYP-D3	Intensity (km mol^{-1})	Sato et al. exp[a]	Riese et al. exp[b]	Kim et al. exp[c]	This work exp
16b	b1	360	1	343	345		
16a	a2	444	0	432	429		
6b	b2	533	179	510	511	515	
4	b1	578	64		575		
6a	a1	640	8	636	636	635	
5	b1	827	27		823	824	
17a	a2	919	0				
10b	b1	925	1		913	911	
1	a1	953	11	954	956	953	
11	b1	996	0		990		
14	b2	1019	5				
12	a1	1037	0	1038	1038	1028	
9a	a1	1134	0	1126	1127	1134	
18b	b2	1157	1				
15	b2	1174	62				
3	b2	1312	1				
19a	a1	1410	67	1460	1436	1440	
19b	b2	1431	0				
8b	b2	1467	137				
8a	a1	1570	16	1554	1554	1547	
2	a1	3031	13				3045 (C4/C6H)
7b	b2	3031	49				3045 (C4/C6H)
13	a1	3103	15				3112 (C5H)
20a	a1	3117	20				3124 (C2H)

[a] Sato et al., *J. Electron. Spectrosc. Relat. Phenom.* **1998**, *97*, 121. [b] M. Riese and J. Grotemeier, *Anal. Bioanal. Chem.* **2006**, *386*, 59. [c] H.J. Kim et al., *Phys. Chem. Chem. Phys.* **2014**, *16*, 1590.

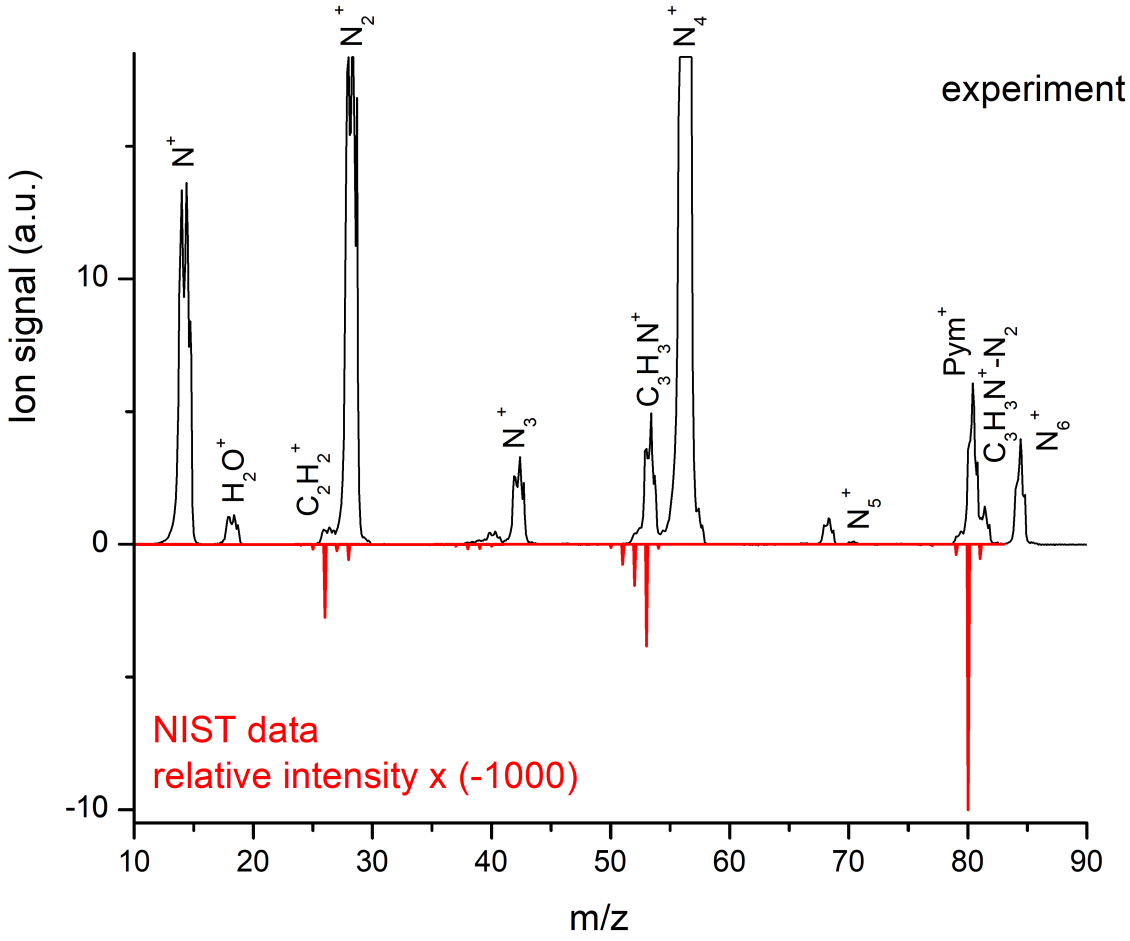

experiment
Ion signal (a.u.)
10
0
-10
10
20
30
40
50
60
70
80
90
m/z
N+
H2O+
C2H2+
N2+
N3+
C3H3N+
N4+
N5+
Pym+
C3H3N+-N2
N6+
NIST data
relative intensity x (-1000)

Figure S1

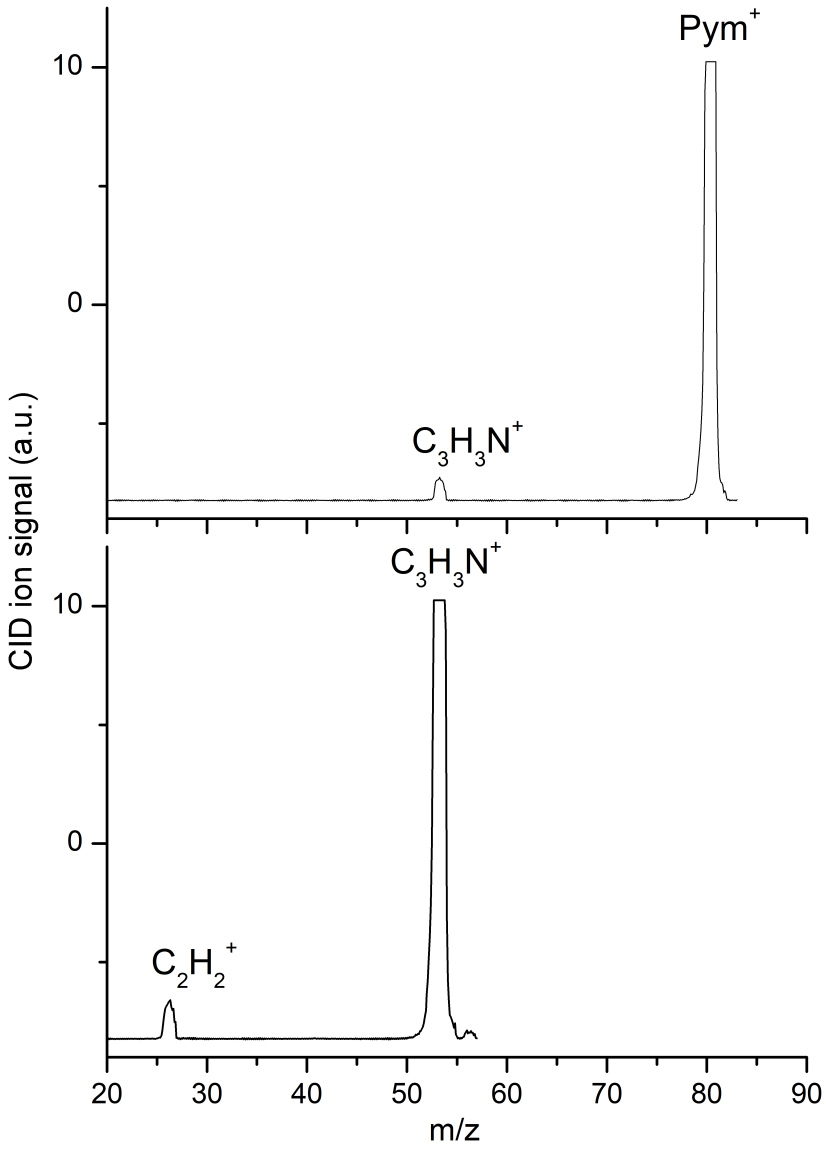
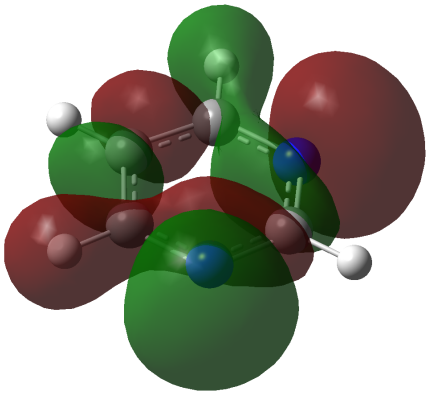
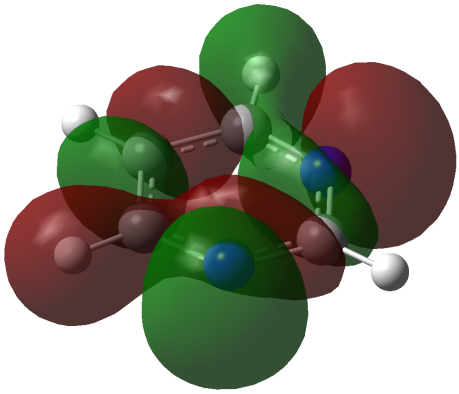

Pym+
10
0
C3H3N+
CID ion signal (a.u.)
C3H3N+
10
0
C2H2+
20
30
40
50
60
70
80
90
m/z

Figure S2

HOMO (Pym)



SOMO (Pym^+)



SOMO-1 (Pym^+)

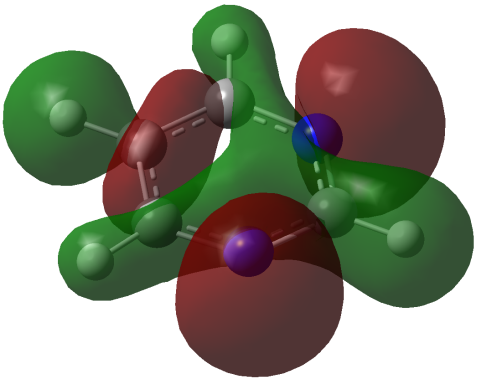


Figure S3

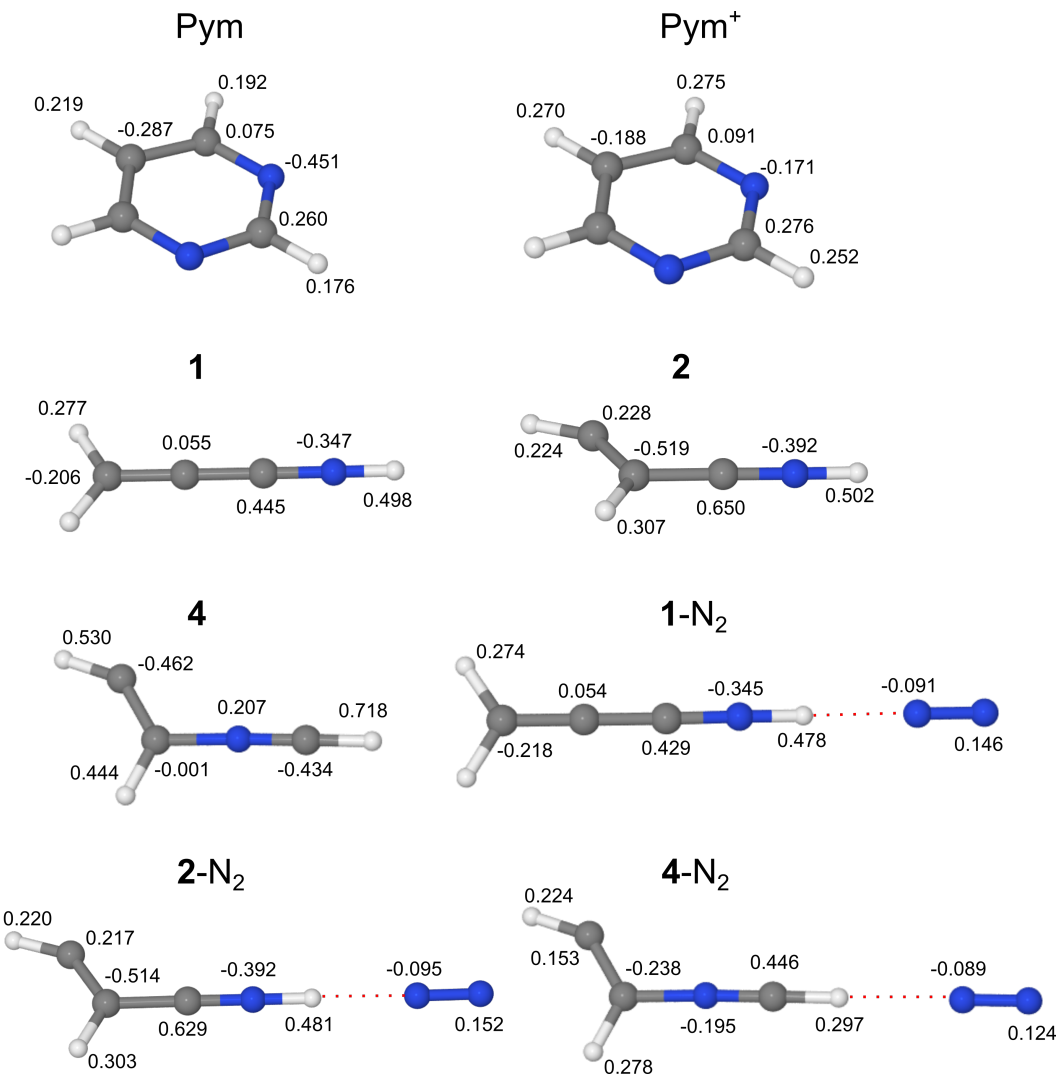

Pym
0.219
0.192
-0.287
0.075
-0.451
0.260
0.176
Pym+
0.270
0.275
-0.188
0.091
-0.171
0.276
0.252
1
0.277
0.055
-0.347
-0.206
0.445
0.498
2
0.228
0.224
-0.519
-0.392
0.650
0.502
0.307
4
0.530
-0.462
0.207
0.718
0.444
-0.001
-0.434
1-N2
0.274
0.054
-0.345
-0.091
-0.218
0.429
0.478
0.146
2-N2
0.220
0.217
-0.514
-0.392
-0.095
0.629
0.481
0.152
0.303
4-N2
0.224
0.153
-0.238
0.446
-0.089
-0.195
0.297
0.124
0.278

Figure S4

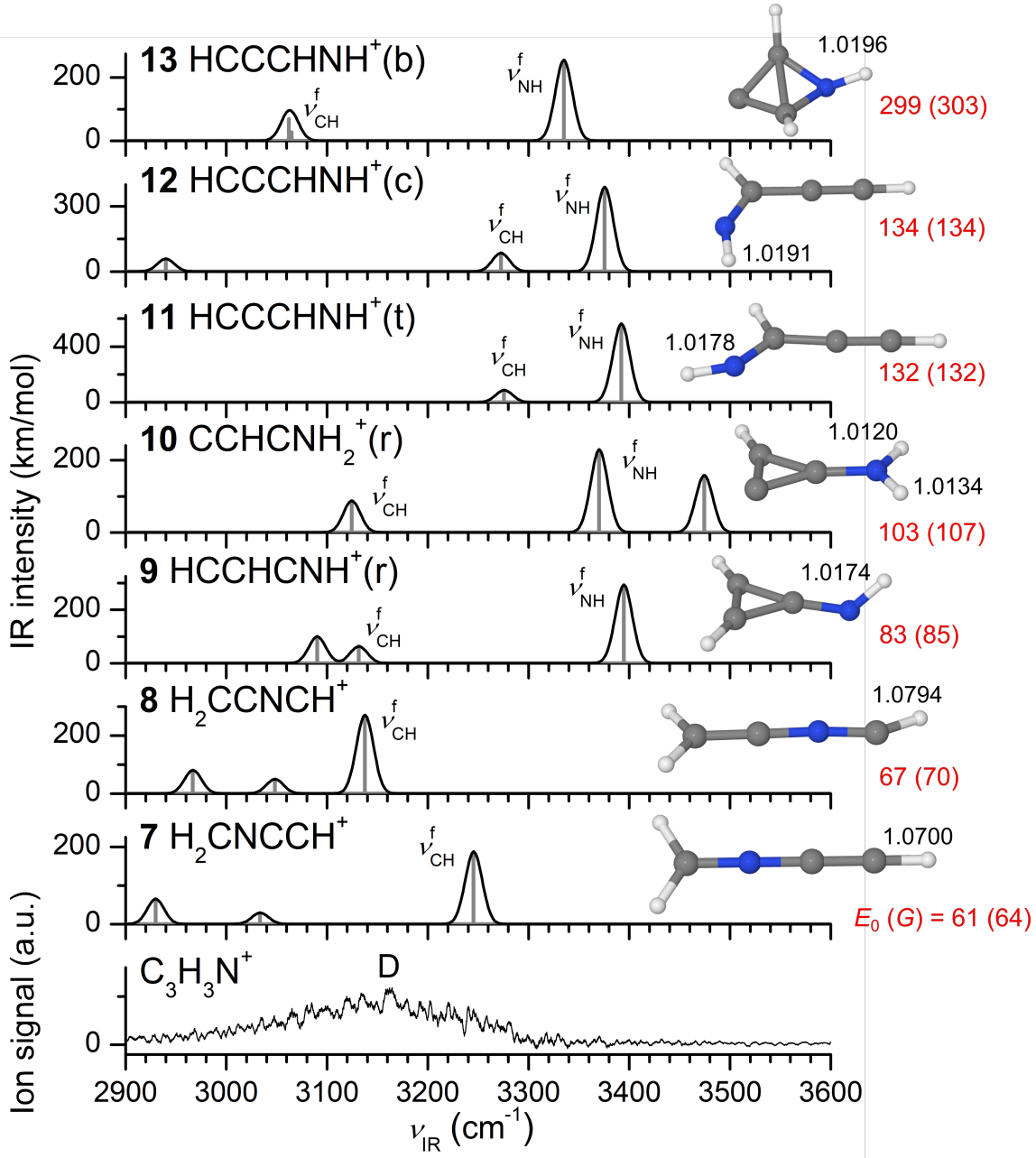

13 HCCCHNH+(b)
1.0196
299 (303)
12 HCCCHNH+(c)
1.0191
134 (134)
11 HCCCHNH+(t)
1.0178
132 (132)
10 CCHCNH2+(r)
1.0120
1.0134
103 (107)
9 HCCHCNH+(r)
1.0174
83 (85)
8 H2CCNCH+
1.0794
67 (70)
7 H2CNCCH+
1.0700
E0 (G) = 61 (64)
C3H3N+
D
IR intensity (km/mol)
Ion signal (a.u.)
νIR (cm-1)

Figure S5

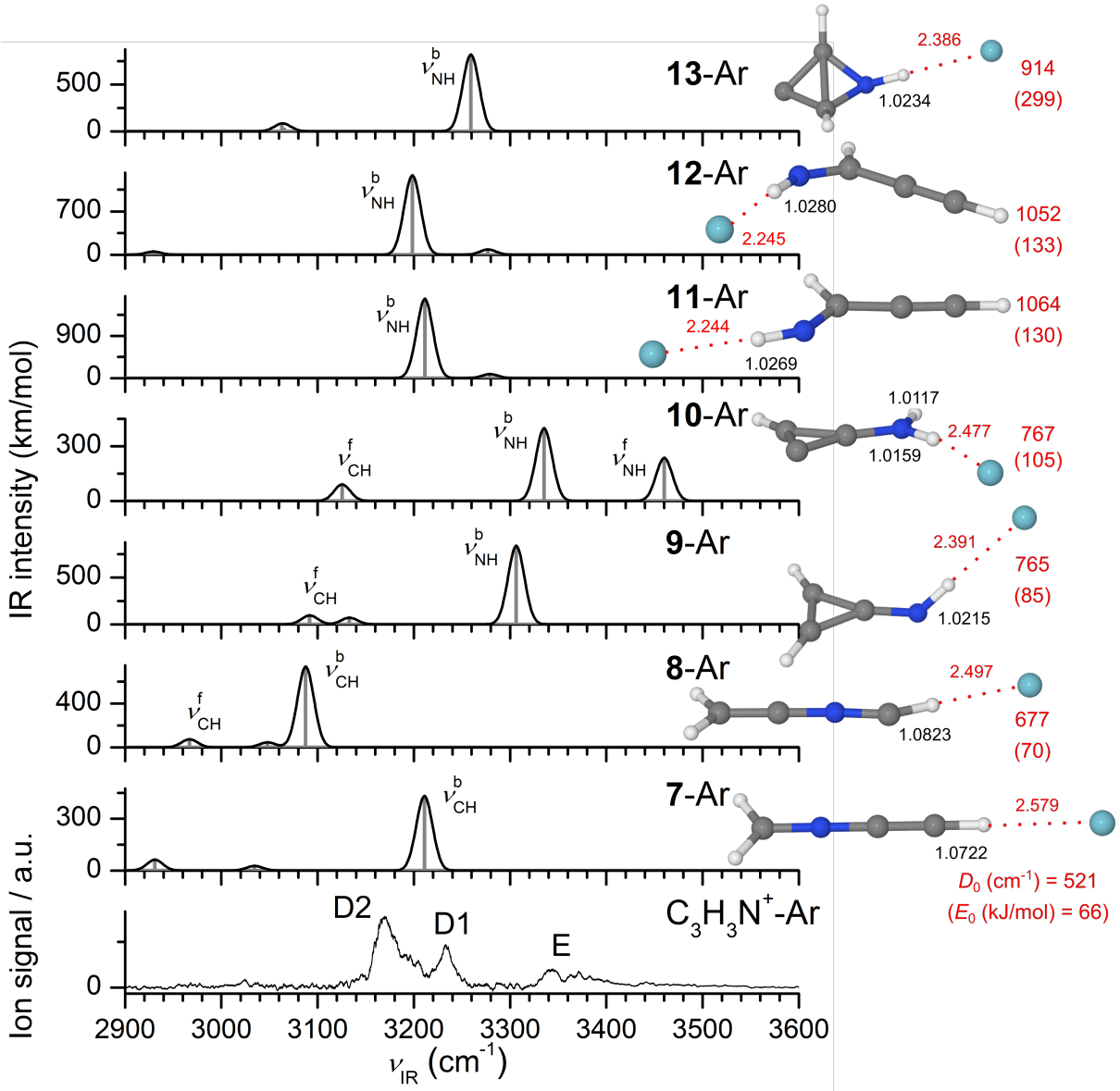

IR intensity (km/mol)
Ion signal / a.u.
13-Ar
12-Ar
11-Ar
10-Ar
9-Ar
8-Ar
7-Ar
C3H3N+-Ar
D2
D1
E
2.386
914
(299)
1.0234
1.0280
2.245
1052
(133)
2.244
1064
(130)
1.0269
1.0117
2.477
767
(105)
1.0159
2.391
765
(85)
1.0215
2.497
677
(70)
1.0823
2.579
1.0722
D0 (cm-1) = 521
(E0 (kJ/mol) = 66)
νIR (cm-1)

Figure S6

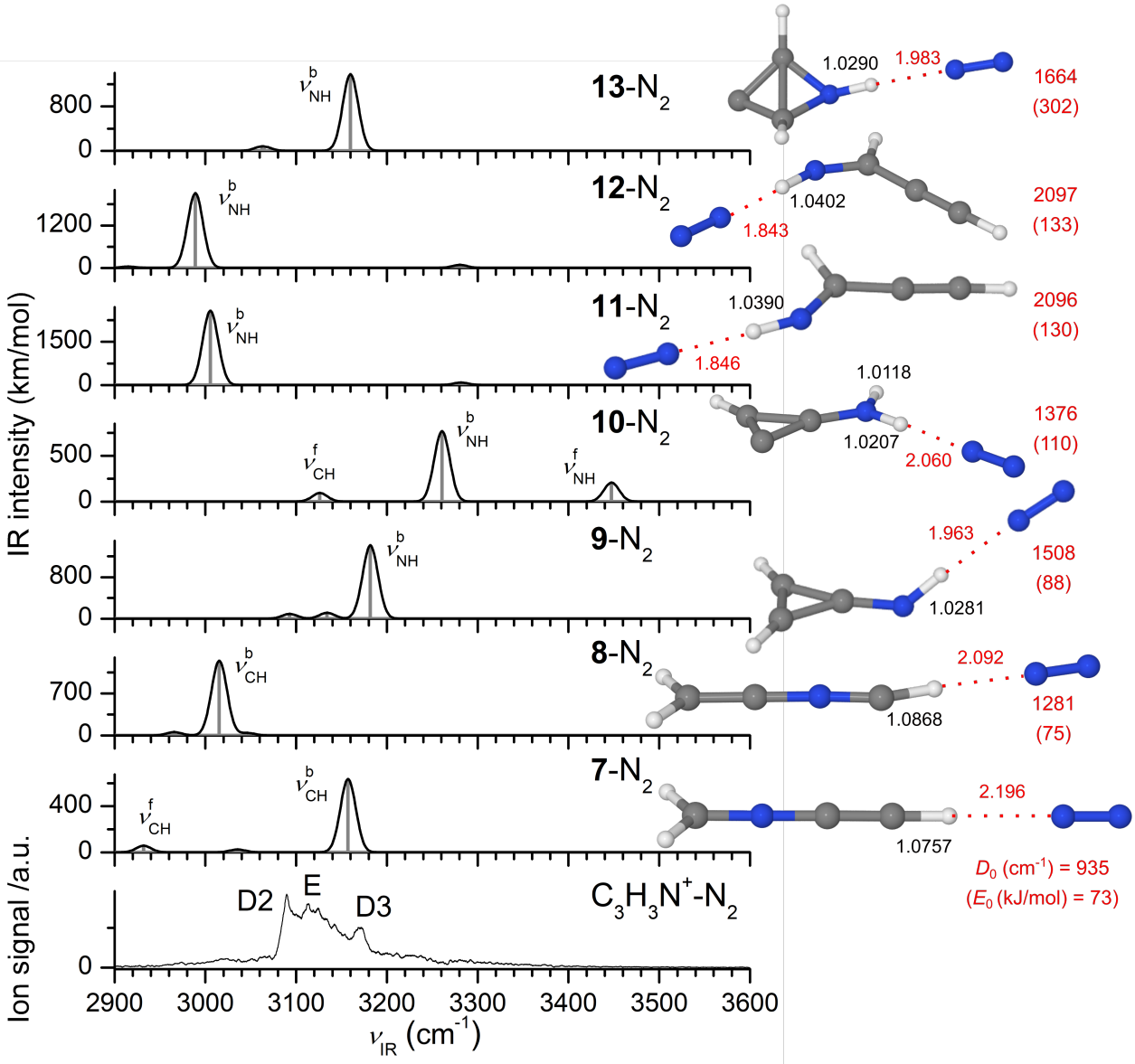

IR intensity (km/mol)
Ion signal /a.u.
ν_{IR} (cm^{-1})
13-N$_2$
12-N$_2$
11-N$_2$
10-N$_2$
9-N$_2$
8-N$_2$
7-N$_2$
C$_3$H$_3$N$^+$-N$_2$
ν^b_{NH}
ν^f_{CH}
ν^b_{CH}
ν^f_{NH}
D2
E
D3
1.0290
1.983
1664
(302)
1.0402
1.843
2097
(133)
1.0390
1.846
2096
(130)
1.0118
1.0207
2.060
1376
(110)
1.963
1.0281
1508
(88)
2.092
1.0868
1281
(75)
2.196
1.0757
D_0 (cm^{-1}) = 935
(E_0 (kJ/mol) = 73)

Figure S7

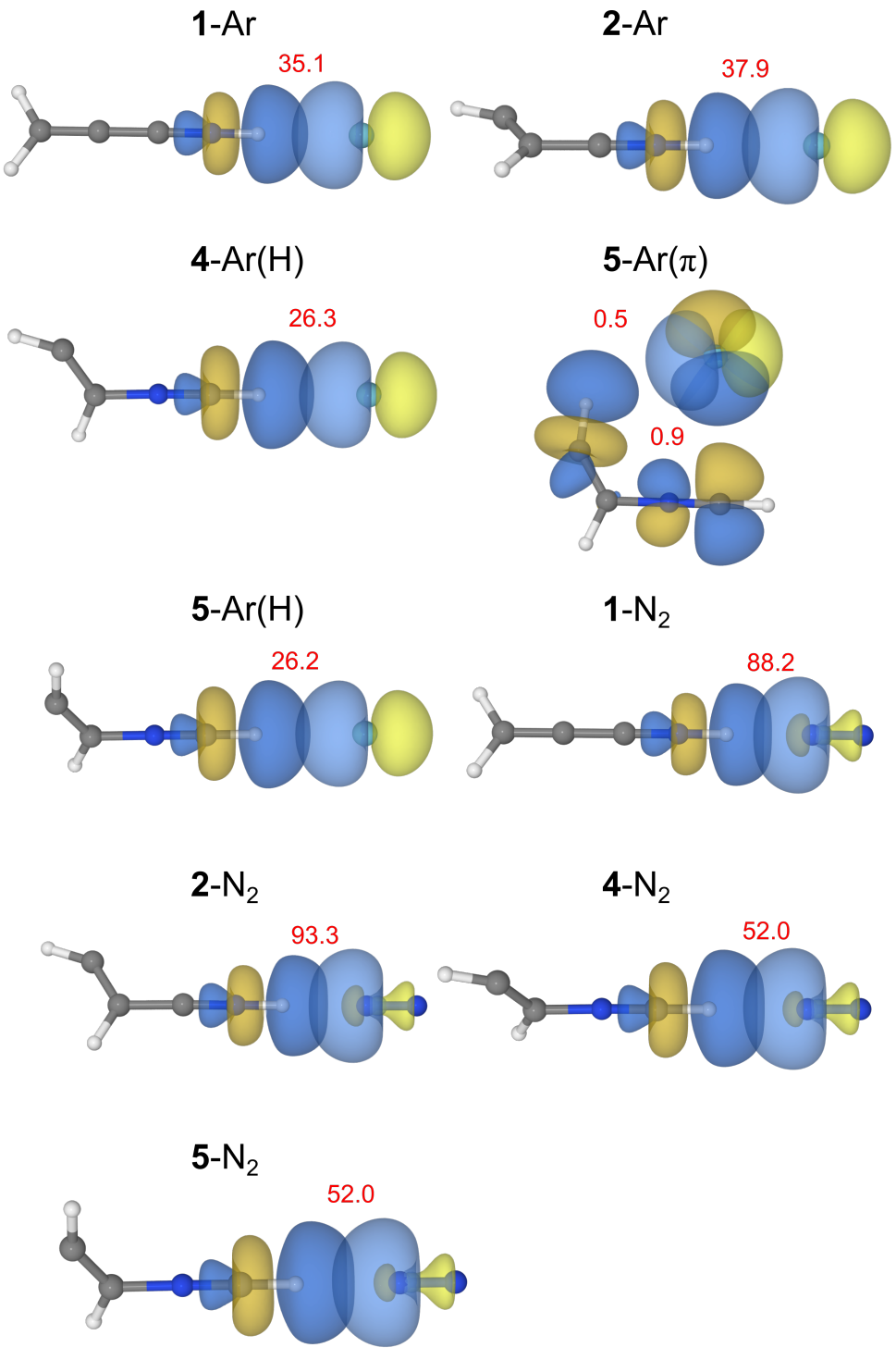

1-Ar
35.1
2-Ar
37.9
4-Ar(H)
26.3
5-Ar(π)
0.5
0.9
5-Ar(H)
26.2
1-N2
88.2
2-N2
93.3
4-N2
52.0
5-N2
52.0

Figure S8

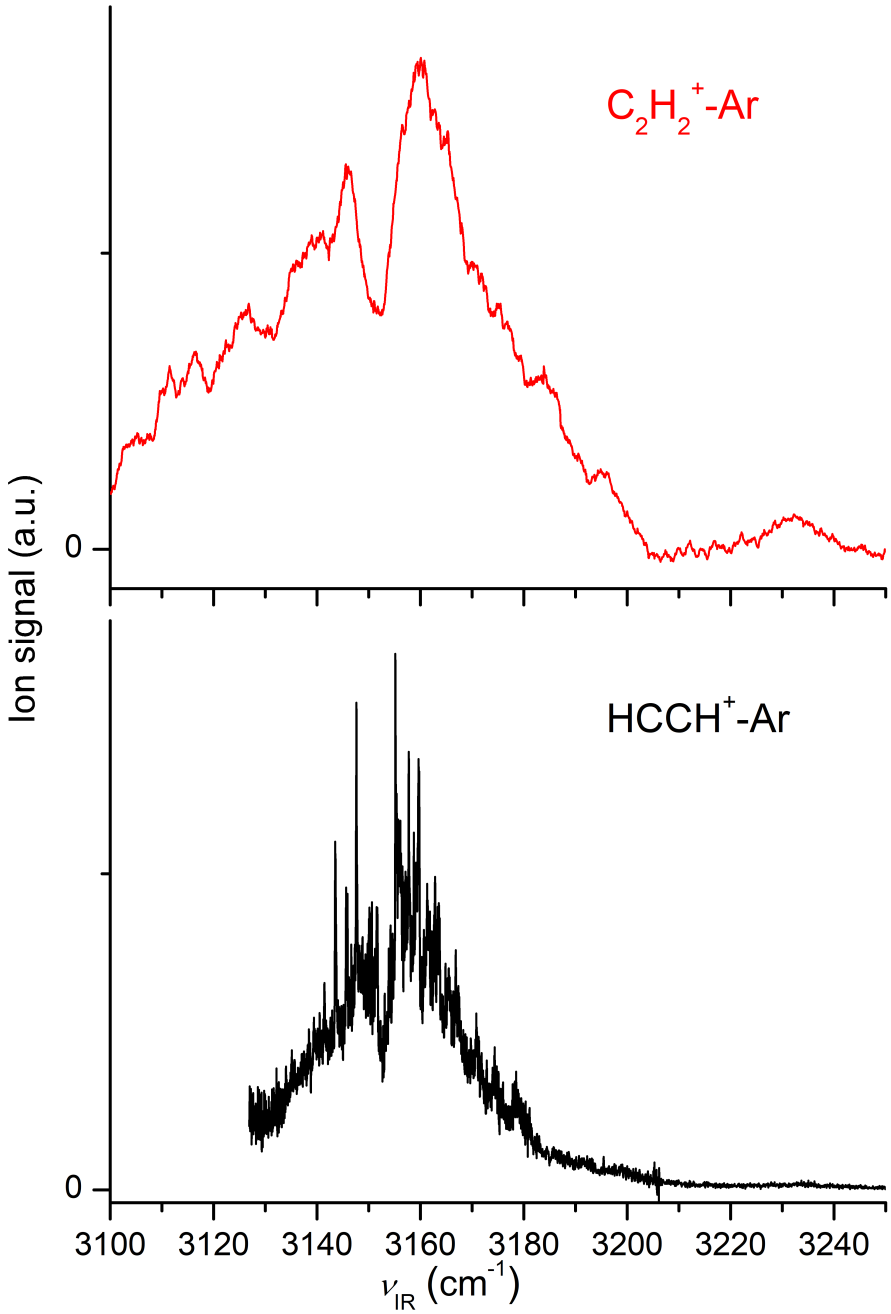

$C_2H_2^+$-Ar
HCCH$^+$-Ar
Ion signal (a.u.)
0
0
3100
3120
3140
3160
3180
3200
3220
3240
ν_{IR} (cm^{-1})

Figure S9

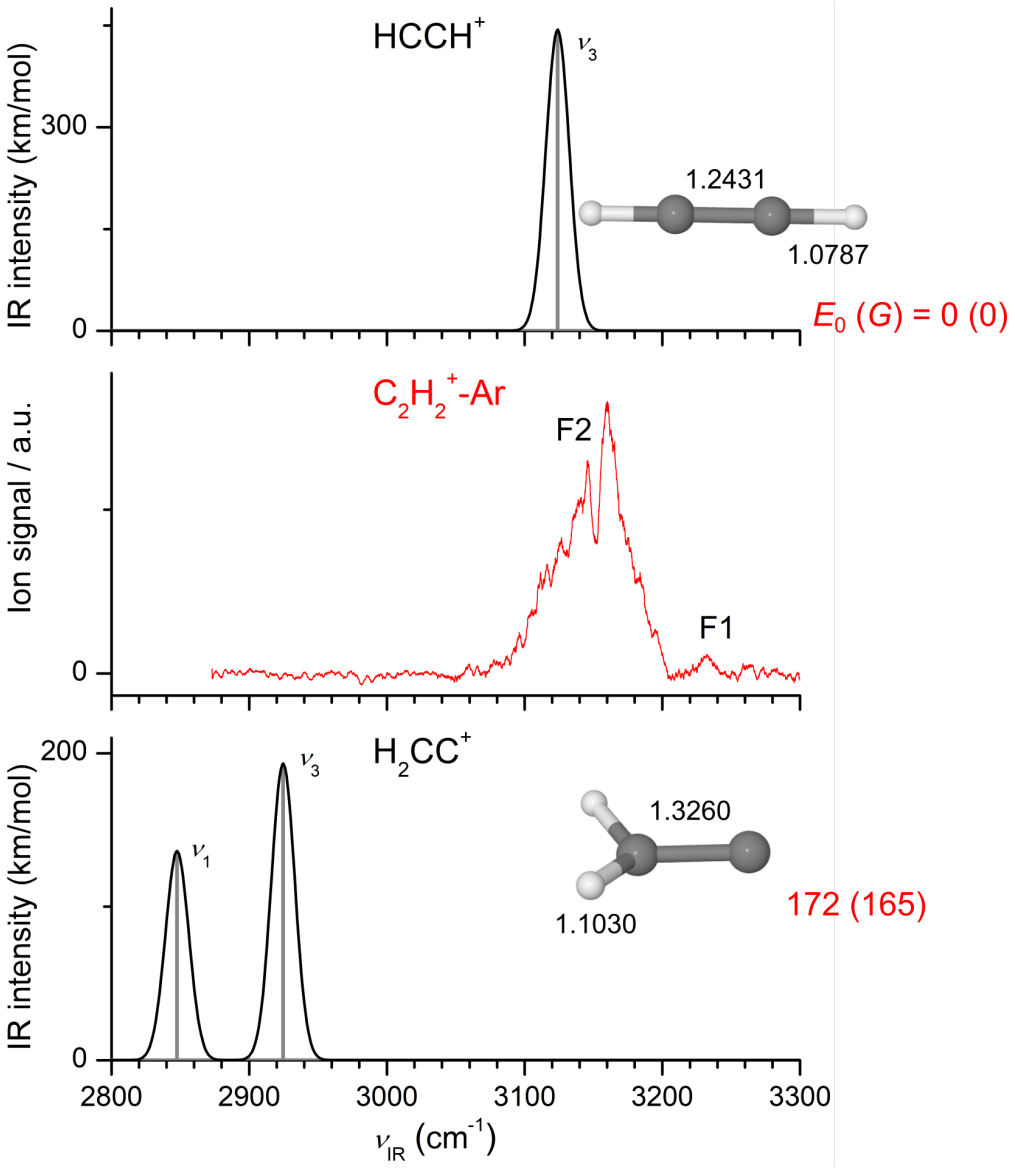

HCCH+
ν3
1.2431
1.0787
E0 (G) = 0 (0)
IR intensity (km/mol)
300
0
C2H2+-Ar
F2
F1
Ion signal / a.u.
0
H2CC+
ν3
ν1
1.3260
1.1030
172 (165)
IR intensity (km/mol)
200
0
2800
2900
3000
3100
3200
3300
νIR (cm-1)

Figure S10

Cartesian coordinates (in Å) and energies (in Hartree) of all relevant structures

Pym

C	0.00000000	0.00000000	-1.30772900
N	0.00000000	1.19231900	-0.71242700
C	0.00000000	1.18110000	0.62104800
C	0.00000000	0.00000000	1.34975300
C	0.00000000	-1.18110000	0.62104800
N	0.00000000	-1.19231900	-0.71242700
H	0.00000000	2.14598500	1.11524000
H	0.00000000	0.00000000	-2.39140000
H	0.00000000	0.00000000	2.43018300
H	0.00000000	-2.14598500	1.11524000

Sum of electronic and zero-point Energies= -264.346942
Sum of electronic and thermal Energies= -264.342759
Sum of electronic and thermal Enthalpies= -264.341815
Sum of electronic and thermal Free Energies= -264.373636

Pym^+

C	0.00000000	0.00000000	-1.40594500
N	0.00000000	1.10782800	-0.68421600
C	0.00000000	1.17085500	0.62987800
C	0.00000000	0.00000000	1.38592700
C	0.00000000	-1.17085500	0.62987800
N	0.00000000	-1.10782800	-0.68421600
H	0.00000000	2.15895100	1.08022100
H	0.00000000	0.00000000	-2.48547800
H	0.00000000	0.00000000	2.46563000
H	0.00000000	-2.15895100	1.08022100

Sum of electronic and zero-point Energies= -264.011742
Sum of electronic and thermal Energies= -264.007432
Sum of electronic and thermal Enthalpies= -264.006487
Sum of electronic and thermal Free Energies= -264.039106

Pym^+-$N_2(\pi)$

C	-0.90100800	-1.33380000	0.00000000
N	-0.90618300	-0.61305700	1.10770000
C	-0.90618300	0.70018400	1.17033300
C	-0.90579400	1.45594000	0.00000000
C	-0.90618300	0.70018400	-1.17033300
N	-0.90618300	-0.61305700	-1.10770000
H	-0.90639600	1.15089600	2.15805700
H	-0.89694100	-2.41305100	0.00000000
H	-0.90479300	2.53552600	0.00000000
H	-0.90639600	1.15089600	-2.15805700
N	2.17039100	-0.19439900	0.00000000

N	3.26048200	-0.23081800	0.00000000

Sum of electronic and zero-point Energies= -373.580705
Sum of electronic and thermal Energies= -373.572380
Sum of electronic and thermal Enthalpies= -373.571436
Sum of electronic and thermal Free Energies= -373.616862

Pym^+-N_2(C4)

C	2.01550200	1.21628700	0.00000000
N	0.69639500	1.12232300	0.00000000
C	0.00000000	0.00714500	0.00000000
C	0.65931600	-1.22162000	0.00000000
C	2.04953600	-1.12922500	0.00000000
N	2.63614900	0.04909800	0.00000000
H	-1.08416200	0.09013600	0.00000000
H	2.53794300	2.16088300	0.00000000
H	0.13471700	-2.16521400	0.00000000
H	2.69325100	-2.00361100	0.00000000
N	-3.45169400	0.02357100	0.00000000
N	-4.54197500	0.04533500	0.00000000

Sum of electronic and zero-point Energies= -373.580324
Sum of electronic and thermal Energies= -373.571923
Sum of electronic and thermal Enthalpies= -373.570978
Sum of electronic and thermal Free Energies= -373.618129

Pym^+-N_2(C2)

C	0.00000000	0.00000000	0.05983900
N	0.00000000	1.10728900	-0.66488000
C	0.00000000	1.17027100	-1.97887000
C	0.00000000	0.00000000	-2.73537900
C	0.00000000	-1.17027100	-1.97887000
N	0.00000000	-1.10728900	-0.66488000
H	0.00000000	2.15837000	-2.42896900
H	0.00000000	0.00000000	1.14058300
H	0.00000000	0.00000000	-3.81502400
H	0.00000000	-2.15837000	-2.42896900
N	0.00000000	0.00000000	3.50051500
N	0.00000000	0.00000000	4.59096700

Sum of electronic and zero-point Energies= -373.580283
Sum of electronic and thermal Energies= -373.571892
Sum of electronic and thermal Enthalpies= -373.570948
Sum of electronic and thermal Free Energies= -373.617368

Pym^+-N_2(C5)

C	0.00000000	0.00000000	-2.77110100
N	0.00000000	1.10784300	-2.04945600
C	0.00000000	1.16983900	-0.73530000
C	0.00000000	0.00000000	0.02265700
C	0.00000000	-1.16983900	-0.73530000
N	0.00000000	-1.10784300	-2.04945600
H	0.00000000	2.15773600	-0.28463500
H	0.00000000	0.00000000	-3.85053000
H	0.00000000	0.00000000	1.10281200
H	0.00000000	-2.15773600	-0.28463500
N	0.00000000	0.00000000	3.54925200
N	0.00000000	0.00000000	4.63983800

Sum of electronic and zero-point Energies= -373.579895
Sum of electronic and thermal Energies= -373.571433
Sum of electronic and thermal Enthalpies= -373.570489
Sum of electronic and thermal Free Energies= -373.617943

Pym^+-$(N_2)_2$(π/π)

C	0.00000000	0.00000000	-1.28565900
N	0.00000000	1.10757300	-0.56585200
C	0.00000000	1.16983000	0.74656400
C	0.00000000	0.00000000	1.50205400
C	0.00000000	-1.16983000	0.74656400
N	0.00000000	-1.10757300	-0.56585200
H	0.00000000	2.15722700	1.19758400
H	0.00000000	0.00000000	-2.36466900
H	0.00000000	0.00000000	2.58154000
H	0.00000000	-2.15722700	1.19758400
N	-3.08320400	0.00000000	-0.15583600
N	-4.17309800	0.00000000	-0.19753900
N	3.08320400	0.00000000	-0.15583600
N	4.17309800	0.00000000	-0.19753900

Sum of electronic and zero-point Energies= -483.149615
Sum of electronic and thermal Energies= -483.137213
Sum of electronic and thermal Enthalpies= -483.136269
Sum of electronic and thermal Free Energies= -483.193360

Pym^+-$(N_2)_2$(C4/π)

C	1.50940800	-0.99908800	-1.24966500
N	2.10143800	-1.26943600	-0.09971600
C	1.52294400	-1.24472700	1.08140000
C	0.17398300	-0.91796400	1.19601800
C	-0.45562200	-0.63723000	-0.01545500
N	0.22812300	-0.69495100	-1.13596400
H	2.14008200	-1.48699500	1.94104900

H	2.02474600	-1.02771400	-2.19742400
H	-0.34225200	-0.88397000	2.14348400
H	-1.50658000	-0.36722300	-0.08034900
N	1.69439900	2.00580800	0.04777300
N	1.96478800	3.05953900	0.12613200
N	-3.81003500	0.21365300	-0.02009800
N	-4.86732500	0.47966500	-0.04392200

Sum of electronic and zero-point Energies= -483.149252
Sum of electronic and thermal Energies= -483.136796
Sum of electronic and thermal Enthalpies= -483.135852
Sum of electronic and thermal Free Energies= -483.195467

Pym^{+}-$(N_2)_2$(C4/C6)

C	0.00000000	0.00000000	2.42238500
N	0.00000000	1.10895100	1.70236500
C	0.00000000	1.17256100	0.38844000
C	0.00000000	0.00000000	-0.36544600
C	0.00000000	-1.17256100	0.38844000
N	0.00000000	-1.10895100	1.70236500
H	0.00000000	2.15983000	-0.06660500
H	0.00000000	0.00000000	3.50176000
H	0.00000000	0.00000000	-1.44498700
H	0.00000000	-2.15983000	-0.06660500
N	0.00000000	4.20917800	-1.27399800
N	0.00000000	5.17504300	-1.78025900
N	0.00000000	-4.20917800	-1.27399800
N	0.00000000	-5.17504300	-1.78025900

Sum of electronic and zero-point Energies= -483.148807
Sum of electronic and thermal Energies= -483.136287
Sum of electronic and thermal Enthalpies= -483.135343
Sum of electronic and thermal Free Energies= -483.195944

H_2CCCNH^{+}

C	0.00000000	0.00000000	-1.91173500
H	0.00000000	0.93066400	-2.47935200
H	0.00000000	-0.93066400	-2.47935200
C	0.00000000	0.00000000	-0.61405600
C	0.00000000	0.00000000	0.70102300
N	0.00000000	0.00000000	1.86261100
H	0.00000000	0.00000000	2.86904100

Sum of electronic and zero-point Energies= -170.490874
Sum of electronic and thermal Energies= -170.485072
Sum of electronic and thermal Enthalpies= -170.484128
Sum of electronic and thermal Free Energies= -170.518278

$HCCHNCH^+$(t)

C	-0.24240000	-1.68886700	0.00000000
H	-0.18050200	-2.76436100	0.00000000
C	0.54466300	-0.64107700	0.00000000
H	-0.80365400	2.70269100	0.00000000
N	0.00000000	0.64058000	0.00000000
C	-0.41024400	1.70166000	0.00000000
H	1.63204100	-0.65268800	0.00000000

Sum of electronic and zero-point Energies= -170.451925
Sum of electronic and thermal Energies= -170.447492
Sum of electronic and thermal Enthalpies= -170.446548
Sum of electronic and thermal Free Energies= -170.478425

$HCCHNCH^+$(c)

C	-0.07875800	-1.73047800	0.00000000
H	-1.07618500	-2.13567800	0.00000000
C	0.62728400	-0.62848400	0.00000000
H	-0.96498900	2.61480800	0.00000000
N	0.00000000	0.62221700	0.00000000
C	-0.49332100	1.64808700	0.00000000
H	1.70994900	-0.56940100	0.00000000

Sum of electronic and zero-point Energies= -170.450228
Sum of electronic and thermal Energies= -170.445764
Sum of electronic and thermal Enthalpies= -170.444819
Sum of electronic and thermal Free Energies= -170.476833

H_2CCHCN^+

C	0.14300100	-1.64028300	0.00000000
H	-0.34986800	-2.60580300	0.00000000
H	1.22687800	-1.60714500	0.00000000
C	-0.61700400	-0.46832400	0.00000000
C	0.00000000	0.77059500	0.00000000
H	-1.70306000	-0.49797900	0.00000000
N	0.52429500	1.81985700	0.00000000

Sum of electronic and zero-point Energies= -170.462614
Sum of electronic and thermal Energies= -170.458146
Sum of electronic and thermal Enthalpies= -170.457202
Sum of electronic and thermal Free Energies= -170.489448

$HCCCHNH^+$(b)

C	0.16566600	-1.18924700	0.00000000
C	0.16566600	-0.05570400	0.84792800
C	0.16566600	-0.05570400	-0.84792800
N	-0.56738900	0.78773400	0.00000000
H	-0.54957800	1.80721700	0.00000000

H	0.76965600	0.24128900	-1.69962000
H	0.76965600	0.24128900	1.69962000

Sum of electronic and zero-point Energies= -170.377169
Sum of electronic and thermal Energies= -170.373473
Sum of electronic and thermal Enthalpies= -170.372528
Sum of electronic and thermal Free Energies= -170.402959

HCCCHNH$^+$(c)

C	0.53786700	1.76206100	0.00000000
H	0.99710900	2.72759500	0.00000000
C	0.00000000	0.68508000	0.00000000
C	-0.63714200	-0.56423500	0.00000000
N	0.04895800	-1.62017300	0.00000000
H	-1.72761000	-0.65708500	0.00000000
H	0.98344600	-2.02673800	0.00000000

Sum of electronic and zero-point Energies= -170.439713
Sum of electronic and thermal Energies= -170.434604
Sum of electronic and thermal Enthalpies= -170.433660
Sum of electronic and thermal Free Energies= -170.467118

HCCCHNH$^+$(t)

C	-0.30148400	1.88446200	0.00000000
H	-0.58791100	2.91427700	0.00000000
C	0.00000000	0.72037000	0.00000000
C	0.45135600	-0.59538200	0.00000000
N	-0.23456000	-1.64738800	0.00000000
H	1.54562100	-0.77430900	0.00000000
H	-0.21501900	-2.66495600	0.00000000

Sum of electronic and zero-point Energies= -170.440624
Sum of electronic and thermal Energies= -170.435497
Sum of electronic and thermal Enthalpies= -170.434552
Sum of electronic and thermal Free Energies= -170.467886

HCCHCNH$^+$(r)

C	-0.97644500	-0.65513400	0.01364100
C	-0.96453700	0.66881600	0.00213300
C	0.27178400	-0.00768200	0.02982000
N	1.53071000	-0.03209400	-0.11719400
H	2.26057600	0.16424200	0.56391400
H	-1.49679200	-1.60251200	0.01383000
H	-1.46356800	1.62693000	-0.03094800

Sum of electronic and zero-point Energies= -170.459410
Sum of electronic and thermal Energies= -170.454975

Sum of electronic and thermal Enthalpies= -170.454031
Sum of electronic and thermal Free Energies= -170.486045

H_2CCNCH^+

C	0.01564800	-1.83550700	0.00000000
H	-0.91125500	-2.40496400	0.00000000
H	0.95705700	-2.38095300	0.00000000
C	0.07327200	1.88538900	0.00000000
H	-0.40462000	2.85326200	0.00000000
C	0.00000000	-0.54219900	0.00000000
N	-0.02495800	0.69808000	0.00000000

Sum of electronic and zero-point Energies= -170.465350
Sum of electronic and thermal Energies= -170.460371
Sum of electronic and thermal Enthalpies= -170.459427
Sum of electronic and thermal Free Energies= -170.491770

H_2CNCCH^+

C	0.00000000	0.00000000	1.77547400
H	0.00000000	0.94536900	2.31893000
H	0.00000000	-0.94536900	2.31893000
C	0.00000000	0.00000000	-0.71127000
N	0.00000000	0.00000000	0.52492600
C	0.00000000	0.00000000	-1.94679200
H	0.00000000	0.00000000	-3.01681400

Sum of electronic and zero-point Energies= -170.467617
Sum of electronic and thermal Energies= -170.462529
Sum of electronic and thermal Enthalpies= -170.461585
Sum of electronic and thermal Free Energies= -170.493787

$CCHCNH_2^+$

C	0.03300200	-1.26444900	0.00000000
C	1.16314100	-0.57771700	0.00000000
C	0.00000000	0.16339600	0.00000000
N	-0.67576300	1.26061300	0.00000000
H	-0.20160300	2.15618500	0.00000000
H	-0.55717000	-2.16858200	0.00000000
H	-1.68774700	1.26072800	0.00000000

Sum of electronic and zero-point Energies= -170.451583
Sum of electronic and thermal Energies= -170.447668
Sum of electronic and thermal Enthalpies= -170.446724
Sum of electronic and thermal Free Energies= -170.477680

$HCCHCNH^+$(c)

C	0.02210600	-1.76010700	0.00000000
H	-0.98225500	-2.15410000	0.00000000
C	0.70043800	-0.62934600	0.00000000
H	-1.08758700	2.44900700	0.00000000
H	1.78743900	-0.57392600	0.00000000
C	0.00000000	0.59368000	0.00000000
N	-0.57898000	1.57909300	0.00000000

Sum of electronic and zero-point Energies= -170.470767
Sum of electronic and thermal Energies= -170.466167
Sum of electronic and thermal Enthalpies= -170.465222
Sum of electronic and thermal Free Energies= -170.497509

$HCCHCNH^+$(t)

C	-0.17330900	-1.73334500	0.00000000
H	-0.08348000	-2.80897300	0.00000000
C	0.59531600	-0.66159700	0.00000000
H	-0.88303400	2.57440000	0.00000000
H	1.68701300	-0.68658100	0.00000000
N	-0.46464800	1.65762500	0.00000000
C	0.00000000	0.61457100	0.00000000

Sum of electronic and zero-point Energies= -170.472100
Sum of electronic and thermal Energies= -170.467496
Sum of electronic and thermal Enthalpies= -170.466552
Sum of electronic and thermal Free Energies= -170.498764

H_2CCCNH^+-Ar

C	0.00000000	0.00000000	-3.92249400
H	0.00000000	0.93038500	-4.49018400
H	0.00000000	-0.93038500	-4.49018400
C	0.00000000	0.00000000	-2.62504500
C	0.00000000	0.00000000	-1.30916800
N	0.00000000	0.00000000	-0.14773800
H	0.00000000	0.00000000	0.86782600
Ar	0.00000000	0.00000000	3.12705200

Sum of electronic and zero-point Energies= -698.055105
Sum of electronic and thermal Energies= -698.047344
Sum of electronic and thermal Enthalpies= -698.046400
Sum of electronic and thermal Free Energies= -698.088527

$HCCHNCH^+$(t)-Ar(H)

C	2.33510800	2.81879600	0.00000000
H	3.06768600	3.60846400	0.00000000
C	1.03431900	2.66204800	0.00000000
H	-0.45394200	-0.62773800	0.00000000
N	0.48386200	1.38278700	0.00000000
C	0.00000000	0.35282300	0.00000000
H	0.29179000	3.45639400	0.00000000
Ar	-1.47273000	-2.83992400	0.00000000

Sum of electronic and zero-point Energies= -698.015629
Sum of electronic and thermal Energies= -698.008724
Sum of electronic and thermal Enthalpies= -698.007780
Sum of electronic and thermal Free Energies= -698.049488

$HCCHNCH^+$(c)-Ar(H)

C	2.40217800	2.79403500	0.00000000
H	3.33577400	2.25807000	0.00000000
C	1.09971200	2.66792200	0.00000000
H	-0.47195800	-0.59133200	0.00000000
N	0.50284800	1.40237700	0.00000000
C	0.00000000	0.38078700	0.00000000
H	0.38526700	3.48338300	0.00000000
Ar	-1.54335400	-2.77906800	0.00000000

Sum of electronic and zero-point Energies= -698.013944
Sum of electronic and thermal Energies= -698.007007
Sum of electronic and thermal Enthalpies= -698.006063
Sum of electronic and thermal Free Energies= -698.047927

$HCCHNCH^+$(c)-Ar(π)

C	-2.08459600	-0.42671300	0.00000000
H	-2.00384200	0.64663000	0.00000000
C	-1.39799300	-1.54129500	0.00000000
H	2.21194900	-1.44108300	0.00000000
N	0.00000000	-1.51067400	0.00000000
C	1.13749300	-1.47702800	0.00000000
H	-1.81260200	-2.54283000	0.00000000
Ar	0.87083700	1.92123400	0.00000000

Sum of electronic and zero-point Energies= -698.012920
Sum of electronic and thermal Energies= -698.005853
Sum of electronic and thermal Enthalpies= -698.004909
Sum of electronic and thermal Free Energies= -698.048315

H_2CCHCN^+-Ar(π)

C	-2.59776800	-0.87092200	-0.36509900
H	-3.37610700	-1.53566600	-0.00913800
H	-2.37588500	-0.85011700	-1.42596000
C	-1.90425400	-0.06513300	0.53376400
C	-0.90659300	0.78446500	0.09040800
H	-2.12674500	-0.07860100	1.59666500
N	-0.07891200	1.52489100	-0.29019700
Ar	2.27126700	-0.40557300	0.01752100

Sum of electronic and zero-point Energies= -698.025087
Sum of electronic and thermal Energies= -698.018218
Sum of electronic and thermal Enthalpies= -698.017274
Sum of electronic and thermal Free Energies= -698.059143

$HCCCHNH^+$(b)-Ar

C	0.37963600	-2.83573100	0.00000000
C	0.37963600	-1.69688300	0.84591900
C	0.37963600	-1.69688300	-0.84591900
N	-0.35064500	-0.85458600	0.00000000
H	-0.35960200	0.16875100	0.00000000
H	0.98504600	-1.39874500	-1.69599600
H	0.98504600	-1.39874500	1.69599600
Ar	-0.33274600	2.55487900	0.00000000

Sum of electronic and zero-point Energies= -697.941334
Sum of electronic and thermal Energies= -697.935199
Sum of electronic and thermal Enthalpies= -697.934254
Sum of electronic and thermal Free Energies= -697.974606

$HCCCHNH^+$(c)-Ar

C	-1.30904300	-2.70670800	0.00000000
H	-1.09191000	-3.75311700	0.00000000
C	-1.57118800	-1.53270800	0.00000000
C	-1.90123400	-0.16881300	0.00000000
N	-1.00332600	0.71141000	0.00000000
H	-2.94459200	0.16421600	0.00000000
H	0.00000000	0.93522300	0.00000000
Ar	2.20825400	1.34017700	0.00000000

Sum of electronic and zero-point Energies= -698.004511
Sum of electronic and thermal Energies= -697.997334
Sum of electronic and thermal Enthalpies= -697.996389
Sum of electronic and thermal Free Energies= -698.038633

$HCCCHNH^+$(t)-Ar

C	-1.94068800	3.28267300	0.00000000
H	-2.28437300	4.29442100	0.00000000
C	-1.53582100	2.15090800	0.00000000
C	-1.16310300	0.80830800	0.00000000
N	0.00000000	0.33769400	0.00000000
H	-1.96216900	0.04123200	0.00000000
H	0.58307100	-0.50764800	0.00000000
Ar	1.75006400	-2.42462200	0.00000000

Sum of electronic and zero-point Energies= -698.005473
Sum of electronic and thermal Energies= -697.998214
Sum of electronic and thermal Enthalpies= -697.997269
Sum of electronic and thermal Free Energies= -698.039351

$HCCHCNH^+$(r)-Ar

C	-2.77075800	-0.38053700	0.49250400
C	-2.57941900	0.81154700	-0.04811100
C	-1.53926700	-0.13787500	-0.14572700
N	-0.45898900	-0.55414000	-0.65292000
H	0.50981200	-0.36022900	-0.39349400
H	-3.37520900	-1.09371200	1.03458200
H	-2.91105800	1.80845700	-0.30070800
Ar	2.79589100	0.09809200	0.13544800

Sum of electronic and zero-point Energies= -698.022898
Sum of electronic and thermal Energies= -698.016142
Sum of electronic and thermal Enthalpies= -698.015198
Sum of electronic and thermal Free Energies= -698.056951

H_2CCNCH^+-Ar

C	3.65342600	1.34059400	0.00000000
H	4.40098900	0.55042900	0.00000000
H	3.99511700	2.37346900	0.00000000
C	0.00000000	0.63217000	0.00000000
H	-0.87248100	-0.00825600	0.00000000
C	2.39053300	1.06043600	0.00000000
N	1.17943000	0.78500100	0.00000000
Ar	-2.89129900	-1.47832400	0.00000000

Sum of electronic and zero-point Energies= -698.028437
Sum of electronic and thermal Energies= -698.020959
Sum of electronic and thermal Enthalpies= -698.020015
Sum of electronic and thermal Free Energies= -698.062652

H_2CNCCH^+-Ar

C	0.00000000	0.00000000	-3.96621000
H	0.00000000	0.94522300	-4.50966300
H	0.00000000	-0.94522300	-4.50966300
C	0.00000000	0.00000000	-1.47950000
N	0.00000000	0.00000000	-2.71564600
C	0.00000000	0.00000000	-0.24350000
H	0.00000000	0.00000000	0.82871500
Ar	0.00000000	0.00000000	3.40752200

Sum of electronic and zero-point Energies= -698.029994
Sum of electronic and thermal Energies= -698.022376
Sum of electronic and thermal Enthalpies= -698.021432
Sum of electronic and thermal Free Energies= -698.064026

$CCHCNH_2^+$-Ar

C	-2.56470400	-1.28557500	0.00000000
C	-1.32934500	-1.75647500	0.00000000
C	-1.45689700	-0.38265000	0.00000000
N	-1.00211900	0.82168400	0.00000000
H	0.00000000	0.98848700	0.00000000
H	-3.64063300	-1.37398900	0.00000000
H	-1.62081600	1.62219500	0.00000000
Ar	2.46566400	0.75331800	0.00000000

Sum of electronic and zero-point Energies= -698.015080
Sum of electronic and thermal Energies= -698.008684
Sum of electronic and thermal Enthalpies= -698.007740
Sum of electronic and thermal Free Energies= -698.049438

$HCCHCNH^+$(c)-Ar

C	2.71181700	2.36423600	0.00000000
H	3.51565400	1.64487300	0.00000000
C	1.39712300	2.45739700	0.00000000
H	-0.55417400	-0.53327700	0.00000000
H	0.85726900	3.40222600	0.00000000
C	0.61974200	1.27990800	0.00000000
N	0.00000000	0.31998100	0.00000000
Ar	-1.78838000	-2.40905200	0.00000000

Sum of electronic and zero-point Energies= -698.035700
Sum of electronic and thermal Energies= -698.028817
Sum of electronic and thermal Enthalpies= -698.027873
Sum of electronic and thermal Free Energies= -698.069012

$HCCHCNH^+$(t)-Ar

C	2.72910600	2.32770700	0.00000000
H	3.59333400	2.97403000	0.00000000
C	1.41365600	2.41284100	0.00000000
H	-0.56455500	-0.55736000	0.00000000
H	0.85914300	3.35332300	0.00000000
N	0.00000000	0.28914400	0.00000000
C	0.64185500	1.23319600	0.00000000
Ar	-1.81086800	-2.42424800	0.00000000

Sum of electronic and zero-point Energies= -698.037026
Sum of electronic and thermal Energies= -698.030138
Sum of electronic and thermal Enthalpies= -698.029194
Sum of electronic and thermal Free Energies= -698.070255

H_2CCCNH^+-N_2

C	0.00000000	0.00000000	-3.67441400
H	0.00000000	0.93010700	-4.24225200
H	0.00000000	-0.93010700	-4.24225200
C	0.00000000	0.00000000	-2.37713100
C	0.00000000	0.00000000	-1.06058000
N	0.00000000	0.00000000	0.10110000
H	0.00000000	0.00000000	1.12957800
N	0.00000000	0.00000000	2.97811000
N	0.00000000	0.00000000	4.06760000

Sum of electronic and zero-point Energies= -280.064767
Sum of electronic and thermal Energies= -280.056152
Sum of electronic and thermal Enthalpies= -280.055208
Sum of electronic and thermal Free Energies= -280.098113

$HCCHNCH^+$(t)-N_2

C	3.38515400	-0.46746700	0.00000000
H	4.45698000	-0.57344000	0.00000000
C	2.30811100	-1.21316100	0.00000000
H	-0.99728200	0.25873700	0.00000000
N	1.04653100	-0.62329200	0.00000000
C	0.00000000	-0.17509800	0.00000000
H	2.28171300	-2.30012500	0.00000000
N	-2.87374000	1.07594900	0.00000000
N	-3.87293400	1.51151200	0.00000000

Sum of electronic and zero-point Energies= -280.023768
Sum of electronic and thermal Energies= -280.015747
Sum of electronic and thermal Enthalpies= -280.014803
Sum of electronic and thermal Free Energies= -280.057757

$HCCHNCH^{+}$(c)-N_2

C	-3.36667300	-0.72258700	0.00000000
H	-3.79990900	0.26280300	0.00000000
C	-2.24244000	-1.39191600	0.00000000
H	0.96321400	0.30246600	0.00000000
N	-1.01135200	-0.72692300	0.00000000
C	0.00000000	-0.20270300	0.00000000
H	-2.15112200	-2.47213800	0.00000000
N	2.78111700	1.24363400	0.00000000
N	3.75059100	1.74187500	0.00000000

Sum of electronic and zero-point Energies= -280.022072
Sum of electronic and thermal Energies= -280.014022
Sum of electronic and thermal Enthalpies= -280.013077
Sum of electronic and thermal Free Energies= -280.056168

H_2CCHCN^{+}-N_2

C	-2.16123900	0.10311800	0.00000000
H	-2.35916100	1.16875400	0.00000000
H	-3.00022000	-0.58367000	0.00000000
C	-0.84245100	-0.35896900	0.00000000
C	-0.57623300	-1.71745900	0.00000000
H	0.00000000	0.33117000	0.00000000
N	-0.34709600	-2.86721600	0.00000000
N	2.50837300	2.56419700	0.00000000
N	1.67285500	1.86353300	0.00000000

Sum of electronic and zero-point Energies= -280.032519
Sum of electronic and thermal Energies= -280.024142
Sum of electronic and thermal Enthalpies= -280.023198
Sum of electronic and thermal Free Energies= -280.068770

$HCCCHNH^{+}$(b)-N_2

C	0.50550600	-2.63610700	0.00000000
C	0.50550600	-1.49112300	0.84469500
C	0.50550600	-1.49112300	-0.84469500
N	-0.21679700	-0.64820300	0.00000000
H	-0.29706900	0.37764400	0.00000000
H	1.11190400	-1.19508900	-1.69473600
H	1.11190400	-1.19508900	1.69473600
N	-0.57612500	2.34054800	0.00000000
N	-0.78220000	3.41089100	0.00000000

Sum of electronic and zero-point Energies= -279.949762
Sum of electronic and thermal Energies= -279.942526

Sum of electronic and thermal Enthalpies= -279.941582
Sum of electronic and thermal Free Energies= -279.983058

$HCCCHNH^{+}(c)\text{-}N_2$

C	0.62398400	-2.88244600	0.00000000
H	0.23349000	-3.87686600	0.00000000
C	1.07514800	-1.76809300	0.00000000
C	1.63833200	-0.48184300	0.00000000
N	0.92634800	0.55215500	0.00000000
H	2.72656000	-0.34837500	0.00000000
H	0.00000000	1.02540500	0.00000000
N	-1.62703300	1.89052400	0.00000000
N	-2.58286200	2.41362600	0.00000000

Sum of electronic and zero-point Energies= -280.014278
Sum of electronic and thermal Energies= -280.006195
Sum of electronic and thermal Enthalpies= -280.005251
Sum of electronic and thermal Free Energies= -280.048580

$HCCCHNH^{+}(t)\text{-}N_2$

C	-2.99556400	-1.94441300	0.00000000
H	-3.73114200	-2.71905100	0.00000000
C	-2.15584800	-1.08488400	0.00000000
C	-1.25141800	-0.02168800	0.00000000
N	0.00000000	-0.09480700	0.00000000
H	-1.65283600	1.00952300	0.00000000
H	0.92308100	0.38219800	0.00000000
N	2.57194800	1.21319300	0.00000000
N	3.55346300	1.68636200	0.00000000

Sum of electronic and zero-point Energies= -280.015186
Sum of electronic and thermal Energies= -280.007007
Sum of electronic and thermal Enthalpies= -280.006063
Sum of electronic and thermal Free Energies= -280.049202

$HCCHCNH^{+}(r)\text{-}N_2$

C	-2.57589500	-0.47971600	0.40626200
C	-2.42691800	0.78442900	0.05403400
C	-1.33182900	-0.09157100	-0.13727100
N	-0.21651300	-0.37487700	-0.64312500
H	0.75682100	-0.21502900	-0.35323300
H	-3.16180900	-1.29230600	0.81097200
H	-2.79920200	1.79176600	-0.06373200
N	2.66120600	0.02071600	0.05923200
N	3.72845600	0.13083500	0.25072800

Sum of electronic and zero-point Energies= -280.031293
Sum of electronic and thermal Energies= -280.023490
Sum of electronic and thermal Enthalpies= -280.022546
Sum of electronic and thermal Free Energies= -280.065672

H_2CCNCH^+-N_2

C	-3.65279000	0.26682200	0.00000000
H	-4.04883900	1.27988000	0.00000000
H	-4.35913100	-0.56062500	0.00000000
C	0.00000000	-0.44608700	0.00000000
H	1.07022600	-0.25709100	0.00000000
C	-2.37694900	0.05080500	0.00000000
N	-1.14955400	-0.15679400	0.00000000
N	3.14253600	0.03046000	0.00000000
N	4.22361400	0.17042000	0.00000000

Sum of electronic and zero-point Energies= -280.036197
Sum of electronic and thermal Energies= -280.027452
Sum of electronic and thermal Enthalpies= -280.026508
Sum of electronic and thermal Free Energies= -280.070830

H_2CNCCH^+-N_2

C	0.00000000	0.00000000	-3.69738900
H	0.00000000	0.94504800	-4.24088500
H	0.00000000	-0.94504800	-4.24088500
C	0.00000000	0.00000000	-1.21067300
N	0.00000000	0.00000000	-2.44678500
C	0.00000000	0.00000000	0.02602500
H	0.00000000	0.00000000	1.10176500
N	0.00000000	0.00000000	3.29773300
N	0.00000000	0.00000000	4.38794100

Sum of electronic and zero-point Energies= -280.036887
Sum of electronic and thermal Energies= -280.028049
Sum of electronic and thermal Enthalpies= -280.027104
Sum of electronic and thermal Free Energies= -280.071279

$CCHCNH_2^+$-N_2

C	-1.97610100	-1.93380600	0.00000000
C	-0.66607800	-2.10816200	0.00000000
C	-1.10506500	-0.79906200	0.00000000
N	-0.93900600	0.47641200	0.00000000
H	0.00000000	0.87647900	0.00000000
H	-3.00287600	-2.26693300	0.00000000

H	-1.72918800	1.10826700	0.00000000
N	1.91320200	1.64033100	0.00000000
N	2.91373600	2.07302400	0.00000000

Sum of electronic and zero-point Energies= -280.022864
Sum of electronic and thermal Energies= -280.015307
Sum of electronic and thermal Enthalpies= -280.014362
Sum of electronic and thermal Free Energies= -280.056912

$HCCHCNH^{+}$(c)-N_2

C	-3.34924000	0.39172200	0.00000000
H	-3.37345500	1.47003800	0.00000000
C	-2.51713800	-0.62974600	0.00000000
H	1.01521800	-0.01459600	0.00000000
H	-2.83769800	-1.66948600	0.00000000
C	-1.12485800	-0.39334300	0.00000000
N	0.00000000	-0.19218600	0.00000000
N	2.82999800	0.29271100	0.00000000
N	3.90476700	0.47122400	0.00000000

Sum of electronic and zero-point Energies= -280.045701
Sum of electronic and thermal Energies= -280.037854
Sum of electronic and thermal Enthalpies= -280.036910
Sum of electronic and thermal Free Energies= -280.079211

$HCCHCNH^{+}$(t)-N_2

C	3.23438200	0.90370200	0.00000000
H	4.25915300	1.24158500	0.00000000
C	2.55203700	-0.22354800	0.00000000
H	-1.03057200	-0.15744600	0.00000000
H	3.00830300	-1.21527100	0.00000000
N	0.00000000	-0.17556300	0.00000000
C	1.14166400	-0.18546500	0.00000000
N	-2.87001800	-0.12464600	0.00000000
N	-3.95932200	-0.10507700	0.00000000

Sum of electronic and zero-point Energies= -280.047040
Sum of electronic and thermal Energies= -280.039189
Sum of electronic and thermal Enthalpies= -280.038245
Sum of electronic and thermal Free Energies= -280.080464

$HCCH^+$

C	0.00000000	0.00000000	0.62152600
H	0.00000000	0.00000000	1.70023200
C	0.00000000	0.00000000	-0.62152600
H	0.00000000	0.00000000	-1.70023200

Sum of electronic and zero-point Energies= -76.924858
Sum of electronic and thermal Energies= -76.922081
Sum of electronic and thermal Enthalpies= -76.921137
Sum of electronic and thermal Free Energies= -76.944514

$HCCH^+$-Ar(π)

C	0.60180200	-1.71273200	0.00000000
H	1.64904300	-1.95729200	0.00000000
C	-0.59975700	-1.42277100	0.00000000
H	-1.66131100	-1.25639200	0.00000000
Ar	0.00000000	1.22370600	0.00000000

Sum of electronic and zero-point Energies= -604.495512
Sum of electronic and thermal Energies= -604.490864
Sum of electronic and thermal Enthalpies= -604.489920
Sum of electronic and thermal Free Energies= -604.523801

$HCCH^+$-Ar(H)

C	0.00000000	0.00000000	-2.92916900
H	0.00000000	0.00000000	-4.00740400
C	0.00000000	0.00000000	-1.68580800
H	0.00000000	0.00000000	-0.60158400
Ar	0.00000000	0.00000000	1.79438100

Sum of electronic and zero-point Energies= -604.489008
Sum of electronic and thermal Energies= -604.483904
Sum of electronic and thermal Enthalpies= -604.482959
Sum of electronic and thermal Free Energies= -604.516840

$HCCH^+$-N_2(π)

C	0.69585300	-1.23236200	0.00000000
H	1.72537700	-0.92817900	0.00000000
C	-0.40476900	-1.79927300	0.00000000
H	-1.37350900	-2.26560600	0.00000000
N	0.00000000	1.00279100	0.00000000
N	-0.29976800	2.05200800	0.00000000

Sum of electronic and zero-point Energies= -186.502261
Sum of electronic and thermal Energies= -186.496385
Sum of electronic and thermal Enthalpies= -186.495441
Sum of electronic and thermal Free Energies= -186.531463

$HCCH^{+}$-N_2(H)

C	0.00000000	0.00000000	-2.76469700
H	0.00000000	0.00000000	-3.84258700
C	0.00000000	0.00000000	-1.52069700
H	0.00000000	0.00000000	-0.42896600
N	0.00000000	0.00000000	1.59669200
N	0.00000000	0.00000000	2.68672400

Sum of electronic and zero-point Energies= -186.497316
Sum of electronic and thermal Energies= -186.491188
Sum of electronic and thermal Enthalpies= -186.490243
Sum of electronic and thermal Free Energies= -186.525248

H_2CC^{+}

C	-0.02551600	-0.49316800	0.00000000
H	0.15309400	-1.01890200	0.95303200
C	-0.02551600	0.83280200	0.00000000
H	0.15309400	-1.01890200	-0.95303200

Sum of electronic and zero-point Energies= -76.859328
Sum of electronic and thermal Energies= -76.856081
Sum of electronic and thermal Enthalpies= -76.855137
Sum of electronic and thermal Free Energies= -76.881625

Ar

HF=-527.5600021

N_2

N	0.00000000	0.00000000	0.54558200
N	0.00000000	0.00000000	-0.54558200

Sum of electronic and zero-point Energies= -109.565010
Sum of electronic and thermal Energies= -109.562650
Sum of electronic and thermal Enthalpies= -109.561706
Sum of electronic and thermal Free Energies= -109.583435