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Supporting Information

Pseudohalide HCN Aggregate Ions: $[N_3(HCN)_3]^-$, $[OCN(HCN)_3]^-$, $[SCN(HCN)_2]^-$ and $[P(CN{\cdot}HCN)_2]^-$

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Content

1 Experimental Details

General: All manipulations were carried out in oxygen- and moisture-free conditions in an argon atmosphere using standard Schlenk or dry-box techniques if not mentioned otherwise. Solvents and reactants were obtained from commercial sources or synthesized as detailed in Table S1.

Table S 1. Origin and purification of used compounds.

Compound	Origin	Purification
Acetone	local trade	dried with CaH_2 and freshly distilled, stored over molecular sieves (3 Å) and distilled again prior to use
Acetonitrile-d_3	euriso-top	dried with CaH_2 and freshly distilled, stored over molecular sieves (3 Å)
H_2O	local trade	distilled twice
HCN	synthesized[1]	-
NaOCP·Dioxane	synthesized[2]	-
NaN_3	Sigma Aldrich (99.0 %)	-
NaOCN	abcr (99.0 %)	-
KSCN	Riedel-de Haën (99.0 %)	-

NMR Spectroscopy: ^{1}H, $^{13}C\{^{1}H\}$ and $^{31}P\{^{1}H\}$ NMR spectra were recorded with a Bruker AVANCE 250 or a Bruker AVANCE 300 spectrometer. The chemical shifts were referenced internally to the deuterated solvent ($^{13}C\{^{1}H\}$: CD_3CN δ_{ref} = 1.3 ppm), to protic impurities in the deuterated solvent (^{1}H: CHD_2CN δ_{ref} = 1.94 ppm) or externally ($^{31}P\{^{1}H\}$: 85 % H_3PO_4 δ_{ref} = 0.0 ppm). All measurements were carried at room temperature unless otherwise denoted.[3]

IR Spectroscopy: A Bruker Alpha FT-IR spectrometer with ATR device was used.

Raman Spectroscopy: A LabRAM HR 800 Horiba Jobin YVON equipped with an Olympus BX41 microscope with variable lenses were used. A red laser (633 nm, 17mW, HeNe-laser) was used. All measurements were carried out at ambient temperature except for hydrogen cyanide products. For these crystalline samples a Linkam THMS600 Temperature Control Stage was used to cool the substances to temperatures, which are denoted in the experimental descriptions.

CHN Analyses: Analysator vario micro cube from Elementar was used.

Melting points are uncorrected (*EZ*)-Melt, Stanford Research Systems. Heating rate 5 $K \cdot min^{-1}$ (clearing-points are reported).

2 Structure Elucidation

X-ray Structure Determination: X-ray quality crystals were selected in Fomblin YR-1800 perfluoroether (Alfa Aesar) for low-temperature applications. Single crystals were measured on a Bruker D8 Quest diffractometer using graphite-monochromated Mo Kα radiation (λ= 0.71073). The structures were solved by direct methods (*SHELXS-2014*)[6] and refined by full-matrix least squares procedures (*SHELXL-2014*).[7] Semi empirical absorption corrections were applied (SADABS/TWINABS).[8] All non-hydrogen atoms were refined anisotropically and hydrogen atoms were included in the refinement at calculated positions using a riding model.

The PCO anion in the asu of [PPN][PCO] · acetone (is_ps279) was found to be disordered, and was split in two parts. The occupancy of each part was refined freely (0.829(3)/0.171(3)). The geometry within part b was restrained to the geometry of part a within an esd of 0.01 (SAME). For the displacement parameters of the atoms within part b of the PCO anion P1b, C1b and O1b, similarity restraints were applied (SIMU, DELU). The atoms C87a, C88a and C89a, as well as all C and O-atoms in part b, were refined isotropically. The acetone molecule in the asu of [PNP][PCO] · acetone (is_ps279, Scheme SX) was found to be disordered, and was split in four parts. The occupancy of each part was refined freely (0.679(3)/0.141(3)/0.133(3)/0.047(3)). The geometry within part b was restrained to the geometry of part a within an esd of 0.01 (SAME). In the same manner, the geometry within part c was restrained to the geometry within b, as well as the geometry within part d was restrained to geometry within part c within an esd of 0.01 (SAME). The atoms in parts b/c/d were refined isotropically. For the displacement parameters of the atoms within part a - d of the acetone molecule similarity restraints were applied (SIMU, DELU). The geometry of the acetone molecule within parts c and d was restrained to be flat within an esd of 0.02 (FLAT). For the atoms C38a/b/c/d, the displacement parameters were restrained to be equal (EADP).

The NCO anion in the asu of [PNP][NCO] · 3 HCN (av_ps291b) was found to be disordered, and was split in two parts. The occupancy of each part was refined freely (0.261(13)/0.239(13)). The geometry within part b was restrained to the geometry of

part a within an esd of 0.01 (SAME). For the displacement parameters of the atoms within part a and b of the NCO anion, similarity restraints were applied (SIMU, DELU).

One HCN molecule in the asu of [PNP][$P(CN)_2$] · 1.98 HCN (av_ps292) was found to be disordered and was split in two parts. The occupancy of each part was refined freely (0.963(11)/0.019(6), part b is half-occupied). The displacement parameters in the atom pairs N3a/N3b, as well as C3a/C3b, were constrained to be equal (EADP).

	$[N(PPh_3)_2][N_3(HCN)_3]$ (**1**)
formula	$C_{39}H_{33}N_7P_2$
M [g mol^{-1}]	661.66
color	colorless
system	monoclinic
space group	*C*2/*c*
a [Å]	16.1472(5)
b [Å]	16.1089(6)
c [Å]	15.3501(5)
α [°]	90
β [°]	116.105(1)
γ [°]	90
V [Å^3]	3585.5(2)
Z	4
$\rho_{calc.}$ [g cm^{-3}]	1.226
μ [mm^{-1}]	0.16
$\lambda_{MoK\alpha}$ [Å]	0.71073
T [K]	123
collected reflexes	35443
independent reflexes	4757
refelxes with $I > 2\sigma(I)$	3987
$R_{int.}$	0.046
F(000)	1384
R_1 (R [$F^2 > 2\sigma(F^2)$])	0.033
wR_2 (F^2)	0.094
GooF	1.04
parameter	270
CCDC #	2024353

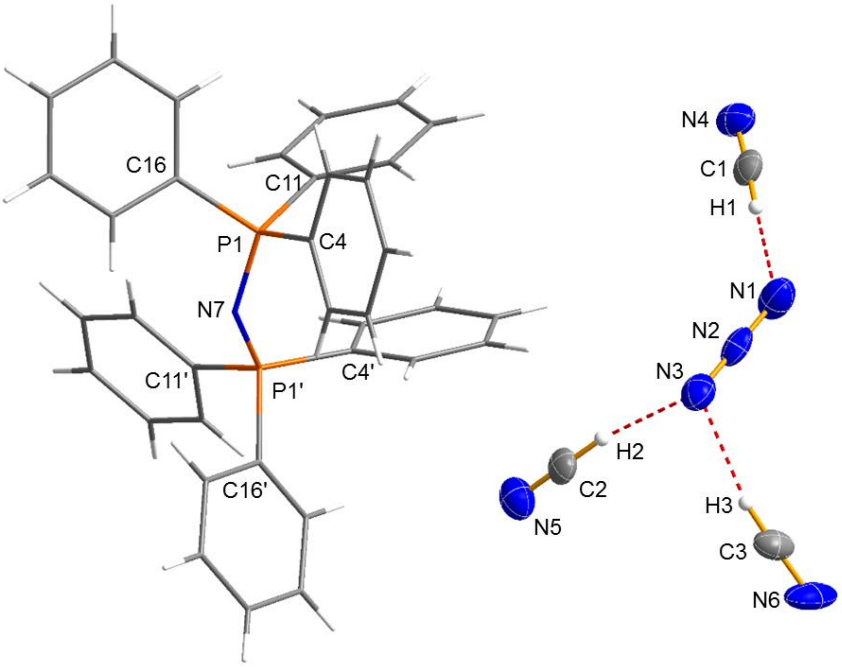


Figure S1. Representation of [PPN][$N_3(HCN)_3$] (**1**) in the crystal structure. Probability of thermal ellipsoids of the ORTEPs are set at 50 % at 173 K.

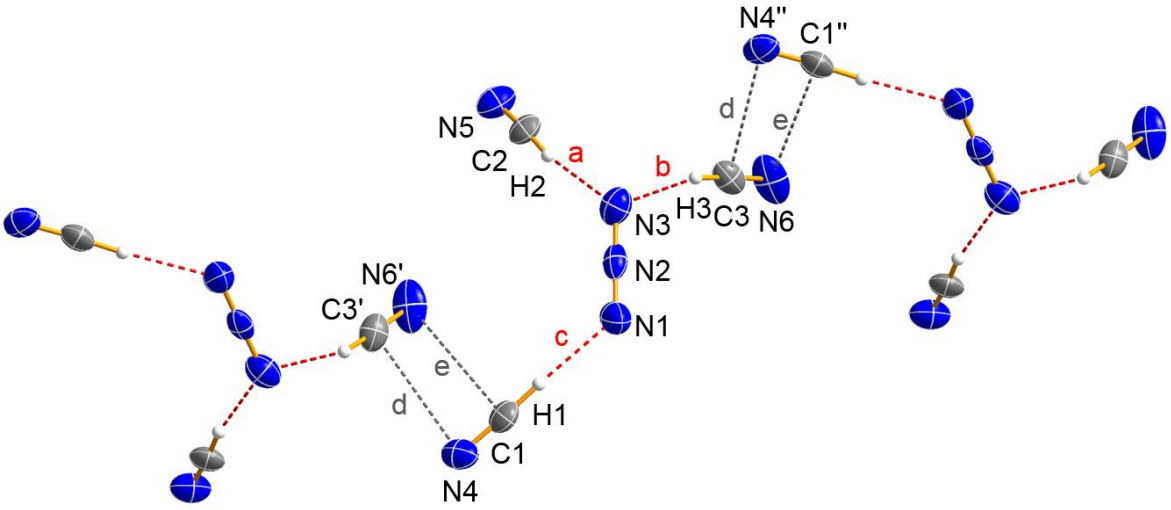


Figure S2. ORTEP representation of the arrangement of the anionic molecular structure of $[N_3(HCN)_3]^-$ in the crystal of **1** along the *c*-axis. Probability of thermal ellipsoids are set at 50 % at 173 K.

	$[N(PPh_3)_2][OCN(HCN)_3]$ (**2**)
formula	$C_{40}H_{33}N_5P_2O$
M [g mol^{-1}]	661.65
color	colorless
system	monoclinic
space group	*C*2/*c*
a [Å]	16.2482(5)
b [Å]	16.0014(5)
c [Å]	15.3207(5)
α [°]	90
β [°]	115.710(1)
γ [°]	90
V [Å^3]	3559.1(4)
Z	4
$\rho_{calc.}$ [g cm^{-3}]	1.225
μ [mm^{-1}]	0.16
$\lambda_{MoK\alpha}$ [Å]	0.71073
T [K]	123
collected reflexes	34657
independent reflexes	6213
refelxes with $I > 2\sigma(I)$	4672
$R_{int.}$	0.043
F(000)	1384
R_1 (R [$F^2 > 2\sigma(F^2)$])	0.041
wR_2 (F^2)	0.104
GooF	1.02
parameter	286
CCDC #	2024351

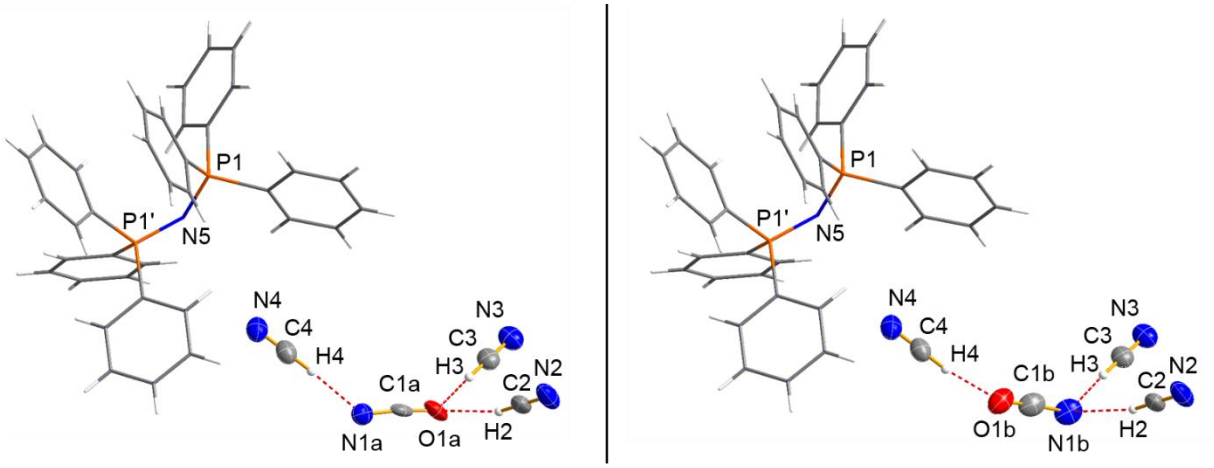


Figure S3. Representation of the molecular structure of an ion pair in the crystal structure of **2**. Two isomers are possible due to disorder (layer B 48 %, layer A 52 %). Probability of thermal ellipsoids are set at 50 % at 173 K.

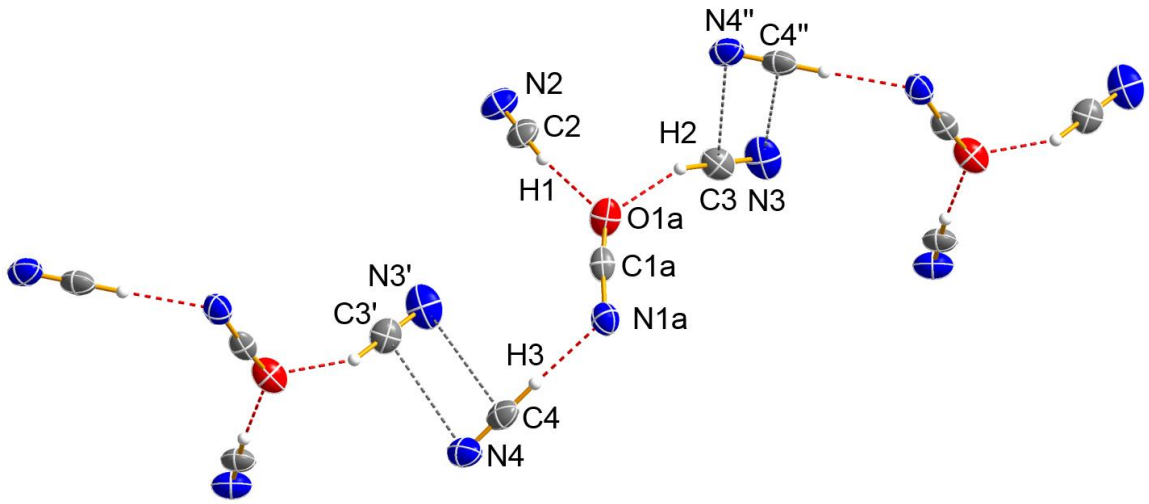


Figure S4. ORTEP representation of the arrangement of the anionic molecular structure of the thermodynamically favored isomer (52 %) of $[OCN(HCN)_3]^-$ in the crystal of **2** along the *c*-axis. Probability of thermal ellipsoids are set at 50 % at 173 K.

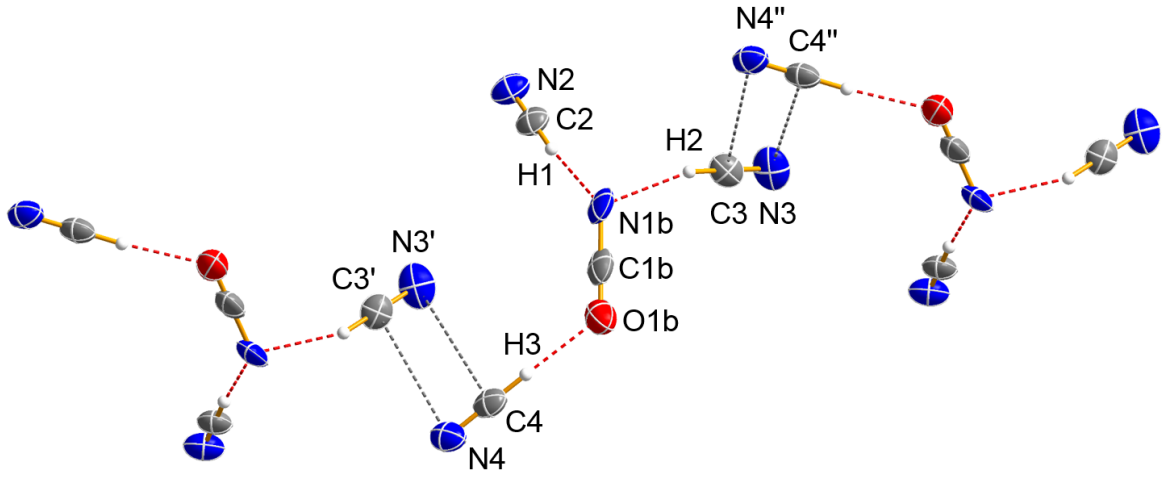


Figure S5. ORTEP representation of the arrangement of the anionic molecular structure of the thermodynamically slightly less favored isomer (48 %) of $[OCN(HCN)_3]^-$ in the crystal of **2** along the *c*-axis. Probability of thermal ellipsoids are set at 50 % at 173 K.

	$[N(PPh_3)_2][SCN(HCN)_2]$ (**3**)
formula	$C_{39}H_{32}N_4P_2S$
M [g mol^{-1}]	650.68
color	colorless
system	monoclinic
space group	$P2_1$
a [Å]	9.0732(3)
b [Å]	19.1434(6)
c [Å]	9.8622(3)
α [°]	90)
β [°]	91.602(1)
γ [°]	90
V [Å^3]	1712.32(9)
Z	2
$\rho_{calc.}$ [g cm^{-3}]	1.262
μ [mm^{-1}]	0.22
$\lambda_{MoK\alpha}$ [Å]	0.71073
T [K]	123
collected reflexes	48620
independent reflexes	12377
refelxes with $I > 2\sigma(I)$	10431
$R_{int.}$	0.043
F(000)	680
R_1 (R [$F^2 > 2\sigma(F^2)$])	0.039
wR_2 (F^2)	0.083
GooF	1.02
parameter	424
CCDC #	2024350

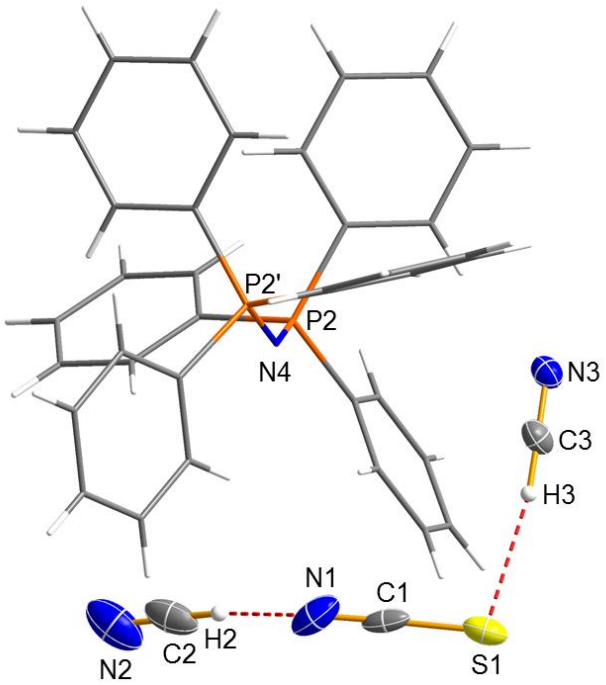


Figure S6. Representation of the molecular structure of an ion pair in the crystal structure of **3**. Probability of thermal ellipsoids are set at 50 % at 173 K.

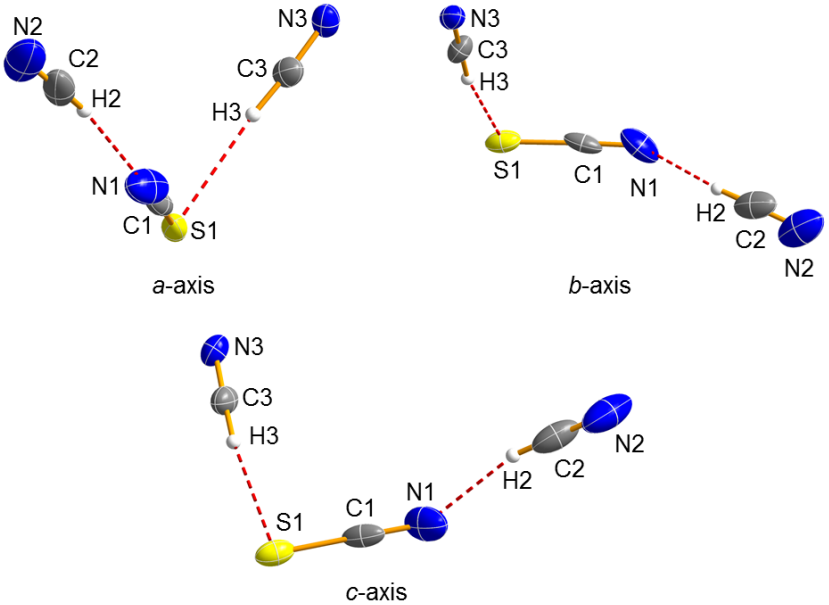


Figure S7. ORTEP representation of different point of views of the anion in the crystal structure of **3**. Probability of thermal ellipsoids are set at 50 % at 173 K.

	$[N(PPh_3)_2][P(CN)_2(HCN)_2]$ (**4**)
formula	$C_{40}H_{32}N_5P_4$
M [g mol^{-1}]	675.14
color	colorless
system	monoclinic
space group	$P2_1/c$
a [Å]	10.9830(8)
b [Å]	12.836(1)
c [Å]	25.301(2)
α [°]	90
β [°]	92.649(2)
γ [°]	90
V [Å^3]	3563.0(5)
Z	4
$\rho_{calc.}$ [g cm^{-3}]	1.259
μ [mm^{-1}]	0.20
$\lambda_{MoK\alpha}$ [Å]	0.71073
T [K]	123
collected reflexes	19960
independent reflexes	6236
refelxes with $I > 2\sigma(I)$	3928
$R_{int.}$	0.096
F(000)	1407
R_1 (R [$F^2 > 2\sigma(F^2)$])	0.053
wR_2 (F^2)	0.119
GooF	1.01
parameter	448
CCDC #	2024352

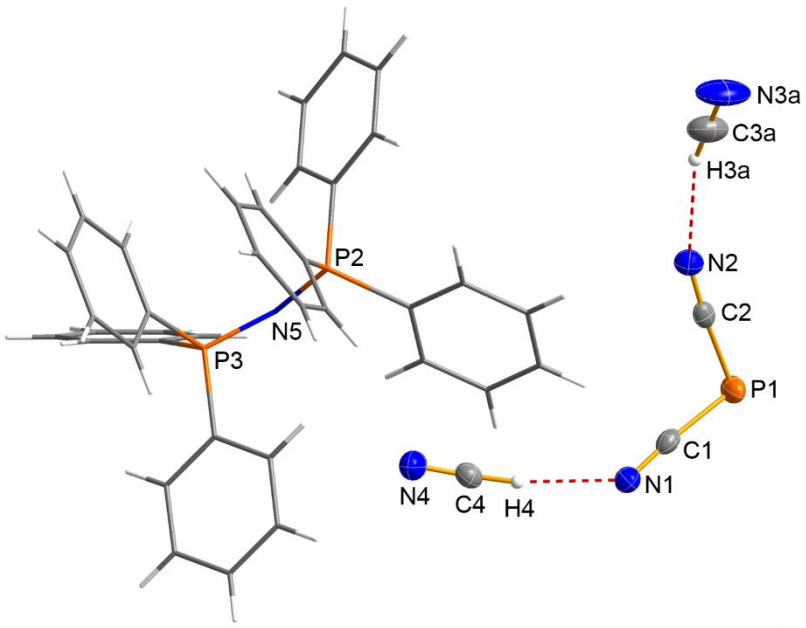


Figure S8. Representation of the molecular structure of an ion pair in the crystal structure of **4**. Probability of thermal ellipsoids are set at 50 % at 173 K.

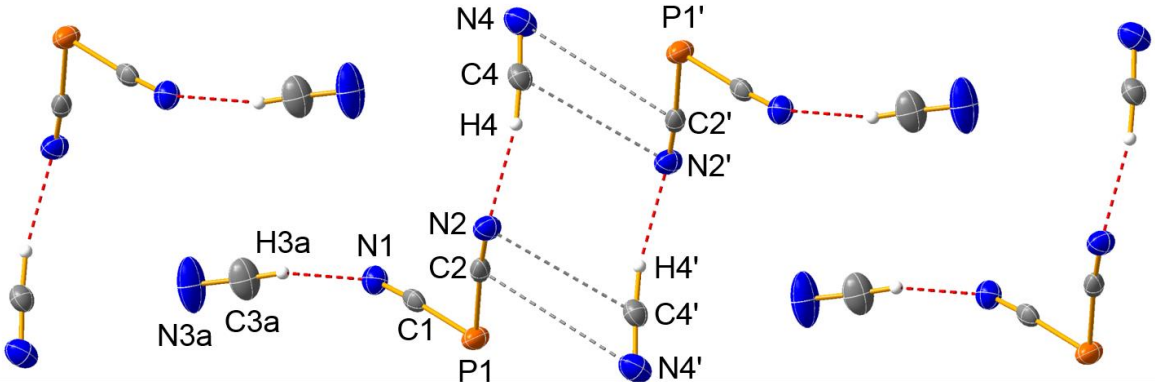


Figure S9. ORTEP representation of the anionic arrangement of the a-layer (96 % probability) in the crystal structure of **4**. Probability of thermal ellipsoids are set at 50 % at 173 K.

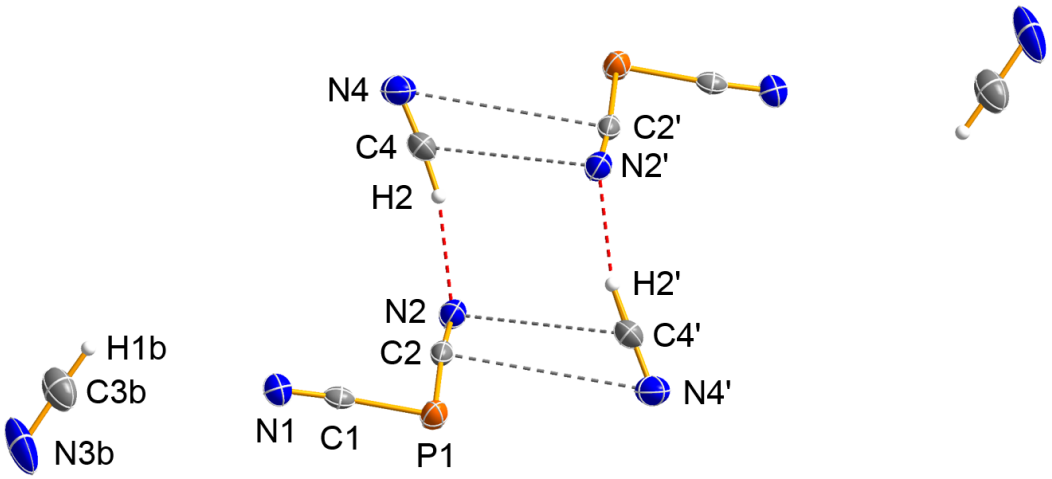


Figure S 10. ORTEP representation of the anionic arrangement of the b-layer (4 % probability) in the crystal structure of **4**. Probability of thermal ellipsoids are set at 50 % at 173 K.

	$[N(PPh_3)_2]OCP\cdot(CH_3)_2CO$ (**5**)
formula	$C_{40}H_{36}NP_2O$
M [g mol^{-1}]	655.61
color	colorless
system	triclinic
space group	$P\bar{1}$
a [Å]	9.5122(6)
b [Å]	10.6129(7)
c [Å]	17.131(1)
α [°]	91.229(2)
β [°]	95.309(2)
γ [°]	91.786(2)
V [Å^3]	1720.6(2)
Z	2
$\rho_{calc.}$ [g cm^{-3}]	1.265
μ [mm^{-1}]	0.21
$\lambda_{MoK\alpha}$ [Å]	0.71073
T [K]	123
collected reflexes	68849
independent reflexes	8300
refelxes with $I > 2\sigma(I)$	5487
$R_{int.}$	0.118
F(000)	688
R_1 (R [$F^2 > 2\sigma(F^2)$])	0.053
wR_2 (F^2)	0.111
GooF	1.03
parameter	489
CCDC #	2024349

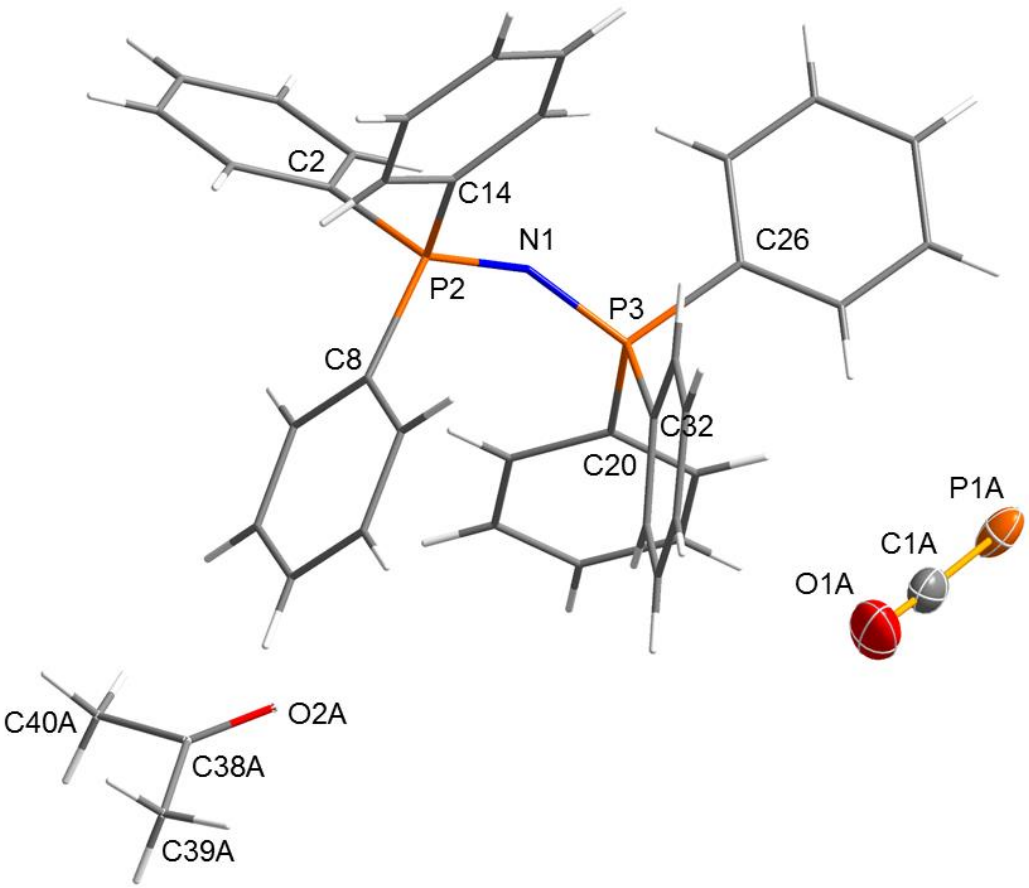
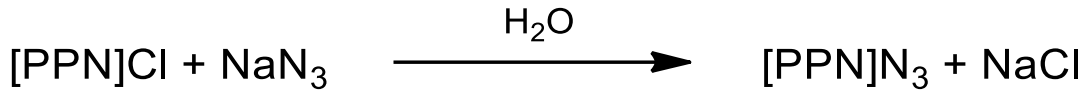


Figure S11. Representation of the molecular structure of an ion pair in the crystal structure of **5**. Probability of thermal ellipsoids are set at 50 % at 173 K. Disorder is not shown for reasons of clarity.

3 Experimental Description

3.1 Starting material synthesis

3.1.1 Synthesis of [PPN]N_3



[PPN]Cl (1.5 g, 2.61 mmol) was dissolved in 11 mL hot water (80 °C). An aqueous solution (5 mL) of NaN_3 (0.34 g, 5.22 mmol, 2 eq.) was added dropwise which immediately resulted in formation of a precipitate of the [PPN]N_3. The suspension was cooled for 30 min to 0 °C with an ice bath and then filtered with a frit (G3). The solid was washed with water (4 x 60 mL) and dried (80 °C, $1 \cdot 10^{-3}$ bar, 3 h). Finally, the salt was dissolved in acetone (ca. 20 mL), filtered (G3 frit) and crystallized from a concentrated solution. The crystals were collected by filtration (G3 frit) and dried (80 °C, $1 \cdot 10^{-3}$ bar, 6 h) leading to colorless [PPN]N_3 (1.24 g, 2.13 mmol) in yields of 82 %.

$C_{36}H_{30}N_4P_2$ (580.60 g/mol): **m.p.** = 213 °C, **dec.** = 315 °C. **EA** found (calc.) %: C 73.78 (74.47); H 5.41 (5.21); 9.59 (9.65). **^{1}H NMR** (297 K, CD_3CN, 250.13 MHz): δ = 7.74 – 7.41 (m, 30 H, Ph-*H*). **^{13}C{^{1}H} NMR** (297 K, CD_3CN, 62.9 MHz): δ = 134.8 – 134.5 (m, *p*-*C*); 133.6 – 133.1 (m, *m*-*C*); 130.7 – 130.2 (m, *o*-*C*); 128.1 (dd, *i*-*C*, $^1J(^{13}C–^{31}P)$ = 127 Hz, $^3J(^{13}C–^{31}P)$ = 2 Hz). **^{39}P{^{1}H} NMR** (297 K, CD_3CN, 101.26 MHz): δ = 20.8 (s, *P*). **IR** (25 °C, ATR, 32 scans, cm^{-1}) $\tilde{\nu}$ = 439 (M), 451 (M), 460 (M), 495 (VS), 532 (VS), 548 (S), 616 (W), 631 (W), 690 (S), 721 (S), 748 (M), 758 (M), 802 (W), 857 (W), 929 (W), 948 (W), 995 (M), 1024 (W), 1111 (S), 1160 (W), 1183 (M), 1261 (S), 1284 (M), 1333 (W), 1434 (M), 1482 (W), 1574 (W), 1587 (W), 1989 (S), 2003 (M), 2959 (W), 2988 (W), 3006 (W), 3050 (W), 3077 (W), 3278 (W), 3295 (W). **Raman** (laser: 633 nm, accumulation time: 8 s ,20 scans, 298 K, cm^{-1}) $\tilde{\nu}$ = 171 (3), 183 (2), 193 (1), 205 (1), 225 (2), 234 (2), 244 (2), 255 (3), 267 (4), 283 (1), 327 (1), 365 (1), 395 (1), 434 (1), 445 (1), 492 (1), 524 (1), 549 (1), 615 (3), 665 (4), 728 (1), 804 (1), 848 (1), 922 (1), 939 (1), 975 (1), 999 (10), 1025 (2), 1032 (4), 1068 (1), 1111 (4), 1164 (1), 1170 (1), 1182 (1), 1191 (1), 1243 (1), 1271 (1), 1323 (2), 1440 (1), 1480

(1), 1575 (2), 1589 (5), 2959 (1), 3007 (1), 3038 (1), 3058 (2), 3066 (3), 3096 (1), 3146 (1), 3175 (1).

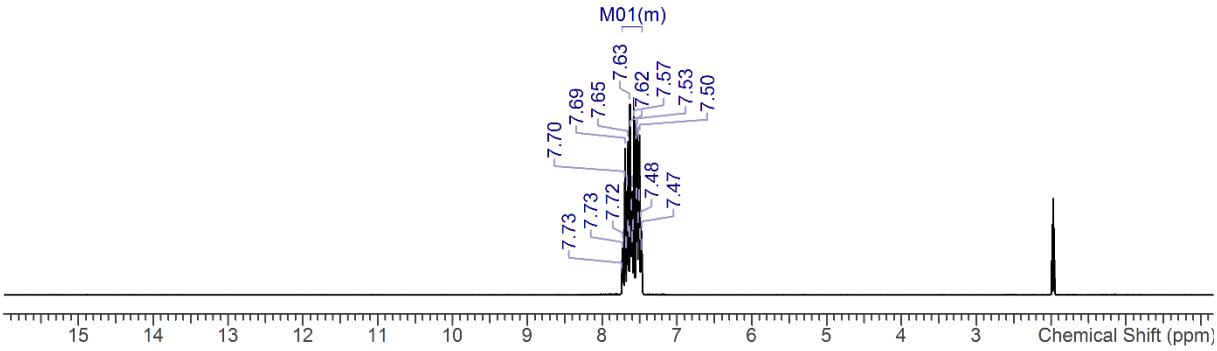


Figure S 12. ^{1}H NMR of $[PPN]N_3$.

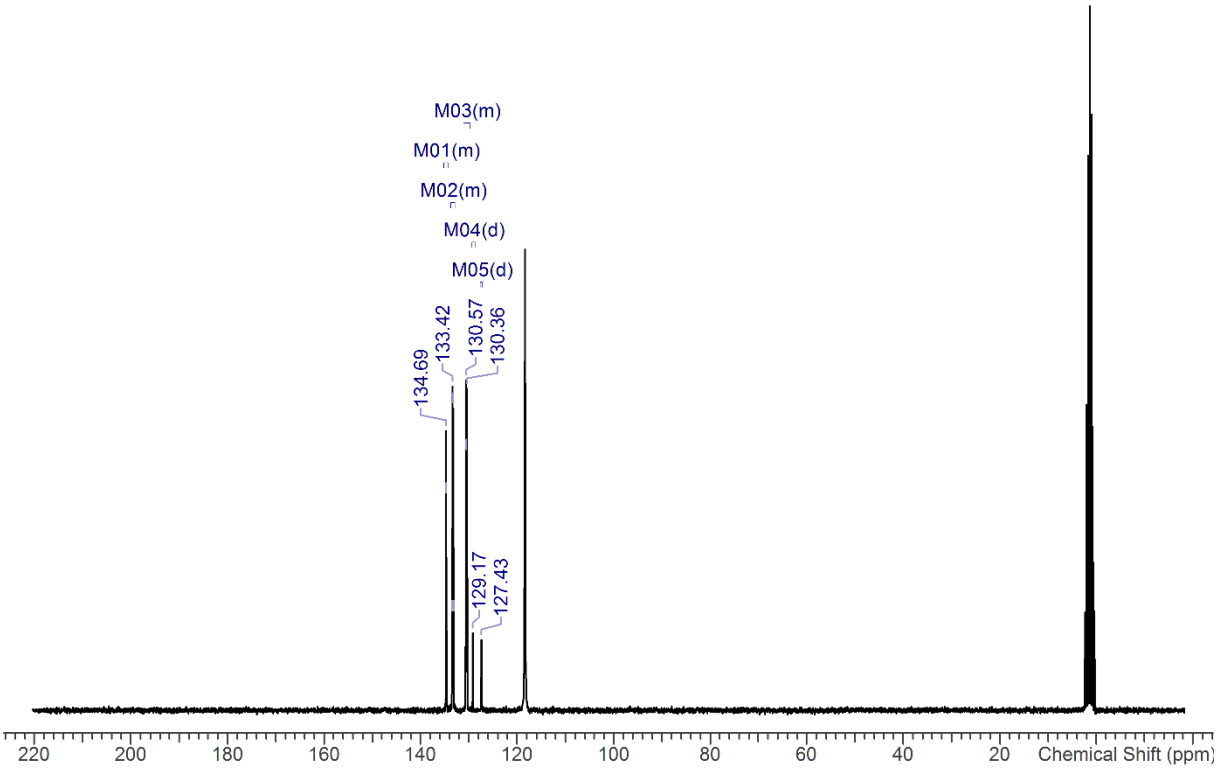


Figure S 13. $^{13}C\{^{1}H\}$ NMR of $[PPN]N_3$.

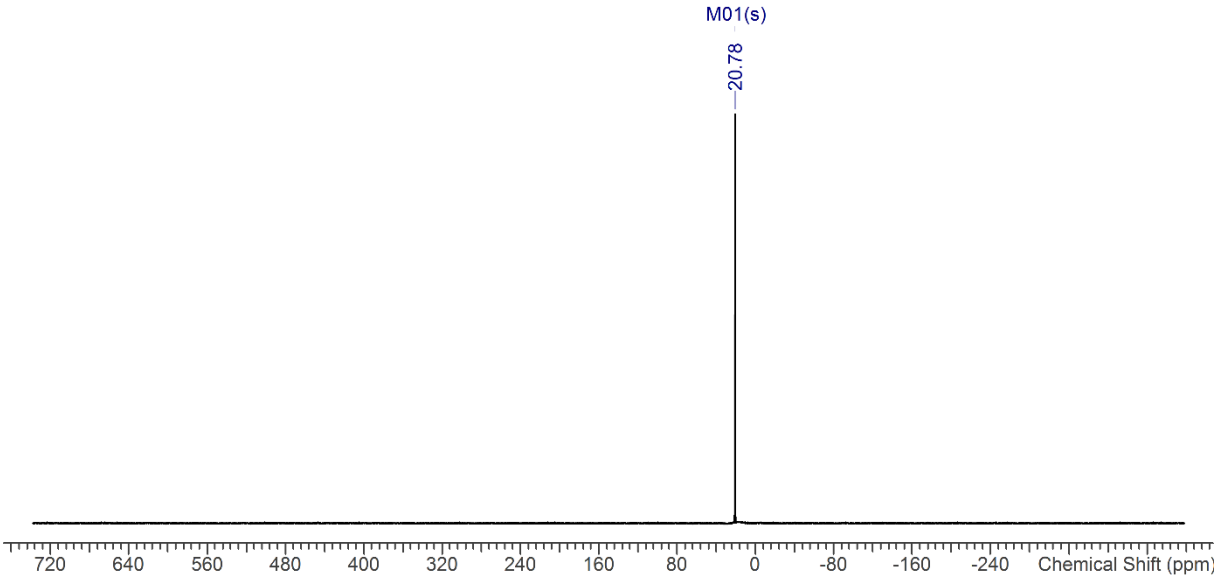


Figure S 14. $^{31}P\{^{1}H\}$ NMR of $[PPN]N_3$.

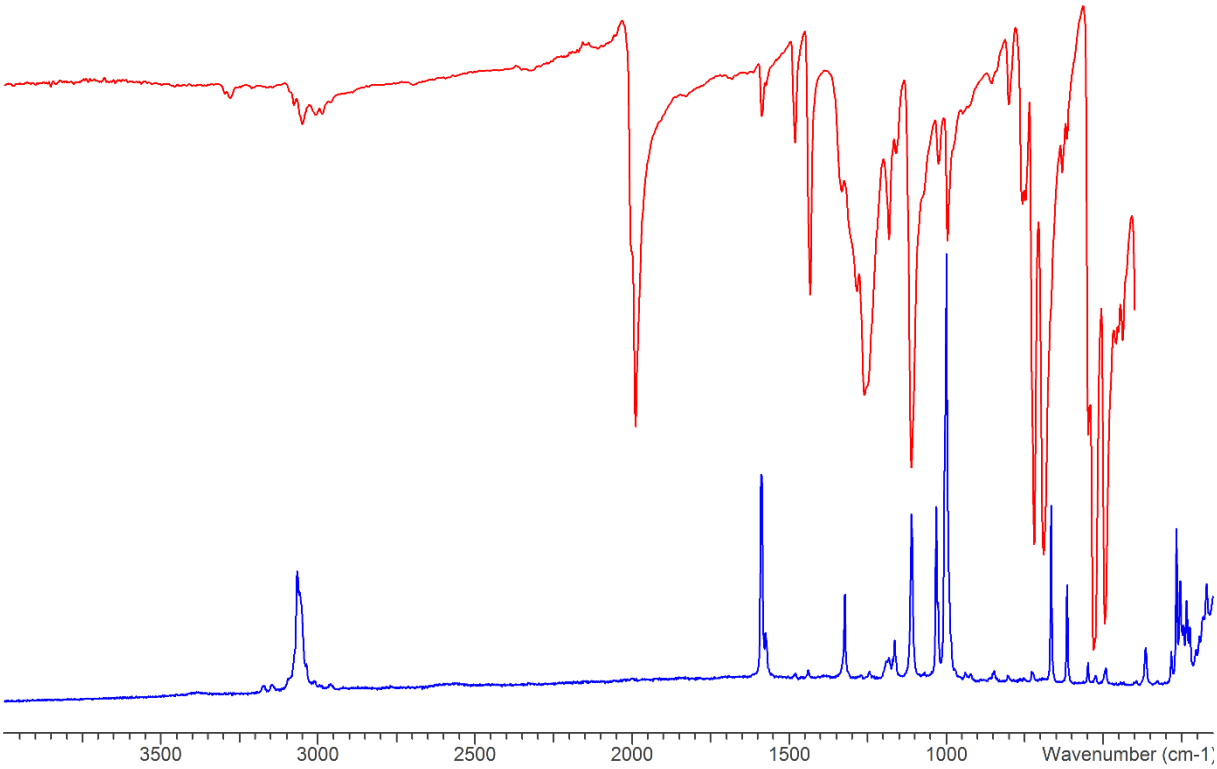
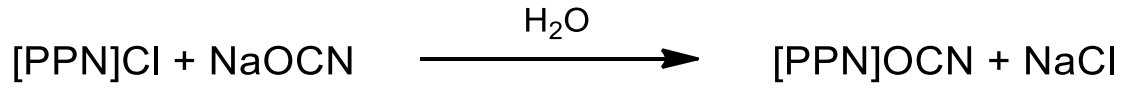


Figure S 15. IR (red) and Raman (blue) spectra of $[PPN]N_3$.

3.1.2 Synthesis of [PPN]OCN



[PPN]Cl (1.5 g, 2.61 mmol) was dissolved in 11 mL hot water (80 °C). An aqueous solution (7 mL) of NaOCN (0.51 g, 7.83 mmol, 3 eq.) was added dropwise which immediately resulted in formation of a precipitate of the [PPN]OCN. The suspension was cooled for 30 min to 0 °C with an ice bath and then filtered with a frit (G3). The solid was washed with water (4 x 60 mL) and dried (80 °C, $1 \cdot 10^{-3}$ bar, 3 h). Finally, the salt was dissolved in acetone (ca. 20 mL), filtered (G3 frit) and crystallized from a concentrated solution. The crystals were collected by filtration (G3 frit) and dried (80 °C, $1 \cdot 10^{-3}$ bar, 6 h) leading to colorless [PPN]OCN (1.16 g, 1.99 mmol) in yields of 76 %.

$C_{37}H_{30}N_2OP_3$ (580.59 g/mol): **m.p.** = 217 °C, **dec.** = 295 °C. **EA** found (calc.) %: C 76.75 (76.54); H 5.08 (5.21); 4.50 (4.82). **^{1}H NMR** (297 K, CD_3CN, 300.13 MHz): δ = 7.74 – 7.41 (m, 30 H, Ph-*H*). **^{13}C{^{1}H} NMR** (297 K, CD_3CN, 62.90 MHz): δ = 134.7 – 134.6 (m, *p*-*C*); 133.5 – 133.1 (m, *m*-*C*); 130.7 – 130.2 (m, *o*-*C*); 128.1 (dd, *i*-*C*, $^{1}J(^{13}C–^{31}P)$ = 127 Hz, $^{3}J(^{13}C–^{31}P)$ = 2 Hz). **^{39}P{^{1}H} NMR** (297 K, CD_3CN, 101.27 MHz): δ = 20.8 (s, *P*). **IR** (25 °C, ATR, 16 scans, cm^{-1}) $\tilde{\nu}$ = 443 (M), 457 (M), 495 (VS), 532 (VS), 620 (M), 688 (S), 721 (S), 744 (W), 764 (W), 795 (W), 841 (VW), 925 (VW), 948 (W), 995 (M), 1026 (W), 1113 (S), 1162 (W), 1185 (W), 1265 (M), 1294 (M), 1436 (M), 1482 (W), 1587 (W), 1673 (VW), 1904 (VW), 2133 (M), 2990 (W), 3019 (W), 3054 (W), 3074 (W), 3309 (VW), 3394 (VW). **Raman** (laser: 633 nm, accumulation time: 8 s ,20 scans, 298 K, cm^{-1}) $\tilde{\nu}$ = 172 (1), 189 (1), 199 (1), 222 (2), 232 (2), 248 (2), 268 (2), 281 (1), 300 (1), 325 (1), 367 (1), 386 (1), 395 (1), 407 (1), 444 (1), 458 (1), 488 (1), 497 (1), 526 (1), 534 (1), 547 (1), 615 (2), 664 (5), 689 (1), 696 (1), 702 (1), 723 (1), 729 (1), 741 (1), 768 (1), 797 (1), 851 (1), 869 (1), 935 (1), 947 (1), 1000 (10), 1021 (2), 1029 (4), 1072 (1), 1110 (4), 1153 (1), 1161 (1), 1181 (1), 1188 (1), 1194 (1), 1272 (1), 1280 (1), 1295 (1), 1323 (1), 1439 (1), 1486 (1), 1575 (1), 1589 (4), 2124 (1), 2134 (2), 2142 (1), 2959 (1), 2992 (1), 3010 (1), 3029 (1), 3049 (2), 3055 (3), 3060 (3), 3070 (2), 3092 (1), 3148 (1), 3174 (1).

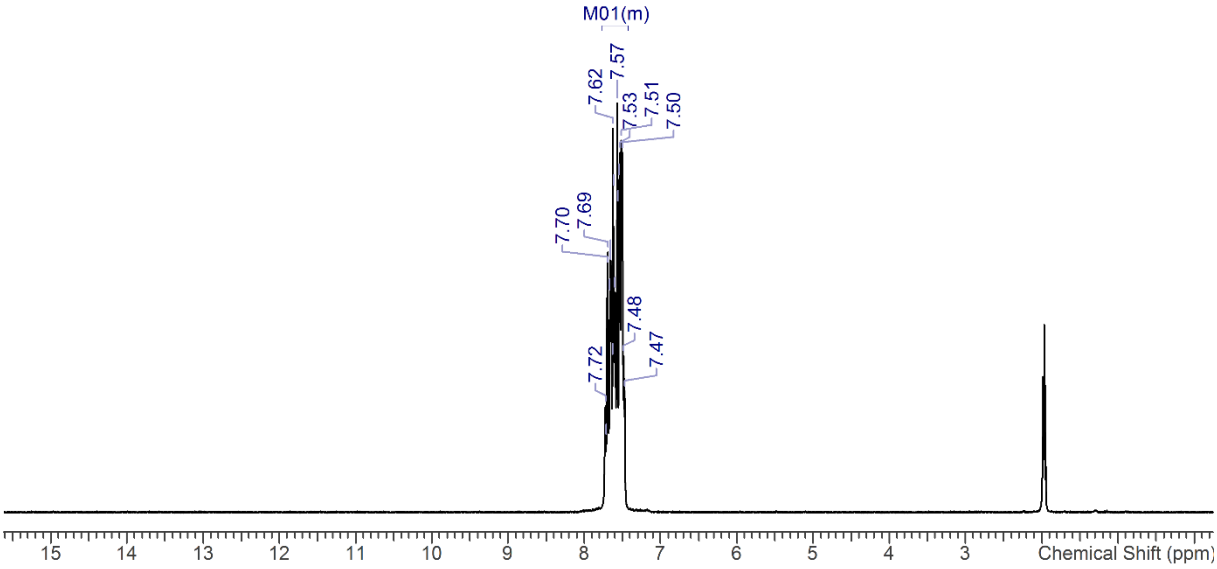


Figure S 16. ^{1}H NMR of [PPN]OCN.

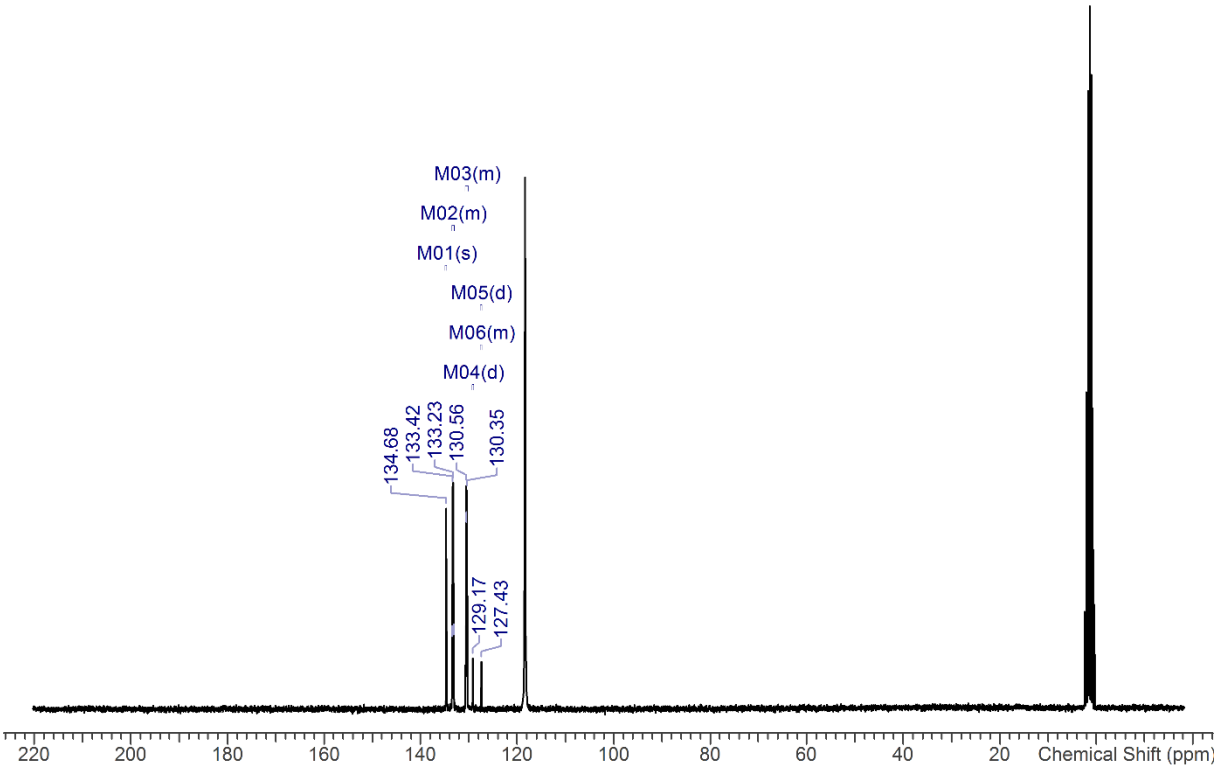


Figure S 17. ^{13}C{^{1}H} NMR of [PPN]OCN.

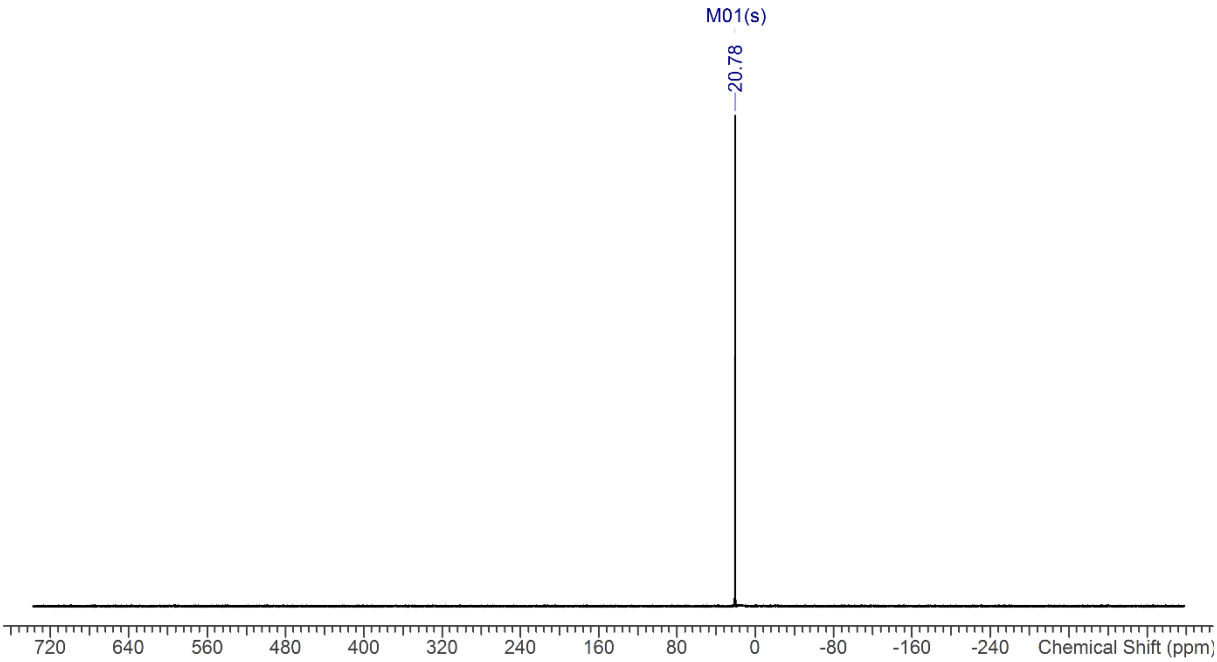


Figure S 18. $^{31}P\{^{1}H\}$ NMR of [PPN]OCN.

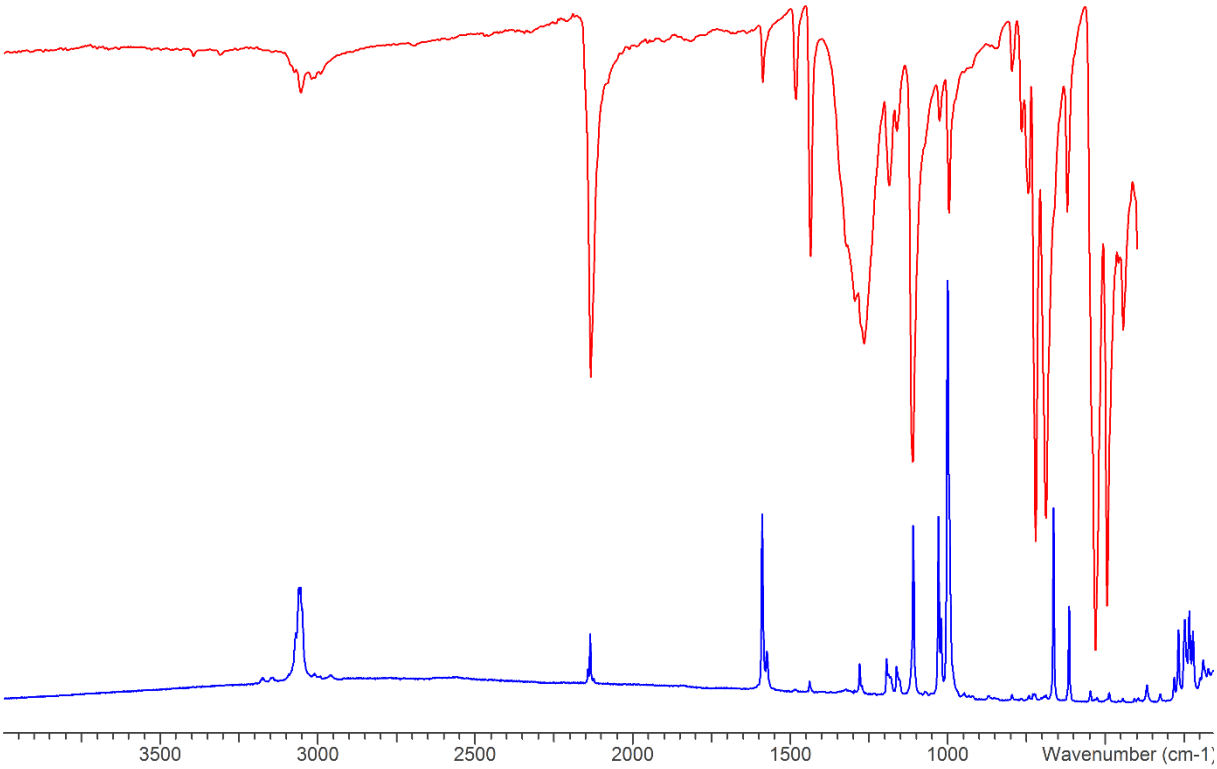
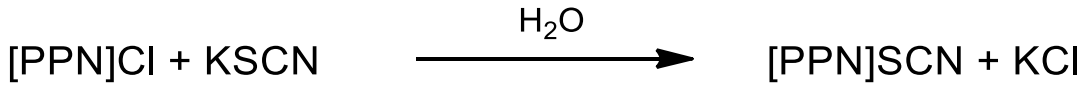


Figure S 19. IR (red) and Raman (blue) spectra of [PPN]OCN.

3.1.3 Synthesis of [PPN]SCN



[PPN]Cl (2.0 g, 3.49 mmol) was dissolved in 20 mL hot water (80 °C). An aqueous solution (5 mL) of KSCN (0.67 g, 6.95 mmol, 2 eq.) was added dropwise which immediately resulted in formation of a precipitate of the [PPN]SCN. The suspension was cooled for 30 min to 0 °C with an ice bath and then filtered with a frit. The solid was washed with water (3 x 40 mL) and dried (80 °C, $1 \cdot 10^{-3}$ bar, 3 h). Finally, the salt was dissolved in acetone (ca. 20 mL), filtered (G3 frit) and crystallized from a concentrated solution. The crystals were collected by filtration (G3 frit) and dried (80 °C, $1 \cdot 10^{-3}$ bar, 6 h) leading to colorless [PPN]SCN (1.30 g, 2.18 mmol) in yields of 62 %.

$C_{37}H_{30}N_2P_2S$ (586.66 g/mol): **m.p.** = 196 °C, **dec.** = 355 °C. **EA** found (calc.) %: C 74.64 (74.48); H 5.05 (5.07); 4.41 (4.70); S 5.19 (5.37). **^{1}H NMR** (297 K, CD_3CN, 300.13 MHz): δ = 7.74 – 7.41 (m, 30 H, Ph-*H*). **^{13}C{^{1}H} NMR** (297 K, CD_3CN, 62.90 MHz): δ = 134.7 – 134.6 (m, *p*-*C*); 133.5 – 133.1 (m, *m*-*C*); 130.7 – 130.2 (m, *o*-*C*); 128.1 (dd, *i*-*C*, $^{1}J(^{13}C–^{31}P)$ = 127 Hz, $^{3}J(^{13}C–^{31}P)$ = 2 Hz). **^{39}P{^{1}H} NMR** (297 K, CD_3CN, 101.27 MHz): δ = 20.8 (s, *P*). **IR** (25 °C, ATR, 16 scans, cm^{-1}) $\tilde{\nu}$ = 433 (M), 457 (M), 490 (VS), 528 (VS), 546 (S), 616 (W), 686 (S), 701 (M), 719 (S), 740 (M), 764 (M), 795 (W), 868 (VW), 923 (W), 995 (M), 1024 (W), 1076 (W), 1111 (S), 1179 (W), 1267 (M), 1286 (M), 1300 (S), 1319 (M), 1434 (M), 1482 (W), 1574 (W), 1587 (W), 1681 (VW), 1805 (VW), 2005 (W), 2050 (M), 2971 (W), 2988 (W), 3013 (W), 3058 (W), 3074 (W), 3087 (W), 3173 (W), 3287 (W). **Raman** (laser: 633 nm, accumulation time: 4 s ,20 scans, 298 K, cm^{-1}) $\tilde{\nu}$ = 179 (2), 191 (2), 200 (1), 223 (2), 233 (3), 251 (2), 266 (3), 279 (1), 361 (1), 486 (1), 492 (1), 526 (1), 543 (1), 550 (1), 614 (3), 662 (3), 691 (1), 723 (1), 729 (1), 737 (1), 756 (1), 762 (1), 792 (1), 861 (1), 924 (1), 939 (1), 999 (10), 1026 (5), 1044 (1), 1054 (1), 1069 (1), 1108 (4), 1153 (1), 1160 (1), 1180 (2), 1192 (1), 1312 (1), 1315 (1), 1338 (1), 1437 (1), 1442 (1), 1480 (1), 1574 (2), 1587 (5), 2052 (2), 2960 (0), 2972 (0), 2990 (0), 3011 (0), 3019 (0), 3057 (3), 3145 (0), 3171 (0).

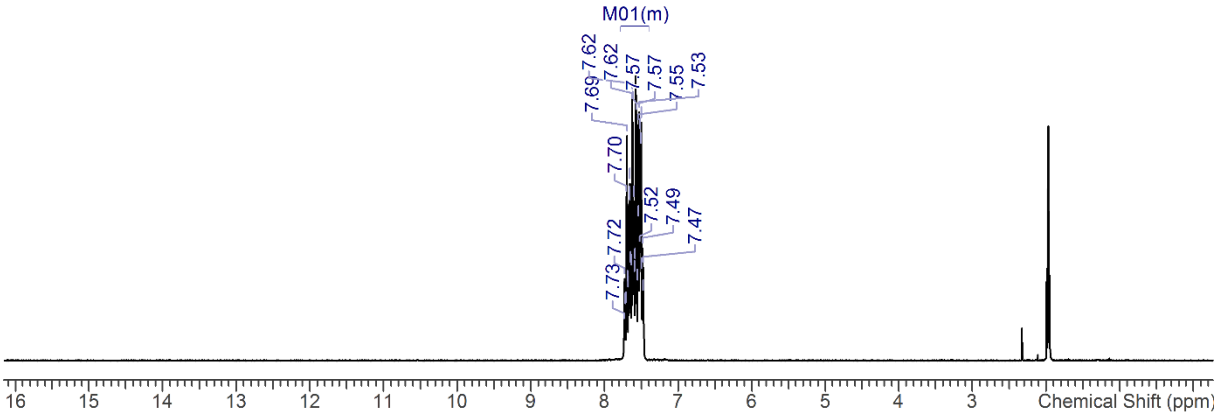


Figure S 20. ^{1}H NMR of [PPN]SCN.

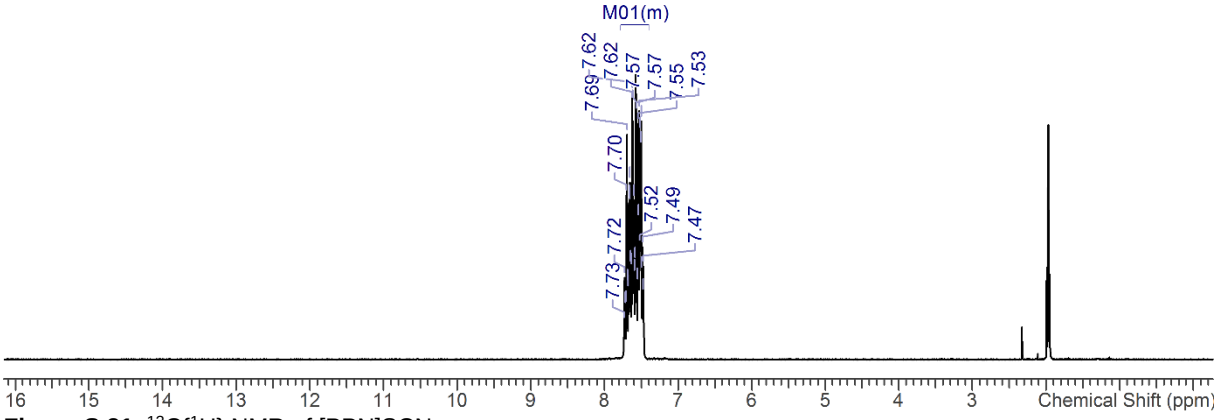


Figure S 21. ^{13}C{^{1}H} NMR of [PPN]SCN.

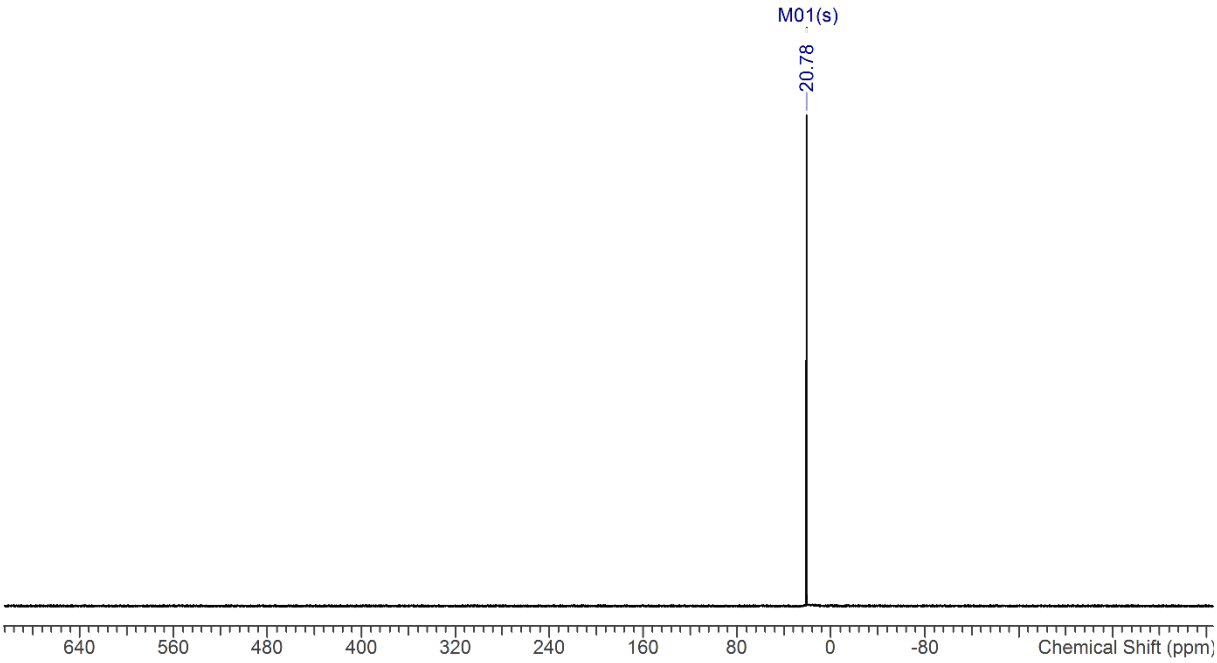


Figure S 22. ^{31}P{^{1}H} NMR of [PPN]SCN.

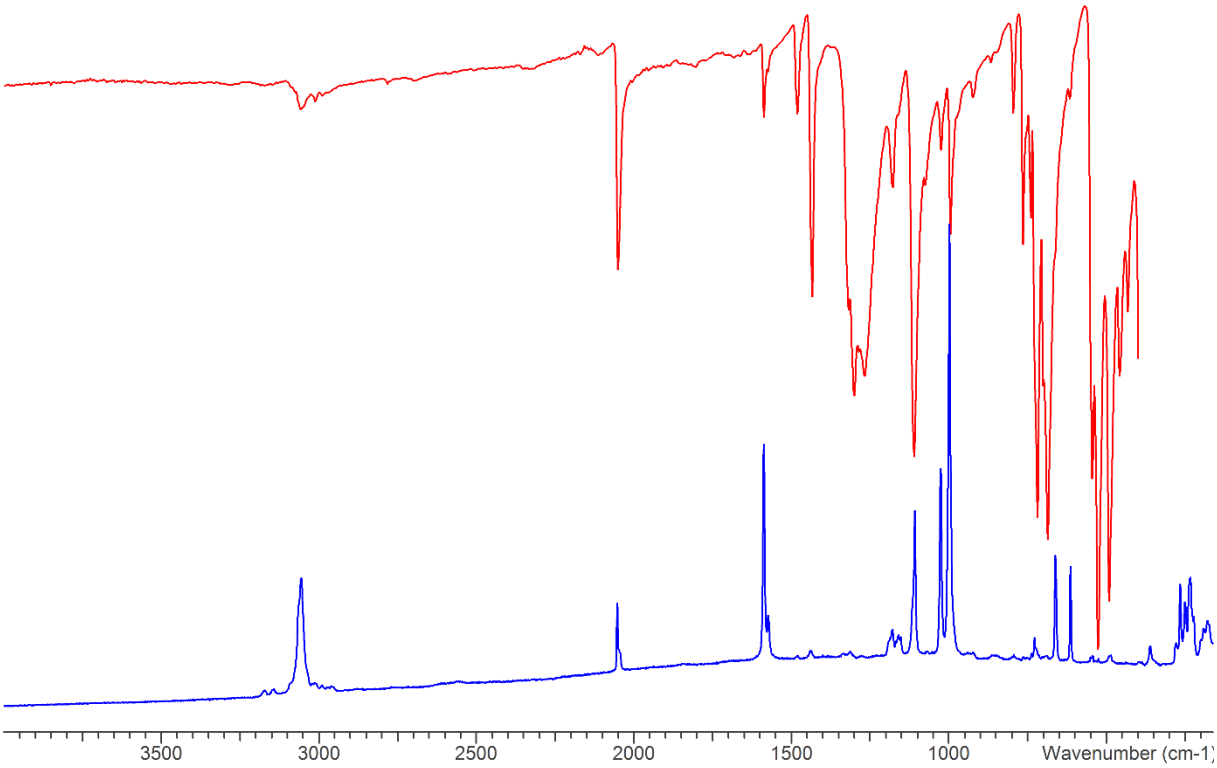
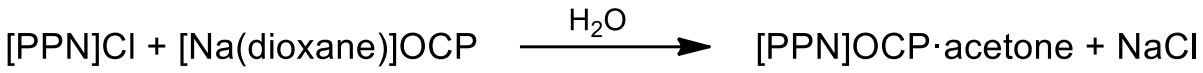


Figure S 23. IR (red) and Raman (blue) spectra of [PPN]SCN.

3.1.4 Synthesis of [PPN]OCP·$(CH_3)_2CO$



μ-Nitrido-bis(triphenylphosphane) chloride [PPN]Cl (1.13 g, 1.97 mmol) was placed in a round bottom flask and was dissolved in 10 mL of hot water (80 °C). NaOCP·0.4dioxane (0.30 g, 2.57 mmol) was suspended in 25 mL of water. The suspension was added quickly within one minute, since decomposition of PCO^- is quickly progressing. As soon as the sodium salt is added, a shiny colorless precipitate was formed which is filtered off with a frit (G3) and washed with water (5 x 60 mL; water from the last fraction was tested with $AgNO_3$ for chloride impurities). The colorless solid was transferred into a Schlenk vessel and dried (60 °C, $1 \cdot 10^{-3}$ mbar, 10 h). The solution turns brownish when 20 mL of acetone was added and minor amounts of a precipitate was formed which was filtered off (G3 frit). Due to fractionalized crystallization of a concentrated solution, [PPN]OCP·$(CH_3)_2CO$ (0.50 g, 0.76 mmol) was obtained in yields of 39 %.

$C_{40}H_{36}NO_2P_3$ (655.64 g/mol): **m.p**. = 189 °C. **EA** found (calc.) %: C 73.75 (73.28); H 4.63 (5.55); 2.75 (2.14). **^{1}H NMR** (297 K, CD_3CN, 300.13 MHz): δ = 7.74 – 7.41 (m, 30 H, Ph-*H*). **^{13}C{^{1}H} NMR** (297 K, CD_3CN, 62.90 MHz): δ = 134.7 – 134.6 (m, *p-C*); 133.5 – 133.1 (m, *m-C*); 130.7 – 130.2 (m, *o-C*); 128.1 (dd, *i-C,* $^1J(^{13}C–^{31}P)$ = 127 Hz, $^3J(^{13}C–^{31}P)$ = 2 Hz). **^{39}P{^{1}H} NMR** (297 K, CD_3CN, 101.27 MHz): δ = 20.8 (s, *P,* $[PPN]^+$), −391.1 (s, *P*, OC*P*$^-$) **IR** (25 °C, ATR, 16 scans, cm^{-1}) $\tilde{\nu}$ = 441 (M), 455 (M), 495 (VS), 528 (VS), 546 (S), 616 (W), 688 (VS), 721 (S), 744 (M), 758 (W), 797 (W), 851 (W), 896 (W), 938 (W), 995 (M), 1022 (M), 1111 (S), 1160 (M), 1181 (M), 1222 (M), 1257 (M), 1282 (M), 1358 (W), 1434 (M), 1480 (W), 1574 (W), 1587 (W), 1616 (W), 1708 (M), 1768 (M), 1791 (M), 2988 (W), 3021 (W), 3052 (W). **Raman** (laser: 633 nm, accumulation time: 8 s ,20 scans, 298 K, cm^{-1}) $\tilde{\nu}$ = 187 (2), 201 (2), 231 (3), 247 (2), 264 (2), 279 (2), 362 (2), 486 (2), 496 (2), 527 (1), 615 (3), 663 (5), 723 (2), 792 (2), 797 (4), 849 (2), 999 (10), 1026 (4), 1107 (4), 1159 (2), 1181 (2), 1437 (2), 1479 (2), 1572 (3), 1586 (5), 1709 (2), 1776 (3), 1794 (4), 2913 (1), 2952 (1), 2988 (1), 3008 (1), 3058 (3), 3143 (1), 3172 (1).

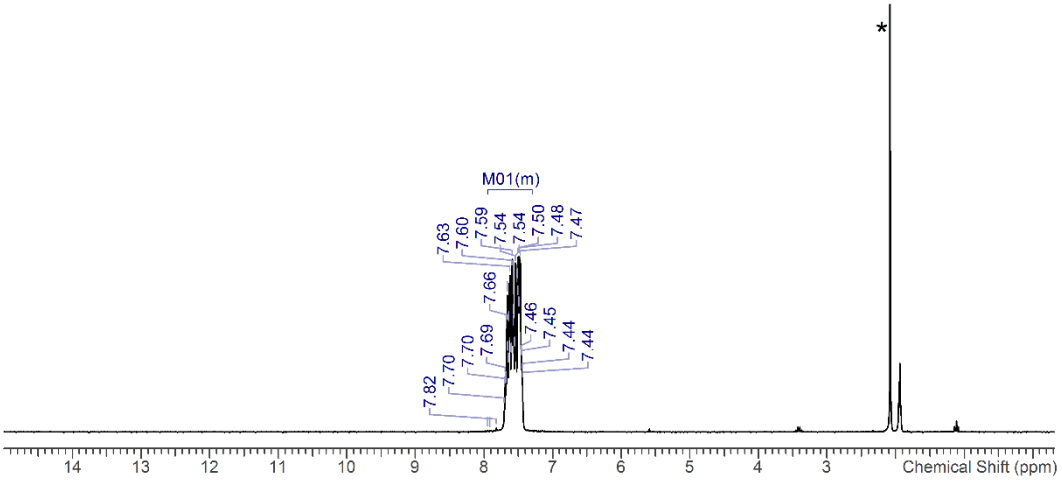


Figure S 24. ^{1}H NMR of [PPN]OCP·$(CH_3)_2CO$.

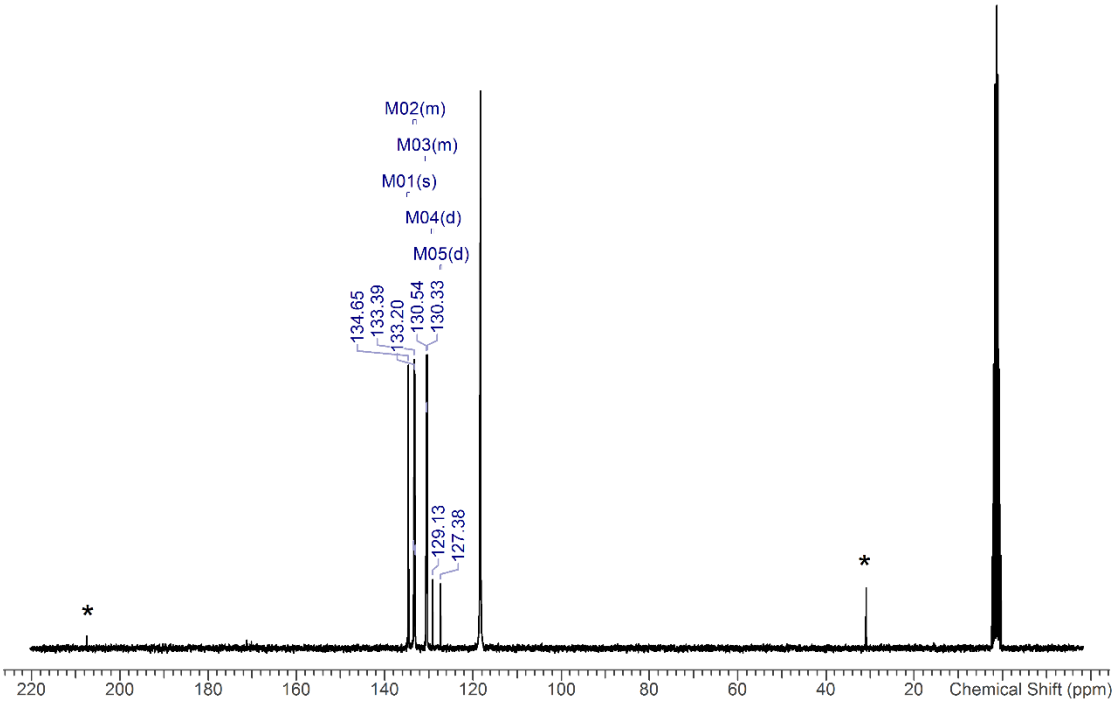


Figure S 25. $^{13}C\{^{1}H\}$ NMR of [PPN]OCP·$(CH_3)_2CO$.

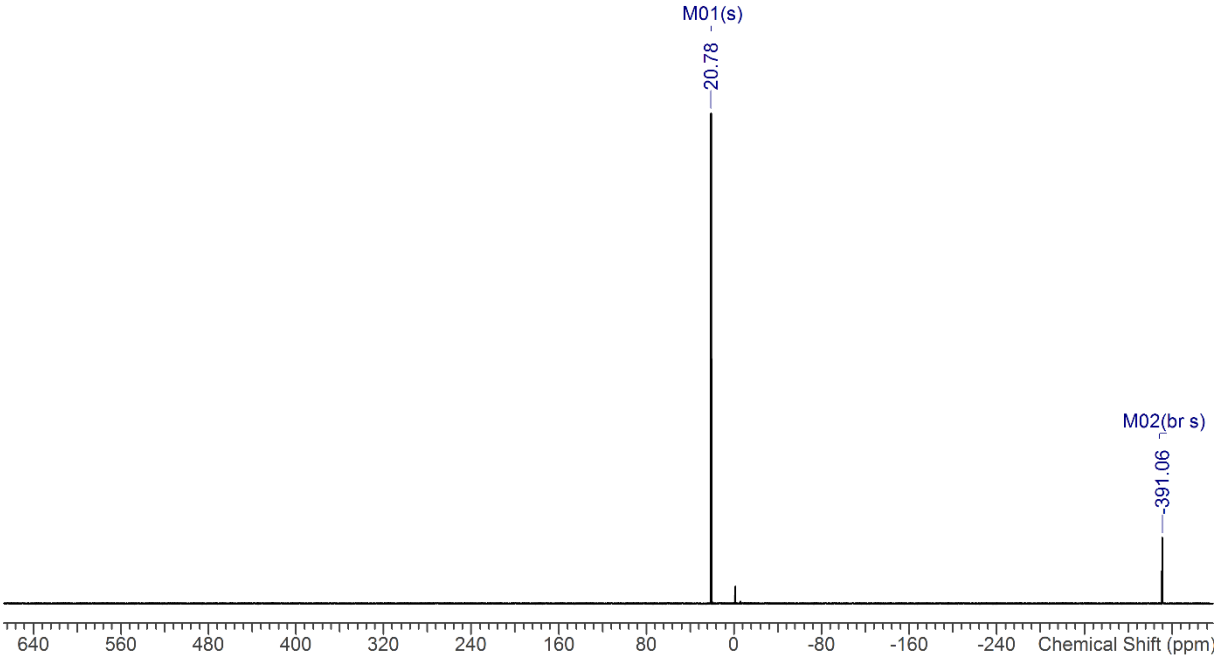


Figure S 26. $^{31}P\{^{1}H\}$ NMR of [PPN]OCP·$(CH_3)_2CO$.

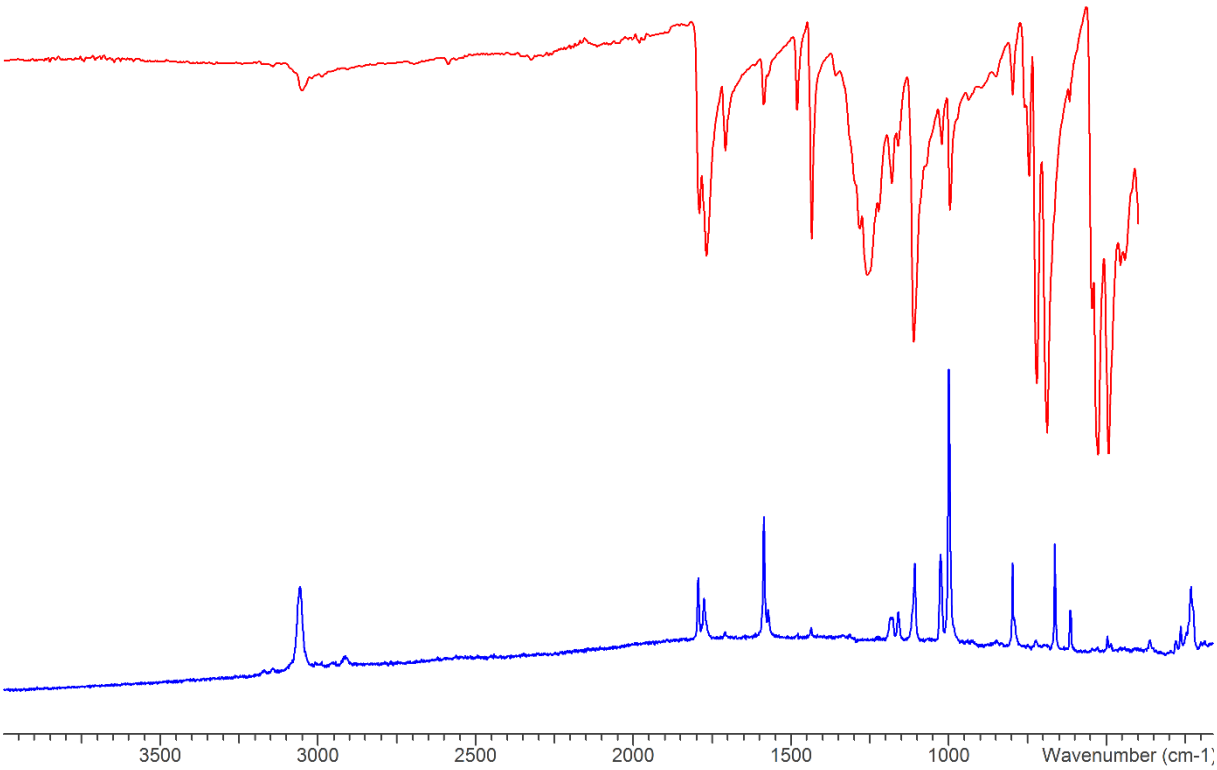
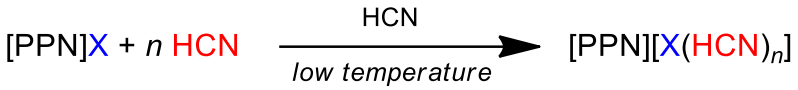


Figure S 27. IR (red) and Raman (blue) spectra of [PPN]OCP·$(CH_3)_2CO$.

3.2 Product synthesis

General annotation: It was not possible to obtain further analytical data like NMR since all obtained HCN solvates were found to be unstable with respect to solvents. Additionally, no IR or EA could be obtained since crystallization was achieved at low-temperatures in Fomblin YR-1800 perfluoropolyether and the solvates were found to be unstable at room temperature (loss of HCN or polymerization). The same applies to the determination of the yield.

3.2.1 Synthesis of [PPN][X(HCN)$_n$] salts



X = N_3, OCN; n = 3 X = SCN; n = 2

3.2.1.1 Synthesis of [PPN][N_3(HCN)$_3$] (**1**)

[PPN]N_3 (0.1 g, 0.17 mmol, 1 eq.) was placed in a Schlenk tube which was cooled to 0 °C afterwards. 120 µL of HCN (80 mg, 2.9 mmol, 17 eq.) which was cooled to 0 °C was transferred onto the salt via a pre-cooled syringe. The mixture was shaken rapidly until complete dissolution of the salt was noticed. During the whole process the liquid remained colorless. Several attempts to obtain crystals by cooling the mixture slowly to −21 °C did not lead to crystallization. However, at −22 °C the liquid started to solidify slowly. **Small** amounts of the solid were transferred to a self-build low-temperature mounting station for crystal picking, which was cooled to −60 °C. Under the microscope evolving gas was observed (subliming HCN). The amount of the colorless solid started to reduce and after one minute colorless crystals were formed. X-ray analysis revealed the formation of [PPN][N_3(HCN)$_3$] (**1**).

$C_{39}H_{33}N_7P_2$ (661.66 g/mol): **Raman** (laser: 633 nm, accumulation time: 6 s ,20 scans, 225 K, cm^{-1}) $\tilde{\nu}$ = 169 (1), 187 (1), 204 (1), 222 (1), 239 (2), 250 (1), 254 (1), 268 (1), 283 (1), 309 (1), 335 (1), 365 (1), 390 (1), 399 (1), 489 (1), 526 (1), 534 (1), 551 (1), 615 (2), 626 (1), 667 (3), 694 (1), 697 (1), 725 (1), 729 (1), 747 (1), 757 (1), 806 (1), 842 (1), 856 (1), 930 (1), 973 (1), 1001 (10), 1027 (4), 1054 (1), 1073 (1), 1090 (1),

1113 (3), 1159 (1), 1165 (1), 1183 (1), 1191 (1), 1230 (1), 1242 (1), 1246 (1), 1275 (1), 1286 (1), 1315 (1), 1322 (1), 1332 (1), 1435 (1), 1440 (1), 1481 (1), 1576 (1), 1588 (4), 2056 (1), 2067 (2), 2077 (1), 2958 (1), 2993 (1), 3013 (1), 3023 (1), 3028 (1), 3061 (3), 3143 (1), 3149 (1), 3178 (1).

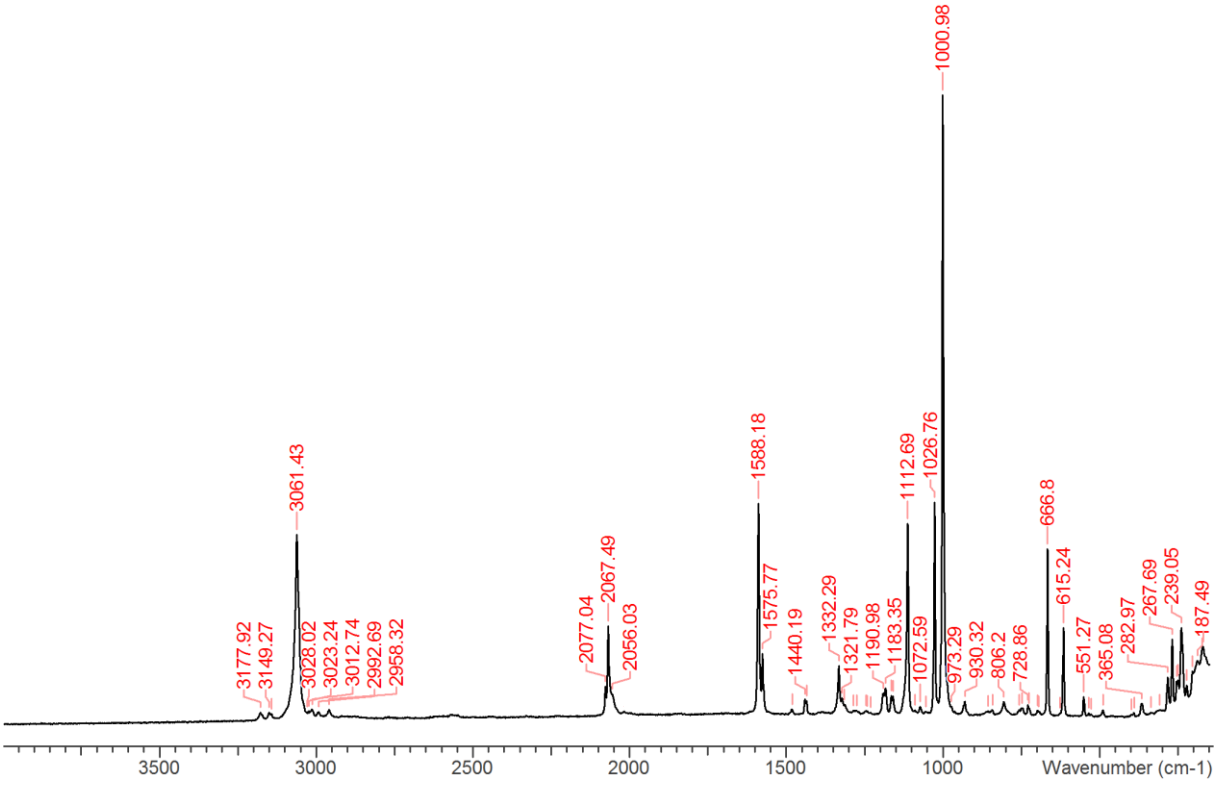


Figure S28. Raman spectrum of **1**.

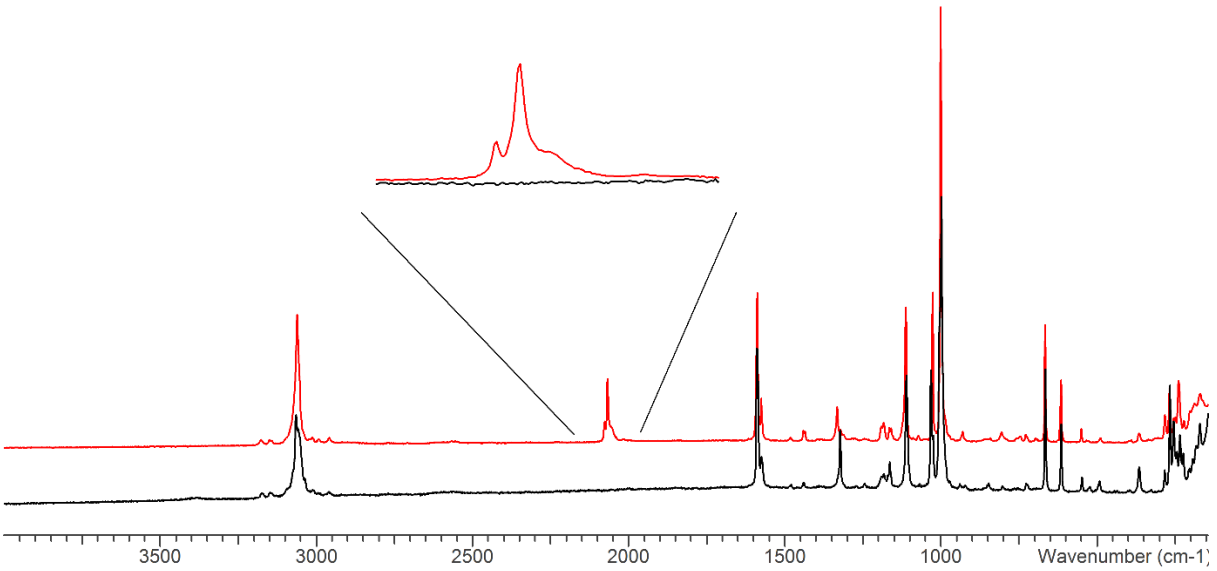


Figure S 29. Raman spectra of **1** (red) and reference material $[PPN]N_3$ (black) for comparison.

3.2.1.2 Synthesis of [PPN][OCN(HCN)$_3$] (**2**)

[PPN]OCN (0.2 g, 0.34 mmol, 1 eq.) was placed in a Schlenk tube which was cooled to 0 °C afterwards. 250 µL of HCN (170 mg, 6.29 mmol, 19 eq.) which was cooled to 0 °C was transferred onto the salt via a pre-cooled syringe. The mixture was shaken rapidly until complete dissolution of the salt was noticed. The solution started to change in color (yellowish to brown) which was fast progressing even at low temperatures with accompanying increase in viscosity. Several attempts to obtain crystals by cooling the mixture slowly to −21 °C did not lead to crystallization. However, at −22 °C the liquid started to solidify slowly. **Small** amounts of the solid were transferred to a self-build low-temperature mounting station for crystal picking, which was cooled to −60 °C. Under the microscope evolving gas was observed (subliming HCN). The amount of the colorless solid started to reduce and after one minute colorless crystals were formed. X-ray analysis revealed the formation of [PPN][OCN(HCN)$_3$] (**2**).

$C_{40}H_{33}N_5P_2O$ (661.65 g/mol): **Raman** (laser: 633 nm, accumulation time: 4 s ,20 scans, 225 K, cm^{-1}) $\tilde{\nu}$ = 157 (1), 169 (2), 183 (1), 202 (1), 220 (1), 237 (2), 248 (1), 252 (1), 266 (2), 279 (1), 364 (1), 389 (1), 395 (1), 432 (1), 462 (1), 487 (1), 533 (1), 548 (1), 615 (2), 630 (1), 665 (4), 695 (1), 722 (1), 727 (1), 755 (1), 804 (1), 842 (1), 849 (1), 858 (1), 922 (1), 928 (1), 972 (1), 999 (10), 1015 (1), 1025 (4), 1070 (1), 1111 (3), 1159 (1), 1163 (1), 1181 (1), 1204 (1), 1252 (1), 1273 (1), 1284 (1), 1293 (1), 1312 (1), 1337 (1), 1434 (1), 1440 (1), 1482 (1), 1571 (1), 1575 (1), 1587 (4), 2060 (1), 2073 (2), 2098 (1),* 2164 (1), 2912 (1), 2958 (1), 2994 (1), 3014 (1), 3022 (1), 3039 (1), 3061 (4), 3080 (1), 3084 (1), 3142 (1), 3149 (1), 3172 (1), 3178 (1).

* (free HCN attached to the surface)

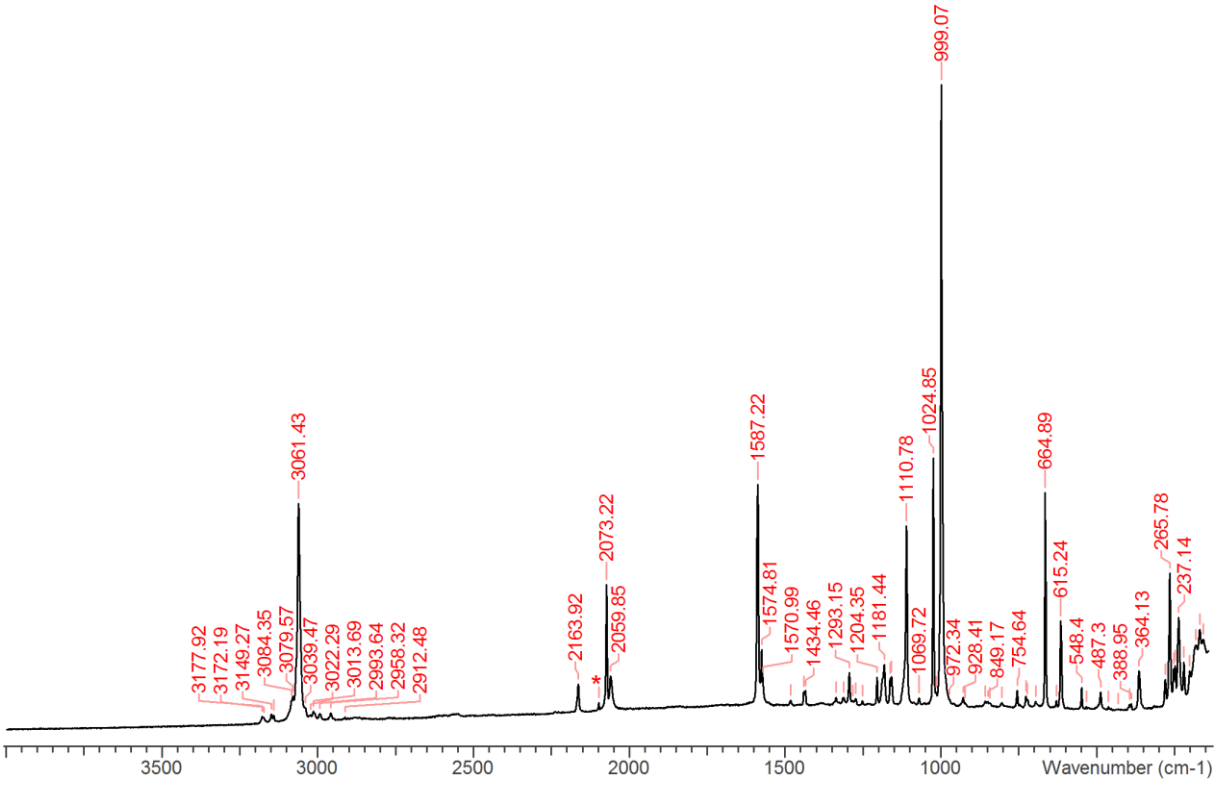


Figure S30. Raman spectrum of **2**. The asterisk marks attached HCN at the crystal surface.

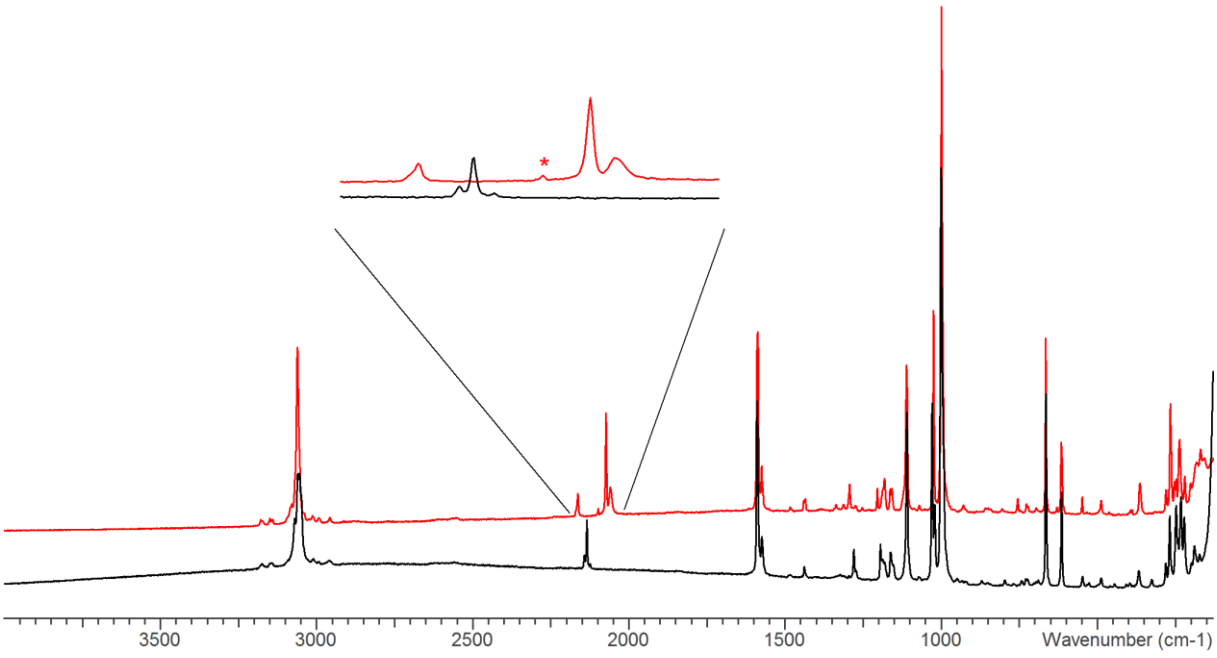


Figure S31. Raman spectra of **2** (red) and reference material [PPN]OCN (black) for comparison. The asterisk marks attached HCN at the crystal surface.

3.2.1.3 Synthesis of [PPN][SCN(HCN)$_2$] (**3**)

[PPN]SCN (0.3 g, 0.49 mmol, 1 eq.) was placed in a Schlenk tube which was cooled to 0 °C afterwards. 300 µL of HCN (200 mg, 7.62 mmol, 16 eq.) which was cooled to 0 °C was transferred onto the salt via a pre-cooled syringe. The mixture was shaken rapidly until complete dissolution of the salt was noticed. The solution started to change the color to yellowish (intensified with time) which was only slowly progressing at low temperatures with accompanying increase in viscosity. Several attempts to obtain crystals by cooling the mixture slowly to −18 °C did not lead to crystallization. However, at −20 °C the liquid started to solidify slowly. **Small** amounts of the solid were transferred to a self-build low-temperature mounting station for crystal picking, which was cooled to −60 °C. Under the microscope evolving gas was observed (subliming HCN). The amount of the colorless solid started to reduce and after one minute colorless crystals were formed. X-ray analysis revealed the formation of [PPN][SCN(HCN)$_2$] (**3**).

$C_{39}H_{32}N_4P_2S$ (650.68 g/mol): **Raman** (laser: 633 nm, accumulation time: 4 s ,20 scans, 245 K, cm^{-1}) $\tilde{\nu}$ = 172 (1), 185 (1), 206 (1), 221 (1), 239 (2), 252 (1), 269 (1), 283 (1), 369 (1), 391 (1), 397 (1), 489 (1), 527 (1), 535 (1), 552 (1), 615 (2), 667 (3), 694 (1), 722 (1), 729 (1), 749 (1), 758 (1), 804 (1), 844 (1), 930 (1), 976 (1), 1000 (10), 1028 (4), 1076 (1), 1089 (1), 1112 (4), 1161 (1), 1182 (1), 1192 (1), 1279 (1), 1286 (1), 1315 (1), 1338 (1), 1343 (1), 1437 (1), 1442 (1), 1483 (1), 1578 (1), 1588 (3), 2051 (2), 2059 (1), 2073 (1), 2959 (1), 2996 (1), 3015 (1), 3022 (1), 3060 (2), 3073 (1), 3097 (1), 3142 (1), 3150 (1), 3153 (1), 3174 (1), 3177 (1).

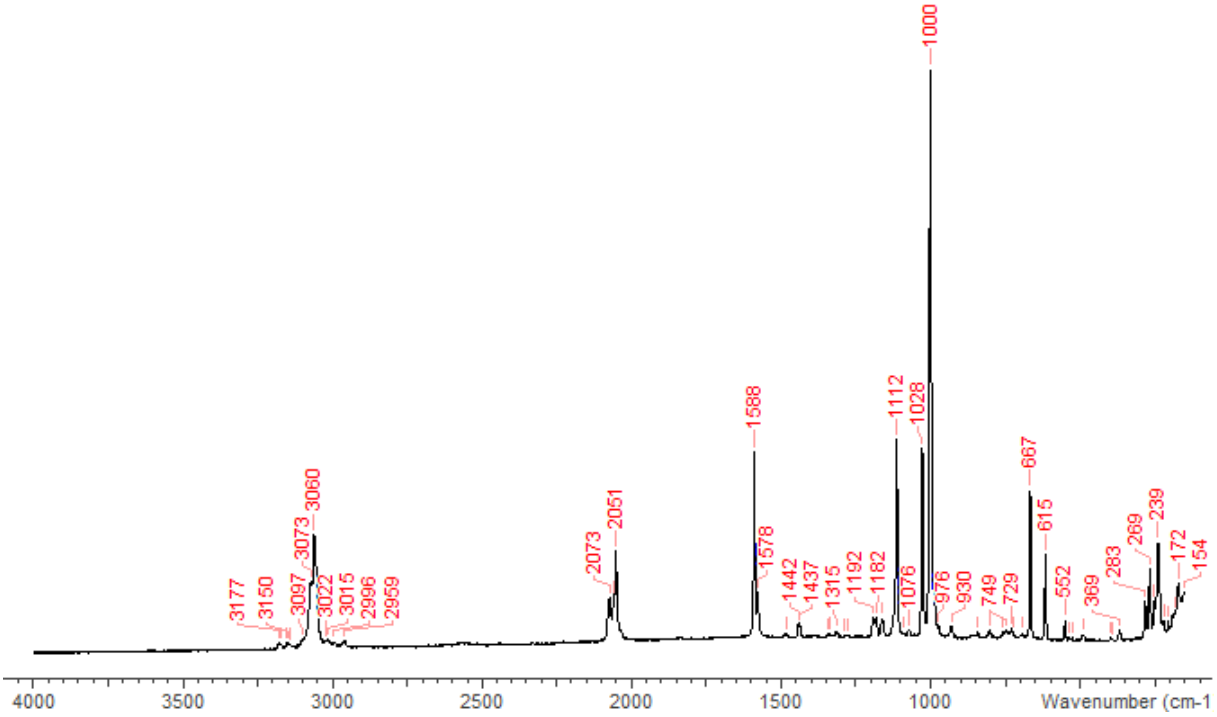


Figure S32. Raman spectrum of **3**.

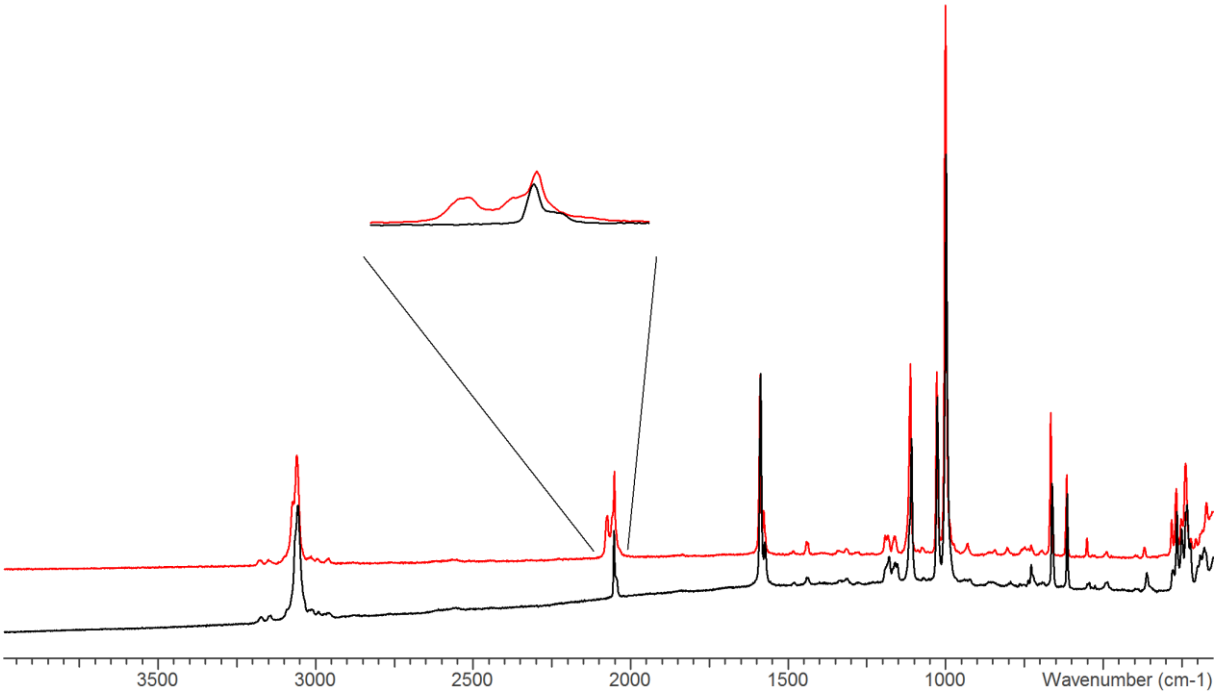
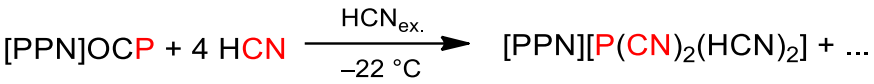


Figure S 33. Raman spectra of **3** (red) and reference material [PPN]SCN (black) for comparison.

3.2.2 Synthesis of [PPN][P(CN·HCN)$_2$] (**4**)



[PPN]OCP·acetone (0.08 g, 0.12 mmol, 1 eq.) was placed in a Schlenk tube which was cooled to 0 °C afterwards. 100 µL of HCN (60 mg, 2.14 mmol, 17 eq.) which was cooled to 0 °C was transferred onto the salt via a pre-cooled syringe. The mixture was shaken rapidly for two minutes but no complete dissolution of the salt was noticed. The liquid phase of the suspension started to change the color (brownish) as soon as HCN was added. Several attempts to obtain crystals by cooling the mixture slowly to −21 °C did not lead to crystallization. However, at −22 °C the upper liquid phase started to solidify slowly. This process was initiated as soon as the solid material of the suspension had settled to the bottom of the flask. **Small** amounts of the solid were transferred to a self-build low-temperature mounting station for crystal picking, which was cooled to −60 °C. Under the microscope evolving gas was observed (subliming HCN). The amount of the colorless solid started to reduce and after one minute colorless crystals were formed. X-ray analysis revealed the formation of [PPN][P(CN)$_2$(HCN)$_2$] (**4**).

$C_{40}H_{32}N_5P_4$ (675.14 g/mol): **Raman** (laser: 633 nm, accumulation time: 4 s ,20 scans, 225 K, cm^{-1}) $\tilde{\nu}$ = 99 (8), 114 (9), 137 (5), 177 (1), 184(1), 195 (1), 205 (1), 226 (2), 236 (3), 252 (2), 267 (2), 285 (1), 344 (1), 361 (1), 386 (1), 392 (1), 402 (1), 413 (1), 447 (1), 459 (1), 491 (1), 526 (1), 536 (1), 547 (1), 614 (2), 633 (1), 664 (4), 693 (1), 725 (1), 745 (1), 803 (1), 842 (1), 848 (1), 852 (1), 866 (1), 927 (1), 939 (1), 1001 (9), 1027 (3), 1031 (3), 1071 (1), 1111 (3), 1162 (1), 1166 (1), 1179 (1), 1192 (1), 1282 (1), 1312 (1), 1337 (1), 1438 (1), 1483 (1), 1576 (1), 1588 (3), 2022 (1), 2025 (1), 2048 (1), 2064 (1), 2074 (1) (shoulder), 2084 (3), 2105 (10), 2958 (1), 2993 (1), 3011 (1), 3048 (1), 3057 (3), 3074 (1), 3089 (1), 3145 (1), 3151 (1), 3175 (1).

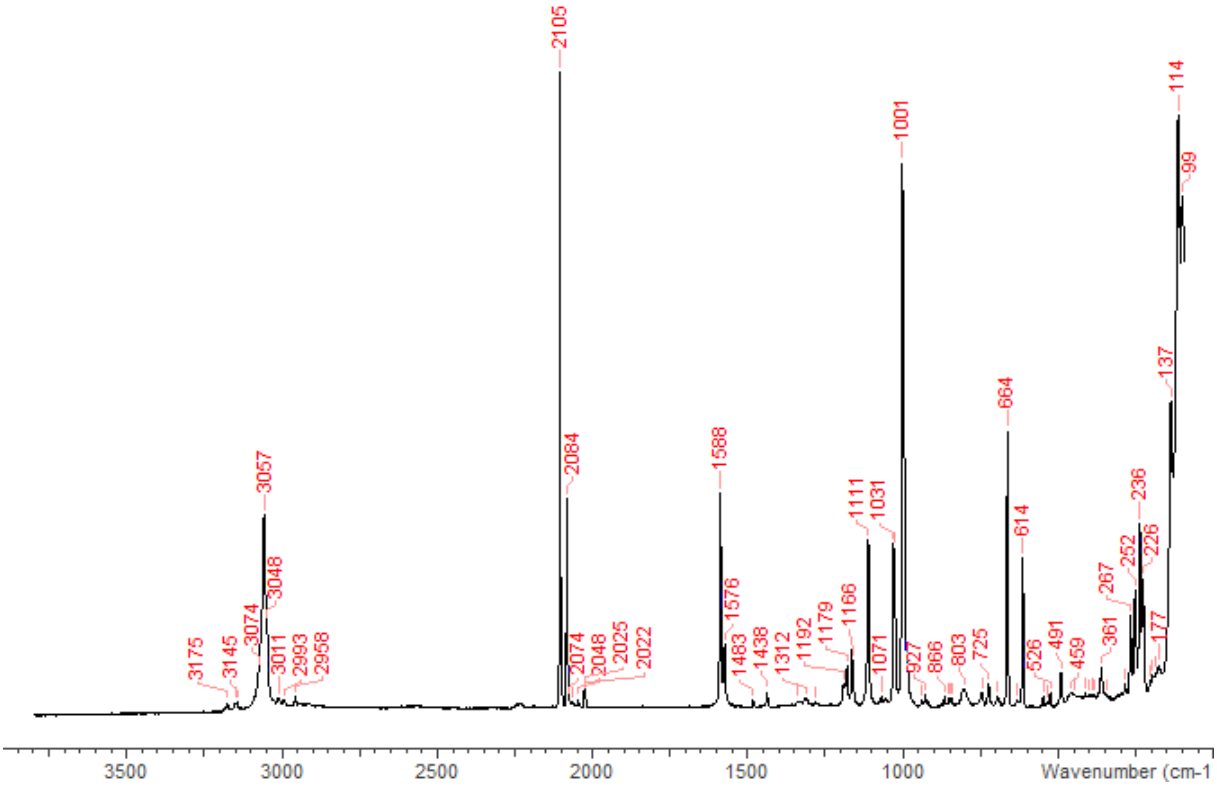


Figure S34. Raman spectrum of **4**.

4 Computational Details

All computations were carried out using Gaussian09.[9]

Method. Just recently we reported on the synthesis of $[CN(HCN)_n]^-$ (n = 2, 3)[5] and used different methods (M06, MP2, CCSD(T) and PBE0) in combination with the Grimme's dispersion model D3BJ and two different basis sets (pVDZ, pVTZ) to optimize the molecular structure of the isomers. We found that the DFT method pbe0[10-12] with Grimme's dispersion model D3BJ[13-14] in conjunction with the aug-cc-pVTZ[15-19] basis set provides good qualitative and quantitative results. Therefore, we decided to use this combination here as well.

Structure. All structures were fully optimized and confirmed as minima by frequency analyses (NIMAG = 0). Cartesian coordinates of all considered species can be found at the end of the document.
All green marked compounds in forthcoming tables represent structures, where proton migration during optimization occurred, while the red marked isomers are the energetically most favored ones.

Note. We would like to point out that all solvates of the type $[X(HCN)_n]^-$ (X = N_3, OCN, SCN) have very flat potentials for the bridging H–C and H–N distances as well as angles and dihedral angles. Therefore, the structure at ambient temperatures can be considered to be highly dynamic. Although the calculated gas phase energy data agree very well with the experimental data, it is difficult to compare the structural data with one another, even if the thermodynamically favored gas phase structural motifs are also observed in the solid state (best isomer). However, there are significant differences in terms of linearity and planarity due to very soft potentials for bending/distortion.

Mono-, Di- and Trisolvates $[N_3(HCN)_n]^-$

Table S2. Absolute energies in a.u and relative energies in kcal/mol. Red: Energetically preferred isomer. Green: Proton migration during optimization.

isomer	symmetry	connectivity	# bonds HC	# bonds HN	# bridge HC	# bridge HN	E0	H298	G298	ΔE0	ΔH298	ΔG298
M1	C1	NCH NNN	1			1	-257.493829	-257.45918	-257.495461	0.00	0.00	0.00
M2	C1	CN HNNN		1		1	-257.485195	-257.451665	-257.488133	5.42	4.72	4.60
D1	C1	NCH NCH NNN	2			2	-350.860038	-350.805475	-350.852547	4.44	3.56	3.82
D2	C1	NCH CNH NNN	1	1	1	1	-350.859157	-350.803245	-350.85063	5.00	4.96	5.02
D3	C1	CNH NC HNNN		2	1	1	-350.850478	-350.79533	-350.841763	10.44	9.93	10.59
D4	C1	CNH CNH NNN		2	1	1	-350.849176	-350.794121	-350.840943	11.26	10.69	11.10
D5	C1	NCH NNN HCN	2			2	-350.866673	-350.810356	-350.859300	0.28	0.50	-0.42
D6	C1	NCH NNN HNC	1	1		2	-350.854605	-350.798904	-350.847106	7.85	7.68	7.23
D7	C1	CNH NNN HNC		2		2	-350.841790	-350.786376	-350.833753	15.89	15.55	15.61
D8	Cs	NCH NNN NCH	2			2	-350.867119	-350.811149	-350.858632	0.00	0.00	0.00
D9	Cs	NCH NNN CNH	1	1		2	-350.855634	-350.800456	-350.847541	7.21	6.71	7.96
D10	Cs	CNH NNN CNH		2		2	-350.843463	-350.788726	-350.835265	14.84	14.07	14.66
T1	C1	NCH NCH NC HNNN	2	1	1	2	-444.224689	-444.147706	-444.205789	6.26	5.70	7.10
T2	C1	NCH NCH CN HNNN	2	1	1	2	-444.222684	-444.145452	-444.203811	7.52	7.12	8.34
T3	C1	NCH CNH NC HNNN	1	2	1	2	-444.215787	-444.140045	-444.197343	11.83	10.51	12.40
T4	C1	NCH CN HCN HNNN	2	1	1	2	-444.221339	-444.14385	-444.202372	8.37	8.12	9.24
T5	C1	CNH NCH NC HNNN	1	2	1	2	-444.210023	-444.133274	-444.190466	15.47	14.76	16.71
T6	C1	CNH NCH CN HNNN	1	2	1	2	-444.208130	-444.13128	-444.188626	16.65	16.01	17.87

isomer	symmetry	connectivity				# bonds HC	# bonds HN	# bridge HC	# bridge HN	E0	H298	G298	ΔE0	ΔH298	ΔG298
T7	**C1**	CNH	CN	HCN	HNNN	1	2	1	2	-444.211039	-444.134254	-444.192194	14.83	14.14	15.63
T8	**C1**	CNH	CN	HNC	HNNN		3	1	2	-444.203278	-444.128009	-444.184739	19.70	18.06	20.31
T9	**C1**	NCH	NCH	NNN	HCN	3			3	-444.229944	-444.152464	-444.212405	2.97	2.72	2.95
T10	**C1**	NCH	NCH	NNN	HNC	2	1		3	-444.217138	-444.139988	-444.199156	11.00	10.54	11.26
T11	**C1**	NCH	CNH	NNN	HCN	2	1	1	2	-444.219798	-444.144272	-444.203538	9.33	7.86	8.51
T12	**C1**	NCH	CNH	NNN	HNC	1	2	1	2	-444.205987	-444.129805	-444.188056	18.00	16.93	18.23
T13	**C1**	CNH	NCH	NNN	HCN	2	1		3	-444.215294	-444.138201	-444.197175	12.16	11.67	12.50
T14	**C1**	CNH	NCH	NNN	HNC	1	2		3	-444.202221	-444.125323	-444.183473	20.13	19.75	21.10
T15	**C1**	CNH	CN	HNNN	HCN	1	2	1	2	-444.208907	-444.132728	-444.192663	16.17	15.10	15.34
T16	**C1**	CNH	CNH	NNN	HNC		3	1	2	-444.192364	-444.117385	-444.174913	26.55	24.73	26.47
T17	**C1**	NCH NCH	NNN	HCN		3			3	-444.234671	-444.156791	-444.217103	0.00	0.00	0.00
T18	**C1**	NCH NCH	NNN	HNC		2	1		3	-444.220891	-444.143293	-444.202734	8.65	8.47	9.02
T19	**C1**	CNH NCH	NNN	HCN		2	1		3	-444.221546	-444.144073	-444.204096	8.24	7.98	8.16
T20	**C1**	CNH NCH	NNN	HNC		1	2		3	-444.207218	-444.129889	-444.18883	17.23	16.88	17.74
T21	**C1**	CNH CNH	NNN	HCN		1	2		3	-444.193128	-444.11602	-444.174384	26.76	25.58	26.81

isomer	symmetry	connectivity	# bonds HC HN	# bridge HC HN	E0	H298	G298	ΔE0	ΔH298	ΔG298
T22	C1	CNH NNN HCN CNH	3	3	-444.207966	-444.130797	-444.190495	16.76	16.31	16.70

Table S3. Reaction energies (pbe0/aug-cc-pVTZ) for the stepwise formation of solvates in kcal/mol (for the thermodynamically most favored isomer).

m1 C1	HCN + N_3^- → monomer$^-$		
E0 H298 G298			
D8 Cs			
E0 H298 G298			
T17 C1			
E0 H298 G298			

Mono-, Di- and Trisolvates $[OCN(HCN)_n]^-$

Table S4. Absolute energies in a.u and relative energies in kcal/mol. Red: Energetically preferred isomer. Green: Proton migration during optimization.

isomer	symmetry	connectivity	# bonds		# bridge			E0	H298	G298	ΔE0	ΔH298	ΔG298
			HC	HN	HC	HN	HS						
M1	Cs	NCH OCN		1			1	-261.384680	-261.349739	-261.386015	4.16	3.99	4.24
M2	Cv	NCH NCO		1		1		-261.391309	-261.356092	-261.392769	0.00	0.00	0.00
M3	Cs	CNH OCN	1				1	-261.373626	-261.339397	-261.375259	11.60	10.48	10.99
M4	Cv	CNH NCO	1			1		-261.383395	-261.350118	-261.38824	4.97	3.75	2.84
d1	C2v	NCH OCN NCH		2			2	-354.754653	-354.698179	-354.745181	6.39	6.65	6.49
d2	C2v	NCH NCO NCH		2		2		-354.764838	-354.708776	-354.755517	0.00	0.00	0.00
d3	Cs	NCH OCN CNH	1	1			2	-354.741617	-354.68545	-354.732731	14.57	14.64	14.30
d4	Cs	NCH NCO CNH	1	1		2		-354.753755	-354.698383	-354.745483	6.95	6.52	6.30
d5	C2v	CNH OCN CNH	2				2	-354.727798	-354.671777	-354.717862	23.24	23.22	23.63
d6	C2v	CNH NCO CNH	1	1		2		-354.741472	-354.686396	-354.732371	14.66	14.04	14.52
d7	Cs	NCH NCH OCN		2		1	1	-354.748698	-354.692734	-354.740558	10.13	10.07	9.39
d8	Cv	NCH NCH NCO		2		2		-354.757843	-354.70212	-354.752183	4.39	4.18	2.09
d9	Cs	NCH CNH OCN	1	1	1		1	-354.739094	-354.684594	-354.731652	16.15	15.17	14.98

isomer	symmetry	connectivity				# bonds		# bridge			E0	H298	G298	ΔE0	ΔH298	ΔG298
						HC	HN	HC	HN	HS						
d10	Cs	NCH	CN	HNCO		1		1	1		-354.756777	-354.701353	-354.74896	5.06	4.66	4.11
d11	Cs	CNH	NCH	OCN		1	1		1	1	-354.734076	-354.678507	-354.725253	19.30	18.99	18.99
d12	C1	CNH	NCH	NCO		1	1		2		-354.747844	-354.693047	-354.739399	10.66	9.87	10.11
d13	Cs	CNH	CNH	OCN		2			1	1	-354.725813	-354.672837	-354.719068	24.49	22.55	22.87
d14	Cs	CNH	CN	HNCO		2		1	1		-354.747109	-354.692434	-354.738961	11.13	10.25	10.39
d15	Cs	NCH	OCN	HCN			2		1	1	-354.761901	-354.705608	-354.754188	1.84	1.99	0.83
d16	Cs	NCH	OCN	HNC		1	1		1	1	-354.752373	-354.696777	-354.744412	7.82	7.53	6.97
d17	Cs	NCH	NCO	HNC		1	1		1	1	-354.748689	-354.692701	-354.740925	10.13	10.09	9.16
d18	Cs	CNH	NCO	HNC			2		1	1	-354.737735	-354.68231	-354.730109	17.01	16.61	15.94
t1	Cs	NCH	NCH	NCH	OCN		3		2	1	-448.109341	-448.032111	-448.090315	13.75	13.35	14.44
t2	C1	NCH	NCH	NC	HNCO		3		3		-448.122008	-448.045377	-448.103335	5.80	5.03	6.27
t3	Cs	NCH	NCH	CNH	OCN	1	2	1	1	1	-448.100884	-448.02592	-448.083475	19.06	17.23	18.73
t4	C1	NCH	NCH	CN	HNCO	1	2	1	2		-448.120586	-448.043753	-448.101839	6.69	6.04	7.21
t5	Cs	NCH	CNH	CN	HOCN	2	1	2		1	-448.090307	-448.015739	-448.072439	25.69	23.62	25.66
t6	Cs	NCH	CN	HCN	HNCO	2	1	2	1		-448.118789	-448.041677	-448.099817	7.82	7.35	8.48
t7	Cs	NCH	CNH	NCH	OCN	1	2	1	1	1	-448.096244	-448.019778	-448.076836	21.97	21.09	22.90
t8	Cs	NCH	CN	HNC	HNCO	1	2	1	2		-448.113117	-448.037708	-448.094882	11.38	9.84	11.57
t9	Cs	CNH	NCH	NCH	OCN	1	2		2	1	-448.093592	-448.01659	-448.073755	23.63	23.09	24.83
t10	Cs	CNH	NCH	NCH	NCO	1	2		3		-448.107340	-448.03094	-448.08797	15.00	14.08	15.91
t11	Cs	CNH	CNH	NCH	OCN	2	1	1	1	1	-448.081424	-448.005459	-448.061575	31.27	30.07	32.47
t12	C1	CNH	CNH	NC	HNCO	2	1	1	2		-448.100534	-448.025653	-448.08218	19.28	17.40	19.54
t13	Cs	CNH	NCH	CNH	OCN	2	1	1	1	1	-448.085522	-448.010922	-448.067422	28.70	26.65	28.80
t14	C1	CNH	NCH	CN	HNCO	2	1	1	2		-448.105999	-448.029517	-448.086554	15.85	14.98	16.80
t15	Cs	CNH	CNH	CNH	OCN	3		2		1	-448.076505	-448.002858	-448.058931	34.35	31.71	34.13
t16	Cs	CNH	CN	HCN	HNCO	3		2	1		-448.108441	-448.032007	-448.089529	14.31	13.41	14.93
t25	C1	NCH	NCH	OCN	HCN		3		2	1	-448.124783	-448.047054	-448.106144	4.06	3.97	4.51
t26	C1	NCH	NCH	NCO	HCN		3		2	1	-448.126697	-448.0492	-448.108297	2.86	2.63	3.16

isomer	symmetry	connectivity	# bonds		# bridge			E0	H298	G298	ΔE0	ΔH298	ΔG298
			HC	HN	HC	HN	HS						
t27	C1	NCH NCH OCN HNC	1	2		2	1	-448.113393	-448.036225	-448.095408	11.21	10.77	11.24
t28	C1	NCH NCH NCO HNC	1	2		2	1	-448.113202	-448.035849	-448.094315	11.33	11.00	11.93
t29	C1	NCH CNH OCN HCN	1	2	1	1	1	-448.113209	-448.036104	-448.094409	11.32	10.84	11.87
t30	C1	NCH CN HNCO HCN	1	2	1	1	1	-448.118795	-448.043472	-448.103907	7.82	6.22	5.91
t31	C1	NCH CNH OCN HNC	2	1	1	1	1	-448.101908	-448.025076	-448.082876	18.41	17.76	19.11
t32	C1	NCH CNH NCO HNC	2	1	1	1	1	-448.104368	-448.028457	-448.086482	16.87	15.64	16.84
t33	C1	CNH NCH OCN HCN	1	2		2	1	-448.109048	-448.031545	-448.08958	13.93	13.70	14.90
t34	C1	CNH NCH NCO HCN	1	2		2	1	-448.112370	-448.035294	-448.09365	11.85	11.35	12.35
t35	C1	CNH NCH OCN HNC	2	1		2	1	-448.098902	-448.021868	-448.079551	20.30	19.78	21.19
t36	C1	CNH NCH NCO HNC	2	1		2	1	-448.098666	-448.021643	-448.079263	20.45	19.92	21.37
t37	C1	CNH CNH OCN HCN	2	1	1	1	1	-448.099211	-448.022666	-448.080116	20.11	19.28	20.84
t38	C1	CNH CN HNCO HCN	2	1	1	1	1	-448.107637	-448.031983	-448.091576	14.82	13.43	13.65
t39	C1	CNH CNH OCN HNC	3		1	1	1	-448.087657	-448.011248	-448.068149	27.36	26.44	28.35
t40	C1	CNH CNH NCO HNC	3		1	1	1	-448.091612	-448.016762	-448.075266	24.87	22.98	23.88
t17	C1	NCH NCO HCN NCH		3		2	1	-448.131251	-448.053385	-448.113325	0.00	0.00	0.00
t18	C2v	NCH OCN HCN NCH		3		1	2	-448.127938	-448.049888	-448.108795	2.08	2.19	2.84
t19	C1	CNH NCO HCN NCH	1	2		2	1	-448.118800	-448.041339	-448.101039	7.81	7.56	7.71
t20	Cs	CNH OCN HCN NCH	1	2		1	2	-448.113659	-448.035773	-448.094858	11.04	11.05	11.59

isomer	symmetry	connectivity	# bonds		# bridge			E0	H298	G298	ΔE0	ΔH298	ΔG298
			HC	HN	HC	HN	HS						
t21	**C2v**	CNH OCN HCN CNH	2	1		1	2	-448.098763	-448.020975	-448.078814	20.39	20.34	21.66
t22	**C1**	CNH NCO HCN CNH	2	1		2	1	-448.105335	-448.028129	-448.087372	16.26	15.85	16.29
t23	**C2v**	CNH OCN HNC CNH	3			1	2	-448.086520	-448.009013	-448.066314	28.07	27.84	29.50
t24	**C1**	CNH NCO HNC CNH	3			2	1	-448.090119	-448.012922	-448.071332	25.81	25.39	26.35
t41	**C1**	CNH OCN HNC NCH	1	2		1	2	-448.101795	-448.024251	-448.082825	18.48	18.28	19.14
t42	**C1**	CNH NCO HNC NCH	1	2		2	1	-448.104011	-448.026607	-448.085554	17.09	16.80	17.43

Table S5. Reaction energies (pbe0/aug-cc-pVTZ) for the stepwise formation of solvates in kcal/mol (for the thermodynamically most favored isomer with two C–H···N H-bridges).

M2 Cv	**HCN + NCO^- → monomer$^-$**		
E0	-25.0		
H298	-24.6		
G298	-17.6		
D2 C2v	**2 HCN + NCO^- → monomer$^-$**	**HCN + monomer$^-$ → dimer$^-$**	
E0	-43.4	-18.4	
H298	-42.4	-17.8	
G298	-27.4	-9.8	
T17 C1	**3 HCN + NCO^- → monomer$^-$**	**2 HCN + monomer$^-$ → dimer$^-$**	**HCN + dimer$^-$ → trimer$^-$**
E0	-57.4	-32.3	-13.9
H298	-55.1	-30.5	-12.7
G298	-34.1	-16.5	-6.7

Table S6. Reaction energies (pbe0/aug-cc-pVTZ) for the stepwise formation of solvates in kcal/mol (for the thermodynamically favored isomer with two C–H···O H-bridges).

M2 Cs	**HCN + OCN^- → monomer$^-$**		
E0	-25.0		
H298	-24.6		
G298	-17.6		
D15 Cs	**2 HCN + OCN^- → monomer$^-$**	**HCN + monomer$^-$ → dimer$^-$**	
E0	-41.6	-16.5	
H298	-40.4	-15.8	
G298	-26.6	-9.0	
T18 C2v	**3 HCN + OCN^- → monomer$^-$**	**2 HCN + monomer$^-$ → dimer$^-$**	**HCN + dimer$^-$ → trimer$^-$**
E0	-55.3	-30.2	-13.7
H298	-52.9	-28.4	-12.5
G298	-31.3	-13.6	-4.7

Mono- and Disolvates of $[SCN(HCN)_n]^-$

Table S7. Absolute energies in a.u and relative energies in kcal/mol. Red: Energetically preferred isomer. Green: Proton migration during optimization.

isomer	symmetry	connectivity	# bonds		# bridge			E0	H298	G298	ΔE0	ΔH298	ΔG298
			HC	HN	HC	HN	HS						
m1	Cs	NCH SCN	1			1		-584.286433	-584.253222	-584.292258	3.68	3.29	2.29
m2	Cs	CNH SCN		1		1		-584.271575	-584.238852	-584.277471	13.00	12.31	11.57
m3	Cv	NCH NCS	1			1		-584.292293	-584.258464	-584.295911	0.00	0.00	0.00
m4	Cv	CNH NCS		1		1		-584.281709	-584.248616	-584.285268	6.64	6.18	6.68
d1	C1	NCH SCN HCN	2			1	1	-677.658853	-677.604223	-677.654479	0.58	0.57	0.29
d2	C1	NCH SCN HNC	1	1		1	1	-677.646998	-677.5928	-677.642335	8.02	7.73	7.91
d3	C1	CNH SCN HNC		2		1	1	-677.631116	-677.577225	-677.626312	17.99	17.51	17.97
d10	C1	CNH SCN HCN	1	1		1	1	-677.643237	-677.588981	-677.638802	10.38	10.13	10.13
d11	C1	NCH NCH SCN	2			1	1	-677.649632	-677.595117	-677.645231	6.37	6.28	6.10
d12	C1	NCH NCH NCS	2			2		-677.656370	-677.601887	-677.644249	2.14	2.03	6.71
d13	C1	NCH CNH SCN	1	1	1		1	-677.635516	-677.581728	-677.631282	15.22	14.68	14.85
d14	C1	NCH CNH NCS	1	1	1	1		-677.647694	-677.595094	-677.639854	7.58	6.29	9.47
d15	C1	CNH CNH SCN		2	1		1	-677.621409	-677.568117	-677.616851	24.08	23.22	23.91
d16	C1	CNH CN HNCS		2	1	1		-677.635536	-677.5838	-677.630625	15.21	13.38	15.26
d17	C1	CNH NCH SCN	1	1		1	1	-677.634703	-677.580443	-677.629629	15.73	15.49	15.89
d18	C1	CNH NCH NCS	1	1		2		-677.641922	-677.58784	-677.632607	11.20	10.85	14.02
d4	C1	NCH SCN NCH	2				2	-677.652662	-677.598171	-677.649815	4.47	4.36	3.22
d5	C1	CNH SCN NCH	1	1			2	-677.636869	-677.582743	-677.633747	14.38	14.05	13.31
d6	C1	CNH SCN CNH		2			2	-677.620820	-677.567012	-677.617322	24.45	23.92	23.61

isomer	symmetry	connectivity	# bonds HC	# bonds HN	# bridge HC	# bridge HN	# bridge HS	E0	H298	G298	ΔE0	ΔH298	ΔG298
d7	Cs	HCN SCN HCN	2		2			-677.659778	-677.605126	-677.654954	0.00	0.00	0.00
d7	C2v	HCN SCN HCN	2		2			-677.659777	-677.605117	-677.654338	0.00	0.01	0.38
d8	Cs	HNC SCN HCN	1	1	2			-677.646767	-677.59248	-677.641764	8.16	7.94	8.28
d9	Cs	HNC SCN HNC		2	2			-677.632291	-677.578329	-677.627037	17.25	16.82	17.52
d9	C2v	HNC SCN HNC		2	2			-677.632291	-677.578321	-677.626382	17.25	16.82	17.93
t1	C1	NCH NCS HCN NCH	3		2		1	-771.023166	-770.947105	-771.009913	0.00	0.00	0.00
t2	C1	NCH SCN HCN NCH	3		1		2	-771.021906	-770.94585	-771.008972	0.79	0.79	0.59
t3	C1	NCH NCH SCN NCH	3				3	-771.015432	-770.939527	-771.003656	4.85	4.76	3.93
t4	C1	NCH NCH SCN HCN	3		2		1	-771.020479	-770.944432	-771.015432	1.69	1.68	2.45
t5	C1	NCH NCH NCS HCN	3		2		1	-771.021581	-770.945606	-771.006863	0.99	0.94	1.91

isomer	symmetry	connectivity	# bonds HC	# bonds HN	# bridge HC	# bridge HN	# bridge HS	E0	H298	G298	ΔE0	ΔH298	ΔG298
t6	C1	NCH NCH SCN NCH	3			1	2	-771.014325	-770.938393	-771.00122	5.55	5.47	5.45
t7	Cs	NCH NCH NCS NCH	3			3		-771.021994	-770.946012	-771.006985	0.74	0.69	1.84
t8	C1	NCH NCH NCH NCS				3		-771.016203	-770.940404	-770.99642	4.37	4.20	8.47
t9	C1	NCH NCH NCH SCN				2	1	-771.009305	-770.933333	-770.99454	8.70	8.64	9.65

Table S8. Reaction energies (pbe0/aug-cc-pVTZ) for the stepwise formation of solvates in kcal/mol (for the thermodynamically most favored isomers).

M3 C1	**HCN + NCS^- ⟶ monomer$^-$**		
***E*0**	−20.2		
***H*298**	−19.4		
***G*298**	−12.0		
D7 Cs	**2 HCN + NCS^- ⟶ dimer$^-$**	**HCN + monomer$^-$ ⟶ dimer$^-$**	
***E*0**	−34.8	−14.6	
***H*298**	−33.4	−14.0	
***G*298**	−19.5	−7.5	
T1 C1	**3 HCN + NCS^- ⟶ trimer$^-$**	**2 HCN + monomer$^-$ ⟶ trimer$^-$**	**HCN + dimer$^-$ ⟶ trimer$^-$**
***E*0**	−46.8	−26.6	−12.0
***H*298**	−45.5	−25.1	−11.1
***G*298**	−24.4	−12.4	−4.9

Table S9. Reaction energies (pbe0/aug-cc-pVTZ) for the stepwise formation of solvates in kcal/mol (for the experimentally observed isomers + solvation of a third HCN solvate).

M3 C1	**HCN + NCS^- ⟶ monomer$^-$**		
***E*0**	−20.2		
***H*298**	−19.4		
***G*298**	−12.0		
D1 C1	**2 HCN + NCS^- ⟶ dimer$^-$**	**HCN + monomer$^-$ ⟶ dimer$^-$**	
***E*0**	−34.2	−14.0	
***H*298**	−32.9	−13.5	
***G*298**	−19.2	−7.2	
T1 C1	**3 HCN + NCS^- ⟶ trimer$^-$**	**2 HCN + monomer$^-$ ⟶ trimer$^-$**	**HCN + dimer$^-$ ⟶ trimer$^-$**
***E*0**	−46.8	−26.6	−12.6
***H*298**	−45.5	−25.1	−11.7
***G*298**	−24.4	−12.4	−5.2

Isomers of $[P(CN{\cdot}HCN)_2]^-$

Table S10. Absolute energies in a.u and relative energies in kcal/mol. Red: Energetically preferred isomer.

isomer	symmetry	connectivity	# bonds HC HN	# bridges HC HN	E0	H298	G298	ΔE0	ΔH298	ΔG298
1	**C2v**	P(CN HCN)$_2$	2	2	-713.582143	-713.516176	-713.572563	0.00	0.00	0.00
2	**Cs**	P(CN)$_2$ HCN HCN	2	2	-713.576392	-713.510526	-713.567165	3.61	3.55	3.39
3	**Cs**	P(NC HCN)$_2$	2	2	-713.514572	-713.449738	-713.506767	42.40	41.69	41.29
4	**Cs**	P(CN HCN) (NC HCN)	2	1 1	-713.546927	-713.481522	-713.538566	22.10	21.75	21.33
5	**Cs**	(NCH)$_2$ P(CN)$_2$	2		-713.572156	-713.506666	-713.565751	6.27	5.97	4.27

Starting compounds

Table S11. Absolute energies of starting materials in a.u.

compound	PG	E^{tot}	H^{298}	G^{298}	Compound	PG	E^{tot}	H^{298}	G^{298}
CN^-	Coov	−92.774938	−92.766741	−92.789078	HN_3	Cs	−164.6669066	−164.643116	−164.670191
N_3^-	Dh	−164.113381	−164.098688	−164.122764	HOCN	Cs	−168.518954	−168.492866	−168.520233
OCN^-	Cv	−168.007184	−167.992658	−168.017542	HNCO	Cs	−168.564999	−168.539289	−168.566347
SCN^-	Cv	−490.915929	−490.903212	−490.929601	HSCN	Cs	−491.422369	−491.400819	−491.430127
OCP^-	Cv	−454.524878	−454.512572	−454.538925	HNCS	Cs	−491.444115	−491.420798	−491.449204
$[P(CN)_2]^-$	C2v	−526.844834	−526.821755	−526.855597	HOCP	Cs	−455.024182	−455.000634	−455.029416
HCN	Cv	−93.344219	−93.324305	−93.347142	HPCO	Cs	−455.057902	−455.037532	−455.066792
CH_2O	Cs	−114.416980	−114.386507	−114.411969					

Reaction energies of X^- + HCN → CN^- + HX

Table S12. Reaction energies (pbe0/aug-cc-pVTZ) in kcal/mol.

reaction	ΔE^{tot}	$\Delta_R H^{298}$	$\Delta_R G^{298}$
N_3^- + HCN → CN^- + HN_3	9.89	8.24	6.67
OCN^- + HCN → CN^- + HNCO	7.20	6.86	5.81
OCN^- + HCN → CN^- + HOCN	36.09	35.99	34.75
SCN^- + HCN → CN^- + HNCS	25.79	25.09	24.13
SCN^- + HCN → CN^- + HSCN	39.43	37.62	36.11
OCP^- + HCN → CN^- + HPCO	22.75	20.46	18.95
OCP^- + HCN → CN^- + HOCP	43.91	43.61	42.40
OCP^- + 2 HCN → $[P(CN)_2]^-$ + CH_2O	−30.43	−29.54	−21.56
OCP^- + 4 HCN → $[P(CN{\cdot}HCN)_2]^-$ + CH_2O	−61.10	−58.29	−35.79
$[P(CN)_2]^-$ + 2 HCN → $[P(CN{\cdot}HCN)_2]^-$	−30.67	−28.75	−14.23

Structural parameter of computed isomers

Table S13. Bond length and bond angles of selected calculated (energetically preferred) isomers.

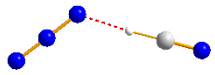
$N_3(HCN)_3$ t17	N1–C1	N1–C2	N3–C3	N1–N2–C3
(non–planar)	2.941 Å	2.941 Å	2.971 Å	174.4°
$OCN(HCN)_3$ t17	N1–C1	N1–C2	O1–C3	C4–O1–C3
(non–planar)	2.933 Å	2.933 Å	2.888 Å	136.2°
$NCO(HCN)_3$ t18	O1–C1	O1–C2	N1–C3	C2–N1–C3
(planar)	2.902 Å	2.902 Å	2.905 Å	180.0°
$SCN(HCN)_2$ d7	N1–C1	N1–C2		
(planar)	2.956 Å	2.956 Å		
NCH–(SCN)–HCN	S1–C1	N1–C2	C1–S1–C3	C3–N1–C2
d1 (planar)	3.408 Å	2.926 Å	92.7°	174.7

Optimized structures (pbe0-D3/aug-cc-pVTZ)

$[N_3(HCN)_n]^-$

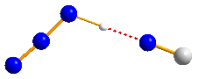
M1

C	1.98560000	-0.00030000	0.00020000
N	-2.57290000	-0.61850000	-0.00010000
N	-1.64370000	0.07800000	0.00010000
N	-0.70820000	0.80050000	-0.00010000
N	3.09700000	-0.30090000	-0.00010000
H	0.88090000	0.28780000	0.00030000



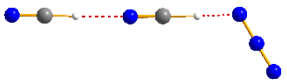
M2

N	-2.32605800	-0.69093200	-0.00006000
N	-1.46361100	0.05573500	0.00006600
N	-0.61442000	0.90255300	0.00005400
H	0.45496200	0.50487300	-0.00020300
N	1.83359600	0.01056400	-0.00037900
C	2.92308300	-0.40838600	0.00040500



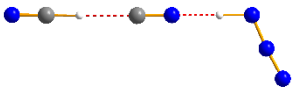
D1

C	-0.00480000	-0.00960000	-4.39274300
C	-0.00160000	-0.00480000	-0.20842900
N	-0.03680000	-0.08320000	4.89344600
N	0.00480000	0.00960000	3.73273800
N	0.05120000	0.11360000	2.55532900
N	0.00000000	0.00000000	-5.54043200
N	-0.01280000	-0.02720000	-1.35751100
H	-0.00800000	-0.01760000	-3.30103300
H	0.00640000	0.01440000	0.92308200



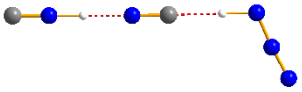
D2

C	-4.18123200	-0.13489600	-0.01688000
N	4.08731800	-0.94528700	0.00055800
N	3.34523500	-0.08479000	0.00754700
N	2.64316500	0.89651800	0.01382100
N	-5.32584000	-0.23673800	0.03123700
H	-3.06484100	-0.03230500	-0.03515000
H	1.58171200	0.65360400	0.00529700
N	0.01924100	0.27933400	-0.01201100
C	-1.13555400	0.13746900	-0.02615400



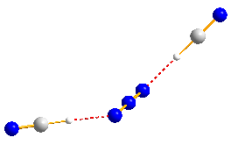
D3

N	-3.96746800	-1.00075700	0.00134700
N	-3.27331400	-0.10186100	-0.00376800
N	-2.61359700	0.90783200	-0.00952100
H	2.84005400	-0.01440600	0.00163500
H	-1.53672000	0.70591200	0.00259500
C	0.14552800	0.39182700	0.01799700
N	1.29222400	0.21171900	0.00428700
N	3.91229800	-0.16790600	-0.00229600
C	5.06208300	-0.33094300	-0.00709200



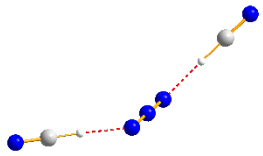
D4

N	-4.38255900	-0.63562500	0.00039600
N	-3.39361900	-0.04726700	-0.00079700
N	-2.39399400	0.56967500	-0.00220600
H	3.07210500	-0.00856100	0.00713600
H	-1.00935400	0.37867300	-0.00143200
N	4.11905700	-0.13148700	0.00143400
C	5.27225100	-0.26384300	-0.00420100
C	1.28425300	0.15545800	0.00299700
N	0.13657600	0.28473100	0.00139100



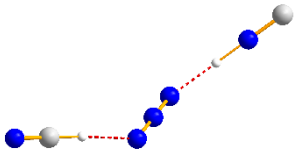
D5

N	-4.93874300	-0.12999800	-0.18173000
H	2.72894700	-0.22011700	0.00273900
N	-0.01020800	-0.03397200	0.17750700
N	-0.98809800	0.59397100	0.20560800
N	0.98387700	-0.64503000	0.15506900
N	4.94013700	0.19733700	-0.18542100
C	3.81652800	-0.02391800	-0.08869300
C	-3.80509500	0.04586100	-0.10806800
H	-2.70629700	0.21230600	-0.01940600



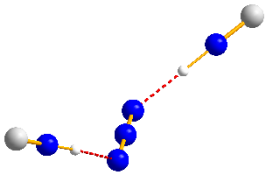
D6

H	2.64763500	-0.20588300	0.03911800
N	-0.12018100	0.09085200	0.10590800
N	-1.11053600	0.71454100	0.06339100
N	0.87922300	-0.50516800	0.15374400
N	4.88040800	0.06181800	-0.12793500
C	3.74355100	-0.08151400	-0.04293000
H	-2.60318700	0.21646200	-0.03377200
C	-4.77729600	-0.30520400	-0.10572100
N	-3.64919700	-0.03208200	-0.06845700



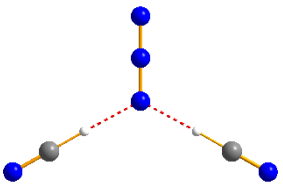
D7

H	-2.21114200	0.10261200	0.02775800
N	0.00166200	1.28068600	0.03078500
N	1.16703400	1.30011900	-0.00932500
N	-1.16536700	1.30318700	-0.01330900
H	2.20770200	0.09225000	-0.05175800
C	3.75325200	-1.50863400	0.01733800
N	2.95750700	-0.66278900	-0.01574000
N	-2.96430100	-0.65770900	-0.00410200
C	-3.74863600	-1.51458600	0.00030300



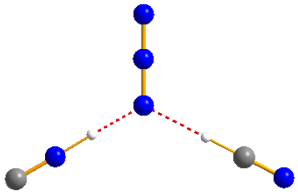
D8

C	-2.05161495	-1.79780401	-0.58847575
C	-6.25727342	0.64821573	-0.58847575
N	-3.45737342	0.64821573	-0.58847575
N	-2.78209911	1.82319303	-0.58847575
N	-2.16821338	2.89135421	-0.58847575
N	-1.48621224	-2.78160473	-0.58847575
N	-7.42497342	0.64821573	-0.58847575
H	-2.65015354	-0.75634686	-0.58847575
H	-5.05607342	0.64821573	-0.58847575



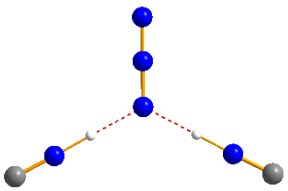
D9

C	-2.21661495	-1.79780401	-0.58847575
N	-3.62237342	0.64821573	-0.58847575
N	-2.94709911	1.82319303	-0.58847575
N	-2.33321338	2.89135421	-0.58847575
N	-1.65121224	-2.78160473	-0.58847575
H	-2.81515354	-0.75634686	-0.58847575
H	-5.22107342	0.64821573	-0.58847575
N	-6.42227342	0.64821573	-0.58847575
C	-7.56227342	0.64821573	-0.58847575



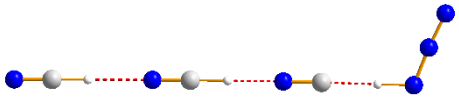
D10

N	-3.52271665	0.47481294	-0.58847575
N	-2.84744234	1.64979024	-0.58847575
N	-2.23355661	2.71795142	-0.58847575
H	-2.71549677	-0.92974965	-0.58847575
H	-5.12141665	0.47481294	-0.58847575
N	-6.32261665	0.47481294	-0.58847575
C	-7.46261665	0.47481294	-0.58847575
C	-1.54891456	-2.95960270	-0.58847575
N	-2.11695818	-1.97120680	-0.58847575



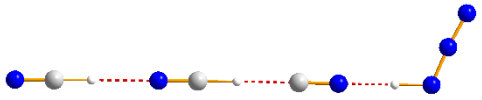
T1

C	2.08232400	-0.14010000	-0.00023800
C	-1.89178700	-0.51466800	0.00007300
N	-5.87590400	1.19836900	0.00000200
N	-5.25695200	0.24595200	0.00001300
N	-4.67988300	-0.81296900	0.00008900
N	-0.73595900	-0.39497700	0.00009100
H	0.95295400	-0.23970000	-0.00010000
H	-3.58797200	-0.69892800	0.00006400
C	6.27337000	0.20984600	0.00008300
N	3.22639200	-0.04046800	-0.00037300
N	7.41715100	0.30211500	0.00026700
H	5.18765700	0.12199900	-0.00009300



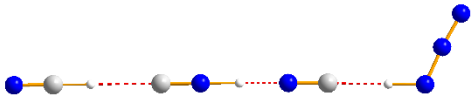
T2

C	-2.14372900	-0.14650100	0.00007800
N	5.85736200	1.21901800	0.00003100
N	5.23436900	0.27129800	-0.00006500
N	4.66831000	-0.79533500	-0.00019700
H	-1.00066500	-0.25001300	0.00014800
H	3.59663200	-0.70095300	-0.00009400
C	-6.33096900	0.21522000	-0.00006100
N	-3.28828800	-0.04430700	0.00001400
N	-7.47447200	0.31128900	-0.00008700
H	-5.24507900	0.12381900	-0.00003700
N	1.95777400	-0.54209900	0.00008600
C	0.80198600	-0.42070100	0.00023500



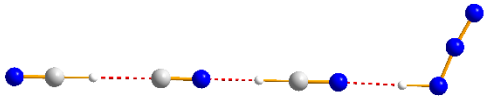
T3

N	5.79490400	1.19747100	-0.00008200
N	5.17314400	0.24946200	0.00022900
N	4.60084900	-0.81520200	0.00068200
H	-0.80733500	-0.25516000	-0.00048200
H	3.52814700	-0.70317100	0.00058300
C	-6.24730200	0.21817400	0.00031100
N	-7.39144400	0.31381200	0.00065600
H	-5.15336300	0.12638100	-0.00003000
C	-3.09850800	-0.04946400	-0.00058400
C	1.76619200	-0.50384600	-0.00012300
N	-1.94491600	-0.15180800	-0.00064200
N	0.61178700	-0.38762500	-0.00051400



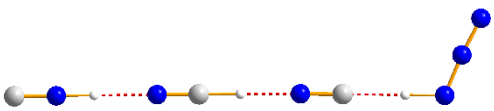
T4

N	5.85452900	1.20517800	0.00003200
N	5.22881200	0.26536400	-0.00007700
N	4.67402600	-0.81597000	-0.00021600
H	-0.47139300	-0.28824100	0.00006100
H	3.63776300	-0.71863300	0.00020200
H	-5.22271400	0.12148900	0.00000200
C	-6.33694900	0.21295400	-0.00006300
C	-3.28128600	-0.03985400	0.00007100
C	0.66848100	-0.39534200	0.00011500
N	-7.48279700	0.30632700	-0.00011400
N	-2.12122900	-0.13861000	0.00009000
N	1.81164000	-0.50531200	0.00014100



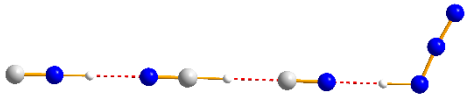
T5

N	5.79336000	1.18751600	0.00004300
N	5.17145900	0.23768000	-0.00008900
N	4.59305100	-0.82123300	-0.00017800
H	-1.00970700	-0.23356000	-0.00005200
H	3.50663000	-0.70526500	0.00012300
H	-5.02409800	0.12439200	-0.00003700
C	1.79446600	-0.51285400	0.00038100
N	0.63889000	-0.39048700	0.00002800
N	-6.05698700	0.21286400	-0.00001600
N	-3.29164600	-0.02639800	-0.00007400
C	-7.21397700	0.31142400	0.00002400
C	-2.14877600	-0.12943000	-0.00007500



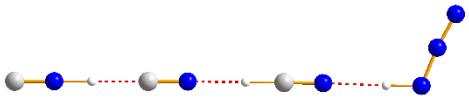
T6

N	5.76640300	1.21116300	0.00004000
N	5.14323300	0.26412400	-0.00008300
N	4.57810300	-0.80376600	-0.00025900
H	-1.04721000	-0.24531100	0.00021200
H	3.51011200	-0.70877100	-0.00008900
H	-5.07480200	0.12679500	-0.00003600
C	0.70264500	-0.41817800	0.00027000
N	1.85732500	-0.54431700	0.00010600
C	-7.26506600	0.32207300	-0.00015500
C	-2.20503800	-0.13580800	0.00013500
N	-6.10846000	0.21919500	-0.00009300
N	-3.34850900	-0.02943200	0.00006300



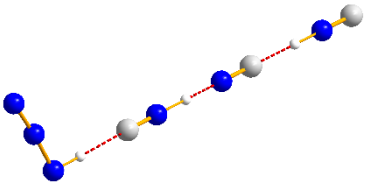
T7

N	5.79137600	1.19396900	-0.00001600
N	5.16382100	0.25580500	0.00004200
N	4.60753600	-0.82545400	0.00013200
H	-0.53730100	-0.28091800	-0.00009900
H	3.57330500	-0.72571300	0.00006300
H	-5.03993400	0.12029800	-0.00000100
C	0.59064300	-0.39004100	-0.00008200
N	1.73286500	-0.50276200	-0.00006700
C	-7.29403400	0.31263500	0.00011900
N	-6.13599400	0.21405900	0.00005400
N	-2.22700800	-0.12344300	-0.00010500
C	-3.38398300	-0.02240900	-0.00007800



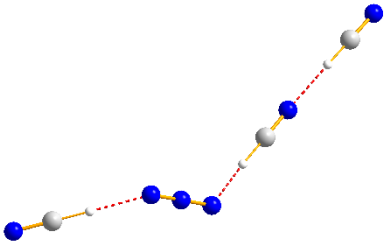
T8

N	5.74509300	1.18011500	-0.00000400
N	5.11763800	0.23955000	-0.00021900
N	4.54985200	-0.83247100	-0.00048800
H	-0.66275800	-0.26555400	0.00094400
H	3.50073300	-0.72046700	-0.00092100
H	-4.94140500	0.12407100	-0.00022100
C	-7.17158300	0.31976600	-0.00058800
N	-6.01417100	0.21844600	-0.00040900
N	-2.06834800	-0.13328100	0.00041500
C	-3.22300800	-0.02864100	0.00010700
C	1.63213800	-0.49314700	0.00052900
N	0.48110000	-0.37606200	0.00069200



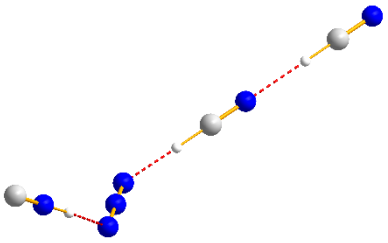
T9

H	4.37642100	-0.30970200	0.21678400
N	1.84369100	0.83970400	0.14707100
N	0.90435000	1.28192400	-0.39701700
N	2.78197900	0.41639800	0.69182000
N	6.38969800	-1.20219000	-0.26674800
C	5.36438700	-0.74814200	-0.01671200
H	-0.67731200	0.77747400	-0.25456200
C	-5.84197900	-0.55929200	0.03930300
H	-4.78445400	-0.30368700	-0.01388900
N	-6.95637000	-0.82729700	0.09472100
N	-2.87862000	0.17595400	-0.11831000
C	-1.77370000	0.48151300	-0.19077500



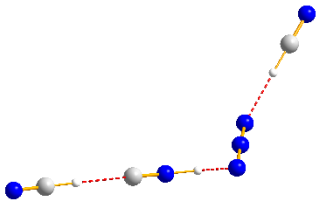
T10

H	-4.21152600	-0.25846800	-0.27188400
N	-1.99669300	0.91915400	-0.10581900
N	-1.03754300	1.22618200	0.48343200
N	-2.95780600	0.63793400	-0.70671600
H	0.58613900	0.72631900	0.29931700
C	5.76584000	-0.53274700	-0.07174400
H	4.70670500	-0.29322300	-0.00510600
N	6.88324800	-0.78382600	-0.14145100
N	2.78248200	0.16396200	0.12536800
C	1.67424900	0.44889500	0.21750800
C	-5.99305500	-1.48346300	0.27491900
N	-5.06847700	-0.84494100	-0.01859000



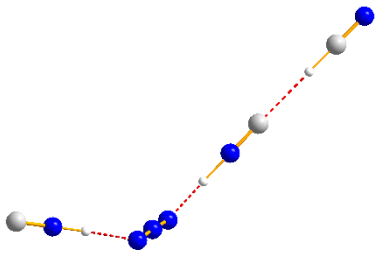
T11

H	4.20880400	-0.43602900	0.17170000
N	1.70340800	1.00690800	0.14963600
N	0.78376700	1.58302600	-0.30886100
N	2.62605800	0.47451700	0.59855700
H	-0.51729800	1.07625500	-0.23234200
C	-5.67576400	-0.73686300	0.03294000
H	-4.63518200	-0.38879100	-0.01692400
N	-6.76418000	-1.09880800	0.08461500
N	6.14876700	-1.48916500	-0.23491000
N	-1.60940000	0.69092900	-0.18445800
C	5.15594200	-0.95223200	-0.02436600
C	-2.69272200	0.28521500	-0.11765600



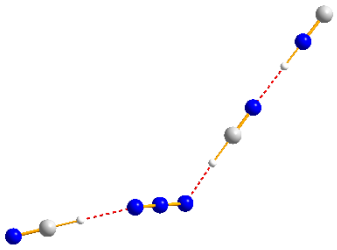
T12

H	-4.07367300	0.37062900	0.24813000
N	-1.86419900	-0.97433800	0.14725700
N	-0.93741700	-1.42290100	-0.41118800
N	-2.79590500	-0.56582400	0.70668600
H	0.45485800	-0.93226200	-0.29473700
C	5.66036600	0.63572800	0.05986800
H	4.60829900	0.33903700	-0.00694400
N	6.76376200	0.94465500	0.12922600
N	1.51604400	-0.60336100	-0.22930400
C	2.61527200	-0.25009300	-0.14259100
C	-5.83677700	1.59575400	-0.30074800
N	-4.91409100	0.95523600	-0.00633700



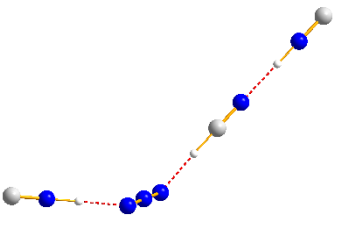
T13

H	4.28656100	-0.31339100	0.20379700
N	1.73011400	0.84690300	0.14912500
N	0.79487900	1.32640400	-0.37283600
N	2.66319800	0.38852000	0.67040200
H	-0.73526000	0.80237800	-0.24293400
H	-4.60613100	-0.31600600	-0.01761900
N	-5.60537400	-0.58798000	0.03496200
N	-2.93493700	0.15167100	-0.11107100
N	6.31547900	-1.16991900	-0.26674700
C	-6.72504100	-0.89016600	0.09271100
C	-1.83737200	0.48049600	-0.18115000
C	5.28096600	-0.73402700	-0.02324300



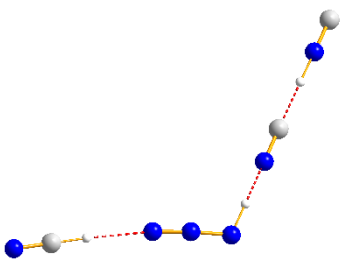
T14

H	-4.12177000	0.25644400	0.26658700
N	-1.88520100	-0.92369200	0.11091000
N	-0.93097500	-1.25354400	-0.47640500
N	-2.84016200	-0.62065900	0.70803900
H	0.64561800	-0.73417900	-0.29872100
H	4.53152200	0.30509900	0.00164300
N	5.53329600	0.55322600	0.07225400
N	2.83919900	-0.12872500	-0.12375200
C	6.65858600	0.82897600	0.15035300
C	1.73745800	-0.43443900	-0.21619200
C	-5.92346200	1.44249200	-0.28288300
N	-4.98628000	0.82346000	0.01221300



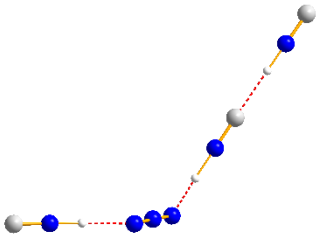
T15

H	4.19604300	-0.53865000	0.00099400
N	1.51521800	1.11090500	0.00144100
N	0.59938300	1.87886500	-0.00180100
N	2.44373800	0.45186400	0.00449000
H	-0.40679300	1.40679800	-0.00183800
H	-4.37404500	-0.44375500	-0.00033100
N	-5.36425500	-0.89184200	0.00025200
C	-6.42416300	-1.36807700	0.00090800
N	-1.78460000	0.76226900	-0.00181100
N	6.18517100	-1.54407100	-0.00181700
C	-2.83239000	0.26389100	-0.00122700
C	5.16025500	-1.02920100	-0.00036400



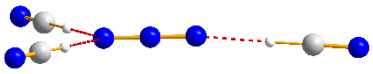
T16

H	3.97106700	-0.38131700	0.23186300
N	1.72883900	0.99367600	0.15141100
N	0.81007500	1.48776300	-0.38798200
N	2.65196000	0.54652500	0.68747600
H	-0.49441500	0.98364200	-0.28672900
H	-4.38530600	-0.35719300	-0.01182200
N	-5.38276300	-0.68229100	0.05644800
C	-6.48622900	-1.03748300	0.13082800
N	-1.58441500	0.60785100	-0.22160500
C	-2.67028000	0.21983300	-0.13462600
C	5.75791100	-1.56591600	-0.30125500
N	4.81919700	-0.94548500	-0.01474800



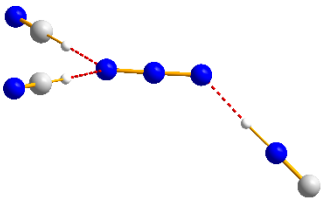
T17

C	2.50621700	-2.41486400	-0.02080000
C	-2.49078700	-2.42980400	-0.02080000
N	0.00307300	-0.87085300	0.00320000
N	0.00000000	0.30707400	0.05920000
N	3.47527100	-3.03170600	-0.02880000
N	-3.45611000	-3.05247300	-0.02880000
H	1.57499100	-1.81727000	-0.01120000
H	-1.56318600	-1.82660700	-0.01120000
C	-0.01511400	4.43251100	-0.02240000
N	-0.00295500	1.46416500	0.11840000
N	-0.01969900	5.58053500	-0.06720000
H	-0.01076200	3.33961900	0.01760000



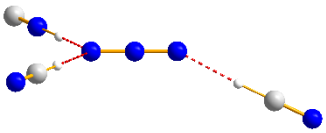
T18

C	-2.25048800	2.48049100	-0.15691500
C	-2.26441400	-2.47447500	-0.15670900
N	-0.65629700	-0.00165200	0.16866200
N	0.45731300	-0.00083400	0.53556600
N	-2.88745700	3.42802100	-0.28010500
N	-2.90715600	-3.41811800	-0.27974700
H	-1.63803400	1.57280900	-0.03598700
H	-1.64642500	-1.57060600	-0.03571000
N	1.55274600	0.00013700	0.92193100
H	3.03816600	-0.00350300	0.19927100
N	4.00490200	-0.00565700	-0.22011400
C	5.06455800	-0.00801100	-0.69486300



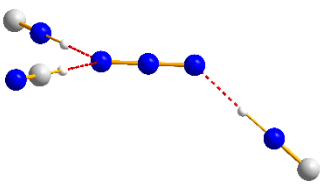
T19

N	-0.88059800	0.13073800	0.12169400
N	0.26923800	0.07483500	0.38076200
H	-1.65448000	1.54747400	-0.02905800
H	-1.87760100	-1.43433900	-0.02588100
N	1.39128100	0.00721700	0.64440300
H	3.20685300	-0.08073600	0.11502500
C	-2.75866500	3.47021700	-0.23922600
N	-2.19001200	2.46305800	-0.13211000
C	4.26932500	-0.13828300	-0.13640900
N	5.38394600	-0.19949800	-0.40406600
N	-3.09812300	-3.31803600	-0.20083800
C	-2.47814200	-2.35536600	-0.11253400



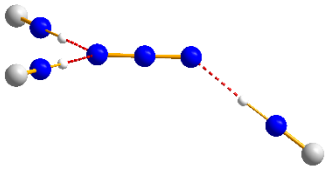
T20

C	-2.38541200	-2.33200700	-0.13995700
N	-0.72425900	0.13317500	0.15432800
N	0.39610700	0.07791800	0.50492400
N	-3.03096700	-3.27538700	-0.24734100
H	-1.53482200	1.55666100	-0.04174100
H	-1.76378400	-1.43178800	-0.03416100
N	1.49196300	0.01192200	0.87143900
H	3.02159800	-0.08783600	0.18410900
N	3.99269100	-0.15477700	-0.20092000
C	5.06551400	-0.23025700	-0.63849700
C	-2.68019000	3.43916500	-0.30379100
N	-2.08588700	2.45022900	-0.17025000



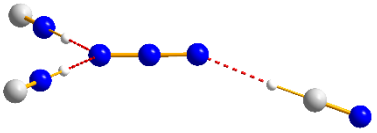
T21

N	-0.81434500	0.00003100	0.14438500
N	0.31660700	-0.00031100	0.47511400
H	-1.65539100	-1.43051100	-0.03827000
H	-1.65496700	1.43087100	-0.03827500
N	1.41769700	-0.00067600	0.81885400
H	2.99472300	-0.00056700	0.16934400
N	3.97455000	-0.00023200	-0.18226200
C	5.06436700	0.00022600	-0.58268400
C	-2.79238200	-3.31698200	-0.27119900
N	-2.20235500	-2.32362000	-0.15266400
N	-2.20170700	2.32411800	-0.15254600
C	-2.79156500	3.31759500	-0.27094300



T22

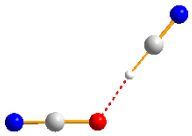
N	-0.96346800	0.00002400	0.10035900
N	0.20056500	-0.00049100	0.31112600
H	-1.77926800	-1.42158000	-0.02329000
H	-1.77835000	1.42215400	-0.02319900
N	1.33134000	-0.00101300	0.52452900
H	3.20213500	-0.00044000	0.08975700
C	-2.88883100	-3.33928600	-0.18773000
N	-2.31697300	-2.33181200	-0.10380000
N	-2.31548300	2.33272400	-0.10367300
C	-2.88667400	3.34058300	-0.18753400
N	5.40191900	-0.00025900	-0.31995800
C	4.27386700	-0.00035400	-0.10862800



$[OCN(HCN)_n]^-$

M1

C	-0.50674500	1.60161100	0.00000000
C	0.56057600	-1.86546600	0.00000000
H	0.00000000	-0.89329200	0.00000000
N	1.12908100	-2.86505100	0.00000000
N	-0.09505500	2.70481700	0.00000000
O	-0.94514600	0.44975700	0.00000000

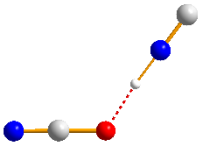


M2

C	0.00000000	0.00000000	1.75209700
C	0.00000000	0.00000000	-2.23166200
H	0.00000000	0.00000000	-1.09198400
N	0.00000000	0.00000000	-3.38305800
O	0.00000000	0.00000000	2.96040000
N	0.00000000	0.00000000	0.56679700

M3

C	-0.56205300	1.44635300	0.00000000
H	0.00000000	-0.83328800	0.00000000
N	0.64384300	-1.71780400	0.00000000
C	1.32389100	-2.65910700	0.00000000
N	-0.22788300	2.57174200	0.00000000
O	-0.93534400	0.26653100	0.00000000

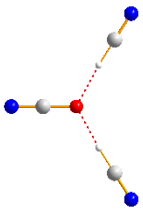


M4

C	0.00000000	0.00000000	1.61807900
H	0.00000000	0.00000000	-0.94638000
O	0.00000000	0.00000000	2.82080300
N	0.00000000	0.00000000	0.43685900
N	0.00000000	0.00000000	-2.10852700
C	0.00000000	0.00000000	-3.27114200

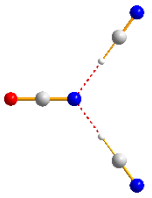
D1

C	0.00000000	0.00000000	1.70457600
C	0.00000000	2.47217600	-0.95112100
C	0.00000000	-2.47217600	-0.95112100
O	0.00000000	0.00000000	0.46370700
N	0.00000000	0.00000000	2.87699300
H	0.00000000	1.53504000	-0.36648500
H	0.00000000	-1.53504000	-0.36648500
N	0.00000000	3.44206600	-1.56640300
N	0.00000000	-3.44206600	-1.56640300



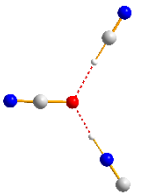
D2

C	0.00000000	0.00000000	1.78974300
H	0.00000000	1.43165600	-0.43498600
H	0.00000000	-1.43165600	-0.43498600
N	0.00000000	0.00000000	0.59743600
O	0.00000000	0.00000000	2.98751800
C	0.00000000	2.33346500	-1.09733800
N	0.00000000	3.26571300	-1.77018800
N	0.00000000	-3.26571300	-1.77018800
C	0.00000000	-2.33346500	-1.09733800



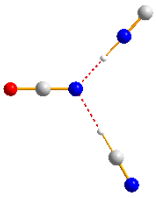
D3

C	-0.31830400	1.64531900	0.00000000
C	-2.08923400	-1.54404400	0.00000000
O	0.00000000	0.44226100	0.00000000
N	-0.62984500	2.77316300	0.00000000
H	-1.31270200	-0.76617400	0.00000000
H	1.48560500	0.03451300	0.00000000
N	-2.89652900	-2.36050100	0.00000000
N	2.49020300	-0.30987300	0.00000000
C	3.58758700	-0.68893300	0.00000000



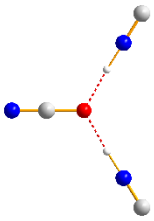
D4

C	-0.40517900	1.70344700	0.00000000
H	-1.14649400	-0.82909800	0.00000000
H	1.42125000	0.00836400	0.00000000
N	2.42945800	-0.41482900	0.00000000
C	3.50896800	-0.84389600	0.00000000
N	0.00000000	0.58195000	0.00000000
O	-0.82896900	2.81942000	0.00000000
C	-1.85238900	-1.68596700	0.00000000
N	-2.59394300	-2.56371100	0.00000000



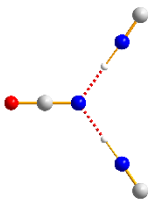
D5

C	0.00000000	0.00000000	1.63662500
O	0.00000000	0.00000000	0.38881800
N	0.00000000	0.00000000	2.80475000
H	0.00000000	1.37550100	-0.38289300
H	0.00000000	-1.37550100	-0.38289300
N	0.00000000	-2.26911100	-0.93959400
C	0.00000000	-3.25434900	-1.55362000
C	0.00000000	3.25434900	-1.55362000
N	0.00000000	2.26911100	-0.93959400



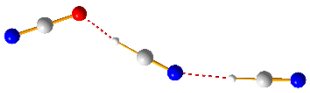
D6

C	0.00000000	0.00000000	1.67849100
H	0.00000000	1.29227300	-0.43764000
H	0.00000000	-1.29227300	-0.43764000
N	0.00000000	-2.16690500	-1.06478400
C	0.00000000	-3.12651500	-1.71890600
C	0.00000000	3.12651500	-1.71890600
N	0.00000000	2.16690500	-1.06478400
N	0.00000000	0.00000000	0.48430400
O	0.00000000	0.00000000	2.86850700



D7

C	0.00000000	0.19987900	0.00000000
C	-4.05719800	0.94706300	0.00000000
C	3.40236300	-0.89005200	0.00000000
O	2.23257400	-1.28856400	0.00000000
H	-2.96724400	0.91955300	0.00000000
H	1.00175400	-0.35517800	0.00000000
N	-5.20455800	0.97004800	0.00000000
N	-1.02313100	0.72330900	0.00000000
N	4.51824800	-0.52152900	0.00000000

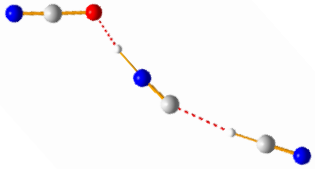


D8

C	0.00000000	0.00000000	-0.22374700
C	0.00000000	0.00000000	-4.38264100
C	0.00000000	0.00000000	3.66522400
H	0.00000000	0.00000000	-3.28714300
H	0.00000000	0.00000000	0.96144000
N	0.00000000	0.00000000	-5.53065800
N	0.00000000	0.00000000	-1.37515300
N	0.00000000	0.00000000	2.48046100
O	0.00000000	0.00000000	4.86876700

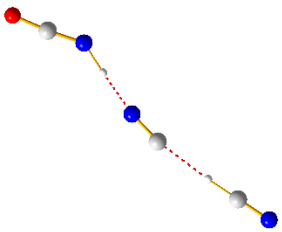
D9

C	3.25925300	0.95575900	0.00000000
H	-3.03304700	-0.70257800	0.00000000
H	1.15042400	0.19898400	0.00000000
C	-3.98260000	-1.25420600	0.00000000
C	-1.15383800	0.12537700	0.00000000
N	-4.96967600	-1.84067500	0.00000000
N	0.00000000	0.22513700	0.00000000
N	4.03407900	1.83309900	0.00000000
O	2.46186300	0.00238600	0.00000000



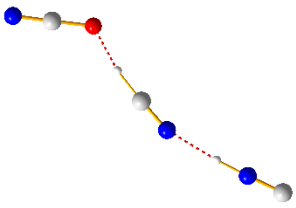
D10

C	2.60739900	-2.35366900	0.00000000
H	-2.34922800	2.22754200	0.00000000
H	0.89794000	-1.05894400	0.00000000
N	1.48420700	-1.97280800	0.00000000
O	3.69269300	-2.82772800	0.00000000
C	-3.27964500	2.84939100	0.00000000
C	-0.79498400	1.06578000	0.00000000
N	-4.23947400	3.48231200	0.00000000
N	0.00000000	0.21681100	0.00000000



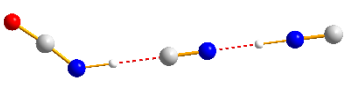
D11

C	2.66122200	-2.15746600	0.00000000
H	-2.23591100	1.98537800	0.00000000
H	0.71619300	-0.68029900	0.00000000
N	3.82542100	-2.31146600	0.00000000
O	1.43310800	-2.01052300	0.00000000
N	-3.16174200	2.45566400	0.00000000
N	-0.75724400	1.08916100	0.00000000
C	-4.20958700	2.95585800	0.00000000
C	0.00000000	0.22587200	0.00000000



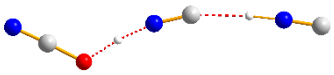
D12

C	-3.41045500	0.03776500	0.00030400
H	2.98140300	0.02266600	-0.00029100
H	-1.38723500	-0.55634800	-0.00005300
N	4.05646200	0.16288000	0.00027800
N	1.43261100	-0.18150000	-0.00093300
C	5.20811100	0.31247000	0.00072000
C	0.28313200	-0.34126600	-0.00114500
N	-2.47052600	-0.69338800	0.00095000
O	-4.40109000	0.68299100	-0.00012400



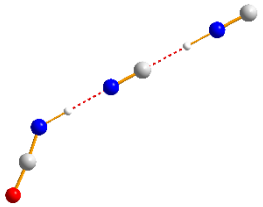
D13

C	-3.25653300	-0.35704200	0.00000000
H	2.90725400	0.48429200	0.00000000
H	-1.10891600	-0.25599300	0.00000000
N	3.95920900	0.35960500	0.00000000
C	5.10588300	0.17378000	0.00000000
C	1.12679200	0.51136500	0.00000000
N	0.00000000	0.24824500	0.00000000
N	-4.31468500	0.13671000	0.00000000
O	-2.14585800	-0.92610600	0.00000000



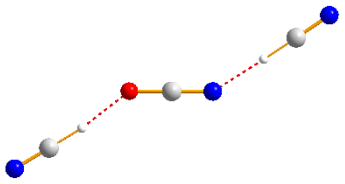
D14

C	-2.71141400	-2.01271300	0.00000000
H	2.46960100	1.74977400	0.00000000
H	-1.40444500	-0.36412400	0.00000000
N	3.44436600	2.27478600	0.00000000
C	4.46748500	2.82648000	0.00000000
N	-2.34222600	-0.88242000	0.00000000
O	-3.17992700	-3.09740900	0.00000000
C	1.02047700	0.97142000	0.00000000
N	0.00000000	0.41942000	0.00000000



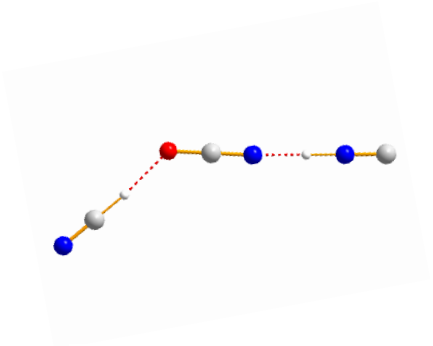
D15

C	1.23777700	3.71870800	0.00000000
H	-0.93585400	-2.60394700	0.00000000
N	1.39253000	4.85839300	0.00000000
O	-0.81763400	-0.87402900	0.00000000
N	-1.35343800	-4.81423400	0.00000000
N	0.79051900	0.90266700	0.00000000
C	-1.13883300	-3.68594000	0.00000000
C	0.00000000	0.02743300	0.00000000
H	1.07598700	2.60718500	0.00000000



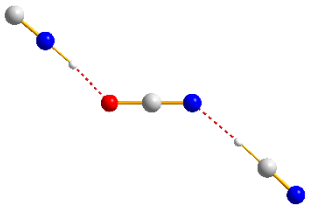
D16

C	-3.58679200	-0.60202200	0.00000000
H	2.62896200	0.11058700	0.00000000
N	-4.58959800	-1.16153900	0.00000000
C	0.00000000	0.64828200	0.00000000
H	-2.62748800	-0.06403700	0.00000000
N	3.70904700	-0.08398800	0.00000000
C	4.85271600	-0.28617100	0.00000000
N	1.14520300	0.38248000	0.00000000
O	-1.18119800	0.92928100	0.00000000



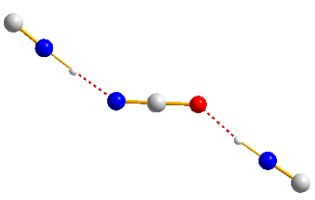
D17

C	0.82583100	-3.67826100	0.00000000
H	-0.69667700	2.50973600	0.00000000
N	0.80105100	-4.82772300	0.00000000
O	-0.82415200	0.97364800	0.00000000
N	0.78262900	-0.80652100	0.00000000
C	0.00000000	0.07250600	0.00000000
H	0.83647000	-2.56052200	0.00000000
N	-0.71943400	3.56731900	0.00000000
C	-0.75854700	4.72743400	0.00000000



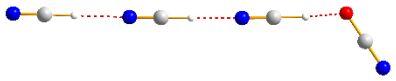
D18

H	-0.39130800	2.60139600	0.00000000
C	0.00000000	0.03264900	0.00000000
H	0.24282100	-2.58717900	0.00000000
N	-0.24510800	3.68159800	0.00000000
C	-0.04963300	4.82644700	0.00000000
N	-0.54004700	1.07722900	0.00000000
O	0.56488800	-1.04308100	0.00000000
N	0.14899000	-3.63008200	0.00000000
C	0.06339000	-4.78756100	0.00000000



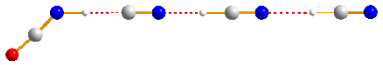
T1

C	0.27475900	1.99793700	0.00000000
C	-0.76334800	-1.98182500	0.00000000
C	1.95999600	5.01383000	0.00000000
O	0.78981700	4.60908200	0.00000000
H	-0.47075300	-0.92136900	0.00000000
H	0.54348100	3.12656500	0.00000000
N	0.00000000	0.88201800	0.00000000
N	3.06791500	5.40219900	0.00000000
C	-1.94383400	-6.07069500	0.00000000
N	-1.07141900	-3.08582000	0.00000000
N	-2.27097300	-7.17010400	0.00000000
H	-1.63536100	-5.03138100	0.00000000



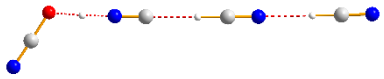
T2

C	1.77943100	-0.43063300	-0.00002700
C	-2.19912500	-0.11306800	0.00005300
C	5.44228900	0.15061500	0.00000000
H	-1.06850600	-0.19904700	0.00001600
H	3.45599500	-0.55605400	-0.00000900
N	0.62186300	-0.33058500	-0.00002600
N	4.54637400	-0.63407000	-0.00001500
O	6.39323100	0.85300000	-0.00000100
C	-6.39366400	0.19509700	-0.00000300
N	-3.34426800	-0.02658800	0.00008700
N	-7.53821000	0.27725300	-0.00007500
H	-5.30723400	0.11697000	0.00006600



T3

C	1.97621300	-4.86934200	0.00000000
H	-0.49033700	0.90137700	0.00000000
H	0.56625700	-3.27471100	0.00000000
C	-0.78533100	1.97713600	0.00000000
C	0.00000000	-0.97367200	0.00000000
N	0.27854300	-2.09749700	0.00000000
N	3.08127500	-5.24661200	0.00000000
O	0.78401000	-4.49789200	0.00000000
C	-1.95667900	6.05175900	0.00000000
N	-1.09252400	3.08239800	0.00000000
N	-2.28212800	7.15181400	0.00000000
H	-1.64936400	5.01045300	0.00000000

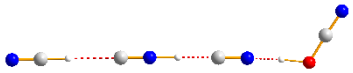


T4

C	-2.26672600	-0.10717900	-0.00184700
C	5.43493500	0.15792200	0.00211400
H	-1.12332700	-0.19068900	-0.00262700
H	3.44333300	-0.52428200	0.00156400
N	4.51457400	-0.59512300	0.00621600
O	6.41341300	0.82010400	-0.00088300
C	-6.46078700	0.18768700	0.00155300
N	-3.41276500	-0.02426800	-0.00108000
N	-7.60559400	0.26647600	0.00256300
H	-5.37383700	0.11277200	0.00060300
C	0.68640000	-0.32731500	-0.00377600
N	1.84429800	-0.42213100	-0.00494900

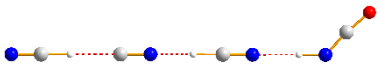
T5

C	2.09803600	-4.66802400	0.00000000
H	-0.46561300	0.71593100	0.00000000
H	0.66397100	-3.26417000	0.00000000
C	0.00000000	-0.83586700	0.00000000
N	0.31723400	-1.94795700	0.00000000
N	3.21146900	-5.00377700	0.00000000
O	0.87838900	-4.35751600	0.00000000
C	-2.13531900	5.91175900	0.00000000
N	-2.49621600	7.00135900	0.00000000
H	-1.79219500	4.87316200	0.00000000
C	-1.14526200	2.88223900	0.00000000
N	-0.79506000	1.77817000	0.00000000



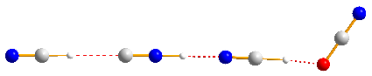
T6

C	-1.93488500	-5.04330700	0.00000000
H	0.00000000	0.62886500	0.00000000
H	-1.86586900	-3.00418300	0.00000000
N	-2.34449800	-3.92058800	0.00000000
O	-1.65457000	-6.18292400	0.00000000
C	2.67903900	5.86508500	0.00000000
N	3.20090300	6.88941000	0.00000000
H	2.17169900	4.86931800	0.00000000
C	-0.52595200	-0.39004500	0.00000000
N	-1.05376100	-1.40972600	0.00000000
N	0.75548900	2.09588700	0.00000000
C	1.28576500	3.13235200	0.00000000



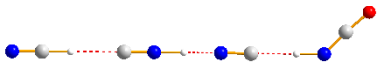
T7

C	2.07118700	-4.82785500	0.00000000
H	-0.46485500	0.78517000	0.00000000
H	0.60955200	-3.03761900	0.00000000
N	3.19028200	-5.17836700	0.00000000
O	0.88554400	-4.46345900	0.00000000
C	-2.10921900	5.96783800	0.00000000
N	-2.46690100	7.05809000	0.00000000
H	-1.77050000	4.93276600	0.00000000
C	-1.11835100	2.89925900	0.00000000
N	-0.77421700	1.79458400	0.00000000
N	0.00000000	-0.79125300	0.00000000
C	0.30593400	-1.89824600	0.00000000



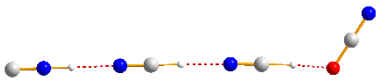
T8

C	3.04303900	-4.40925700	0.00000000
H	-0.67804600	0.65772800	0.00000000
H	1.37967300	-3.15266000	0.00000000
N	1.89310000	-4.09474500	0.00000000
O	4.14789400	-4.82228400	0.00000000
C	-3.29399000	5.45037700	0.00000000
N	-3.84588300	6.45716600	0.00000000
H	-2.76630200	4.48770400	0.00000000
N	-1.22275300	1.66128300	0.00000000
C	-1.77649900	2.67844100	0.00000000
C	0.54583000	-1.62025800	0.00000000
N	0.00000000	-0.59660800	0.00000000



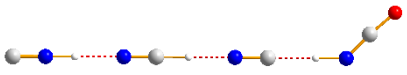
T9

C	2.10449400	-4.84516300	0.00000000
H	-0.52417500	0.95831900	0.00000000
H	0.62031900	-3.02861300	0.00000000
N	3.22797900	-5.18482600	0.00000000
O	0.91733900	-4.49136200	0.00000000
H	-1.75716000	4.80876700	0.00000000
N	0.00000000	-0.80012700	0.00000000
C	0.31253800	-1.90607900	0.00000000
C	-2.44718000	6.88602500	0.00000000
C	-0.85449500	2.01148600	0.00000000
N	-2.08039500	5.78401400	0.00000000
N	-1.20041800	3.10305400	0.00000000



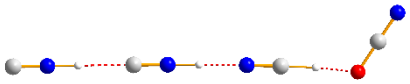
T10

C	2.93017300	-4.48560500	0.00000000
H	-0.75275800	0.85723800	0.00000000
H	1.29309900	-3.16720800	0.00000000
N	1.79204400	-4.13378600	0.00000000
O	4.02532100	-4.92910700	0.00000000
H	-2.59656000	4.44134000	0.00000000
C	0.51893400	-1.65719600	0.00000000
N	0.00000000	-0.61764000	0.00000000
N	-3.07243300	5.36228700	0.00000000
C	-3.60576200	6.39374100	0.00000000
C	-1.27483800	1.87500700	0.00000000
N	-1.79923800	2.89568300	0.00000000



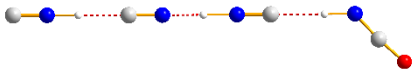
T11

C	2.23911600	-4.63260200	0.00000000
H	-0.52089100	0.81957100	0.00000000
H	0.70330100	-2.93564300	0.00000000
N	3.37419900	-4.92499000	0.00000000
O	1.03529400	-4.32968100	0.00000000
H	-1.91215200	4.67284500	0.00000000
N	0.00000000	-0.70798400	0.00000000
C	0.35131000	-1.80152700	0.00000000
C	-2.68033000	6.73311400	0.00000000
N	-2.27368900	5.64485600	0.00000000
N	-0.87490100	1.82168200	0.00000000
C	-1.26540800	2.90863700	0.00000000



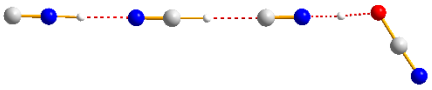
T12

C	-5.29066600	0.14740900	0.00020200
H	0.77371100	-0.22322500	-0.00046800
H	-3.36727600	-0.57041200	0.00037200
N	-4.41158800	-0.66150700	0.00054900
O	-6.23162400	0.85176200	-0.00006900
H	5.05298000	0.12032700	-0.00005900
C	-1.52693400	-0.41868200	0.00000700
N	-0.37444800	-0.31883600	-0.00023000
N	6.12584300	0.20431200	0.00029200
C	7.28414900	0.29470300	0.00079300
N	2.17551500	-0.10806500	-0.00074700
C	3.33117100	-0.01544700	-0.00072600



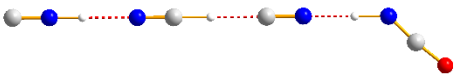
T13

C	2.10789100	4.69878700	0.00000000
H	-0.53897400	-0.92843900	0.00000000
H	0.65012300	3.20445400	0.00000000
N	3.22531800	5.03273300	0.00000000
O	0.89817000	4.37816000	0.00000000
H	-1.76043700	-4.78362400	0.00000000
C	-2.44240000	-6.86693100	0.00000000
N	-2.08050300	-5.76343200	0.00000000
N	-1.21645300	-3.09581400	0.00000000
C	-0.87227000	-2.00240000	0.00000000
C	0.00000000	0.88394600	0.00000000
N	0.31515300	1.99821600	0.00000000



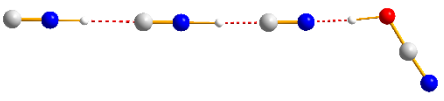
T14

C	5.34326500	-0.15107600	0.00011000
H	-1.17023000	0.18538100	-0.00012600
H	3.35821100	0.53073800	0.00011600
N	4.42508400	0.60537100	0.00019600
O	6.32002900	-0.81453600	-0.00004500
H	-5.20370500	-0.11507100	0.00002200
N	-6.23839500	-0.19030700	0.00006100
C	-7.39653900	-0.27411900	0.00008000
C	-2.32796200	0.09779100	-0.00006500
C	0.58834700	0.32295600	-0.00018900
N	-3.47305900	0.01201400	-0.00000300
N	1.74534500	0.42176900	-0.00015000



T15

C	2.26572600	4.47324500	0.00000000
H	-0.49665000	-0.70219400	0.00000000
H	0.77790600	3.16819200	0.00000000
N	3.39202500	4.75732700	0.00000000
O	1.02882000	4.22391600	0.00000000
H	-1.93368200	-4.58985700	0.00000000
C	-2.72045800	-6.65682200	0.00000000
N	-2.30668300	-5.57137500	0.00000000
C	0.00000000	0.72283200	0.00000000
N	0.36525400	1.81861800	0.00000000
N	-0.89197900	-1.80177800	0.00000000
C	-1.29334400	-2.88709200	0.00000000

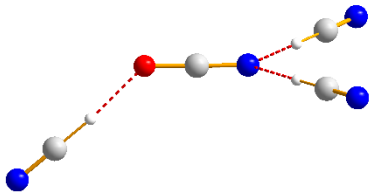


T16

C	3.12248800	-4.32615400	0.00000000
H	-0.55722300	0.40121300	0.00000000
H	1.45622900	-3.15582600	0.00000000
N	1.95732400	-4.05773400	0.00000000
O	4.22987900	-4.71289600	0.00000000
H	-2.78948100	4.32784600	0.00000000
N	-3.33445700	5.28223500	0.00000000
C	-3.91106100	6.29132700	0.00000000
C	0.00000000	-0.58720800	0.00000000
N	0.56249400	-1.58742500	0.00000000
N	-1.38962700	1.87292600	0.00000000
C	-1.96454400	2.88202200	0.00000000

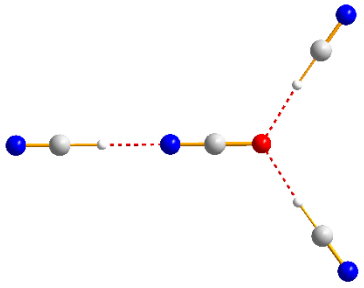
T17

C	2.42912300	2.30316800	-0.17429700
C	-0.46272200	-0.00027600	0.61884300
C	-4.20797500	0.00009500	-0.27722400
N	3.11716700	3.20803700	-0.34027000
N	-5.26520300	0.00031200	-0.72437600
H	-3.20072700	-0.00011200	0.15024000
H	1.76107900	-1.43561200	-0.01159700
H	1.76111900	1.43580000	-0.01149000
N	0.66692700	-0.00004700	0.26359400
O	-1.61254300	-0.00052000	0.98833600
N	3.11729200	-3.20775300	-0.34050200
C	2.42917400	-2.30294700	-0.17448200



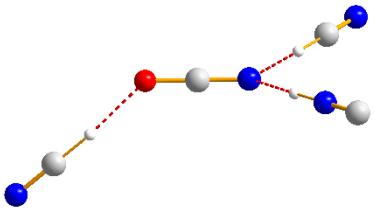
T18

C	0.00000000	2.43579200	2.42123900
C	0.00000000	-2.43579200	2.42123900
C	0.00000000	0.00000000	-0.38385500
C	0.00000000	0.00000000	-4.46209400
N	0.00000000	3.37082700	3.08698000
N	0.00000000	-3.37082700	3.08698000
N	0.00000000	0.00000000	-5.61125700
H	0.00000000	0.00000000	-3.35270800
H	0.00000000	1.54111600	1.78945800
H	0.00000000	-1.54111600	1.78945800
N	0.00000000	0.00000000	-1.55670700
O	0.00000000	0.00000000	0.84408100



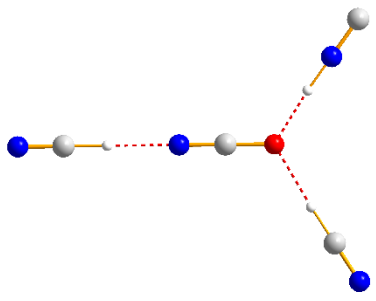
T19

C	-2.44997900	-2.19099200	-0.16060400
C	0.41781700	0.08707800	0.58849000
C	4.21249400	-0.04842000	-0.25923400
N	-3.10543000	-3.12198200	-0.31007100
N	5.28187000	-0.06519900	-0.67554000
H	3.19615100	-0.03295100	0.13784000
H	-1.71642600	1.40650600	-0.01115500
H	-1.81232700	-1.30555900	-0.01367700
N	-2.39535600	2.21317500	-0.18408400
C	-3.12235700	3.10025600	-0.36662900
N	-0.71244400	0.18672400	0.24893300
O	1.56303500	-0.03056800	0.94002400



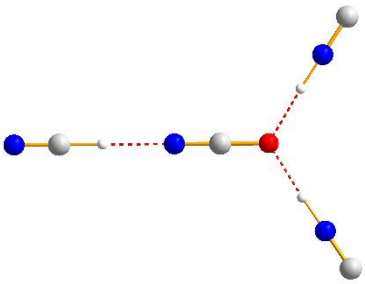
T20

C	-1.67702300	-2.98220400	0.00000000
C	0.00000000	0.34175500	0.00000000
C	-1.13304600	4.27275700	0.00000000
N	-2.43705900	-3.84204400	0.00000000
N	-1.45391600	5.37596400	0.00000000
H	-0.82477200	3.21027500	0.00000000
H	1.86800100	-1.29333800	0.00000000
H	-0.95210800	-2.16580300	0.00000000
N	-0.32443900	1.46636700	0.00000000
O	0.33088700	-0.84460000	0.00000000
N	2.85217600	-1.64790100	0.00000000
C	3.94414500	-2.04248000	0.00000000



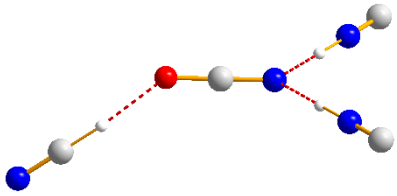
T21

C	0.00000000	0.00000000	-0.28179900
C	0.00000000	0.00000000	-4.38539900
N	0.00000000	0.00000000	-5.53411600
H	0.00000000	0.00000000	-3.28169900
H	0.00000000	1.40179200	1.78753800
H	0.00000000	-1.40179200	1.78753800
N	0.00000000	2.27123900	2.35893000
C	0.00000000	3.24206500	2.99572700
N	0.00000000	-2.27123900	2.35893000
C	0.00000000	-3.24206500	2.99572700
N	0.00000000	0.00000000	-1.45028900
O	0.00000000	0.00000000	0.95336300



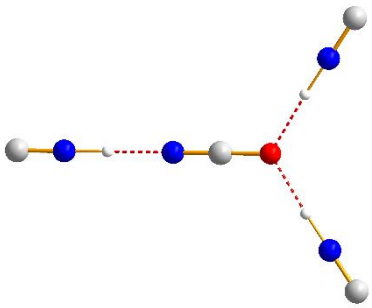
T22

C	0.33844600	-0.00041600	0.56367400
C	4.18137000	-0.00106100	-0.24054600
N	5.26013000	-0.00143000	-0.63166500
H	3.15839100	-0.00065100	0.13212800
H	-1.76168000	1.30951200	-0.01827200
H	-1.76350500	-1.30921700	-0.01782200
N	-2.37974200	2.15453800	-0.17379600
C	-3.04208000	3.09415200	-0.33776400
N	-0.79957500	-0.00086000	0.22901000
O	1.48736100	0.00007600	0.90878700
N	-2.38310900	-2.15320700	-0.17360900
C	-3.04707200	-3.09159900	-0.33801600



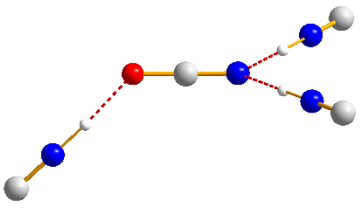
T23

C	0.00000000	0.00000000	-0.37356100
H	0.00000000	0.00000000	-3.15420000
H	0.00000000	1.40756500	1.71878600
H	0.00000000	-1.40756500	1.71878600
N	0.00000000	2.26499400	2.30141700
C	0.00000000	3.22563500	2.95355100
N	0.00000000	-2.26499400	2.30141700
C	0.00000000	-3.22563500	2.95355100
N	0.00000000	0.00000000	-1.54071500
O	0.00000000	0.00000000	0.85724600
N	0.00000000	0.00000000	-4.21625400
C	0.00000000	0.00000000	-5.37727400



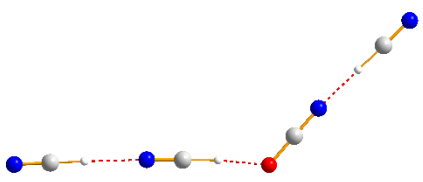
T24

C	0.45166100	0.00024000	0.60789100
H	3.01408500	0.00076500	0.16963200
H	-1.66683800	-1.30855100	-0.01880700
H	-1.66934800	1.30834000	-0.01849700
N	-2.29604700	-2.13797200	-0.17789100
C	-2.97688800	-3.06358600	-0.34542000
N	-2.30029500	2.13643100	-0.17769500
C	-2.98308700	3.06059900	-0.34525700
N	3.94384300	0.00138200	-0.28702600
C	4.98642800	0.00233500	-0.79762900
N	-0.67390400	0.00085800	0.24369100
O	1.59227900	-0.00037200	0.99282700



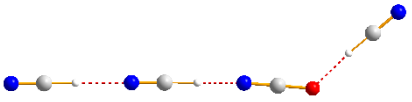
T25

C	-1.77643600	0.56226400	0.00041500
C	1.82666000	0.96880700	-0.00005500
C	-5.80642100	-0.69232200	-0.00040400
C	5.43314900	-0.87450800	-0.00027000
N	-6.90940200	-1.00831400	-0.00003000
N	-2.86226200	0.19108800	0.00052300
N	2.83957300	0.37178100	0.00039300
N	6.47212700	-1.36661800	0.00006400
H	-4.76156000	-0.39074200	-0.00068400
H	-0.71769700	0.92933300	0.00024600
H	4.42603800	-0.39500300	-0.00045400
O	0.77640700	1.59442600	-0.00048400



T26

C	1.92339600	0.16234200	-0.00000400
C	-1.97795300	0.77715100	-0.00006300
C	6.08242200	-0.35839300	0.00002700
C	-5.49788100	-0.60820200	-0.00001100
N	7.22174400	-0.49631300	-0.00000700
N	3.06296200	0.01369700	0.00010100
N	-6.47074600	-1.21833000	0.00002200
H	4.99942200	-0.22687200	0.00006800
H	0.78836700	0.31354900	-0.00010400
H	-4.56673300	-0.02237500	-0.00000600
O	-3.16543800	1.03257900	0.00019100
N	-0.82502500	0.53489900	-0.00028400

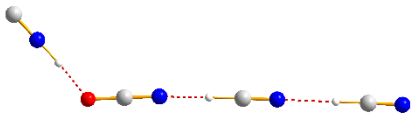


T27

C	1.87705300	-0.19354800	-0.00211100
C	-1.95157800	0.19137100	-0.00222900
C	6.07930200	-0.03193200	0.00124200
N	7.21433000	0.13481400	0.00468900
N	3.00990000	-0.37265600	-0.00274700
H	5.00459500	-0.18737100	-0.00124300
H	0.78614900	-0.00155800	-0.00077800
H	-4.60190000	-0.14460200	0.00064700
N	-5.69037600	-0.11204000	0.00257200
C	-6.85055100	-0.05944200	0.00465200
N	-3.07075200	-0.16650000	-0.00285300
O	-0.79448900	0.56369000	-0.00244700

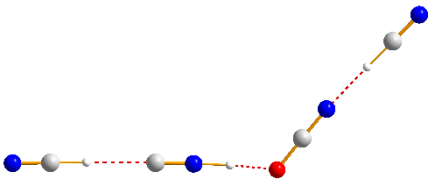
T28

C	-1.84008300	0.17225400	-0.01733400
C	2.08108100	0.78233600	-0.00002600
C	-6.00820500	-0.34117700	0.00765900
N	-7.14796300	-0.47440600	0.01644800
N	-2.97908900	0.02331000	-0.01390400
H	-4.92576100	-0.21395900	-0.00067000
H	-0.71343900	0.32351600	-0.01990600
H	4.43853800	-0.00542600	0.01072300
O	3.27406200	1.03253700	0.02264600
N	0.92799400	0.55637500	-0.02173000
N	5.27042000	-0.65341400	0.00470100
C	6.18531200	-1.36799300	-0.00195300



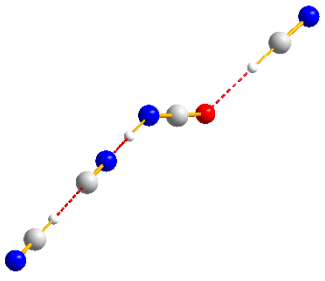
T29

C	-1.72579300	0.99366700	-0.00013900
C	5.74293200	-0.76791700	-0.00008100
N	6.83438900	-1.12309300	-0.00022100
H	4.70395500	-0.42689600	0.00008100
H	0.62249400	1.05395800	0.00013300
H	-4.31448000	-0.44303900	-0.00021600
N	-2.72228500	0.37621200	0.00005700
O	-0.69210500	1.65639200	-0.00027800
C	-5.30727300	-0.94006100	-0.00008700
N	-6.33632600	-1.45171100	0.00006600
N	1.64143900	0.66837000	0.00034700
C	2.72419300	0.26037800	0.00038600



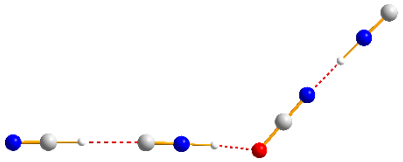
T30

C	1.74640500	0.45223400	0.00948900
C	-6.07571200	-0.22228100	-0.13525800
N	-7.21726300	-0.30155500	-0.23985100
H	-4.97291000	-0.14549300	-0.03393200
H	-0.47467700	0.18762000	0.38248700
H	4.58356600	-0.02191300	-0.18034300
C	5.61854300	-0.34096700	-0.09217800
N	6.71153800	-0.67691900	0.00169400
N	-1.84701800	0.07957300	0.26593400
C	-2.99977400	-0.00586000	0.15088400
N	0.68060700	0.28215800	0.47586500
O	2.85402400	0.62477900	-0.41141500



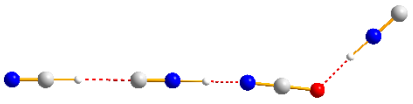
T31

C	-1.82488200	0.92844900	-0.00056200
C	5.72540200	-0.69862200	-0.00018500
N	6.82583000	-1.02457100	-0.00109400
H	4.67897800	-0.38562800	0.00069100
H	0.56454500	0.99514400	0.00029000
H	-4.20575600	-0.42486200	-0.00002700
N	1.58036600	0.63696700	0.00107400
C	2.67236900	0.25485300	0.00197300
N	-5.15727600	-0.92598900	0.00003900
C	-6.18711400	-1.46236600	0.00009900
N	-2.82285400	0.31602500	-0.00023700
O	-0.79186100	1.58305600	-0.00092300



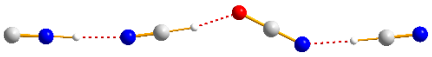
T32

C	-1.95836400	0.73082300	0.00011100
C	6.00725400	-0.32985100	0.00102100
N	7.14899100	-0.45117800	0.00213100
H	4.91527800	-0.21311300	-0.00004100
H	0.58779900	0.30077200	-0.00247500
H	-4.38710600	-0.00748500	0.00133500
N	1.71908500	0.15475000	-0.00233000
C	2.86859100	0.01498100	-0.00194500
N	-0.81076600	0.48993100	-0.00264600
O	-3.14264100	0.99247000	0.00279800
N	-5.24406100	-0.60604000	0.00067200
C	-6.19541200	-1.27131600	-0.00018600



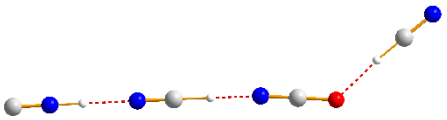
T33

C	1.77586800	0.13839600	-0.01077000
H	-4.85569400	-0.14708400	-0.00007200
H	-0.84899800	0.18739900	-0.01898400
H	4.58625900	-0.26653000	-0.00122300
N	2.82796600	-0.38778900	-0.01779900
O	0.68647200	0.69138600	-0.00235200
C	5.69704300	-0.16119200	0.01080600
C	-1.95679300	0.01316400	-0.02083900
C	-7.04793400	-0.07069700	0.02711600
N	-5.88766000	-0.11609700	0.01243000
N	-3.09265000	-0.14131100	-0.01795700
N	6.84056700	-0.04378900	0.02350100



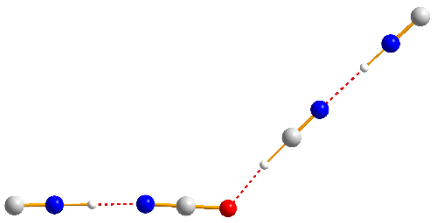
T34

C	-1.87534600	0.75216300	0.00010600
H	4.84243200	-0.22465000	-0.00001800
H	0.84634200	0.28344200	-0.00011400
H	-4.49348400	-0.00612500	0.00005900
C	-5.43666400	-0.56918000	0.00001800
C	1.99413000	0.13271800	-0.00033700
C	7.02730800	-0.49042500	0.00031300
N	5.87461200	-0.35069100	0.00018900
N	3.13326900	-0.01291500	-0.00050700
N	-6.42328400	-1.15656100	0.00000800
N	-0.72543300	0.49589800	0.00010900
O	-3.05825100	1.02069500	0.00011000



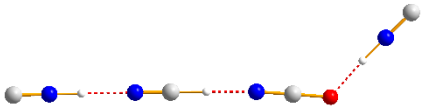
T35

C	1.82723400	0.90553500	0.00013000
H	-4.57584700	-0.35919300	0.00001600
H	-0.72975900	0.85606700	-0.00009900
H	4.23803100	-0.35409100	0.00003300
C	-1.79176200	0.50227700	-0.00022000
C	-6.68655600	-0.95375800	0.00019600
N	-5.56825500	-0.64076600	0.00009500
N	-2.88087400	0.14554000	-0.00035300
N	5.21154800	-0.82733700	-0.00004700
C	6.25748900	-1.33181500	-0.00003700
N	2.84854100	0.32793200	0.00015600
O	0.76905300	1.51077700	0.00008500



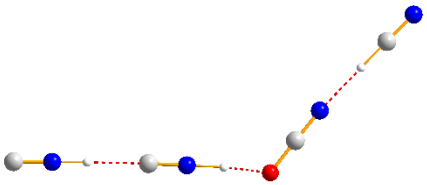
T36

C	-1.98088200	0.76668400	0.00005100
H	4.76690000	-0.21442400	-0.00003900
H	0.77229800	0.29733200	0.00043200
H	-4.36051300	0.01040900	-0.00021400
C	1.90909700	0.14499500	0.00021900
C	6.95039300	-0.47524600	-0.00022000
N	5.79735700	-0.33809300	-0.00012200
N	3.04737000	-0.00273900	0.00001500
N	-0.83068100	0.52508300	0.00066900
O	-3.16922700	1.03192100	-0.00048600
N	-5.20218300	-0.62076300	-0.00012700
C	-6.12992700	-1.31861500	0.00006000



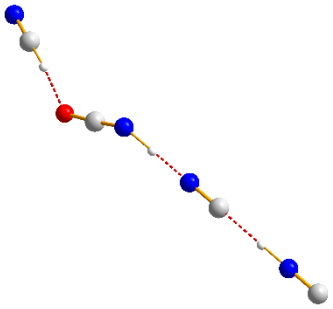
T37

C	1.61588300	0.99618300	0.00041100
H	-4.51434400	-0.43594900	-0.00020800
H	-0.69199100	1.03956800	-0.00048500
H	4.22851100	-0.41764400	0.00164700
C	-6.59582200	-1.17025300	0.00052500
N	-5.49956800	-0.78610300	0.00013500
N	2.61647400	0.38745200	0.00129400
O	0.57611600	1.65300500	-0.00026400
C	-2.79070200	0.20245400	-0.00077100
N	-1.71679500	0.62790700	-0.00074700
N	6.26208100	-1.39765100	-0.00089800
C	5.22623200	-0.90026000	0.00027900



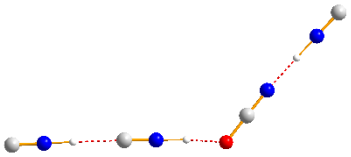
T38

C	-1.65450600	0.52047300	0.10271900
H	4.77237500	-0.18704600	-0.00391300
H	0.50100000	0.47017600	-0.33230800
H	-4.51316500	-0.14121700	0.16537200
C	6.98791900	-0.52263600	0.16856200
N	5.84240600	-0.34928200	0.07962800
C	3.09709100	0.06906500	-0.13668700
N	1.95524800	0.24790400	-0.23246600
N	-6.63418700	-0.74512900	-0.17133400
C	-5.54343900	-0.43535200	0.00211700
N	-0.59757600	0.63900600	-0.40210900
O	-2.75548000	0.44016300	0.55431800



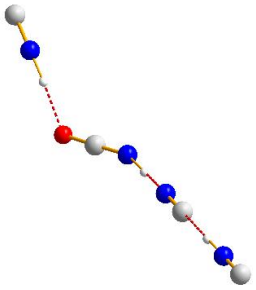
T39

C	-1.71722200	0.93448500	-0.00011600
H	4.49002300	-0.39505200	0.00010700
H	0.63572100	0.98455300	0.00000700
H	-4.11955300	-0.40326000	0.00015800
C	6.58749400	-1.07372000	-0.00008900
N	5.48144700	-0.71868000	-0.00001800
C	2.73934400	0.20418700	0.00008000
N	1.65583300	0.60401800	0.00015000
N	-5.07300800	-0.89239200	0.00011600
C	-6.10850900	-1.41768100	-0.00000700
O	-0.67880400	1.58393100	0.00004200
N	-2.71890000	0.32972300	-0.00022100



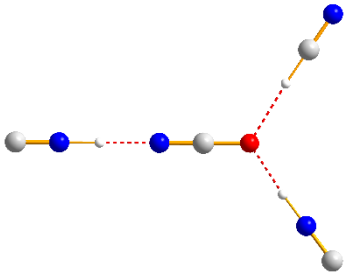
T40

C	1.77226800	-0.59844300	0.00568000
H	-4.68908500	0.18289600	-0.02758600
H	-0.44563200	-0.27449600	0.33788200
H	4.34268300	0.01958600	-0.17188700
C	-6.90847800	0.40638900	-0.21946800
N	-5.75666300	0.29098100	-0.12007300
C	-2.98031500	0.00662000	0.12239600
N	-1.83239100	-0.11522600	0.22814600
N	0.69218700	-0.41301100	0.42210300
O	2.89342700	-0.79825400	-0.36994300
N	5.26184200	0.47384100	-0.07678900
C	6.29815800	0.98575800	0.03262900



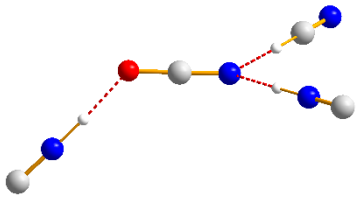
T41

C	0.43189900	0.06469900	0.00270900
H	3.19250500	-0.08844600	0.00179100
H	-1.84203700	-1.41426000	-0.00056800
H	-1.60055100	1.53237200	-0.00054700
N	-2.17595200	2.40047000	-0.00090100
C	-2.81868000	3.36745000	-0.00126800
N	4.25785900	-0.14839800	-0.00084800
C	5.41702100	-0.21477000	-0.00388900
C	-2.49920900	-2.28331900	-0.00080600
N	-3.19305700	-3.19718100	-0.00104200
N	1.59898700	-0.00248300	0.00578700
O	-0.79387100	0.12489000	-0.00026600



T42

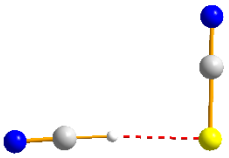
C	0.53213700	0.10727400	0.62715500
H	3.05652100	-0.02343900	0.17309600
H	-1.70401400	-1.30587000	-0.01127100
H	-1.63991000	1.40293600	-0.01450600
N	-2.33954800	2.18199800	-0.19166200
C	-3.09641800	3.04275200	-0.37841500
N	3.97934100	-0.04489900	-0.30631700
C	5.00956800	-0.06895600	-0.84085600
N	-0.58749400	0.19970500	0.26236300
O	1.67111300	-0.00279900	1.01435400
C	-2.34501700	-2.18539300	-0.15631500
N	-3.00703200	-3.11184600	-0.30317900



$[SCN(HCN)_n]^-$

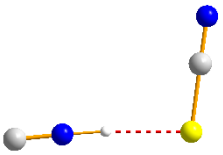
M1

C	-0.53890000	-2.15660000	0.00000000
C	-0.16670000	1.59480000	0.00000000
H	0.00000000	-1.19430000	0.00000000
N	-1.06760000	-3.17640000	0.00000000
N	-1.15640000	2.21490000	0.00000000
S	1.23760000	0.70600000	0.00000000



M2

C	-0.16046500	1.61600000	0.00000000
H	0.00000000	-1.20123000	0.00000000
N	-1.04918900	2.37147000	0.00000000
S	1.11859500	0.55073100	0.00000000
N	-0.49903800	-2.12848400	0.00000000
C	-1.01619100	-3.16789300	0.00000000



M3

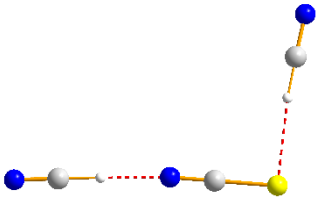
C	0.00000000	0.00000000	1.06058700
N	0.00000000	0.00000000	-4.14219900
N	0.00000000	0.00000000	-0.11107100
C	0.00000000	0.00000000	-2.99248600
S	0.00000000	0.00000000	2.70254600
H	0.00000000	0.00000000	-1.87645700

M4

C	0.00000000	0.00000000	0.95471500
N	0.00000000	0.00000000	-0.21559200
S	0.00000000	0.00000000	2.59103700
H	0.00000000	0.00000000	-1.75403700
N	0.00000000	0.00000000	-2.84261100
C	0.00000000	0.00000000	-4.00390500

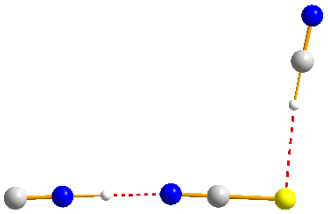
D1

C	-3.04380000	1.31950500	0.00009100
C	0.07749300	-0.94146400	0.00010700
C	3.85935300	0.61813700	-0.00008200
N	-3.67425400	2.27903000	0.00006100
N	4.93757200	1.01507900	-0.00036700
N	1.12586200	-0.42596500	0.00020600
H	2.82206200	0.23254400	0.00017000
H	-2.46457600	0.38822000	0.00011400
S	-1.40250200	-1.66717700	-0.00001700



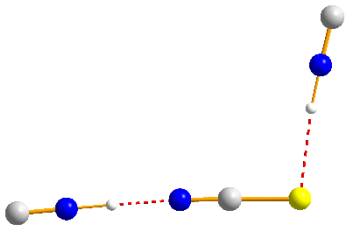
D2

H	2.42413500	0.34587100	-0.00002500
C	3.06244800	1.23522200	-0.00000900
H	-2.70814500	0.26912900	-0.00005000
S	1.24982700	-1.66749300	0.00002400
C	-0.20906500	-0.91083100	-0.00003200
N	-1.24565900	-0.37449500	-0.00004500
N	-3.68991300	0.68978900	-0.00002400
C	-4.75961200	1.14126300	0.00005900
N	3.75330900	2.15198600	0.00000900



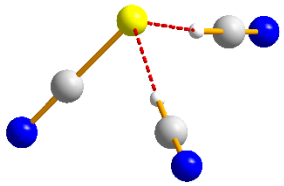
D3

H	2.45279600	0.32207100	0.00006100
H	-2.75232200	0.23258100	0.00002100
S	1.31768900	-1.49218200	-0.00000400
C	-0.17980700	-0.80779200	-0.00000800
N	-1.24528900	-0.33494000	0.00000900
N	-3.75291700	0.59578900	0.00000000
C	-4.84656100	0.98561400	-0.00000500
N	3.07830500	1.15235500	0.00002000
C	3.80233500	2.06015000	-0.00002200



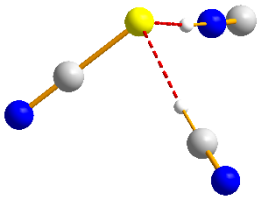
D4

C	-0.00006400	1.46886800	-0.07025400
H	2.05906900	-0.48287900	0.13756100
C	3.03711300	-0.83889400	-0.20251400
H	-2.05851600	-0.48323200	0.13714900
C	-3.03676800	-0.83903900	-0.20279000
N	0.00028900	2.36512500	-0.81551500
N	4.06122000	-1.23410800	-0.53847000
N	-4.06103600	-1.23400400	-0.53855000
S	-0.00034700	0.18383800	0.98914900



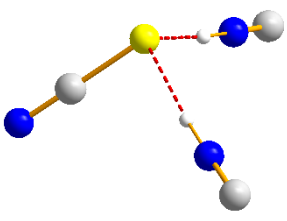
D5

C	0.00641100	1.59071400	-0.11694400
H	1.93904000	-0.51354600	0.12720600
H	-1.89337900	-0.51637700	0.15845800
C	-2.85902300	-0.93308200	-0.13951000
N	-0.11002200	2.48323200	-0.85569600
N	-3.87067700	-1.38998200	-0.43148400
S	0.15310500	0.31352300	0.94527500
N	2.81663000	-0.96037100	-0.21117500
C	3.79480300	-1.47706500	-0.56381000



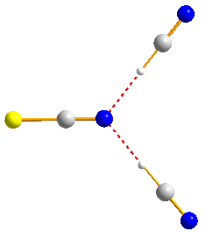
D6

C	-0.00227100	1.68110700	-0.11745100
H	-1.80328200	-0.54814700	0.13419900
H	1.80520700	-0.54588600	0.13349600
N	-0.00425500	2.61867300	-0.80607400
S	0.00052600	0.34409200	0.88290700
N	-2.68096800	-1.01558000	-0.16519400
C	-3.66094100	-1.55449900	-0.47726400
C	3.66368000	-1.55089600	-0.47766700
N	2.68334400	-1.01248000	-0.16586400



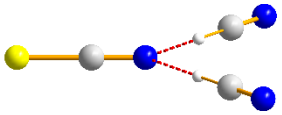
D7_*Cs*

C	-0.00728300	1.32639800	0.00000000
S	-0.01744300	2.95476400	0.00000000
H	-1.44575200	-1.01072200	0.00000000
C	-2.29818200	-1.71005800	0.00000000
H	1.45782500	-0.99520300	0.00000000
N	0.00000000	0.14893900	0.00000000
N	-3.18597900	-2.43868400	0.00000000
C	2.31781600	-1.68523500	0.00000000
N	3.21353800	-2.40410200	0.00000000



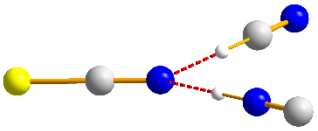
D7_*C2v*

C	0.00000000	0.00000000	1.33267200
S	0.00000000	0.00000000	2.96116900
H	0.00000000	1.44723100	-1.00415200
C	0.00000000	2.29991900	-1.70260800
H	0.00000000	-1.44723100	-1.00415200
C	0.00000000	-2.29991900	-1.70260800
N	0.00000000	0.00000000	0.15527300
N	0.00000000	3.18858200	-2.43014600
N	0.00000000	-3.18858200	-2.43014600



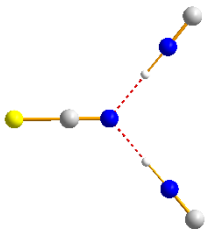
D8

C	-1.15260100	-0.62327900	0.00000000
S	-2.74736600	-0.93022800	0.00000000
H	0.39948100	1.49934100	0.00000000
C	0.63959100	2.56793100	0.00000000
H	1.50461900	-0.98572600	0.00000000
N	0.00000000	-0.38410500	0.00000000
N	0.89122800	3.68793200	0.00000000
N	2.49424600	-1.37192700	0.00000000
C	3.57224800	-1.80353000	0.00000000



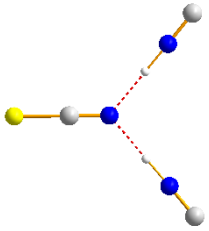
D9_*Cs*

C	-0.03885900	-1.25172400	0.00000000
S	-0.09229300	-2.86925600	0.00000000
H	1.32316500	0.95063900	0.00000000
H	-1.25855500	1.03011700	0.00000000
N	0.00000000	-0.07285800	0.00000000
N	-2.04737900	1.72530400	0.00000000
C	-2.92651900	2.48366500	0.00000000
C	3.07728100	2.29913700	0.00000000
N	2.15318600	1.59625000	0.00000000



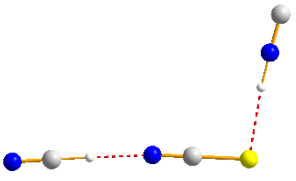
D9_*C2v*

C	0.00000000	0.00000000	1.25503900
S	0.00000000	0.00000000	2.87353800
H	0.00000000	1.28962200	-0.99161700
H	0.00000000	-1.28962200	-0.99161700
N	0.00000000	0.00000000	0.07558400
N	0.00000000	-2.09767200	-1.66410100
C	0.00000000	-2.99874200	-2.39627300
C	0.00000000	2.99874200	-2.39627300
N	0.00000000	2.09767200	-1.66410100



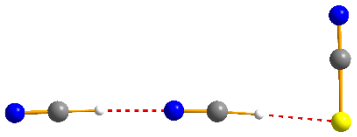
D10

H	-2.51843300	0.34663300	-0.00006200
H	2.88456600	0.21217100	-0.00000500
S	-1.44083500	-1.48344300	0.00001600
C	0.07410100	-0.82637200	0.00004700
N	1.14916200	-0.37300300	0.00002600
N	-3.11607200	1.20115300	-0.00003300
C	-3.80736600	2.13404500	0.00000000
C	3.93728000	0.54755400	-0.00002200
N	5.03307200	0.89255200	-0.00004100



D11

C	2.96736500	0.69312500	-0.00098000
H	-3.52480200	0.02582800	0.00171200
C	-4.60957300	0.11307500	-0.00120900
N	-5.75364800	0.20065600	-0.00419200
N	-1.55744000	-0.18786900	0.00672800
N	3.05582000	1.85711100	-0.00017300
S	2.81301200	-0.96215800	-0.00205200
C	-0.41999000	-0.33769400	0.00427400
H	0.67667800	-0.53163200	0.00205200

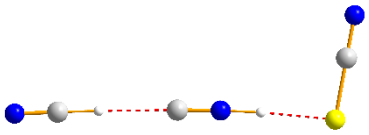


D12

C	2.90805600	-0.00010700	-0.00000400
H	-4.16724300	-0.00010300	0.00001200
C	-5.25766000	0.00032300	0.00000400
N	-6.40525600	0.00076900	0.00000500
N	-2.21056100	-0.00078000	0.00000500
C	-1.06173100	-0.00073800	-0.00005600
H	0.07640700	-0.00067700	-0.00004800
N	1.73589400	-0.00057200	0.00005900
S	4.54489400	0.00050000	-0.00000700

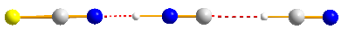
D13

C	3.10184500	0.63580000	-0.00086800
H	-3.63118900	0.07027300	0.00163800
C	-4.71949000	0.17448600	-0.00105100
N	-5.86241100	0.27994300	-0.00343200
H	0.65465300	-0.51388000	0.00189300
C	-1.54773900	-0.17307100	0.00613800
N	-0.40146900	-0.32990500	0.00374700
N	3.46136100	1.74444900	-0.00017400
S	2.59915500	-0.95256800	-0.00186500



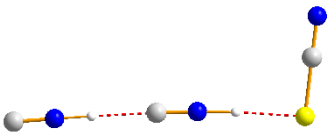
D14

C	-2.79540800	0.00256200	0.00013400
H	4.13379900	0.00344700	0.00003100
C	5.23303100	-0.00810300	0.00007500
N	6.38121700	-0.02042500	0.00011700
H	-0.22689200	0.01917600	-0.00025700
N	-1.62525000	0.01484100	0.00089600
S	-4.42399800	-0.01381000	-0.00017800
C	2.08204600	0.02030100	-0.00044400
N	0.92389800	0.02126700	-0.00037200



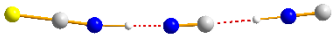
D15

C	-3.00075300	0.62439200	0.00005300
H	3.45644300	0.07241000	-0.00111600
H	-0.58034800	-0.51032100	0.00021900
C	1.62596700	-0.14963100	-0.00036100
N	0.48250300	-0.31165400	0.00015600
N	-3.36685700	1.73044900	0.00000700
S	-2.48813500	-0.96142200	0.00006200
C	5.65111500	0.29540600	0.00113400
N	4.49522400	0.18115700	-0.00088600



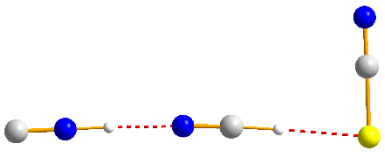
D16

C	-2.68556900	-0.04466300	0.00051700
H	3.89390900	-0.01598400	-0.00108600
H	-0.39432800	-0.22417100	0.00021600
C	2.18939200	-0.16750500	-0.00140000
N	1.03165400	-0.22735100	-0.00064000
C	6.12415100	0.22551400	0.00102200
N	4.96956800	0.09596500	-0.00026000
N	-1.52874300	-0.20210000	0.00177700
S	-4.28592400	0.15590500	-0.00038100



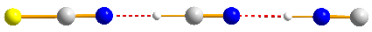
D17

C	2.86853200	0.68500500	0.00007000
H	-3.36981400	0.02523800	0.00063600
H	0.60667700	-0.52829400	0.00056500
C	-5.55785500	0.20697800	-0.00069000
N	-4.40047900	0.11392300	0.00010800
N	-1.62773300	-0.16337800	0.00049800
C	-0.49230000	-0.32018600	0.00044700
N	2.95755600	1.84869100	-0.00010500
S	2.70921600	-0.97014800	-0.00022900



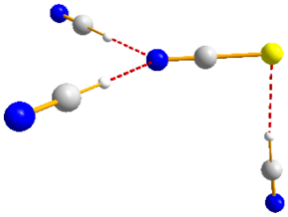
D18

C	-2.80698700	0.00593900	-0.00039400
H	4.00924700	0.00122300	0.00036700
H	-0.01549200	0.02244700	-0.00010300
C	6.20902000	-0.02255200	-0.00058500
N	5.04796000	-0.00966500	-0.00002700
N	-1.63479700	0.02191900	-0.00120200
S	-4.44174600	-0.01572100	0.00025600
N	2.28135500	0.01701400	0.00095000
C	1.13339400	0.02044500	0.00057700



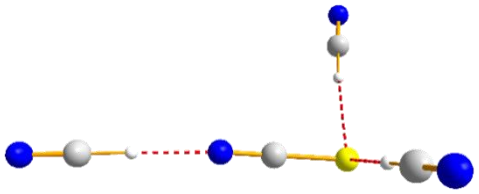
T1

C	0.03566943	1.40503191	-0.65978334
H	2.95676563	0.13657894	1.37090395
C	3.51486454	-0.35017123	2.15015032
N	4.11013542	-0.86934121	2.98129811
S	1.65341001	1.27331036	-0.44890814
H	-2.06094039	2.96167741	-0.06327280
C	-2.59002715	3.78963394	0.36034872
H	-2.05302969	0.19937143	-1.79546950
C	-2.58152454	-0.54247146	-2.35695175
N	-1.12668195	1.49967643	-0.81130131
N	-3.14785369	-1.33742198	-2.95862983
N	-3.15699060	4.67686286	0.81429678



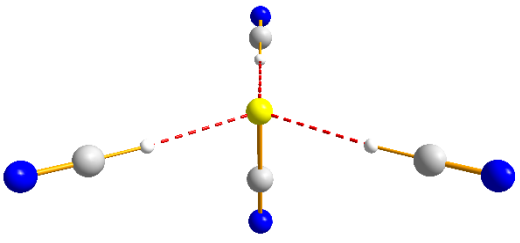
T2

C	-0.00009395	1.39282337	-0.00702091
H	2.05906900	-0.48287900	0.13756100
C	3.03711300	-0.83889400	-0.20251400
H	-2.05851600	-0.48323200	0.13714900
C	-3.03676800	-0.83903900	-0.20279000
N	4.06122000	-1.23410800	-0.53847000
N	-4.06103600	-1.23400400	-0.53855000
S	-0.00037695	0.10779337	1.05238209
C	0.00125769	4.82459681	-2.86062976
N	0.00160505	5.70652998	-3.59398013
N	0.00025341	2.27475654	-0.74037128
H	0.00089392	3.90098903	-2.09262587



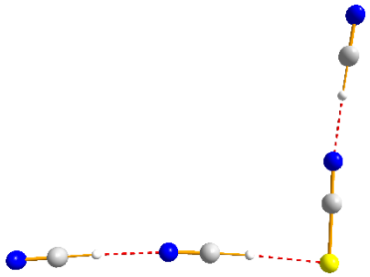
T3

C	-0.01705442	1.46919926	-0.12476662
H	2.05906900	-0.48287900	0.13756100
C	3.03711300	-0.83889400	-0.20251400
H	-2.05851600	-0.48323200	0.13714900
C	-3.03676800	-0.83903900	-0.20279000
N	-0.01670142	2.36545626	-0.87002762
N	4.06122000	-1.23410800	-0.53847000
N	-4.06103600	-1.23400400	-0.53855000
S	-0.01733742	0.18416926	0.93463638
C	0.99982621	0.16433756	4.19813809
N	1.34112234	0.15768329	5.29316397
H	0.67549075	0.17066115	3.15752936



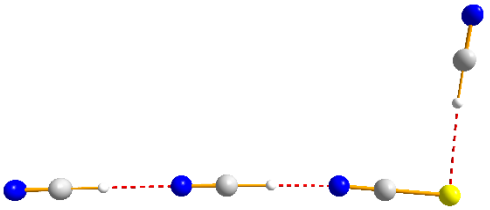
T4

H	-3.71285117	0.04022350	0.00122169
C	-4.79762217	0.12747050	-0.00169931
N	-1.55744000	-0.18786900	0.00672800
S	2.80362731	-1.08565190	-0.00213762
C	-0.41999000	-0.33769400	0.00427400
H	0.67667800	-0.53163200	0.00205200
N	-5.94127219	0.21501897	-0.00468120
C	3.29995902	5.06975470	0.00205435
N	3.38687258	6.21345677	0.00284729
N	3.04489386	1.71333316	-0.00027268
C	2.95798031	0.56963110	-0.00106562
H	3.20893847	3.87200848	0.00122394



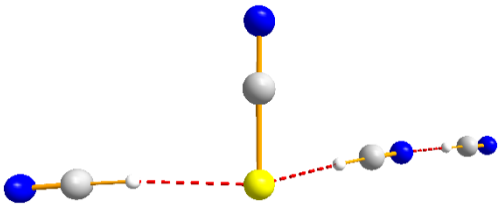
T5

N	-1.55744000	-0.18786900	0.00672800
S	2.79855798	-1.15235954	-0.00218387
C	-0.41999000	-0.33769400	0.00427400
H	0.67667800	-0.53163200	0.00205200
C	3.29488969	5.00304706	0.00200810
N	3.03982453	1.64662552	-0.00031893
C	2.95291098	0.50292346	-0.00111187
H	3.20386914	3.80530084	0.00117769
C	3.62943491	9.40535272	0.00506026
N	3.38180325	6.14674912	0.00280104
N	3.71631816	10.54865593	0.00585293
H	3.54531744	8.29844456	0.00429283



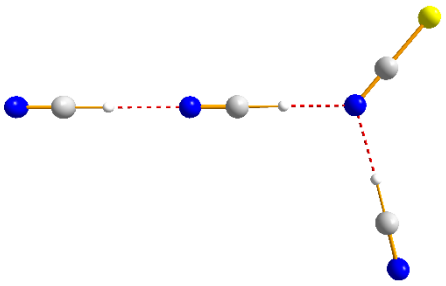
T6

C	-0.00006400	1.46886800	-0.07025400
H	1.94563904	-0.43910515	0.17477144
C	2.92368304	-0.79512015	-0.16530356
H	-2.05851600	-0.48323200	0.13714900
C	-3.03676800	-0.83903900	-0.20279000
N	0.00028900	2.36512500	-0.81551500
N	-4.06103600	-1.23400400	-0.53855000
S	-0.00034700	0.18383800	0.98914900
C	6.95568762	-2.35111445	-1.48799360
N	3.99526830	-1.20865652	-0.51683469
N	7.97892129	-2.74599142	-1.82366311
H	5.94271304	-1.96019657	-1.15568956



T7

C	0.00000000	0.00000000	1.33267200
S	0.00000000	0.00000000	2.96116900
H	0.00000000	1.33693077	-0.91385049
C	0.00000000	2.18961877	-1.61230649
H	0.00000000	-1.44723100	-1.00415200
C	0.00000000	-2.29991900	-1.70260800
N	0.00000000	0.00000000	0.15527300
N	0.00000000	-3.18858200	-2.43014600
C	0.00000000	5.71063729	-4.49492316
N	0.00000000	6.59814597	-5.22151613
H	-0.00000000	4.78119054	-3.73399598
N	0.00000000	3.11906552	-2.37323367

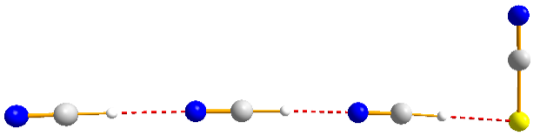


T8

C	2.90805600	-0.00010700	-0.00000400
H	-4.35514299	-0.00002997	0.00001216
C	-5.44555999	0.00039603	0.00000416
N	-2.21056100	-0.00078000	0.00000500
C	-1.06173100	-0.00073800	-0.00005600
H	0.07640700	-0.00067700	-0.00004800
N	1.73589400	-0.00057200	0.00005900
S	4.54489400	0.00050000	-0.00000700
C	-9.33375969	0.00190713	0.00000755
N	-10.48215961	0.00235344	0.00000855
H	-8.13255978	0.00144030	0.00000651
N	-6.59255990	0.00084179	0.00000516

T9

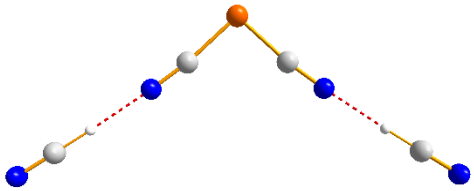
C	2.96736500	0.69312500	-0.00098000
H	-3.71285117	0.04022350	0.00122169
C	-4.79762217	0.12747050	-0.00169931
N	-1.55744000	-0.18786900	0.00672800
N	3.05582000	1.85711100	-0.00017300
S	2.81301200	-0.96215800	-0.00205200
C	-0.41999000	-0.33769400	0.00427400
H	0.67667800	-0.53163200	0.00205200
C	-8.67446612	0.42424988	-0.01180759
N	-9.81811615	0.51179835	-0.01478948
H	-7.47677440	0.33256443	-0.00868479
N	-5.94127219	0.21501897	-0.00468120



$[P(CN)_2(HCN)_2]^-$

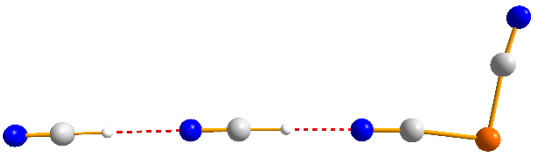
1

P	0.00000000	0.00000000	2.11142300
C	0.00000000	1.29913100	0.92070000
C	0.00000000	-1.29913100	0.92070000
N	0.00000000	2.23920100	0.23869300
N	0.00000000	-2.23920100	0.23869300
H	0.00000000	-3.82123700	-0.80679400
C	0.00000000	-4.75237600	-1.38553000
H	0.00000000	3.82123700	-0.80679400
C	0.00000000	4.75237600	-1.38553000
N	0.00000000	-5.73014300	-1.98725000
N	0.00000000	5.73014300	-1.98725000



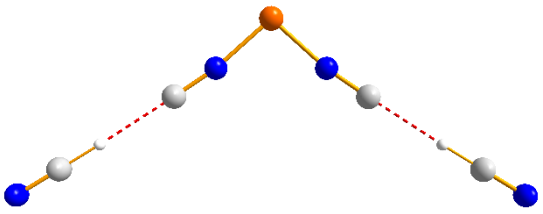
2

P	-0.84473500	-3.69482000	0.00000000
C	-0.41036200	-1.99114600	0.00000000
C	-2.59183600	-3.41811900	0.00000000
N	0.00000000	-0.90290000	0.00000000
N	-3.75216400	-3.36772500	0.00000000
H	0.62432800	0.76045700	0.00000000
C	1.03368200	1.79494300	0.00000000
N	1.46123200	2.85941300	0.00000000
H	2.22852000	4.70342800	0.00000000
C	2.65456200	5.70294600	0.00000000
N	3.10549000	6.75788000	0.00000000



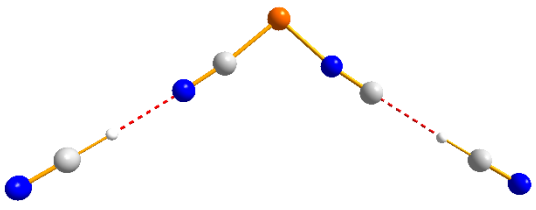
3

P	-1.68322800	1.20320500	0.00000000
H	2.99906000	2.73704700	0.00000000
C	4.01040700	3.16601800	0.00000000
H	-1.61900700	-3.72353000	0.00000000
C	-1.69716200	-4.81931200	0.00000000
N	5.06560700	3.61881400	0.00000000
N	-1.78372100	-5.96429200	0.00000000
N	0.00000000	1.57651400	0.00000000
C	1.09750800	1.98208000	0.00000000
C	-1.52079500	-1.67995200	0.00000000
N	-1.49208300	-0.51026500	0.00000000



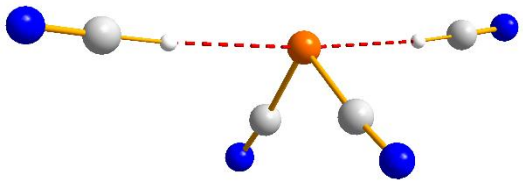
4

P	-1.69461600	1.19610100	0.00000000
C	-1.51274500	-0.55329900	0.00000000
N	-1.51713900	-1.71667700	0.00000000
H	2.99515800	2.74350300	0.00000000
C	4.00015100	3.18468000	0.00000000
H	-1.59414500	-3.60369600	0.00000000
C	-1.66461500	-4.69866700	0.00000000
N	5.04930500	3.65109000	0.00000000
N	-1.74274900	-5.84421200	0.00000000
N	0.00000000	1.55502100	0.00000000
C	1.09259200	1.96764100	0.00000000



5

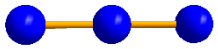
P	0.00000300	0.46933700	0.00000000
C	0.00000300	-0.70983200	1.32155400
C	0.00000300	-0.70983200	-1.32155400
N	0.00000300	-1.37920200	2.26894900
N	0.00000300	-1.37920200	-2.26894900
H	2.51903900	0.56702500	0.00000000
C	3.60332000	0.67900600	0.00000000
H	-2.51905200	0.56693800	0.00000000
C	-3.60333000	0.67893000	0.00000000
N	4.74181400	0.82182200	0.00000000
N	-4.74182100	0.82177500	0.00000000



Starting compounds

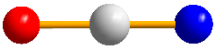
N_3^-

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.17426300
N	0.00000000	0.00000000	-1.17426300



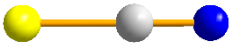
OCN^-

C	0.00000000	0.00000000	-0.06980000
O	0.00000000	0.00000000	1.15140000
N	0.00000000	0.00000000	-1.25610000



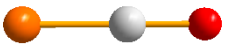
SCN^-

C	0.00000000	0.00000000	-0.63192800
S	0.00000000	0.00000000	1.02573900
N	0.00000000	0.00000000	-1.80289300



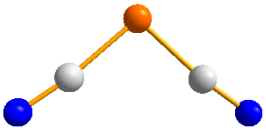
OCP^-

C	0.00000000	0.00000000	-0.50970500
O	0.00000000	0.00000000	-1.70270100
P	0.00000000	0.00000000	1.11198900



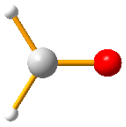
$[P(CN)_2]^-$

P	0.00000000	0.00000000	0.97654000
C	0.00000000	-1.31760800	-0.20261800
C	0.00000000	1.31760800	-0.20261800
N	0.00000000	-2.26841200	-0.87262100
N	0.00000000	2.26841200	-0.87262100



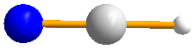
CH_2O

C	-0.00000500	0.52515500	0.00000000
H	0.94012200	1.11061500	0.00000000
H	-0.94004500	1.11077200	0.00000000
O	-0.00000500	-0.67154000	0.00000000



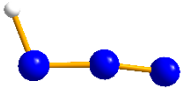
HCN

C	0.00000000	0.00000000	-0.49658000
H	0.00000000	0.00000000	-1.56418000
N	0.00000000	0.00000000	0.64909400



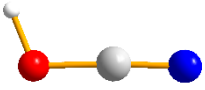
HN_3

N	0.20085900	-1.21355800	0.00000000
N	0.00000000	-0.10904800	0.00000000
N	-0.05480600	1.11838600	0.00000000
H	-1.02237100	1.42954500	0.00000000



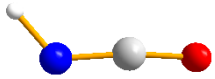
HOCN

C	0.00000000	0.17863400	0.00000000
O	0.14295900	-1.10458600	0.00000000
N	-0.06097900	1.32964300	0.00000000
H	-0.71682000	-1.54261000	0.00000000



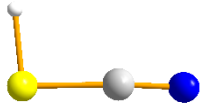
HNCO

C	0.00000000	0.04904200	0.00000000
O	-0.48492400	1.10421000	0.00000000
N	0.36514600	-1.10363100	0.00000000
H	1.32336900	-1.40251600	0.00000000



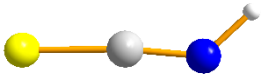
HSCN

C	0.00000000	0.69299000	0.00000000
S	0.06773500	-0.99516800	0.00000000
N	0.02659900	1.84649400	0.00000000
H	-1.26995300	-1.16071200	0.00000000



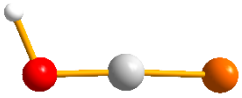
HNCS

C	0.00000000	0.49357400	0.00000000
S	-0.02905400	-1.07380700	0.00000000
N	0.14049300	1.68290800	0.00000000
H	-0.51859400	2.43910600	0.00000000



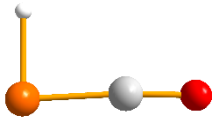
HOCP

C	0.00000000	0.37329100	0.00000000
O	0.04856800	1.66600500	0.00000000
P	0.02985800	-1.17459300	0.00000000
H	-0.83642000	2.05111000	0.00000000



HPCO

C	0.00000000	0.58869200	0.00000000
O	0.03808000	1.73698600	0.00000000
P	0.07009900	-1.09082600	0.00000000
H	-1.35612900	-1.06564400	0.00000000



5 References

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