

## Supporting Information:

### **Interstellar Formation of Nitrogen Heteroaromatics [Indole, C<sub>8</sub>H<sub>7</sub>N; Pyrrole, C<sub>4</sub>H<sub>5</sub>N; Aniline, C<sub>6</sub>H<sub>5</sub>NH<sub>2</sub>] – Key Precursors to Amino Acids and Nucleobases**

Jia Wang,<sup>1,2</sup> Anatoliy A. Nikolayev,<sup>3</sup> Joshua H. Marks,<sup>1,2</sup> Andrew M. Turner,<sup>1,2</sup> Sankhabrata Chandra,<sup>1,2</sup> N. Fabian Kleimeier,<sup>1,2</sup> Leslie A. Young,<sup>4</sup> Alexander M. Mebel,<sup>5\*</sup> Ralf I. Kaiser<sup>1,2\*</sup>

<sup>1</sup> *W. M. Keck Research Laboratory in Astrochemistry, University of Hawaii at Manoa, Honolulu, HI 96822, United States*

<sup>2</sup> *Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, USA*

<sup>3</sup> *Samara National Research University, Samara 443086, Russia*

<sup>4</sup> *Department of Space Studies, Southwest Research Institute, Boulder, CO 80302, USA.*

<sup>5</sup> *Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, United States*

\*Corresponding Authors:

Alexander M. Mebel, [mebela@fiu.edu](mailto:mebela@fiu.edu)

Ralf I. Kaiser, [ralfk@hawaii.edu](mailto:ralfk@hawaii.edu)

## Methods and Materials

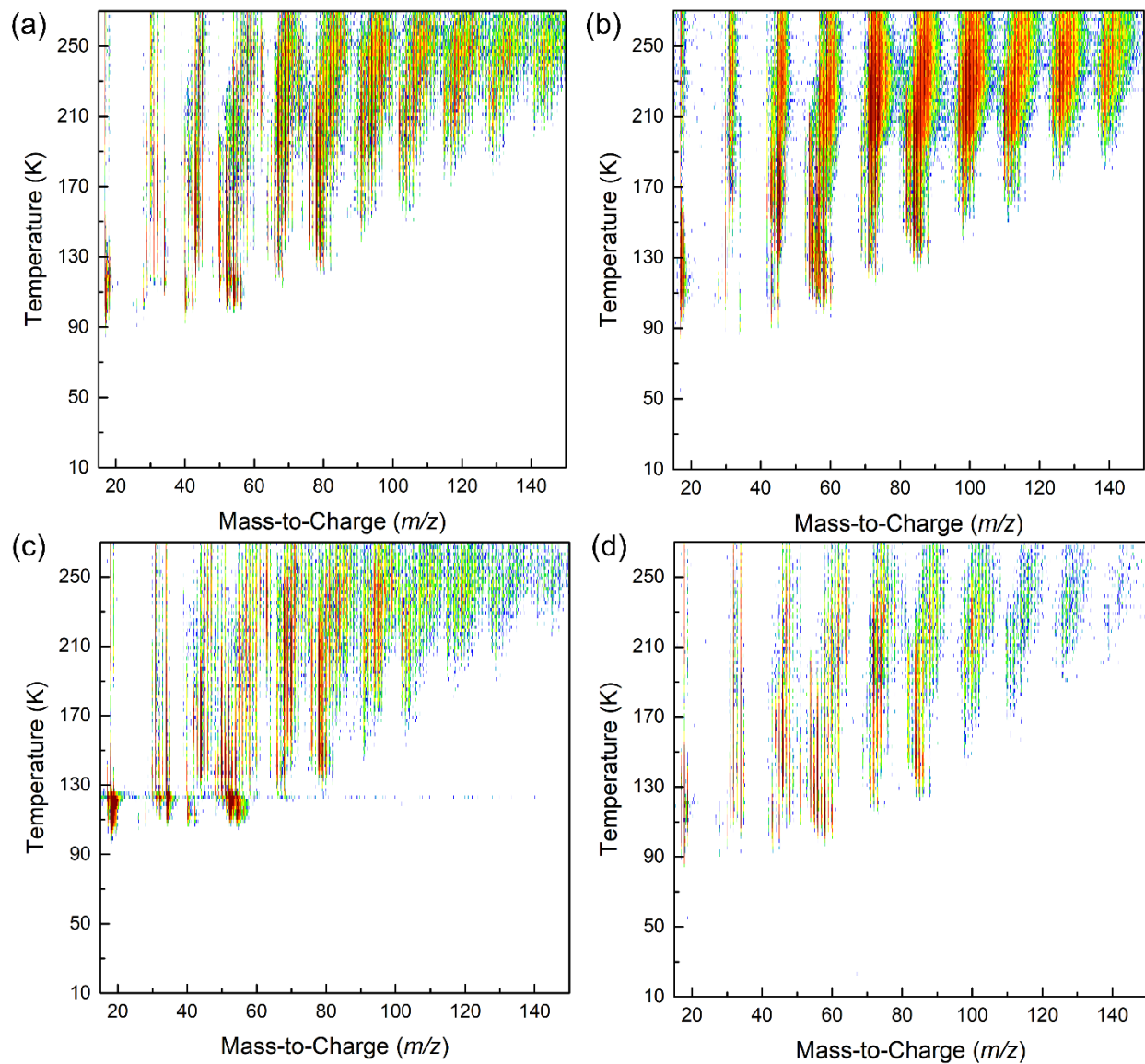
**Experimental.** The experiments were carried out in a contamination-free ultrahigh vacuum chamber operated at base pressures of a few  $10^{-11}$  Torr using magnetically suspended turbomolecular pumps (Osaka, TG1300MUCWB and TG420MCAB) backed by an oil-free scroll pump (Edwards, GVSP30).<sup>1,2</sup> A polished silver substrate was interfaced to a closed-cycle helium cryostat (Sumitomo Heavy Industries, RDK415E) that can be moved vertically via an adjustable bellows (McAllister, BLT86) and rotated horizontally via a rotatable flange (Thermionics Vacuum Products, RNN-600/FA/MCO). After cooling the substrate to  $4.6 \pm 0.1$  K, acetylene ( $\text{C}_2\text{H}_2$ ; 99.9%, Airgas) and ammonia ( $\text{NH}_3$ ; 99.999%, Matheson) were deposited onto the substrate surface through separate glass capillary arrays at partial pressures of  $1.2 \times 10^{-8}$  Torr for  $\text{C}_2\text{H}_2$  and  $0.8 \times 10^{-8}$  Torr for  $\text{NH}_3$ . A dry ice ethanol slush bath was used to remove the traces of acetone ( $\text{CH}_3\text{COCH}_3$ ) in the acetylene.<sup>3</sup> The formulae of interested ion signals were verified using isotopically substituted ice mixtures including  $^{13}\text{C}_2\text{H}_2\text{-NH}_3$  ( $^{13}\text{C}_2\text{H}_2$ ; >99  $^{13}\text{C}\%$ , Cambridge Isotope),  $\text{C}_2\text{H}_2\text{-}^{15}\text{NH}_3$  ( $^{15}\text{NH}_3$ ; >98  $^{15}\text{N}\%$ , Sigma Aldrich), and  $^{13}\text{C}_2\text{H}_2\text{-}^{15}\text{NH}_3$ . To measure the ice thickness, a photodiode recorded interference fringes between helium-neon laser (632.8 nm) reflections of the ice surface and silver substrate during the ice deposition.<sup>4</sup> The ice thickness and the acetylene-to-ammonia ratio were determined to be  $1,000 \pm 100$  nm and 1.0: ( $1.0 \pm 0.2$ ), respectively.<sup>5</sup> After deposition, each ice was then processed with energetic electrons (5 keV; SPECS EQ 22/35) at a  $70^\circ$  angle of incidence at a current of 100 nA for 60 minutes, which correspond to doses of  $5.0 \pm 0.8$  eV per  $\text{C}_2\text{H}_2$  molecule and  $3.5 \pm 0.6$  eV per  $\text{NH}_3$  molecule,<sup>5</sup> simulating the irradiation of interstellar ices by secondary electrons generated in the track of GCRs in cold molecular clouds aged around  $2 \times 10^7$  years.<sup>6</sup> The average penetration depth ( $350 \pm 30$  nm) of the energetic electrons is significantly less than the ice thickness ( $1,000 \pm 100$  nm), preventing energetic electron-initiated interactions between the substrate and ice mixtures. A Fourier transform infrared (FTIR) spectrometer (Thermo Electron, Nicolet 6700) monitored the infrared spectra of ice mixtures before, during, and after irradiation with a spectral resolution of  $4 \text{ cm}^{-1}$ .

After irradiation, the ice was heated from 5 K to 300 K at a rate of  $1 \text{ K minute}^{-1}$  (temperature-programmed desorption, TPD) to release molecules into the gas phase. A cryogenic silicon diode sensor (Lakeshore DT-670) was used to measure the temperature of the silver substrate, which was precisely regulated between 5 K and 300 K, with a precision of  $\pm 0.1$  K, by a programmable

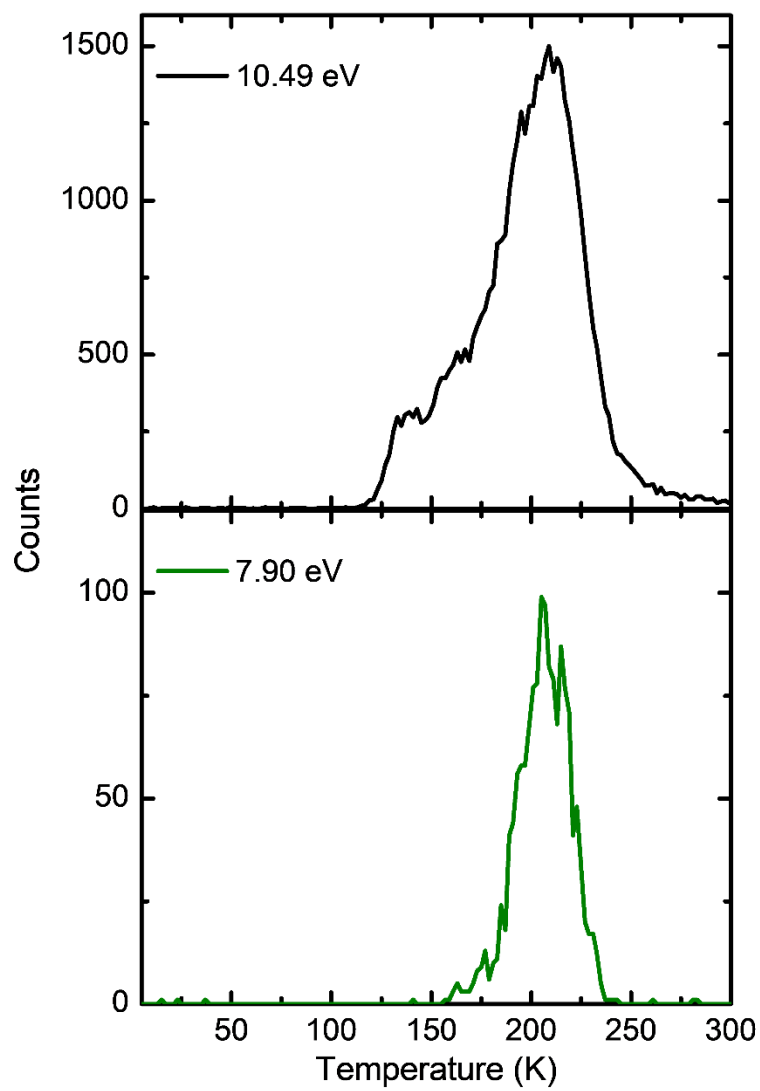
temperature controller (Lakeshore 336). During the TPD, subliming molecules were ionized by vacuum ultraviolet (VUV) single-photon ionization (SPI); individual isomers were selectively ionized by two-photon resonance-enhanced multiphoton ionization (REMPI). Tunable VUV photons were generated through the non-resonant (10.49 eV) or resonant (7.90 eV, and 8.10 – 8.27 eV) four-wave mixing method with the detailed parameters listed in Table S2. The synchronized laser beams were generated from two dye lasers (Sirah Lasertechnik GmbH, Cobra-Stretch) pumped by two pulsed (30 Hz) Nd: YAG lasers (Spectra-Physics, Quanta Ray Pro 250 and 270). Xenon (Specialty Gases, 99.999%) or krypton (Specialty Gases, 99.999%) gas was used as a nonlinear medium. The ultraviolet (UV) photons were generated via the frequency doubling process in a dye laser pumped by the third harmonic (355 nm) of a Nd:YAG laser. To determine the [1 + 1] REMPI wavelengths of aniline (**4**) and indole (**2**), separate experiments were performed with processed C<sub>2</sub>H<sub>2</sub>-NH<sub>3</sub> ice under the same experimental conditions. During the TPD, the laser wavelengths were scanned over the relevant wavelength ranges; the wavelengths were calibrated with a wavelength meter (Coherent, Wavemaster). Wavelengths at 283.817 nm (4.369 eV) and 293.842 nm (4.219 eV) were found to produce the strongest signals for aniline (Figure S3) and indole (**2**) (Figure S4), respectively, and therefore they were used to detect aniline (**4**) and indole (**2**) molecules in separate irradiation experiments. The ionization laser beam was separated spatially by a biconvex lithium fluoride lens (Korth Kristalle, R<sub>1</sub> = R<sub>2</sub> = 131.2 mm) in an off-axis geometry and passed 2.0 ± 0.5 mm over the ice surface to ionize the subliming molecules. The resulting ions were then detected by a reflectron time-of-flight mass spectrometer (ReToF-MS; Jordan-TOF products) equipped with two microchannel plates in chevron geometry. The ion signals were amplified by a preamplifier (Ortec 9305), shaped in a discriminator (Advanced Research Instruments Corp., F100-TD), and finally recorded by a multichannel scaler (FAST ComTec, MCS6A). The ionization laser was synchronized with the multichannel scaler through a digital delay pulse generator (Quantum Composers, 9518). During TPD, each recorded spectrum was integrated over 3600 sweeps (2 minutes) in bins of 3.2 ns width. The resolving power ( $m/\Delta m$ ) of this instrument was measured to be around 360 in the considered range. It is worth noting that a blank experiment was performed with C<sub>2</sub>H<sub>2</sub>-NH<sub>3</sub> ice under identical conditions but without electron irradiation; no ion signals at the mass-to-charge ratios ( $m/z$ ) of 67, 93, and 117 were observed (Figure S7). An additional experiment with C<sub>2</sub>H<sub>2</sub>-hydrogen cyanide (HCN, 5% seeded

in helium) ice irradiated with a lower dose (20 nA, 15 minutes) was recorded at a photon energy of 10.49 eV (Figure S12).

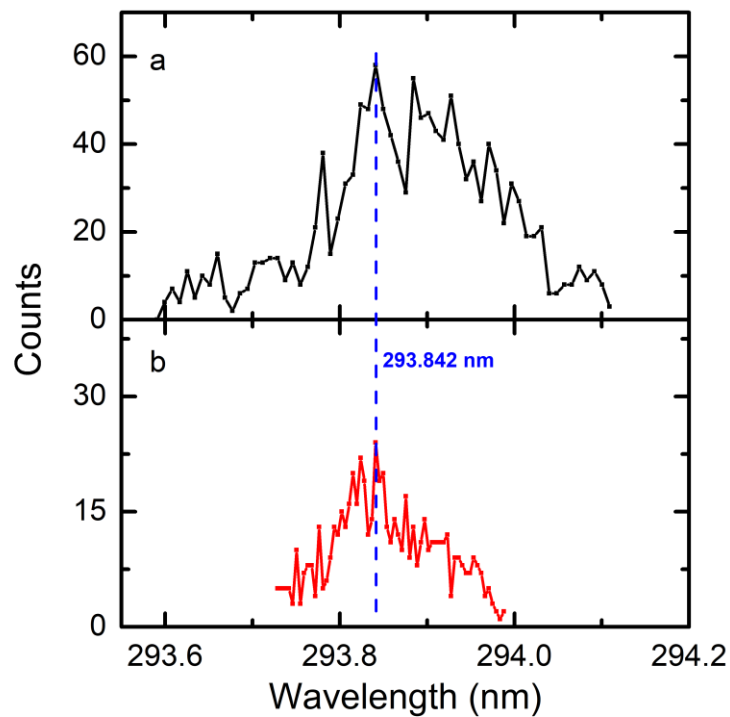
**Computational.** Geometry optimization of various reactants, products, intermediates, and transition states involved in the variety of considered radical-molecule and radical-radical reactions leading to the formation of pyrrole, indole, and aniline were carried out using density functional theory with the  $\omega$ B97X-D functional by Chai and Head-Gordon<sup>7</sup> and 6-311G(d,p) basis set. Vibrational frequencies for each stationary structure were evaluated at the same  $\omega$ B97X-D/6-311G(d,p) level of theory to verify whether the structure is a local minimum or a first-order saddle point (transition state) and to obtain the zero-point vibrational energy (ZPE) correction. Following the optimization, single-point energies were further improved using either explicitly correlated coupled cluster calculations with single and double excitations and perturbative treatment of triple excitations, CCSD(T)-F12,<sup>8,9</sup> with Dunning's cc-pVTZ-F12 basis set<sup>10</sup> (for the pyrrole and aniline formation reactions), or employing the G3(MP2,CC) model chemistry scheme<sup>11-13</sup> (for indole formation). Relative energies computed at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) + ZPE( $\omega$ B97X-D/6-311G(d,p)) and G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) + ZPE( $\omega$ B97X-D/6-311G(d,p)) levels of theory are anticipated to be accurate within 4 and 8 kJ mol<sup>-1</sup>, respectively<sup>13,14</sup>. All electronic structure calculations were performed using the Gaussian 09 and Molpro 2015 program packages<sup>15,16</sup>. Besides the potential energy surfaces presented in Figures 5–6, our electronic structure calculations reveal other reaction pathways leading to the formation of pyrrole (**3**) (Figures S13–S19) and indole (**2**) (Figures S20–S25). The computed Cartesian coordinates and vibrational frequencies of optimized structures (reactants, products, intermediates, and transition states) are listed in Table S3, which includes 88 reaction intermediates and 93 transition states. It is worth noting that gas-phase calculations may overestimate the reaction barrier because nearby molecules could participate in the reactions in the ice phase,<sup>17-19</sup> in particular, to be directly involved in the H transfer processes (Figures S13, S14, S16, S18, and S19).



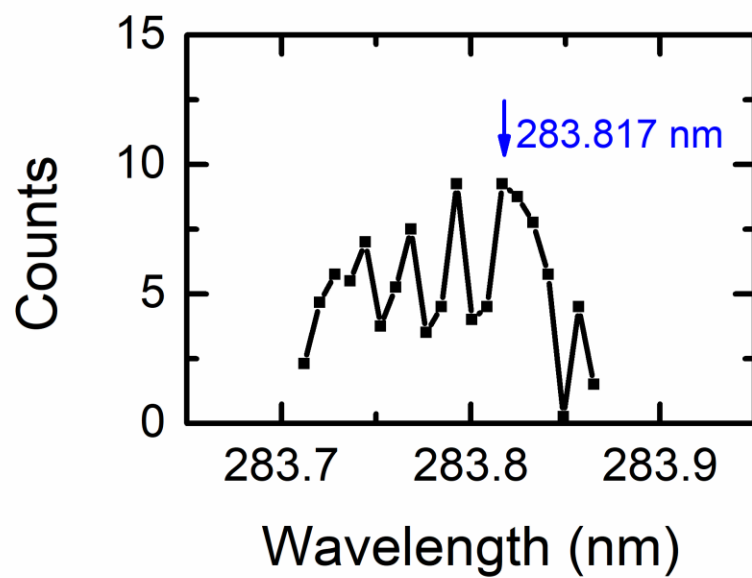
**Figure S1.** Photoionization reflectron time-of-flight mass spectrometric data. PI-ReToF-MS data as a function of temperature and mass-to-charge ( $m/z$ ) during the TPD of the irradiated acetylene–ammonia ices. Data were collected at a photon energy of 10.49 eV for  $\text{C}_2\text{H}_2\text{--NH}_3$  (a),  $^{13}\text{C}_2\text{H}_2\text{--NH}_3$  (b),  $\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  (c), and  $^{13}\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  ices (d).



**Figure S2.** TPD profiles of  $m/z = 67$  measured at 10.49 eV and 7.90 eV in irradiated  $C_2H_2-NH_3$  ice.

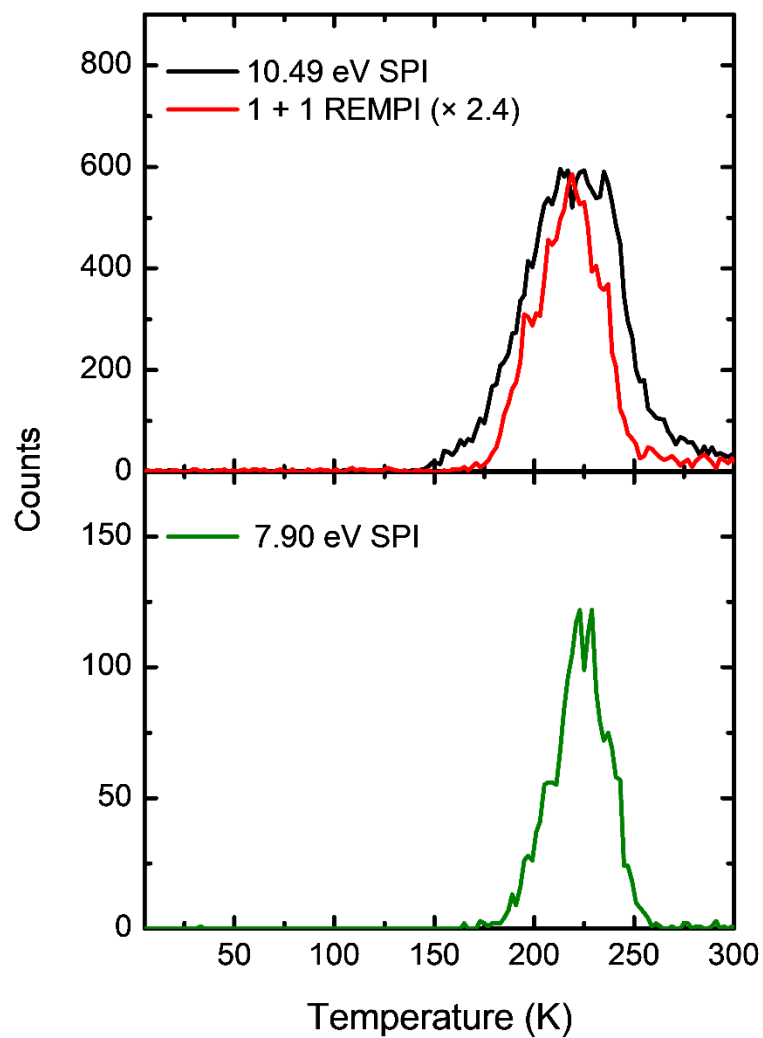


**Figure S3.** Resonance-enhanced multiphoton ionization (REMPI) scan from 293.59–294.11 nm recorded in irradiated  $\text{C}_2\text{H}_2\text{-NH}_3$  ice during sublimation from 193–205 K (a). A precise scan was performed to determine the wavelength ( $\lambda = 293.842$  nm) at the maximum signal (b), which corresponds to the  $\text{S}_1 \leftarrow \text{S}_0$  transition origin ( $0^0$ ) band of aniline.

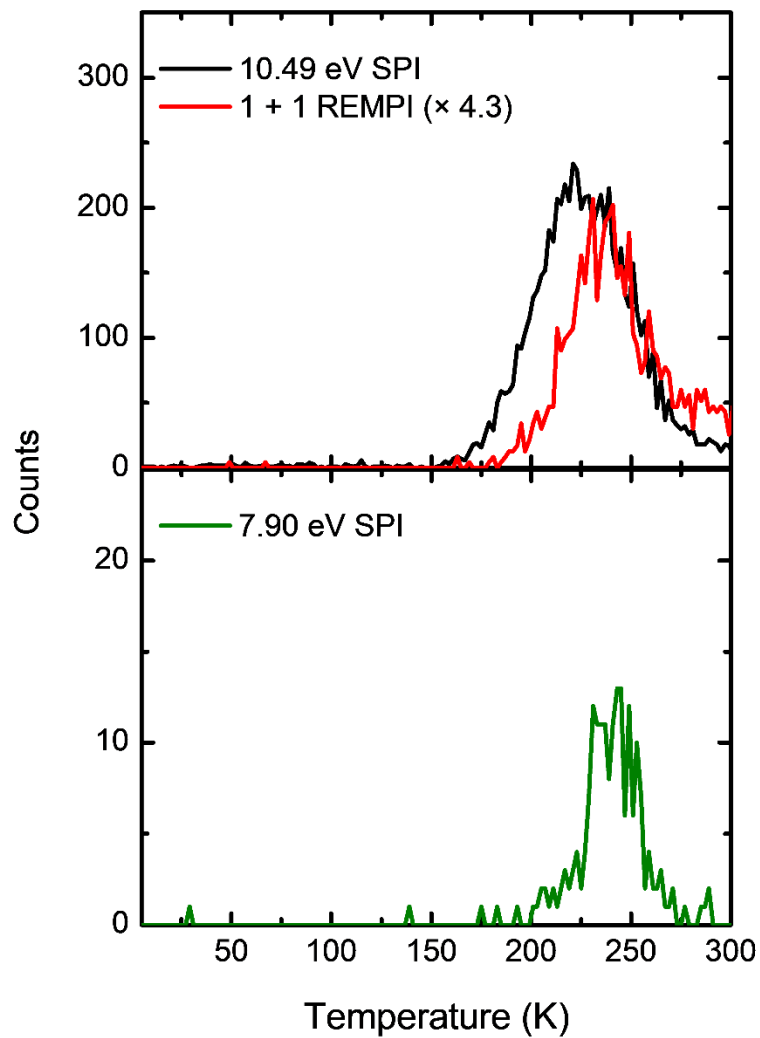


**Figure S4.** REMPI scan from 283.65–283.87 nm recorded in irradiated  $\text{C}_2\text{H}_2\text{-NH}_3$  ice during sublimation from 206–268 K. The arrow indicates the wavelength ( $\lambda = 283.817$  nm) at the maximum signal, which corresponds to the  $S_1 \leftarrow S_0$  transition origin ( $0^0$ ) band of indole.

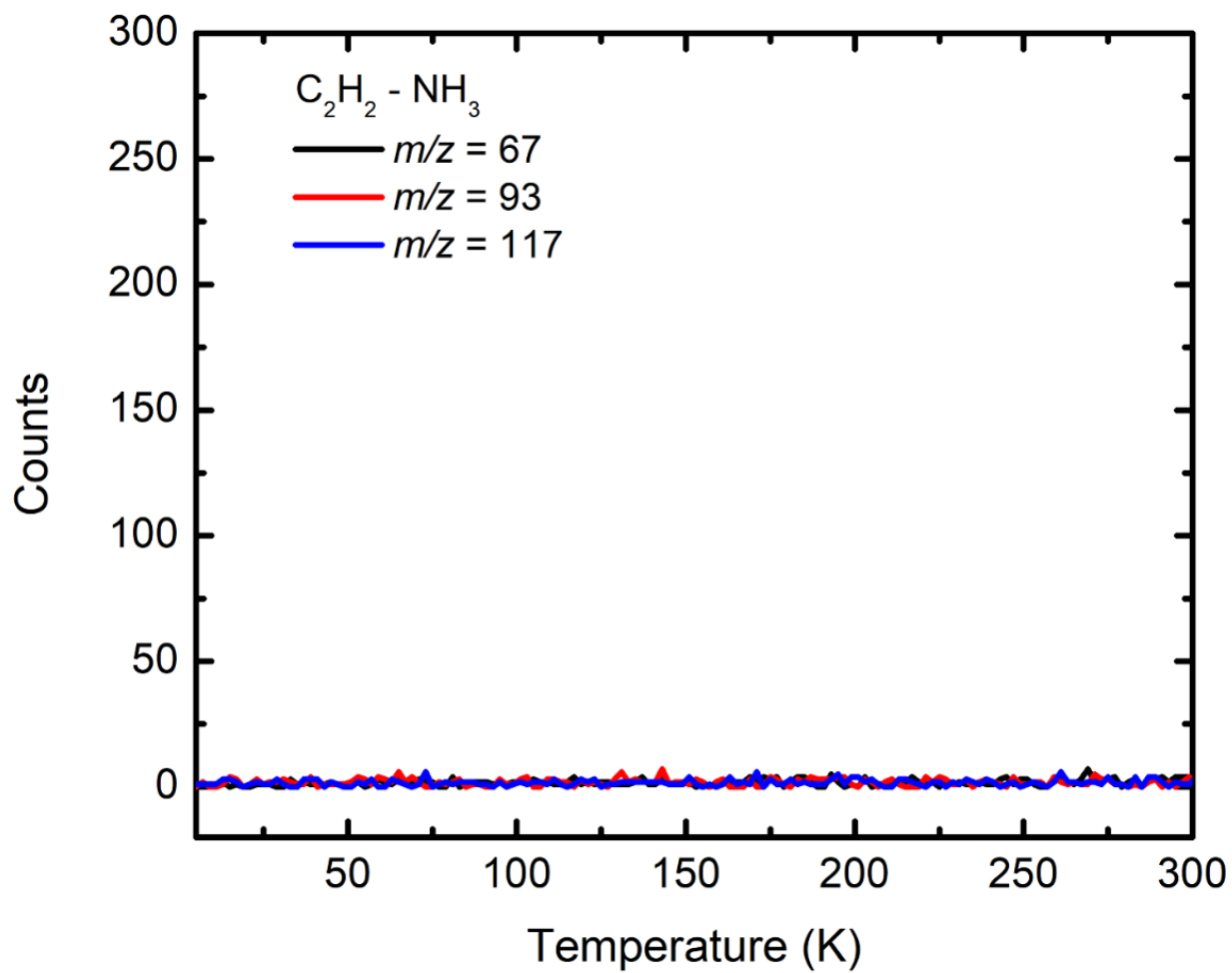




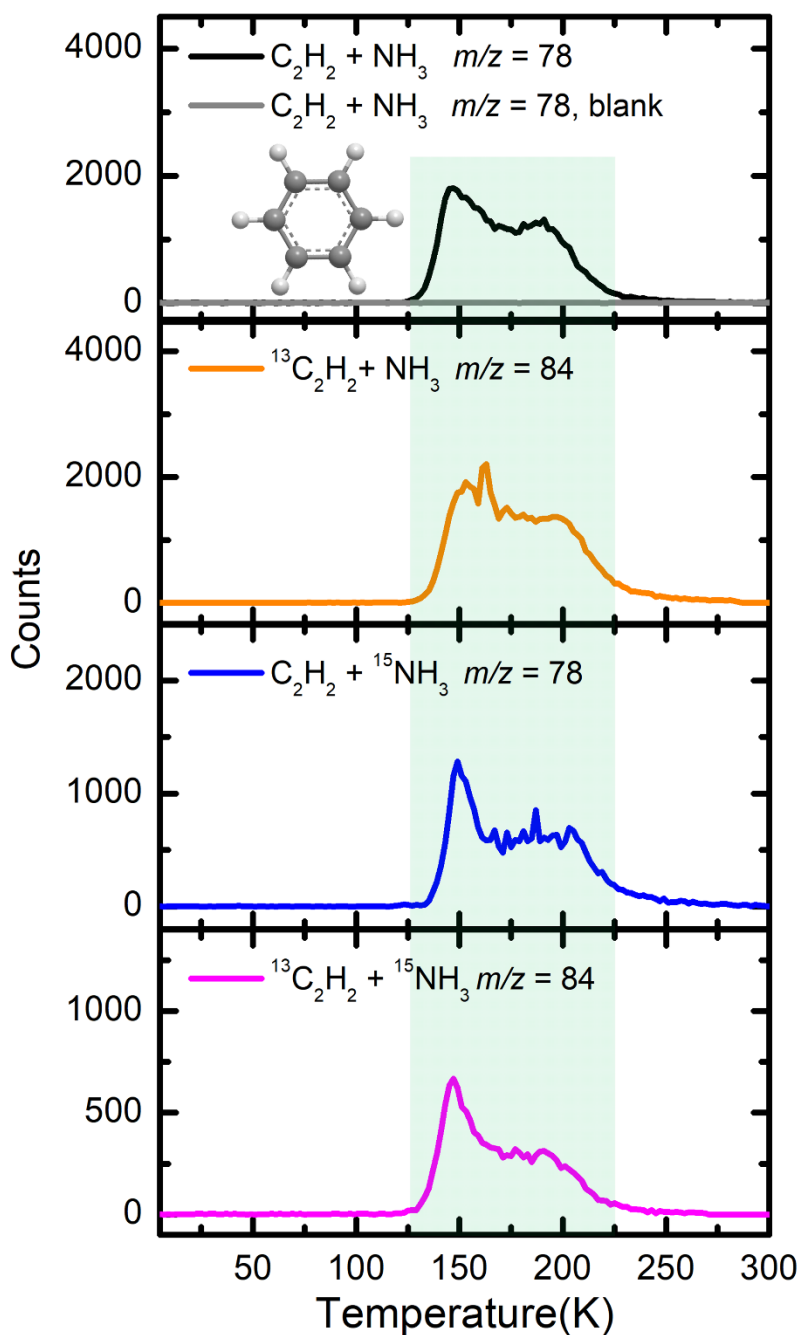
**Figure S5.** TPD profiles of  $m/z = 93$  measured at 10.49 eV and 7.90 eV, and the REMPI wavelength of 293.842 nm in irradiated  $C_2H_2-NH_3$  ice.



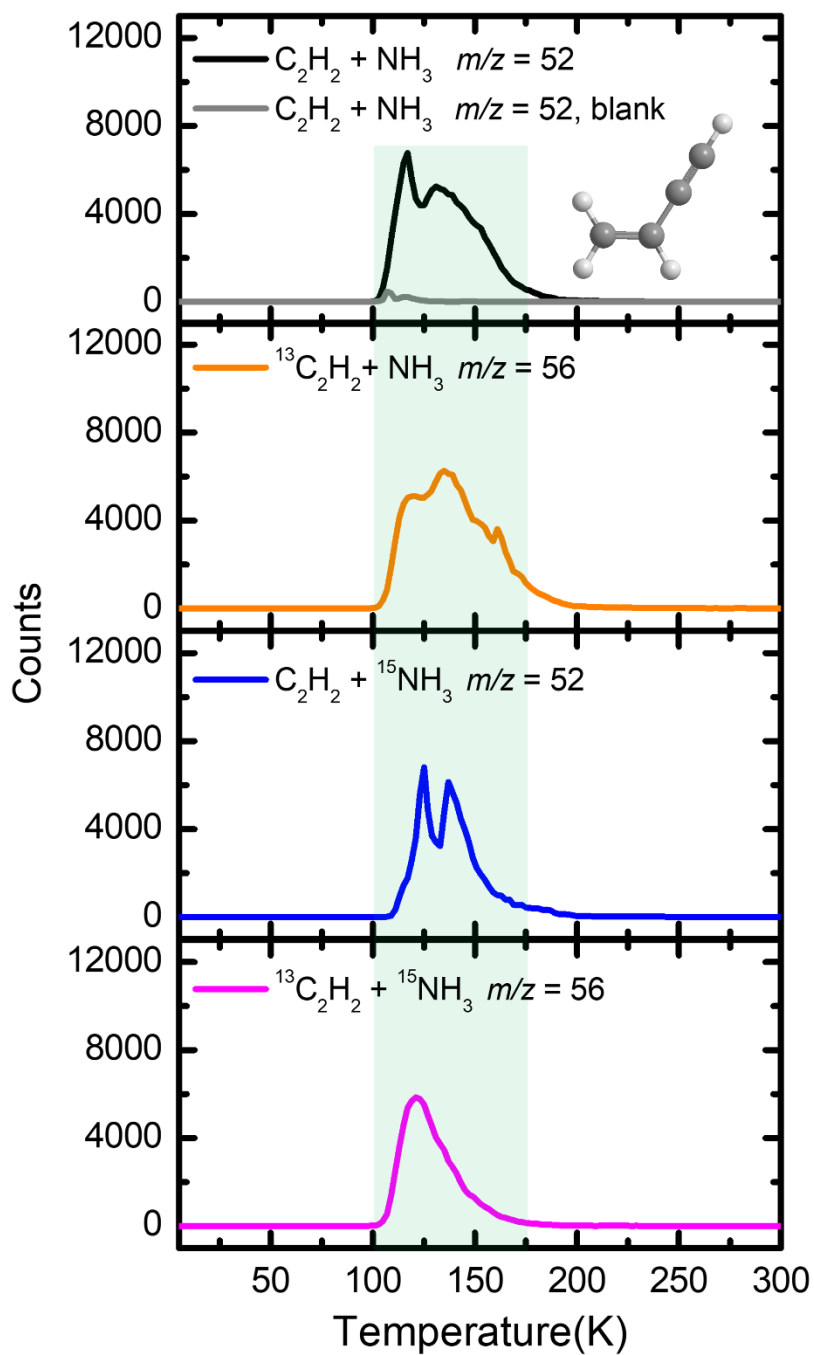
**Figure S6.** TPD profiles of  $m/z = 117$  measured at 10.49 eV and 7.90 eV, and the REMPI wavelength of 283.817 nm in irradiated  $C_2H_2-NH_3$  ice.



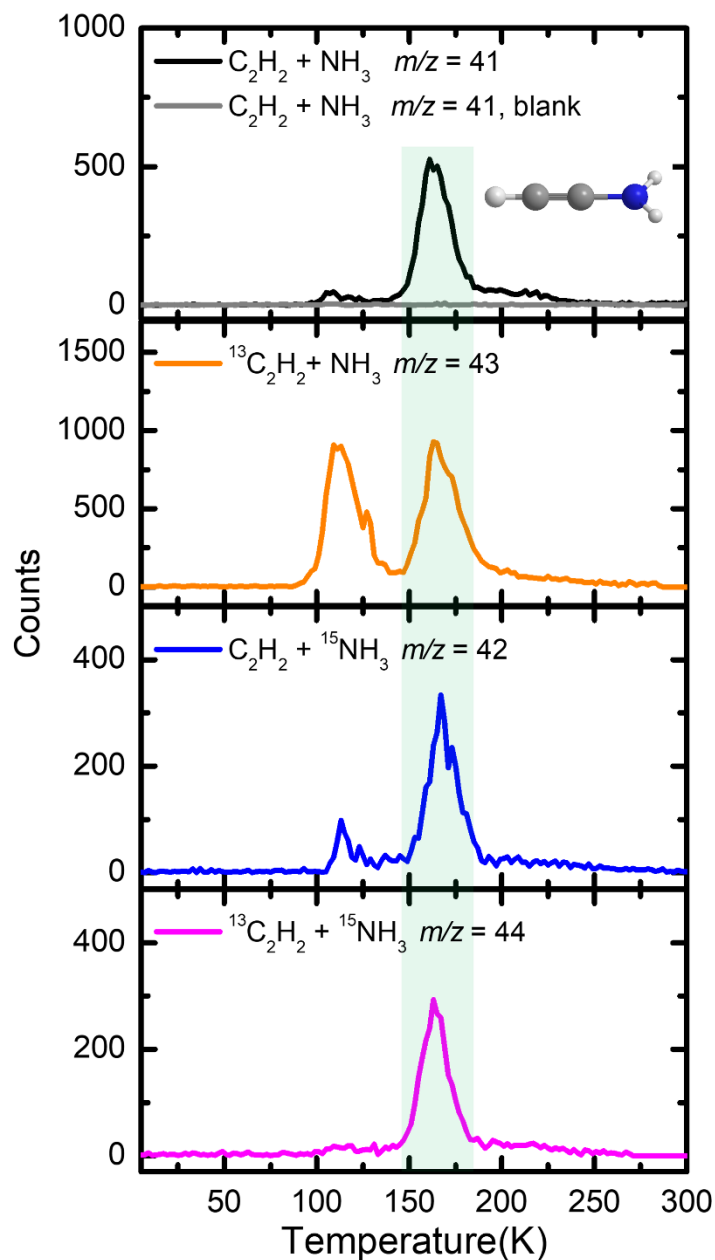
**Figure S7.** TPD profiles measured as a function of temperature for the blank experiment in  $C_2H_2-NH_3$  ice recorded at a photon energy of 10.49 eV.



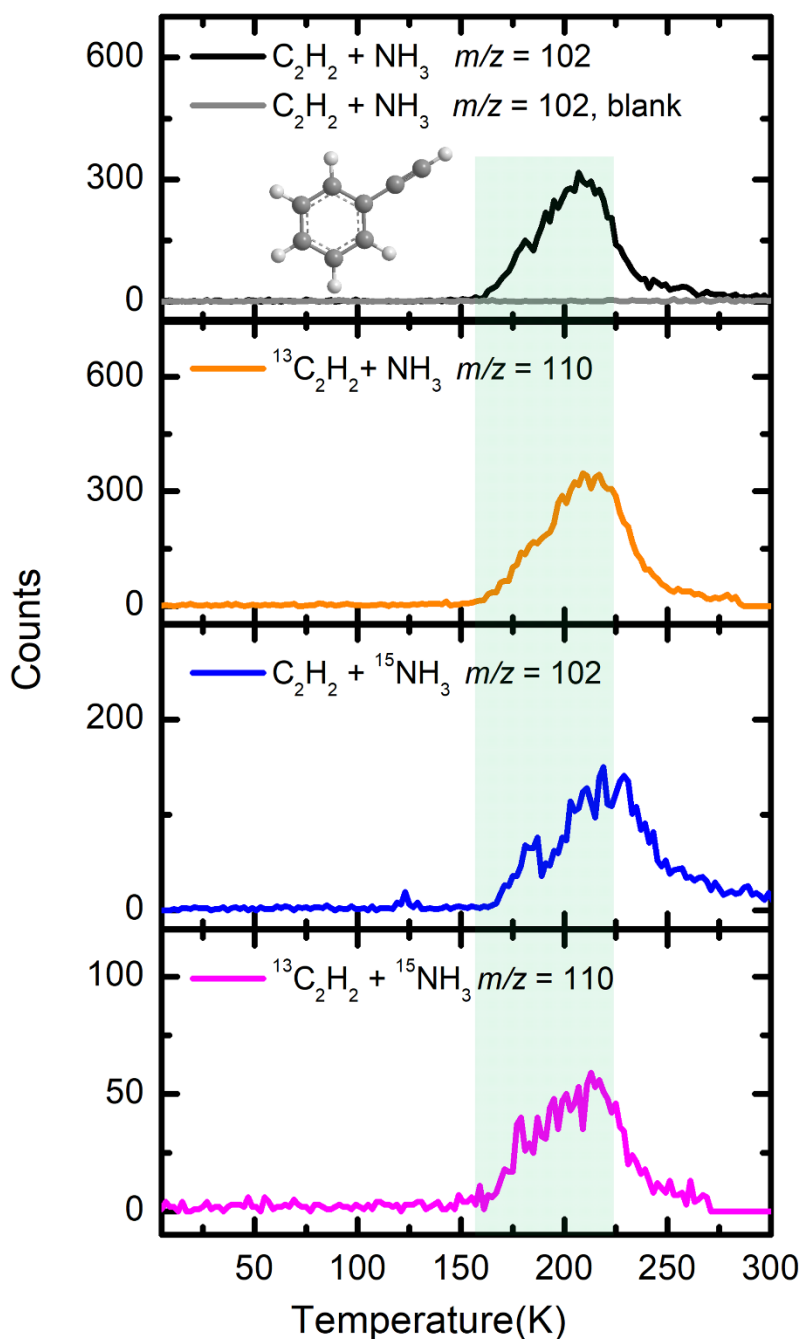
**Figure S8.** Ion signals during TPD of acetylene–ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated  $\text{C}_2\text{H}_2\text{--NH}_3$  ( $m/z = 78$ ),  $^{13}\text{C}_2\text{H}_2\text{--NH}_3$  ( $m/z = 84$ ),  $\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  ( $m/z = 78$ ), and  $^{13}\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  ( $m/z = 84$ ) ices, confirming the formula  $\text{C}_6\text{H}_6$ . The shaded region indicates the range of sublimation temperature of benzene (**1**) in processed acetylene ices.<sup>20,21</sup>



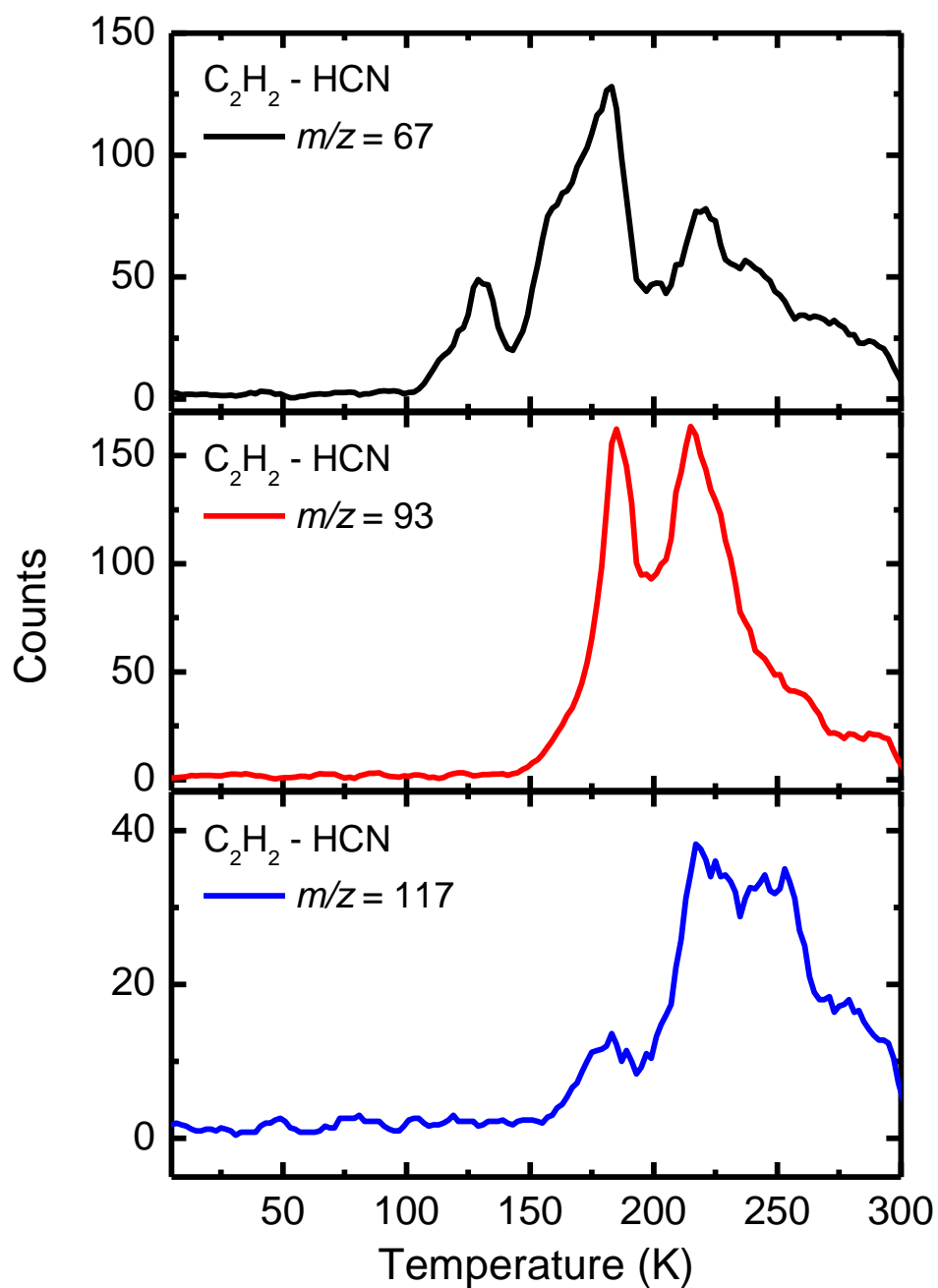
**Figure S9.** Ion signals during TPD of acetylene–ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated  $\text{C}_2\text{H}_2\text{-NH}_3$  ( $m/z = 52$ ),  $^{13}\text{C}_2\text{H}_2\text{-NH}_3$  ( $m/z = 56$ ),  $\text{C}_2\text{H}_2\text{-}^{15}\text{NH}_3$  ( $m/z = 52$ ), and  $^{13}\text{C}_2\text{H}_2\text{-}^{15}\text{NH}_3$  ( $m/z = 56$ ) ices, confirming the formula  $\text{C}_4\text{H}_4$ . The shaded region indicates the range of sublimation temperature of vinylacetylene (**5**) in processed acetylene ices.<sup>20</sup>



**Figure S10.** Ion signals during TPD of acetylene–ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated  $\text{C}_2\text{H}_2\text{--NH}_3$  ( $m/z = 41$ ),  $^{13}\text{C}_2\text{H}_2\text{--NH}_3$  ( $m/z = 43$ ),  $\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  ( $m/z = 42$ ), and  $^{13}\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  ( $m/z = 44$ ) ices, confirming the formula  $\text{C}_2\text{H}_3\text{N}$ . The shaded region indicates the sublimation event of ethynylamine (6) in processed acetylene–ammonia ices.<sup>5</sup>

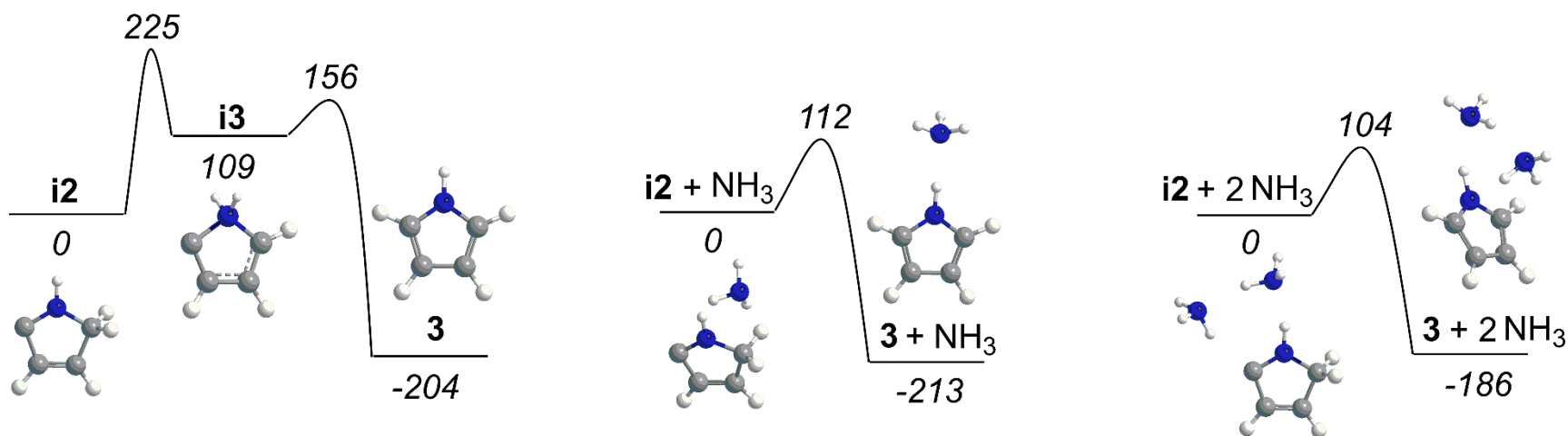


**Figure S11.** Ion signals during TPD of acetylene–ammonia ices. TPD profiles were recorded at 10.49 eV from irradiated  $\text{C}_2\text{H}_2\text{--NH}_3$  ( $m/z = 102$ ),  $^{13}\text{C}_2\text{H}_2\text{--NH}_3$  ( $m/z = 110$ ),  $\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  ( $m/z = 102$ ), and  $^{13}\text{C}_2\text{H}_2\text{--}^{15}\text{NH}_3$  ( $m/z = 110$ ) ices, confirming the formula  $\text{C}_8\text{H}_6$ . The shaded region indicates the range of sublimation temperature of phenylacetylene (7) in processed acetylene ices.<sup>20</sup>

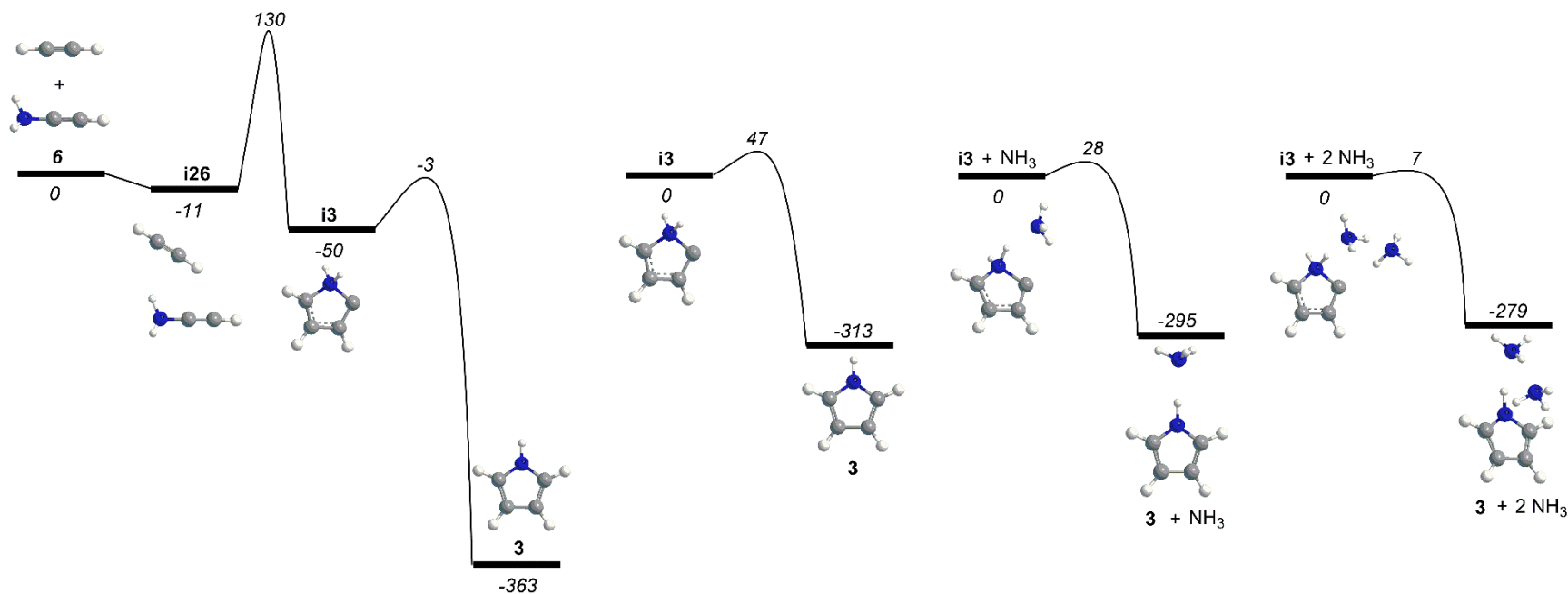


**Figure S12.** TPD profiles measured as a function of temperature for the irradiated (20 nA, 15 minutes) experiment in  $C_2H_2$ -HCN ice recorded at a photon energy of 10.49 eV.

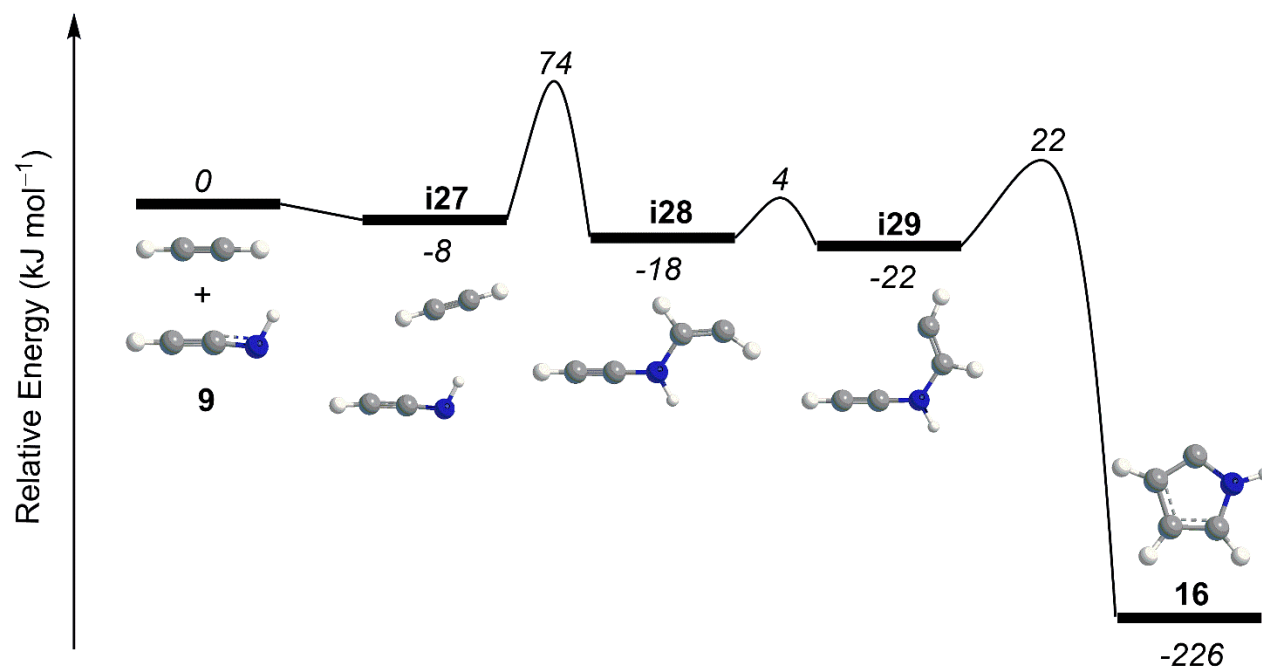




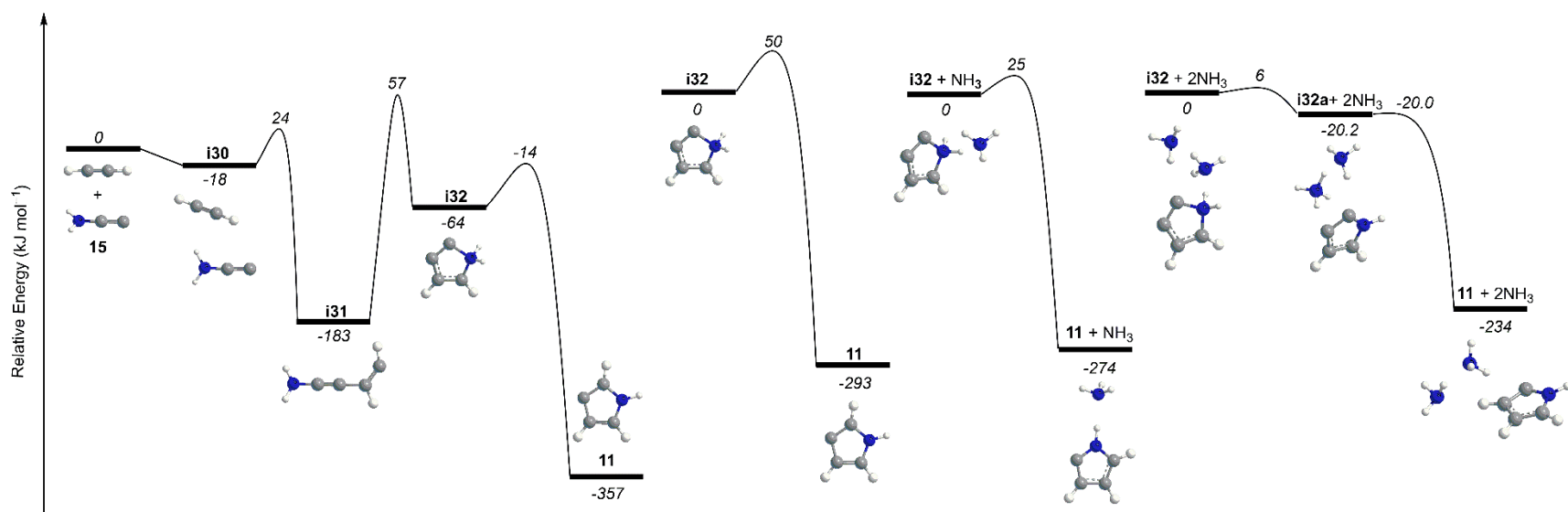
**Figure S13.** Potential energy surface for formation of pyrrole (**3**) from **i2** calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory. Adding ammonia ( $\text{NH}_3$ ) molecules into the reaction results in a reduction of the barrier to form pyrrole (**3**). Relative energies (italics) are shown in  $\text{kJ mol}^{-1}$ .



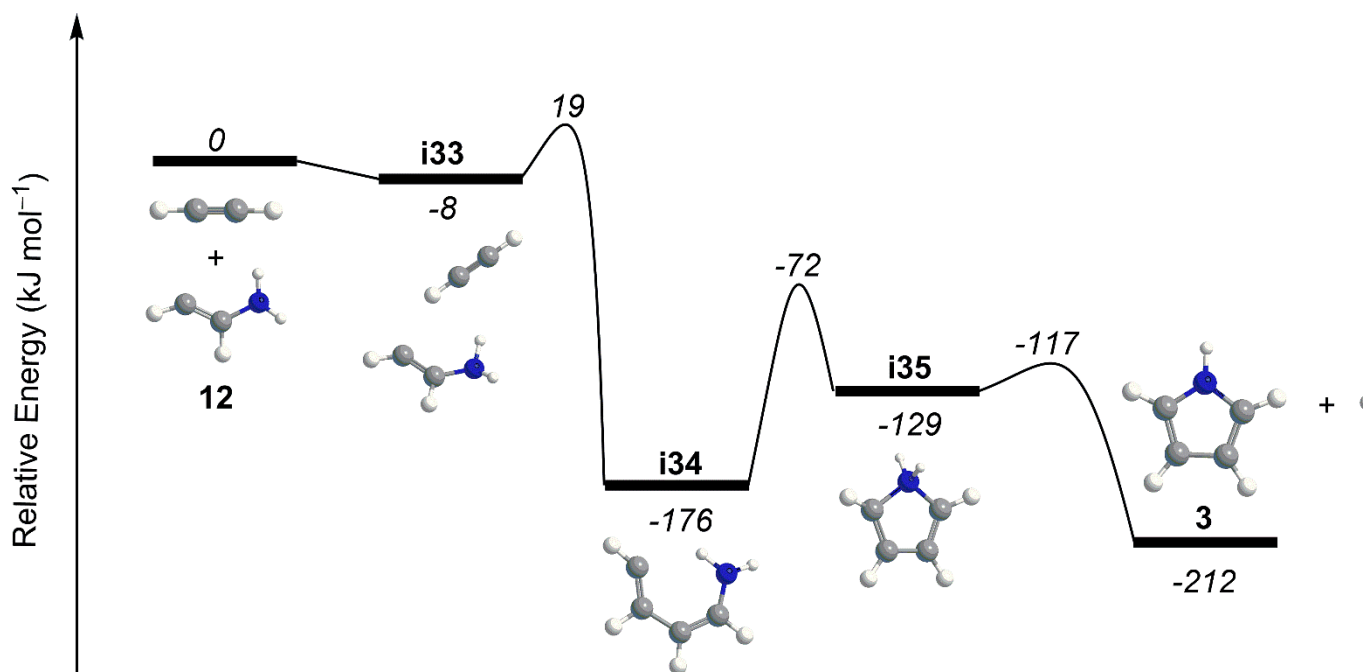
**Figure S14.** Potential energy surface for the bimolecular reaction of acetylene ( $C_2H_2$ ) with ethynylamine (**6**) calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory. Adding ammonia molecules into the reaction results in a reduction of the barrier to form pyrrole (**3**). Relative energies (italics) are shown in  $\text{kJ mol}^{-1}$ .



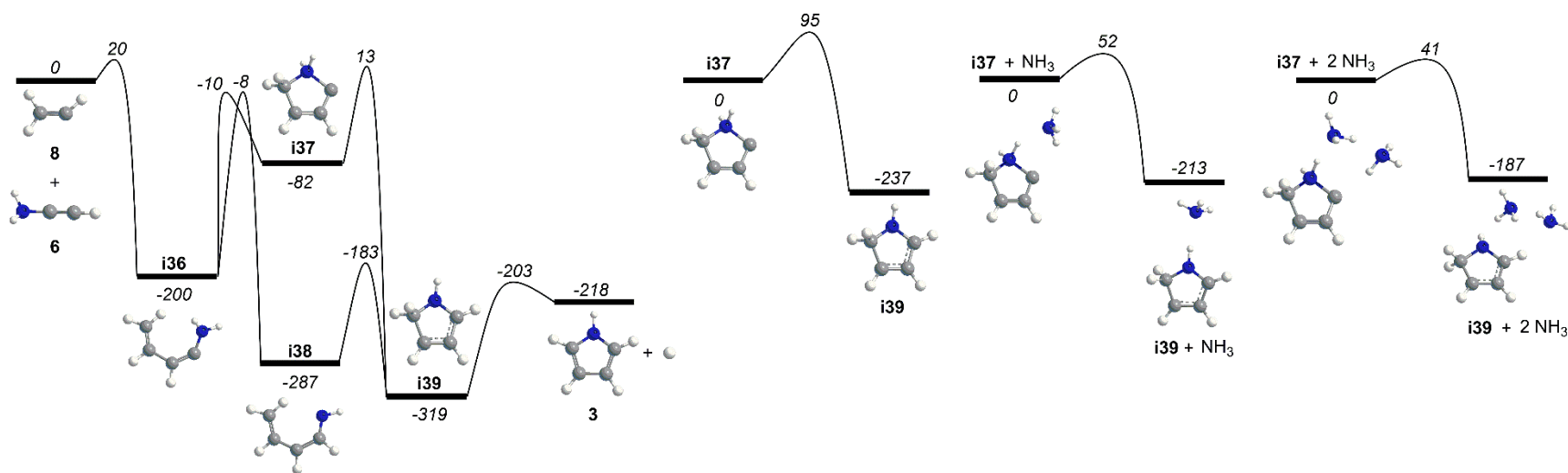
**Figure S15.** Potential energy surface for the reaction of acetylene (C<sub>2</sub>H<sub>2</sub>) with the ethynylamidogen (**9**) radical, leading to the formation of 2-pyrrolyl (C<sub>4</sub>H<sub>4</sub>N, **16**) radical. Relative energies (italics) were calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory.



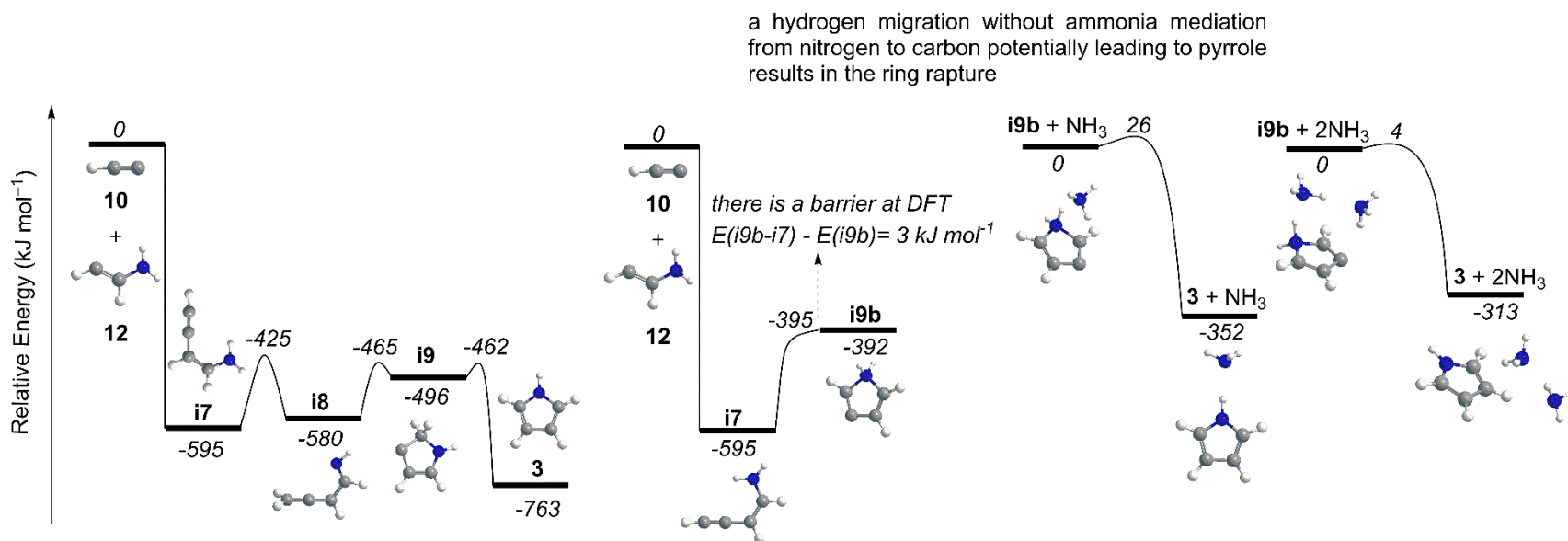
**Figure S16.** Potential energy surface for the reaction of acetylene (C<sub>2</sub>H<sub>2</sub>) with the aminoethynyl (**15**) radical, leading to the formation of 3-pyrrolyl (C<sub>4</sub>H<sub>4</sub>N, **11**) radical. Relative energies (italics) were calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory. Adding ammonia molecules into the reaction results in a reduction of the barrier to form 3-pyrrolyl (**11**).



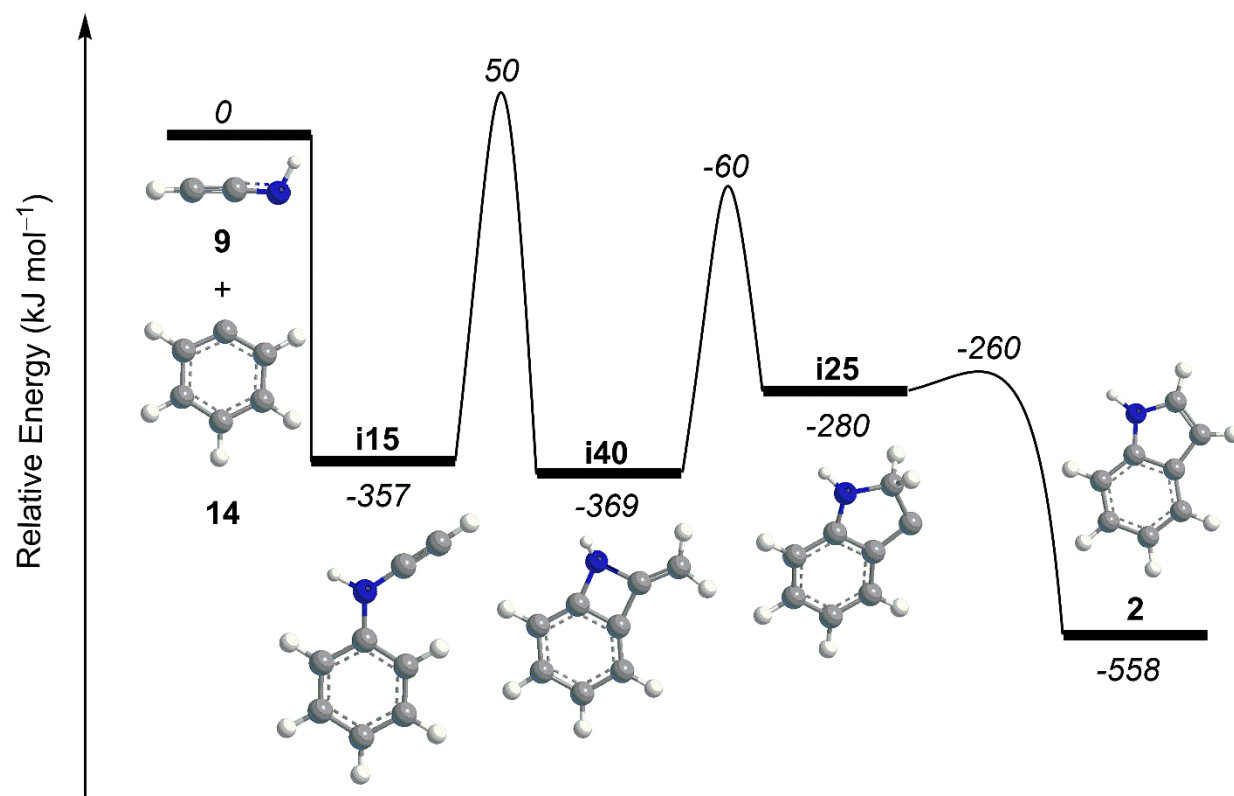
**Figure S17.** Potential energy surface for the reaction of acetylene (C<sub>2</sub>H<sub>2</sub>) with the 2-aminoethenyl (**12**) radical calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory.



**Figure S18.** Potential energy surface for the reaction of the vinyl (**8**) radical with ethynylamine (**6**) calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory. Adding ammonia (NH<sub>3</sub>) molecules into the reaction results in a reduction of the barrier from **i37** to **i39**. Relative energies (*italics*) are shown in  $\text{kJ mol}^{-1}$ .

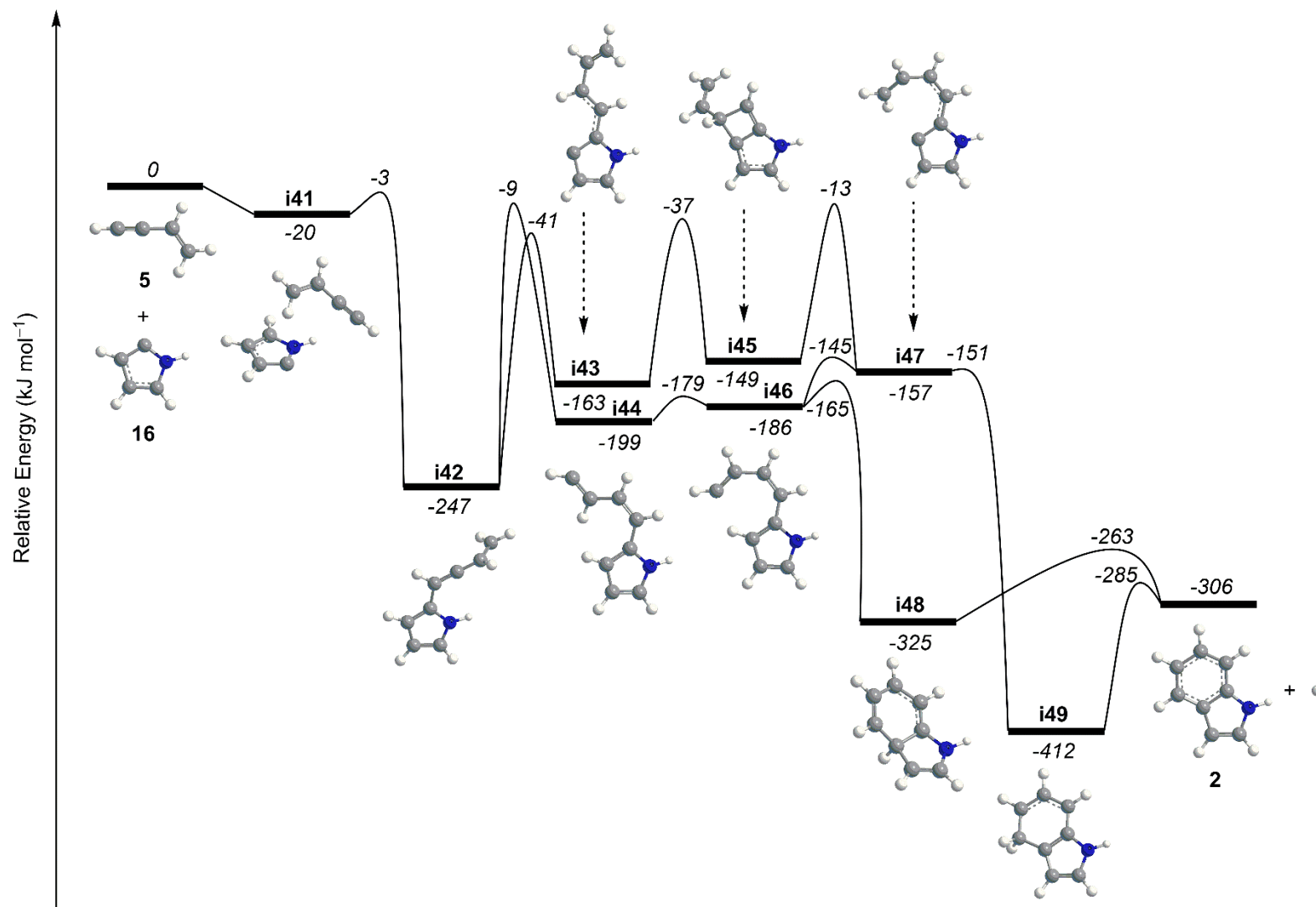


**Figure S19.** Potential energy surface for the reaction of the ethynyl (**10**) plus 2-aminoethenyl ( $\text{NH}_2\text{CHCH}$ , **12**) calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory. Direct participation of ammonia ( $\text{NH}_3$ ) molecules in the reaction creates a possibility for a hydrogen atom to be transferred from the nitrogen atom to the “bare” carbon atom. Relative energies (italics) are shown in  $\text{kJ mol}^{-1}$ .

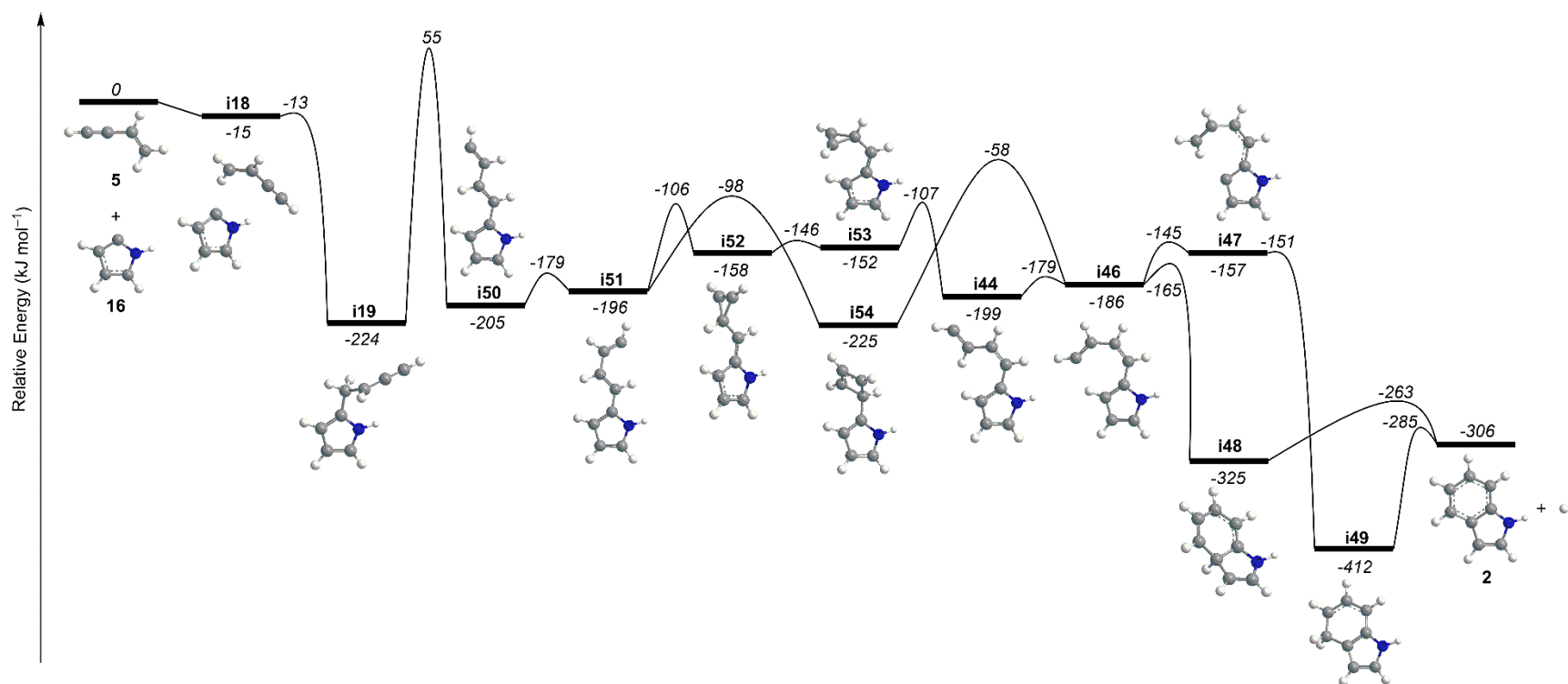


**Figure S20.** Potential energy surface for the reaction of ethynylamidogen (**9**) and phenyl (**14**) radicals calculated at the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level of theory.

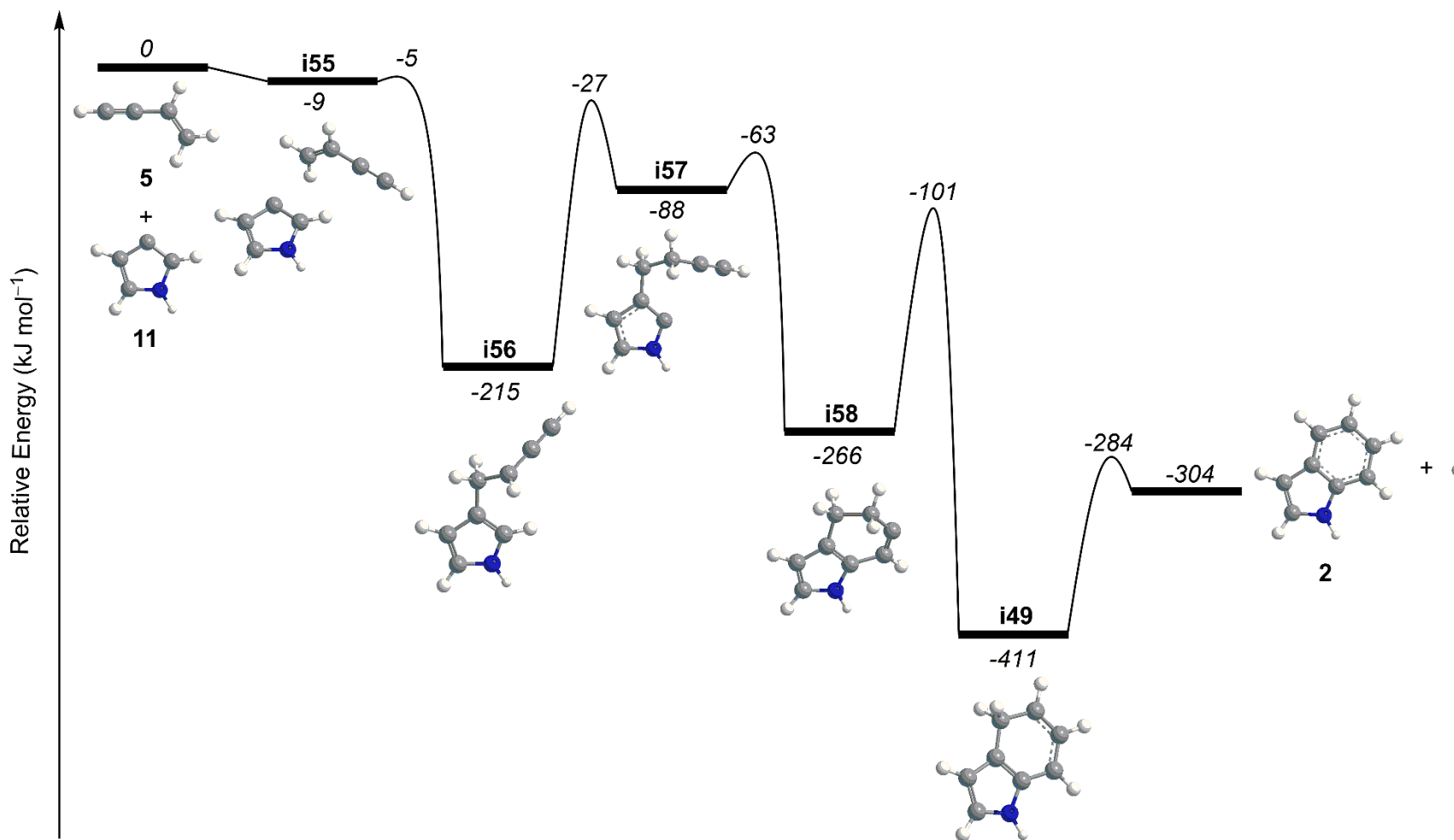




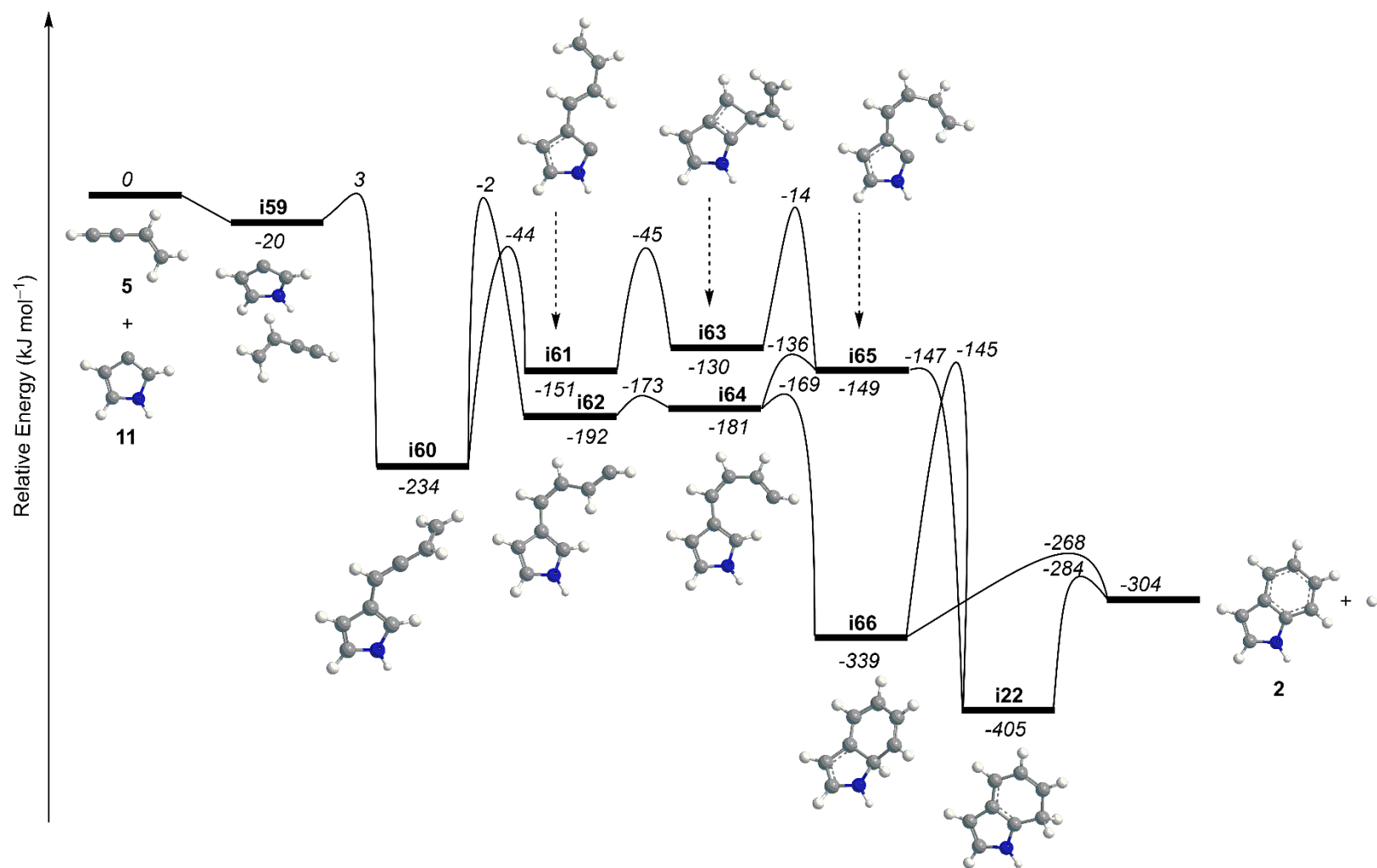
**Figure S21.** Potential energy surface for the reaction of vinylacetylene (**5**) with the 2-pyrrolyl (**16**) radical calculated at the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level of theory.



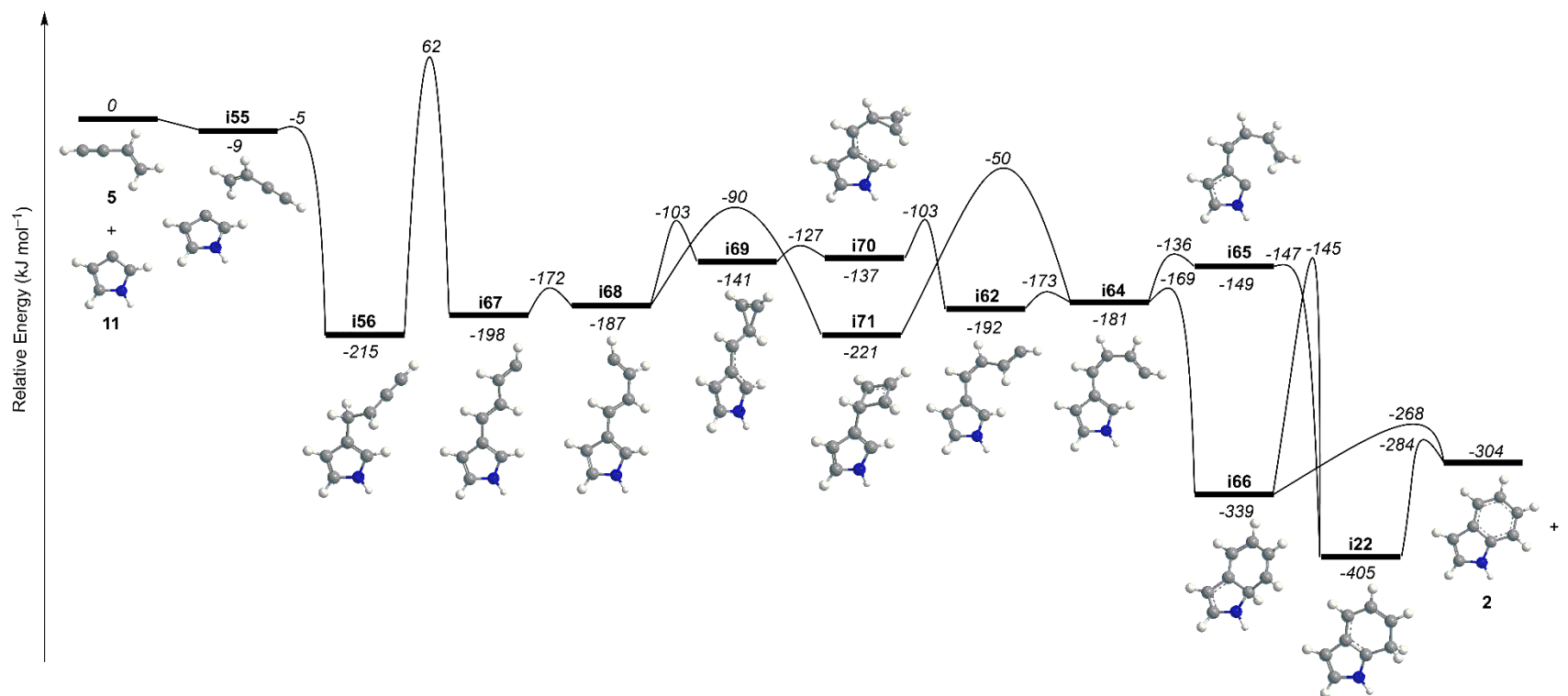
**Figure S22.** Potential energy surface for the reaction of vinylacetylene (**5**) with the 2-pyrrolyl (**16**) radical calculated at the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level of theory.



**Figure S23.** Potential energy surface for the reaction of vinylacetylene (**5**) with the 3-pyrrolyl (**11**) radical calculated at the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level of theory.



**Figure S24.** Potential energy surface for the bimolecular reaction of vinylacetylene (**5**) with the 3-pyrrolyl (**11**) radical calculated at the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level of theory.



**Figure S25.** Potential energy surface for the reaction of the vinylacetylene (**5**) with the 3-pyrrolyl (**11**) radical calculated at the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level of theory.

**Table S1.** Absorption peaks observed in C<sub>2</sub>H<sub>2</sub>-NH<sub>3</sub> ice before and after electron irradiation (100 nA, 60 minutes) at 5 K. Assignment labels: stretching ( $\nu$ ) and bending ( $\delta$ ).

Pristine ice, absorptions before irradiation (cm <sup>-1</sup> )	
<b>C<sub>2</sub>H<sub>2</sub></b>	Assignment <sup>20-23</sup>
3236	$\nu_3$
1947	$\nu_2$
1375	$\nu_4 + \nu_5$
805, 753	$\nu_5$
<b>NH<sub>3</sub></b>	Assignment <sup>24,25</sup>
3380	$\nu_3$
3303	2 $\nu_4$
3165	$\nu_1$
1629	$\nu_4$
1087	$\nu_2$
New absorptions after irradiation (cm <sup>-1</sup> )	
	Assignment <sup>20,26-31</sup>
2974	$\nu_6 + \nu_7$ (C <sub>4</sub> H <sub>4</sub> )/ $\nu_{11}$ (C <sub>2</sub> H <sub>4</sub> )/ $\nu_{10}$ (C <sub>2</sub> H <sub>6</sub> )
2792	$\nu$ (C-H)
2109	$\nu_5$ (C <sub>4</sub> H <sub>4</sub> )
2054	$\nu$ (C=C=N)
1506	$\nu$ (ring)/ $\delta$ (NH <sub>2</sub> )/ $\dot{\text{N}}\text{H}_2$
1435	$\nu_{12}$ (C <sub>2</sub> H <sub>4</sub> )
1304	$\nu_9$ (C <sub>6</sub> H <sub>6</sub> )/ $\nu_4$ (CH <sub>4</sub> )
1274	$\delta$ (NH)
961	$\delta$ (C=CH) <sub>aromatic</sub>

**Table S2.** Parameters for the generation of vacuum ultraviolet (VUV;  $3\omega_1$  or  $2\omega_1 - \omega_2$ ) and ultraviolet (UV;  $\omega_2$ ) lights. The uncertainty of photon wavelengths is less than 0.001 nm.

Photon energy (eV)	10.49 ( $3\omega_1$ )	8.10 – 8.27 ( $2\omega_1 - \omega_2$ )	7.90 ( $2\omega_1 - \omega_2$ )	4.219 ( $\omega_2$ )	4.368 ( $\omega_2$ )
Nonlinear medium for four-wave mixing	Xenon	Krypton	Xenon	–	–
$\omega_1$ wavelength (nm)	355	202.316	249.628	–	–
Nd:YAG 1 output (nm)	355	532	355	–	–
Dye laser 1 output (nm)	–	606.948	499.256	–	–
$\omega_2$ wavelength (nm)	–	298 – 311 <sup>a</sup>	609.696	293.842 <sup>a</sup>	283.817 <sup>a</sup>
Nd:YAG 2 output (nm)	–	532	532	532	532
Dye laser 2 output (nm)	–	596 – 622	609.696	587.684	567.634

<sup>a</sup> obtained through frequency doubling process.

**Table S3.** Cartesian coordinates and vibrational frequencies of optimized structures (reactants, products, intermediates, and transition states) calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level and the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level.

### Reactants and products

#### *Acetylene*

##### Cartesian coordinates

C	0.000000	0.000000	0.598192
C	0.000000	0.000000	-0.598192
H	0.000000	0.000000	1.662187
H	0.000000	0.000000	-1.662187

##### Vibrational frequencies

675.1455 675.1455 768.9518  
 768.9518 2088.336 3423.093  
 3530.67

#### *Ammonia*

##### Cartesian coordinates

N	0.000000	0.000000	0.114745
H	0.000000	0.938582	-0.267738
H	0.812836	-0.469291	-0.267738
H	-0.812836	-0.469291	-0.267738

##### Vibrational frequencies

1064.784 1682.874 1682.998  
 3507.326 3634.768 3635

#### *Benzene (1)*

##### Cartesian coordinates

C	1.379003	0.175768	-0.000001
C	0.841743	-1.106425	-0.000001
C	-0.537179	-1.282193	0.000000
C	-1.379003	-0.175768	0.000000
C	-0.841743	1.106425	0.000000
C	0.537179	1.282193	0.000000
H	2.454596	0.312944	0.000005
H	1.498509	-1.969296	0.000001
H	-0.957019	-2.281974	0.000002
H	-2.454596	-0.312944	-0.000001
H	-1.498509	1.969296	0.000001
H	0.957019	2.281974	0.000002

##### Vibrational frequencies

413.1913 414.2282 625.9993



627.3443	686.819	730.0167
862.6288	877.5347	991.8031
1004.368	1027.099	1028.037
1029.236	1070.853	1074.961
1178.398	1203.341	1210.547
1340.871	1384.089	1523.176
1528.737	1670.821	1672.722
3184.327	3191.905	3197.115
3208.994	3213.669	3222.537

### ***Indole (2)***

#### **Cartesian coordinates**

N	1.558908	-1.076624	-0.000036
C	2.378381	0.029070	-0.000025
C	1.621948	1.161607	0.000008
C	0.248178	0.745771	0.000035
C	-0.978770	1.422864	0.000013
C	-2.149074	0.690308	-0.000019
C	-2.125626	-0.715717	-0.000014
C	-0.932876	-1.412053	0.000012
C	0.247307	-0.666896	0.000028
H	1.871417	-2.030209	0.000156
H	3.451125	-0.087050	-0.000059
H	1.996585	2.172995	-0.000014
H	-1.006300	2.507032	0.000014
H	-3.104374	1.202587	-0.000048
H	-3.061841	-1.262273	-0.000036
H	-0.915768	-2.496435	0.000015

#### **Vibrational frequencies**

213.4478	246.5963	403.472
413.1689	431.2457	555.8567
590.8125	622.4174	623.2906
726.8646	755.6784	782.6987
788.8756	862.2803	879.8249
892.6123	916.9751	951.5005
990.926	1042.761	1092.459
1123.951	1152.724	1180.769
1233.504	1273.145	1317.391
1377.747	1391.005	1469.091
1501.149	1547.195	1581.2
1652.483	1696.432	3191.383
3198.7	3209.364	3221.297
3259.988	3280.178	3724.61

***Pyrrole (3)***

**Cartesian coordinates**

N	-1.116972	-0.004172	-0.000235
C	-0.334469	1.118024	-0.000025
C	0.976135	0.714387	-0.000020
C	0.981639	-0.707082	-0.000113
C	-0.326101	-1.120471	-0.000137
H	-2.120677	-0.007958	0.000731
H	-0.771207	2.103680	0.000761
H	1.836312	1.365623	0.000243
H	1.846599	-1.351918	0.000611
H	-0.755452	-2.109368	0.001067

**Vibrational frequencies**

501.1219	636.2196	647.7327
703.8612	740.4986	856.0911
885.0829	903.8719	905.6801
1038.571	1073.724	1103.861
1175.942	1192.966	1314.851
1440.203	1489.491	1527.269
1600.285	3250.215	3262.821
3283.781	3289.152	3720.48

***Aniline (4)***

**Cartesian coordinates**

N	2.326736	0.000038	-0.074118
C	0.935255	-0.000002	-0.009595
C	0.220266	1.202364	-0.006262
C	-1.166695	1.196673	0.003633
C	-1.873485	0.000001	0.008999
C	-1.166699	-1.196672	0.003655
C	0.220264	-1.202366	-0.006235
H	2.768317	-0.835174	0.276196
H	2.768304	0.834934	0.276968
H	0.759134	2.144805	-0.016063
H	-1.699343	2.141484	0.007535
H	-2.956773	0.000002	0.017456
H	-1.699348	-2.141483	0.007576
H	0.759118	-2.144817	-0.016009

**Vibrational frequencies**

221.6451	286.2772	388.5944
419.5718	509.8614	541.8018
593.953	638.0537	708.7131

768.8114	834.9846	842.9233
892.2601	978.3354	994.9788
1016.042	1062.631	1080.285
1145.391	1184.894	1214.905
1325.84	1350.43	1375.493
1515.543	1552.463	1662.408
1667.595	1693.027	3182.513
3183.668	3199.841	3206.076
3223.716	3606.929	3707.891

### *Vinylacetylene (5)*

#### **Cartesian coordinates**

C	-1.899901	-0.173838	0.000001
C	-0.734772	0.118044	-0.000001
C	0.642282	0.494146	-0.000004
C	1.648571	-0.378115	0.000004
H	-2.929811	-0.438232	0.000002
H	0.844856	1.561434	0.000006
H	2.677071	-0.037282	-0.000004
H	1.470807	-1.447336	-0.000009

#### **Vibrational frequencies**

223.9837	308.3506	563.9499
676.5628	702.8568	706.388
894.6541	963.0477	1010.796
1117.303	1332.419	1445.456
1706.094	2243.637	3165.339
3181.842	3262.931	3487.017

### *Ethynylamine (6)*

#### **Cartesian coordinates**

N	0.128010	-1.182754	0.000000
C	-0.061211	1.360347	0.000000
C	0.000000	0.161386	0.000000
H	-0.205880	-1.635867	-0.837650
H	-0.205880	-1.635867	0.837650
H	-0.117042	2.420609	0.000000

#### **Vibrational frequencies**

378.103	457.0034	520.4194
610.5933	714.7365	1097.72
1207.987	1649.646	2277.598
3495.49	3587.772	3679.068

### *Phenylacetylene (7)*

**Cartesian coordinates**

C	-0.119132	-1.207129	0.000149
C	-1.506056	-1.203155	-0.000033
C	-2.202394	-0.000058	-0.000037
C	-1.506328	1.203124	-0.000004
C	0.586783	-0.000013	0.000051
C	2.019228	0.000048	-0.000004
C	3.219987	0.000088	-0.000046
C	-0.119329	1.207103	0.000021
H	0.428652	-2.141832	-0.000257
H	-2.045047	-2.143573	-0.000099
H	-3.286444	-0.000185	-0.000104
H	-2.045401	2.143499	-0.000018
H	4.283296	0.000145	-0.000094
H	0.428390	2.141893	-0.000008

**Vibrational frequencies**

137.2745	155.4812	366.7227
412.9701	474.7877	541.5413
555.6264	639.4061	663.8127
703.3922	711.5259	781.6306
782.0688	868.2194	948.2836
1002.296	1019.549	1023.236
1060.86	1112.24	1188.054
1211.568	1234.385	1320.032
1357.334	1488.024	1539.473
1648.272	1679.345	2244.399
3196.38	3205.343	3214.876
3222.268	3227.896	3483.02

***Vinyl (8)*****Cartesian coordinates**

C	0.705695	-0.145126	0.000043
C	-0.586139	0.030185	0.000008
H	1.596176	0.468312	-0.000193
H	-1.031826	1.027826	0.000019
H	-1.281689	-0.806492	-0.000133

**Vibrational frequencies**

714.0075	840.4995	933.957
1052.702	1393.892	1668.571
3080.482	3173.723	3244.261

***Ethynylamidogen (9)*****Cartesian coordinates**

N	0.199650	-1.209956	0.000000
C	-0.091959	1.273331	0.000000
C	0.000000	0.039543	0.000000
H	-0.671255	-1.740382	0.000000
H	-0.174542	2.332835	0.000000

**Vibrational frequencies**

391.4586 439.0174 482.5993  
492.8083 1089.818 1234.455  
1951.013 3473.279 3515.849

***Ethynyl (10)***

**Cartesian coordinates**

C	0.000000	0.000000	0.728771
C	0.000000	0.000000	-0.472490
H	0.000000	0.000000	-1.537681

**Vibrational frequencies**

479.621 479.621 2105.446  
3467.291

***3-pyrrolyl (11)***

**Cartesian coordinates**

N	-0.692252	0.807233	0.000165
C	0.672571	0.879890	0.000039
C	1.183526	-0.399846	-0.000164
C	0.053919	-1.241083	-0.000154
C	-1.095874	-0.509447	0.000047
H	-1.309487	1.599771	0.000317
H	1.180231	1.831633	0.000103
H	2.226314	-0.672027	-0.000303
H	-2.136147	-0.787091	0.000116

**Vibrational frequencies**

472.9041 555.0542 644.482  
669.2904 751.4329 848.2296  
868.6323 893.6301 1044.395  
1082.379 1169.544 1192.876  
1247.526 1400.868 1465.722  
1508.184 1558.444 3264.466  
3282.734 3287.616 3710.187

***2-aminoethenyl (12)***

**Cartesian coordinates**

N	-1.144817	-0.151780	-0.089763
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C	1.278259	-0.300036	0.025044
C	0.146671	0.368942	-0.005115
H	-1.840419	0.387918	0.401533
H	-1.205423	-1.133662	0.135339
H	2.329501	-0.067096	0.000136
H	0.180477	1.461862	-0.028242

### **Vibrational frequencies**

350.9439	473.396	546.6063
672.718	801.6183	830.63
1098.624	1232.48	1318.862
1652.527	1716.459	3088.343
3292.939	3590.155	3695.205

### ***Amino (13)***

#### **Cartesian coordinates**

N	0.000000	0.000000	0.143152
H	0.000000	0.801064	-0.501032
H	0.000000	-0.801064	-0.501032

#### **Vibrational frequencies**

1529.3416	3392.5823	3484.1199
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### ***Phenyl (14)***

#### **Cartesian coordinates**

C	0.000000	1.318531	0.000008
C	1.208548	0.629476	0.000001
C	1.221224	-0.768106	0.000011
C	0.000000	-1.393561	0.000033
C	-1.221224	-0.768106	0.000011
C	-1.208548	0.629476	0.000001
H	0.000000	2.402524	0.000151
H	2.146711	1.174245	-0.000154
H	2.155250	-1.318632	-0.000115
H	-2.155250	-1.318632	-0.000115
H	-2.146711	1.174245	-0.000154

#### **Vibrational frequencies**

402.9057	428.6025	603.4573
623.5396	680.8597	726.6003
828.7893	903.511	984.5328
992.4926	1008.27	1030.581
1058.743	1083.794	1180.029
1186.905	1310.543	1328.027
1471.488	1486.828	1608.889

1662.023 3187.815 3193.394  
3204.981 3208.334 3220.585

***Aminoethynyl (15)***

**Cartesian coordinates**

N -0.004320 -1.059142 0.000000  
C 0.006831 1.520722 0.000000  
C 0.000000 0.242827 0.000000  
H -0.005374 -1.583651 0.862850  
H -0.005374 -1.583651 -0.862850

**Vibrational frequencies**

285.9247 322.3054 514.9335  
1129.881 1152.854 1646.472  
2057.592 3567.927 3674.262

***2-pyrrolyl (16)***

**Cartesian coordinates**

N -1.064904 -0.445145 0.000032  
C -0.687321 0.882032 0.000087  
C 0.681667 0.925787 0.000017  
C 1.177639 -0.417923 -0.000085  
C 0.060537 -1.197019 -0.000073  
H -2.006708 -0.792243 0.000052  
H -1.423562 1.669346 0.000166  
H 1.284010 1.821557 0.000037  
H 2.205452 -0.739903 -0.000158

**Vibrational frequencies**

373.8766 503.5496 627.709  
709.4518 761.0483 860.9699  
879.454 893.6414 1027.084  
1071.113 1126.558 1190.207  
1259.544 1387.159 1438.875  
1487.524 1580.363 3248.38  
3281.974 3288.353 3721.472

***Phenylethynyl (17)***

**Cartesian coordinates**

C 0.045775 1.219540 0.013382  
C 1.426126 1.212650 -0.006714  
C 2.115813 -0.000010 -0.017253  
C 1.426105 -1.212662 -0.006715  
C 0.045755 -1.219531 0.013384  
C -0.671544 0.000009 0.023596

C	-2.068345	0.000016	0.040729
C	-3.340546	-0.000008	-0.055969
H	-0.510694	2.148691	0.019942
H	1.973361	2.147570	-0.015716
H	3.199878	-0.000024	-0.035097
H	1.973339	-2.147581	-0.015717
H	-0.510719	-2.148680	0.019947

### **Vibrational frequencies**

109.121	143.9347	246.8164
390.712	476.4153	484.9854
507.448	629.6306	687.8436
783.453	788.1472	862.7349
967.323	1013.887	1014
1029.06	1049.789	1112.732
1182.9	1188.033	1227.958
1322.98	1353.082	1478.244
1508.72	1612.226	1638.882
1988.97	3202.807	3213.566
3220.99	3230.08	3233.759

### ***2-ethynylphenyl (18)***

#### **Cartesian coordinates**

C	2.042478	-0.071590	-0.000012
C	3.242552	-0.077665	-0.000138
C	0.611950	-0.044191	0.000122
C	-0.098674	1.168226	0.000066
C	-1.486709	1.169338	0.000005
C	-2.200959	-0.024898	-0.000080
C	-1.522494	-1.246478	-0.000058
C	-0.154485	-1.193515	0.000242
H	4.305832	-0.089762	-0.000159
H	0.455537	2.100040	0.000016
H	-2.017623	2.113934	-0.000091
H	-3.285416	-0.011930	-0.000228
H	-2.060287	-2.187652	-0.000411

### **Vibrational frequencies**

134.285	152.1005	362.984
419.6871	467.5995	524.2418
553.1206	635.1337	668.6079
707.7231	707.8756	755.1998
776.0236	870.1455	964.1584
997.0964	1005.034	1053.838



1131.872	1181.193	1230.858
1261.052	1322.018	1453.837
1491.351	1600.44	1667.172
2248.818	3195.473	3205.052
3212.683	3225.013	3483.441

## Intermediates

*i1*

### Cartesian coordinates

C	1.702481	-0.867979	-0.015081
C	1.341575	0.413456	0.034922
N	-2.086606	-0.521561	-0.104387
C	-0.025430	0.941968	-0.017985
C	-1.104734	0.191484	-0.006517
H	0.974166	-1.667444	-0.112524
H	2.746098	-1.152002	0.036125
H	2.113003	1.173077	0.121069
H	-2.532200	-0.790271	0.771394
H	-0.178176	2.013995	-0.057385

### Vibrational frequencies

63.6979	147.0411	421.9808
439.4693	537.8321	681.3255
715.5785	874.8834	924.676
942.9165	1011.969	1032.406
1067.822	1168.965	1351.021
1443.706	1457.27	1709.998
2138.447	3153.326	3177.39
3210.213	3249.516	3521.053

*i2*

### Cartesian coordinates

C	0.662715	0.957050	0.000027
C	-0.823468	0.848144	0.000030
N	1.030155	-0.456284	-0.000205
C	-1.158629	-0.448515	-0.000031
C	0.042245	-1.335599	0.000168
H	1.050965	1.468114	0.887922
H	1.051069	1.468797	-0.887445
H	-1.479017	1.709393	0.000011
H	1.996806	-0.740865	0.000094
H	-2.168079	-0.837934	-0.000313

### Vibrational frequencies

370.0682	459.2703	718.4605
745.2103	830.9494	862.4973
962.8502	970.0482	999.4173
1004.056	1018.624	1122.484
1167.717	1293.468	1333.188
1364.673	1463.279	1512.648
1622.933	3058.503	3101.29
3221.651	3246.753	3659.528

### *i3*

#### **Cartesian coordinates**

N	0.981586	-0.581262	0.000037
C	-1.224799	-0.206955	-0.000070
C	-0.416202	-1.299351	-0.000057
H	1.480681	-0.924752	-0.819355
H	1.480595	-0.924794	0.819463
H	-2.304336	-0.283406	-0.000129
C	-0.521760	1.072569	0.000001
C	0.798616	0.869018	0.000065
H	-0.986145	2.050514	0.000002
H	1.642980	1.539583	0.000126

#### **Vibrational frequencies**

330.7959	535.3667	637.9702
656.3801	755.4084	800.1407
855.6273	890.7059	960.0267
975.9631	1025.965	1124.811
1139.489	1147.325	1212.343
1352.889	1512.226	1601.184
1667.79	3225.079	3238.813
3277.805	3504.244	3568.934

### *i4*

#### **Cartesian coordinates**

C	2.559979	-0.242879	-0.076285
C	1.405147	0.080807	0.009449
N	-2.293483	-0.129583	-0.074159
C	0.052948	0.511012	0.100650
C	-0.987152	-0.324886	0.127434
H	3.577856	-0.539604	-0.150231
H	-2.963309	-0.775874	0.305709
H	-2.624525	0.493076	-0.796746
H	-0.121185	1.585159	0.192897

#### **Vibrational frequencies**

161.6514	194.0814	232.0806
370.3277	437.3246	537.5451
558.2615	630.5023	698.8906
782.1758	981.1996	1115.421
1221.662	1316.657	1642.967
1712.933	2234.083	3099.703
3487.543	3580.925	3715.84

*i5*

**Cartesian coordinates**

C	2.121698	-0.569416	-0.037771
C	1.168685	0.165547	0.001355
N	-1.708311	-0.721229	0.046235
C	0.017573	1.003687	0.047618
C	-1.216521	0.504591	-0.097858
H	2.972736	-1.205089	-0.076962
H	-2.503032	-1.022712	-0.489932
H	-1.219648	-1.420759	0.590467
H	0.159513	2.070712	0.172718

**Vibrational frequencies**

130.6581	277.4076	327.9636
357.5233	484.8107	523.0174
629.7223	656.892	697.0277
802.4514	971.7997	1102.076
1158.694	1373.948	1627.297
1683.072	2212.267	3197.75
3484.952	3551.612	3717.04

*i6*

**Cartesian coordinates**

C	-1.000004	-0.694878	-0.000003
C	0.235091	-1.194960	-0.000024
N	-0.801507	0.751396	0.000021
C	1.278947	-0.196122	-0.000016
C	0.754860	1.058220	0.000012
H	-1.982291	-1.137137	-0.000001
H	-1.180080	1.220537	-0.821515
H	-1.180064	1.220507	0.821582
H	2.339629	-0.397239	-0.000030

**Vibrational frequencies**

336.9159	544.7477	623.3001
623.9609	730.3596	750.3533
829.2177	871.1613	998.2957

1055.348	1127.105	1145.846
1208.521	1258.856	1470.75
1593.095	1635.209	3256.964
3286.256	3498.561	3566.207

*i7*

**Cartesian coordinates**

C	2.153677	-0.487420	0.004119
C	1.175503	0.215633	0.001365
N	-1.492258	-0.901978	-0.064778
C	-0.007178	1.001179	0.005455
C	-1.231547	0.437871	0.003121
H	3.031613	-1.086560	0.000128
H	-2.383974	-1.227642	0.262551
H	-0.716645	-1.527855	0.090365
H	0.082932	2.079006	0.003608
H	-2.110845	1.073312	0.012427

**Vibrational frequencies**

146.3628	270.1539	375.2718
411.8161	488.5052	610.0686
620.9127	700.7592	710.3976
713.5904	969.4399	982.9693
1106.086	1189.001	1324.905
1435.746	1646.407	1722.18
2217.951	3194.827	3227.536
3485.095	3612.571	3742.589

*i8*

**Cartesian coordinates**

C	-2.161289	-0.443208	0.000037
C	-1.057800	0.237245	-0.000028
N	1.579162	-0.942865	-0.000056
C	0.055937	0.925024	-0.000064
C	1.398604	0.312671	0.000071
H	-2.632122	-0.742860	-0.930434
H	-2.632191	-0.742541	0.930578
H	2.575545	-1.154319	0.000072
H	0.000805	2.010185	-0.000200
H	2.221120	1.039202	0.000275

**Vibrational frequencies**

92.8515	152.3929	346.5927
418.7581	513.3616	737.2766
823.7469	876.7872	905.7569

934.7155	1008.648	1129.31
1136.04	1234.728	1379.417
1446.132	1484.785	1728.347
2071.558	3047.194	3153.56
3177.191	3237.308	3517.28

***i9***

**Cartesian coordinates**

C	1.058120	-0.536281	-0.000009
C	-0.202154	-1.337469	0.000002
N	0.676415	0.888294	-0.000017
C	-1.198002	-0.353166	0.000003
C	-0.644890	0.934387	0.000008
H	1.661663	-0.760472	-0.885740
H	1.661455	-0.760458	0.885867
H	1.283299	1.690807	0.000022
H	-2.266926	-0.526782	-0.000077
H	-1.152847	1.894018	0.000032

**Vibrational frequencies**

273.6518	430.0321	562.3233
769.4489	797.6613	872.1557
878.0469	906.906	960.5088
1005.386	1092.311	1169.588
1181.116	1201.728	1250.214
1363.847	1403.935	1483.161
1589.304	3067.538	3115.818
3202.725	3221.038	3682.945

***i9b***

**Cartesian coordinates**

C	1.214768	0.130564	0.000000
C	0.815542	-1.135213	0.000000
N	0.000000	1.137397	0.000000
C	-0.672598	-1.027359	0.000000
C	-1.142155	0.224765	0.000000
H	2.162591	0.651022	0.000000
H	0.009545	1.735146	0.826695
H	0.009545	1.735146	-0.826695
H	-1.338265	-1.884310	0.000000
H	-2.136759	0.644666	0.000000

**Vibrational frequencies**

357.3871	468.6032	497.1051
656.7494	661.3871	786.0959

821.4932	839.3158	988.9299
990.9668	997.1436	1124.302
1141.557	1158.491	1264.295
1339.27	1540.769	1593.048
1619.971	3197.384	3245.841
3267.96	3465.386	3542.68

### *ii0*

#### **Cartesian coordinates**

C	-0.204135	1.238204	-0.258137
C	-1.002593	-0.026154	-0.423847
C	-0.162597	-1.257128	-0.249682
C	1.161407	-1.206038	0.050654
C	1.834400	0.029421	0.209873
C	1.119036	1.239974	0.055642
N	-2.172470	-0.113028	0.473779
H	-0.741130	2.175145	-0.376641
H	-1.423004	-0.045043	-1.442669
H	-0.679184	-2.205464	-0.346507
H	1.715433	-2.130030	0.179846
H	2.888987	0.047623	0.455828
H	1.638176	2.183050	0.192794
H	-1.855470	0.002988	1.431282
H	-2.809621	0.653256	0.282596

#### **Vibrational frequencies**

93.3238	275.2226	318.0654
398.3086	445.2934	537.9635
588.0224	619.0193	703.7917
758.5601	810.0234	843.8518
888.1413	979.5542	988.6002
990.9675	998.5382	1038.878
1100.313	1117.52	1171.444
1179.106	1207.28	1311.867
1352.254	1380.198	1421.448
1465.64	1561.572	1623.598
1659.817	2969.87	3174.079
3188.069	3195.559	3208.563
3219.713	3515.198	3602.172

### *iii*

#### **Cartesian coordinates**

C	1.412090	0.000011	-0.012756
C	2.616470	0.000007	-0.007844
C	-0.016190	0.000006	-0.006271

C	-0.729351	1.205180	-0.002952
C	-2.116341	1.200677	0.004510
C	-2.816648	-0.000008	0.008553
C	-2.116329	-1.200686	0.004515
C	-0.729339	-1.205175	-0.002944
N	3.963095	0.000004	-0.067892
H	-0.185442	2.142465	-0.007218
H	-2.653231	2.142766	0.006715
H	-3.900591	-0.000013	0.014310
H	-2.653210	-2.142780	0.006724
H	-0.185422	-2.142455	-0.007202
H	4.405037	0.839094	0.276623
H	4.405021	-0.839176	0.276426

### **Vibrational frequencies**

87.4094	88.0317	94.2774
275.3092	323.1305	408.513
413.6261	452.8027	535.4198
556.7081	579.0886	641.4173
712.0649	730.2958	774.7131
862.1199	932.6997	994.8059
1011.201	1020.443	1052.674
1085.314	1111.119	1185.794
1204.868	1213.322	1314.29
1357.79	1368.199	1486.655
1547.232	1643.714	1651.128
1680.626	2386.575	3192.117
3199.76	3211.281	3217.34
3224.523	3588.101	3681.32

### ***i12***

#### **Cartesian coordinates**

C	-2.578877	-0.528340	-0.029517
C	-2.309317	0.833713	-0.045685
C	-0.997894	1.288693	-0.016340
C	0.070436	0.389705	0.030121
C	-0.212291	-0.980379	0.050262
C	-1.522444	-1.431944	0.019236
N	3.513930	-0.548958	0.049418
C	1.446110	0.907191	0.061598
C	2.522980	0.158876	-0.002369
H	-3.602116	-0.884897	-0.052673
H	-3.123005	1.549495	-0.080964
H	-0.797532	2.355091	-0.030204
H	0.601031	-1.697548	0.097754

H	-1.720442	-2.497903	0.037887
H	3.932324	-0.785239	-0.849149
H	1.600019	1.978613	0.127586

**Vibrational frequencies**

46.8709	115.5217	210.6329
342.2463	413.8508	428.5258
462.8184	477.6024	626.1019
636.9626	671.1904	712.6174
783.7837	845.6799	856.5009
883.0504	929.6544	992.8844
1012.787	1021.628	1024.829
1063.569	1113.199	1148.345
1186.573	1217.02	1224.519
1325.892	1364.962	1435.069
1504.812	1550.634	1654.347
1682.057	2142.686	3186.079
3188.941	3199.218	3200.688
3208.896	3221.058	3517.56

***i13***

**Cartesian coordinates**

C	1.981491	-0.811687	-0.264584
C	2.120490	0.625256	-0.031669
C	1.046262	1.408462	0.185320
C	-0.262699	0.789593	0.172718
C	-0.350236	-0.675660	0.448103
C	0.811138	-1.442753	-0.106095
N	-1.725275	-0.945175	0.021674
C	-1.477525	1.223143	-0.223377
C	-2.459773	0.114837	-0.289046
H	2.857949	-1.365400	-0.582199
H	3.109163	1.064230	-0.103977
H	1.137225	2.486110	0.255744
H	-0.336606	-0.829701	1.541791
H	0.714588	-2.511191	-0.265064
H	-2.136906	-1.856854	0.147444
H	-1.723384	2.241877	-0.493672

**Vibrational frequencies**

164.4852	185.889	338.6885
394.4453	491.4295	519.2063
534.83	591.9683	697.4991
706.3675	726.2358	795.2073
864.5025	883.076	897.2849



916.4682	979.2635	1001.54
1012.32	1020.359	1072.097
1114.978	1157.777	1186.444
1206.288	1239.107	1280.902
1331.053	1377.854	1408.158
1449.545	1490.955	1623.374
1636.101	1717.048	2978.278
3188.557	3197.957	3210.649
3218.951	3227.46	3650.88

#### *il4*

##### **Cartesian coordinates**

C	2.140830	-0.700417	-0.000006
C	0.934008	-1.398310	0.000001
C	-0.221394	-0.647991	0.000003
C	-0.255182	0.742622	-0.000002
C	0.959675	1.425103	-0.000009
C	2.143343	0.693558	-0.000011
H	3.077845	-1.243778	-0.000008
H	0.913814	-2.482750	0.000005
H	0.982534	2.508677	-0.000013
H	3.092258	1.218410	-0.000016
N	-1.609202	-1.096020	0.000011
C	-1.653598	1.169971	0.000002
C	-2.573028	0.174424	0.000008
H	-1.852932	-1.647666	0.820137
H	-1.852938	-1.647680	-0.820104
H	-1.944094	2.213164	-0.000002

##### **Vibrational frequencies**

184.4761	218.8045	377.4195
379.287	424.6881	538.553
570.6976	597.7453	636.6408
734.9038	743.3243	754.3159
790.6197	857.1382	873.8052
894.5343	904.4661	954.1488
1006.68	1048.148	1122.409
1155.53	1168.426	1172.291
1186.39	1207.929	1262.735
1309.853	1365.674	1494.791
1515.029	1566.858	1614.321
1661.725	1689.032	3196.687
3203.041	3215.458	3216.259
3226.113	3507.335	3572.813

***il5*****Cartesian coordinates**

C	-2.525514	0.552967	0.000086
C	-2.266599	-0.812566	0.000151
C	-0.962457	-1.283030	0.000049
C	0.104725	-0.383220	-0.000102
C	-0.148038	0.987615	-0.000149
C	-1.459051	1.443338	-0.000070
C	3.500276	0.563095	0.000371
N	1.414140	-0.882842	-0.000082
C	2.516774	-0.126160	-0.000281
H	-3.545320	0.918358	0.000157
H	-3.085695	-1.522830	0.000281
H	-0.769233	-2.351348	0.000141
H	0.680113	1.686078	-0.000277
H	-1.644778	2.511564	-0.000141
H	4.372978	1.167999	0.000558
H	1.532265	-1.882167	-0.000473

**Vibrational frequencies**

62.3602	133.1268	220.5619
262.9631	350.7191	419.4927
453.8979	466.7019	511.9297
531.5486	634.3429	656.5879
709.1232	739.1392	768.0778
836.6225	846.0732	908.5133
986.6969	1004.566	1017.847
1061.479	1108.759	1145.111
1186.222	1215.382	1292.394
1342.579	1365.035	1470.021
1539.165	1557.197	1669.768
1684.77	2272.529	3184.106
3197.687	3208.328	3220.846
3227.262	3495.969	3665.543

***il6*****Cartesian coordinates**

C	-2.091734	0.724387	-0.154058
C	-2.086774	-0.711475	-0.038423
C	-0.936459	-1.425016	0.107410
C	0.281677	-0.698648	0.117349
C	0.318620	0.762072	0.250874
C	-0.953222	1.443235	-0.054322
C	1.769861	1.079491	-0.066269

N	1.524046	-1.089011	-0.094944
C	2.518824	-0.059184	-0.176462
H	-3.038097	1.224310	-0.323524
H	-3.033083	-1.236543	-0.105834
H	-0.938659	-2.508764	0.120660
H	0.444420	0.907185	1.353945
H	-0.965376	2.525615	-0.112076
H	2.164244	2.082194	0.029741
H	1.773468	-2.060093	-0.214898

### Vibrational frequencies

173.09	202.6425	352.7139
405.4604	531.2087	534.9688
554.4575	596.5501	642.1932
713.6317	723.9636	790.4399
803.7371	823.8555	875.7259
882.7324	927.5244	982.0401
990.6691	1005.533	1013.863
1056.288	1116.433	1175.801
1190.909	1208	1243.52
1331.128	1397.299	1425.684
1456.708	1476.078	1550.795
1604.791	1693.195	2870.886
3196.514	3205.212	3217.368
3224.24	3232.975	3640.027

*il7*

### Cartesian coordinates

C	2.143259	0.695873	-0.000003
C	2.135815	-0.696220	0.000006
C	0.936633	-1.406097	0.000000
C	-0.230752	-0.665879	-0.000007
C	-0.247821	0.723347	0.000001
C	0.949252	1.417094	-0.000003
C	-1.697470	1.131981	0.000002
N	-1.586690	-1.096206	-0.000008
C	-2.515267	-0.151164	0.000031
H	3.089810	1.223901	0.000008
H	3.075439	-1.236536	0.000022
H	0.926451	-2.490201	0.000012
H	-1.981011	1.728762	-0.874095
H	0.963828	2.501583	-0.000004
H	-1.981017	1.728964	0.873983
H	-1.828560	-2.076645	-0.000030

**Vibrational frequencies**

193.439	207.868	353.6283
388.0755	425.6009	542.3043
578.9726	623.6437	705.5948
760.0154	764.2434	782.2174
868.0982	870.221	900.3262
906.2973	937.0438	961.6194
1005.025	1048.633	1132.008
1145.323	1184.198	1201.567
1227.302	1248.253	1316.7
1334.187	1372.421	1409.725
1461.749	1508.652	1539.49
1675.933	1692.598	3059.329
3095.375	3195.606	3202.917
3212.7	3224.069	3631.61

***i18*****Cartesian coordinates**

C	-1.990446	1.225387	0.089274
C	-2.980573	0.277457	0.071146
C	-2.372534	-1.003866	-0.120307
C	-1.036290	-0.743615	-0.209276
N	-0.785976	0.579871	-0.083240
H	-2.037396	2.295723	0.209355
H	-4.037643	0.466202	0.182979
H	-2.862544	-1.961125	-0.183774
H	0.125947	1.008313	-0.115248
C	2.707701	1.703854	0.084046
C	2.564114	0.523834	-0.098799
C	2.370032	-0.869018	-0.341736
C	1.707326	-1.669713	0.494712
H	2.860098	2.742683	0.254888
H	2.774321	-1.256430	-1.271685
H	1.565538	-2.718187	0.263835
H	1.297531	-1.302193	1.427971

**Vibrational frequencies**

38.5702	47.0104	62.1243
76.1559	96.7392	148.2271
234.0167	349.9845	459.4281
554.0833	571.0984	633.6425
702.6567	717.1909	720.09
733.2061	769.4812	863.6231
880.8245	895.8899	897.6606
1003.662	1023.171	1038.637

1082.618	1118.135	1131.806
1194.334	1277.055	1326.582
1394.526	1447.519	1451.354
1488.563	1580.758	1691.397
2231.933	3170.964	3184.37
3252.314	3269.799	3278.676
3285.037	3479.18	3653.751

***i19***

**Cartesian coordinates**

C	2.125431	1.263015	0.055215
C	2.856330	0.107872	0.153634
C	1.951170	-0.978018	0.001234
C	0.697926	-0.451201	-0.190936
N	0.818751	0.913427	-0.155818
H	2.422965	2.297098	0.120879
H	3.920708	0.045391	0.318010
H	2.188689	-2.030867	0.024815
H	0.047985	1.554257	-0.236049
C	-3.713060	0.774728	-0.140773
C	-2.754174	0.105814	0.204025
C	-1.663774	-0.644891	0.569409
C	-0.629596	-1.113655	-0.414955
H	-4.562391	1.342987	-0.434562
H	-1.502660	-0.856710	1.621386
H	-0.481854	-2.193464	-0.310703
H	-0.986219	-0.934671	-1.434165

**Vibrational frequencies**

19.8364	50.6303	161.2995
191.1323	308.0973	362.0236
401.7322	490.2271	514.5583
542.2933	625.2343	638.5207
665.2371	680.2963	729.6567
746.6146	807.8142	877.96
894.1547	905.8724	984.1814
1029.022	1053.082	1123.709
1144.61	1148.676	1203.079
1264.436	1298.889	1318.516
1415.602	1462.907	1475.722
1498.896	1524.119	1638.795
2026.27	3051.356	3097.702
3190.96	3251.199	3265.052
3285.183	3472.997	3696.943

***i20*****Cartesian coordinates**

C	-1.968316	-1.205846	0.003013
C	-2.737687	-0.106208	0.311747
C	-1.866881	0.991874	0.168456
C	-0.620578	0.588460	-0.218840
N	-0.708905	-0.784659	-0.320992
C	2.781881	-1.432886	0.017231
C	2.347735	-0.331685	0.217072
C	1.808711	1.010593	0.429285
C	0.629909	1.350903	-0.506943
H	-2.224587	-2.253607	-0.009189
H	-3.777517	-0.109554	0.594915
H	1.485699	1.108632	1.469879
H	0.075223	-1.384766	-0.519863
H	3.192197	-2.400760	-0.143939
H	2.615209	1.733333	0.271679
H	0.400817	2.412618	-0.398769
H	0.946655	1.195491	-1.543897

**Vibrational frequencies**

43.273	99.7961	132.3979
194.1259	312.3045	364.163
365.2601	506.9607	549.4173
609.2557	638.1629	674.3734
693.9304	709.0446	718.9438
836.8256	844.9505	889.6745
915.913	974.9392	1010.652
1045.049	1096.364	1147.258
1190.512	1216.159	1248.764
1299.891	1356.952	1371.264
1422.02	1464.507	1474.334
1490.682	1510.021	1617.175
2243.917	3058.285	3062.317
3108.48	3128.514	3259.557
3279.564	3482.83	3675.012

***i21*****Cartesian coordinates**

C	-1.720469	1.080805	0.054947
C	-2.401158	-0.109528	0.090635
N	-1.482457	-1.128647	0.017521
C	-0.224251	-0.606632	-0.053497
C	-0.336157	0.765226	-0.039508
C	0.881753	1.586580	-0.138135

C	2.028267	0.945633	-0.005328
C	2.235413	-0.496801	0.299338
C	1.061135	-1.344184	-0.257571
H	-2.163974	2.063471	0.102316
H	-3.455541	-0.315464	0.178040
H	-1.705305	-2.107936	0.026087
H	0.812474	2.655100	-0.314702
H	3.179345	-0.866849	-0.108622
H	2.289600	-0.614264	1.389716
H	1.216579	-1.516478	-1.330843
H	1.056819	-2.323640	0.230080

### Vibrational frequencies

132.7684	221.7734	255.2135
379.7357	391.0401	463.0701
495.192	581.6789	638.1408
664.7575	705.9731	725.0007
762.0697	838.2333	866.2207
877.1145	920.3071	932.5229
993.004	1027.167	1091.025
1115.351	1186.827	1190.551
1204.803	1220.894	1292.087
1327.902	1343.367	1391.017
1458.069	1471.704	1492.509
1522.446	1543.145	1627.518
1705.364	3021.31	3028.69
3089.621	3096.947	3188.456
3260.12	3285.908	3713.41

### *i22*

#### Cartesian coordinates

N	-1.563830	-1.066109	-0.000068
C	-2.419313	0.013757	-0.000120
C	-1.670642	1.156016	0.000001
C	-0.294561	0.760007	0.000130
C	-0.273145	-0.626730	0.000067
C	0.929103	1.491879	0.000122
C	2.135366	0.767296	-0.000118
C	0.953918	-1.469138	0.000202
C	2.182423	-0.601008	-0.000177
H	-1.850219	-2.028772	-0.000219
H	-3.488051	-0.127624	-0.000247
H	-2.053953	2.164591	0.000002
H	0.968476	-2.140370	-0.874156
H	0.930266	2.574523	0.000216

H	3.072018	1.315659	-0.000333
H	0.968627	-2.139729	0.875081
H	3.140764	-1.107987	-0.000510

**Vibrational frequencies**

133.1089	220.7678	274.7435
385.3056	467.6087	503.3496
503.3654	598.5214	626.2908
653.5806	673.4051	724.912
744.8995	765.2524	869.8615
885.3511	924.5399	944.7
947.177	966.4468	1071.283
1096.256	1117.647	1183.611
1189.637	1200.757	1245.383
1279.093	1365.481	1382.633
1438.067	1461.318	1472.626
1497.247	1538.258	1588.521
1622.734	2960.179	2968.578
3177.374	3198.437	3216.113
3255.503	3279.941	3712.998

***i23***

**Cartesian coordinates**

C	-1.867357	-0.594154	0.002918
C	-3.063190	-0.721031	-0.010409
C	-0.451870	-0.400594	0.008187
C	0.069853	0.910963	0.010340
C	1.460824	1.073843	0.000190
C	2.303284	-0.023531	-0.008688
C	1.789476	-1.318267	-0.005549
C	0.417631	-1.495685	0.002813
N	-0.770758	2.002195	0.068961
H	-4.117585	-0.858165	-0.013581
H	1.874792	2.076919	0.006812
H	3.376267	0.133435	-0.016850
H	2.452627	-2.174303	-0.010853
H	-0.009926	-2.491488	0.001273
H	-1.733759	1.835791	-0.178440
H	-0.399020	2.873183	-0.269900

**Vibrational frequencies**

122.6125	152.2703	226.7346
364.2214	381.9108	387.1482
468.3434	484.4109	515.5498
564.2917	580.2357	602.0317



624.4936	739.6834	748.8255
757.968	767.3743	864.919
870.4828	960.882	992.759
1063.145	1090.991	1169.114
1192.624	1227.381	1301.158
1352.517	1355.569	1504.299
1544.799	1643.161	1665.261
1690.712	2229.787	3189.149
3203.12	3213.1	3226.639
3481.019	3614.922	3728.71

### *i24*

#### **Cartesian coordinates**

C	1.834088	-0.369233	-0.000002
C	3.124777	-0.460306	0.000029
C	0.516632	-0.293798	-0.000019
C	-0.172483	1.034562	-0.000008
C	-1.639869	0.979229	0.000023
C	-2.311753	-0.183084	0.000021
C	-1.626795	-1.463114	-0.000008
C	-0.286315	-1.515120	-0.000023
N	0.520161	2.109552	-0.000027
H	3.682952	-0.487523	-0.930930
H	-2.169305	1.927128	0.000048
H	-3.396738	-0.177735	0.000040
H	-2.212796	-2.374272	-0.000008
H	0.240792	-2.462009	-0.000041
H	3.682904	-0.487545	0.931016
H	-0.098623	2.920280	-0.000015

#### **Vibrational frequencies**

43.8786	140.3165	178.2156
324.5079	390.0804	445.0254
459.9607	478.4293	570.8295
591.6271	594.8652	697.4922
743.0804	774.1092	846.0584
867.246	884.9701	906.1996
992.8769	999.775	1003.485
1012.784	1089.677	1174.614
1208.47	1251.162	1264.024
1383.98	1413.639	1460.603
1482.829	1642.23	1673.172
1733.925	2051.401	3140.976
3184.853	3199.238	3209.671

3223.823 3223.988 3497.744

***i25***

**Cartesian coordinates**

C	-2.180489	-0.665976	0.000018
C	-2.097710	0.748347	0.000121
C	-0.902994	1.429084	0.000036
C	0.275670	0.656671	-0.000143
C	0.226592	-0.773467	-0.000085
C	-1.033501	-1.416856	-0.000077
C	2.401488	-0.152180	0.000170
N	1.557163	1.047981	-0.000344
C	1.516361	-1.355410	-0.000005
H	-3.154838	-1.138755	0.000027
H	-3.020900	1.319404	0.000269
H	-0.874496	2.512486	0.000119
H	-1.058256	-2.500712	-0.000131
H	3.052969	-0.175787	-0.881699
H	3.051419	-0.175852	0.883242
H	1.871457	2.002067	0.000375

**Vibrational frequencies**

132.6969	214.3821	269.8982
355.5716	412.3745	452.4197
547.8742	551.9225	609.3625
762.686	765.8848	771.1062
790.2553	859.3434	863.1028
900.1066	963.2748	996.0798
1012.231	1018.881	1031.265
1147.735	1165.207	1184.864
1205.017	1253.17	1312.803
1333.395	1380.334	1393.945
1446.898	1492.202	1559.738
1620.942	1697.277	3050.001
3091.219	3187.395	3209.842
3213.125	3229.457	3703.119

***i26***

**Cartesian coordinates**

N	-0.916243	-1.294915	0.052375
C	-2.019475	1.003332	0.040995
C	-1.498209	-0.079740	0.027581
H	0.071024	-1.270833	0.275563
H	-1.109326	-1.866475	-0.756947
H	-2.514495	1.941780	0.085385

C	1.731222	0.669600	-0.124173
C	2.708635	0.004536	0.068429
H	0.844023	1.241797	-0.285803
H	3.589432	-0.568229	0.238190

### **Vibrational frequencies**

56.9391	62.8232	91.4994
123.5705	153.4879	390.9734
466.8054	523.5801	648.4025
699.0631	708.0244	731.0722
798.2959	810.554	1101.568
1222.283	1652.222	2081.604
2271.017	3396.273	3492.82
3513.784	3561.441	3661.171

### ***i27***

#### **Cartesian coordinates**

N	-0.911355	1.330572	0.000008
C	-2.095497	-0.872550	-0.000034
C	-1.482371	0.203794	-0.000007
H	0.107280	1.238048	0.000240
H	-2.698178	-1.747995	-0.000079
C	2.614985	0.063079	-0.000071
C	1.733875	-0.747917	0.000067
H	3.406765	0.774452	-0.000123
H	0.937666	-1.456948	0.000174

### **Vibrational frequencies**

55.5285	75.4991	84.7167
144.6458	265.2216	388.2124
463.2919	495.2643	499.1427
704.7186	722.0106	800.755
825.0053	1108.135	1236.741
1938.032	2083.525	3411.213
3469.247	3477.831	3520.947

### ***i28***

#### **Cartesian coordinates**

N	-0.045064	0.504200	0.000092
C	2.397156	-0.194403	-0.000061
C	1.244695	0.143335	0.000005
H	-0.266603	1.485947	-0.000015
H	3.417643	-0.488013	-0.000115
C	-1.097694	-0.423692	0.000055
C	-2.380862	-0.150938	-0.000083

H	-0.749002	-1.453688	0.000169
H	-3.066358	0.680546	-0.000181

**Vibrational frequencies**

51.7159	179.9626	357.6055
401.7932	456.7266	505.3531
576.322	610.1542	744.5962
776.6292	873.5463	1078.52
1224.365	1290.474	1470.289
1698.262	2275.091	3168.301
3293.376	3498.252	3666.819

***i29***

**Cartesian coordinates**

N	-0.035331	0.868742	-0.000020
C	2.099148	-0.508358	0.000005
C	1.095066	0.149190	-0.000003
C	-1.310148	0.296232	0.000004
C	-1.584325	-0.987419	0.000001
H	0.037600	1.870661	0.000071
H	2.988889	-1.087838	0.000011
H	-2.108976	1.038823	0.000017
H	-2.468635	-1.600710	0.000002

**Vibrational frequencies**

128.0328	152.2298	229.3893
394.1578	474.1729	536.1078
609.1225	637.5218	739.0143
818.075	866.0022	977.8898
1222.97	1313.292	1516.498
1712.056	2276.253	3124.426
3300.311	3496.061	3691.56

***i30***

**Cartesian coordinates**

N	-0.929914	-1.158547	0.000158
C	-2.015209	1.177467	-0.000332
C	-1.509994	0.004359	0.000053
C	2.488505	-0.129879	-0.000276
C	1.659742	0.735925	0.000347
H	-1.463087	-2.015684	-0.000082
H	0.084155	-1.214772	0.000229
H	3.253682	-0.869964	-0.000847
H	0.896383	1.483019	0.000845

**Vibrational frequencies**

68.9301	78.5561	105.5091
185.9156	214.2595	314.7817
352.3513	556.6144	704.7189
722.4234	809.8845	836.6045
1136.927	1170.488	1631.624
2059.401	2075.022	3397.351
3508.371	3512.575	3655.456

***i31*****Cartesian coordinates**

N	-2.399706	0.163144	-0.075067
C	0.119557	-0.228970	-0.004799
C	-1.071524	-0.046425	-0.007897
H	-2.711465	1.062055	0.260262
H	-2.973403	-0.597908	0.255539
C	2.452331	0.468990	0.004853
C	1.526392	-0.467135	0.007410
H	2.490816	1.549015	-0.006859
H	1.831459	-1.513926	0.019125

**Vibrational frequencies**

110.1905	148.9875	195.5874
340.5402	453.9977	523.5649
566.1844	686.8802	754.988
866.3746	925.2816	1203.049
1262.473	1306.883	1648.996
1658.695	2375.985	3120.289
3253.05	3592.267	3686.281

***i32*****Cartesian coordinates**

N	-0.795880	0.746296	0.000035
C	0.084390	-1.269168	-0.000019
C	-1.149334	-0.794430	0.000027
C	0.664458	0.909764	-0.000009
C	1.184317	-0.324905	-0.000042
H	-1.241383	1.152733	0.821466
H	-1.241434	1.152753	-0.821360
H	1.108932	1.893036	-0.000011
H	2.242055	-0.550160	-0.000078

**Vibrational frequencies**

305.9141	493.7638	567.6765
655.9753	728.7904	766.2387

835.3373 949.4413 962.0774  
1051.764 1112.919 1134.615  
1148.675 1329.929 1497.944  
1592.441 1626.281 3235.28  
3267.561 3500.332 3569.381

### *i33*

#### **Cartesian coordinates**

N 0.973493 1.215571 -0.188095  
C 1.586593 -1.135691 -0.258317  
C 1.690984 0.094336 0.205077  
H 0.813068 1.888687 0.544619  
H 0.130334 1.018285 -0.707990  
H 2.139782 -2.054820 -0.158836  
H 2.449687 0.300884 0.965521  
C -2.786095 0.066991 -0.043326  
C -1.788439 -0.554631 0.186740  
H -3.679195 0.609474 -0.243876  
H -0.886393 -1.097538 0.376183

#### **Vibrational frequencies**

51.7619 69.7204 83.2574  
112.1023 162.9276 370.1169  
481.7732 544.8754 682.591  
702.5647 712.6341 804.8798  
810.4602 826.7557 845.2793  
1108.035 1244.757 1324.985  
1658.651 1710.789 2076.3  
3081.272 3288.021 3371.895  
3506.651 3590.472 3696.563

### *i34*

#### **Cartesian coordinates**

N 1.387963 -0.876445 -0.054250  
C -0.026154 1.083482 -0.005140  
C 1.176327 0.472545 -0.004978  
C -1.522699 -0.917174 -0.015127  
C -1.300954 0.384066 0.016752  
H 0.589131 -1.472253 0.124535  
H 2.275235 -1.226162 0.262319  
H -0.046748 2.164948 -0.010144  
H 2.080947 1.072583 -0.000822  
H -2.385754 -1.566513 -0.024889  
H -2.187673 1.025002 0.079711

**Vibrational frequencies**

188.2946	236.6384	326.9767
416.9851	433.8797	544.0562
622.937	700.8968	730.4724
845.4477	897.8074	966.6436
978.9733	1124.332	1189.417
1268.43	1330.946	1451.218
1624.896	1649.248	1725.072
3054.697	3184.633	3230.722
3255.274	3542.761	3720.814

***i35*****Cartesian coordinates**

N	-1.163437	-0.000126	0.030522
C	1.035098	0.699128	0.018541
C	-0.265264	1.182285	-0.091244
C	-0.264990	-1.182371	-0.091606
C	1.035200	-0.698920	0.018497
H	-1.878114	-0.000141	-0.695583
H	-1.664610	-0.000362	0.932738
H	1.911753	1.328753	0.051104
H	-0.689015	2.141452	0.160311
H	-0.688312	-2.141361	0.161483
H	1.912093	-1.328194	0.051168

**Vibrational frequencies**

268.6474	313.0924	427.4146
546.7707	720.4059	778.023
805.5896	846.4239	890.1828
968.874	969.6083	1079.563
1094.022	1130.867	1157.365
1218.089	1310.656	1421.464
1501.059	1512.711	1637.677
3190.258	3237.246	3251.926
3268.637	3275.291	3463.79

***i36*****Cartesian coordinates**

C	1.500603	-0.948105	-0.082388
C	1.305667	0.366086	0.064054
H	0.690495	-1.635063	-0.299963
H	2.497783	-1.367595	-0.020411
H	2.179547	0.990225	0.240166
N	-1.658420	-0.658578	0.064056
C	0.039500	1.103207	0.003739

C	-1.178260	0.574256	-0.140731
H	-2.541201	-0.928504	-0.334383
H	-1.332539	-1.207160	0.849923
H	0.109796	2.185484	0.048225

**Vibrational frequencies**

111.2143	191.9516	287.8191
366.482	395.7531	468.4369
650.1394	705.7208	834.1038
926.695	927.9004	1036.211
1054.136	1135.067	1154.296
1334.966	1385.285	1445.422
1632.39	1660.784	1709.261
3153.076	3166.879	3182.027
3252.06	3550.773	3705.261

***i37***

**Cartesian coordinates**

C	0.908077	0.803360	0.000039
C	-0.559346	1.084019	-0.000033
N	0.922456	-0.705042	-0.000035
C	-1.268791	-0.111855	0.000004
C	-0.548101	-1.306407	0.000040
H	1.438517	1.174015	-0.883879
H	1.438387	1.173903	0.884084
H	-0.961295	2.087227	-0.000055
H	1.394527	-1.087484	-0.813838
H	1.394682	-1.087575	0.813633
H	-2.353047	-0.139483	0.000004

**Vibrational frequencies**

59.0037	422.1573	515.2199
602.7373	733.4272	766.3
831.3209	918.3782	930.838
966.4717	993.2997	1073.57
1135.87	1143.544	1215.776
1283.824	1320.289	1387.994
1411.292	1505.147	1646.926
3036.761	3071.851	3206.901
3247.188	3532.362	3593.569

***i38***

**Cartesian coordinates**

N	1.430666	-0.912760	-0.000010
C	0.020300	1.037751	0.000001



C	1.291230	0.367370	0.000005
C	-1.571931	-0.866074	0.000006
C	-1.267782	0.462418	-0.000006
H	-0.790887	-1.614177	0.000026
H	2.419747	-1.155425	-0.000001
H	0.070380	2.122436	0.000002
H	2.156516	1.042007	0.000026
H	-2.608118	-1.185100	0.000001
H	-2.093199	1.170792	-0.000020

### **Vibrational frequencies**

160.4934	284.3844	322.0995
414.2569	565.6806	678.8743
766.2175	842.9517	923.5301
934.5526	1020.713	1070.6
1096.027	1172.817	1252.148
1284.388	1395.184	1431.384
1490.364	1559.825	1620.511
3046.476	3159.051	3171.149
3193.275	3288.793	3516.858

### ***i39***

#### **Cartesian coordinates**

C	1.148625	0.389149	0.020070
C	-0.101958	1.220690	-0.008415
N	0.626535	-0.972778	-0.105018
C	-1.194384	0.376722	0.014820
C	-0.754264	-0.940911	0.013560
H	1.844409	0.621994	-0.798167
H	1.710629	0.517399	0.961670
H	-0.107295	2.299911	-0.028284
H	1.138786	-1.725635	0.323439
H	-2.232437	0.676805	0.012654
H	-1.327951	-1.854932	0.023599

#### **Vibrational frequencies**

268.9579	459.5879	525.2713
561.3912	628.887	798.1764
851.3241	885.0427	945.3073
973.294	1000.594	1065.298
1119.178	1165.123	1183.645
1302.115	1335.832	1404.406
1467.587	1501.287	1526.71
2938.978	3003.014	3237.111
3256.089	3269.113	3665.591

*i40*

**Cartesian coordinates**

C	2.012464	1.044162	0.006503
C	2.327695	-0.311756	0.040360
C	1.348285	-1.319618	0.024470
C	0.056971	-0.853381	-0.019960
C	-0.272412	0.502571	-0.028321
C	0.681676	1.490924	-0.032028
C	-2.898164	0.658405	0.064757
N	-1.300367	-1.293094	-0.141356
C	-1.702808	0.099715	-0.028341
H	2.816250	1.770941	0.015980
H	3.372290	-0.601264	0.076119
H	1.612467	-2.369432	0.044929
H	-2.992972	1.733114	0.144666
H	0.445635	2.548276	-0.046711
H	-3.800505	0.059065	0.062239
H	-1.672842	-1.955177	0.527624

**Vibrational frequencies**

127.8078	245.5763	260.3149
389.3408	457.0766	516.0753
530.4303	567.7945	644.1039
665.7486	741.7787	765.6528
784.1695	814.8924	846.9182
878.7476	885.7543	947.8219
950.3303	996.9736	1023.166
1070.751	1136.47	1174.929
1197.029	1251.942	1275.072
1331.091	1402.874	1436.954
1492.282	1510.362	1683.979
1696.59	1802.694	3172.851
3191.256	3206.129	3217.365
3223.752	3268.552	3590.598

*i41*

**Cartesian coordinates**

N	0.753058	0.921891	-0.416442
C	1.426237	-0.027184	-1.155968
C	2.429799	-0.536717	-0.374125
C	2.373105	0.105607	0.904945
C	1.314381	0.960005	0.813932
C	-2.663771	1.484254	0.051239
C	-2.436568	0.303585	0.014687

C	-2.201779	-1.104173	-0.054115
C	-1.118242	-1.703596	0.437476
H	-0.135687	1.330731	-0.658082
H	1.121148	-0.263669	-2.162333
H	3.148889	-1.283146	-0.675868
H	3.034513	-0.037972	1.743073
H	-2.878626	2.524465	0.109750
H	-2.974816	-1.685559	-0.548302
H	-0.999478	-2.776630	0.345518
H	-0.326327	-1.152141	0.932916

### Vibrational frequencies

24.235	53.9048	64.7416
100.5582	116.5974	151.9275
247.547	335.2023	458.3587
569.5039	608.7695	637.1357
675.3729	708.863	712.9731
718.5992	768.1419	863.0633
882.6733	893.9833	899.3538
1012.827	1023.546	1030.05
1079.081	1116.974	1129.925
1192.447	1266.714	1324.491
1390.518	1439.473	1451.869
1484.508	1578.796	1701.569
2231.029	3160.991	3180.628
3256.818	3259.983	3282.916
3289.137	3478.808	3670.719

*i42*

### Cartesian coordinates

N	0.925713	-0.884051	-0.148475
C	2.245283	-1.224779	-0.055352
C	2.965647	-0.073577	0.146440
C	2.040934	1.000496	0.175965
C	0.781803	0.471135	-0.009406
C	-0.511785	1.140277	-0.063964
C	-1.664826	0.556638	-0.252691
C	-2.843609	-0.068837	-0.445877
C	-3.659023	-0.566887	0.565764
H	0.161394	-1.521567	-0.292303
H	2.563891	-2.251221	-0.140348
H	4.036256	-0.009967	0.261170
H	2.262026	2.047509	0.317202
H	-0.477817	2.221678	0.068748
H	-3.178353	-0.183161	-1.476583

H	-4.596520	-1.053138	0.329240
H	-3.377410	-0.468563	1.606926

### **Vibrational frequencies**

54.9773	64.1247	149.7049
185.1435	265.8835	347.7045
431.9738	529.981	541.5088
567.4392	636.1602	673.7792
731.6801	736.8292	760.9461
808.9925	852.3149	901.1264
905.1176	921.2643	953.8122
991.5361	1056.985	1083.305
1125.118	1146.457	1192.049
1243.315	1311.101	1318.401
1398.868	1467.689	1493.139
1495.285	1518.434	1633.445
1919.623	3128.215	3139.141
3171.285	3255.567	3267.928
3277.147	3286.436	3697.131

### ***i43***

#### **Cartesian coordinates**

N	1.651358	1.051058	-0.157110
C	2.921949	0.572574	-0.029477
C	2.860936	-0.788622	0.194058
C	1.493319	-1.094958	0.187222
C	0.729662	0.027981	-0.025775
C	-0.694731	0.261227	-0.120317
C	-1.629203	-0.697577	-0.162914
C	-3.070309	-0.449658	-0.212441
C	-3.700183	0.578778	0.355375
H	1.413795	2.010506	-0.342486
H	3.775676	1.227306	-0.106416
H	3.698409	-1.451344	0.339340
H	-1.307955	-1.736354	-0.186436
H	-1.009743	1.302119	-0.173275
H	-3.659828	-1.188409	-0.751271
H	-4.770319	0.711706	0.248122
H	-3.168175	1.308594	0.957807

#### **Vibrational frequencies**

46.5045	96.0549	118.4941
196.2427	235.5878	314.2166
425.5364	466.8339	536.6213
606.8324	642.9136	673.7582

696.6059	793.6381	850.307
879.3602	885.7371	950.6723
977.5256	985.3523	997.9903
1035.108	1087.798	1114.861
1135.678	1197.454	1248.819
1315.94	1343.683	1355.703
1421.943	1459.72	1463.741
1496.015	1593.863	1705.918
1727.619	3152.276	3154.198
3160.856	3172.349	3248.18
3266.371	3285.884	3697.524

*i44*

**Cartesian coordinates**

N	1.808396	0.894007	-0.270557
C	2.757875	-0.085744	-0.294859
C	2.168989	-1.250988	0.128742
C	0.811214	-0.960342	0.407191
C	0.600384	0.380416	0.141455
C	-0.559689	1.246422	0.274413
C	-1.852818	0.907890	0.154043
C	-2.360182	-0.402456	-0.242411
C	-3.623450	-0.764466	-0.193014
H	1.947188	1.841029	-0.576706
H	3.769172	0.121812	-0.605269
H	2.661937	-2.203759	0.241194
H	0.077826	-1.639891	0.811343
H	-0.339110	2.286160	0.507535
H	-1.628178	-1.115678	-0.633341
H	-4.200043	-1.643076	-0.444751
H	-2.601512	1.670961	0.340533

**Vibrational frequencies**

56.6284	100.1811	185.0822
209.5747	274.676	361.8998
457.3799	501.0313	603.1715
634.5957	644.5528	698.3308
732.616	761.2537	792.1029
817.3178	839.2007	890.4335
905.2202	906.9773	989.5727
1005.616	1070.673	1100.833
1139.6	1153.461	1249.485
1260.909	1279.625	1311.272
1434.057	1479.737	1480.283

1517.783	1622.515	1660.725
1718.176	3076.163	3148.397
3190.019	3251.017	3256.407
3269.475	3286.866	3704.956

*i45*

**Cartesian coordinates**

C	1.478060	-1.327374	0.048927
C	2.461852	-0.438339	-0.378600
N	1.982275	0.864906	-0.348423
C	0.690475	0.798509	0.092225
C	0.365113	-0.529761	0.341500
C	-0.547492	1.321899	0.483201
C	-1.049473	-0.109565	0.808891
C	-2.204077	-0.663340	0.029673
C	-2.922753	0.013102	-0.855852
H	1.607505	-2.396487	0.119197
H	3.470334	-0.638379	-0.705233
H	2.507862	1.677724	-0.613365
H	-0.991383	2.301120	0.578971
H	-1.208099	-0.284268	1.879865
H	-2.441148	-1.707170	0.228900
H	-3.744895	-0.450737	-1.389341
H	-2.706322	1.053068	-1.079826

**Vibrational frequencies**

71.9488	151.9094	158.3791
262.519	337.9995	434.3287
464.7447	475.0683	582.9858
617.1491	620.1849	675.0355
699.1274	759.2406	837.5982
859.9038	882.7912	933.9011
961.6447	997.0286	1038.85
1051.212	1080.937	1099.516
1130.767	1195.522	1206.913
1273.048	1314.587	1332.449
1350.904	1419.604	1451.134
1485.833	1521.275	1602.997
1736.494	3046.956	3142.306
3156.801	3238.254	3253.218
3256.729	3279.274	3723.012

*i46*

**Cartesian coordinates**

N	1.731017	-0.962485	-0.107952
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C	2.684728	0.007575	-0.123476
C	2.058093	1.217329	0.056143
C	0.673402	0.960894	0.176651
C	0.478638	-0.406688	0.065219
C	-0.666834	-1.283864	0.116639
C	-1.989846	-1.037689	0.058777
C	-2.719586	0.214600	-0.104203
C	-2.287523	1.458494	-0.084969
H	1.902756	-1.943100	-0.244587
H	3.727063	-0.232497	-0.259816
H	2.543097	2.179531	0.103589
H	-0.105985	1.685437	0.351710
H	-0.401766	-2.336662	0.203077
H	-2.630462	-1.912534	0.111348
H	-3.794490	0.082138	-0.271412
H	-2.743753	2.431175	-0.202930

### **Vibrational frequencies**

31.0765	107.8494	175.5827
227.379	236.6488	418.5995
464.0056	492.2024	615.3287
629.4395	634.4309	697.652
743.1205	754.3234	773.2464
830.3624	885.9378	893.6624
899.0955	908.7621	979.7074
993.8684	1017.245	1075.013
1138.132	1156.519	1249.576
1272.255	1304.145	1328.439
1440.654	1480.519	1492.977
1516.437	1620.737	1651.839
1709.121	3054.822	3143.974
3183.514	3246.911	3253.722
3267.131	3286.127	3705.19

### ***i47***

#### **Cartesian coordinates**

C	2.009415	1.271511	-0.050882
C	2.678660	0.065485	-0.092677
N	1.766951	-0.943739	-0.015135
C	0.480845	-0.433261	0.071751
C	0.650712	0.931548	0.036192
C	-0.654212	-1.323322	0.148059
C	-1.963466	-1.054705	-0.006200
C	-2.609540	0.227131	-0.261462
C	-2.231662	1.425406	0.189394

H	2.455720	2.251558	-0.094566
H	3.733562	-0.140587	-0.185975
H	1.989891	-1.923694	-0.051056
H	-0.392304	-2.367899	0.305023
H	-2.632357	-1.911170	0.009093
H	-3.511515	0.169744	-0.868254
H	-2.782242	2.319596	-0.080366
H	-1.393926	1.549867	0.866989

### Vibrational frequencies

64.3746	77.2176	155.3492
208.4553	239.3554	401.5464
442.5794	468.9271	583.5847
618.2632	637.4383	690.4986
715.9476	800.4508	809.0554
856.6153	884.8858	937.8154
947.7632	993.0247	1004.644
1027.309	1096.593	1114.617
1147.408	1200.146	1250.104
1279.603	1341.123	1401.68
1444.25	1463.882	1486.517
1506.905	1594.911	1687.364
1716.755	3143.169	3151.708
3157.64	3177.914	3244.792
3264.841	3284.667	3695.529

*i48*

### Cartesian coordinates

N	1.549301	-1.123657	0.011660
C	0.237492	-0.719585	0.184005
C	0.257936	0.766490	0.427440
C	-0.991036	1.427304	-0.074037
C	-2.127978	0.691270	-0.200374
C	-2.135433	-0.721350	-0.042294
C	-0.921540	-1.431757	0.064695
C	1.638996	1.141691	-0.062631
C	2.331443	0.014592	-0.244141
H	1.762192	-2.005592	-0.424526
H	0.270537	0.913427	1.532698
H	-0.990471	2.500594	-0.226641
H	-3.056070	1.186001	-0.467612
H	-3.067895	-1.264158	-0.134878
H	-0.904739	-2.511339	-0.043131
H	2.031687	2.145222	-0.119834
H	3.370375	-0.110492	-0.513670



**Vibrational frequencies**

149.1073	202.5236	358.4694
393.9104	478.765	522.7119
537.8631	551.067	581.7882
666.9839	695.1791	716.9755
749.1358	841.309	855.7258
866.7443	878.3549	920.0336
961.1457	1000.974	1047.198
1059.865	1114.731	1128.017
1138.799	1169.273	1230.028
1260.039	1271.012	1326.545
1360.317	1397.667	1440.526
1460.077	1565.141	1649.076
1674.377	2806.154	3185.804
3188.739	3207.489	3221.95
3247.975	3271.995	3667.708

*i49***Cartesian coordinates**

N	1.614089	-1.064737	0.000003
C	0.295741	-0.675122	0.000026
C	0.274849	0.719346	0.000017
C	-1.016494	1.473145	0.000045
C	-2.207730	0.556073	-0.000047
C	-2.107243	-0.803929	-0.000032
C	-0.863709	-1.478354	0.000042
C	1.616530	1.162547	-0.000018
C	2.417936	0.043064	-0.000033
H	1.935809	-2.015657	-0.000025
H	-1.069281	2.145076	0.870761
H	-1.069230	2.145265	-0.870524
H	-3.188160	1.019963	-0.000129
H	-3.016588	-1.396175	-0.000084
H	-0.809829	-2.559996	0.000063
H	1.967177	2.183577	-0.000025
H	3.492198	-0.049512	-0.000064

**Vibrational frequencies**

126.8114	233.7246	269.9953
387.4216	454.9212	494.1314
506.7614	597.6794	620.9932
639.131	673.9448	711.3409
746.2854	748.5178	852.6095
884.7926	920.2892	941.2937

943.2587	967.1412	1061.949
1079.423	1128.671	1190.324
1199.865	1216.424	1242.68
1263.033	1356.597	1389.277
1422.858	1442.558	1458.823
1504.245	1538.336	1570.113
1625.194	2982.488	2992.571
3179.387	3203.995	3218.158
3252.784	3280.588	3719.026

### *i50*

#### **Cartesian coordinates**

C	-2.720388	0.944946	-0.002202
C	-2.967881	-0.406499	0.030259
N	-1.765184	-1.049273	0.018341
C	-0.736203	-0.137418	-0.016582
C	-1.317341	1.117030	-0.032403
C	4.177382	0.448723	0.038326
C	3.084960	-0.282233	-0.016508
C	1.720045	0.224010	0.022166
C	0.644144	-0.573769	-0.035796
H	-3.468064	1.722401	-0.007743
H	-3.896139	-0.953735	0.059502
H	-1.642839	-2.046165	0.048156
H	-0.784738	2.054537	-0.071357
H	5.243911	0.278520	0.023649
H	1.596807	1.299728	0.103495
H	0.804090	-1.649249	-0.107447
H	3.194961	-1.369870	-0.100195

#### **Vibrational frequencies**

40.9138	109.6171	115.3905
177.9536	297.9553	356.0742
369.3199	496.8737	513.5866
622.8497	635.8373	686.8425
732.9345	771.1476	812.0804
821.6552	839.4104	891.6456
899.0878	906.0077	989.673
1002.759	1069.592	1138.049
1142.027	1154.803	1232.842
1267.797	1306.151	1332.618
1366.261	1473.028	1488.226
1510.401	1621.385	1664.567
1722.909	3050.223	3144.483

3186.965 3260.211 3264.568  
3271.369 3288.379 3706.261

*i51*

**Cartesian coordinates**

C	2.796129	0.718981	0.074945
C	2.841744	-0.650938	-0.031199
N	1.557517	-1.107269	-0.069918
C	0.673725	-0.056162	0.003592
C	1.433694	1.095410	0.098753
C	-3.746823	-0.715162	0.204979
C	-3.139089	0.410064	-0.102438
C	-1.696325	0.666359	-0.107843
C	-0.754802	-0.283900	-0.025075
H	3.649841	1.375675	0.134812
H	3.678159	-1.329379	-0.077896
H	1.288161	-2.071358	-0.158666
H	1.042964	2.097022	0.190076
H	-4.764363	-1.072261	0.263104
H	-3.770760	1.259488	-0.383426
H	-1.396315	1.706318	-0.196342
H	-1.079829	-1.322539	0.023482

**Vibrational frequencies**

31.4607	88.2551	121.8618
164.9471	239.9427	331.674
427.6699	499.9289	522.2595
615.4547	634.5335	683.2239
735.4901	762.8069	813.3744
831.1851	877.1276	894.7655
900.2383	905.8378	989.3139
995.1053	1033.561	1058.831
1133.669	1146.023	1238.112
1269.426	1299.18	1342.079
1358.259	1469.728	1486.263
1506.998	1624.688	1649.017
1720.373	3062.289	3147.013
3187.697	3254.926	3264.723
3267.505	3285.574	3705.971

*i52*

**Cartesian coordinates**

C	2.597594	0.911825	-0.000023
C	2.837978	-0.445648	0.000080
N	1.632684	-1.087480	0.000075

C	0.591945	-0.170601	-0.000031
C	1.204404	1.098336	-0.000092
C	-0.750724	-0.555006	-0.000042
C	-1.876439	0.388682	-0.000224
C	-3.198691	0.010909	-0.643621
C	-3.198501	0.011398	0.643866
H	3.353287	1.681839	-0.000061
H	3.766064	-0.994359	0.000150
H	1.506650	-2.083526	0.000140
H	0.682053	2.041834	-0.000164
H	-0.991854	-1.615199	0.000045
H	-1.595357	1.441634	-0.000651
H	-3.697745	-0.180238	-1.578488
H	-3.697287	-0.179004	1.579028

### Vibrational frequencies

57.1894	101.704	141.9126
247.8954	337.0983	411.2969
422.6834	443.7423	610.4776
624.3701	626.8742	688.189
713.8881	763.4066	768.3574
783.337	886.3362	887.8065
894.9868	928.2491	983.0562
1025.778	1051.252	1058.582
1092.519	1134.878	1148.462
1178.795	1230.674	1300.622
1352.054	1406.714	1437.346
1506.685	1509.698	1573.229
1740.05	3105.585	3164.021
3260.751	3262.826	3272.112
3286.54	3312.196	3713.278

### *i53*

#### Cartesian coordinates

C	2.097181	-1.189539	-0.000003
C	2.696866	0.050839	0.000223
N	1.711227	0.994076	0.000158
C	0.457756	0.396595	-0.000115
C	0.704829	-0.991575	-0.000208
C	-0.711440	1.168369	-0.000306
C	-2.102477	0.682031	-0.000503
C	-2.525600	-0.627217	-0.643215
C	-2.526083	-0.626271	0.643907
H	2.613944	-2.136706	-0.000014
H	3.738835	0.327863	0.000433

H	1.860256	1.987068	0.000260
H	-0.051330	-1.757859	-0.000347
H	-0.587309	2.247935	-0.000190
H	-2.831150	1.493047	-0.001346
H	-2.633424	-1.150826	-1.577992
H	-2.634602	-1.148439	1.579408

### **Vibrational frequencies**

55.7366	108.2337	159.6206
251.5189	291.9974	404.0192
445.3727	539.8416	590.7933
614.2211	645.2902	689.6248
708.2345	755.5933	783.7983
788.5521	882.9466	884.3654
890.0895	912.3986	963.9429
1025.581	1031.047	1068.925
1071.302	1130.499	1151.306
1193.28	1237.284	1304.639
1393.773	1413.327	1435.054
1502.587	1509.497	1572.717
1739.383	3101.633	3172.617
3259.286	3263.292	3279.484
3304.742	3312.741	3711.337

### ***i54***

#### **Cartesian coordinates**

C	-2.310275	0.964084	0.211702
C	-2.612195	-0.362120	0.038708
N	-1.435626	-1.030857	-0.169280
C	-0.380797	-0.156292	-0.132334
C	-0.900356	1.095301	0.104403
C	1.028035	-0.615628	-0.296659
C	1.958786	-0.501072	0.921158
C	2.792484	0.385765	0.246098
C	2.018743	0.375782	-0.910811
H	-3.022995	1.753977	0.391190
H	-3.557901	-0.879521	0.040617
H	-1.351868	-2.019440	-0.327424
H	-0.321240	2.001987	0.191198
H	1.057112	-1.604359	-0.770796
H	1.920782	-0.923926	1.915125
H	3.709116	0.894069	0.518705
H	2.049834	0.878296	-1.867246

#### **Vibrational frequencies**

31.0513	128.1936	149.5768
317.5221	381.8443	429.8453
494.7457	552.0131	570.7659
638.0742	689.9981	721.724
791.0998	816.461	887.6107
899.5437	919.0639	930.8568
935.4245	962.7713	964.3526
1007.874	1051.142	1129.701
1149.163	1150.797	1189.795
1208.006	1230.553	1287.173
1328.681	1371.785	1464.986
1469.404	1501.196	1522.374
1635.798	3048.627	3217.728
3245.137	3253.465	3260.504
3267.311	3285.841	3708.658

*i55*

**Cartesian coordinates**

N	-2.073247	-1.218196	0.01219
C	-3.051953	-0.263662	-0.01067
C	-2.456514	0.978620	0.01298
C	-1.071259	0.718540	0.05037
C	-0.832620	-0.623463	0.05075
H	-2.237202	-2.209168	0.00278
H	-4.095814	-0.534143	-0.04250
H	-2.963286	1.929930	0.00328
H	0.081940	-1.193370	0.07276
C	3.106448	-1.576433	-0.16568
C	2.758903	-0.455654	0.09550
C	2.342026	0.865978	0.43363
C	1.688747	1.669254	-0.40735
H	3.424412	-2.562639	-0.40423
H	2.566729	1.196255	1.44325
H	1.384280	2.662304	-0.10068
H	1.448998	1.359124	-1.41724

**Vibrational frequencies**

24.814	42.326	49.2582
60.0943	95.9461	113.8933
226.8519	331.2929	474.3211
564.7978	566.1047	644.6955
661.6997	678.4108	702.4978
706.3738	779.8225	847.7506
865.4646	894.2177	897.0746

969.9936	1009.548	1057.537
1086.723	1113.198	1170.783
1189.908	1260.074	1319.506
1403.2	1440.773	1467.933
1507.911	1561.98	1689.486
2235.181	3173.289	3188.804
3260.828	3271.605	3280.712
3283.222	3484.167	3706.891

### *i56*

#### **Cartesian coordinates**

N	-2.246657	-1.157742	0.020894
C	-2.892902	0.041383	-0.088546
C	-1.940220	1.025856	-0.141348
C	-0.665471	0.397035	-0.062246
C	-0.893279	-0.953830	0.039289
H	-2.695450	-2.052667	0.091715
H	-3.969160	0.098640	-0.115707
H	-2.128328	2.085424	-0.229176
H	-0.197308	-1.774037	0.117438
C	3.900658	-0.583713	-0.402958
C	2.882330	-0.145724	0.103632
C	1.730365	0.349173	0.663565
C	0.677651	1.077112	-0.116659
H	4.790365	-0.966119	-0.841373
H	1.556094	0.183686	1.722304
H	0.568665	2.089854	0.293346
H	1.006934	1.195663	-1.153174

#### **Vibrational frequencies**

33.5497	39.8668	172.1474
199.8989	279.3432	370.2768
401.8505	495.5014	496.8532
536.9895	617.734	646.3446
649.3488	684.8617	710.6961
730.3652	794.6988	863.8831
886.2624	915.7202	985.9844
1043	1094.948	1099.942
1156.953	1174.483	1207.232
1249.117	1307.211	1333.836
1423.861	1443.583	1481.951
1500.236	1543.031	1633.43
2029.794	3025.421	3088.907
3183.84	3253.803	3274.639

3282.167 3475.092 3723.586

*i57*

**Cartesian coordinates**

N	-1.847112	-1.287129	0.150229
C	-2.691338	-0.206004	0.025164
C	-1.913429	0.908922	-0.143203
C	-0.534379	0.516227	-0.123777
C	-0.571860	-0.834642	0.071832
C	2.807052	-1.430756	-0.292485
C	2.395428	-0.363947	0.071351
C	1.890084	0.939257	0.497286
C	0.661073	1.401037	-0.302539
H	-2.123536	-2.237106	0.318846
H	-3.761435	-0.323290	0.083324
H	-2.276608	1.918761	-0.269638
H	1.633311	0.888111	1.560055
H	3.171821	-2.375775	-0.614721
H	2.691352	1.677323	0.392434
H	0.406767	2.415556	0.018254
H	0.932317	1.465764	-1.361927

**Vibrational frequencies**

20.0889	75.9607	150.8868
189.0993	260.2513	355.7903
365.2829	414.6963	527.137
566.2038	630.078	668.5909
681.3296	697.5302	707.9197
837.3303	855.4576	901.4578
907.7343	992.2605	1018.307
1056.73	1083.033	1127.825
1184.946	1220.058	1266.572
1290.709	1364.527	1376.395
1407.523	1442.442	1474.173
1488.391	1524.914	1612.691
2246.11	3050.07	3055.986
3095.233	3102.375	3243.993
3279.651	3487.578	3724.042

*i58*

**Cartesian coordinates**

N	1.658821	0.991994	0.044960
C	2.397961	-0.161167	0.100052
C	1.532312	-1.227076	0.026198
C	0.219737	-0.698949	-0.065773



C	0.332310	0.673767	-0.053719
C	-0.819019	1.571424	-0.146142
C	-1.992270	0.980531	0.001248
C	-2.254850	-0.449910	0.310427
C	-1.122995	-1.345088	-0.261331
H	2.030548	1.922255	0.114356
H	3.471238	-0.129732	0.195193
H	1.815862	-2.268672	0.037846
H	-0.698631	2.634424	-0.330770
H	-2.299131	-0.558014	1.402550
H	-3.221387	-0.776948	-0.081571
H	-1.170807	-2.327436	0.215415
H	-1.298550	-1.501027	-1.333498

### **Vibrational frequencies**

136.0472	211.1695	272.9133
379.3066	389.7347	463.4436
482.2429	583.2536	637.2812
664.0422	703.8921	725.5798
762.8313	820.4949	855.788
876.8456	917.6077	929.493
989.1394	1026.581	1077.435
1113.959	1178.793	1190.851
1216.097	1225.518	1284.576
1324.006	1341.11	1389.492
1460.677	1467.478	1495.047
1503.687	1544.516	1625.286
1697.964	3024.326	3031.042
3096.231	3101.736	3182.251
3250.197	3281.633	3714.921

### ***i59***

#### **Cartesian coordinates**

N	-1.091306	0.931768	-0.463112
C	-1.554146	-0.176903	-1.112560
C	-2.283281	-0.939099	-0.224532
C	-2.213144	-0.238246	0.995737
C	-1.480386	0.904169	0.856684
C	2.417700	1.690088	-0.161870
C	2.045143	0.566988	0.053321
C	1.575203	-0.756873	0.315577
C	2.298979	-1.848584	0.076089
H	-0.423272	1.580870	-0.843723
H	-1.329538	-0.346222	-2.153652
H	-2.792914	-1.863489	-0.441801

H	-1.200278	1.679981	1.548481
H	2.777869	2.674305	-0.342401
H	0.572794	-0.835822	0.729129
H	1.898521	-2.831749	0.291959
H	3.299555	-1.789488	-0.336885

**Vibrational frequencies**

16.2646	32.1827	67.5802
87.0093	95.8846	155.3431
230.1745	338.9688	508.1175
559.1593	570.4965	644.16
678.6751	687.0203	701.476
716.2367	766.7735	859.1781
871.3519	892.9112	895.7802
978.9492	1040.431	1048.64
1083.421	1119.604	1176.126
1193.398	1250.868	1337.356
1401.188	1446.639	1465.817
1506.112	1556.956	1703.543
2232.394	3159.645	3172.527
3256.959	3261.885	3280.456
3290.163	3484.064	3693.169

***i60***

**Cartesian coordinates**

N	-2.318860	-1.147962	0.044281
C	-2.955277	0.046659	-0.156802
C	-2.000735	1.028631	-0.172861
C	-0.735199	0.403664	0.026632
C	-0.973592	-0.946746	0.157245
C	0.559370	1.091818	0.079140
C	1.723409	0.530743	0.258268
C	2.913059	-0.075154	0.443906
C	3.734766	-0.553488	-0.571919
H	-2.772524	-2.041737	0.101060
H	-4.025590	0.099684	-0.272165
H	-2.177527	2.084260	-0.312811
H	-0.287347	-1.762633	0.318140
H	0.521725	2.175272	-0.047138
H	3.250787	-0.191352	1.473388
H	4.679691	-1.027729	-0.340291
H	3.448001	-0.456789	-1.611807

**Vibrational frequencies**

42.2695	64.974	142.7924
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194.7071	267.4636	353.4262
425.1142	509.456	541.835
569.8352	645.8181	652.0839
721.02	722.0831	750.411
791.3059	841.9673	882.9471
913.6533	922.9242	951.0981
996.2197	1081.252	1099.448
1105.325	1173.481	1191.98
1225.481	1309.875	1342.323
1404.472	1453.286	1493.428
1497.261	1546.444	1625.009
1925.374	3109.167	3138.975
3170.605	3256.269	3275.481
3279.433	3285.052	3719.652

### *i61*

#### **Cartesian coordinates**

N	2.649224	-0.815759	0.000164
C	2.911054	0.568146	0.000077
C	1.721087	1.214548	-0.000107
C	0.715238	0.190269	-0.000122
C	1.352017	-1.153091	0.000020
C	-0.670530	0.381155	-0.000161
C	-1.572175	-0.662856	-0.000155
C	-3.006735	-0.542206	-0.000044
C	-3.721258	0.597857	0.000235
H	3.384869	-1.503682	0.000279
H	3.921206	0.951933	0.000143
H	1.572309	2.283864	-0.000206
H	-1.145091	-1.660581	-0.000207
H	-1.036807	1.405778	-0.000156
H	-3.553018	-1.481568	-0.000187
H	-4.804206	0.573908	0.000300
H	-3.256017	1.577729	0.000425

#### **Vibrational frequencies**

46.5126	110.2585	136.6532
227.0077	259.5334	259.6438
438.7327	511.2901	551.0699
600.414	632.343	731.7808
740.5529	788.4084	879.9521
884.174	916.7159	919.3147
930.6425	982.5223	1001.987
1034.817	1036.374	1073.494

1093.404	1177.655	1242.38
1277.256	1318.751	1339.968
1362.387	1419.906	1449.952
1491.636	1498.267	1596.789
1649.593	3155.449	3160.606
3171.757	3197.81	3240.687
3250.592	3263.042	3666.121

## *i62*

### **Cartesian coordinates**

C	-1.870258	0.961219	0.337997
C	-2.750119	-0.085791	0.317464
N	-2.080921	-1.182804	-0.154347
C	-0.785467	-0.854309	-0.430487
C	-0.607577	0.481206	-0.127627
C	0.594119	1.295346	-0.284976
C	1.875092	0.916932	-0.160099
C	2.339329	-0.402824	0.262581
C	3.582900	-0.825650	0.202157
H	-2.086567	1.966816	0.665051
H	-3.788910	-0.143676	0.599281
H	-2.487808	-2.088724	-0.301297
H	-0.106034	-1.568837	-0.865799
H	0.408978	2.338656	-0.528366
H	1.585744	-1.071581	0.691392
H	4.123137	-1.721291	0.473873
H	2.649790	1.651489	-0.355765

### **Vibrational frequencies**

56.6883	94.4838	190.7428
213.7479	272.8608	365.8085
458.489	514.9675	595.5045
633.056	646.1859	688.8737
714.1667	759.583	780.5225
814.4709	832.6325	868.0056
888.0475	914.7404	983.2895
1013.316	1087.833	1100.845
1116.701	1180.672	1244.818
1264.212	1275.923	1330.724
1419.37	1454.003	1499.478
1543.744	1620.966	1659.196
1720.196	3072.711	3161.727
3190.77	3253.171	3259.557
3277.913	3285.436	3723.014

*i63*

**Cartesian coordinates**

N	1.429442	-1.235804	0.076618
C	2.469602	-0.426496	-0.364989
C	2.078704	0.893023	-0.390824
C	0.717596	0.886638	0.049772
C	0.374732	-0.418560	0.315881
C	-0.572370	1.364884	0.451024
C	-1.039965	-0.070936	0.800994
C	-2.191014	-0.671424	0.047634
C	-2.923121	-0.029208	-0.851981
H	1.477208	-2.234943	0.164782
H	3.416243	-0.868600	-0.634254
H	2.704530	1.718056	-0.692660
H	-1.037582	2.328695	0.592950
H	-1.173466	-0.238010	1.877268
H	-2.416231	-1.711140	0.280785
H	-3.743740	-0.517321	-1.365891
H	-2.718044	1.006370	-1.104374

**Vibrational frequencies**

51.7997	123.393	159.5004
254.9667	329.4605	337.9864
450.757	465.9278	604.2005
614.771	621.7669	684.1878
722.643	758.2316	841.4433
861.1196	884.0262	939.2899
969.738	996.6583	1041.236
1060.236	1071.322	1095.757
1135.868	1194.865	1197.334
1278.97	1316.616	1334.376
1358.803	1452.089	1458.883
1498.482	1534.752	1583.03
1737.14	3038.581	3137.901
3154.928	3239.101	3250.711
3258.815	3280.946	3715.025

*i64*

**Cartesian coordinates**

N	1.979223	1.143625	-0.063005
C	2.688084	-0.013290	0.136906
C	1.796817	-1.047060	0.134267
C	0.486205	-0.502783	-0.065059
C	0.652355	0.865353	-0.188170
C	-0.706263	-1.324945	-0.125232

C	-2.018790	-1.030613	-0.060561
C	-2.247223	1.480758	0.084246
C	-2.703626	0.245871	0.118238
H	2.378270	2.062887	-0.124077
H	3.758186	0.001337	0.265222
H	2.033238	-2.091429	0.271902
H	-0.072985	1.639686	-0.378410
H	-0.481375	-2.385636	-0.215047
H	-2.693913	-1.879430	-0.112181
H	-2.683547	2.461715	0.211932
H	-3.777799	0.145755	0.313886

### **Vibrational frequencies**

34.1658	108.2032	169.2403
228.8747	238.6702	411.8795
466.4908	517.6432	606.8924
628.5858	644.1176	682.6579
726.566	754.3506	765.4044
822.9749	879.5348	888.9571
898.5057	912.5286	975.626
1009.564	1014.576	1095.836
1104.611	1176.315	1247.157
1280.328	1299.374	1339.997
1425.663	1469.362	1498.224
1547.057	1615.1	1654.234
1708.758	3050.987	3155.741
3185.483	3241.195	3256.32
3259.685	3284.569	3719.779

### ***i65***

#### **Cartesian coordinates**

N	-1.890364	-1.190500	-0.069607
C	-2.671385	-0.050180	-0.039066
C	-1.832364	1.024905	0.029045
C	-0.476473	0.545027	0.043268
C	-0.589951	-0.823583	-0.075629
C	0.703914	1.380001	0.124202
C	1.997054	1.040021	-0.032121
C	2.541208	-0.289502	-0.272369
C	2.126677	-1.431044	0.287247
H	-2.230133	-2.125500	-0.207777
H	-3.745660	-0.109644	-0.109540
H	-2.131922	2.061800	0.074469
H	0.491650	2.436728	0.266127
H	2.719456	1.851848	-0.051563

H	3.379166	-0.332349	-0.966499
H	2.579927	-2.379937	0.023392
H	1.377982	-1.443319	1.071183

**Vibrational frequencies**

70.4274	108.5128	146.443
218.7613	244.4311	391.3159
424.2911	486.8383	563.7417
603.9249	621.2425	680.4117
722.4432	804.2601	811.8232
860.4684	896.0855	929.6381
953.848	979.3788	1016.637
1034.12	1081.421	1099.251
1112.579	1195.682	1259.286
1291.046	1335.594	1377.319
1433.561	1441.285	1469.177
1525.519	1586.924	1677.938
1709.006	3145.814	3160.97
3165.036	3184.755	3246.49
3251.98	3278.622	3712.544

***i66***

**Cartesian coordinates**

N	1.586430	-1.078308	-0.114776
C	2.333951	0.081156	-0.204213
C	1.569699	1.201035	-0.070386
C	0.227874	0.785989	0.161941
C	0.273489	-0.699358	0.419375
C	-0.990896	1.438002	0.073307
C	-2.160028	0.690658	-0.027501
C	-0.939369	-1.418766	-0.078261
C	-2.099493	-0.731431	-0.192338
H	2.029370	-1.897379	0.271500
H	3.389990	0.020459	-0.429397
H	1.909437	2.213449	-0.229718
H	0.315546	-0.834212	1.524944
H	-1.024669	2.519143	-0.011026
H	-3.117045	1.190732	-0.114635
H	-0.889211	-2.489597	-0.240302
H	-3.009793	-1.258140	-0.459476

**Vibrational frequencies**

156.9335	191.1313	362.84
408.4019	502.8262	528.2811
538.6616	551.9228	595.8246

679.1964	707.3175	767.0203
784.8008	852.7908	861.1276
877.7528	908.8191	916.2119
977.1707	1000.494	1058.781
1069.515	1105.656	1129.655
1159.698	1179.323	1233.084
1269.626	1295.636	1330.238
1381.003	1389.511	1435.964
1468.922	1543.939	1579.458
1634.911	2804.764	3184.205
3189.93	3206.568	3217.417
3238.589	3263.826	3645.249

*i67*

**Cartesian coordinates**

N	2.625250	-0.920699	-0.000010
C	2.984582	0.400347	0.000185
C	1.834433	1.141706	0.000125
C	0.729767	0.236865	-0.000101
C	1.266737	-1.035404	-0.000193
C	-0.673112	0.623076	-0.000214
C	-1.730401	-0.199974	0.000112
C	-3.108160	0.275773	-0.000080
C	-4.184256	-0.480574	0.000221
H	3.266487	-1.693313	-0.000058
H	4.020188	0.698640	0.000351
H	1.773967	2.219480	0.000252
H	0.788707	-2.001617	-0.000419
H	-0.858496	1.695912	-0.000589
H	-3.240643	1.364139	-0.000512
H	-5.254107	-0.331777	0.000160
H	-1.590388	-1.277464	0.000557

**Vibrational frequencies**

30.0648	110.8253	116.6086
181.5966	293.7786	367.5032
369.843	506.8411	515.355
631.1421	646.6176	676.1074
715.5695	766.4167	798.1089
818.1201	844.1146	871.9696
901.763	913.1569	998.0872
1003.016	1094.319	1107.553
1143.123	1176.515	1226.394
1259.398	1316.603	1336.547



1359.018	1437.69	1494.664
1541.297	1618.454	1664.177
1723.358	3049.494	3149.903
3172.673	3252.543	3258.488
3274.296	3281.894	3720.165

***i68***

**Cartesian coordinates**

N	-2.692810	-0.721555	0.110908
C	-2.869120	0.625913	-0.057242
C	-1.629525	1.201437	-0.122319
C	-0.657802	0.162793	0.005637
C	-1.361879	-1.015344	0.155494
C	0.785702	0.346150	-0.018695
C	1.701788	-0.615285	-0.193736
C	3.152734	-0.399470	-0.169352
C	3.792238	0.638391	0.323041
H	-3.432657	-1.392444	0.213302
H	-3.854281	1.058820	-0.117954
H	-1.424037	2.252280	-0.258690
H	-1.016398	-2.024630	0.311671
H	1.136169	1.368504	0.109175
H	1.377945	-1.634817	-0.386584
H	3.758415	-1.200602	-0.607078
H	4.819701	0.956258	0.422831

**Vibrational frequencies**

33.2454	90.6101	126.1579
174.8854	233.6582	347.8573
419.0084	512.5137	520.1042
621.5944	646.4256	669.1218
719.378	758.7051	801.2333
830.826	877.1273	878.9477
911.5732	913.6512	997.3534
1010.795	1031.199	1101.374
1107.144	1174.485	1233.46
1267.463	1312.928	1342.214
1360.628	1436.724	1496.96
1544.038	1621.863	1655.908
1720.836	3062.244	3163.526
3174.619	3257.702	3264.459
3279.004	3285.794	3719.643

***i69***

**Cartesian coordinates**

N	2.522318	-0.874083	-0.000044
C	2.847715	0.458675	0.000053
C	1.689962	1.178048	0.000085
C	0.586203	0.251139	-0.000001
C	1.162712	-1.021739	-0.000070
C	-0.785734	0.592408	-0.000001
C	-1.887283	-0.375582	-0.000170
C	-3.219847	-0.028100	0.643645
C	-3.219986	-0.027706	-0.643493
H	3.183063	-1.629237	-0.000049
H	3.877071	0.779813	0.000078
H	1.608966	2.254306	0.000106
H	0.709173	-1.999061	-0.000098
H	-1.051488	1.645742	0.000049
H	-1.588581	-1.424503	-0.000447
H	-3.718279	0.163818	1.578703
H	-3.718601	0.164852	-1.578318

### **Vibrational frequencies**

54.9202	89.0832	143.6989
267.0443	333.3497	410.5084
417.1327	441.544	604.9065
619.7267	623.5295	653.1073
686.8177	752.6321	764.1946
774.2692	859.2435	882.6953
901.6734	928.6923	986.6033
1022.932	1047.535	1074.486
1095.037	1109.896	1173.125
1176.087	1227.242	1303.394
1345.037	1405.162	1470.17
1494.192	1543.27	1578.627
1740.167	3095.055	3173.021
3255.113	3262.056	3278.56
3289.288	3311.554	3722.397

### ***i70***

#### **Cartesian coordinates**

N	2.033851	-1.117697	-0.000003
C	2.698636	0.081947	0.000009
C	1.769746	1.078556	0.000004
C	0.459394	0.476333	-0.000010
C	0.682550	-0.904474	-0.000014
C	-0.754506	1.207946	-0.000010
C	-2.125337	0.676387	0.000003
C	-2.505461	-0.648999	-0.643654

C	-2.505439	-0.649001	0.643672
H	2.471437	-2.020685	-0.000001
H	3.776141	0.122742	0.000021
H	1.973585	2.138535	0.000010
H	-0.009151	-1.728445	-0.000028
H	-0.663496	2.289650	-0.000012
H	-2.885358	1.458199	0.000012
H	-2.608834	-1.174149	-1.578327
H	-2.608778	-1.174144	1.578353

### **Vibrational frequencies**

62.1344	101.2413	151.94
271.7853	285.034	410.435
441.672	525.307	572.2291
622.0273	637.8005	668.2676
696.052	758.3417	763.2135
772.1543	857.9914	882.8417
896.2189	908.103	964.2089
1021.219	1027.132	1070.204
1096.625	1103.334	1170.379
1188.299	1231.419	1302.677
1386.494	1424.302	1459.621
1496.13	1535.454	1581.237
1737.781	3101.239	3185.314
3255.114	3259.241	3282.126
3304.597	3308.736	3722.888

### ***i71***

#### **Cartesian coordinates**

N	2.202653	-0.961004	0.069279
C	2.630886	0.336187	0.012238
C	1.519681	1.136893	-0.061791
C	0.374368	0.292195	-0.049608
C	0.836758	-1.001317	0.032162
H	2.801436	-1.764751	0.123915
H	3.680862	0.579938	0.027552
H	1.517743	2.215035	-0.121212
H	0.297251	-1.934494	0.066333
C	-1.059240	0.716710	-0.104087
C	-1.993544	0.213616	1.005186
C	-2.786786	-0.466721	0.084754
C	-2.005424	-0.087219	-1.003598
H	-1.125650	1.797916	-0.264744
H	-1.987509	0.335453	2.079480
H	-3.687060	-1.062163	0.179348

H -2.015828 -0.281969 -2.067161

**Vibrational frequencies**

14.7147	123.1724	148.4713
315.9667	385.3922	426.4752
500.9378	549.8318	564.6196
647.9099	676.8849	705.7978
790.1262	800.7926	860.6769
909.083	913.9378	919.6277
935.5356	949.7793	958.1085
1001.641	1082.382	1098.838
1157.127	1171.874	1187.345
1206.639	1226.595	1308.982
1326.901	1364.776	1444.949
1465.496	1494.75	1542.234
1625.244	3068.934	3210.528
3237.576	3252.279	3253.648
3275.375	3279.991	3721.674

**Transition states**

*i1 - i2*

**Cartesian coordinates**

C	-0.912904	1.023991	0.060564
C	-1.126812	-0.359077	-0.009601
N	1.145373	0.698725	-0.227313
C	-0.037590	-1.219626	0.026093
C	1.165837	-0.507289	0.121175
H	-0.473406	1.464102	0.949621
H	-1.600473	1.686638	-0.459260
H	-2.106614	-0.753824	-0.259618
H	1.743111	1.377677	0.234163
H	-0.111416	-2.293661	-0.063106

**Vibrational frequencies**

-606.872	402.5393	558.2762
596.3095	669.0316	721.2089
798.6082	841.4211	934.7428
958.1409	1022.486	1087.15
1112.471	1140.933	1207.226
1395.057	1449.035	1532.267
1685.724	3142.519	3199.449
3218.945	3251.759	3565.75

### *i2 – i3*

#### **Cartesian coordinates**

C	0.666767	0.969907	-0.029017
C	-0.710791	0.949352	-0.005639
N	1.005767	-0.496748	-0.013686
C	-1.159621	-0.384142	-0.012844
C	-0.121740	-1.328746	-0.020045
H	1.103602	0.171153	0.980623
H	1.406140	1.711969	-0.284642
H	-1.321674	1.840193	0.044779
H	1.929613	-0.825934	-0.258041
H	-2.205745	-0.658376	0.018353

#### **Vibrational frequencies**

-1612.78	577.9274	587.0062
648.8493	784.022	843.18
859.7155	869.9743	895.8858
959.4134	1024.806	1081.375
1123.121	1205.781	1262.722
1341.288	1382.801	1430.72
1542.748	2261.045	3224.978
3243.008	3284.843	3637.587

### *i3 – pyrrole (3)*

#### **Cartesian coordinates**

N	1.034419	-0.426938	0.000822
C	-1.175996	-0.321456	0.000872
C	-0.211665	-1.306738	-0.095894
C	-0.644647	1.002134	-0.007110
C	0.712608	0.928765	-0.007619
H	1.906805	-0.787891	-0.359846
H	0.742767	-1.105088	0.906725
H	-2.231417	-0.550916	0.056820
H	-1.212247	1.922097	0.018343
H	1.471358	1.694135	0.030712

#### **Vibrational frequencies**

-1299.91	538.9385	597.0165
670.8703	738.2924	777.6936
856.3227	879.2623	882.9838
953.2961	1052.498	1102.766
1136.305	1183.333	1215.434
1383.831	1440.253	1471.793
1604.058	2313.662	3232.786
3246.417	3279.799	3642.406

*i4 – i5*

**Cartesian coordinates**

C	-2.429152	-0.480796	-0.027583
C	-1.370673	0.090118	0.005331
C	-0.121473	0.790844	0.030145
H	-3.363095	-0.987042	-0.054965
H	-0.179033	1.881328	0.058743
N	2.208486	-0.427581	-0.002945
C	1.045763	0.180354	0.013394
H	3.026980	0.003007	-0.408102
H	2.308964	-1.387346	0.297214

**Vibrational frequencies**

-402.565	169.4052	173.5646
268.4313	413.0704	444.826
521.4801	604.1645	715.8553
723.3933	892.2387	1091.131
1106.393	1321.645	1641.693
1880.755	2221.711	3076.175
3485.666	3536.661	3626.807

*i5 – i6*

**Cartesian coordinates**

C	-0.395539	1.173223	0.000025
C	0.893646	0.991688	-0.000015
N	-1.158189	-0.423303	0.000008
C	1.190015	-0.466782	0.000005
C	0.067765	-1.176226	-0.000024
H	-1.170465	1.919734	-0.000050
H	-1.720000	-0.595867	0.830210
H	-1.719991	-0.595771	-0.830219
H	2.182458	-0.896397	0.000053

**Vibrational frequencies**

-739.458	271.1856	375.3746
596.0392	658.0922	659.72
754.8777	889.54	965.2704
973.0457	1021.611	1128.738
1158.345	1258.408	1580.128
1586.553	1608.382	3240.719
3316.404	3504.668	3592.189

*i6 – 3-pyrrolyl (11)*

**Cartesian coordinates**

C	-1.014668	-0.656009	-0.007552
C	0.229132	-1.197240	-0.003633
N	-0.793306	0.718169	0.001345
C	1.246218	-0.222668	0.000236
C	0.695137	1.047843	-0.100376
H	-1.999002	-1.092142	0.033594
H	-1.453196	1.397381	-0.353137
H	-0.238652	1.235643	0.911057
H	2.309085	-0.399629	0.067029

**Vibrational frequencies**

-1388.48	554.1844	585.5934
666.7726	728.3598	773.1
837.3829	842.117	863.7101
1096.975	1105.162	1167.831
1209.938	1312.917	1381.4
1452.797	1551.401	2256.591
3260.608	3283.047	3630.91

***i7 – i8*****Cartesian coordinates**

C	1.583014	0.590485	0.092352
C	1.067670	-0.565989	-0.010870
N	-0.943357	1.049725	-0.051021
C	-0.125814	-1.201755	-0.053453
C	-1.177720	-0.228927	-0.048841
H	2.308379	1.157055	-0.467973
H	0.469507	1.141161	0.402155
H	-1.749674	1.618628	0.175424
H	-0.321724	-2.216351	0.258833
H	-2.185894	-0.611454	0.113582

**Vibrational frequencies**

-1458.84	341.6874	384.9475
522.6393	592.7844	614.5794
736.2002	770.1798	776.8306
858.0609	1015.079	1050.519
1150.542	1191.016	1330.728
1368.372	1426.455	1535.225
1699.205	1931.745	3134.074
3250.811	3293.796	3602.219

***i8 – i9*****Cartesian coordinates**

C	-1.153690	-0.708483	-0.000120
C	-1.139773	0.668695	0.000130
N	0.752619	-1.004104	0.000275
C	0.088640	1.229688	-0.000064
C	1.137532	0.220467	-0.000052
H	-1.420432	-1.234465	-0.914980
H	-1.420921	-1.234780	0.914427
H	1.454175	-1.734453	-0.000573
H	0.328758	2.285834	0.000073
H	2.193832	0.484392	-0.000241

### Vibrational frequencies

-484.895	302.297	488.9303
685.3483	694.8688	727.1114
792.6171	893.6858	995.3835
1016.996	1035.659	1040.206
1125.583	1147.455	1302.73
1378.554	1418.951	1562.417
1667.738	3133.397	3159.335
3208.325	3212.469	3600.615

### *i9* – pyrrole (3)

#### Cartesian coordinates

C	1.095370	-0.347331	-0.021628
C	0.039891	-1.328726	-0.104309
N	0.577194	0.951398	-0.018292
C	-1.126907	-0.480185	0.003267
C	-0.777574	0.843262	0.000918
H	2.143659	-0.498733	-0.247800
H	0.873044	-0.986234	0.999185
H	1.097161	1.810079	0.039385
H	-2.145960	-0.839654	0.029923
H	-1.392942	1.732635	0.037865

### Vibrational frequencies

-893.764	435.3519	585.4728
616.5848	806.8557	835.0183
900.3948	910.9479	956.2193
1051.671	1063.683	1126.207
1135.55	1179.321	1247.293
1345.396	1398.916	1505.233
1544.401	2272.969	3226.464
3227.865	3247.404	3690.305

### *i7* – *i9b*



**Cartesian coordinates**

C	-1.100888	-0.688440	-0.000001
C	-1.263873	0.596926	0.000001
N	0.637929	-1.011002	0.000000
C	0.076676	1.219491	0.000000
C	1.102717	0.358721	0.000000
H	-1.613707	-1.635107	-0.000001
H	0.926864	-1.526646	0.828167
H	0.926870	-1.526649	-0.828163
H	0.241100	2.291885	0.000000
H	2.165575	0.553343	-0.000001

**Vibrational frequencies**

-387.047	287.4508	470.9893
590.7168	638.5279	726.3111
734.6217	785.7766	968.473
987.5805	1021.485	1052.462
1146.376	1163.513	1180.585
1362.125	1593.615	1628.963
1635.096	3201.828	3253.472
3309.169	3497.774	3584.209

***Benzene (1) + amino (13) – i10*****Cartesian coordinates**

C	0.228809	1.177128	0.523906
C	0.864174	-0.079018	0.717013
C	0.094994	-1.253474	0.475043
C	-1.145883	-1.163348	-0.114406
C	-1.705970	0.087090	-0.408184
C	-1.018168	1.251351	-0.072766
N	2.155390	-0.121787	-0.827781
H	0.747251	2.082997	0.818708
H	1.697711	-0.142895	1.404453
H	0.528948	-2.218995	0.704693
H	-1.703377	-2.066671	-0.336396
H	-2.684459	0.148057	-0.870175
H	-1.471569	2.218877	-0.257201
H	1.454079	-0.151868	-1.574470
H	2.435949	0.864628	-0.818789

**Vibrational frequencies**

-585.253	136.3242	163.2273
190.0394	396.0845	420.532
609.801	616.5975	678.3798
728.5064	778.3953	844.5637

857.0946	901.4735	961.5977
996.0042	1007.757	1019.226
1039.272	1052.633	1063.124
1177.717	1187.678	1205.04
1329.781	1379.919	1494.191
1510.692	1549.051	1602.012
1629.482	3185.932	3193.34
3201.525	3213.778	3215.723
3226.733	3413.96	3513.154

***i10 – aniline (4) + H***

**Cartesian coordinates**

C	0.198501	1.216726	-0.019704
C	0.928092	0.000008	0.100555
C	0.198516	-1.216718	-0.019658
C	-1.180646	-1.203347	-0.040859
C	-1.885426	-0.000006	-0.027488
C	-1.180663	1.203341	-0.040875
N	2.321072	-0.000047	-0.045373
H	0.741902	2.155616	-0.028994
H	0.807948	0.000080	1.799279
H	0.741929	-2.155601	-0.028884
H	-1.718594	-2.143971	-0.082257
H	-2.968406	-0.000015	-0.045993
H	-1.718618	2.143960	-0.082285
H	2.697959	-0.835104	-0.462955
H	2.698123	0.835348	-0.462126

**Vibrational frequencies**

-1219.6	120.4088	200.4818
365.879	418.4749	494.1412
516.1561	528.1903	559.7245
629.594	674.1649	685.306
770.1666	814.771	836.0693
907.6397	976.8084	991.9922
1005.66	1050.248	1076.843
1147.491	1179.434	1208.886
1305.371	1332.597	1372.59
1509.126	1523.387	1612.63
1657.773	1671.558	3188.642
3190.731	3204.345	3208.999
3225.593	3616.047	3718.046

***i11 – i12***

**Cartesian coordinates**

C	-1.424572	0.022075	-0.180515
C	-2.659177	0.026561	-0.068473
C	-0.006988	0.012729	-0.090985
C	0.693672	-1.202724	-0.052404
C	2.076673	-1.209943	0.034002
C	2.783564	-0.013025	0.079174
C	2.098808	1.196737	0.036139
C	0.715775	1.214863	-0.048436
N	-3.990211	-0.137131	0.056465
H	0.139836	-2.133101	-0.093055
H	2.606381	-2.155160	0.064660
H	3.865276	-0.023110	0.147037
H	2.645749	2.132077	0.068331
H	0.179383	2.155615	-0.085363
H	-2.748427	-0.079129	1.081938
H	-4.423256	0.779082	0.170182

### Vibrational frequencies

-1379.49	82.0757	88.268
206.5947	253.4214	304.9239
356.4886	407.3446	416.5765
478.3479	517.966	522.2995
637.9407	710.2887	729.8801
779.2767	863.587	944.869
1001.099	1020.609	1021.264
1040.834	1068.451	1111.732
1162.711	1187.713	1212.549
1315.551	1350.754	1356.826
1486.098	1538.91	1639.537
1672.637	2196.414	2734.638
3195.327	3203.92	3213.241
3220.478	3226.559	3505.26

### *i12 – i13*

#### Cartesian coordinates

C	2.105475	-0.725763	-0.241073
C	2.113966	0.699161	-0.152833
C	0.978287	1.388642	0.147409
C	-0.252298	0.681586	0.283395
C	-0.227816	-0.762170	0.428920
C	0.987954	-1.438063	0.065627
N	-1.955842	-0.967173	-0.325915
C	-1.498513	1.211186	-0.048592
C	-2.458338	0.197535	-0.188221
H	3.023805	-1.242527	-0.496323

H	3.033607	1.234949	-0.358507
H	0.968804	2.472976	0.153786
H	-0.715040	-1.174320	1.314153
H	1.021851	-2.520627	0.114553
H	-2.460083	-1.772203	0.033992
H	-1.674347	2.259280	-0.248052

### **Vibrational frequencies**

-547.942	177.6952	216.3503
357.0414	439.6254	518.6792
557.0323	565.8172	600.1755
652.0934	736.3319	752.7208
817.2044	834.8485	860.7355
894.3145	921.5001	977.3209
1004.585	1014.115	1032.436
1131.703	1148.056	1173.11
1193.301	1204.676	1264.639
1319.073	1384.18	1418.685
1473.759	1497.483	1574.948
1594.014	1679.155	3109.682
3192.08	3199.937	3211.596
3221.168	3238.017	3559.921

### ***i13 – i14***

#### **Cartesian coordinates**

C	2.116148	-0.717288	-0.077467
C	2.120984	0.701694	0.005559
C	0.961994	1.430394	0.067876
C	-0.283237	0.753843	0.041553
C	-0.243100	-0.660778	0.085176
C	0.942045	-1.420062	-0.062578
N	-1.692278	-1.023919	0.018373
C	-1.631692	1.157825	-0.086953
C	-2.530816	0.087657	-0.098428
H	3.057930	-1.246558	-0.158426
H	3.075267	1.216233	-0.005873
H	0.989234	2.513719	0.086431
H	-0.972438	-1.027234	1.087350
H	0.920513	-2.502013	-0.119098
H	-1.996162	-1.978463	-0.110848
H	-1.942357	2.192048	-0.156570

#### **Vibrational frequencies**

-1596.86	201.7258	236.8812
368.4437	428.5849	532.3453

560.8529	585.3464	614.2125
704.591	745.7504	751.1044
761.6924	845.0591	857.7571
878.799	909.5312	968.3676
1008.205	1026.707	1040.712
1099.097	1165.332	1180.015
1195.042	1210.388	1275.549
1326.91	1347.353	1400.684
1426.185	1492.461	1518.977
1618.638	1667.175	2138.982
3198.798	3207.411	3217.915
3226.578	3229.068	3645.479

***i14 – indole (2)***

**Cartesian coordinates**

C	2.127673	-0.713032	0.005367
C	0.934706	-1.410515	0.009724
C	-0.238467	-0.660912	-0.006141
C	-0.255740	0.739193	-0.015346
C	0.969395	1.423805	-0.006999
C	2.140363	0.692822	0.001340
N	-1.574356	-1.079914	-0.001059
C	-1.632108	1.163463	0.003617
C	-2.521942	0.127047	-0.080251
H	3.066388	-1.254368	0.008445
H	0.915142	-2.494422	0.020184
H	0.992779	2.507487	-0.005780
H	3.093796	1.208892	0.007367
H	-2.366410	-0.832131	0.862090
H	-1.876319	-1.942583	-0.432448
H	-1.948157	2.195288	0.079689

**Vibrational frequencies**

-1555.81	205.1332	240.2522
390.7853	431.5996	504.3466
547.5729	586.3633	614.5045
652.3738	729.5202	765.2198
768.7836	786.3635	854.5208
880.6555	900.2822	910.2779
964.8833	1007.034	1043.604
1129.11	1151.441	1159.943
1186.484	1254.047	1273.428
1317.267	1372.86	1416.834
1467.375	1517.965	1546.268

1653.896 1685.917 2266.945  
3197.38 3205.521 3215.856  
3225.341 3235.82 3638.962

***il5 – il6***

**Cartesian coordinates**

C 2.174157 0.683171 0.157711  
C 2.109952 -0.725111 0.115026  
C 0.917190 -1.383351 -0.083015  
C -0.255452 -0.622488 -0.185860  
C -0.207087 0.795195 -0.260561  
C 1.045440 1.432080 -0.062047  
C -2.035057 1.065825 0.260722  
N -1.526603 -1.097096 -0.030013  
C -2.496505 -0.154965 0.169241  
H 3.127504 1.169340 0.326366  
H 3.015647 -1.301621 0.265910  
H 0.867883 -2.466648 -0.070048  
H -0.847548 1.240185 -1.047340  
H 1.106327 2.512309 -0.127465  
H -2.400306 2.062267 0.078129  
H -1.699106 -2.078302 0.117232

**Vibrational frequencies**

-529.909 167.691 224.0751  
377.9881 431.2813 493.701  
557.5927 570.8754 602.7161  
623.2823 630.6653 707.3407  
761.2539 765.8647 786.9729  
861.7135 874.6986 963.637  
1004.621 1014.242 1031.908  
1056.156 1094.08 1172.196  
1180.666 1193.174 1291.498  
1312.015 1396.117 1430.946  
1506.384 1511.431 1582.408  
1625.782 1670.393 2934.039  
3194.751 3200.923 3212.466  
3223.44 3311.085 3660.84

***il6 – il7***

**Cartesian coordinates**

C -2.119176 0.702452 -0.090843  
C -2.096444 -0.722145 -0.022052  
C -0.922434 -1.421860 0.064138  
C 0.277541 -0.687065 0.071432

C	0.288696	0.752705	0.127591
C	-0.974748	1.436095	-0.037118
C	1.764491	1.093443	-0.075126
N	1.558274	-1.075803	-0.054086
C	2.520873	-0.065699	-0.112165
H	-3.075130	1.203277	-0.189515
H	-3.036483	-1.260255	-0.061721
H	-0.910448	-2.505766	0.069834
H	0.725517	0.989000	1.171181
H	-0.999030	2.519020	-0.067474
H	2.133211	2.105899	0.011649
H	1.821647	-2.048112	-0.110497

### Vibrational frequencies

-617.009	204.8155	248.6284
373.5829	439.4946	535.7299
557.1762	595.6097	612.6828
722.8818	741.252	766.9787
788.1136	798.7996	869.7971
873.0237	906.5823	972.4321
1007.807	1020.591	1063.593
1079.952	1102.962	1174.286
1198.573	1203.844	1268.59
1335.009	1347.359	1415.573
1442.596	1489.2	1527.256
1608.663	1684.021	2596.831
3197.54	3206.384	3218.191
3225.407	3249.663	3648.851

### *i17 – indole (2)*

#### Cartesian coordinates

C	2.142071	0.703652	0.005650
C	2.121536	-0.700913	0.007906
C	0.934978	-1.409878	-0.001365
C	-0.251771	-0.673258	-0.008310
C	-0.246138	0.729959	-0.009718
C	0.963922	1.426491	-0.001920
C	-1.645941	1.111678	-0.037216
N	-1.569009	-1.083280	-0.004464
C	-2.480797	-0.051552	-0.094482
H	3.094573	1.220154	0.009179
H	3.061499	-1.241362	0.018145
H	0.928169	-2.493773	0.000719
H	0.977763	2.510702	-0.006500
H	-2.035431	2.113524	-0.165561

H	-2.415657	0.702262	0.967273
H	-1.855012	-2.045625	0.044724

**Vibrational frequencies**

-1204.47	207.1687	245.3289
397.9885	431.2648	549.17
569.1956	588.5446	626.5997
668.6708	755.2237	778.7689
780.6503	842.0045	872.1547
902.0687	934.7201	966.2479
1004.168	1044.08	1084.881
1146.961	1169.445	1194.551
1239.451	1264.484	1289.894
1320.874	1372.716	1377.104
1446.566	1514.509	1539.685
1657.167	1692.204	2154.094
3196.287	3204.629	3214.941
3225.245	3232.519	3697.656

***i18 – i19***

**Cartesian coordinates**

C	-1.992105	-1.275514	0.046534
C	-2.943513	-0.289151	0.004865
C	-2.275754	0.975798	-0.019340
C	-0.945004	0.672145	0.006789
N	-0.757040	-0.667609	0.048766
H	-2.085531	-2.349178	0.072937
H	-4.011988	-0.443302	-0.007488
H	-2.725518	1.954358	-0.051431
H	0.138660	-1.128108	0.069589
C	2.909732	-1.555944	-0.197177
C	2.587371	-0.432521	0.088678
C	2.169803	0.880448	0.449745
C	1.478087	1.678413	-0.375346
H	3.219029	-2.539519	-0.458598
H	2.396143	1.200073	1.461894
H	1.169689	2.666784	-0.058889
H	1.267091	1.390115	-1.397865

**Vibrational frequencies**

-92.5269	41.942	50.0534
75.1151	105.3299	166.5461
228.0585	360.7032	480.3921
559.7829	567.0592	634.8388
684.6569	709.0247	713.5088



721.7072	772.67	853.3869
876.6526	891.8045	898.5745
968.9828	1002.79	1034.669
1076.768	1114.854	1134.243
1193.64	1271.202	1316.305
1391.572	1440.683	1449.806
1485.132	1578.206	1653.005
2221.922	3170.419	3186.713
3247.355	3269.709	3273.613
3279.854	3481.508	3670.496

### *i19 – i20*

#### **Cartesian coordinates**

C	-2.785790	-0.196903	-0.288764
C	-2.058144	-1.309821	0.065380
C	-0.733352	-0.841656	0.258257
C	-0.693946	0.499767	0.031129
N	-1.954287	0.901298	-0.307592
C	3.703487	-0.495629	-0.645835
C	2.713690	-0.226587	-0.016826
C	1.517993	0.065558	0.710995
C	0.616355	1.201574	0.180476
H	-3.832758	-0.098908	-0.531145
H	-2.445364	-2.311252	0.162627
H	0.676184	-0.908075	0.584411
H	-2.240761	1.834761	-0.543570
H	4.581977	-0.730547	-1.196569
H	1.678771	0.105239	1.788648
H	0.581857	2.035156	0.888978
H	0.998342	1.586715	-0.769111

#### **Vibrational frequencies**

-1880.95	51.9388	133.1444
183.9122	240.2215	363.7052
404.9119	467.1954	487.2949
566.5507	615.713	644.6212
658.8887	703.1555	708.1311
721.9347	859.4073	864.4731
889.6055	927.64	993.1058
1028.483	1081.152	1094.714
1138.855	1188.858	1208.398
1248.375	1262.591	1323.55
1356.926	1431.108	1488.218
1504.563	1515.484	1614.405

1668.225 2207.775 3055.914  
3095.295 3132.686 3259.502  
3278.742 3482.717 3708.157

***i20 – i21***

**Cartesian coordinates**

C -1.822281 1.200255 0.070470  
C -2.510997 0.010480 0.131162  
N -1.610798 -1.015063 0.011744  
C -0.336821 -0.511428 -0.126467  
C -0.463063 0.850178 -0.099725  
C 1.693241 1.722172 -0.143528  
C 2.202353 0.640793 0.089307  
C 2.125994 -0.794081 0.361216  
C 0.870498 -1.375360 -0.329737  
H -2.253838 2.185949 0.144229  
H -3.564196 -0.184933 0.259559  
H -1.848665 -1.991611 0.019599  
H 1.543564 2.757837 -0.345101  
H 3.019924 -1.322047 0.019475  
H 2.055510 -0.935797 1.444510  
H 1.079075 -1.479229 -1.400588  
H 0.690675 -2.382785 0.059920

**Vibrational frequencies**

-402.784 86.8034 133.2894  
231.413 293.3263 342.7147  
395.6026 465.9677 534.7017  
612.9805 637.9454 690.1643  
692.4941 709.8038 739.0448  
847.7134 853.8995 879.0224  
924.0963 988.1056 1017.652  
1028.91 1108.659 1139.569  
1189.31 1218.353 1227.131  
1286.787 1349.219 1377.016  
1440.165 1468.808 1476.366  
1491.695 1509.31 1606.578  
2094.459 3042.061 3060.511  
3086.378 3109.24 3255.99  
3275.668 3447.99 3700.725

***i21 – i22***

**Cartesian coordinates**

C -1.693211 1.124177 -0.049957  
C -2.410878 -0.037268 -0.064994

N	-1.527220	-1.093937	-0.003996
C	-0.251728	-0.620317	0.040524
C	-0.308754	0.766872	0.018707
C	0.907229	1.521072	0.138871
C	2.105123	0.891038	-0.203443
C	2.183936	-0.518653	-0.163490
C	0.996989	-1.430035	0.149096
H	-2.102098	2.121758	-0.090082
H	-3.473625	-0.209155	-0.121422
H	-1.788001	-2.064087	-0.006250
H	0.884914	2.555959	0.462599
H	3.041699	-0.994914	-0.635688
H	1.002618	-2.251255	-0.578363
H	1.090880	-1.900347	1.137885
H	2.861917	0.218283	0.667412

### **Vibrational frequencies**

-1595.93	108.164	219.2578
262.6788	382.593	477.1701
493.5499	525.2504	570.1071
629.7542	654.8736	680.8351
709.4016	738.0973	760.9685
836.7586	871.0673	911.7994
925.8838	973.0952	1077.076
1095.804	1111.397	1180.999
1200.534	1237.658	1241.352
1287.22	1335.271	1365.867
1385.087	1449.365	1463.926
1473.299	1526.455	1535.649
1611.684	2164.575	3005.741
3047.907	3141.267	3186.42
3262.675	3286.187	3713.038

### ***i22 – indole (2)***

#### **Cartesian coordinates**

N	-1.553096	1.072717	-0.070324
C	-2.396227	-0.014898	-0.010823
C	-1.660742	-1.160037	0.037348
C	-0.280074	-0.769556	0.011749
C	-0.255422	0.637433	-0.056835
C	0.934694	-1.470075	0.035024
C	2.123002	-0.761180	-0.023105
C	0.945353	1.372838	-0.053060
C	2.132798	0.635443	-0.093155
H	-1.844295	2.033256	-0.075955

H	-3.466194	0.122851	-0.013735
H	-2.052983	-2.163556	0.084170
H	0.941684	-2.553061	0.087616
H	3.066256	-1.295116	-0.023855
H	0.939979	1.926452	1.754802
H	0.949347	2.437445	-0.255648
H	3.077591	1.162900	-0.147986

### **Vibrational frequencies**

-819.968	202.218	232.7716
298.7785	373.31	409.5088
436.0032	495.318	552.279
590.214	619.4892	628.7945
730.3406	759.2546	779.5671
802.6613	880.1217	889.1619
899.3364	919.1978	975.4413
1007.404	1038.32	1095.089
1122.113	1143.067	1180.311
1232.673	1265.989	1313.056
1374.566	1390.477	1469.176
1497.872	1534.31	1574.421
1631.291	1672.252	3194.948
3201.119	3211.39	3223.453
3262.101	3282.303	3724.476

### ***i23 – i24***

#### **Cartesian coordinates**

C	1.621971	-1.047301	-0.065211
C	2.772119	-0.551910	0.150704
C	0.315858	-0.666145	-0.140700
C	0.211200	0.806051	-0.098456
C	-1.137673	1.314722	-0.017284
C	-2.215164	0.488826	0.032150
C	-2.080868	-0.929058	0.062777
C	-0.840965	-1.481670	0.002761
N	1.292892	1.541659	-0.034166
H	3.743547	-0.621765	-0.309727
H	-1.273933	2.390692	-0.039358
H	-3.209147	0.922982	0.060323
H	-2.963033	-1.552905	0.131712
H	-0.706522	-2.556650	0.020500
H	2.388475	0.525845	0.580941
H	1.091493	2.499098	0.234332

#### **Vibrational frequencies**

-1295.17	147.7519	185.9516
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285.3147	391.8924	442.1419
500.2995	539.5257	542.8887
569.8365	580.6024	700.3796
737.4251	745.2156	761.863
798.5263	840.7412	856.8418
888.5561	978.1008	1002.697
1030.448	1103.291	1154.467
1212.607	1246.649	1320.698
1343.398	1371.969	1420.714
1514.442	1526.739	1579.033
1697.069	1852.793	1947.899
3188.098	3204.516	3211.308
3228.002	3294.373	3573.349

### *i24 – i25*

#### **Cartesian coordinates**

C	1.543955	-1.240272	-0.000005
C	2.586887	-0.374798	-0.000015
C	0.286008	-0.739235	0.000006
C	0.270668	0.747460	0.000008
C	-1.023851	1.391913	-0.000005
C	-2.151780	0.642355	-0.000011
C	-2.137135	-0.797306	0.000001
C	-0.958359	-1.459305	0.000008
N	1.426641	1.323454	0.000015
H	3.134825	-0.185734	-0.920383
H	3.134861	-0.185747	0.920334
H	-1.078557	2.475150	-0.000022
H	-3.114223	1.144800	-0.000025
H	-3.079038	-1.331914	0.000004
H	-0.914877	-2.542203	0.000024
H	1.432153	2.336598	0.000036

#### **Vibrational frequencies**

-460.411	142.1193	196.6137
330.88	420.4945	480.4621
515.4339	550.7167	557.0368
644.8018	651.2545	715.2959
762.1879	764.703	781.6345
855.2971	890.9487	971.2532
977.0436	998.5799	1006.475
1014.75	1092.592	1148.054
1201.179	1228.35	1272.815
1368.067	1400.683	1427.984

1491.886	1562.943	1613.292
1668.734	1728.658	3140.576
3186.131	3204.093	3210.809
3223.509	3228.07	3590.338

***i25 – indole (2)***

**Cartesian coordinates**

C	2.162022	-0.678077	0.008619
C	2.110901	0.727686	0.015394
C	0.915364	1.419574	0.002792
C	-0.257915	0.658271	-0.023132
C	-0.236584	-0.754830	-0.015311
C	0.997490	-1.418234	-0.004881
C	-2.361409	-0.105985	0.003285
N	-1.566134	1.056913	-0.043889
C	-1.580633	-1.313261	-0.095090
H	3.125590	-1.173392	0.017187
H	3.040852	1.286172	0.028178
H	0.894239	2.503366	0.004460
H	1.013667	-2.502179	-0.009677
H	-2.300381	-0.706084	1.047759
H	-3.417633	-0.015767	-0.224257
H	-1.888799	1.998636	0.093514

**Vibrational frequencies**

-777.739	198.3117	235.9162
368.2086	412.2526	435.0824
552.678	568.7592	603.1456
620.5982	765.0315	773.6087
781.7804	861.5182	877.8885
898.9868	953.804	981.8424
1010.55	1040.63	1068.291
1119.187	1150.087	1177.115
1232.689	1253.198	1293.112
1312.425	1368.585	1387.505
1439.021	1492.044	1542.845
1638.663	1692.954	2329.333
3191.62	3207.433	3213.225
3215.567	3226.339	3696.714

***i26 – i3***

**Cartesian coordinates**

N	1.176626	-0.842883	-0.000042
C	0.221101	1.333128	0.000064
C	1.169426	0.508067	0.000188

H	1.544980	-1.276882	0.836604
H	1.543578	-1.276380	-0.837568
H	0.036418	2.391443	-0.000755
C	-1.416152	0.276815	0.000033
C	-1.275652	-0.950784	0.000023
H	-2.145748	1.065035	0.000025
H	-1.407950	-2.006389	0.000144

### **Vibrational frequencies**

-564.203	187.8549	208.1918
262.365	447.976	488.5769
539.2022	606.8452	700.7887
714.2379	742.0725	763.5871
890.0457	973.0256	1167.238
1180.712	1640.409	1843.592
1953.208	3318.671	3344.515
3464.248	3565.031	3655.059

### ***i27 – i28***

#### **Cartesian coordinates**

N	0.159147	-0.929177	-0.147343
C	2.194526	0.558149	0.054728
C	1.220066	-0.147325	-0.097355
H	-0.141053	-1.093826	-1.105940
H	3.063775	1.157647	0.169891
C	-1.400145	-0.020589	0.574809
C	-2.067983	0.566978	-0.275830
H	-1.249616	-0.292317	1.598984
H	-2.465918	0.989457	-1.169641

### **Vibrational frequencies**

-741.204	77.7697	156.1272
311.701	441.6802	483.0281
509.6919	517.7982	638.1043
702.8756	746.3373	791.1369
949.897	1092.051	1198.207
1835.634	2097.614	3365.625
3458.858	3487.207	3530.495

### ***i28 – i29***

#### **Cartesian coordinates**

N	-0.052775	0.789559	-0.227630
C	2.148106	-0.438567	0.126500
C	1.105856	0.130386	-0.055555
H	-0.165226	1.243647	-1.121499

H	3.073482	-0.932571	0.290096
C	-1.274079	0.271729	0.356937
C	-1.846997	-0.817571	-0.081289
H	-1.677570	0.855961	1.179413
H	-1.658571	-1.569820	-0.834158

### **Vibrational frequencies**

-182.497	164.9651	310.1004
402.6628	481.2011	540.8217
567.5611	744.9217	762.7226
859.9582	913.6553	1016.494
1180.113	1303.284	1440.948
1663.411	2266.124	3172.879
3260.266	3495.185	3626.445

### ***i29 – 2-pyrrolyl (16)***

#### **Cartesian coordinates**

N	0.258294	-1.080200	-0.052401
C	-1.541406	0.511484	0.017257
C	-0.998270	-0.595951	0.000434
C	1.204355	-0.042072	0.001246
C	0.759014	1.200785	0.011610
H	0.487040	-2.017557	0.224556
H	-2.275946	1.280980	-0.036255
H	2.249627	-0.334886	0.008344
H	1.189066	2.187390	-0.013109

### **Vibrational frequencies**

-461.379	261.2755	358.1603
450.4221	509.0293	533.7082
646.527	704.1429	746.3784
840.0155	877.3599	1064.069
1164.104	1256.666	1447.245
1658.161	1991.789	3183.863
3301.775	3454.21	3710.607

### ***i30 – i31***

#### **Cartesian coordinates**

N	-2.156463	0.401067	0.00000
C	-0.076050	-1.106783	0.00000
C	-1.049621	-0.304401	0.00000
C	1.874568	0.915152	0.00000
C	1.968694	-0.295946	0.00000
H	-2.626042	0.629457	0.86143
H	-2.626042	0.629458	-0.86143



H	1.634150	1.951718	0.00000
H	2.407632	-1.266236	0.00000

**Vibrational frequencies**

-458.348	15.0382	93.3235
233.9455	263.6186	337.0115
374.4529	496.2829	586.2826
676.8248	768.1702	829.0835
1139.062	1148.154	1643.248
1952.592	2034.337	3417.996
3503.043	3594.797	3704.211

***i31 – i32***

**Cartesian coordinates**

N	-1.185029	0.645115	-0.000034
C	0.097824	-1.240050	-0.000042
C	-1.064074	-0.729895	0.000091
C	0.982988	0.975512	0.000069
C	1.257728	-0.309898	-0.000010
H	-1.585726	1.055292	0.837132
H	-1.585366	1.055149	-0.837447
H	1.546804	1.895728	-0.000015
H	2.272701	-0.695991	-0.000082

**Vibrational frequencies**

-503.778	168.5684	355.9837
489.0846	507.1543	585.7536
646.8546	737.7657	840.7373
845.4931	989.992	1116.241
1133.123	1191.879	1575.991
1614.529	1738.396	3172.916
3271.274	3530.276	3624.938

***i32 – 3-pyrrolyl (11)***

**Cartesian coordinates**

N	0.754795	0.759179	-0.000781
C	-0.104373	-1.241669	0.006746
C	1.145361	-0.742017	-0.089744
C	-0.629835	0.920047	-0.011095
C	-1.184442	-0.326451	-0.003700
H	1.395062	1.452847	-0.363457
H	1.287020	0.217918	0.898977
H	-1.083776	1.898721	0.029406
H	-2.242132	-0.543192	0.027305

**Vibrational frequencies**

-1357.31	529.0305	545.2846
619.2897	693.7299	751.3529
825.8286	865.6192	910.2099
1058.397	1119.566	1149.887
1175.952	1356.844	1404.071
1446.391	1559.644	2280.436
3249.288	3270.41	3629.959

***i33 – i34*****Cartesian coordinates**

N	-1.385237	-1.026961	0.079650
C	-0.383402	1.176779	-0.146066
C	-1.412265	0.349673	-0.127895
H	-2.186875	-1.391811	0.569665
H	-0.512592	-1.361826	0.462390
H	-0.303456	2.217312	-0.419560
H	-2.410016	0.738937	-0.345489
C	2.028427	-0.562371	-0.349296
C	1.644898	0.259840	0.457102
H	2.210377	-1.234501	-1.154556
H	1.633277	0.877083	1.326941

**Vibrational frequencies**

-439.832	67.4141	125.3156
148.6041	260.2879	393.7617
517.6273	565.3414	588.5465
685.3875	707.2392	752.5524
784.7148	870.6993	881.0653
1105.255	1244.665	1325.019
1646.016	1713.433	1949.655
3090.632	3265.797	3400.122
3490.172	3586.706	3695.5

***i34 – i35*****Cartesian coordinates**

N	-1.014730	-0.791457	0.033442
C	0.215476	1.186264	-0.059445
C	-1.027231	0.645618	-0.003948
C	0.869546	-1.064013	-0.122294
C	1.271645	0.227986	0.026711
H	-1.229938	-1.232143	-0.851599
H	-1.625505	-1.186411	0.751437
H	0.378225	2.256365	-0.033078
H	-1.956648	1.171106	0.165350

H	1.294114	-1.956139	0.333276
H	2.266252	0.512292	0.354374

**Vibrational frequencies**

-695.84	277.9548	527.0034
554.4973	602.6066	637.9898
725.3617	774.7135	819.9692
906.91	962.3691	1007.969
1029.701	1060.238	1139.317
1207.656	1222.417	1401.786
1479.791	1588.032	1650.628
3156.823	3189.977	3219.668
3240.818	3421.963	3596.452

***i35 – pyrrole (3) + H***

**Cartesian coordinates**

N	-1.117199	-0.000011	-0.013482
C	1.028603	0.710225	-0.025230
C	-0.267699	1.137934	0.088213
C	-0.267687	-1.137924	0.088244
C	1.028605	-0.710208	-0.025230
H	-1.769427	-0.000034	-1.162418
H	-1.927268	-0.000027	0.592772
H	1.894144	1.350960	-0.094296
H	-0.701113	2.122833	0.048360
H	-0.701006	-2.122858	0.048276
H	1.894135	-1.350958	-0.094302

**Vibrational frequencies**

-1745.05	383.7555	565.9351
592.5174	641.3082	783.6832
821.3563	835.8139	856.0707
877.8617	915.9655	1020.652
1046.22	1078.349	1146.616
1156.771	1289.836	1316.436
1340.439	1451.681	1519.06
1579.576	3253.571	3266.867
3291.048	3295.709	3597.61

***ethynylamine (6) + vinyl (8) – i37***

**Cartesian coordinates**

C	1.824604	-0.918962	-0.077042
C	1.772523	0.380271	0.085132
H	0.920846	-1.499033	-0.255684
H	2.764622	-1.471990	-0.044737

H	2.552800	1.113291	0.261931
N	-1.898248	-0.765887	0.020585
C	-0.396369	1.289766	-0.061271
C	-1.221073	0.395554	-0.021857
H	-2.723409	-0.815735	-0.557972
H	-2.040216	-1.147243	0.944064
H	-0.065015	2.302141	-0.041470

**Vibrational frequencies**

-400.268	42.0892	90.7558
133.0716	209.0613	261.1168
365.1445	438.4221	544.8049
623.6251	723.4873	807.0467
899.3219	951.5486	1095.221
1101.629	1197.183	1397.538
1646.342	1663.452	2171.434
3087.962	3172.069	3196.552
3438	3587.372	3681.462

***i36 – i37***

**Cartesian coordinates**

C	0.835811	1.056712	-0.127897
C	1.199556	-0.292431	0.077905
N	-1.084555	0.676972	0.134689
C	0.140142	-1.236207	-0.067348
C	-1.132119	-0.733197	-0.101408
H	1.313498	1.837028	0.465265
H	0.588843	1.389333	-1.134959
H	2.129851	-0.567770	0.560689
H	-1.428913	0.912800	1.066922
H	-1.599359	1.224599	-0.545559
H	0.327623	-2.304065	-0.042689

**Vibrational frequencies**

-739.75	228.1859	467.4355
513.2401	631.8362	715.3788
781.9037	866.4838	880.243
927.215	985.2992	1018.996
1032.253	1072.7	1109.694
1187.501	1284.256	1360.891
1456.359	1513.152	1610.836
3095.882	3163.367	3201.981
3217.112	3470.767	3602.408

***i36 – i38***

**Cartesian coordinates**

C	1.528367	-0.940091	-0.052955
C	1.341733	0.374879	0.060574
N	-1.688351	-0.779166	-0.050184
C	0.054374	1.078498	-0.029010
C	-1.129028	0.484801	0.028667
H	0.705155	-1.620020	-0.245016
H	2.520263	-1.368032	0.033913
H	2.204063	1.014684	0.232637
H	-2.299816	0.267817	-0.431996
H	-2.159390	-0.987905	0.834336
H	0.075506	2.159100	-0.116238

**Vibrational frequencies**

-2069.19	102.2196	181.5725
277.4673	400.001	426.3186
659.4128	734.1204	844.3997
917.3809	956.2785	1031.894
1049.507	1083.969	1116.994
1125.611	1331.874	1364.976
1449.55	1690.756	1720.964
2392.009	3156.114	3169.252
3198.249	3251.185	3463.802

***i37 – i39*****Cartesian coordinates**

C	0.928705	0.790587	0.009925
C	-0.540590	1.082488	-0.007488
N	0.926486	-0.685623	0.020388
C	-1.260677	-0.084898	-0.007768
C	-0.493538	-1.269255	-0.081226
H	1.467414	1.163547	-0.872598
H	1.443823	1.182616	0.895938
H	-0.938481	2.087653	0.009569
H	1.621042	-1.188541	-0.514885
H	0.459994	-1.438161	0.831648
H	-2.342588	-0.121286	0.026951

**Vibrational frequencies**

-1753.89	242.3731	489.2452
581.6574	638.3219	723.0461
787.9117	836.1551	922.8577
942.116	977.4516	1019.799
1086.119	1112.236	1125.903
1204.787	1325.269	1351.403

1425.519 1451.814 1500.237  
2320.057 3001.502 3035.327  
3220.085 3246.29 3618.503

***i38 – i39***

**Cartesian coordinates**

N 0.930156 -0.934813 0.086465  
C 0.049009 1.197430 -0.101047  
C 1.172678 0.347950 -0.014865  
C -1.073202 -0.893116 -0.089001  
C -1.144045 0.510074 0.067392  
H 1.700269 -1.577468 0.223022  
H 0.144276 2.273965 -0.062335  
H 2.182608 0.746934 0.061417  
H -1.691106 -1.533218 0.539923  
H -0.862697 -1.321223 -1.062955  
H -2.011079 0.980669 0.520800

**Vibrational frequencies**

-647.519 203.4579 454.3633  
557.2841 624.0565 668.4908  
787.8175 826.59 898.1934  
945.9783 1007.454 1047.007  
1072.106 1101.907 1137.509  
1205.835 1320.478 1429.517  
1465.447 1518.94 1555.561  
3115.651 3152.195 3175.933  
3196.371 3236.045 3591.376

***i39 – pyrrole (3) + H***

**Cartesian coordinates**

C 1.121277 0.087116 0.112288  
C 0.249658 1.169156 0.089270  
N 0.350994 -1.050776 0.094884  
C -1.058428 0.656937 -0.036725  
C -0.963797 -0.716291 -0.040923  
H 1.727308 0.155944 -1.721687  
H 2.164553 0.045561 0.379185  
H 0.542743 2.206215 0.129607  
H 0.715283 -1.985166 0.051513  
H -1.972369 1.224132 -0.116167  
H -1.726733 -1.472761 -0.130103

**Vibrational frequencies**

-643.676 319.2177 353.8252

524.534	625.3526	653.093
737.8363	782.1736	878.9623
890.9369	902.5578	918.9818
1046.931	1066.677	1100.916
1177.364	1186.025	1315.882
1425.891	1472.326	1520.999
1573.489	3258.317	3268.261
3279.272	3287.295	3719.882

***i15 – i40***

**Cartesian coordinates**

C	-2.049484	0.990621	-0.062225
C	-2.289339	-0.386074	-0.110223
C	-1.270211	-1.339471	-0.038911
C	0.011299	-0.832645	0.080102
C	0.237529	0.544496	0.130661
C	-0.755924	1.499359	0.064844
C	2.929404	0.853658	-0.238926
N	1.333538	-1.248490	0.160808
C	1.865699	0.110306	0.033144
H	-2.884780	1.676747	-0.130188
H	-3.312564	-0.729082	-0.215485
H	-1.480941	-2.399541	-0.097608
H	1.284473	0.734485	0.939627
H	-0.551839	2.561175	0.105921
H	3.812160	0.247126	-0.485145
H	1.724884	-1.992984	-0.393584

**Vibrational frequencies**

-875.842	133.7217	206.5644
272.6982	314.2598	381.0701
407.1435	507.4261	538.7402
604.2559	648.4878	683.0718
761.4941	768.7475	812.0086
865.8378	871.3388	903.725
957.4424	995.5597	1001.172
1006.142	1030.408	1142.002
1156.671	1186.247	1242.66
1274.367	1334.268	1401.046
1480.733	1512.561	1581.373
1668.655	1691.868	2225.537
3074.766	3201.67	3218.128
3229.704	3238.425	3671.218

***i25 – i40***

**Cartesian coordinates**

C	-2.119634	-0.764569	0.086490
C	-2.167647	0.629508	0.178560
C	-1.013526	1.414292	0.091389
C	0.149425	0.705367	-0.124306
C	0.212810	-0.677488	-0.243728
C	-0.924036	-1.456694	-0.125030
C	2.470883	-0.429655	0.608530
N	1.545994	0.962879	-0.202172
C	1.668252	-0.632939	-0.510673
H	-3.045067	-1.322598	0.177574
H	-3.126446	1.114693	0.320915
H	-1.050065	2.494502	0.168501
H	-0.908982	-2.537166	-0.207594
H	3.465210	-0.009745	0.475480
H	2.241402	-0.773618	1.623978
H	1.942824	1.566842	-0.911036

**Vibrational frequencies**

-761.675	164.3229	242.6667
371.583	412.951	445.972
541.4354	567.4435	584.4178
663.0818	730.0593	765.069
789.6172	834.988	850.1083
879.4233	913.6005	950.7015
999.1873	1025.407	1090.972
1102.675	1124.082	1146.877
1175.911	1189.601	1244.922
1304.913	1355.5	1418.765
1481.92	1511.691	1548.98
1658.844	1690.193	3055.005
3176.129	3189.286	3201.675
3212.328	3219.059	3592.495

***i41 – i42*****Cartesian coordinates**

N	-0.781105	0.671921	-0.165180
C	-2.005658	1.300759	-0.135316
C	-2.962143	0.338198	0.056750
C	-2.306149	-0.930002	0.148544
C	-0.975832	-0.656996	0.002414
C	1.211707	-1.825507	0.075256
C	1.994292	-0.926804	-0.132629
C	2.781190	0.225820	-0.396845
C	2.964079	1.209272	0.490378



H	0.114516	1.111056	-0.292939
H	-2.090321	2.368849	-0.255019
H	-4.025560	0.510898	0.127801
H	-2.765482	-1.893321	0.298751
H	0.698205	-2.733996	0.284536
H	3.236970	0.286709	-1.381076
H	3.567842	2.074167	0.243254
H	2.522657	1.163749	1.479642

**Vibrational frequencies**

-207.232	37.1267	56.0677
65.877	106.6338	129.8858
229.2564	342.8397	484.3625
564.6191	567.8634	636.7564
687.607	697.4436	712.6702
715.1799	782.1959	860.1733
876.8599	898.0944	903.0535
971.4742	1025.944	1042.341
1080.572	1115.696	1133.593
1194.123	1276.05	1322.996
1398.214	1442.643	1451.462
1485.889	1582.397	1672.578
2158.998	3162.25	3180.62
3250.871	3261.825	3270.203
3281.862	3465.042	3696.761

***i42 – i43***

**Cartesian coordinates**

N	1.964616	1.044450	0.006089
C	2.913009	0.072022	0.226755
C	2.303367	-1.168227	0.193586
C	0.947075	-0.917656	-0.100670
C	0.759112	0.436447	-0.176093
C	-0.634950	0.853312	-0.306145
C	-1.418646	-0.225519	-0.280215
C	-2.830527	-0.485522	-0.258365
C	-3.693115	0.138324	0.553763
H	2.146378	2.032385	-0.011027
H	3.953942	0.331842	0.341627
H	2.805935	-2.114404	0.317937
H	-0.442897	-1.189389	-0.224293
H	-0.982625	1.871653	-0.444700
H	-3.196834	-1.259460	-0.929748
H	-4.753767	-0.084703	0.524565
H	-3.354380	0.881838	1.267319

**Vibrational frequencies**

-2120.28	66.2408	91.4527
158.4636	225.7571	327.6476
381.8446	440.2905	487.011
570.5022	586.9074	671.0322
685.8209	700.7161	761.9393
866.2009	868.1137	891.5067
954.0567	982.0018	1012.181
1022.896	1043.062	1096.875
1102.712	1133.102	1194.913
1231.937	1324.865	1341.271
1432.611	1440.636	1479.089
1521.898	1578.372	1646.232
1682.915	1751.069	3151.114
3161.611	3199.62	3250.655
3258.718	3277.801	3705

***i42 – i44*****Cartesian coordinates**

N	1.839382	-0.981374	0.137367
C	2.863050	-0.077073	0.185926
C	2.331535	1.167539	-0.041782
C	0.936909	1.004333	-0.230131
C	0.649057	-0.340645	-0.108271
C	-0.599694	-1.085923	-0.200004
C	-1.810199	-0.551798	-0.070332
C	-2.501968	0.693879	0.188067
C	-3.746587	0.225553	0.090876
H	1.930711	-1.968185	0.302526
H	3.877854	-0.389626	0.371542
H	2.885065	2.092644	-0.080961
H	0.222770	1.777778	-0.465159
H	-0.523082	-2.153823	-0.388260
H	-2.116990	1.684095	0.400220
H	-4.755425	0.618386	0.175171
H	-3.129198	-1.006835	-0.162746

**Vibrational frequencies**

-2294.89	38.8006	96.8544
127.4551	220.6602	291.7623
403.65	419.0098	492.057
633.7138	663.4549	697.2261
710.8196	732.0346	774.0274
803.2018	843.4324	891.0365

899.2539	913.7915	932.0316
986.2957	1027.929	1062.251
1070.446	1134.626	1144.718
1203.867	1248.498	1299.574
1378.823	1471.65	1483.655
1510.886	1602.12	1627.531
1733.626	1936.841	3167.25
3186.659	3229.97	3257.973
3273.817	3287.886	3708.433

### *i43 – i45*

#### **Cartesian coordinates**

C	-1.932249	-1.287719	0.169671
C	-2.745169	-0.169046	0.218442
N	-1.996917	0.976460	0.078832
C	-0.686122	0.589910	-0.072886
C	-0.615859	-0.796023	-0.004818
C	0.606711	1.064069	-0.315012
C	1.296622	-0.118574	-0.749944
C	2.646307	-0.444549	-0.301181
C	3.161277	-0.007957	0.851200
H	-2.275145	-2.306095	0.265889
H	-3.814852	-0.104654	0.355618
H	-2.371156	1.906464	0.024713
H	1.076489	1.996330	-0.025820
H	0.985248	-0.562378	-1.686663
H	3.243140	-1.088925	-0.941688
H	4.178601	-0.241345	1.143466
H	2.566985	0.584713	1.539832

#### **Vibrational frequencies**

-496.121	88.6822	134.7879
200.6109	278.215	340.9922
422.7637	470.1688	577.029
619.5899	656.2818	681.9804
713.4272	735.608	753.7853
798.3499	878.3913	881.13
967.754	975.5071	1005.402
1044.049	1059.365	1093.604
1126.362	1161.536	1183.462
1256.602	1321.436	1338.525
1400.914	1441.233	1452.574
1479.944	1501.317	1595.564
1690.597	3152.72	3167.01

3211.955 3215.55 3248.681  
3248.77 3269.921 3714.262

***i44 – i46***

**Cartesian coordinates**

N	-1.795616	0.903543	0.153493
C	-2.716335	-0.097950	0.079709
C	-2.037433	-1.274663	-0.124957
C	-0.658019	-0.965724	-0.174177
C	-0.522656	0.399906	0.000360
C	0.607763	1.312007	0.025169
C	1.909210	1.049449	-0.119560
C	2.527731	-0.281784	-0.342094
C	2.834912	-1.138862	0.596410
H	-2.009647	1.874788	0.296970
H	-3.770902	0.101147	0.181737
H	-2.484641	-2.251209	-0.225258
H	0.153115	-1.660278	-0.312050
H	0.340434	2.357561	0.170027
H	2.601865	1.886814	-0.101572
H	2.775711	-0.531109	-1.382182
H	3.292336	-2.116786	0.652723

**Vibrational frequencies**

-113.077 43.6151 147.1634  
173.2752 263.9121 340.0395  
488.2869 504.7519 540.383  
634.7728 665.1472 681.8917  
737.5173 749.4234 765.3116  
828.6844 835.0633 891.7969  
905.1277 905.6938 980.5874  
999.846 1025.277 1076.664  
1136.007 1156.549 1237.574  
1254.135 1255.803 1317.402  
1428.02 1480.326 1485.377  
1513.827 1625.597 1689.288  
1742.957 3026.483 3147.906  
3176.589 3252.295 3256.406  
3283.419 3296.945 3705.685

***i45 – i47***

**Cartesian coordinates**

C	-1.701352	-1.145928	-0.595442
C	-2.395833	-0.429553	0.363433
N	-1.700752	0.705072	0.712174

C	-0.533644	0.707764	-0.010793
C	-0.515884	-0.412145	-0.831997
C	0.639952	1.441766	-0.235871
C	1.512032	0.492415	-0.850653
C	2.153088	-0.626333	-0.146534
C	2.351002	-0.697649	1.169507
H	-2.037850	-2.066488	-1.045680
H	-3.349436	-0.644512	0.823008
H	-1.972748	1.348726	1.433294
H	0.753031	2.518607	-0.285760
H	2.062689	0.806755	-1.741453
H	2.533589	-1.418192	-0.786769
H	2.844677	-1.553612	1.613918
H	2.015140	0.091187	1.834319

### **Vibrational frequencies**

-554.932	79.0662	140.9596
189.3654	265.3956	321.8073
430.8152	454.4359	597.5703
612.4613	650.8569	668.2928
686.3339	748.7308	794.5322
863.3614	877.3667	907.4859
930.6741	938.6486	981.6474
1040.339	1068.512	1095.31
1128.791	1140.025	1160.203
1274.164	1323.008	1343.23
1399.808	1432.375	1451.013
1476.948	1498.104	1594.625
1693.784	3097.989	3156.911
3175.744	3198.663	3250.932
3251.95	3272.758	3710.363

### ***i46 – i47***

#### **Cartesian coordinates**

N	1.745010	-0.969863	-0.000002
C	2.614748	0.080742	0.000005
C	1.892159	1.253389	0.000003
C	0.534866	0.871989	-0.000007
C	0.444637	-0.505120	-0.000007
C	-0.693895	-1.379952	-0.000004
C	-1.996100	-1.024103	0.000004
C	-2.571039	0.311868	0.000006
C	-1.936417	1.484780	-0.000003
H	2.011389	-1.939109	-0.000001
H	3.681581	-0.080831	0.000013

H	2.302546	2.250367	0.000008
H	-0.679427	1.478422	-0.000005
H	-0.472267	-2.444844	-0.000005
H	-2.719312	-1.833146	0.000008
H	-3.660930	0.337240	0.000011
H	-2.412396	2.459388	-0.000009

**Vibrational frequencies**

-1392.32	86.0853	177.6506
282.0555	288.5188	399.5006
460.3963	480.8267	484.9741
613.6189	629.7878	676.8703
704.4739	724.6345	788.2351
820.2789	858.9426	907.6866
926.1002	946.6334	965.7831
988.0554	1012.854	1101.911
1118.619	1152.708	1214.081
1267.343	1270.383	1321.477
1420.25	1453.099	1484.791
1491.067	1514.896	1620.07
1652.313	1708.056	3130.945
3158.774	3197.747	3212.08
3262.347	3282.115	3704.617

***i46 – i48***

**Cartesian coordinates**

N	1.466366	-1.046274	-0.355770
C	2.381121	-0.023534	-0.389896
C	1.851343	1.060822	0.244944
C	0.520806	0.710462	0.658148
C	0.316821	-0.624575	0.267659
C	-0.902345	-1.375081	0.307168
C	-2.099584	-0.778418	0.093265
C	-2.257265	0.597771	-0.358051
C	-1.332491	1.547852	-0.275406
H	1.542503	-1.900009	-0.880268
H	3.343290	-0.160064	-0.858073
H	2.353598	1.998104	0.423860
H	0.011208	1.163789	1.494182
H	-0.854011	-2.453791	0.429989
H	-2.994122	-1.392481	0.117437
H	-3.198664	0.814492	-0.867711
H	-1.338790	2.562079	-0.656012

**Vibrational frequencies**

-447.082	126.4905	168.7558
277.144	328.0692	436.9335
469.3177	487.5509	612.6553
623.3026	640.8112	680.8413
750.3669	764.1927	799.7735
835.3192	886.7423	888.1446
917.6877	922.0664	975.3956
992.9909	1022.86	1063.435
1132.926	1150.719	1199.95
1243.789	1273.193	1283.911
1410.002	1444.22	1463.99
1537.529	1559.081	1606.382
1656.051	3100.037	3164.37
3189.763	3222.273	3244.091
3258.64	3279.315	3704.266

#### *i47 – i49*

##### **Cartesian coordinates**

C	-1.854103	1.241480	0.084306
C	-2.570527	0.062035	0.110958
N	-1.701506	-0.982593	-0.006994
C	-0.405185	-0.508740	-0.103223
C	-0.502654	0.865050	-0.024098
C	0.739301	-1.379350	-0.168011
C	2.018192	-0.995695	0.053684
C	1.829004	1.440695	-0.284825
C	2.401441	0.372162	0.316993
H	-2.268266	2.234347	0.158203
H	-3.630638	-0.106899	0.222077
H	-1.961086	-1.953231	0.028090
H	0.537441	-2.438530	-0.308073
H	2.776957	-1.767312	0.143596
H	2.068330	2.451295	0.025366
H	1.311028	1.336731	-1.230112
H	3.143960	0.535918	1.095111

##### **Vibrational frequencies**

-289.581	117.5194	168.1769
259.982	274.1103	407.1065
464.7247	471.4319	612.2138
617.3986	626.3628	685.6024
730.8882	793.0086	816.607
847.4471	864.7416	911.5199
955.3033	979.4629	987.6101

1012.826	1090.57	1112.539
1143.364	1194.664	1242.45
1256.2	1299.492	1393.38
1437.194	1449.827	1482.394
1507.759	1574.355	1610.346
1658.723	3148.788	3162.628
3166.275	3185.442	3253.949
3257.282	3275.852	3699.83

***i48 – indole (2) + H***

**Cartesian coordinates**

N	1.547950	-1.095916	-0.019259
C	0.239852	-0.691466	0.045517
C	0.246047	0.739435	0.135158
C	-0.988196	1.418011	-0.068737
C	-2.149820	0.685017	-0.096697
C	-2.131241	-0.722568	-0.018577
C	-0.938640	-1.425860	0.022073
C	1.631395	1.144885	-0.060218
C	2.369370	0.011686	-0.112495
H	1.854838	-2.048315	-0.097459
H	0.295289	0.806811	1.805312
H	-1.005448	2.499359	-0.136339
H	-3.102231	1.192198	-0.200152
H	-3.068637	-1.266113	-0.039541
H	-0.926894	-2.510040	0.009717
H	2.007438	2.154873	-0.079686
H	3.437391	-0.112205	-0.203183

**Vibrational frequencies**

-1145.95	206.3557	240.4718
381.5225	404.1403	433.1101
498.9729	548.0191	559.7067
592.0794	621.4488	640.7632
731.1935	754.3705	765.6839
805.9191	869.1573	886.1951
898.4199	907.5993	942.9902
991.0245	1037.074	1092.21
1121.499	1151.185	1176.874
1222.608	1272.286	1307.498
1357.745	1385.068	1451.673
1489.827	1537.153	1596.849
1623.71	1677.416	3192.54
3200.754	3212.778	3221.825



3263.312 3284.741 3719.287

***i49 – indole (2) + H***

**Cartesian coordinates**

N	-1.599853	-1.072251	0.037422
C	-2.396489	0.046774	-0.016766
C	-1.615036	1.163444	-0.070722
C	-0.255967	0.719368	-0.052696
C	-0.280811	-0.688479	0.015775
C	0.883535	-1.459249	0.036166
C	2.095362	-0.791308	-0.031017
C	2.154651	0.604097	-0.100169
C	0.993378	1.380442	-0.053943
H	-1.930705	-2.018998	0.073433
H	-3.471325	-0.046977	-0.012640
H	-1.967405	2.181791	-0.112667
H	0.842611	-2.541505	0.088308
H	3.118818	1.094986	-0.157054
H	1.074374	1.899888	1.771957
H	1.043782	2.447727	-0.235547
H	3.017085	-1.361685	-0.037509

**Vibrational frequencies**

-836.245	204.5972	235.2252
290.5279	375.3909	410.275
420.8296	490.096	552.554
595.5268	620.643	626.6073
730.395	759.9687	779.6862
800.4358	876.9727	881.5099
894.0686	918.1284	972.9434
1018.337	1039.94	1088.356
1122.881	1144.661	1181.796
1232.043	1268.564	1306.377
1376.494	1389.801	1471.055
1493.478	1529.807	1572.153
1632.477	1672.693	3192.082
3201.712	3209.669	3221.709
3261.342	3281.242	3722.671

***i19 – i50***

**Cartesian coordinates**

C	2.595261	0.968005	-0.171769
C	2.885744	-0.376918	-0.152884
N	1.714602	-1.059050	-0.018887
C	0.659871	-0.177605	0.056617

C	1.194070	1.095793	-0.049968
C	-4.033600	0.219349	-0.468106
C	-2.878800	-0.032904	-0.021008
C	-1.728550	0.255277	0.722629
C	-0.711453	-0.603715	0.202433
H	3.314614	1.765017	-0.274939
H	3.829383	-0.892971	-0.228851
H	1.630133	-2.058410	0.043210
H	0.617780	2.008159	-0.062842
H	-4.878475	-0.027577	-1.075652
H	-1.607607	1.028263	1.475095
H	-0.861044	-1.676132	0.325805
H	-1.942246	-0.816693	-0.777290

### **Vibrational frequencies**

-2155.79	74.191	88.2182
176.7397	223.0023	310.6253
394.3225	409.7879	487.6432
511.1807	523.6193	578.7749
633.4212	668.4734	730.4361
743.8391	762.9049	820.9312
839.9458	903.394	904.5211
997.3265	1012.298	1059.606
1095.252	1135.558	1150.952
1164.503	1242.505	1299.857
1325.888	1438.638	1466.493
1480.799	1511.274	1521.506
1621.902	1810.342	3121.472
3181.546	3255.373	3267.362
3284.504	3386.033	3710.015

### ***i50 – i51***

#### **Cartesian coordinates**

C	-2.766275	0.824316	-0.119770
C	-2.908131	-0.542094	-0.122227
N	-1.663407	-1.088389	-0.001843
C	-0.712895	-0.098666	0.073350
C	-1.385163	1.105623	0.004463
C	3.982542	-0.108583	-0.641758
C	3.130530	0.067368	0.334573
C	1.702727	0.448275	0.162450
C	0.697217	-0.426121	0.203506
H	-3.567772	1.542496	-0.193691
H	-3.787159	-1.161548	-0.196939
H	-1.462668	-2.072925	0.008525

H	-0.928067	2.081993	0.049349
H	5.027905	-0.365716	-0.741742
H	3.487803	-0.051536	1.365305
H	1.496977	1.505251	0.011196
H	0.933525	-1.480004	0.343369

**Vibrational frequencies**

-175.697	54.1544	94.3057
137.8535	272.5889	320.2014
405.8302	467.0706	505.6712
632.2224	643.0186	677.3347
729.9713	770.6848	803.1279
821.335	845.8424	892.9853
896.117	907.5336	996.0984
1000.217	1065.866	1067.605
1135.423	1145.27	1238.898
1242.468	1302.305	1326.739
1354.308	1470.882	1488.749
1508.101	1628.154	1686.811
1749.191	3039.805	3152.851
3168.155	3255.137	3257.155
3270.339	3286.171	3706.85

***i51 – i52***

**Cartesian coordinates**

C	2.633663	0.895982	0.071081
C	2.846161	-0.461679	0.137168
N	1.632151	-1.078382	0.047820
C	0.625450	-0.144769	-0.077290
C	1.244188	1.101528	-0.064248
C	-0.744397	-0.537272	-0.190912
C	-1.803556	0.337292	-0.349061
C	-3.225048	-0.095091	-0.433705
C	-3.329095	0.150807	0.826670
H	3.398265	1.655550	0.117311
H	3.757565	-1.028072	0.240287
H	1.484957	-2.071905	0.066993
H	0.738739	2.051701	-0.138031
H	-0.966543	-1.599095	-0.112181
H	-1.592573	1.390624	-0.506564
H	-3.826708	-0.462639	-1.259491
H	-3.902959	0.131719	1.738720

**Vibrational frequencies**

-723.667	66.3853	95.6949
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155.4244	225.1033	328.627
355.4485	427.0609	480.6035
572.1966	624.9505	663.1783
678.4931	725.7211	770.1827
783.5041	805.8067	867.3782
893.0396	903.6121	929.2659
998.2468	1052.339	1073.396
1136.286	1145.032	1174.458
1238.304	1276.658	1308.005
1338.772	1452.275	1460.203
1503.261	1535.893	1599.633
1723.474	3163.422	3164.629
3178.604	3258.711	3271.002
3285.964	3288.254	3707.811

### *i51 – i54*

#### **Cartesian coordinates**

C	-2.516329	0.815433	0.339602
C	-2.699910	-0.509834	0.016293
N	-1.481023	-1.046511	-0.265045
C	-0.499898	-0.089204	-0.136013
C	-1.131682	1.079190	0.253011
C	0.896041	-0.367327	-0.369209
C	2.615267	-0.588118	0.920285
C	3.046061	0.251657	-0.045366
C	1.843207	0.634218	-0.696371
H	-3.293542	1.508671	0.620361
H	-3.598592	-1.103961	-0.030093
H	-1.316406	-1.996389	-0.548657
H	-0.629726	2.008957	0.472206
H	1.146027	-1.392979	-0.620430
H	3.086673	-1.214019	1.672609
H	4.061880	0.562363	-0.273584
H	1.594308	1.596851	-1.130483

#### **Vibrational frequencies**

-624.978	84.2994	115.8074
156.768	372.2784	400.2379
433.4821	506.2782	582.3149
633.8786	668.3419	696.9407
720.384	745.7892	775.1638
832.8783	842.3627	892.0437
904.9307	905.3345	917.557
1004.468	1060.357	1064.935

1135.37	1145.628	1170.499
1240.051	1255.657	1307.371
1363.116	1446.088	1482.439
1489.293	1504.734	1537.742
1624.53	3163.627	3172.735
3195.658	3205.008	3259.218
3269.141	3284.394	3708.041

### *i52 – i53*

#### **Cartesian coordinates**

C	2.283267	1.080485	0.018201
C	2.739308	-0.196264	-0.240150
N	1.674684	-1.048152	-0.175263
C	0.511550	-0.351441	0.121826
C	0.899855	1.000067	0.244372
C	-0.735513	-0.954626	0.252030
C	-1.970560	-0.183132	0.558945
C	-2.445522	0.935940	-0.340954
C	-3.129576	-0.152685	-0.409746
H	2.893221	1.970210	0.041138
H	3.731743	-0.555587	-0.460835
H	1.714951	-2.039696	-0.327523
H	0.231121	1.810091	0.488064
H	-0.811485	-2.034540	0.150593
H	-2.203755	-0.105533	1.625329
H	-2.258173	1.940737	-0.676864
H	-3.937260	-0.718691	-0.840204

#### **Vibrational frequencies**

-54.3622	99.5718	140.1054
236.8084	326.169	375.7637
431.1661	514.6747	593.3307
613.6562	660.2849	701.9476
719.3796	737.6335	780.3046
842.6559	880.6631	889.5596
890.7537	911.1135	966.3444
1014.419	1033.783	1052.478
1059.614	1126.546	1144.52
1218.485	1225.916	1293.06
1364.193	1398.671	1416.256
1488.32	1505.765	1567.147
1743.771	3047.629	3159.001
3252.113	3274.674	3277.359
3284.244	3325.745	3715.29

*i44 – i53*

**Cartesian coordinates**

C	2.098811	-1.203033	-0.060499
C	2.700905	0.019281	0.127758
N	1.723278	0.968742	0.136161
C	0.482956	0.390013	-0.048395
C	0.709837	-0.979623	-0.170552
C	-0.694313	1.199508	-0.072551
C	-2.004706	0.782587	-0.248966
C	-2.449396	-0.616814	-0.480784
C	-2.750042	-0.670150	0.770689
H	2.605731	-2.153982	-0.110226
H	3.738801	0.281078	0.256521
H	1.875956	1.955158	0.249556
H	-0.051944	-1.728426	-0.307139
H	-0.544387	2.262984	0.097421
H	-2.760685	1.556981	-0.318188
H	-2.429356	-1.256057	-1.358475
H	-3.061366	-1.229537	1.637193

**Vibrational frequencies**

-710.674	60.8989	117.3284
163.0068	233.158	306.3963
412.9059	483.4287	523.3266
605.932	627.6058	664.4155
679.7452	732.6921	756.7748
778.6965	812.603	869.2607
893.0119	901.8441	918.6341
962.306	1020.329	1056.881
1127.271	1143.639	1152.247
1249.323	1256.57	1304.212
1408.489	1443.151	1462.629
1508.346	1527.389	1598.17
1722.273	3153.719	3159.966
3188.885	3260.839	3278.822
3288.599	3289.507	3709.934

*i46 – i54*

**Cartesian coordinates**

C	2.239118	0.940998	-0.247896
C	2.477996	-0.408909	-0.270043
N	1.329318	-1.041110	0.126671
C	0.347475	-0.117644	0.382369
C	0.895553	1.128208	0.168866
C	-0.977655	-0.521964	0.857692

C	-1.882108	-0.617922	-1.156247
C	-2.430827	0.472647	-0.589384
C	-2.124582	0.300672	0.793666
H	2.955696	1.711323	-0.486834
H	3.366519	-0.966458	-0.518456
H	1.190481	-2.035928	0.140653
H	0.379812	2.064196	0.315503
H	-0.935391	-1.283425	1.642390
H	-1.732169	-0.980776	-2.169618
H	-2.990562	1.272143	-1.066970
H	-2.809430	0.450181	1.622509

### Vibrational frequencies

-685.224	56.1621	122.1899
173.8398	280.4473	371.2269
450.9208	484.3741	579.4585
632.285	657.9826	713.5861
726.8637	740.8624	796.3405
820.1241	882.9233	888.2053
904.2771	906.6738	951.3065
991.8901	1058.602	1063.246
1112.873	1142.645	1152.089
1243.806	1260.239	1294.878
1415.828	1432.773	1472.388
1490.061	1519.467	1527.044
1627.745	3085.534	3158.141
3186.425	3194.891	3257.132
3269.29	3282.985	3707.365

### *i55 – i56*

#### Cartesian coordinates

N	-2.108613	-1.230147	0.100601
C	-2.995464	-0.198909	-0.040998
C	-2.288865	0.981385	-0.114644
C	-0.932237	0.606790	-0.011894
C	-0.821372	-0.745049	0.121195
H	-2.362380	-2.199099	0.176185
H	-4.058520	-0.378618	-0.080451
H	-2.708342	1.967785	-0.229980
H	0.037695	-1.388474	0.219367
C	3.211310	-1.444202	-0.280851
C	2.746787	-0.388706	0.060846
C	2.191444	0.848771	0.492833
C	1.467968	1.649746	-0.301709
H	3.632278	-2.369063	-0.593753

H	2.350056	1.110825	1.534281
H	1.075663	2.587662	0.070665
H	1.316418	1.421054	-1.349198

**Vibrational frequencies**

-108.15	34.1861	58.3196
66.4784	91.6956	168.7454
231.0765	364.6825	476.5817
567.4106	574.0887	645.2328
680.5686	686.655	694.2332
725.3502	776.7231	848.6333
857.004	896.3201	900.1022
961.6073	1006.233	1048.619
1085.19	1118.848	1168.018
1187.5	1248.335	1318.112
1402.338	1442.507	1468.162
1508.075	1561.837	1652.137
2226.351	3172.489	3189.875
3258.328	3272.013	3277.302
3285.338	3486.16	3709.656

***i56 – i57***

**Cartesian coordinates**

N	-1.991945	-1.237983	0.070284
C	-2.809345	-0.179085	-0.257021
C	-2.051049	0.966619	-0.309945
C	-0.714235	0.586957	-0.006505
C	-0.722476	-0.761684	0.202465
C	3.731770	-0.512338	-0.604269
C	2.728974	-0.226110	-0.003688
C	1.518025	0.083972	0.690190
C	0.634490	1.225871	0.143422
H	-2.281249	-2.196160	0.142850
H	-3.862239	-0.330610	-0.437849
H	-2.425876	1.952656	-0.539502
H	0.685011	-0.879708	0.540353
H	4.622075	-0.757433	-1.131248
H	1.651308	0.113005	1.772610
H	0.629711	2.068122	0.841722
H	1.027945	1.590801	-0.808815

**Vibrational frequencies**

-1788.76	50.7341	124.5473
174.4043	244.5287	365.3832
402.749	433.1868	477.2247



559.7475	597.4308	642.9082
668.2701	705.5821	717.4152
722.9921	852.2895	862.0361
903.8638	928.2629	994.3496
1027.263	1075.936	1078.672
1132.827	1189.626	1219.857
1247.897	1271.134	1331.346
1355.752	1437.31	1447.965
1496.811	1521.737	1605.251
1659.672	2204.013	3062.515
3101.236	3126.114	3252.857
3273.333	3481.461	3723.556

### *i57 – i58*

#### **Cartesian coordinates**

N	-1.754122	1.106485	-0.041900
C	-2.507484	-0.038504	-0.171794
C	-1.659098	-1.108416	-0.048274
C	-0.337861	-0.607161	0.162970
C	-0.457442	0.758528	0.177548
C	1.631674	1.743425	0.120707
C	2.155570	0.672262	-0.129067
C	2.137380	-0.766042	-0.380619
C	0.929322	-1.387210	0.363059
H	-2.107927	2.044502	-0.085240
H	-3.572558	0.007926	-0.334170
H	-1.944869	-2.149052	-0.102874
H	1.475788	2.777474	0.325484
H	2.037967	-0.926030	-1.459111
H	3.067291	-1.243536	-0.060742
H	0.797131	-2.414748	0.013248
H	1.173656	-1.443218	1.429527

#### **Vibrational frequencies**

-398.492	72.8325	135.442
232.043	299.5451	343.887
396.1271	446.9239	534.3928
593.8257	633.1433	676.6287
680.2564	717.391	747.6249
843.1436	849.4717	893.3566
913.9627	986.8471	1007.197
1026.591	1079.404	1118.462
1181.336	1219.387	1250.202
1290.16	1342.721	1370.979

1415.02	1443.413	1474.084
1486.54	1512.929	1599.733
2095.563	3048.042	3061.313
3101.601	3111.004	3242.35
3276.792	3447.726	3721.319

***i58 – i49***

**Cartesian coordinates**

N	-1.632086	1.036577	-0.03155
C	-2.408896	-0.086781	-0.04515
C	-1.582722	-1.191033	-0.00491
C	-0.255748	-0.718564	0.02563
C	-0.304314	0.681018	0.01346
C	0.836272	1.506461	0.10729
C	2.099368	0.932912	-0.18651
C	2.209157	-0.471051	-0.11823
C	1.051700	-1.440741	0.10195
H	-1.972457	1.980928	-0.06304
H	-3.484499	-0.020573	-0.08413
H	-1.911289	-2.219168	0.00067
H	0.744564	2.560581	0.35014
H	3.130125	-0.918709	-0.49167
H	2.774979	0.275509	0.76997
H	1.117011	-2.210955	-0.67624
H	1.157266	-1.976976	1.05402

**Vibrational frequencies**

-1402.97	88.7998	216.544
268.5882	385.9488	479.7169
489.0827	503.6732	584.5073
624.3191	644.2735	694.6451
720.5887	734.9178	761.2866
847.3845	861.018	912.2868
920.6684	970.1634	1066.937
1078.46	1125.372	1198.339
1207.051	1238.478	1253.991
1271.822	1339.54	1370.47
1395.67	1428.147	1461.171
1475.509	1505.054	1544.707
1578.116	2168.086	3023.866
3051.707	3130.177	3178.411
3253.836	3280.319	3713.519

***i59 – i60***

**Cartesian coordinates**

N	2.182707	-1.249310	0.001797
C	3.043650	-0.189859	-0.072979
C	2.307734	0.974314	-0.045724
C	0.959731	0.565373	0.052821
C	0.885851	-0.795053	0.079099
C	-1.221622	1.731960	0.230551
C	-2.026289	0.888880	-0.093627
C	-2.862446	-0.179649	-0.509878
C	-3.364276	-1.098097	0.320459
H	2.459721	-2.214721	0.002879
H	4.109599	-0.341647	-0.141716
H	2.704374	1.976082	-0.092950
H	0.045143	-1.466412	0.141300
H	-0.691187	2.596065	0.552744
H	-3.084067	-0.228076	-1.572471
H	-3.996656	-1.895406	-0.051274
H	-3.159878	-1.067931	1.384578

### **Vibrational frequencies**

-210.238	12.1477	37.2349
57.222	81.6405	114.6697
226.6014	333.7453	483.1769
563.4937	583.1009	646.1139
663.7613	685.8318	691.0507
703.919	769.0561	848.8014
857.1462	897.5937	902.563
957.5149	1016.067	1045.756
1083.624	1115.812	1167.762
1185.659	1247.026	1321.359
1400.837	1443.828	1470.311
1509.113	1563.509	1676.127
2158.307	3165.715	3179.317
3258.358	3264.592	3277.109
3281.307	3470.602	3714.124

### ***i60 – i61***

#### **Cartesian coordinates**

N	2.192111	-1.075530	0.243142
C	2.829072	0.142644	0.404992
C	1.958469	1.144769	0.056115
C	0.758512	0.498398	-0.340404
C	0.968661	-0.882042	-0.312102
C	-0.646651	0.826045	-0.494377
C	-1.408070	-0.268736	-0.340415
C	-2.796208	-0.532041	-0.133965

C	-3.591915	0.213636	0.653143
H	2.669308	-1.960281	0.277583
H	3.869039	0.191194	0.692527
H	2.155569	2.203455	0.128344
H	-0.392557	-1.208906	-0.374314
H	-1.023854	1.814992	-0.739898
H	-3.210074	-1.416762	-0.613277
H	-4.640575	-0.027782	0.786366
H	-3.202851	1.076761	1.182756

### Vibrational frequencies

-1852.3	84.8584	115.8038
165.8529	258.0464	309.7041
403.4472	455.4966	571.5874
589.8727	627.193	659.4509
697.2788	739.3893	755.9177
866.387	891.5243	912.8911
944.8097	979.6453	1007.394
1025.404	1077.5	1087.05
1095.924	1124.346	1185.457
1258.325	1318.945	1339.307
1378.817	1433.468	1438.62
1501.108	1546.281	1610.054
1639.475	1780.321	3155.036
3165.112	3181.782	3248.073
3255.598	3268.779	3687.502

### *i60 – i62*

#### Cartesian coordinates

C	1.905529	1.060225	-0.184333
C	2.863219	0.082404	-0.210639
N	2.248855	-1.109914	0.057513
C	0.911868	-0.909475	0.256005
C	0.654734	0.437181	0.106694
C	-0.631591	1.127565	0.221671
C	-1.824678	0.560434	0.085317
C	-2.489183	-0.694720	-0.207008
C	-3.745680	-0.260700	-0.106872
H	2.066982	2.112236	-0.363523
H	3.923544	0.137250	-0.396732
H	2.713500	-1.997057	0.125608
H	0.256630	-1.723411	0.520529
H	-0.587666	2.193986	0.422927
H	-2.082985	-1.671241	-0.444964
H	-4.741662	-0.680615	-0.212842

H -3.155642 0.980767 0.181403

**Vibrational frequencies**

-2278.81 40.7885 96.6263  
120.0296 230.1558 286.2089  
408.5442 416.0579 499.8108  
643.698 650.5299 694.3728  
703.4394 723.2772 769.3177  
795.6711 856.8289 887.5834  
905.1919 914.7446 926.8359  
986.3242 1025.741 1061.793  
1098.866 1106.361 1175.56  
1204.054 1245.615 1313.813  
1374.092 1436.814 1497.186  
1542.685 1604.494 1622.544  
1737.059 1933.606 3178.113  
3178.866 3221.056 3256.852  
3279.652 3285.714 3721.074

***i61 – i63***

**Cartesian coordinates**

N 1.838385 -1.212020 -0.132066  
C 2.746329 -0.154979 -0.197761  
C 2.084339 1.031864 -0.101879  
C 0.699621 0.678445 0.044558  
C 0.574981 -0.722053 -0.013637  
C -0.606448 1.099115 0.299953  
C -1.286110 -0.086644 0.760568  
C -2.630311 -0.436846 0.313860  
C -3.134921 -0.033437 -0.854872  
H 2.090387 -2.179490 -0.231834  
H 3.803896 -0.348937 -0.301106  
H 2.541126 2.009005 -0.104947  
H -1.092995 2.041800 0.075805  
H -0.984384 -0.488881 1.719333  
H -3.227355 -1.070207 0.965017  
H -4.147385 -0.280413 -1.152950  
H -2.536861 0.548464 -1.549598

**Vibrational frequencies**

-378.131 87.2545 133.2922  
203.2597 298.7109 338.187  
485.3479 536.4851 590.5341  
633.6277 679.286 700.441  
707.4613 742.8554 781.3188

809.2345	879.7939	891.9345
966.5489	973.3647	1015.783
1042.553	1057	1078.355
1111.217	1175.152	1181.539
1259.097	1329.863	1339.557
1370.146	1426.46	1443.826
1459.287	1566.054	1585.921
1695.62	3152.675	3167.06
3206.27	3208.723	3248.984
3252.178	3277.965	3703.051

### ***i62 – i64***

#### **Cartesian coordinates**

N	-1.954871	-1.208132	0.095444
C	-2.723641	-0.082143	-0.030985
C	-1.875143	0.987007	-0.114036
C	-0.535488	0.495131	-0.033778
C	-0.632231	-0.877359	0.093591
C	0.641954	1.356119	-0.072755
C	1.932401	1.054726	0.090135
C	2.808765	-1.188553	-0.533188
C	2.510389	-0.285866	0.365317
H	-2.310135	-2.144525	0.165531
H	-3.799789	-0.138250	-0.051657
H	-2.165014	2.021765	-0.218954
H	0.133639	-1.629426	0.167412
H	0.411718	2.405013	-0.245846
H	2.655461	1.865711	0.052818
H	3.251916	-2.175139	-0.539752
H	2.744264	-0.502593	1.416536

#### **Vibrational frequencies**

-111.044	42.0804	142.0268
176.3488	259.0249	345.334
499.0057	516.6944	540.5519
646.8094	659.734	671.458
712.5352	745.9315	763.2928
824.7429	830.2233	871.5618
897.0907	913.1201	975.6609
1017.408	1024.671	1087.474
1107.737	1179.065	1239.855
1254.799	1262.377	1332.622
1419.01	1451.205	1496.756
1542.909	1621.32	1687.555

1743.838	3021.263	3153.571
3176.789	3250.562	3257.164
3285.263	3303.292	3718.129

***i63 – i65***

**Cartesian coordinates**

N	-1.562260	-1.047138	-0.625066
C	-2.344152	-0.456256	0.381567
C	-1.780137	0.709708	0.774894
C	-0.568030	0.816382	-0.004914
C	-0.507221	-0.266710	-0.951918
C	0.637169	1.459016	-0.086444
C	1.529938	0.549454	-0.798094
C	2.211451	-0.549720	-0.141571
C	2.173716	-0.842637	1.167223
H	-1.852480	-1.861432	-1.139539
H	-3.254809	-0.931508	0.717598
H	-2.140813	1.358635	1.557284
H	0.911392	2.447725	0.268183
H	2.018866	0.905931	-1.705557
H	2.829545	-1.161005	-0.795027
H	2.722928	-1.687757	1.563896
H	1.584793	-0.256042	1.864165

**Vibrational frequencies**

-474.055	62.5445	98.8967
151.1058	206.8851	298.4845
476.7285	569.3046	612.0249
624.9646	633.1332	709.3413
737.2275	744.5402	761.244
835.2101	885.9282	897.7764
911.6623	943.8259	978.2975
1036.481	1053.65	1060.467
1103.515	1128.108	1177.287
1232.736	1292.018	1334.967
1366.625	1417.337	1427.544
1442.695	1597.792	1615.356
1645.36	3127.796	3156.746
3167.966	3191.437	3247.55
3256.705	3274.78	3686.31

***i64 – i65***

**Cartesian coordinates**

N	1.825290	1.170421	-0.000077
C	2.628201	0.048342	0.000097

C	1.817777	-1.050154	0.000131
C	0.456081	-0.594197	-0.000028
C	0.526456	0.783409	-0.000134
C	-0.731971	-1.411156	-0.000102
C	-2.022755	-1.015423	-0.000075
C	-1.908284	1.498556	0.000014
C	-2.560795	0.335521	0.000125
H	2.150817	2.120115	-0.000143
H	3.702986	0.135833	0.000193
H	2.145098	-2.079204	0.000260
H	-0.671796	1.468934	-0.000402
H	-0.550002	-2.482834	-0.000185
H	-2.771913	-1.800555	-0.000126
H	-2.360732	2.484103	0.000323
H	-3.649758	0.391267	0.000460

### **Vibrational frequencies**

-1263.59	75.7371	181.2403
273.9676	276.242	399.8291
453.0037	477.4223	482.9292
596.5119	627.2643	677.4407
694.681	724.2616	798.089
816.5287	861.3998	887.2924
912.1131	948.5015	952.1093
999.3258	1018.192	1082.957
1112.908	1129.334	1220.137
1270.521	1299.543	1325.341
1403.968	1437.806	1467.563
1498.786	1545.925	1610.903
1657.138	1711.684	3128.932
3169.42	3197.994	3213.309
3249.504	3279.083	3718.583

### ***i64 – i66***

#### **Cartesian coordinates**

N	1.816150	-0.961414	0.290223
C	2.388747	0.067521	-0.410902
C	1.498413	1.108097	-0.451666
C	0.319559	0.693660	0.226661
C	0.539102	-0.622326	0.664314
C	-0.949164	1.378835	0.313544
C	-2.129560	0.758885	0.108454
C	-1.321889	-1.547706	-0.319277
C	-2.268268	-0.620705	-0.355306
H	2.265913	-1.830719	0.510968



H	3.369401	-0.033273	-0.847826
H	1.646540	2.048307	-0.960130
H	0.073345	-1.126567	1.495102
H	-0.939694	2.454064	0.469214
H	-3.040326	1.347067	0.160869
H	-1.325589	-2.567393	-0.686387
H	-3.224288	-0.859150	-0.828304

### **Vibrational frequencies**

-364.152	117.058	164.5887
272.1659	303.4923	430.5515
455.6	468.1292	593.861
634.5587	637.4554	682.0593
742.5821	760.6106	783.8782
807.9667	888.4475	898.6379
916.81	921.2307	979.3535
991.9996	1016.649	1092.165
1100.934	1175.358	1203.843
1260.081	1269.785	1302.799
1398.155	1439.664	1490.514
1539.065	1561.783	1605.795
1674.906	3092.319	3169.673
3193.089	3214.471	3256.499
3264.548	3278.045	3722.727

### ***i22 – i65***

#### **Cartesian coordinates**

N	1.800586	1.161879	-0.072515
C	2.600974	0.033217	-0.066217
C	1.784161	-1.056927	0.019260
C	0.426863	-0.589031	0.066569
C	0.499835	0.789909	-0.049031
C	-0.761203	-1.403324	0.141846
C	-2.038055	-0.993381	-0.045558
C	-1.846391	1.446559	0.304286
C	-2.422067	0.377073	-0.287148
H	2.129579	2.101692	-0.203929
H	3.672055	0.110357	-0.166673
H	2.104630	-2.088044	0.048882
H	-0.589448	-2.469524	0.264634
H	-2.808857	-1.753533	-0.133677
H	-2.107566	2.457075	0.011225
H	-1.273940	1.338374	1.217478
H	-3.195260	0.545877	-1.034380

**Vibrational frequencies**

-199.019	97.3654	171.3478
245.2653	275.7546	401.9812
450.4513	511.6312	588.692
608.5652	616.0642	674.4244
729.1449	805.5337	812.0425
863.7987	866.705	912.7279
948.3253	976.9591	1006.017
1020.98	1079.421	1092.736
1109.129	1197.918	1242.692
1286.958	1308.409	1374.339
1429.537	1433.123	1457.083
1524.243	1569.582	1624.507
1667.069	3144.178	3161.843
3165.957	3185.678	3245.655
3251.318	3275.589	3710.145

***i22 – i66*****Cartesian coordinates**

N	1.593752	-1.079903	-0.075138
C	2.392045	0.028814	-0.109826
C	1.644169	1.166672	-0.017068
C	0.266209	0.777359	0.093798
C	0.275786	-0.660794	0.154358
C	-0.929592	1.474260	0.066618
C	-2.154687	0.715197	-0.062777
C	-0.999526	-1.453056	0.018703
C	-2.184087	-0.643523	-0.118897
H	1.926083	-2.020147	0.034524
H	3.462565	-0.077229	-0.205419
H	2.021896	2.175067	-0.076230
H	-0.305540	-1.087222	1.161592
H	-0.946868	2.555640	0.044836
H	-3.088782	1.257651	-0.158671
H	-0.960169	-2.518782	-0.151575
H	-3.127353	-1.155222	-0.272541

**Vibrational frequencies**

-3401.36	161.1858	203.7743
251.5592	325.8193	377.596
475.8229	528.7769	533.8137
584.2505	601.2067	662.1267
718.7921	744.7061	763.9731
777.5113	867.5867	889.2202
899.384	965.2552	997.2556

1015.55	1094.189	1113.218
1143.681	1181.214	1199.705
1230.639	1266.267	1316.118
1374.81	1426.602	1431.728
1482.634	1498.889	1582.87
1635.011	2233.856	3188.939
3209.722	3228.131	3246.095
3253.326	3275.126	3721.301

***i66 – indole (2) + H***

**Cartesian coordinates**

N	1.563310	-1.067032	-0.083411
C	2.367490	0.045849	-0.089252
C	1.609282	1.178277	-0.039111
C	0.244094	0.765158	0.035147
C	0.248626	-0.664786	0.121238
C	-0.983166	1.436334	0.018703
C	-2.150004	0.699876	-0.014356
C	-0.944756	-1.407400	-0.072677
C	-2.126619	-0.711157	-0.087806
H	1.895667	-1.999123	0.087429
H	3.439991	-0.059073	-0.149788
H	1.980982	2.190004	-0.076546
H	0.253255	-0.707247	1.832088
H	-1.013962	2.520057	0.004515
H	-3.106098	1.210206	-0.030363
H	-0.919512	-2.488763	-0.139037
H	-3.063172	-1.249742	-0.175734

**Vibrational frequencies**

-1028.98	213.8488	231.0279
383.0114	412.6863	448.049
512.1488	545.9072	565.9965
594.5746	623.3671	661.0966
736.5646	757.4359	771.7426
806.9484	869.7326	890.8347
894.4313	909.2093	955.0578
990.7	1035.92	1091.441
1128.658	1153.691	1178.008
1229.414	1266.506	1308.698
1361.26	1388.877	1461.791
1482.3	1538.171	1566.752
1622.398	1670.948	3194.376
3201.97	3213.03	3223.222

3258.662 3278.604 3712.083

***i56 – i67***

**Cartesian coordinates**

N	-2.486959	-0.954013	-0.136452
C	-2.903469	0.353561	-0.142382
C	-1.795046	1.146238	-0.040185
C	-0.655137	0.286931	0.038354
C	-1.130786	-1.008931	-0.036418
H	-3.091528	-1.751721	-0.217938
H	-3.949290	0.603702	-0.217156
H	-1.785472	2.225080	-0.010011
H	-0.596651	-1.945587	-0.051679
C	4.035489	-0.285342	-0.450866
C	2.891729	0.030567	-0.013828
C	1.729429	-0.190566	0.735316
C	0.739210	0.668427	0.172744
H	4.881170	-0.077083	-1.072404
H	1.583983	-0.928546	1.518964
H	0.921475	1.740114	0.234452
H	1.976514	0.806826	-0.805472

**Vibrational frequencies**

-2155.46	70.7439	79.0822
172.3666	227.3971	309.357
394.5107	415.8886	499.673
517.6897	523.2868	573.8453
645.5497	654.5329	718.0734
726.7542	762.0985	805.5397
837.9286	874.3815	909.2635
994.1551	1013.877	1080.451
1101.854	1109.531	1159.936
1170.901	1234.913	1312.32
1332.039	1421.027	1466.379
1488.63	1498.306	1561.773
1612.79	1813.069	3137.458
3173.688	3260.096	3279.825
3286.697	3382.539	3715.65

***i67 – i68***

**Cartesian coordinates**

N	2.653213	-0.845180	-0.065586
C	2.941468	0.492797	-0.069558
C	1.753716	1.172213	-0.030492
C	0.700463	0.210058	0.003354

C	1.302046	-1.030827	-0.025521
C	-0.725705	0.520663	0.054477
C	-1.711783	-0.336171	0.318251
C	-3.149306	0.049571	0.350601
C	-4.000219	-0.131532	-0.625761
H	3.333583	-1.582169	-0.108815
H	3.959119	0.846644	-0.100221
H	1.635679	2.245220	-0.019217
H	0.872413	-2.019533	-0.039975
H	-0.984018	1.558480	-0.146305
H	-1.488206	-1.376705	0.544754
H	-3.515628	0.503750	1.280139
H	-5.049515	0.059942	-0.803359

### Vibrational frequencies

-181.16	40.5977	97.2631
146.5275	274.4494	331.868
392.8098	475.2001	504.1224
641.3186	644.4876	661.0545
705.0515	768.0211	786.7034
821.8351	847.5002	862.5258
902.7392	914.0688	998.5973
1008.943	1066.677	1095.794
1106.545	1176.804	1233.687
1250.006	1309.366	1336.472
1349.904	1436.753	1496.822
1540.575	1624.635	1686.126
1748.756	3034.22	3149.779
3158.798	3247.839	3255.277
3281.025	3284.848	3718.368

### *i68 – i69*

#### Cartesian coordinates

N	-2.542548	-0.871850	0.04729
C	-2.860462	0.457775	0.13676
C	-1.696524	1.170588	0.06852
C	-0.615672	0.240429	-0.06948
C	-1.191351	-1.020950	-0.07734
C	0.777557	0.588832	-0.17361
C	1.817354	-0.305989	-0.35463
C	3.249171	0.095443	-0.43150
C	3.331438	-0.203106	0.81892
H	-3.203740	-1.626504	0.07732
H	-3.883274	0.781437	0.24236
H	-1.605314	2.245296	0.11100

H	-0.742779	-1.998158	-0.15194
H	1.024503	1.641515	-0.06514
H	1.586034	-1.349187	-0.55077
H	3.859353	0.489556	-1.23805
H	3.893993	-0.219126	1.73847

**Vibrational frequencies**

-717.6	57.8342	94.2292
153.9602	233.3548	345.4841
351.8523	417.762	484.1564
568.9153	635.4104	649.8693
683.7325	707.5834	765.9656
772.4591	809.8769	867.0209
867.8109	909.6653	934.0475
995.4062	1048.212	1092.114
1106.468	1166.7	1176.489
1234.826	1272.904	1310.596
1344.664	1420.581	1493.971
1502.964	1556.653	1598.816
1725.033	3162.438	3170.118
3178.198	3255.933	3277.557
3282.341	3285.832	3718.802

***i68 – i71***

**Cartesian coordinates**

N	-2.415487	0.812396	0.301943
C	-2.723463	-0.494179	0.015135
C	-1.554977	-1.147628	-0.258937
C	-0.490790	-0.200615	-0.141905
C	-1.070005	1.000659	0.218380
C	0.926139	-0.434470	-0.351403
C	2.649753	-0.508896	0.952819
C	3.058889	0.269148	-0.070925
C	1.841588	0.570565	-0.742333
H	-3.081555	1.517897	0.560680
H	-3.743528	-0.842482	0.029250
H	-1.455453	-2.188670	-0.525839
H	-0.613617	1.951488	0.442858
H	1.211266	-1.464937	-0.529746
H	3.138901	-1.071553	1.743270
H	4.066573	0.584900	-0.327683
H	1.563005	1.499085	-1.231377

**Vibrational frequencies**

-619.706	79.6628	118.8136
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154.6351	386.1194	397.884
435.5721	515.1791	579.8734
645.6905	663.8749	683.4984
714.4237	729.0014	777.9058
817.5341	842.0909	874.6819
903.9763	911.4926	914.8721
1003.879	1056.705	1092.591
1104.802	1163.21	1174.737
1235.064	1254.779	1322.668
1361.284	1428.163	1480.696
1491.67	1520.006	1566.15
1618.48	3158.06	3185.527
3194.06	3195.78	3260.402
3280.824	3284.81	3715.52

### *i69 – i70*

#### **Cartesian coordinates**

N	2.204139	1.024843	0.030632
C	2.740200	-0.209291	-0.244413
C	1.735790	-1.128966	-0.203992
C	0.509461	-0.437509	0.110362
C	0.859866	0.909802	0.247435
C	-0.773347	-1.004515	0.251394
C	-1.990644	-0.206657	0.555782
C	-2.416611	0.956293	-0.315397
C	-3.126920	-0.111087	-0.437025
H	2.722971	1.882773	0.071025
H	3.793309	-0.325706	-0.444932
H	1.837684	-2.189105	-0.378250
H	0.254701	1.765070	0.497935
H	-0.873270	-2.082605	0.162548
H	-2.250531	-0.159046	1.618644
H	-2.203175	1.966428	-0.618967
H	-3.937423	-0.640122	-0.907298

#### **Vibrational frequencies**

-53.0403	94.866	141.773
253.8344	320.2085	371.5612
455.3022	494.8932	573.7737
623.6438	649.2945	672.2398
705.6376	737.8816	773.6768
841.8876	879.7019	881.8778
899.3941	911.2125	972.395
1012.115	1037.645	1053.219

1100.642	1100.951	1167.083
1219.082	1225.948	1299.292
1358.274	1390.616	1453.008
1492.031	1532.923	1578.965
1741.649	3033.594	3170.197
3257.779	3271.418	3279.706
3282.914	3319.586	3723.74

### *i62 – i70*

#### **Cartesian coordinates**

N	2.023398	-1.133740	-0.060686
C	2.705477	0.043599	0.105156
C	1.788521	1.054461	0.132226
C	0.484427	0.478201	-0.026580
C	0.682704	-0.891808	-0.139911
C	-0.736547	1.238218	-0.045520
C	-2.034350	0.780912	-0.227083
C	-2.436418	-0.624364	-0.504198
C	-2.704783	-0.711072	0.753000
H	2.444674	-2.043691	-0.106757
H	3.779940	0.060223	0.190363
H	2.003828	2.105672	0.249855
H	-0.022763	-1.696728	-0.250776
H	-0.622240	2.303033	0.136462
H	-2.815590	1.532006	-0.279566
H	-2.428332	-1.232529	-1.403914
H	-2.997488	-1.300689	1.606591

#### **Vibrational frequencies**

-701.104	61.1915	122.8166
173.8483	242.2535	299.3211
420.5596	490.5708	516.0715
604.2039	637.605	653.7011
680.4696	716.0804	756.8146
776.4532	806.7668	874.0098
877.7426	908.4951	930.9628
956.3611	1018.16	1095.485
1106.436	1138.934	1179.878
1243.141	1256.482	1322.686
1408.058	1422.935	1488.662
1498.466	1556.345	1599.294
1722.07	3151.349	3168.943
3188.871	3256.71	3277.053
3283.548	3304.239	3721.491



*i64 – i71*

**Cartesian coordinates**

N	2.150627	0.939053	-0.105899
C	2.507920	-0.367994	-0.291099
C	1.412511	-1.143847	-0.018550
C	0.342616	-0.271045	0.339206
C	0.842032	1.010066	0.287684
H	2.766840	1.725507	-0.200153
H	3.505686	-0.637041	-0.598306
H	1.363770	-2.220020	-0.086353
H	0.363408	1.951240	0.503720
C	-1.008317	-0.680034	0.759294
C	-1.927766	-0.426175	-1.230694
C	-2.445977	0.572648	-0.495094
C	-2.134087	0.168275	0.841355
H	-0.988676	-1.558311	1.410381
H	-1.786458	-0.631096	-2.288578
H	-2.987257	1.453247	-0.831469
H	-2.825294	0.171738	1.679442

**Vibrational frequencies**

-701.851	49.4391	130.2543
170.4309	293.4601	366.018
452.3366	474.1968	586.7101
638.2486	646.9462	703.4451
710.3877	743.4428	783.2912
808.5062	859.452	888.1518
903.2526	911.8677	944.1024
984.5386	1059.674	1077.976
1095.224	1139.361	1171.022
1240.408	1252.803	1313.781
1408.319	1423.039	1464.777
1493.068	1524.423	1550.508
1621.855	3093.037	3153.637
3176.799	3191.155	3254.515
3280.608	3283.725	3721.632

*Reaction steps with extra ammonia molecules*

1)

*i2 + NH<sub>3</sub>*

**Cartesian coordinates**

C	0.397016	-0.285947	1.159658
C	0.866534	0.990408	0.556783
N	0.464271	-1.163821	-0.004157

C	1.107375	0.790454	-0.746889
C	0.832072	-0.617860	-1.150981
H	-0.644115	-0.209115	1.494563
H	1.030688	-0.641309	1.979018
H	0.968945	1.907862	1.121868
H	0.171082	-2.125764	0.059338
H	1.452954	1.539840	-1.446885
N	-2.505741	0.213393	-0.105967
H	-3.398221	-0.226141	-0.297934
H	-2.639202	1.212960	-0.204777
H	-1.869821	-0.067672	-0.845751

### Vibrational frequencies

35.4321	71.4887	89.5409
158.5417	174.1515	227.7499
374.2394	464.2956	719.7899
744.1377	832.3217	863.9683
965.8086	971.2871	1002.229
1004.145	1022.432	1089.089
1126.682	1195.539	1302.681
1337.416	1368.8	1443.826
1514.795	1618.339	1673.508
1687.966	3045.45	3100.516
3216.521	3239.988	3506.298
3626.454	3642.349	3658.904

### *i2 + NH<sub>3</sub> – pyrrole (3) + NH<sub>3</sub>*

#### Cartesian coordinates

C	-0.285554	0.445891	1.093218
C	-0.761436	-0.841145	0.755917
N	-0.410801	1.174338	-0.108912
C	-0.959909	-0.862539	-0.618857
C	-0.708113	0.423588	-1.205728
H	1.110656	-0.015882	0.667236
H	-0.337198	0.933887	2.059303
H	-0.858512	-1.658346	1.460212
H	-0.148297	2.143622	-0.178419
H	-1.253642	-1.734150	-1.190219
N	2.006742	-0.269883	-0.145274
H	2.775578	0.387384	-0.100940
H	2.343697	-1.220766	-0.060266
H	1.486204	-0.161709	-1.024904

### Vibrational frequencies

-1082.82	175.6353	195.6927
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265.3575	432.1453	469.7818
586.7273	611.6169	674.3764
724.0266	772.7104	846.8163
868.8377	906.6337	936.9374
1032.085	1053.583	1103.966
1132.297	1232.629	1275.67
1340.256	1388.417	1453.65
1472.584	1503.119	1568.61
1655.127	1706.82	3201.788
3208.824	3229.628	3376.221
3587.073	3662.807	3666.175

***Pyrrole (3) + NH<sub>3</sub>***

**Cartesian coordinates**

C	-0.585064	-1.112578	0.000007
C	-1.899706	-0.711786	0.000057
N	0.202358	0.002168	-0.000033
C	-1.902392	0.708145	0.000055
C	-0.589272	1.113915	0.000003
H	3.564553	-0.142021	-0.932551
H	-0.151659	-2.100335	-0.000253
H	-2.760718	-1.362404	0.000022
H	1.223914	0.003781	0.000279
H	-2.765852	1.355510	0.000016
N	3.193810	0.000221	-0.000080
H	3.564444	-0.736783	0.588761
H	3.570425	0.876026	0.344040
H	-0.159672	2.103326	-0.000250

**Vibrational frequencies**

29.2729	50.1472	62.138
180.6241	276.9531	302.1805
629.8918	638.773	715.7773
737.3557	825.8811	891.1997
892.4632	904.5808	920.9019
1044.289	1081.47	1103.974
1108.236	1196.448	1219.821
1335.531	1441.242	1528.261
1529.485	1618.387	1678.353
1679.107	3243.62	3254.532
3268.346	3276.843	3427.251
3518.424	3643.724	3645.267

***i2 + 2 NH<sub>3</sub>***

**Cartesian coordinates**

N	0.384972	0.458218	0.000098
C	0.395323	-0.858736	0.000503
C	1.690329	1.103093	-0.000416
C	1.848736	-1.188227	0.000355
C	2.598528	-0.078228	-0.000169
H	-0.495454	1.000332	0.000063
H	1.817168	1.735319	-0.886419
H	1.817569	1.736027	0.885017
H	2.223968	-2.203313	0.000614
H	3.678083	0.000639	-0.000447
N	-2.290560	1.573786	0.000287
H	-2.659450	0.611598	0.000049
H	-2.662600	2.046468	0.815936
H	-2.662601	2.046954	-0.815080
N	-2.727689	-1.399456	-0.000393
H	-1.699042	-1.462485	0.000082
H	-3.061518	-1.903621	0.813420
H	-3.060690	-1.903172	-0.814823

**Vibrational frequencies**

33.0113	74.7515	99.0718
154.4523	183.4263	199.1697
232.7614	248.8419	290.8677
360.6117	398.8889	456.0546
507.9403	600.4547	711.2985
840.571	861.1992	958.0317
970.3599	975.7095	1003.732
1032.638	1070.332	1123.085
1165.921	1175.837	1206.326
1296.698	1355.733	1416.708
1457.696	1592.249	1627.695
1658.561	1681.363	1718.538
1730.8	3055.617	3096.523
3218.527	3221.739	3244.718
3298.752	3333.383	3561.116
3568.403	3631.299	3637.689

***i2 + 2 NH<sub>3</sub> – pyrrole (3) + 2 NH<sub>3</sub>*****Cartesian coordinates**

N	0.641612	-0.440013	1.140769
C	0.249484	-1.372857	0.243791
C	1.413024	0.619032	0.600629
C	0.964838	-0.977504	-0.939507
C	1.702976	0.168193	-0.714455

H	0.265163	-0.402559	2.073482
H	0.239179	1.381261	0.161168
H	2.082533	1.187469	1.238156
H	0.910448	-1.510216	-1.880442
H	2.331278	0.703746	-1.415949
N	-0.907693	1.751968	-0.232855
H	-1.590105	0.952441	-0.164748
H	-1.246778	2.537177	0.312134
H	-0.838146	2.036699	-1.203967
N	-2.597157	-0.560286	-0.068096
H	-1.786536	-1.186224	0.098478
H	-3.262166	-0.708576	0.683047
H	-3.044134	-0.874082	-0.922834

### Vibrational frequencies

-1165.99	43.3262	134.27
160.9605	206.4274	236.0046
291.3893	307.6539	413.958
435.968	526.053	545.8227
601.6541	651.0327	713.2891
724.2884	770.5645	848.0175
871.4913	905.6764	945.1583
1032.193	1052.749	1109.498
1130.88	1226.239	1262.797
1341.285	1365.119	1396.817
1458.811	1494.132	1508.299
1555.27	1651.275	1692.369
1714.477	1733.619	2941.75
3182.889	3186.213	3210.978
3232.423	3554.317	3555.701
3629.479	3639.035	3664.406

### *Pyrrole (3) + 2 NH<sub>3</sub>*

#### Cartesian coordinates

N	-0.162224	-0.867513	-0.025889
C	-0.843866	-0.507050	1.099706
C	-0.849561	-0.439763	-1.123816
C	-1.997294	0.140022	0.719540
C	-2.000945	0.182558	-0.699778
H	0.815475	-1.179373	-0.036361
H	0.698702	1.660342	0.771616
H	-0.471082	-0.617402	-2.118392
H	-2.759166	0.520127	1.382844
H	-2.766037	0.602437	-1.334775
N	1.362896	1.876889	0.033340

H	2.560398	0.134682	0.015678
H	0.827256	1.789354	-0.824867
H	1.614809	2.853664	0.131341
N	2.729973	-0.876523	-0.010647
H	-0.460594	-0.744933	2.079750
H	3.299212	-1.078919	-0.823944
H	3.276513	-1.124554	0.805578

**Vibrational frequencies**

55.1256	61.5227	71.4473
143.8167	181.273	183.3674
215.0028	227.2016	263.2587
345.2602	374.9086	521.5999
637.8159	642.4723	726.5667
748.8268	839.9487	886.6105
893.0394	896.6776	962.1063
1043.489	1077.696	1104.763
1151.539	1161.937	1197.61
1221.81	1335.648	1439.178
1527.366	1529.096	1617.767
1667.939	1669.99	1710.461
1723.46	3247.556	3258.791
3273.077	3281.143	3344.326
3396.387	3501.84	3581.654
3607.19	3633.358	3642.735

2)

$i3 + NH_3$

**Cartesian coordinates**

N	0.110630	-0.533455	0.636067
C	-1.187641	1.126917	-0.103498
C	-0.041016	1.004739	0.615082
C	-1.766422	-0.149137	-0.518332
C	-0.998713	-1.149639	-0.076599
H	0.168230	-0.823125	1.610854
H	1.053220	-0.701987	0.208919
H	-1.631345	2.082494	-0.352237
H	-2.671091	-0.280494	-1.098362
H	-1.075921	-2.221255	-0.170139
N	2.668545	-0.015377	-0.391048
H	3.574885	-0.142978	0.042699
H	2.812199	0.060288	-1.391190
H	2.278349	0.871600	-0.065596

**Vibrational frequencies**

58.408	128.6633	174.0734
234.8591	311.8244	452.4989
515.2012	558.5855	670.6288
708.2952	803.2856	809.3786
868.5644	925.0964	961.9374
986.6156	1033.634	1127.327
1143.451	1180.105	1216.21
1316.477	1356.346	1514.036
1638.243	1665.817	1672.664
1693.656	3042.582	3223.529
3236.696	3275.361	3440.026
3539.754	3593.076	3648.764

*i3 + NH<sub>3</sub> – pyrrole (3) + NH<sub>3</sub>*

**Cartesian coordinates**

N	0.112314	-0.647351	0.678112
C	-0.958937	1.158831	-0.012768
C	0.066656	0.827673	0.832070
C	-1.603373	-0.007074	-0.591888
C	-0.970248	-1.101992	-0.129686
H	0.283422	-1.153051	1.539299
H	1.302345	-0.565399	-0.018042
H	-1.260329	2.177644	-0.224099
H	-2.434737	-0.012515	-1.284848
H	-1.144707	-2.153813	-0.301847
N	2.268350	0.028413	-0.481084
H	3.194498	-0.307931	-0.244979
H	2.185488	0.194794	-1.477821
H	2.004780	0.888209	0.046775

**Vibrational frequencies**

-991.445	45.6946	199.4668
264.6427	386.1657	446.1929
589.763	658.4343	679.8398
720.2598	796.4379	849.81
870.7731	881.451	914.1784
920.6587	1009.277	1075.237
1134.369	1216.207	1244.448
1299.767	1376.886	1476.237
1546.542	1631.299	1648.673
1691.573	1757.312	3151.928
3209.398	3228.027	3257.211
3562.57	3591.469	3652.877

***Pyrrole (3) + NH<sub>3</sub>***

**Cartesian coordinates**

N	0.202387	0.002464	0.005401
C	-1.902512	0.707973	-0.002910
C	-0.589504	1.113995	0.002207
C	-1.899457	-0.712118	-0.002900
C	-0.584713	-1.112458	0.002224
H	1.223968	0.004258	0.007692
H	3.556770	-0.749907	-0.578567
H	-2.765932	1.355500	-0.006097
H	-2.760038	-1.363413	-0.006076
H	-0.149917	-2.099649	0.004235
N	3.193301	0.000250	-0.001901
H	3.575629	-0.121010	0.928831
H	3.565804	0.867829	-0.370430
H	-0.158978	2.103054	0.004187

**Vibrational frequencies**

47.193	48.8703	70.1951
180.8137	280.7123	308.3389
629.787	638.0619	707.2158
737.0214	822.8168	892.3841
893.7454	902.5814	923.7
1038.042	1077.003	1104.908
1110.077	1196.897	1222.559
1332.924	1437.596	1528.723
1531.133	1619.226	1677.122
1681.937	3243.494	3256.204
3274.789	3281.439	3429.52
3517.343	3642.315	3643.522

***i3 + 2 NH<sub>3</sub>***

**Cartesian coordinates**

N	0.519882	0.468927	0.704717
C	1.433179	-1.272404	-0.349334
C	0.297416	-0.998077	0.342651
C	2.348875	-0.138106	-0.435003
C	1.814447	0.904925	0.207690
H	0.433239	0.560079	1.715545
H	1.642026	-2.236158	-0.795787
H	3.306622	-0.125723	-0.939272
H	2.159437	1.914323	0.367358
H	-0.296309	1.021130	0.282567
N	-1.739658	1.640678	-0.424482
H	-2.237990	2.431097	-0.032243



H	-1.632774	1.813190	-1.418004
H	-2.323701	0.794246	-0.314903
N	-2.803830	-1.081856	0.035786
H	-3.343780	-1.379290	0.840854
H	-3.093534	-1.664536	-0.741959
H	-1.811493	-1.300633	0.227681

### Vibrational frequencies

45.6546	67.6403	123.0406
166.6019	196.8222	238.5848
251.9268	263.8324	327.4975
406.2126	491.5606	534.149
561.6542	642.1149	680.279
762.1482	819.8224	827.5613
876.9719	938.5143	973.8351
989.2957	1037.314	1122.72
1196.432	1201.333	1221.05
1234.091	1351.174	1419.817
1516.848	1647.949	1654.575
1670.871	1683.955	1721.368
1728.763	2640.813	3220.049
3225.559	3236.138	3271.638
3276.733	3535.83	3557.121
3565.701	3629.967	3638.806

### *i3* + 2 *NH*<sub>3</sub> – pyrrole (3) + 2 *NH*<sub>3</sub>

#### Cartesian coordinates

N	-0.555016	-0.396676	0.869562
C	-1.125064	1.287218	-0.444031
C	-0.140407	0.964751	0.448444
C	-2.162839	0.273424	-0.520675
C	-1.837437	-0.723905	0.321063
H	-0.426108	-0.575771	1.858999
H	-1.144335	2.206470	-1.016458
H	-3.047157	0.297520	-1.144480
H	-2.331664	-1.654470	0.556879
H	0.320653	-1.055761	0.222541
N	1.256598	-1.527531	-0.575836
H	1.554897	-2.485714	-0.436569
H	0.920066	-1.420607	-1.527179
H	2.049601	-0.859778	-0.427146
N	2.874776	0.714615	0.066622
H	3.482818	0.796462	0.874070
H	3.245948	1.333591	-0.645872
H	1.935266	1.076262	0.333976

**Vibrational frequencies**

-930.585	42.3986	79.5533
152.1068	181.5147	228.1516
287.7753	313.278	388.6121
443.0385	545.4117	568.1255
590.9049	669.9394	697.3748
737.5713	803.6325	847.974
878.5305	891.1118	922.1063
926.4323	1005.14	1062.613
1132.947	1219.445	1235.666
1289.55	1326.225	1372.229
1484.221	1533.086	1633.35
1642.33	1671.662	1709.025
1720.737	1739.866	3025.724
3132.627	3206.756	3222.473
3261.898	3552.948	3558.904
3585.662	3629.626	3642.724

***Pyrrrole (3) + 2 NH<sub>3</sub>*****Cartesian coordinates**

N	0.164639	-0.869815	0.042946
C	1.997775	0.125844	-0.723051
C	0.847125	-0.533900	-1.089928
C	1.998680	0.201967	0.694903
C	0.848444	-0.413589	1.131426
H	-0.812658	-1.182641	0.058843
H	2.759664	0.492541	-1.393839
H	2.761204	0.639661	1.320878
H	0.468117	-0.568148	2.129133
H	-0.882554	1.863531	0.831710
N	-1.366857	1.877556	-0.060178
H	-1.619599	2.840826	-0.248231
H	-0.660232	1.611496	-0.741237
H	-2.556916	0.130881	-0.022041
N	-2.727128	-0.879748	0.019397
H	-3.302951	-1.068898	0.831252
H	-3.267399	-1.140413	-0.797095
H	0.466612	-0.796718	-2.064629

**Vibrational frequencies**

56.7607	64.5025	73.3663
117.4016	167.8376	181.7735
201.5116	221.4788	264.1089
309.7767	372.1533	518.5299

638.051	641.6542	726.4422
748.0802	840.1548	886.9301
893.1463	896.3007	963.7564
1043.621	1078.035	1104.885
1149.429	1161.988	1198.034
1222.069	1336.12	1439.579
1527.244	1529.961	1617.919
1667.522	1670.799	1695.717
1722.354	3247.551	3258.501
3272.841	3281.149	3344.808
3396.299	3501.875	3581.646
3607.962	3635.447	3642.812

### *i37 + NH<sub>3</sub>*

#### **Cartesian coordinates**

N	0.144729	-0.532952	0.637257
C	-1.178645	1.163861	-0.083704
C	0.032216	1.025884	0.596202
C	-1.814239	-0.001974	-0.493871
C	-0.981602	-1.184032	-0.112599
H	0.156768	-0.806783	1.615180
H	-1.586620	2.148602	-0.284115
H	-2.741800	-0.089655	-1.042070
H	-1.491404	-1.911774	0.527329
H	-0.569130	-1.728421	-0.970115
H	1.083790	-0.743759	0.247726
N	2.717284	-0.004675	-0.379224
H	3.604400	-0.069175	0.105522
H	2.915214	0.087973	-1.368485
H	2.248309	0.853955	-0.073367

#### **Vibrational frequencies**

46.9649	106.5947	168.2594
173.8724	249.1587	344.3351
442.105	520.6771	548.5135
669.7547	747.5794	840.2998
854.008	937.5135	949.5601
991.8522	1005.725	1074.996
1144.75	1151.913	1174.934
1287.824	1321.901	1363.209
1399.973	1421.254	1499.77
1661.181	1685.186	1696.635
3033.503	3073.06	3181.778
3202.442	3242.287	3399.645

3555.878 3582.746 3645.323

***i37 + NH<sub>3</sub> - i39 + NH<sub>3</sub>***

**Cartesian coordinates**

N	0.204827	-0.663281	0.521064
C	-0.985011	1.208660	0.020520
C	0.203343	0.838978	0.658533
C	-1.745438	0.151996	-0.452889
C	-1.051356	-1.132953	-0.122509
H	0.335611	-1.085447	1.433643
H	-1.266040	2.248213	-0.109257
H	-2.681387	0.203687	-0.992750
H	-1.625180	-1.770718	0.563323
H	-0.825380	-1.743459	-1.008093
H	1.455053	-0.651442	-0.121079
N	2.418558	0.027838	-0.400837
H	3.291709	-0.204517	0.055514
H	2.562656	0.212464	-1.385682
H	1.860029	0.839233	0.100862

**Vibrational frequencies**

-1158.01	76.9257	193.9245
338.6186	361.0405	450.0169
463.0018	579.5608	605.1681
740.7289	780.5691	806.7917
860.5987	905.2642	943.963
966.7982	1002.574	1045.294
1080.217	1170.892	1188.791
1230.269	1306.651	1347.514
1396.512	1426.436	1507.023
1550.273	1623.454	1713.483
1769.972	2396.527	2994.93
3019.555	3201.616	3233.685
3556.737	3564.597	3665.229

***i39 + NH<sub>3</sub>***

**Cartesian coordinates**

N	0.208103	-0.010589	-0.412961
C	-1.825808	0.800528	0.182331
C	-0.514177	1.130598	-0.141238
C	-1.951336	-0.575571	0.199108
C	-0.606883	-1.178829	-0.096197
H	1.214944	-0.034821	-0.261722
H	-2.613204	1.516867	0.369563
H	-2.842057	-1.150826	0.402376

H	-0.193728	-1.728687	0.769989
H	-0.625464	-1.891849	-0.934674
H	3.753585	0.283008	-0.636296
N	3.197307	0.013169	0.166410
H	3.555156	-0.874744	0.498216
H	3.364605	0.696516	0.895683
H	-0.062477	2.106120	-0.241297

### Vibrational frequencies

45.6125	60.6353	104.4608
170.4546	225.9677	264.8877
278.5659	526.3575	563.3064
646.7166	718.9836	826.3825
865.8423	878.7632	953.3669
976.6869	1010.454	1073.2
1089.442	1123.753	1165.088
1206.949	1304.569	1358.402
1418.582	1495.824	1535.674
1546.762	1679.638	1683.116
2907.015	2976.297	3232.79
3247.99	3263.039	3478.412
3518.982	3645.598	3646.53

### *i37 + 2 NH<sub>3</sub>*

#### Cartesian coordinates

N	0.474249	0.464588	0.713614
C	1.455439	-1.297147	-0.323727
C	0.276256	-1.030113	0.369848
C	2.344755	-0.240312	-0.476509
C	1.769638	0.984465	0.158312
H	0.437140	0.551923	1.724856
H	1.651012	-2.286062	-0.723781
H	3.296723	-0.247346	-0.988481
H	2.383441	1.407831	0.960884
H	1.549574	1.791775	-0.550581
N	-1.842653	1.638283	-0.405889
H	-0.351767	0.996839	0.333821
H	-2.369908	2.389916	0.023236
H	-1.776880	1.846058	-1.396065
H	-2.385541	0.763715	-0.308060
N	-2.811629	-1.133658	0.019304
H	-3.349732	-1.451448	0.817904
H	-3.084642	-1.714111	-0.766157
H	-1.815712	-1.334940	0.215672

**Vibrational frequencies**

38.9896	50.2604	106.5807
146.8249	185.3736	197.8088
240.3505	260.513	284.8415
344.8096	419.5219	478.2041
500.3532	557.6361	635.5418
708.0326	767.0743	848.2633
867.5649	934.3429	951.2456
1002.149	1008.695	1073.646
1162.484	1179.215	1200.468
1232.966	1293.12	1324.192
1388.618	1410.407	1474.919
1502.159	1653.086	1675.635
1705.696	1721.035	1731.318
2925.5	3029.863	3066.149
3201.879	3219.37	3244.986
3272.658	3550.808	3556.035
3565.729	3629.339	3637.961

***i37 + 2 NH<sub>3</sub> – i39 + 2 NH<sub>3</sub>*****Cartesian coordinates**

N	0.610432	0.343529	1.006212
C	0.847540	-1.180368	-0.613274
C	0.056391	-0.905475	0.511234
C	1.912487	-0.295535	-0.777952
C	1.944615	0.599923	0.422257
H	0.565998	0.439239	2.010451
H	0.641764	-2.004368	-1.289348
H	2.696518	-0.331376	-1.522585
H	2.746742	0.313385	1.127849
H	2.090965	1.666182	0.196666
N	-1.324212	1.402027	-0.675229
H	-0.566479	1.264837	0.058119
H	-1.658866	2.357414	-0.715007
H	-0.899832	1.140764	-1.561209
H	-2.121836	0.590755	-0.360032
N	-2.703901	-0.601002	0.201026
H	-3.302998	-0.522381	1.015925
H	-3.126109	-1.268808	-0.435154
H	-1.708307	-0.968788	0.496662

**Vibrational frequencies**

-571.569	53.4048	74.2382
132.0025	244.5027	282.524
332.0827	362.6223	384.8186

437.707	545.4863	562.8183
584.9432	663.6009	713.0068
763.9464	796.8855	858.5564
887.5079	912.3398	958.3124
963.9984	1003.533	1063.646
1076.042	1168.295	1189.748
1294.677	1304.326	1363.326
1403.386	1429.284	1452.584
1509.773	1535.513	1574.824
1684.116	1708.766	1755.997
1810.854	2218.675	2780.452
2911.433	2995.524	3185.417
3231.456	3539.908	3543.348
3613.472	3631.722	3637.467

### ***i39 + 2 NH<sub>3</sub>***

#### **Cartesian coordinates**

N	0.575507	0.266434	0.874214
C	1.333441	-1.047965	-0.815710
C	0.287563	-0.841078	0.071031
C	2.359041	-0.162181	-0.539667
C	1.977150	0.649449	0.664696
H	0.238787	0.240480	1.824307
H	1.325985	-1.783906	-1.607161
H	3.304819	-0.070006	-1.051986
H	2.594416	0.396512	1.544356
H	2.073048	1.732714	0.511738
N	-1.851518	1.677353	-0.634609
H	-0.996150	1.468229	-0.120920
H	-2.105734	2.639256	-0.444159
H	-1.618500	1.617273	-1.619152
H	-2.821552	-0.107910	-0.000289
N	-2.998683	-1.065517	0.314678
H	-3.647737	-1.017070	1.091579
H	-3.481403	-1.542316	-0.438434
H	-0.686285	-1.310498	0.148042

#### **Vibrational frequencies**

30.271	41.8644	65.7461
122.1164	134.4179	145.7809
160.1645	190.8399	210.478
281.5023	318.4753	354.1078
482.7729	531.8864	583.6597
603.2324	788.7825	811.4066
855.9214	920.6439	949.7677

979.1195	1005.009	1077.363
1112.976	1121.57	1137.525
1173.321	1190.352	1307.544
1349.364	1402.661	1454.549
1506.911	1532.211	1665.324
1677.309	1703.637	1722.391
2938.831	3010.81	3205.789
3244.103	3262.466	3415.272
3464.162	3576.033	3594.744
3631.9	3637.922	3642.295

***i9b* + NH<sub>3</sub>**

**Cartesian coordinates**

C	-0.434379	1.173076	0.384953
C	-1.202028	1.003032	-0.696379
N	-0.009095	-0.152116	1.035708
C	-1.376844	-0.480445	-0.734483
C	-0.728243	-1.134419	0.236744
H	0.010003	2.035124	0.866347
H	1.015754	-0.250371	0.832973
H	-0.200479	-0.219789	2.033849
H	-1.972498	-0.999539	-1.478616
H	-0.625975	-2.180183	0.485985
N	2.375843	-0.095231	-0.419438
H	1.749375	0.337002	-1.095411
H	3.129584	0.560766	-0.251800
H	2.775966	-0.919048	-0.852228

**Vibrational frequencies**

75.7763	103.2277	115.2902
253.3543	351.3028	366.4334
499.2825	504.8019	665.8936
690.1576	701.1234	808.7287
839.5269	926.9423	979.6392
992.4895	1011.554	1134.841
1149.183	1192.221	1256.816
1326.714	1346.071	1525.411
1585.18	1615.06	1673.761
1682.132	3031.995	3197.633
3223.247	3262.249	3496.692
3524.855	3613.752	3648.049

***i9b* + NH<sub>3</sub> – pyrrole (3) + NH<sub>3</sub>**

**Cartesian coordinates**

C	0.323995	1.159545	-0.439546
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C	0.930932	1.017298	0.764400
N	0.025272	-0.129956	-1.089297
C	1.207061	-0.439495	0.787697
C	0.732949	-1.083585	-0.300891
H	-0.107679	2.025970	-0.930815
H	-1.184086	-0.251633	-0.489131
H	0.088338	-0.217716	-2.098283
H	1.729887	-0.950376	1.590188
H	0.746034	-2.121771	-0.603932
N	-2.010809	-0.169145	0.445385
H	-1.411779	0.318136	1.122247
H	-2.803261	0.422507	0.224881
H	-2.328315	-1.053988	0.822273

### Vibrational frequencies

-1017.48	164.0811	197.5985
219.0264	430.9	507.7228
582.7794	611.7739	681.413
717.3914	753.216	803.1826
842.5943	873.2088	934.2835
954.0085	1012.152	1060.077
1125.695	1237.434	1290.625
1306.541	1353.028	1486.658
1546.328	1581.852	1596.509
1671.052	1773.429	3177.902
3189.595	3234.017	3403.982
3560.217	3585.808	3655.423

### *Pyrrrole (3) + NH<sub>3</sub>*

#### Cartesian coordinates

C	-0.589359	1.113949	0.002144
C	-1.902420	0.708100	-0.002824
N	0.202384	0.002314	0.005234
C	-1.899552	-0.711991	-0.002811
C	-0.584861	-1.112508	0.002156
H	-0.158703	2.102952	0.004077
H	3.557099	-0.750364	-0.577717
H	1.223966	0.004019	0.007441
H	-2.760221	-1.363170	-0.005885
H	-0.150192	-2.099755	0.004110
N	3.193305	0.000236	-0.001835
H	-2.765753	1.355743	-0.005921
H	3.575372	-0.120134	0.929122
H	3.565759	0.867560	-0.371012

**Vibrational frequencies**

47.1614	48.4414	70.2146
180.811	280.5373	308.2735
629.7872	638.062	707.214
737.0211	822.8152	892.3847
893.7462	902.582	923.6989
1038.041	1077.004	1104.899
1110.053	1196.896	1222.559
1332.924	1437.596	1528.723
1531.131	1619.227	1677.104
1681.944	3243.494	3256.203
3274.793	3281.441	3429.52
3517.341	3642.329	3643.504

***i9b* + 2 NH<sub>3</sub>****Cartesian coordinates**

C	0.707085	-0.250647	1.221399
C	0.848130	-1.386929	0.526236
N	1.017853	0.986218	0.406593
C	1.390315	-0.899605	-0.775488
C	1.504706	0.432139	-0.844467
H	0.302544	-0.028946	2.201184
H	0.063487	1.451576	0.221042
H	1.666090	1.641296	0.840830
H	1.665130	-1.549629	-1.599687
H	1.834830	1.108658	-1.618742
N	-1.577684	1.681065	-0.170541
H	-1.906886	0.699328	-0.209959
H	-2.150370	2.165358	0.511995
H	-1.768201	2.104569	-1.071929
N	-2.255235	-1.248825	-0.179331
H	-1.340083	-1.565163	0.159332
H	-2.947063	-1.610278	0.468086
H	-2.415436	-1.715716	-1.065277

**Vibrational frequencies**

45.2517	84.9458	106.3821
168.9925	185.6667	224.6146
260.8085	280.4756	356.75
433.1245	454.569	484.4846
532.7942	636.6039	694.8349
715.0014	748.606	827.5062
851.9202	954.6555	984.6924
1000.527	1022.529	1135.039
1184.809	1208.402	1260.115

1267.291	1346.722	1412.965
1531.64	1611.177	1623.885
1663.122	1684.211	1711.306
1733.856	2570.571	3196.957
3222.163	3231.579	3259.821
3382.852	3517.045	3561.92
3565.43	3628.939	3634.439

***i9b + 2 NH<sub>3</sub> – pyrrole (3) + 2 NH<sub>3</sub>***

**Cartesian coordinates**

C	0.650210	-0.293424	1.227326
C	0.450627	-1.425879	0.521663
N	1.218430	0.802852	0.412590
C	1.084214	-1.094860	-0.778719
C	1.561354	0.162163	-0.823151
H	0.329544	0.002290	2.220439
H	0.153544	1.410330	0.131129
H	1.945915	1.378406	0.828108
H	1.156797	-1.781026	-1.616350
H	2.062697	0.730523	-1.594012
N	-1.092383	1.751667	-0.220680
H	-1.648752	0.858850	-0.231037
H	-1.527112	2.386827	0.440060
H	-1.141150	2.174156	-1.141341
N	-2.449637	-0.801185	-0.141933
H	-1.613406	-1.311192	0.189904
H	-3.182859	-0.959144	0.540927
H	-2.748516	-1.251362	-1.000384

**Vibrational frequencies**

-946	52.2602	124.8758
145.9663	202.0897	229.2262
296.4892	302.7531	427.0411
438.7598	534.075	545.7166
585.0717	658.1304	694.4672
702.8469	762.6495	804.9935
852.1609	903.5709	941.3845
958.6461	1010.256	1054.824
1128.143	1225.956	1230.776
1295.291	1351.782	1364.927
1505.393	1558.118	1599.513
1631.349	1661.588	1713.002
1733.148	1755.919	2967.293
3191.32	3198.266	3242.31
3247.985	3540.136	3554.873

3555.971 3627.876 3635.641

***Pyrrole (3) + 2 NH<sub>3</sub>***

**Cartesian coordinates**

C	1.145347	-0.721145	0.972393
C	0.294715	-0.765160	-0.103857
N	2.264897	-0.024400	0.601443
C	0.931732	-0.058929	-1.163832
C	2.144570	0.383838	-0.698690
H	1.047253	-1.133032	1.964052
H	-0.983352	1.309781	0.287282
H	3.058102	0.152050	1.190670
H	0.541490	0.097207	-2.157838
H	2.927914	0.944809	-1.182797
N	-1.884653	1.776888	0.346827
H	-2.889393	-0.091427	0.006139
H	-1.940905	2.207781	1.262076
H	-1.879263	2.523655	-0.337919
N	-3.091009	-1.080845	-0.153193
H	-0.688140	-1.220138	-0.126025
H	-3.765093	-1.370499	0.545836
H	-3.551441	-1.153312	-1.053097

**Vibrational frequencies**

31.5012	39.0804	48.3969
73.7789	98.8258	131.3393
141.64	159.8554	187.8819
261.3377	317.8211	457.1939
497.6169	643.7488	649.8733
719.312	773.8765	874.9177
882.9811	909.6617	975.8173
1049.989	1086.336	1095.74
1112.9	1123.195	1170.616
1189.9	1326.132	1442.332
1485.712	1523.001	1598.79
1666.888	1680.776	1685.27
1721.26	3216.24	3255.17
3272.47	3279.199	3433.757
3495.851	3582.718	3616.097
3635.785	3643.584	3720.951

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