Supporting Information

Trapping of Brønsted acids with biradicals

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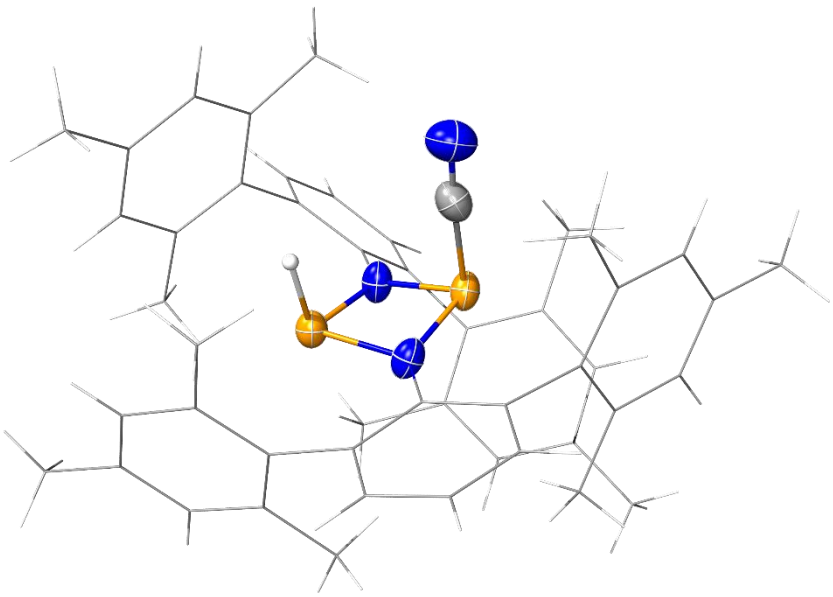


This file includes:

1 Experimental

General Information. If not stated otherwise, all manipulations were carried out under oxygen- and moisture-free conditions under an inert atmosphere of argon using standard Schlenk or Drybox techniques. Solvents and reactants were obtained from commercial sources or synthesized as detailed in Table S1.

Table S1: Origin and purification of solvents and reactants.

Substance	Origin	Purification[1]
C_6H_6, $C_6H_5CH_3$	local trade	purified according to literature procedure dried over Na/benzophenone freshly distilled prior to use
Et_2O, THF	local trade	dried over Na/benzophenone freshly distilled prior to use
n-hexane	local trade	dried over Na/benzophenone/tetraglyme freshly distilled prior to use
PCl_3	Merck, for synthesis	dried over P_4O_{10} freshly distilled and degassed (freeze-pump-thaw)
$P(SiMe_3)_3$	synthesized[2]	
NEt_3	Sigma Aldrich, 99 %	dried over Na freshly distilled prior to use
DBU	Merck, for synthesis	distilled
Mg	abcr, 99.8 %, for Grignards	used as received
$TerNH_2$	synthesized[3,4]	re-crystallized as described in the literature
stearic acid	Roth, ≥ 98 %	re-crystallized from *n*-hexane
NaCl	Chemsolute, 99 %	
NaCN	Merck, 95.0 %	
NaN_3	Aldrich, 99.0 %	
NaNCO	abcr, 97 %	
KNCS	Riedel-de Haen, 98.5 %	
Me_3SiCl	Merck	dried over CaH_2 freshly distilled prior to use
Me_3SiCN	Acros	distilled, recondensed
Me_3SiN_3	synthesized[5]	
Me_3SiNCO	synthesized[5]	
Me_3SiNCS	synthesized[5]	

Substance	Origin	Purification[1]
Me_3SiNSO	synthesized[5]	
$[Na(dioxane)_x]PCO$	synthesized[6]	
$[Ph_4P]Cl$	J&K Scientific GmbH, 99 %	
$[nBu_3NMe][CO_3Me]$	synthesized[7]	
$KHSO_4$	Roth, ≥ 99 %	
H_2SO_4	Chemsolute, 95 %	
CaH_2	Acros Organics, 93 %	
$Ag[B(C_6F_5)_4]$	synthesized[8]	
$[(Et_2O)_2H][B(C_6F_5)_4]$ Jutzi acid	synthesized[9]	
CD_2Cl_2	Euriso-Top, 99.5 %	dried over P_4O_{10} and CaH_2 freshly distilled prior to use
C_6D_6, $C_6D_5CD_3$	Euriso-Top, 99.5 %	dried over Na freshly distilled prior to use
THF-d_8	Euriso-Top, 99.5 %	dried over Na distilled and stored over molecular sieves (4 Å)
Sodium piece	Aldrich, 99 %	
Benzophenon	Aldrich, 99 %	
Tetraglyme	Alfa Aesar, ≥ 95 %	

NMR spectra were recorded on Bruker spectrometers (AVANCE 250, AVANCE 300 or AVANCE 500) and were referenced internally to the deuterated solvent ($^{13}C\{^1H\}$: CD_2Cl_2 δ_{ref} = 54.0 ppm, C_6D_6 δ_{ref} = 128.4 ppm, $C_6D_5CD_3$ δ_{ref} = 20.4 ppm, THF-d_8 $\delta_{ref,1}$ = 25.4 ppm, $\delta_{ref,2}$ = 67.6 ppm), to protic impurities in the deuterated solvent (^1H: $CDHCl_2$ δ_{ref} = 5.32 ppm, C_6HD_5 δ_{ref} = 7.16 ppm, $C_6D_5CHD_2$ δ_{ref} = 2.08 ppm, THF-d_7 $\delta_{ref,1}$ = 1.73 ppm, $\delta_{ref,2}$ = 3.58 ppm) or externally ($^{14}N\{^1H\}$: CH_3NO_2 δ_{ref} = 0 ppm, ^{15}N: CH_3NO_2 δ_{ref} = 0 ppm, ^{17}O: H_2O δ_{ref} = 0 ppm, ^{31}P: 85 % H_3PO_4 δ_{ref} = 0 ppm). All measurements were carried at ambient temperature unless stated otherwise. ^{15}N NMR shifts were derived from ^1H-^{15}N HMBC NMR spectra. NMR signals were assigned using experimental data (e.g. chemical shifts, coupling constants, integrals where applicable) in conjunction with computed NMR data (GIAO method, cf. Computational details, p. 80).

IR spectra of crystalline samples were recorded on a Bruker Alpha II FT-IR spectrometer equipped with an ATR unit at ambient temperature under argon atmosphere.

Raman spectra of crystalline samples were recorded using a LabRAM HR 800 Horiba Jobin YVON Raman spectrometer equipped with an Olympus BX41 microscope with variable lenses. The samples were excited by a red laser (633 nm, 17 mW, air-cooled HeNe laser). All measurements were carried out at ambient temperature unless stated otherwise.

Elemental analyses were obtained using an Elementar vario Micro cube CHNS analyser.

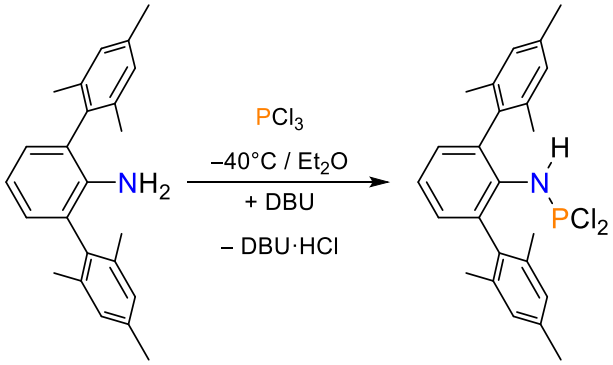
Melting points (uncorrected) were determined using a Stanford Research Systems EZ Melt at a heating rate of 20 °C/min.

DSC analyses were carried out at a heating rate of 5 °C/min using a Mettler-Toledo DSC 823e.

Mass spectra were recorded on a Thermo Electron MAT 95-XP sector field mass spectrometer using crystalline samples.

2 Syntheses of starting materials

2.1 Synthesis of TerN(H)PCl_2



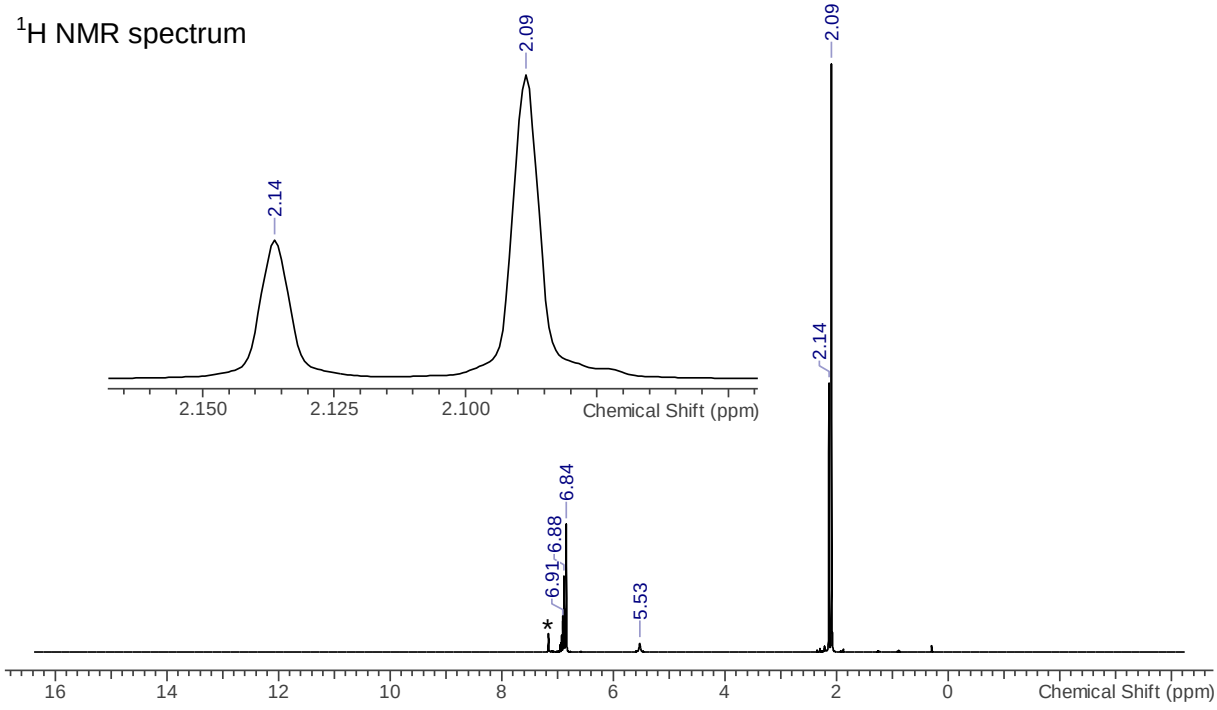
TerN(H)PCl_2 is synthesized according to a slightly modified literature procedure.[3]

PCl_3 (7.07 g, 51.4 mmol) is added to a solution of $TerNH_2$[3,4] (11.38 g, 34.5 mmol) in Et_2O (150 mL) at −40 °C (isopropanol bath). Afterwards, DBU (5.25 g, 34.5 mmol) is added dropwise over a period of 10 minutes, whereupon the reaction mixture is allowed to warm to ambient temperature. The mixture is stirred for 20 hours. Afterwards, the solvent is removed *in vacuo* ($1 \cdot 10^{-3}$ mbar, 50 °C (water bath), 1 h), the remaining white solids are extracted with *n*-hexane (150 mL) and the insoluble residue is separated by filtration. The extraction process is repeated four to five times by back-condensation of the solvent. Finally, the solvent of the filtrate is removed *in vacuo* ($1 \cdot 10^{-3}$ mbar, 50 °C (water bath), 1 h), yielding the product as a colourless, crystalline solid (13.2 g, 30.7 mmol, 89 %).

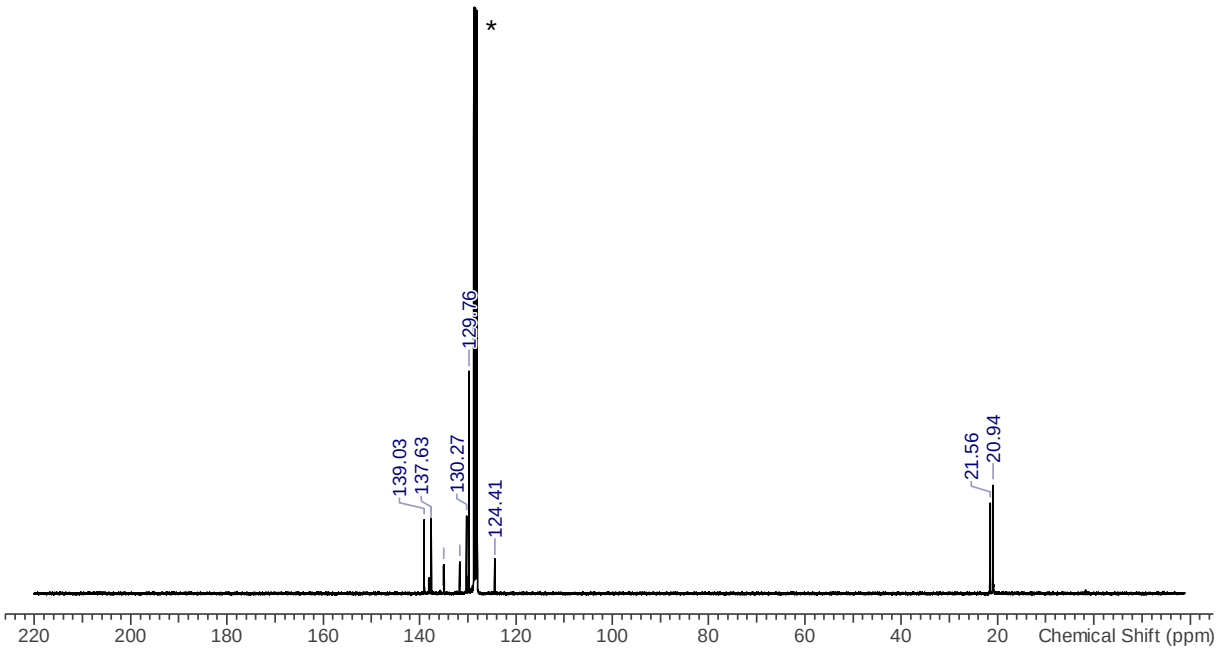
TerN(H)PCl_2 (430.36 g·mol^{-1}): **mp**. 154 °C. **^{1}H NMR** (298 K, CD_2Cl_2, 250.13 MHz): δ = 2.09 (s, 12H, *o*-CH_3), 2.14 (s, 6H, *p*-CH_3), 5.53 (s, 1H, N*H*), 6.84 (s, 4H, Mes *m*-C*H*), 6.88 (m, 2H, *m*-C*H*), 6.91 (m, 1H, *p*-C*H*). **^{13}C{^{1}H} NMR** (298 K, CD_2Cl_2, 75.5 MHz): δ = 20.9 (d, $J(^{13}C,^{31}P)$ = 1.5 Hz, *o*-CH_3), 21.6 (s, *p*-CH_3), 124.4 (s, *C*H), 129.8 (s, *C*H), 130.3 (s, *C*H), 131.7 (d, *C*, $J(^{13}C,^{31}P)$ = 3.8 Hz), 134.9 (d, *C*, $J(^{13}C,^{31}P)$ = 3.0 Hz), 137.6 (d, *C*, $J(^{13}C,^{31}P)$ = 5.1 Hz), 137.8 (d, *C*, $J(^{13}C,^{31}P)$ = 4.1 Hz), 139.0 (s, *C*). **^{31}P{^{1}H} NMR** (298 K, CD_2Cl_2, 121.5 MHz): δ = 159.4 (s, TerN(H)*P*Cl_2). **IR** (ATR, 32 scans, cm^{-1}): $\tilde{\nu}$ = 3327 (m), 3030 (w), 2972 (m), 2943 (w), 2914 (m), 2852 (w), 2731 (w), 1610 (m),

1570 (w), 1487 (w), 1431 (s), 1421 (s), 1373 (m), 1356 (s), 1261 (m), 1240 (w), 1217 (s), 1182 (w), 1163 (w), 1101 (w), 1070 (m), 1032 (m), 1009 (m), 970 (w), 947 (m), 918 (s), 852 (vs), 820 (m), 796 (s), 775 (m), 754 (vs), 741 (m), 735 (m), 715 (w), 642 (s), 596 (w), 577 (w), 567 (w), 557 (m), 532 (m). **Raman** (633 nm, 6mW, 20 s, 20 acc, cm^{-1}): $\tilde{\nu}$ = 3331 (1), 3092 (1), 3054 (2), 3016 (1), 2972 (1), 2944 (2), 2915 (5), 2855 (2), 2731 (1), 1612 (4), 1582 (3), 1482 (1), 1440 (2), 1383 (2), 1359 (1), 1305 (10), 1284 (2), 1266 (1), 1217 (5), 1181 (2), 1165 (1), 1071 (5), 1008 (2), 947 (2), 820 (1), 799 (1), 734 (1), 655 (3), 644 (4), 595 (1), 577 (9), 559 (2), 520 (2), 512 (2), 501 (2), 490 (4), 478 (7), 440 (10), 401 (5), 372 (2), 329 (4), 272 (8), 263 (7), 220 (6), 214 (7), 195 (2), 188 (2), 150 (4).

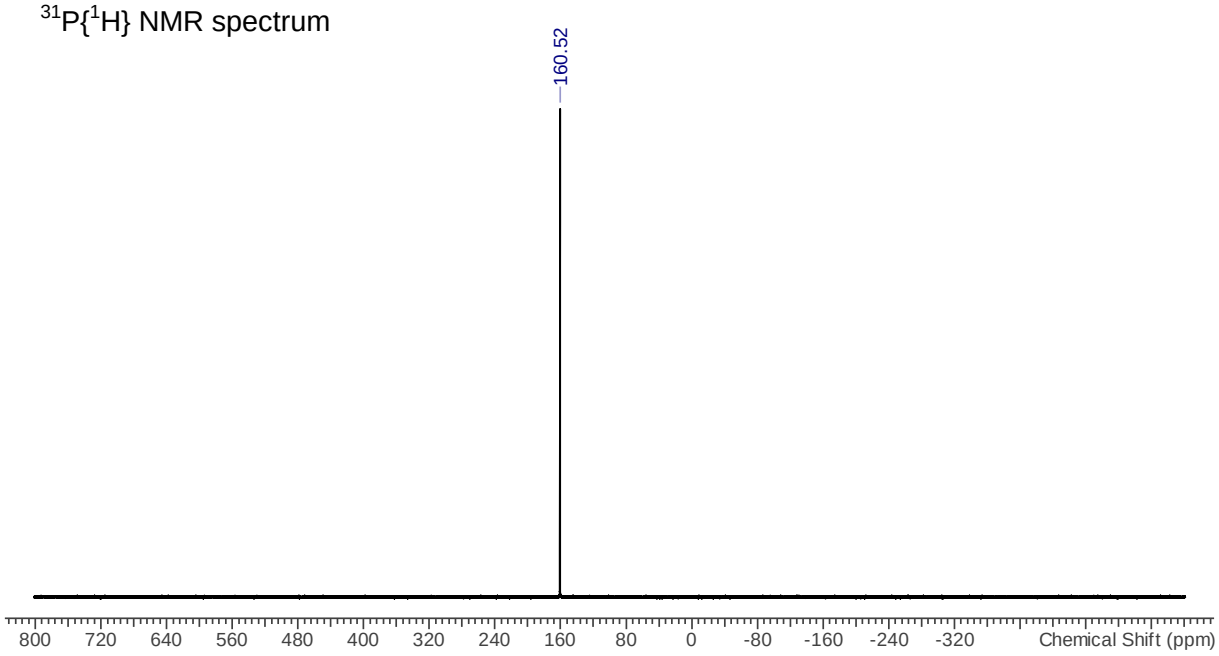
Figure S1: NMR, IR and Raman spectra of TerN(H)PCl_2 in C_6D_6 (solvent signals indicated by asterisk).



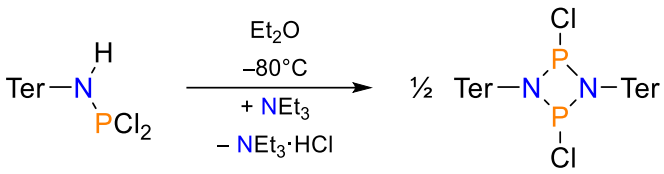
$^{13}C\{^{1}H\}$ NMR spectrum



$^{31}P\{^{1}H\}$ NMR spectrum



2.2 Synthesis of [ClP(μ-NTer)]$_2$



[ClP(μ-NTer)]$_2$ is synthesized according to a modified literature procedure.[4]

A stirred solution of TerN(H)PCl$_2$ (13.2 g, 30.7 mmol) in Et$_2$O (100 mL) is cooled to −80 °C (isopropanol bath). NEt$_3$ (4.86 g, 48 mmol) is added quickly. The mixture is warmed to ambient temperature and stirred overnight, resulting in a slightly yellowish suspension. All volatiles are removed *in vacuo* ($1\cdot10^{-3}$ mbar, 50 °C (water bath), 1 h), and the solid residue is extracted with Et$_2$O (300 mL) in a Soxhlet apparatus (under argon atmosphere) for 20 hours. The solvent of the extract is removed *in vacuo* ($1\cdot10^{-3}$ mbar, 40 °C, 1 h), whereupon the product is obtained as a white powder (9.8 g, 12.4 mmol, 81 %).

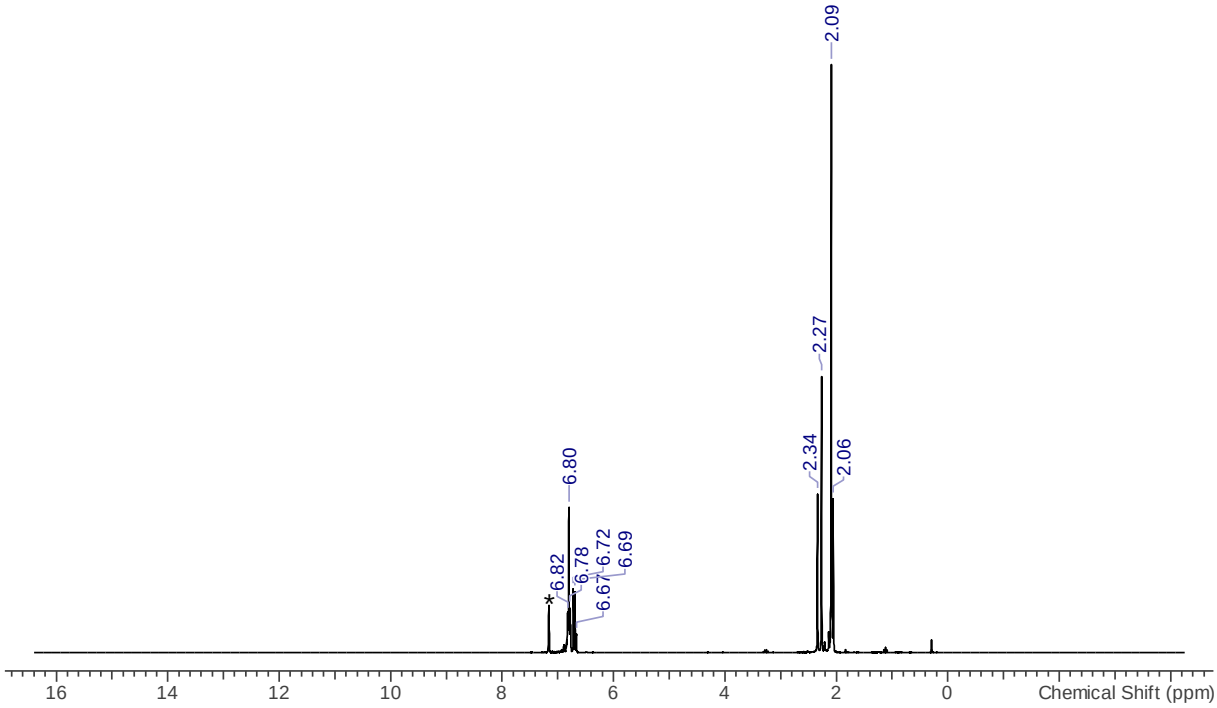
Note: A mixture of the *cis* and *trans* isomers is obtained (approx. ratio: 2:1).

[ClP(μ-NTer)]$_2$ (787.79 g·mol^{-1}): **mp.** 285 °C. **^{1}H NMR** (298 K, C$_6$D$_6$, 300.13 MHz): δ = 2.06 (d, 12H, *trans*, *o*-C*H*$_3$, J(^{31}P,^{1}H) = 1.7 Hz), 2.09 (s, 12H, *cis, o*-C*H*$_3$), 2.27 (s, 6H, *cis*, *p*-C*H*$_3$), 2.34 (s, 6H, *trans*, *p*-C*H*$_3$), 6.67-6.82 (14H, *cis*/*trans*, C*H*). **^{13}C{^{1}H} NMR** (298 K, CD$_2$Cl$_2$, 75.5 MHz): δ = 21.0 (s, *o*-*C*H$_3$), 21.3 (t, *o*-*C*H$_3$, ^2J(^{13}C,^{31}P) = 2.7 Hz), 21.8 (s, *p*-*C*H$_3$), 21.9 (t, *p*-*C*H$_3$, ^2J(^{13}C,^{31}P) = 3.7 Hz), 123.7 (s, *C*H), 124.8 (s, *C*H), 128.8 (s, *C*H), 129.1 (s, *C*H), 131.3 (s, *C*H), 131.6 (s, *C*H), 132.4 (t, *C*, J(^{13}C,^{31}P) = 1.9 Hz), 134.4 (s, *C*), 134.6 (s, *C*), 135.2 (t, *C*, J(^{13}C,^{31}P) = 2.8 Hz), 135.7 (t, *C*, J(^{13}C,^{31}P) = 2.9 Hz), 136.1 (t, *C*, J(^{13}C,^{31}P) = 2.8 Hz), 137.9 (s, *C*), 138.3 (t, *C*, J(^{13}C,^{31}P) = 4.4 Hz), 138.8 (t, *C*, J(^{13}C,^{31}P) = 3.5 Hz), 138.9 (t, *C*, J(^{13}C,^{31}P) = 3.5 Hz). **^{31}P{^{1}H} NMR** (298 K C$_6$D$_6$, 121.5 MHz): δ = 226.6 (s, *cis*, [Cl*P*(μ-NTer)]$_2$), 263.5 (s, *trans*, [Cl*P*(μ-NTer)]$_2$). **IR** (ATR, 32 scans, cm^{-1}): $\tilde{\nu}$ = 3001 (w), 2962 (w), 2943 (w), 2912 (m), 2852 (w), 2727 (w), 1610 (m), 1581 (w), 1483 (w), 1450 (m), 1410 (s), 1375 (m), 1261 (m), 1223 (vs), 1084 (m), 1030 (m), 1007 (m), 951 (w), 906 (s), 891 (vs), 841 (s), 795 (s), 762 (m), 746 (s), 700 (s), 650 (w), 586 (w), 575 (m), 557 (m), 552 (m), 534 (m). **Raman** (633 nm, 6mW, 20 s, 20 acc, cm^{-1}): $\tilde{\nu}$ = 3047 (2), 3013 (2), 2918 (10), 2855 (2), 2732 (1), 1612 (4), 1583 (3), 1485 (1), 1431 (2), 1378 (2), 1305 (5), 1287 (2), 1166 (1), 1094

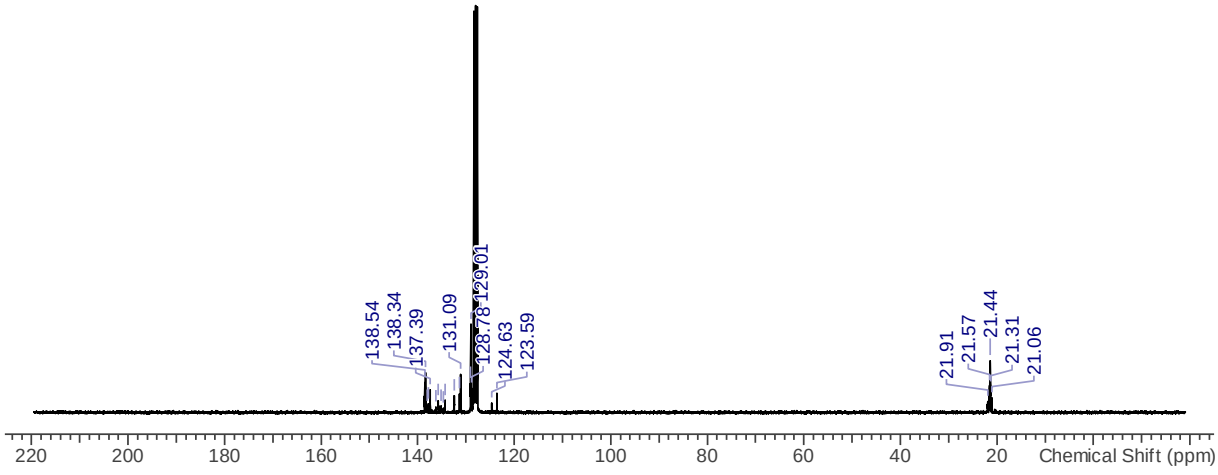
(1), 1007 (1), 942 (1), 740 (1), 577 (4), 562 (2), 540 (3), 524 (2), 483 (1), 438 (2), 387 (1), 338 (1), 264 (1), 227 (2), 203 (2).

Figure S2: NMR, IR and Raman spectra of $[TerNPCl]_2$ in C_6D_6 (solvent signals indicated by asterisk).

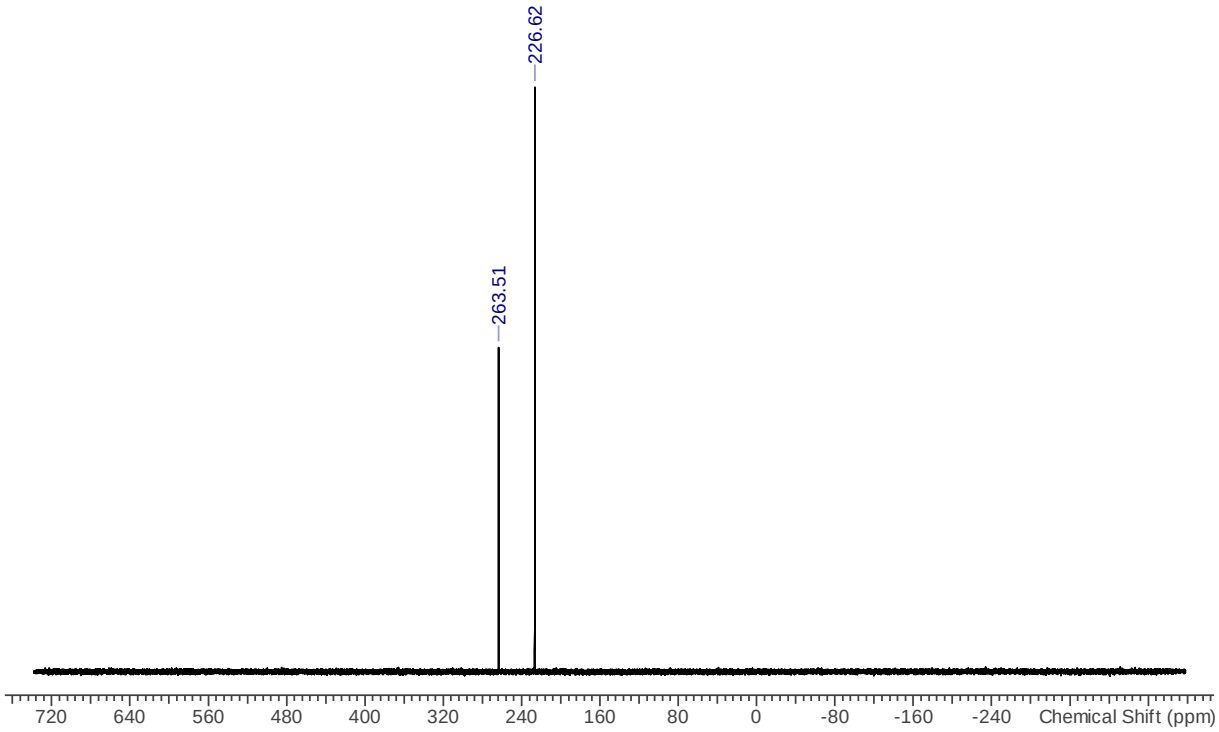
^{1}H NMR spectrum



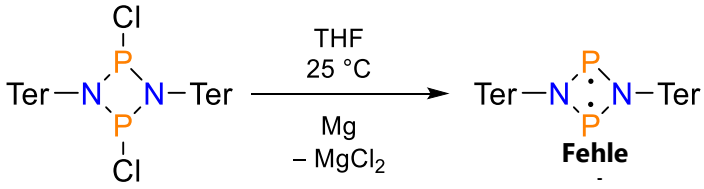
^{13}C{^{1}H} NMR spectrum



$^{31}P\{^{1}H\}$ NMR spectrum



2.3 Synthesis of [P(μ-NTer)]$_2$ (1)



[P(μ-NTer)$_2$] is synthesized according to a modified literature procedure.[10,11]

Mg turnings can be activated by stirring for several days under argon atmosphere using a glass covered magnetic stir bar.

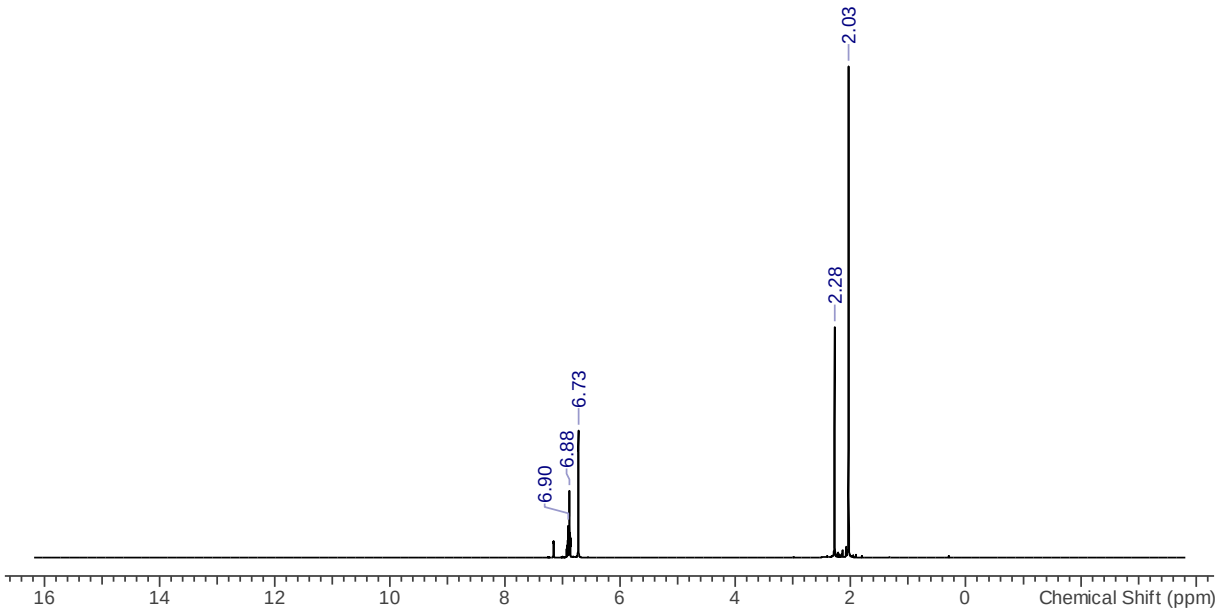
[ClP(μ−NTer)]$_2$ (0.85 g, 1.08 mmol) and Mg turnings (0.40 g, 17 mmol) are combined in a Schlenk flask. *Attention: It is paramount to ensure that no grease finds its way into the reaction vessel.* THF is added (20 mL) and the reaction mixture is stirred at ambient temperature. The colorless mixture gradually turns orange. The progress of the reaction must be monitored by ^{31}P NMR spectroscopy, as over-reduction occurs very quickly. When the reaction is completed, the solvents are removed *in vacuo*, and the solid residue is dried ($1\cdot10^{-3}$ mbar, 40 °C (water bath), 30 min). Benzene (10 mL) is added, and the insoluble material is separated by filtration. If necessary, the cloudy

suspension is filtered a second time over a celite-packed frit. The intensively orange filtrate is concentrated to incipient crystallization. After crystallization overnight at ambient temperature, orange crystals of the product are obtained. The supernatant is removed by syringe and re-crystallized, yielding a second crop of product. The isolated crystals are dried *in vacuo* ($1 \cdot 10^{-3}$ mbar, 40 °C (water bath)). Yield: 0.65 g (0.91 mmol, 84 %).

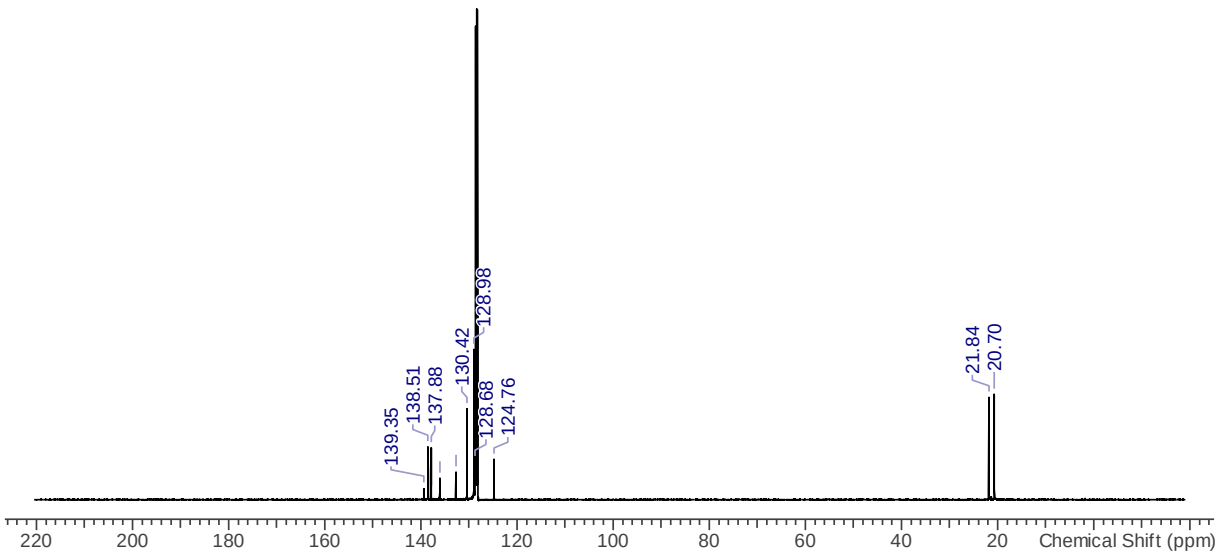
[P(*μ*-NTer)]$_2$ (716.89 g·mol^{-1}): **mp.** 224 °C (dec.). **^{1}H NMR** (298 K, C_6D_6, 300.13 MHz): *δ* = 2.04 (s, 24H, *o*-C*H*$_3$), 2.28 (s, 12H, *m*-C*H*$_3$), 6.73 (s, 8H, Mes *m*-C*H*), 6.73 (s, 4H, Mes *m*-C*H*), 6.89 (m, 2H, *m*-C*H*), 7.16 (m, 1H, *p*-C*H*). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 62.89 MHz): *δ* = 18.5 (t, *o*-*C*H$_3$, *J*(^{13}C,^{31}P) = 2.3 Hz), 19.7 (s, *p*-*C*H$_3$), 122.6 (s, *C*H), 126.8 (s, *C*H), 128.3 (s, *C*H), 130.6 (t, *C*, *J*(^{13}C,^{31}P) = 1.6 Hz), 133.9 (t, *C*, *J*(^{13}C,^{31}P) = 3.2 Hz), 135.7 (s, *C*), 136.35 (t, *C*, *J*(^{13}C,^{31}P) = 3.4 Hz), 137.2 (m, *C*, *J*(^{13}C,^{31}P) = 2.3 Hz). **^{14}N{^{1}H} NMR** no signals observed**. ^{31}P{^{1}H} NMR** (298 K, C_6D_6, 121.5 MHz): *δ* = 276.3 (s, [*P*(*μ*-NTer)]$_2$). **Raman** (633 nm, 6mW, 20 s, 20 acc., cm^{-1}): $\tilde{\nu}$ = 3083 (1), 3045 (1), 3005 (1), 2944 (2), 2916 (3), 2857 (1), 2731 (1), 1612 (5), 1582 (4), 1482 (2), 1429 (3), 1383 (2), 1376 (3), 1305 (7), 1284 (4), 1244 (1), 1189 (1), 1164 (1), 1093 (2), 1030 (1), 1007 (2), 971 (1), 943 (1), 910 (1), 895 (1), 851 (1), 738 (3), 709 (1), 590 (4), 578 (10), 563 (4), 547 (2), 540 (2), 533 (2), 523 (3), 514 (2), 486 (2), 475 (1), 455 (1), 435 (3), 423 (4), 398 (1), 381 (2), 371 (2), 339 (3), 315 (1), 265 (3), 248 (2), 239 (4), 226 (3), 200 (3), 156 (5).

Figure S3: NMR, IR and Raman spectra of $[TerNP]_2$ in C_6D_6 (solvent signals indicated by asterisk).

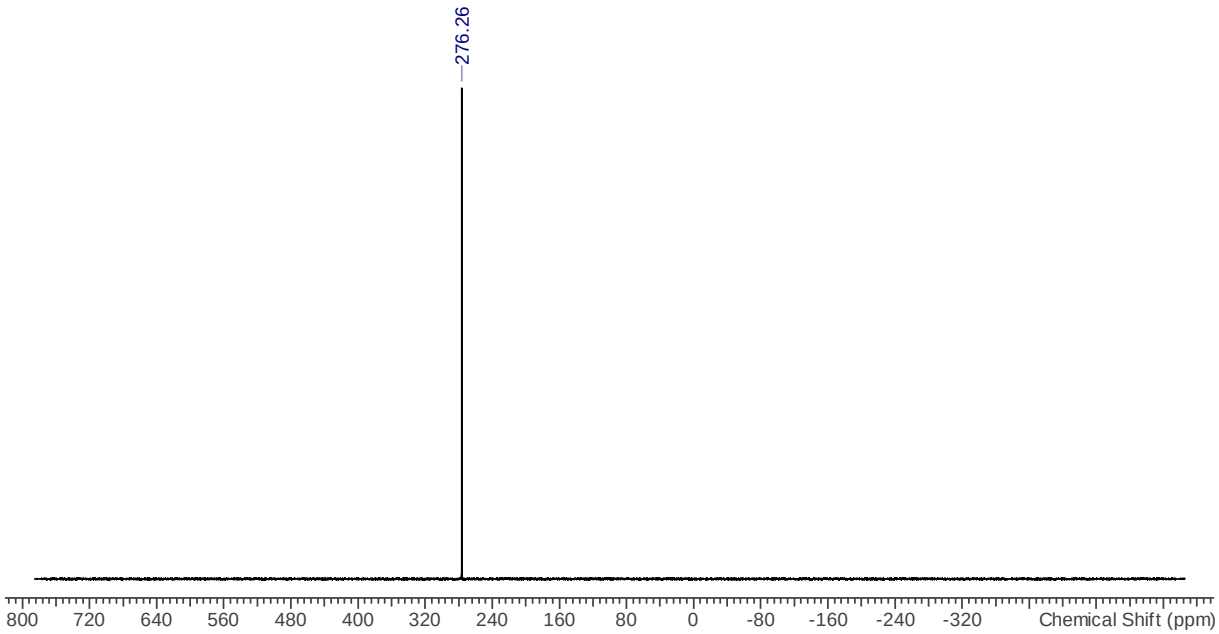
^{1}H NMR spectrum



$^{13}C\{^1H\}$ NMR spectrum



$^{31}P\{^{1}H\}$ NMR spectrum



2.4 Synthesis of hydrogen cyanide (HCN)

2.4.1 Method A

This product is synthesized according to a modified literature procedure.[12]

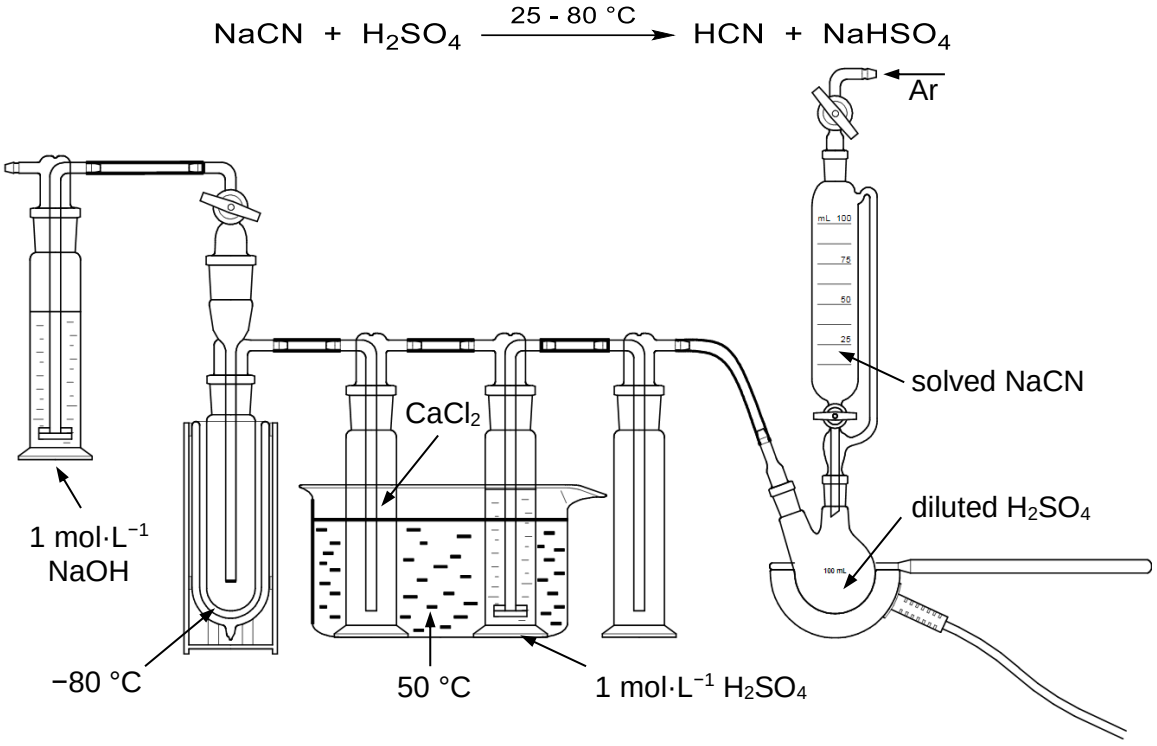


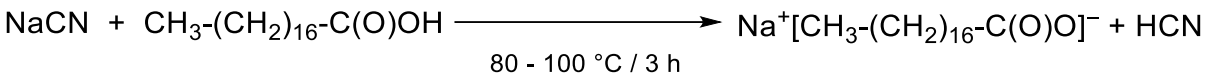
Figure S4: Apparatus for the synthesis of pure HCN.

This reaction is carried out under atmospheric conditions in a two-neck flask equipped with a gas inlet, a dropping funnel and a gas outlet. 95 % H_2SO_4 (22.91 g) is diluted with H_2O (15 mL) and heated to 50 °C (water bath). Sodium cyanide NaCN (11.45 g, 0.22 mol) is dissolved in H_2O (20 mL) and added dropwise over a period of 30 minutes to the H_2SO_4. The evolving gas is bubbled through a flask containing 1 mol·L^{-1} H_2SO_4 and subsequently dried using a column of $CaCl_2$, both of which are heated to 50 °C (water bath). Finally, the gas is passed through a cold trap (−80 °C, isopropanol bath) equipped with a pressure relief valve to collect the hydrogen cyanide HCN. A slow stream of Ar is passed through the apparatus to assist the collection of HCN gas. When the addition of NaCN is completed, the reaction vessel is heated to 80 - 90 °C (oil bath) for approximately 1 h. After completion of the reaction the cold trap containing the hydrogen cyanide is separated from the apparatus and the HCN is condensed into a flask filled with P_4O_{10} (~1 g) to remove any moisture. After warming up to ambient

temperature it is re-condensed into a clean flask and stored under argon atmosphere. Yield: 3.57 g (0.13 mol, 59 %) **See** Fehler! Verweisquelle konnte nicht gefunden w erden.**4.**

2.4.2 Method B

This product is synthesized according to a modified literature procedure.[13]



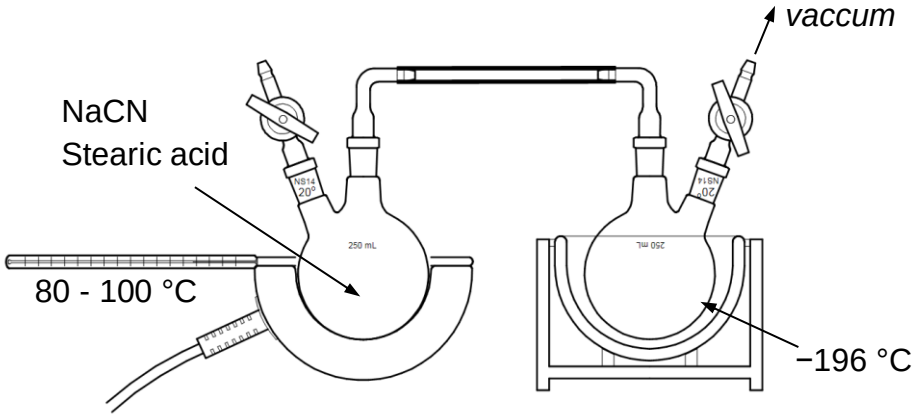


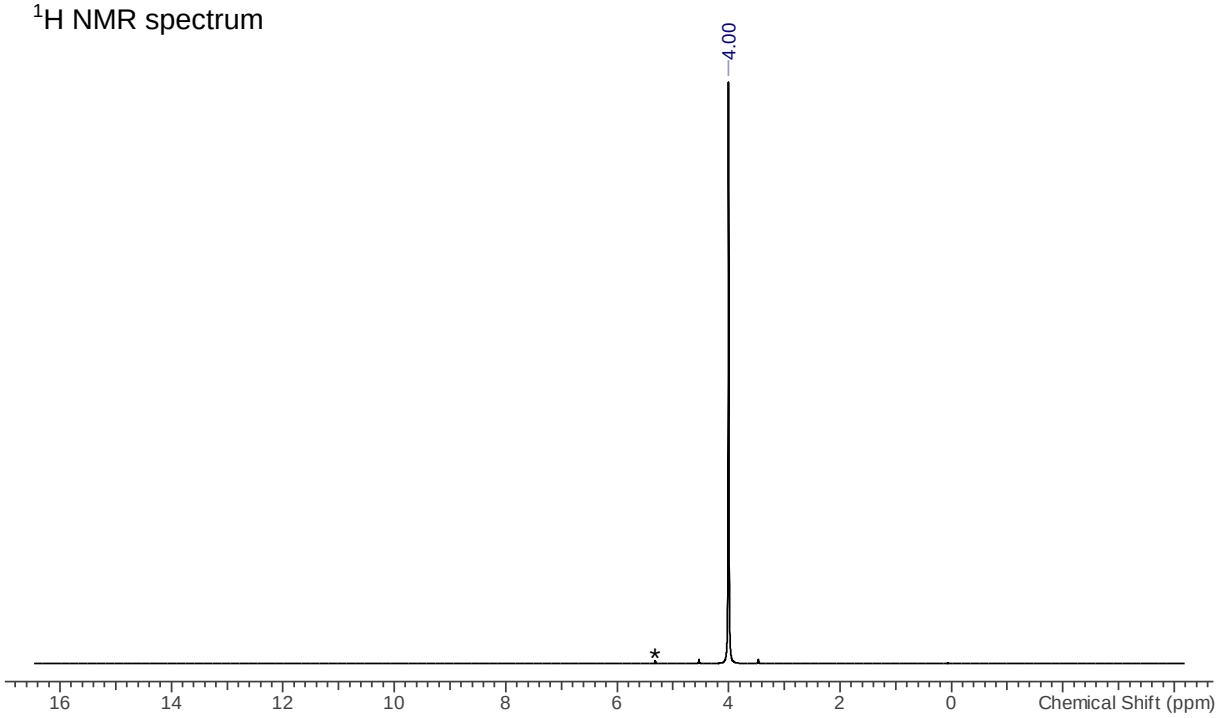
Figure S5: Apparatus for the synthesis of pure HCN with stearic acid.

In a Schlenk flask connected to a second flask acting as a condenser, stearic acid (25.60 g, 89.99 mmol) and NaCN (3.69 g, 71.53 mmol) are combined and then heated *in vacuo* ($1 \cdot 10^{-3}$ mbar) to 80 °C (oil bath) for 1.5 h. Afterwards, the temperature is raised to 100 °C (oil bath), which is maintained for another 1.5 h. The condenser is cooled the whole time using liquid nitrogen to collect the HCN gas. After completion of the reaction, the flask containing the hydrogen cyanide HCN is separated from the apparatus. Yield: 1.08 g (39.88 mol, 56 %). See **Fehler! Verweisquelle konnte nicht g efunden werden.**5.

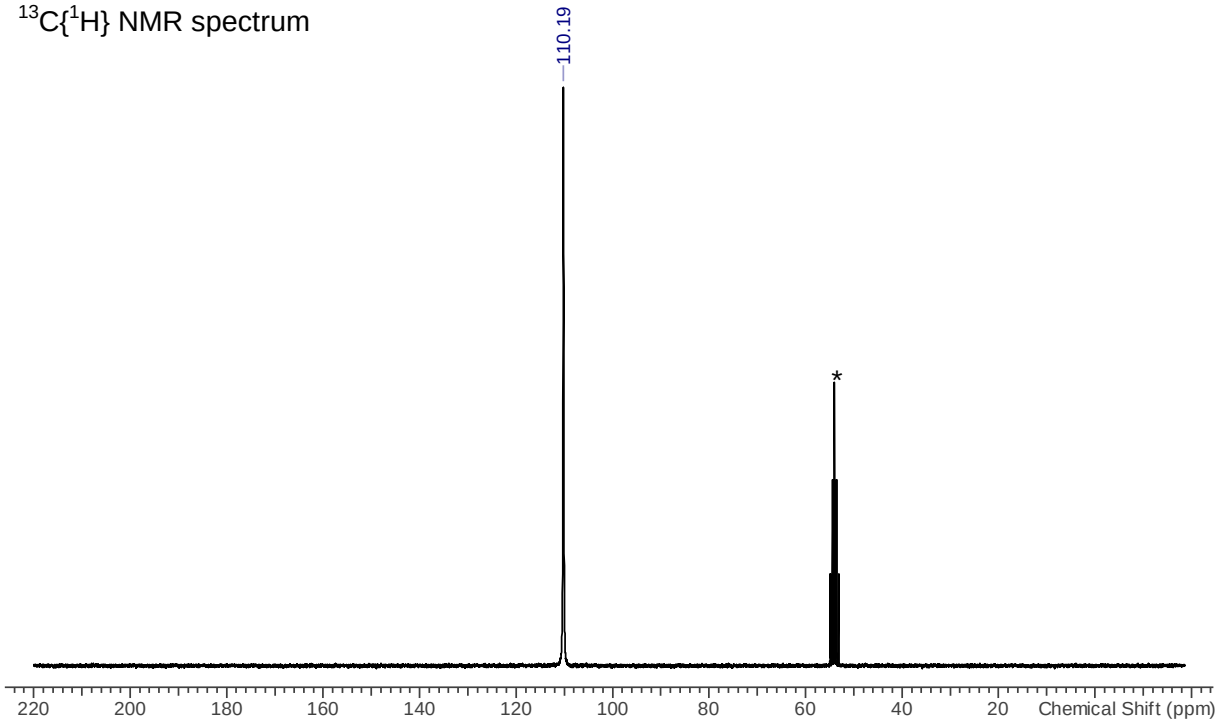
HCN (27.03 g·mol^{-1}): **mp.** −13 °C. **^{1}H NMR** (298 K, CD_2Cl_2, 250.1 MHz): δ = 4.00 (s, 1H, *H*CN, $^{1}J(^{1}H,^{13}C)$ = 266 Hz). **^{13}C{^{1}H} NMR** (298 K, CD_2Cl_2, 62.9 MHz): δ = 110.1 (s, HC*N*). **^{14}N{^{1}H} NMR** (298 K, CD_2Cl_2, 36.1 MHz): δ = −125.0 (s, HC*N*, $\Delta\nu_{1/2}$ = 50 Hz). **Raman** (633 nm, 6 mW, 20 s, 20 acc., 273 K, cm^{-1}): $\tilde{\nu}$ = 3151 (1), 2097 (10), 2063 (1), 1600 (1), 809 (1).

Figure S6: NMR and Raman spectra of HCN in CD_2Cl_2 (solvent signals indicated by asterisk).

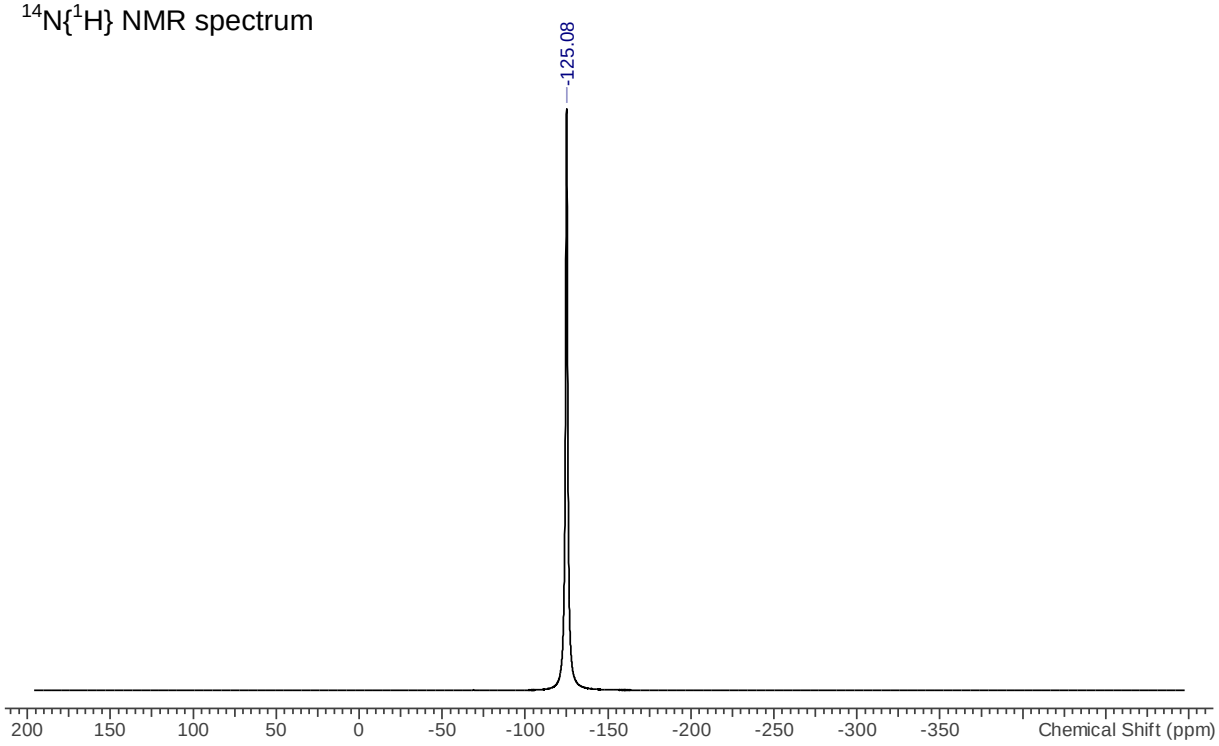
^{1}H NMR spectrum



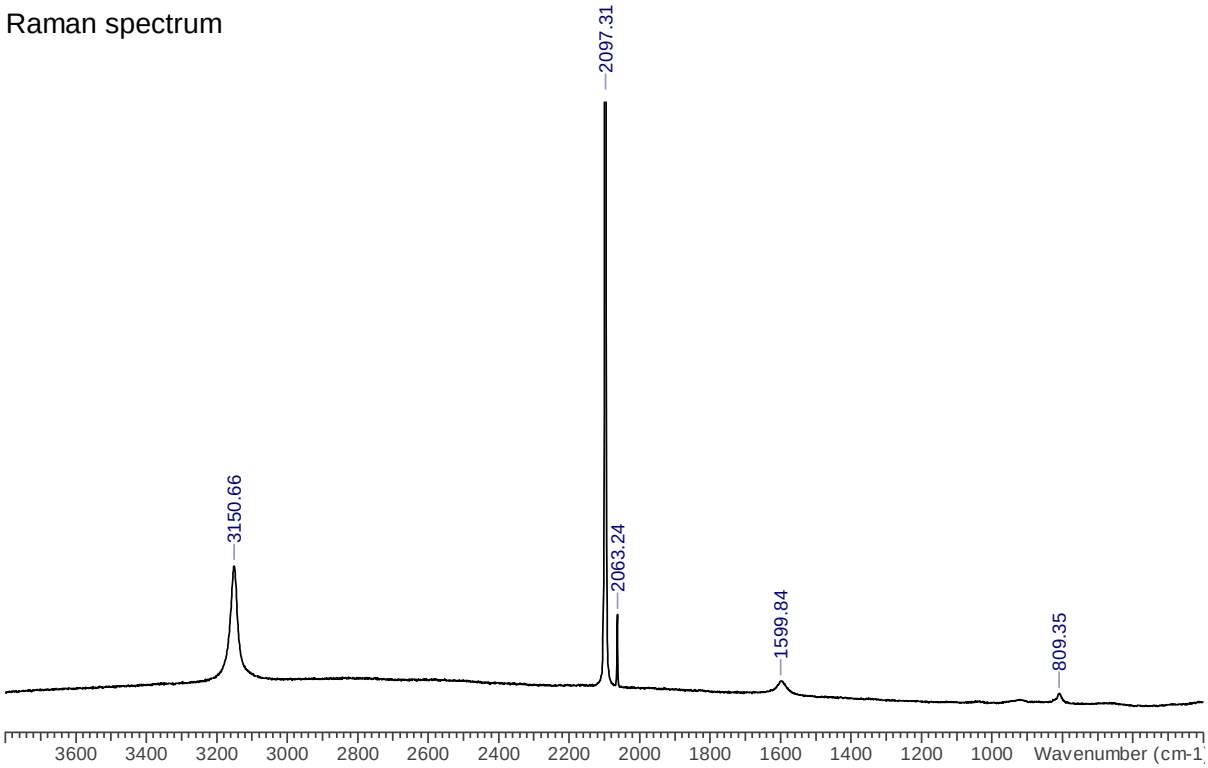
^{13}C{^{1}H} NMR spectrum



$^{14}N\{^{1}H\}$ NMR spectrum

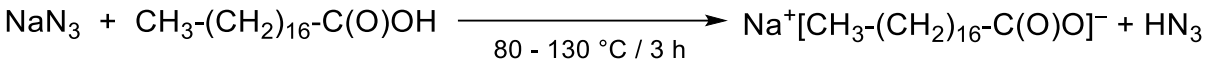


Raman spectrum



2.5 Synthesis of hydrogen azide (HN_3)

HN_3 is synthesized according to a modified literature procedure.[13] In general, it is not isolated, but condensed directly onto a frozen reaction mixture at −196 °C (Fehler! Verweisquelle konnte nicht gefunden werden.).



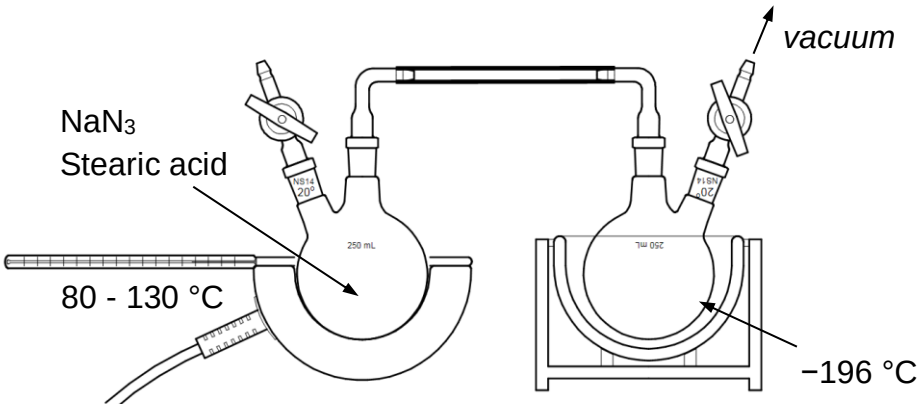


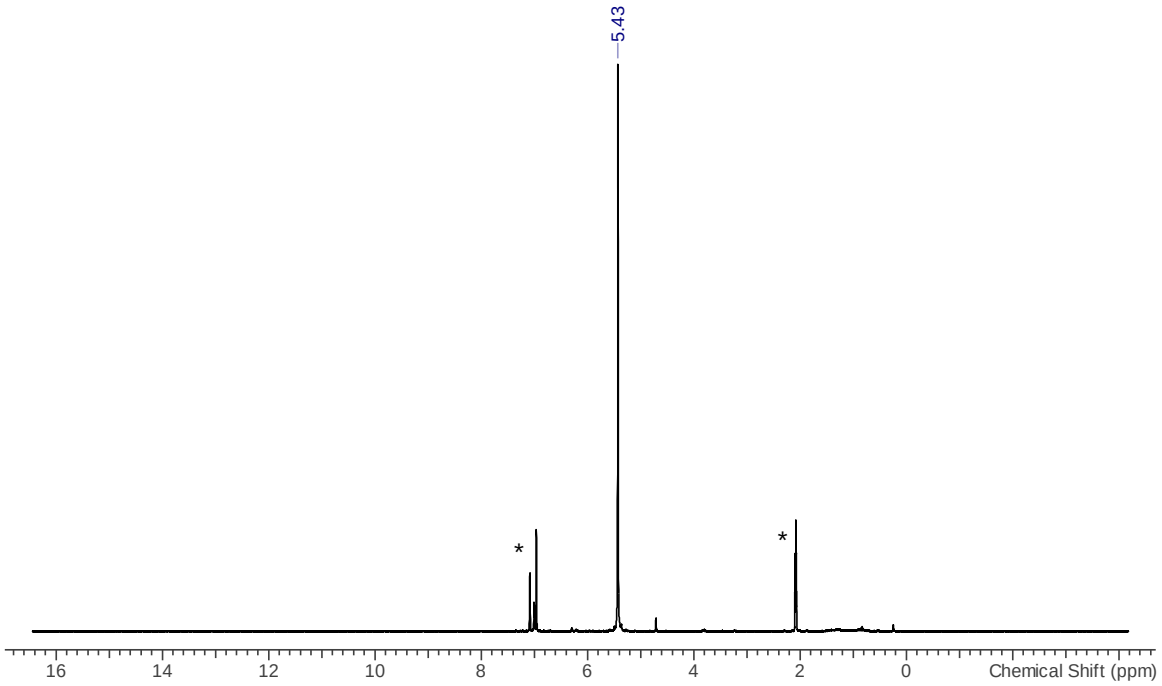
Figure S7: Apparatus for the synthesis of pure HN3 with stearic acid.

In a Schlenk flask connected to a second flask acting as a condenser, stearic acid (728 mg, 2.56 mmol) and sodium azide NaN_3 (75 mg, 1.16 mmol) are combined and then heated *in vacuo* ($1 \cdot 10^{-3}$ mbar) to 80 °C (oil bath) for 0.5 h. Afterwards, the temperature is raised to 100 °C (oil bath) for 1 h and then to 130 °C (oil bath) for 1.5 h. The condenser is cooled the whole time using liquid nitrogen. After completion of the reaction, the flask containing the hydrogen azide HN_3 is separated from the apparatus.

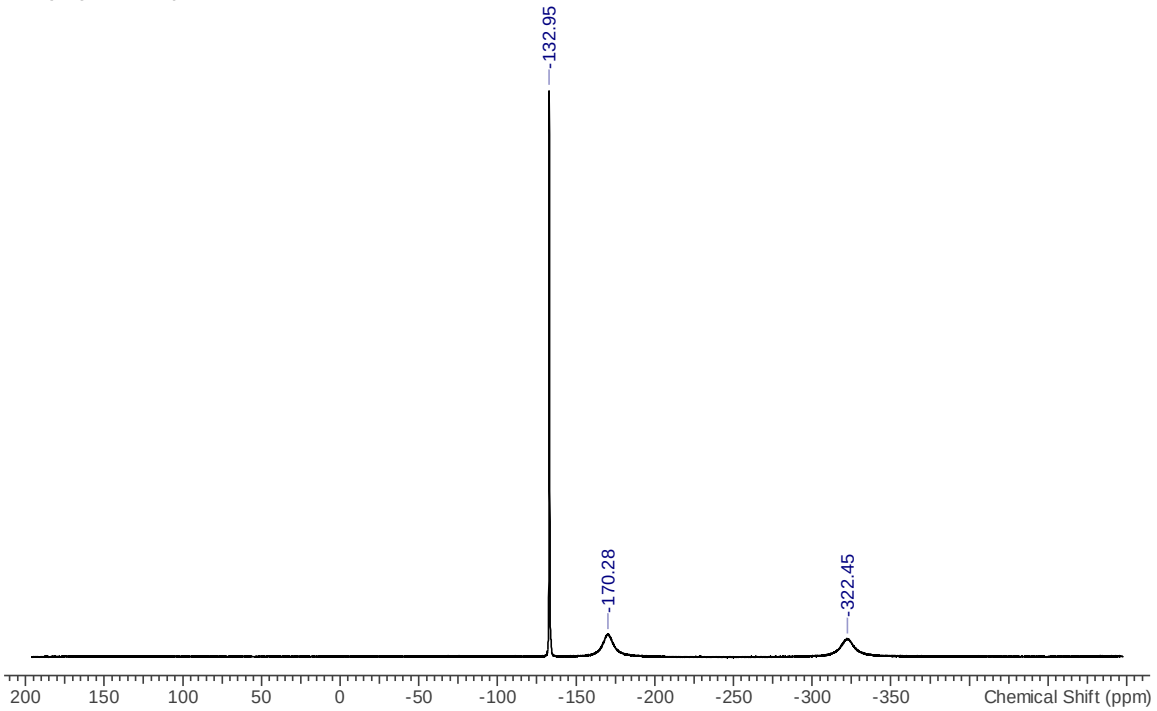
HN_3 (43.03 g·mol^{-1}): **^{1}H NMR** (298 K, C_7D_8, 300.1 MHz): δ = 5.43 (s, 1H, *H*N_3). **^{14}N{^{1}H} NMR** (298 K, C_7D_8, 36.1 MHz): δ = −322.4 (s, H*N*NN, $\Delta\nu_{1/2}$ = 340 Hz), −170.3 (s, HNN*N*, $\Delta\nu_{1/2}$ = 265 Hz), −133.0 (s, HN*N*N, $\Delta\nu_{1/2}$ = 13 Hz).

Figure S8: NMR spectra of HN_3 in toluene-d_8 (solvent signals indicated by asterisk).

^{1}H NMR spectrum

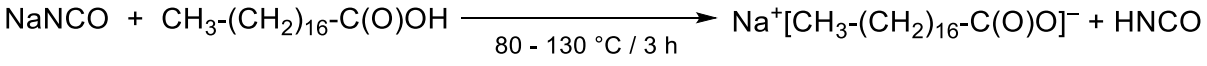


^{14}N{^{1}H} NMR spectrum



2.6 Synthesis of hydrogen cyanate (HNCO)

HNCO is synthesized according to a modified literature procedure.[13] In general, it is not isolated, but condensed directly onto a frozen reaction mixture at −196 °C.



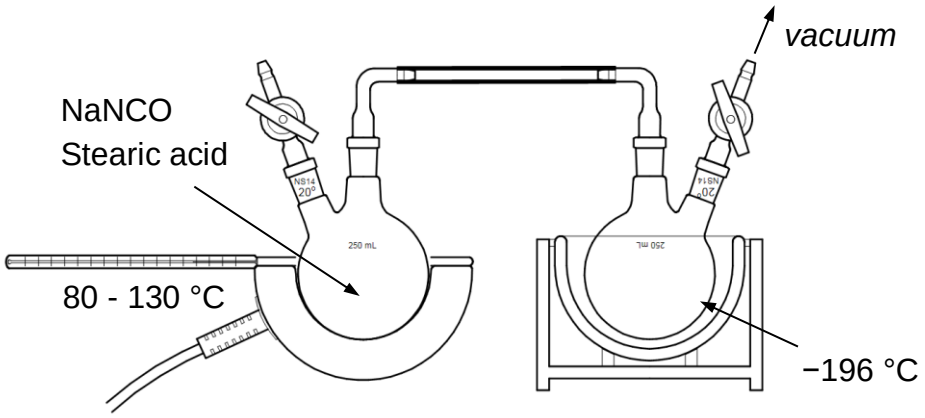
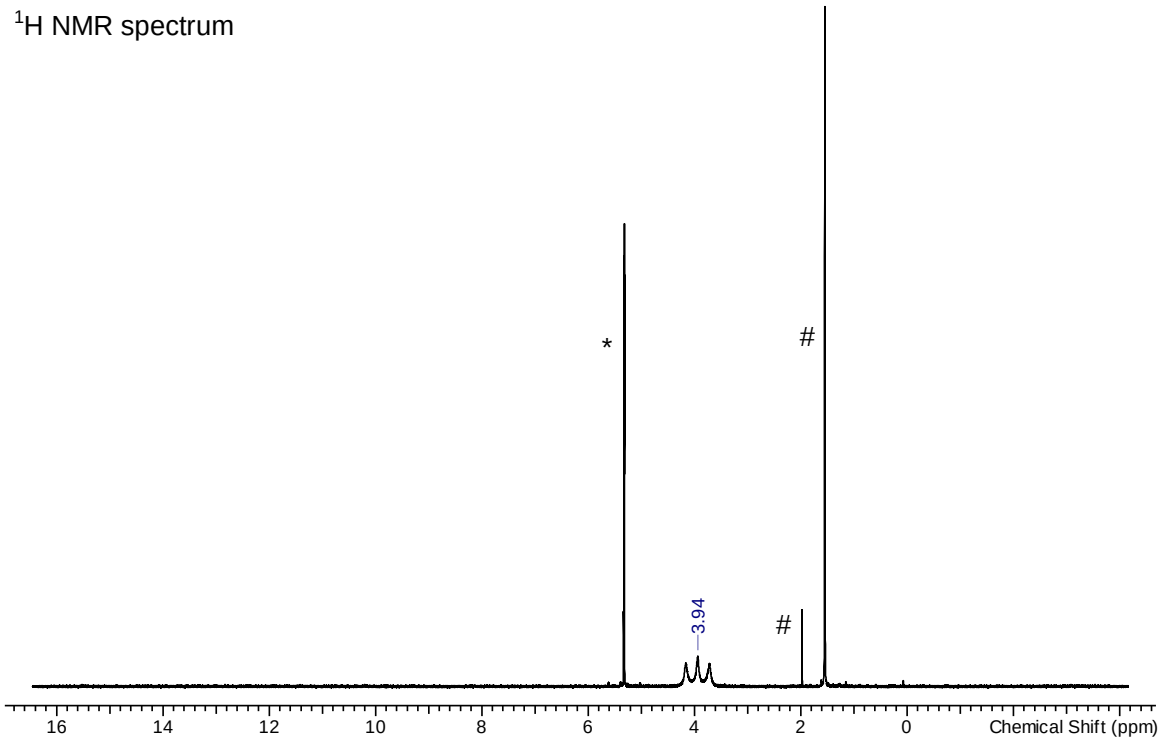


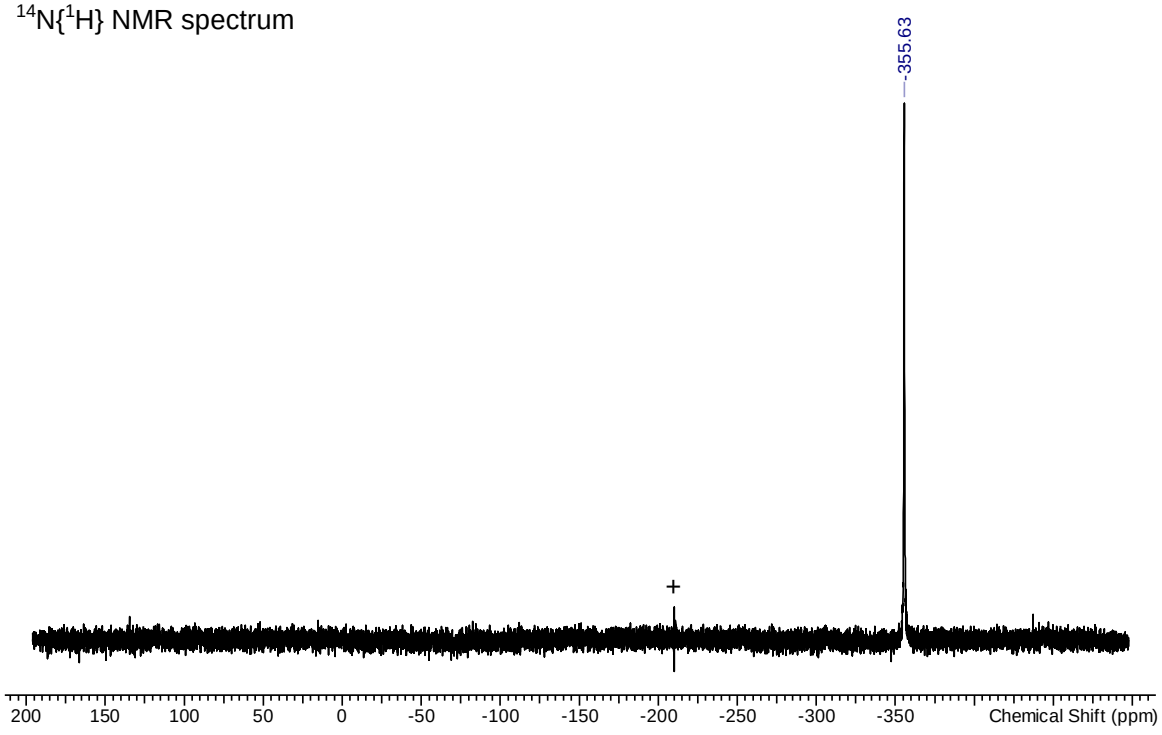
Figure S9: Apparatus for the synthesis of pure HNCO with stearic acid.

In a Schlenk flask connected to a second flask acting as a condenser, stearic acid (601 mg, 2.11 mmol) and sodium cyanate NaNCO (121 mg, 1.58 mmol) are combined and heated *in vacuo* ($1 \cdot 10^{-3}$ mbar) to 80 °C (oil bath) for 0.5 h. Afterwards, the temperature is raised to 100 °C (oil bath) for 1 h and then to 130 °C (oil bath) for 1.5 h. The condenser is cooled the whole time using liquid nitrogen. After completion of the reaction, the flask containing the hydrogen cyanate HNCO is separated from the apparatus.

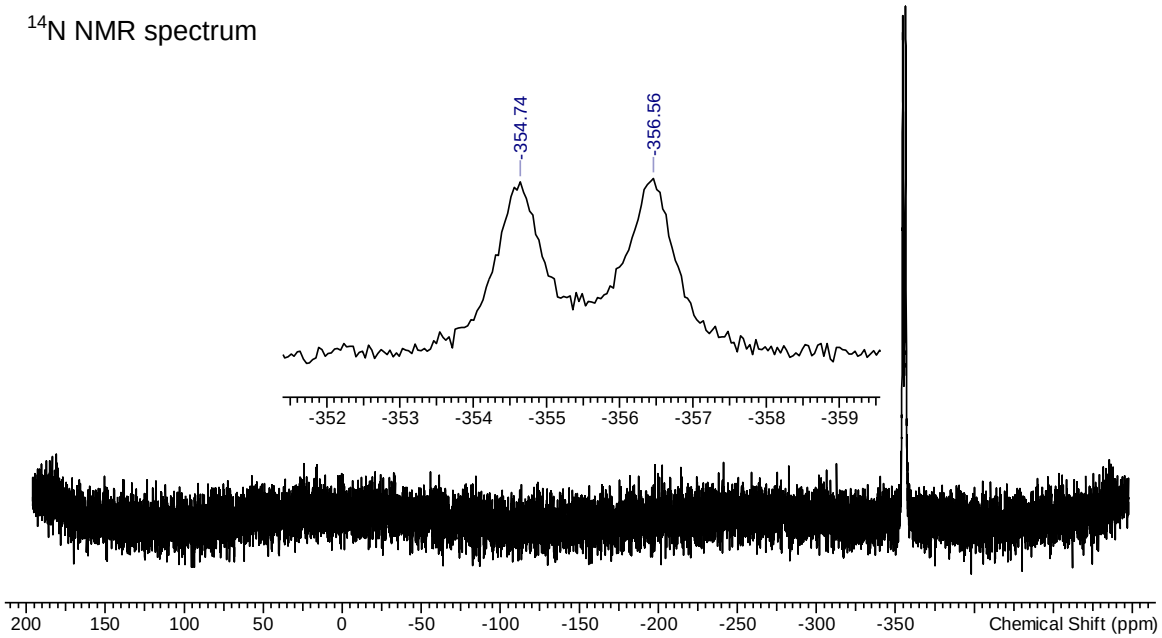
HNCO (43.02 g·mol^{-1}): **^{1}H NMR** (298 K, CD_2Cl_2, 300.13 MHz): δ = 3.94 (t, 1H, *H*NCO, $^{1}J(^{1}H,^{14}N)$ = 66 Hz). **^{13}C{^{1}H} NMR** (298 K, CD_2Cl_2, 75.5 MHz): δ = not observed. **^{14}N{^{1}H} NMR** (298 K, CD_2Cl_2, 36.1 MHz): δ = −355.6 (s, H*N*CO). **^{14}N NMR** (298 K, CD_2Cl_2, 36.1 MHz): δ = −355.6 (s, H*N*CO, $^{1}J(^{14}N,^{1}H)$ = 66 Hz). **Raman** (633 nm, 8 mW, 20 s, 20 acc., 233 K, cm^{-1}): 1384 (10), 1319 (2), 1280 (4).

Figure S10: NMR and Raman spectra of HNCO in CD_2Cl_2 (solvent signals indicated by asterisk, unknown impurities indicated by rhomb).

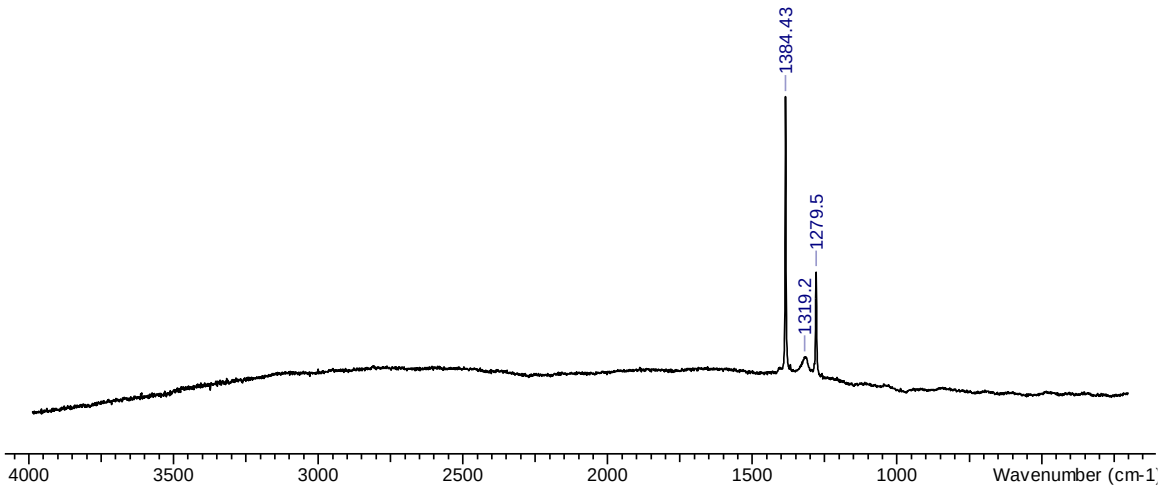




^{14}N NMR spectrum

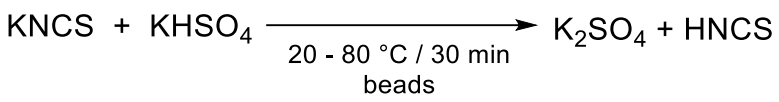


Raman spectrum



2.7 Synthesis of hydrogen thiocyanate (HNCS)

HNCS is synthesized according to a modified literature procedure.[14] It is not isolated, but condensed directly onto a frozen reaction mixture at −196 °C.



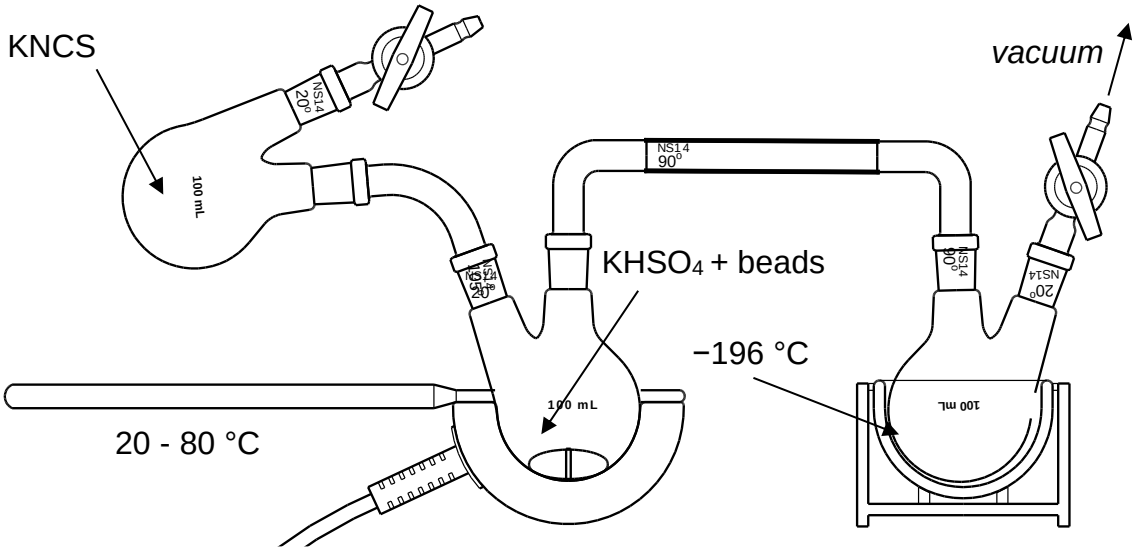
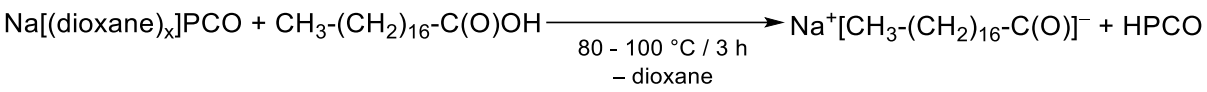


Figure S11: Apparatus for the synthesis of pure HNCS with KHSO4.

Potassium bisulfate $KHSO_4$ (16.23 g, 0.12 mol), glass beads and potassium thiocyanate KNCS (4.62 g, 0.05 mol) are weighed in two separate flasks. Under vacuum ($1 \cdot 10^{-3}$ mbar), the KNCS is added to the $KHSO_4$ at ambient temperature. Trituration of the two solids forms thiocyanic acid, which is condensed into a third flask at −196 °C. The reaction flask is slowly heated to 80 °C (oil bath). After about 30 minutes, when the solids begin to turn yellow, the reaction is stopped and the flask containing the condensed HNCS is removed from the apparatus.

2.8 Synthesis of phosphorus-containing analogue of Isocyanic Acid (HPCO)

HPCO is synthesized according to a modified literature procedure.[13] It is not isolated, but condensed directly onto a frozen reaction mixture at −196 °C.



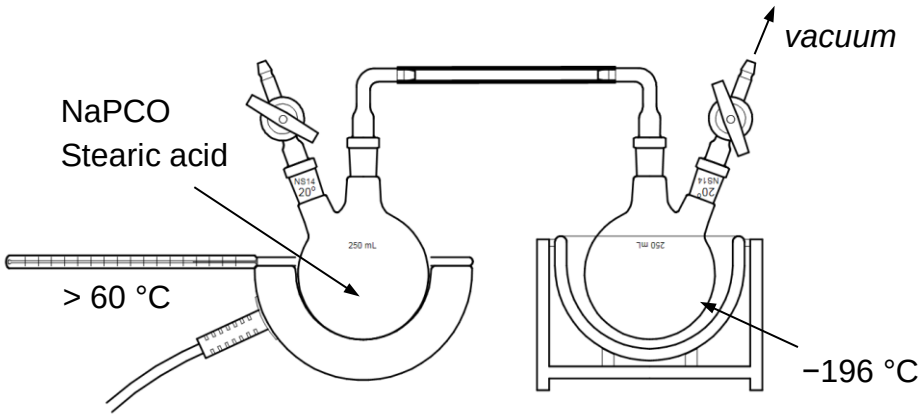


Figure S12: Apparatus for the synthesis of pure HNCO with stearic acid.

In a Schlenk flask connected to a second flask acting as a condenser, stearic acid (480 mg, 1.69 mmol) and sodium cyanate $[Na(dioxane)_x]PCO$ (95 mg, 0.56 mmol) are combined and heated *in vacuo* ($1 \cdot 10^{-3}$ mbar) to 70 °C (oil bath) for 3 h. The condenser is cooled the whole time using liquid nitrogen. After completion of the reaction, the flask containing the product is separated from the apparatus and an orange polymer could be observed. Also when attempting to trap HPCO with $[P(\mu\text{-NTer})]_2$, the formation of an insoluble orange polymer ($[PCO]_x$) was observed.

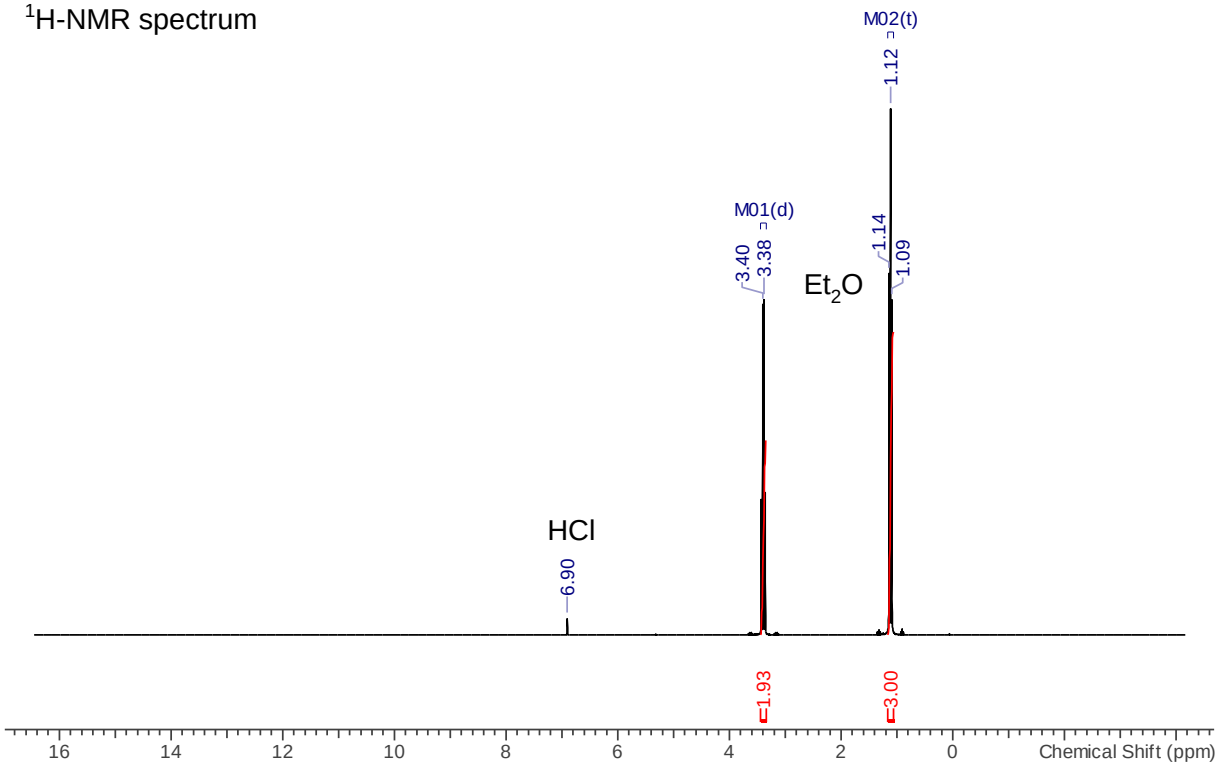
2.9 Synthesis of $Et_2O \cdot HCl$

$$2NaCl + H_2SO_4 \xrightarrow{2h,\ 0\ °C} 2\ HCl + Na_2SO_4$$

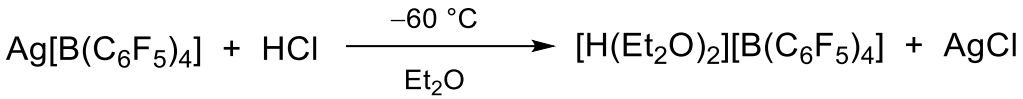
In a 100 mL three-necked flask equipped with a 100 mL dropping funnel HCl is evolved by the reaction of sodium chloride NaCl (32.6 g, 558 mmol) and sulfuric acid H_2SO_4 (60 mL, 95 %). H_2SO_4 is added dropwise over a period of 2 h to the pure NaCl which is cooled to 0 °C (isopropanol bath). The evolving gas is passed through a P_4O_{10} column and bubbled through a flask containing conc. H_2SO_4. Finally, the gas is passed through a flask equipped with an inlet pipe and a pressure relief. The flask contains diethyl ether (250 mL) and is cooled to 0 °C (isopropanol bath). The reaction is complete when the reaction flask is removed from the ice bath and no gas flow can be detected through the inlet pipe (c(HCl) = 6.15 mol·L^{-1}).

HCl (36.46 g·mol^{-1}): **^{1}H NMR** (298 K, CD_2Cl_2, 300.13 MHz): δ = 1.12 (t, 6H, $O(CH_2C\mathit{H}_3)_2$, $^3J(^1H,^1H)$ = 7.0 Hz), 3.39 (q, 4H, $O(C\mathit{H}_2CH_3)_2$, $^3J(^1H,^1H)$ = 7.0 Hz), 6.90 (s, 1H, *H*Cl).

^{1}H-NMR spectrum



2.10 Synthesis of Jutzi's acid $[H(Et_2O)_2][B(C_6F_5)_4]$

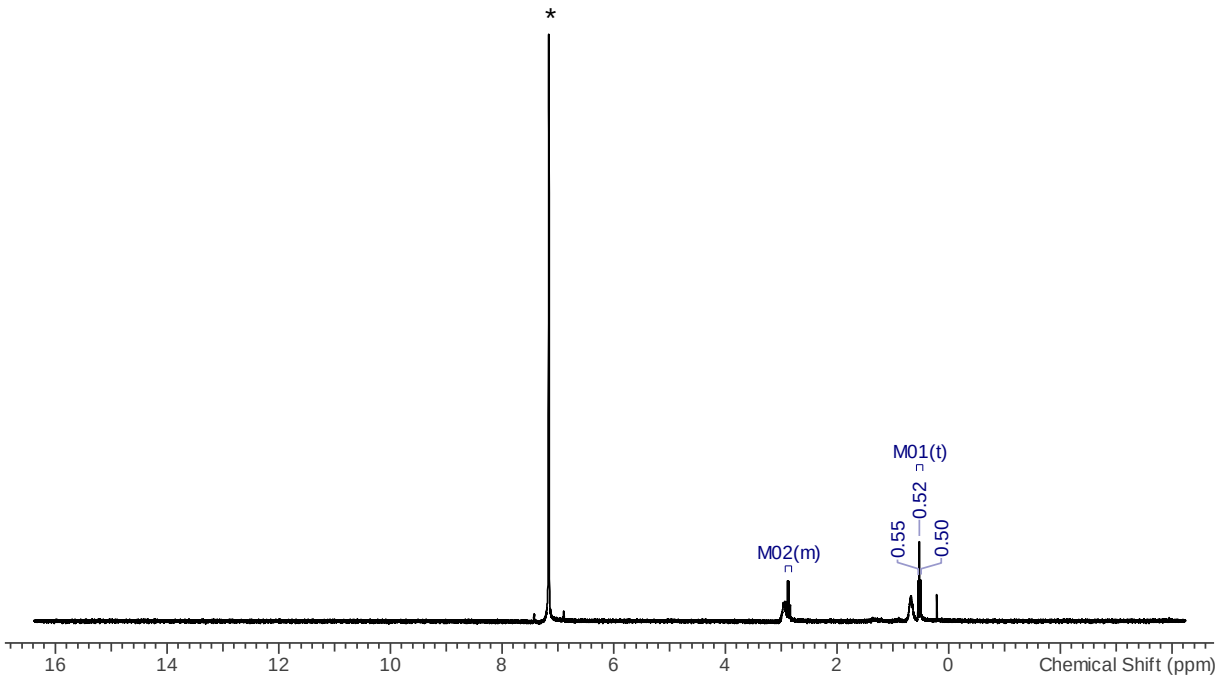


$[H(Et_2O)_2][B(C_6F_5)_4]$ is synthesized according to a modified literature procedure.[9]

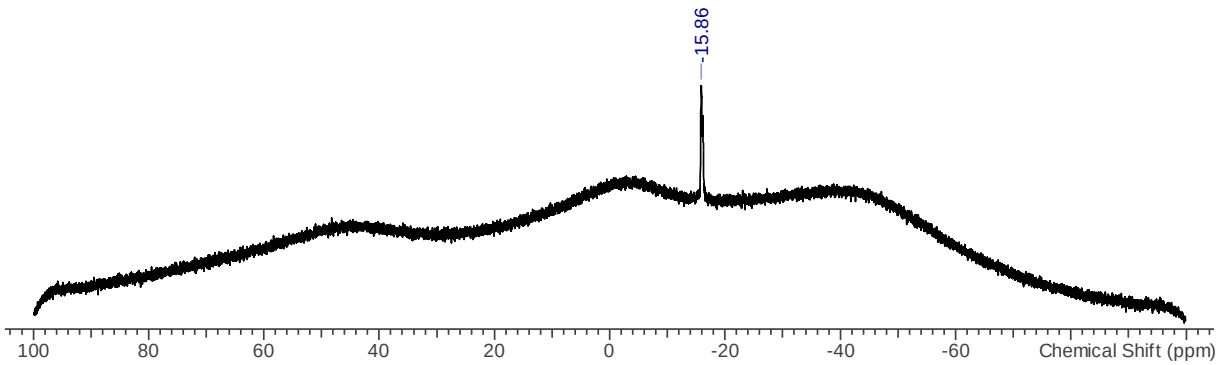
In a 100 mL flask silver tetrakis(pentafluorophenyl)borate $Ag[B(C_6F_5)_4]$ (3.22 g, 4.09 mmol) is suspended in diethyl ether (50 mL). The reaction mixture is cooled to −60 °C (isopropanol bath). To the stirred grey suspension, HCl in ether (6 mol·L^{-1}, 7 mL) is added *via* syringe. The formation of a light grey suspension and a white solid could be observed. The suspension is allowed to warm to room temperature overnight. All volatile components are removed ($1\cdot10^{-3}$ mbar, 30 °C (water bath), 2 h). Fresh diethyl ether is added (50 mL) resulting in a champagne coloured solution and a white precipitate. The solution is filtered (G4) and concentrated to incipient crystallisation. The solution is slowly (24 h) cooled to −80 °C (refrigerator with oil bath) resulting in the deposition of colourless crystals. The supernatant is removed by syringe and discarded. The remaining crystals are dried *in vacuo* ($1\cdot10^{-3}$ mbar, 40 °C (water bath), 3 h), yielding 2.28 g (2.75 mmol, 67 %) of $[H(Et_2O)_2][B(C_6F_5)_4]$.

$[H(Et_2O)_2][B(C_6F_5)_4]$] (828.30 g·mol^{-1}): **mp**. 156 °C (dec.). **EA** calc. (found), %: C, 46.40 (46.82); H, 2.56 (2.74). **^{1}H NMR** (298 K, C_6D_6, 300.1 MHz): δ = 0.52 (t, $^3J(^1H,^1H)$ = 7.2 Hz, 12H, CH_3), 2.87 (q, $^3J(^1H,^1H)$ = 7.2 Hz, 8H, CH_2). **^{11}B NMR** (298 K, C_6D_6, 96.3 MHz): δ = −15.9 (s, 1B, $[B(C_6F_5)_4]^-$). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 75.5 MHz): No signals observed. **^{19}F NMR** (298 K, C_6D_6, 282.4 MHz): δ = −132.3 (br dd, $^3J(^{19}F,^{19}F)$ = 105 Hz, $^4J(^{19}F,^{19}F)$ = 10 Hz, 2F), −162.6 (br dt, $^3J(^{19}F,^{19}F)$ = 296 Hz, $^4J(^{19}F,^{19}F)$ = 21 Hz, 1F), −166.9 (br dt, $^3J(^{19}F,^{19}F)$ = 259 Hz, $^4J(^{19}F,^{19}F)$ = 17 Hz, 2F). **Raman** (633 nm, 8 mW, 10 s, 10 acc., 298 K, cm^{-1}): fluorescence, 2953 (2), 1645 (7), 1451 (7), 1325 (8), 1229 (8), 1134 (8), 1048 (8), 947 (8), 855 (9), 821 (9), 701 (9), 619 (9), 584 (10), 490 (10), 477 (10), 449 (9), 424 (10), 392 (9), 358 (9), 312 (9), 252 (8).

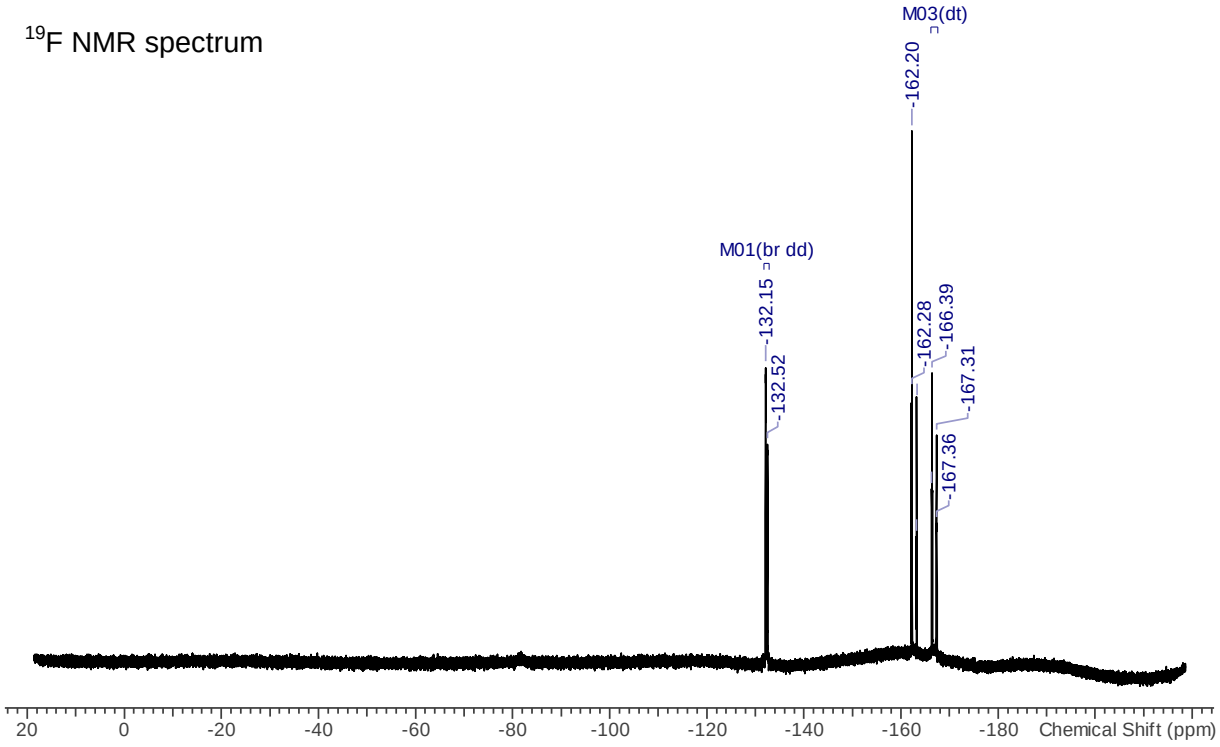
^{1}H NMR spectrum



^{11}B NMR spectrum

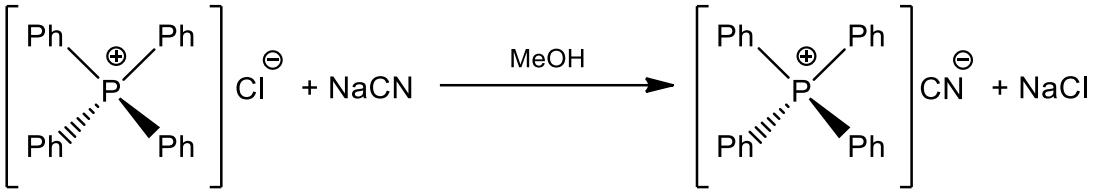


^{19}F NMR spectrum



2.11 Synthesis of [Ph4P]CN

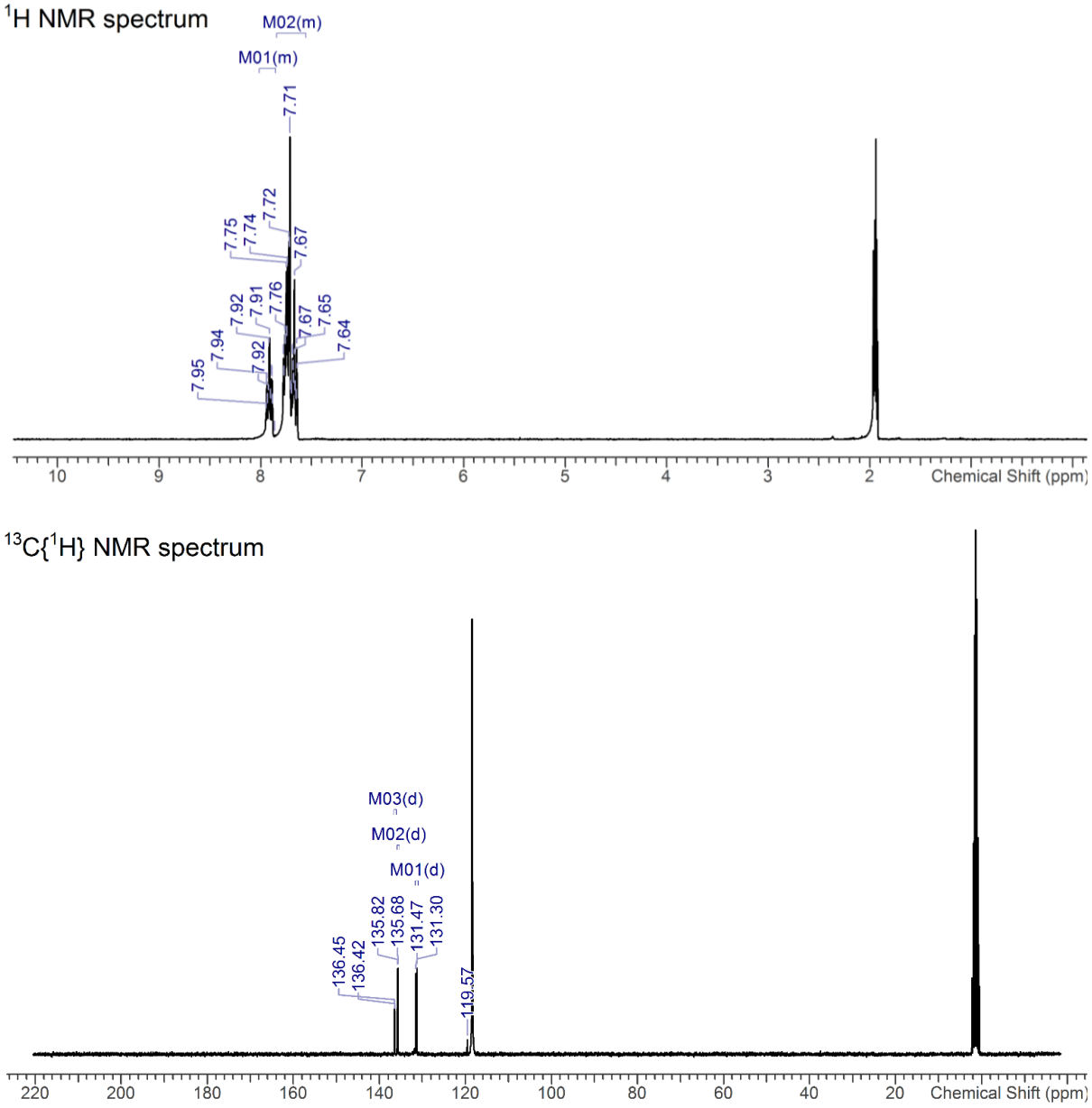
[PPh4]CN is synthesized according to a modified literature procedure.[15]



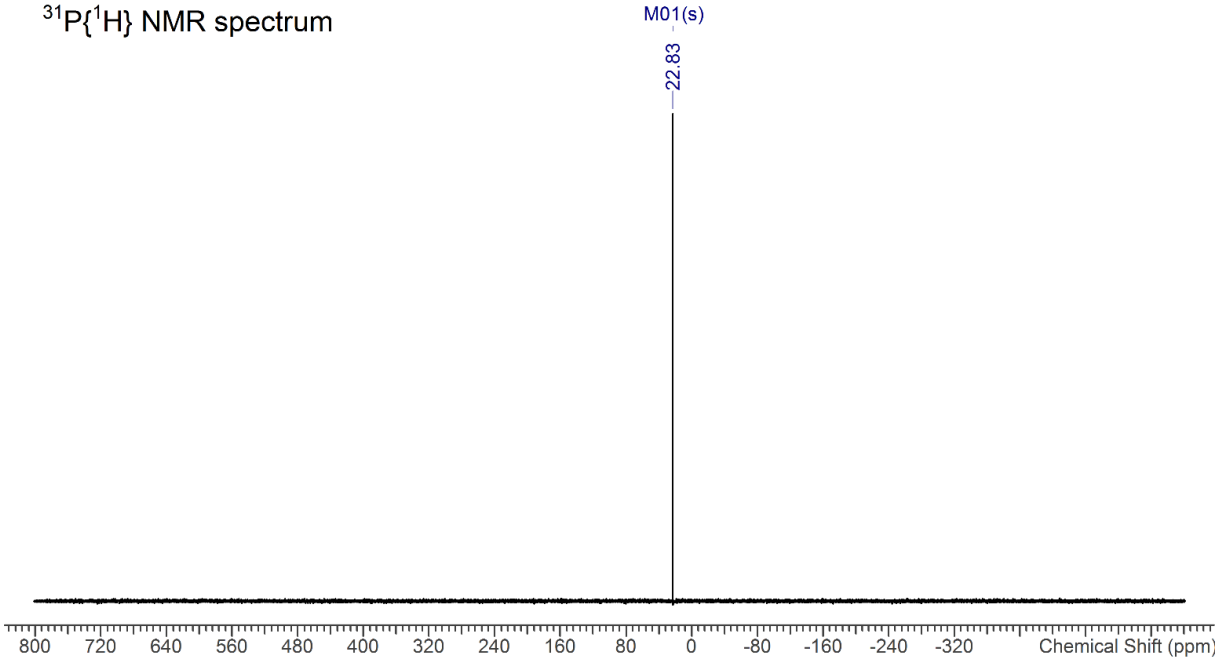
[PPh4]Cl (3.40 g, 9.08 mmol) is placed in a Schlenk flask along with NaCN (1.34 g, 27.30 mmol). MeOH (11 mL) is added which resulted in a suspension. The mixture is stirred for 24 h at room temperature and the solvent is removed *in vacuo* and the remaining solid is dried ($1 \cdot 10^{-3}$ mbar, 100 °C (oil bath), 2 h). Afterwards, the residue is suspended in 9 mL of acetonitrile. The suspension is filtered and the solvent is removed *in vacuo* ($1 \cdot 10^{-3}$ mbar, 50 °C (water bath), 1 h). Crystals could be obtained by recrystallization from a benzene (8 mL) and acetonitrile (3 mL) mixture, leading to slightly pink crystals (0.50 g, 1.37 mmol) in yields of 15 %.

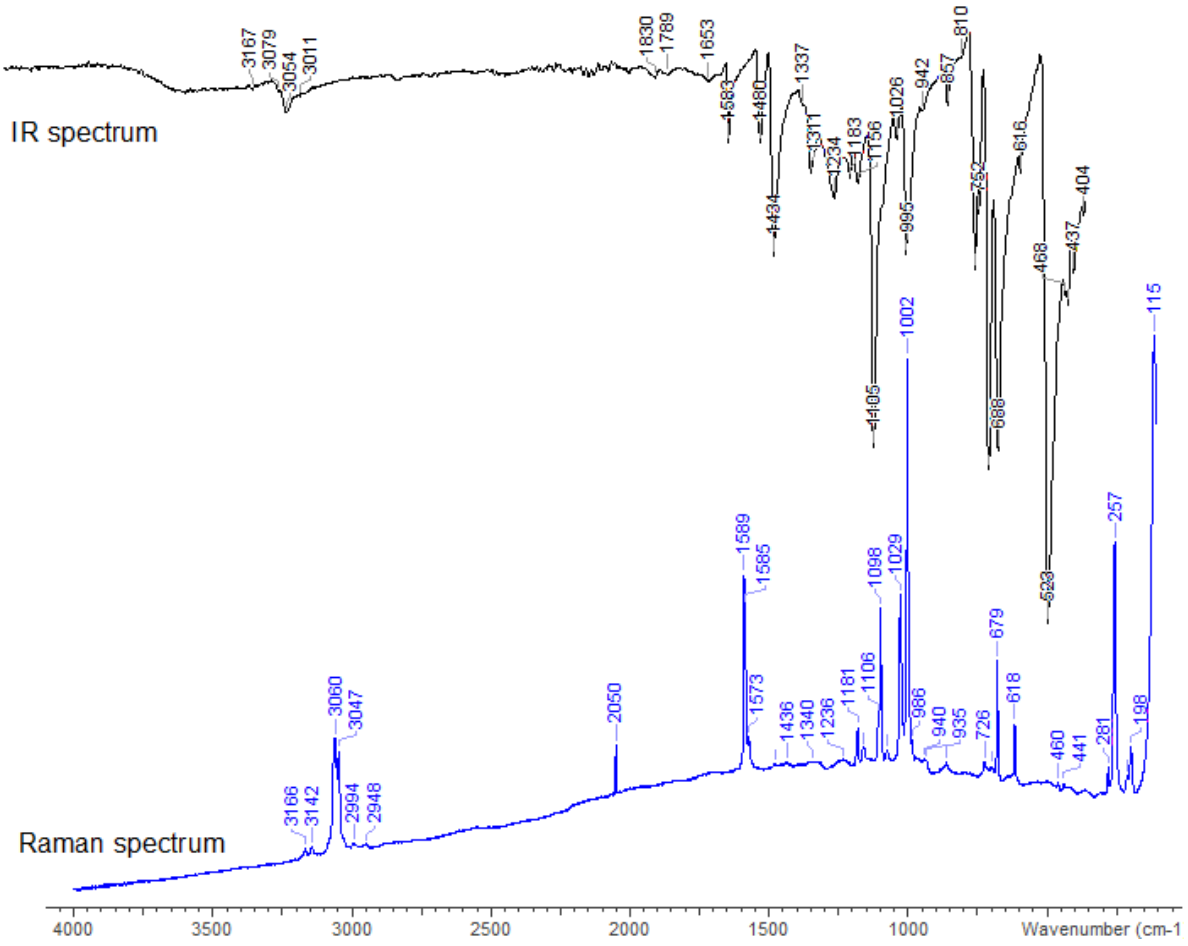
$C_{25}H_{20}NP$ (365.41 g/mol): **mp.** 220 °C (dec.). **EA** calc. (found), %: C, 82.17 (81.06); H, 5.52 (5.73); N, 3.83 (3.86). **^{1}H NMR** (297 K, CD_3CN, 300.13 MHz): δ = 7.72 (m, 16 H, *o*-Ph, *m*-Ph); 7.92 (m, 4 H, *p*-Ph). **^{13}C{^{1}H} NMR** (297 K, CD_3CN, 125.8 MHz): δ = 119.6 (d, *i*-C, $^{1}J(^{13}C,^{31}P)$ = 88 Hz); 131.4 (d, *o*-C, $^{2}J(^{13}C,^{31}P)$ = 13 Hz); 135.7 (d, 8 *m*-C, $^{3}J(^{13}C,^{31}P)$ = 10 Hz); 136.4 (d, *p*-C, $^{4}J(^{13}C,^{31}P)$ = 3 Hz); *n.o.* (CN^-). **^{31}P{^{1}H} NMR** (297 K, CD_3CN, 121.5 MHz): δ = 22.8 (s, $[PPh_4]^+$). **IR** (ATR, 32 scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 404 (S), 437 (M), 457 (M), 616 (S), 688 (W), 719 (W), 764 (M), 810 (VS), 857 (S), 942 (S), 995 (S), 1026 (S), 1105 (W), 1156 (S), 1181 (S), 1234 (S), 1311 (S), 1434 (S), 1480 (S), 1583 (S), 1653 (VS), 1789 (VS), 1830 (VS), 3011 (S), 3054 (S), 3167 (VS). **Raman** (633 nm, 8 mW, 30 s, 4 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 115 (10), 198 (3), 211 (2), 257 (6), 281 (2), 441 (2), 460 (2), 618 (3), 679 (4), 698 (2), 726 (2), 863 (2), 935 (2), 940 (2), 986 (3), 1002 (10), 1029 (5), 1075 (3), 1098 (5), 1106 (3), 1160 (3), 1181 (3), 1236 (2), 1340 (2), 1436 (2), 1476 (2), 1573 (3), 1585 (5), 1589 (6), 2050 (3), 2948 (1), 2994 (1), 3047 (3), 3060 (3), 3142 (1), 3166 (1).

Figure S13: NMR, Raman and IR spectra of $[Ph_4P]CN$ in CD_3CN.



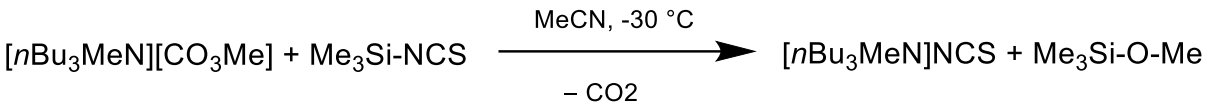
$^{31}P\{^{1}H\}$ NMR spectrum





2.12 Synthesis of [*n*Bu$_3$NMe]NCS

[*n*Bu$_3$NMe]NCS is synthesized according to a modified literature procedure.[16]

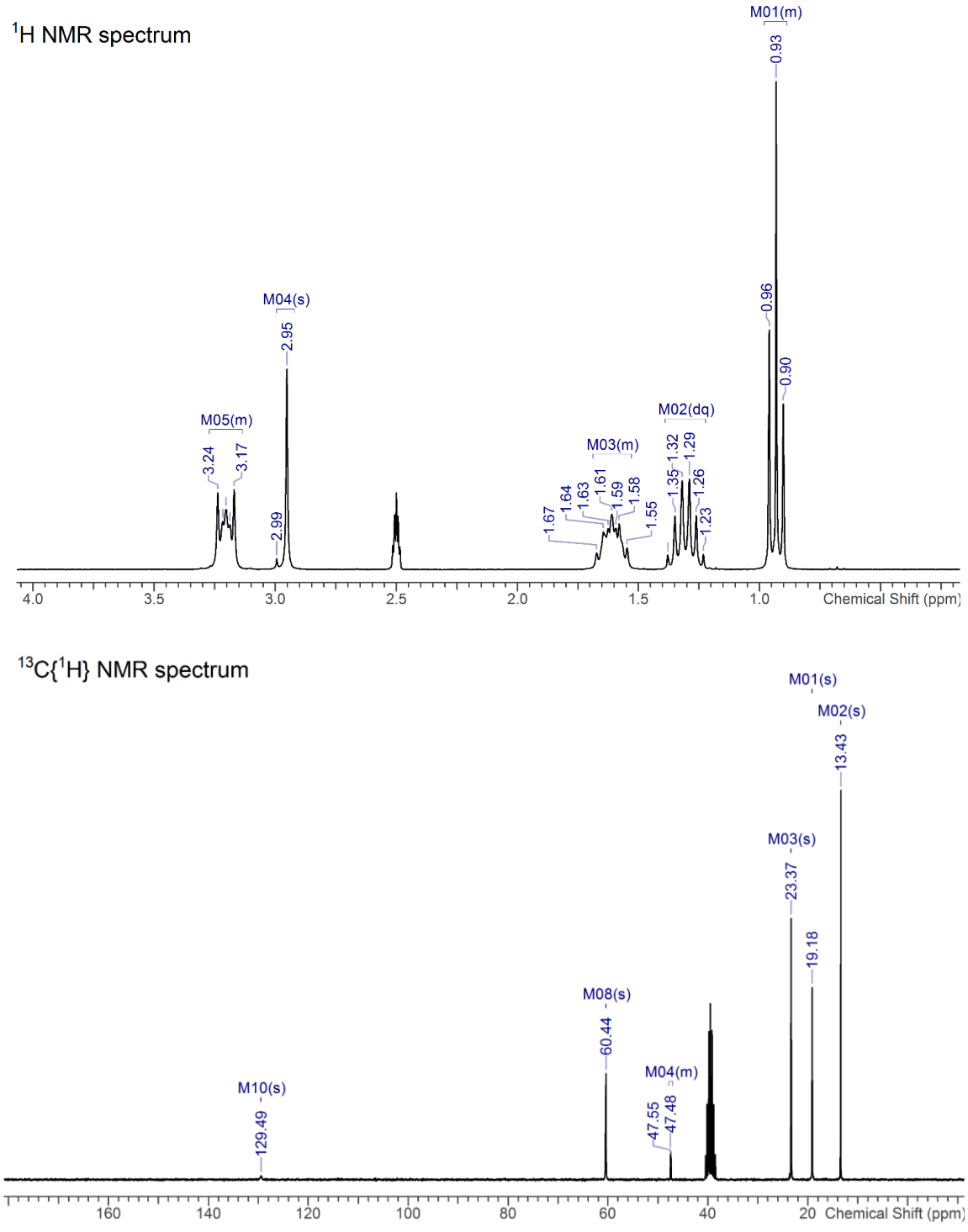


In a three-neck round-bottom flask equipped with a stir bar, tributylmethylammonium carbonate (0.43 g, 1.55 mmol, 1 eq.) is dissolved in acetonitrile (5 mL). Me_3Si–NCS (0.22 g, 1.67 mmol, 1.1 eq.) are added via syringe over a period of 20 min to the carbonate solution at −30 °C (cooled with a isopropanol bath). The mixture is stirred for 30 minutes, warmed up to ambient temperature and allowed to stir for additional 30 minutes. All volatiles are removed *in vacuo* ($1\cdot10^{-3}$ mbar, 50 °C (water bath), 1 h). To the resulting residue, diethyl ether (15 mL) is added, stirred and dried in vacuuo ($1\cdot10^{-3}$ mbar, 50 °C (water bath), 1 h). This procedure is repeated 3 times and helps to remove acetonitrile from the residue. Finally, the solid is dried *in vacuo* ($1\cdot10^{-3}$ mbar, 60 °C (water bath), 2 h), yielding in 0.39 g of colorless [*n*Bu$_3$MeN]SCN (1.50 mmol, 97 %).

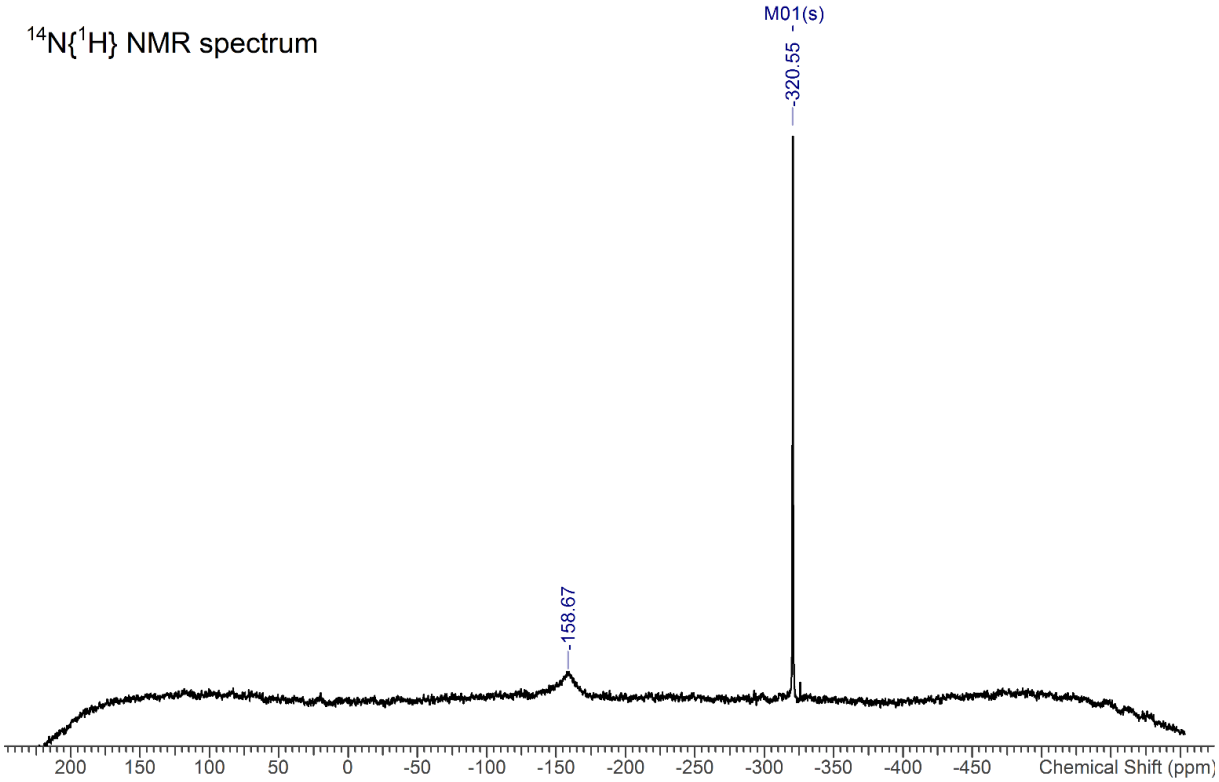
$C_{14}H_{30}NS$ (258.47 g·mol^{-1}): **mp.** 100 °C, 207 °C (dec.). **EA** found % (calc.) C, 65.06 (65.68); H, 11.70 (11.97); N, 10.84 (10.52); S, 12.41 (12.65). **^{1}H NMR** (298 K, $(CD_3)_2SO$, 300.13 MHz) δ = 0.92 (t, 9H, C*H*$_3$CH$_2$, $^3J(^1H,^1H)$ = 7 Hz), 1.29 (sex, 6H, NCH$_2$CH$_2$C*H*$_2$, $^3J(^1H,^1H)$ = 7 Hz), 1.68-1.51 (m, 6H, NCH$_2$C*H*$_2$), 2.94 (s, 3H, NC*H*$_3$), 3.27-3.12 (m, 6H, NC*H*$_2$). **^{13}C{^{1}H} NMR** (297 K, $(CD_3)_2SO$, 74.5 MHz) δ = 13.4 (s, 3C, *C*H$_3$CH$_2$), 19.1 (s, 3C, CH$_3$*C*H$_2$), 23.3 (s, 3C, NCH$_2$*C*H$_2$), 47.3 (t, 1C, N*C*H$_3$, $^1J(^{13}C,^{14}N)$ = 4 Hz), 60.4 (t, 3C, N*C*H$_2$, $^1J(^{13}C,^{14}N)$ = 2 Hz), 129.7-129.1 (m, 1C, S*C*N). **^{14}N{^{1}H} NMR** (300 K, $(CD_3)_2SO$, 36.1 MHz) δ = –158.9 (s, 1N, SC*N*, $\Delta\nu^{1/2}$ = 160 Hz), –320.4 (s, 1N, [*n*Bu$_3$*N*Me]). **IR** (ATR-IR, 8 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 425 (w), 439 (w), 464 (w), 486 (w), 501 (w), 515 (w), 536 (w), 561 (w), 577 (w), 600 (w), 610 (w), 618 (w), 631 (w), 641 (w), 651 (w), 670 (w), 688 (w), 736 (m), 754 (w), 798 (w), 833 (w), 892 (m), 923 (w), 969 (w), 1004 (w), 1016 (w), 1033 (w), 1066 (w), 1107 (w), 1167 (w), 1195 (w), 1241 (w), 1253 (w), 1286 (w), 1346 (w), 1360 (w), 1385 (w), 1461 (m), 2010 (w), 2051 (vs), 2793 (w), 2875 (w), 2937 (m), 2962 (m), 3022 (w). **Raman** (633 nm, 8 mW, 20 s, 10 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 274 (1), 309 (1), 367 (1), 438 (1), 507 (1), 525 (1), 575 (1), 736 (2), 780 (1), 805 (1), 879 (2), 903 (2), 923 (1), 942 (1), 970 (1), 1004 (1), 1035

(1), 1066 (2), 1107 (2), 1133 (1), 1156 (1), 1165 (1), 1193 (1), 1259 (1), 1275 (1), 1287 (1), 1325 (2), 1348 (2), 1395 (2), 1448 (4), 1491 (2), 2056 (9), 2751 (2), 2783 (2), 2874 (8), 2916 (8), 2938 (10), 2963 (8), 3016 (4). **MS** (CI^+, m/z (%)): 17 = 200 ([nBu$_3$NMe]$^+$); 458 ([nBu$_3$NMe]$_2$[SCN]$^+$); CI^-: m/z = 316 ([nBu$_3$NMe][SCN]$_2^-$).

F**igure S14:** NMR, Raman and IR spectra of [nBu3NMe]NCS in dmso-d_6.

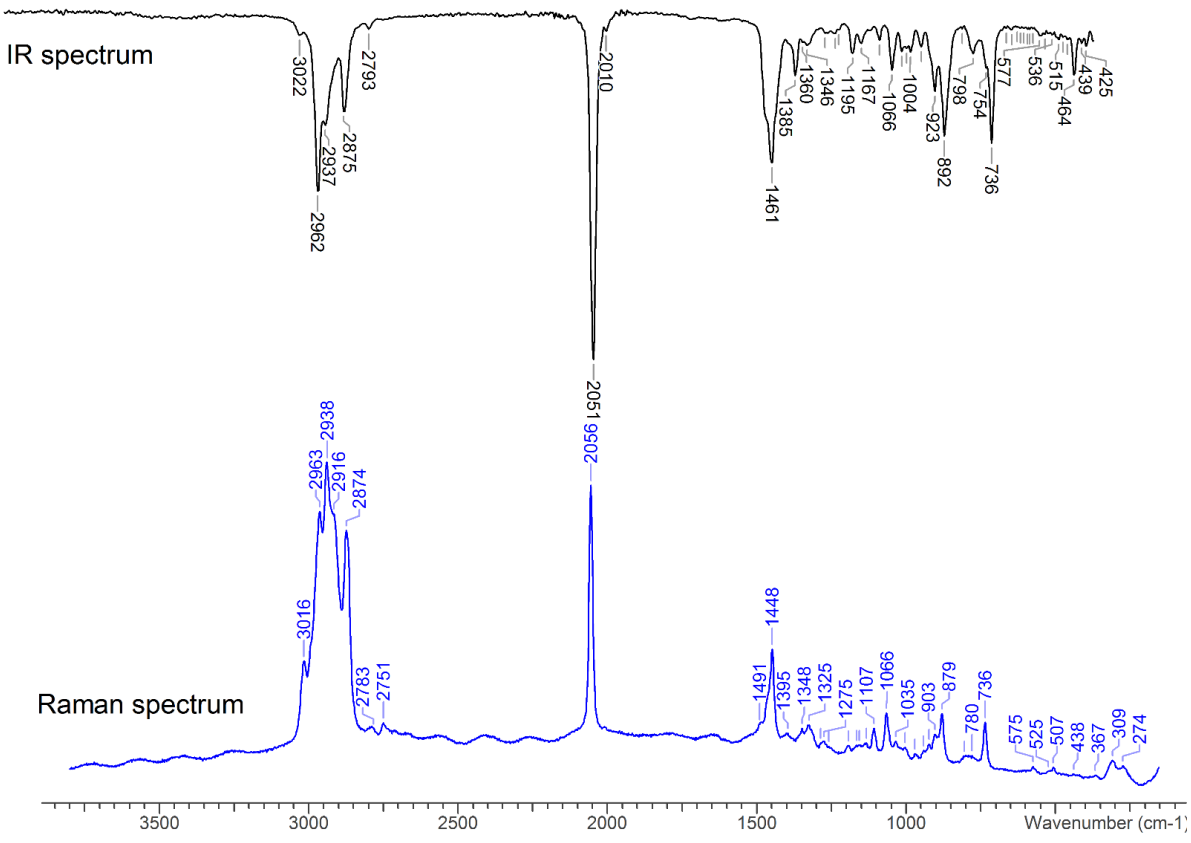


$^{14}N\{^{1}H\}$ NMR spectrum



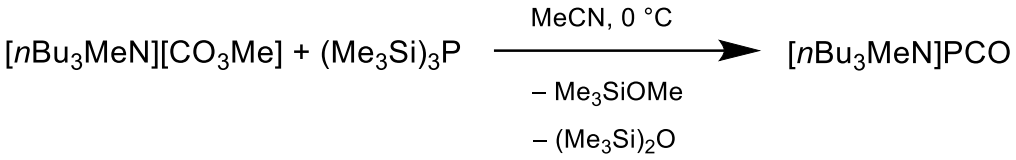
IR spectrum

Raman spectrum



2.13 Synthesis of [*n*Bu$_3$NMe]PCO

[*n*Bu$_3$NMe]PCO is synthesized according to a modified literature procedure.[17]

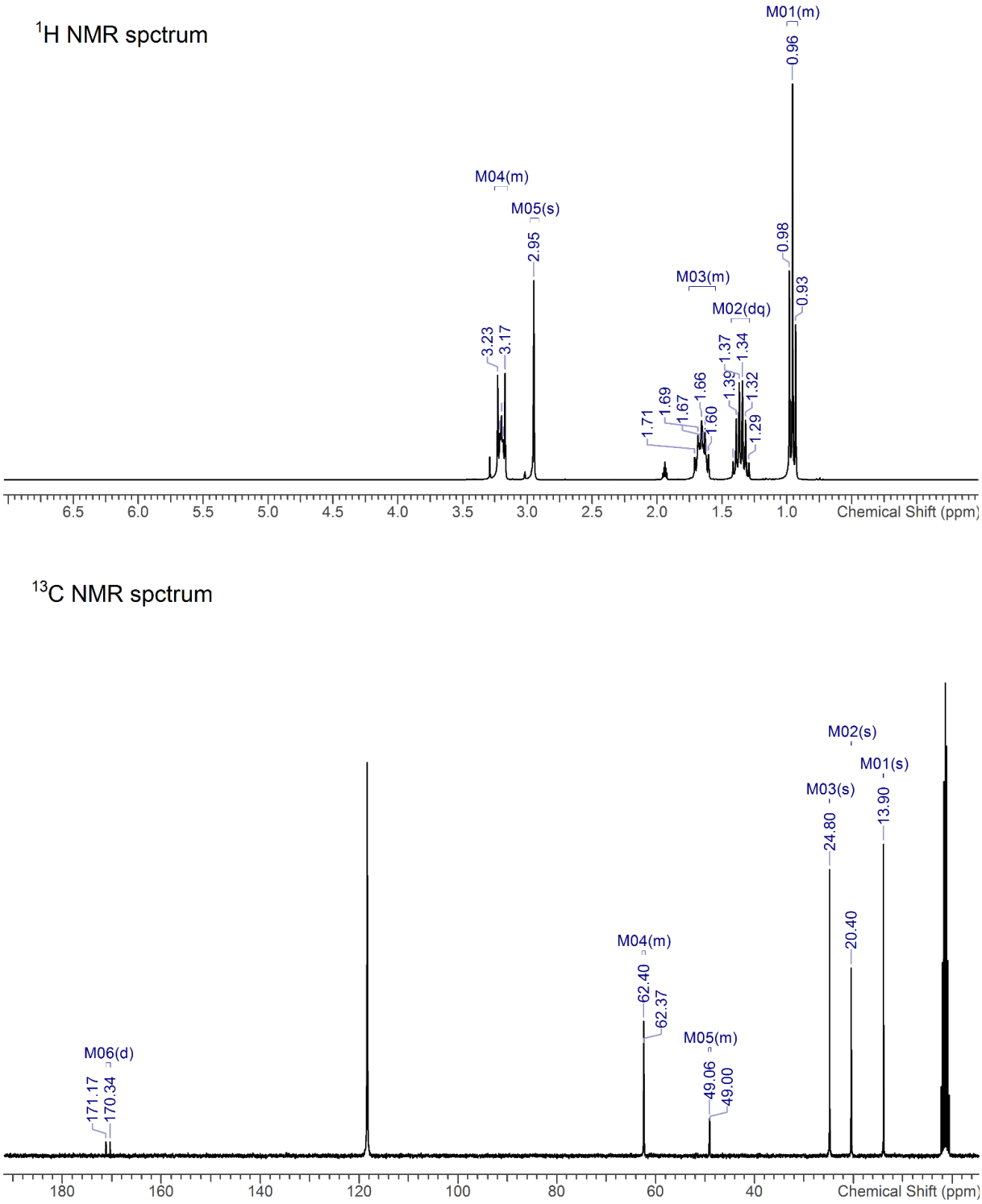


[*n*Bu$_3$MeN][CO$_3$Me] (0.81 g, 2.93 mmol) is placed in a Schlenk vessel and acetonitrile (8 mL) is added. The colorless solution is cooled to 0 °C (isopropanol bath) and (Me$_3$Si)$_3$P (0.74 g, 2.95 mmol) is added within 10 min via syringe. The solution turns yellowish and small amounts of a precipitate formed. The mixture is stirred at 0 °C (isopropanol bath) for additional 30 min and is then allowed to warm up to room temperature. After stirring the mixture for 20 h the precipitate is filtered off and all volatiles are removed *in vacuo* ($1\cdot10^{-3}$ mbar, 50 C (water bath), 2 h) leading to a highly viscous yellow oil. The residue is washed with three portions of Et$_2$O (15 mL each) which lead to the pale yellowish solid [*n*Bu$_3$MeN]PCO (0.67 g, 2.60 mmol) in yields of 89 %.

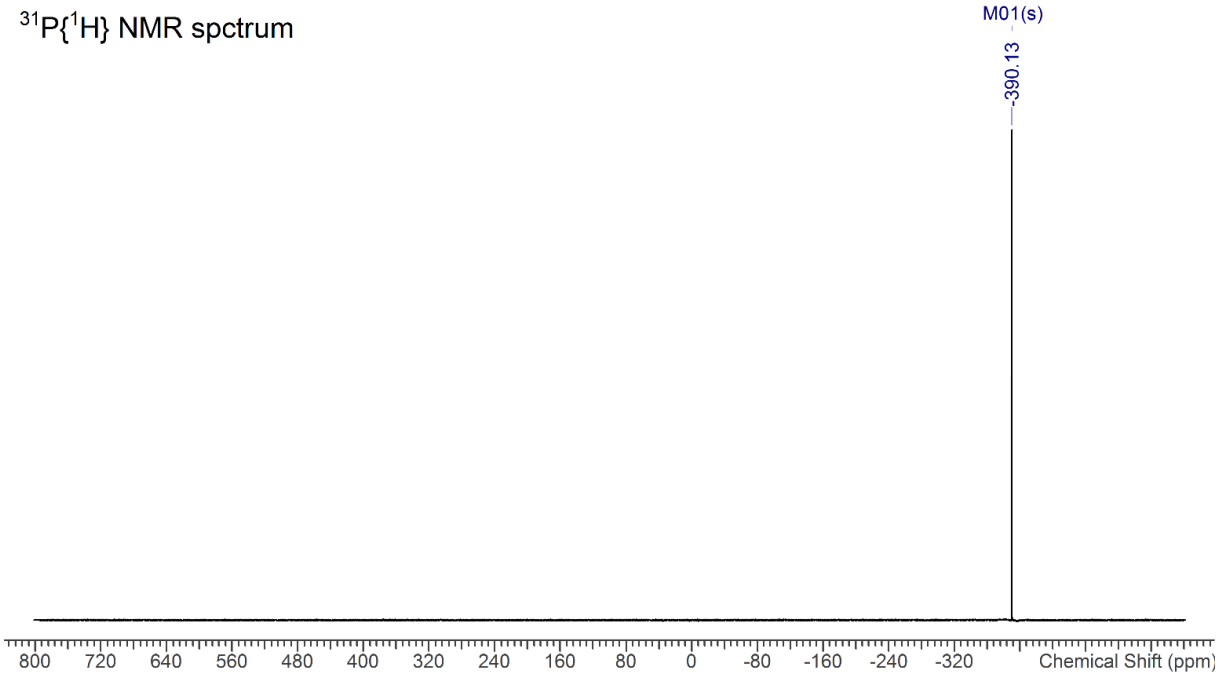
C$_{14}$H$_{30}$NOP (259.37 g·mol^{-1}): **mp.** 94 °C, 178 °C (dec.). **EA** calc. (found) %: C, 64.83 (64.30); H, 11.66 (11.12); N, 5.40 (5.54). **^{1}H NMR** (298 K, CD$_3$CN, 250.13 MHz) δ = 3.40-3.09 (m, 6H, NC*H$_2$*); 2.94 (s, 3H, NC*H$_3$*); 1.84-1.53 (m, 6H, NCH$_2$C*H$_2$*); 1.51-1.25 (m, 6H, NCH$_2$CH$_2$C*H$_2$*); 1.16-0.87 (m, 9H, C*H$_3$*CH$_2$). **^{13}C{^{1}H} NMR** (297 K, CD$_3$CN, 62.9 MHz) δ = 170.8 (d, O*C*P, ^1J(^{13}C,^{31}P) = 63 Hz); 62.4 (t, N*C*H$_2$, ^1J(^{13}C,^{14}N) = 3 Hz); 49.1 (t, N*C*H$_3$, ^1J(^{13}C,^{14}N) = 4 Hz); 24.8 (s, 3C, NCH$_2$*C*H$_2$); 20.4 (t, CH$_3$*C*H$_2$, ^1J(^{13}C,^{14}N) = 2 Hz); 13.9 (s, *C*H$_3$CH$_2$). **^{31}P{^{1}H} NMR** (297 K, CD$_3$CN, 101.3 MHz) δ = −390.5 (s, OC*P*). **IR** (ATR-IR, 32 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 420 (w), 429 (w), 441 (w), 455 (w), 495 (m), 523 (w), 548 (w), 684 (w), 738 (m), 754 (w), 802 (w), 837 (w), 890 (m), 923 (w), 940 (w), 971 (w), 1001 (w), 1016 (w), 1032 (w), 1065 (w), 1107 (w), 1168 (w), 1195 (w), 1259 (w), 1290 (w), 1337 (w), 1379 (m), 1461 (m), 1560 (w), 1630 (m), 1692 (w), 1768 (vs), 1795 (s), 2592 (w), 2666 (w), 2875 (m), 2936 (m), 2959 (m). **Raman** (633 nm, 8 mW, 20 s, 20 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 274 (1), 308 (1), 367 (1), 427 (1), 437 (1), 500 (1), 567 (1), 576 (1), 737 (1), 803 (10), 883 (2), 904 (1), 925 (1), 943 (1), 971 (1), 988 (1), 1000 (1), 1037 (1), 1069 (1), 1109 (1), 1136 (1), 1161 (1), 1196 (1), 1257 (1),

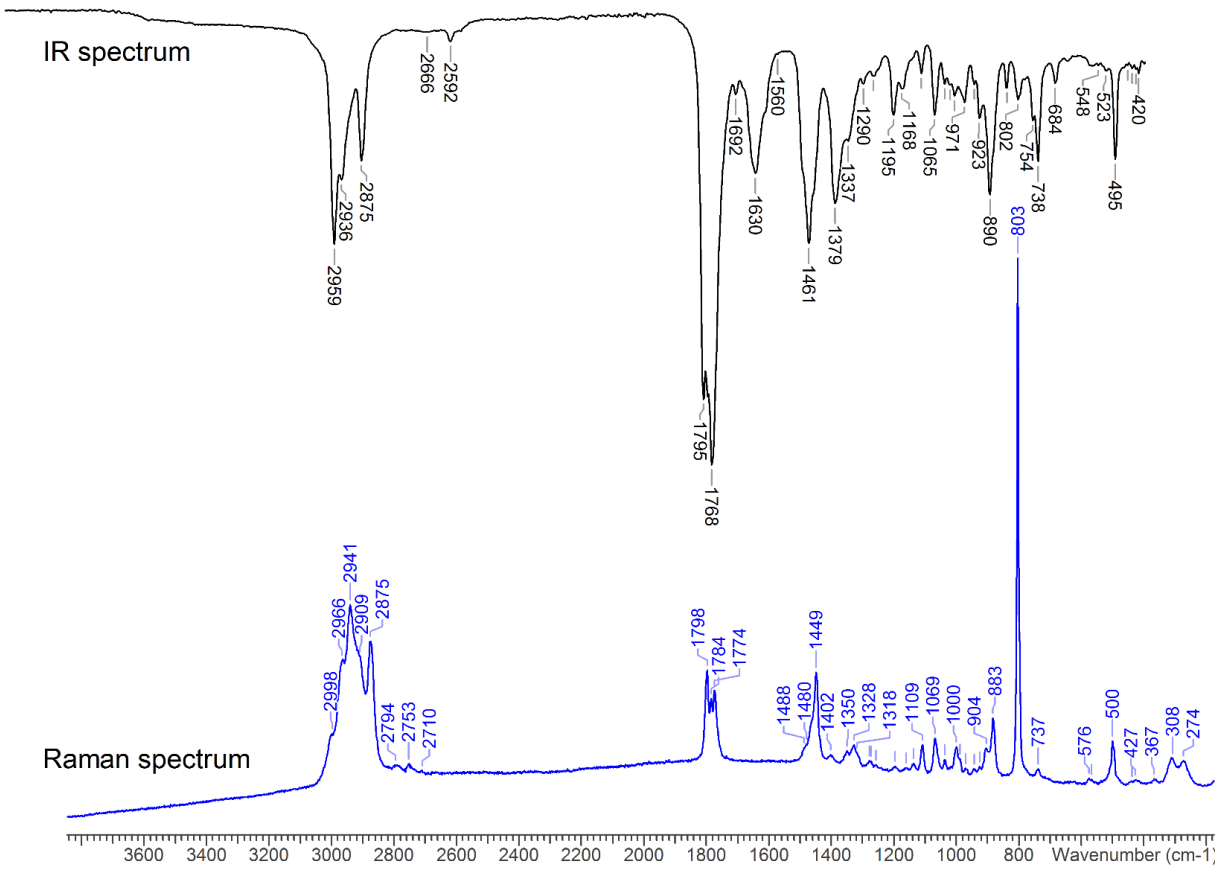
1272 (1), 1278 (1), 1318 (1), 1328 (1), 1350 (1), 1402 (1), 1449 (3), 1480 (1), 1488 (1), 1774 (2), 1784 (2), 1798 (3), 2710 (1), 2753 (1), 2794 (1), 2875 (3), 2909 (3), 2941 (4), 2966 (3), 2998 (2).

Figure S15: NMR, Raman and IR spectra of [nBu3NMe]PCO in CD_3CN.



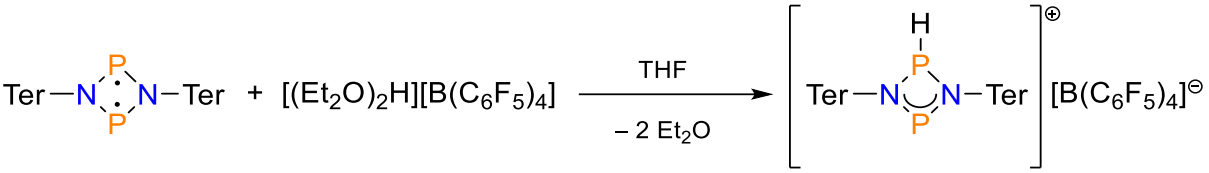
$^{31}P\{^{1}H\}$ NMR spctrum





3 Syntheses of compounds

3.1 Synthesis of [HP(μ-NTer)$_2$P][B(C$_6$F$_5$)$_4$] (2)

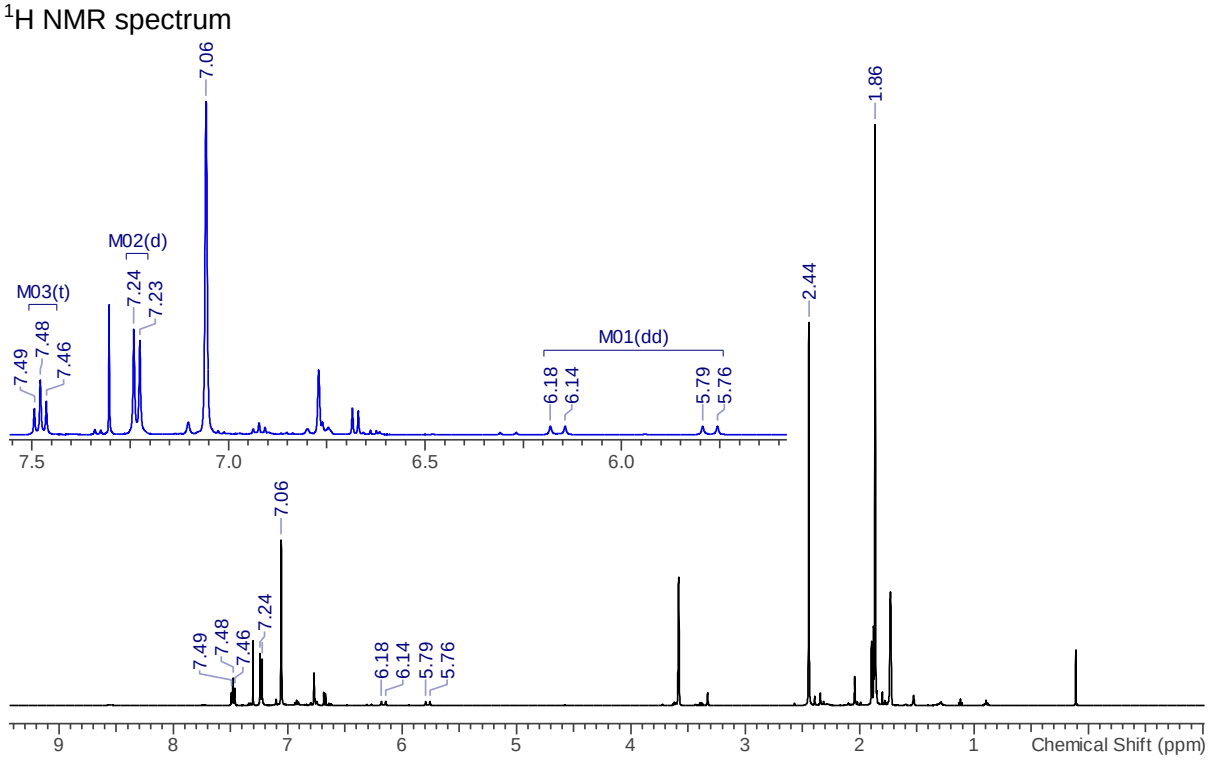


[P(μ-NTer)]$_2$ (82 mg, 0.11 mmol) and Jutzi acid (115.5 mg, 0.14 mmol) are placed in a flask and dissolved in benzene (4 mL). The formation of a clear solution can be observed which separates in two phases: an upper yellow phase and a lower red viscous phase. The mixture is concentrated to 2 mL and cooled down to 5°C (water bath in a refrigerator). Red crystals can be observed in the lower phase. The structure elucidation identified the crystals as [HP(μ-NTer)$_2$P][B(C$_6$F$_5$)$_4$] (**2**). The supernatant is removed by syringe and discarded. The remaining crystals are dried ($1\cdot10^{-3}$ mbar, 40 °C (water bath), 2 h), yielding 71 mg (0.05 mmol, 44 %) of **2**.

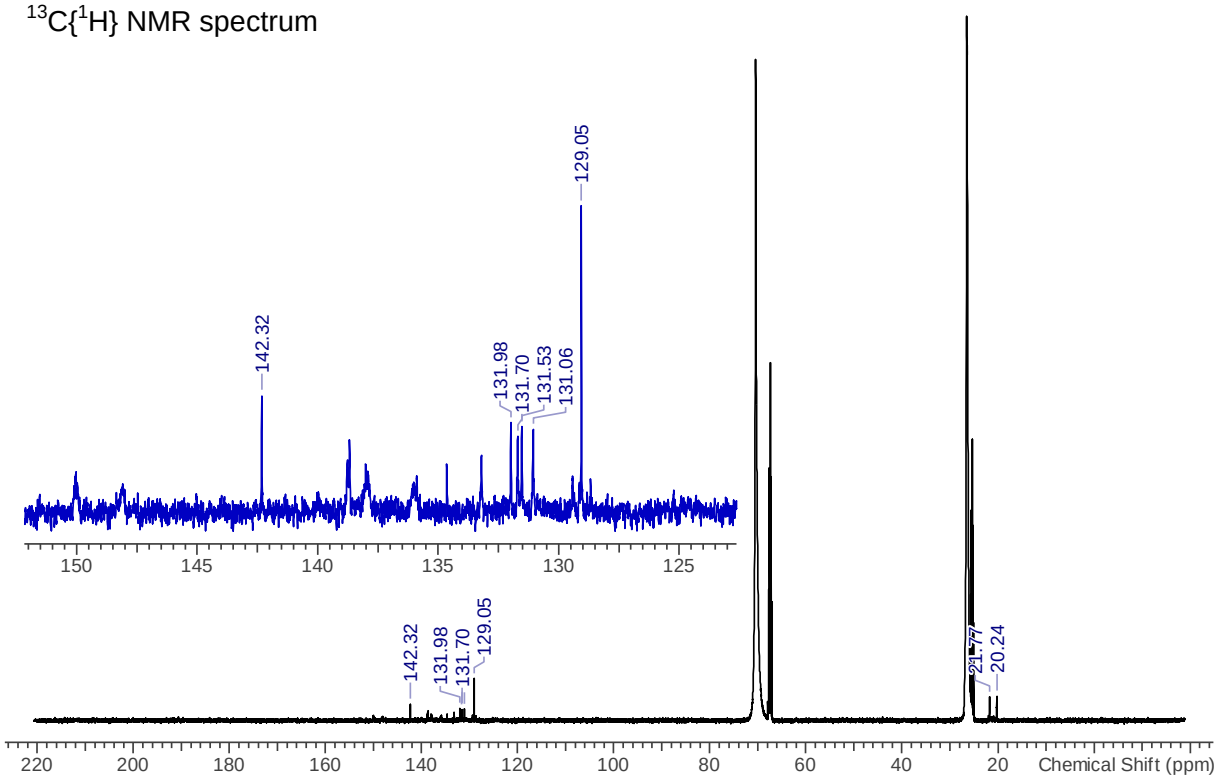
[HP(μ-NTer)$_2$P][B(C$_6$F$_5$)$_4$] (1396.94 g·mol^{-1}): **mp**. 223 °C (dec.). **EA** calc. (found), %: C, 61.91 (62.15); H, 3.68 (3.95); N, 2.01 (1.71). **^{1}H NMR** (298 K, THF-d$_8$, 500.13 MHz): δ = 1.86 (s, 24H, *o*-C*H*$_3$), 2.44 (s, 12H, *p*-C*H*$_3$), 5.97 (dd, 1H, P*H*, $^3J(^1H,^{31}P)$ = 17 Hz, $^1J(^1H,^{31}P)$ = 195 Hz), 7.05 (s, 8H, *m*-C*H*$_{Mes}$), 7.23 (d, 4H, *m*-C*H*$_{Ar}$, $^3J(^1H,^1H)$ = 7.72 Hz), 7.48 (t, 2H, *p*-C*H*$_{Ar}$, $^3J(^1H,^1H)$ = 7.72 Hz). **^{11}B NMR** (298K, C$_6$H$_5$F, 160.5 MHz): δ = −16.1 (s, 1B, [B(C$_6$F$_5$)$_4$]$^-$). **^{13}C{^{1}H} NMR** (298 K, THF-d$_8$, 125.8 MHz): δ = 20.07 (s, *o*-*C*H$_3$), 21.6 (s, *p*-*C*H$_3$), 128.9 (s, C$_6$H$_6$), 130.9 (s), 131.4, 131.5 (s), 131.8 (s), 142.2 (s). **^{14}N{^{1}H} NMR** (298 K, C$_6$D$_6$, 36.1 MHz): δ = not observed. **^{19}F NMR** (298K, THF-d$_8$, 470.6 MHz): δ = −132.7 (br), −165.0 (t, J = 20.3 Hz), −168.5 (t, J = 18.3 Hz). **^{31}P NMR** (298 K, C$_6$D$_6$, 202.5 MHz): δ = 168.9 (dd, 1P, *P*H, $^1J(^{31}P,^1H)$ = 195 Hz, $^2J(^{31}P,^{31}P)$ = 51 Hz), 339.6 (dd, 1P, *P*NPH, $^2J(^{31}P,^{31}P)$ = 51 Hz, $^3J(^{31}P,^1H)$ = 17 Hz). **IR** (ATR-IR, 32 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 2980 (w), 2924 (w), 2918 (w), 2854 (w), 2739 (w), 1642 (w), 1611 (w), 1568 (w), 1558 (w), 1541 (w), 1513 (m), 1459 (vs), 1418 (m), 1381 (m), 1339 (w), 1298 (w), 1276 (m), 1226 (m), 1164 (w), 1084 (s), 1032 (w), 975 (vs), 915 (m), 888 (w), 859 (m), 851 (m), 839 (m), 797 (m), 773 (m), 754 (m), 727 (w), 703 (w), 682 (m),

659 (m), 610 (m), 602 (m), 593 (w), 573 (m), 560 (m), 548 (w), 534 (w), 511 (w), 497 (w), 478 (w), 447 (w), 437 (w), 427 (w), 416 (w), 406 (w). **Raman** (633 nm, 8 mW, 20 s, 20 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 3069 (3), 2951 (3), 2925 (3), 2860 (3), 2277 (4), 1646 (4), 1612 (4), 1584 (5), 1482 (4), 1465 (4), 1424 (8), 1377 (4), 1334 (4), 1311 (5), 1290 (9), 1281 (8), 1230 (4), 1194 (3), 1094 (4), 1085 (4), 1009 (4), 993 (5), 962 (3), 955 (3), 924 (3), 866 (4), 843 (4), 822 (3), 803 (3), 779 (4), 756 (3), 734 (3), 704 (3), 652 (3), 594 (5), 585 (4), 574 (4), 562 (4), 536 (4), 522 (10), 493 (4), 475 (3), 449 (3), 423 (4). **MS** (CI^+, m/z (%)): 330 (100) $[TerNH_3]^+$, 389 (15) $[TerN_2P]^+$.

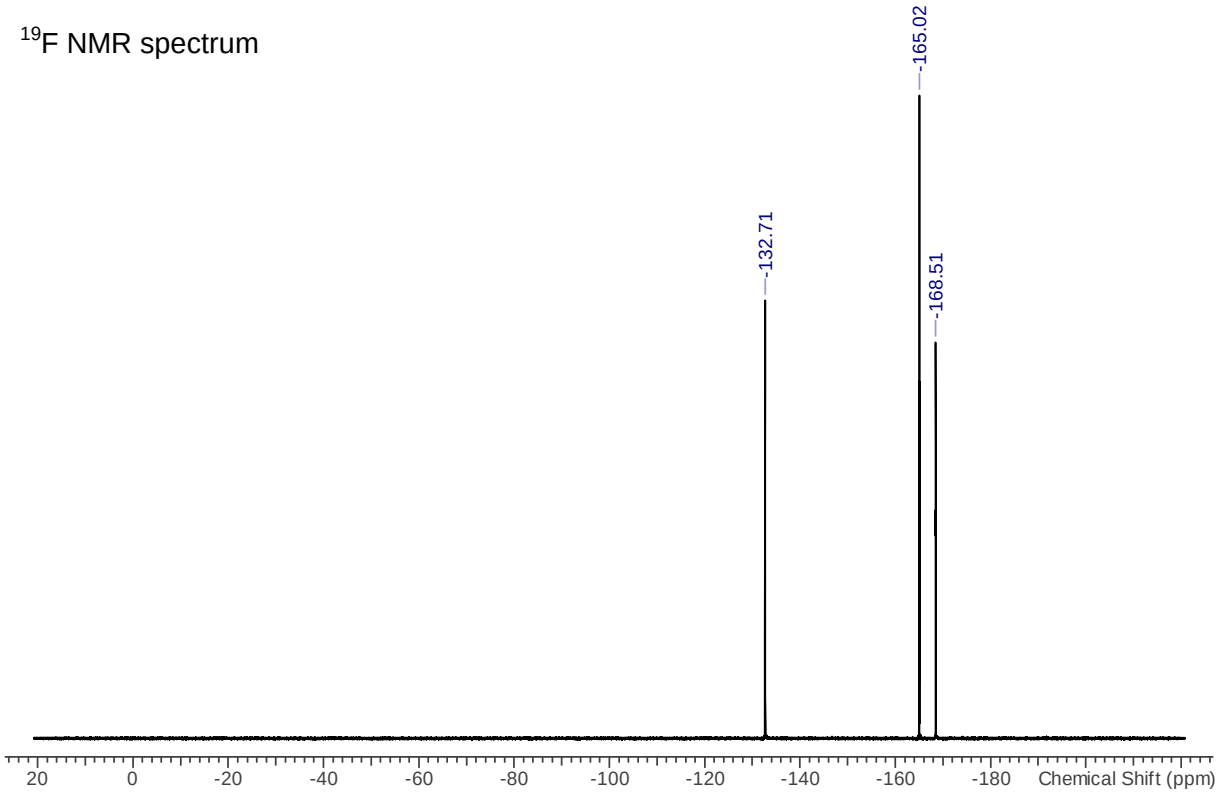
Figure S16: Raman, IR and NMR spectra of **2** in THF-d_8.



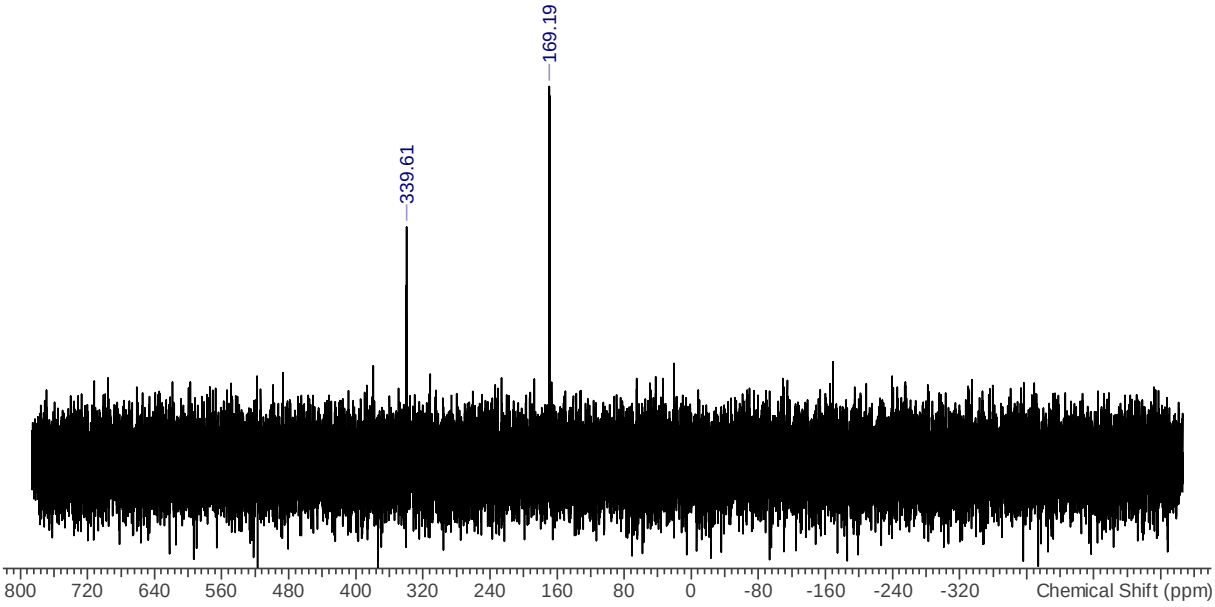
$^{13}C\{^{1}H\}$ NMR spectrum

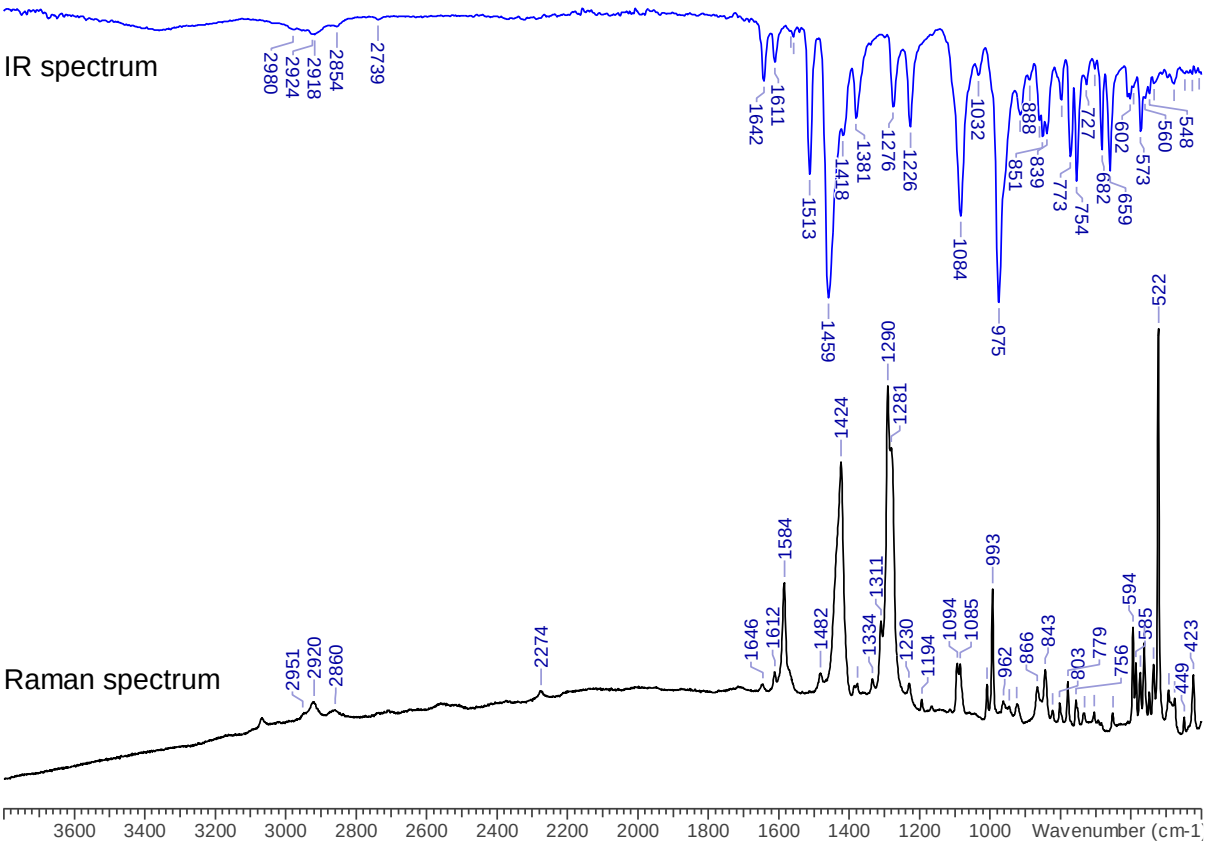


^{19}F NMR spectrum

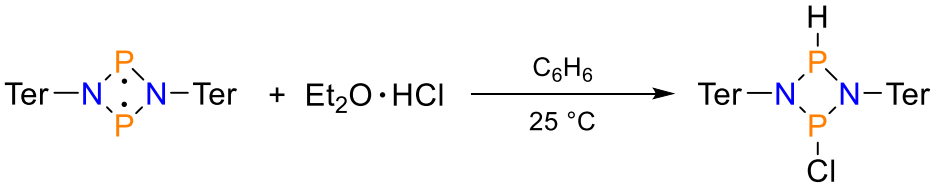


$^{31}P\{^{1}H\}$ NMR spectrum





3.2 Synthesis of [HP(μ-NTer)$_2$PCl] (3Cl)

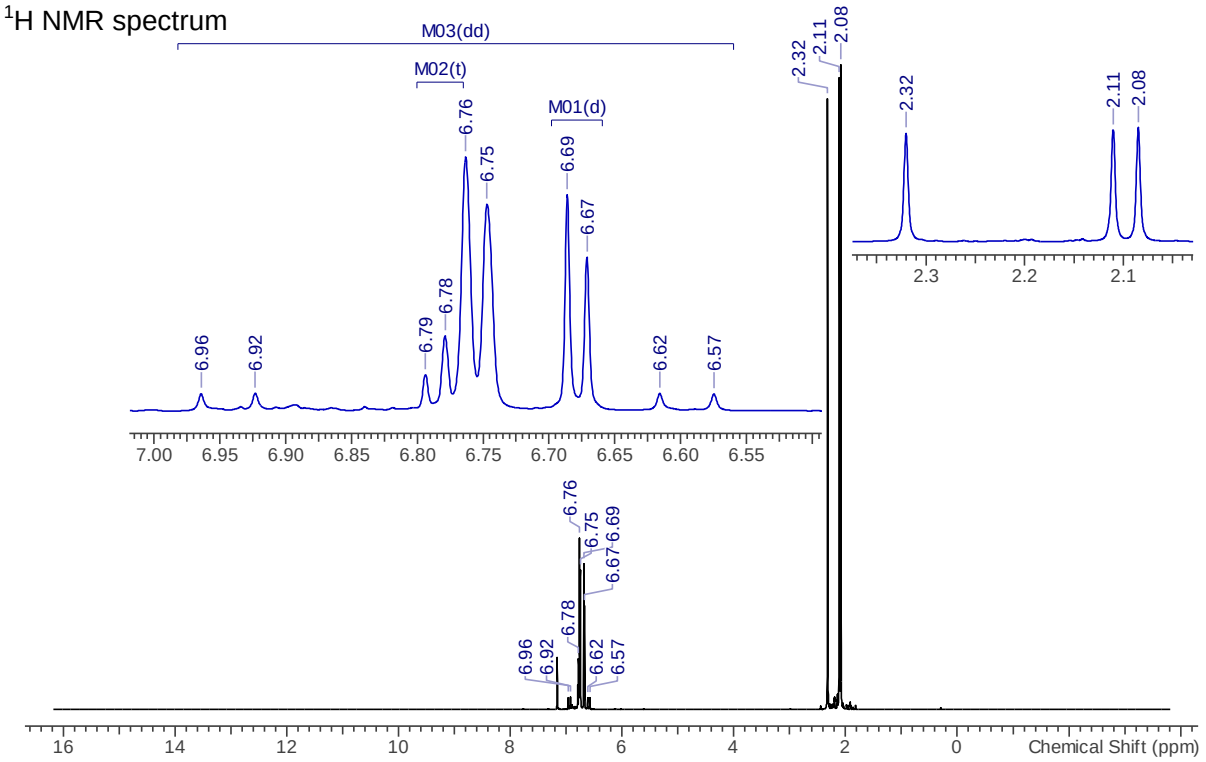


[P(μ-NTer)]$_2$ (248 mg, 0.35 mmol) is dissolved in C_6H_6 (10 mL) at ambient temperature. Under vigorous stirring HCl in Et_2O (60 µL, 6.15 mol·L^{-1}, 0.37 mmol) is added. Upon addition of HCl the reaction mixture turns colourless. All volatile components are removed (1·10^{-3} mbar, 40 °C (water bath), 2 h). Single crystals suitable for X-ray structure elucidation can be grown from benzene overnight by cooling from 50 °C (oil bath) to ambient temperature. The structure elucidation identified the crystals as [HP(μ-NTer)$_2$PCl] (**3Cl**). The supernatant is removed by syringe and discarded. The remaining crystals are dried (1·10^{-3} mbar, 40 °C (water bath), 2 h), yielding 143 mg (0.19 mmol, 55 %) of **3Cl**.

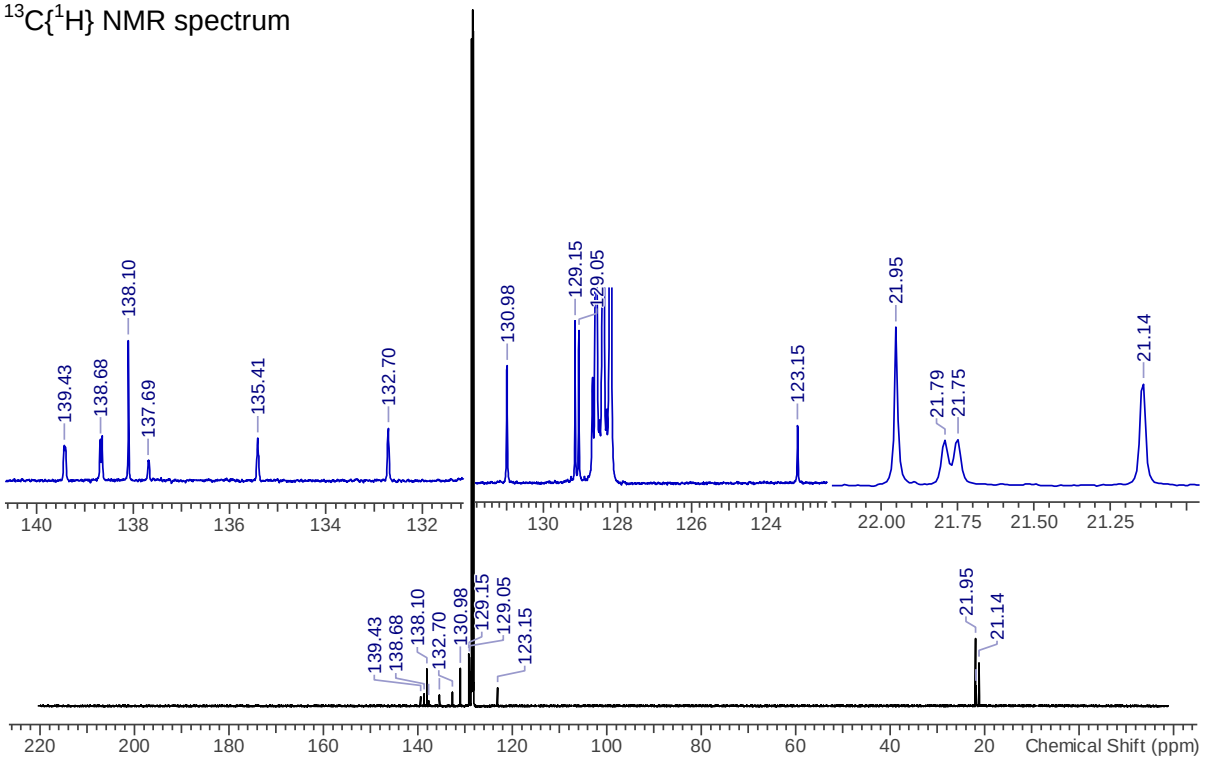
[HP(μ-NTer)$_2$PCl] (753.35 g·mol^{-1}): **mp**. >145 °C (dec.). **EA** calc. (found), %: C, 76.53 (76.12); H, 6.82 (6.56); N, 3.72 (3.39). **^{1}H NMR** (298 K, C_6D_6, 500.13 MHz): *δ* = 2.08 (s, 6H, Mes, *o*-C*H*$_3$), 2.11 (s, 6H, Mes, *o*-C*H*$_3$), 2.32 (s, 6H, Mes, *p*-CH$_3$), 6.68 (d, 2H, *m*-C*H*, ^3J(^{1}H,^{1}H) = 7.5 Hz), 6.75 (s, 2H, Mes, m-C*H*), 6.76 (s, 2H, Mes, m-C*H*), 6.77 (dd, 1H, *H*P(μ-NTer)$_2$PCl, ^1J(^{1}H,^{31}P) = 174 Hz, ^3J(^{1}H,^{31}P) = 20.5 Hz), 6.78 (t, 1H, *p*-C*H*, ^3J(^{1}H,^{1}H) = 7.5 Hz). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 75.5 MHz): *δ* = 21.2 (s, *C*H$_3$,), 21.8 (d, *o*-*C*H$_3$, *J*(^{13}C,^{31}P) = 5.5 Hz), 22.0 (s, *C*H$_3$), 123.2 (s, *C*H), 129.1 (s, *C*H), 129.2 (s, *C*H), 131.0 (s, *C*H), 132.7 (s, *C*), 135.4 (s, *C*), 137.7 (s, *C*), 138.1 (s, *C*), 138.7 (s, *C*), 139.4 (s, *C*). **^{14}N{^{1}H} NMR** (298 K, C_6D_6, 36.1 MHz): *δ* = not observed. **^{31}P NMR** (298 K, C_6D_6, 202.5 MHz): *δ* = 169.7 (dd, H*P*(μ-NTer)$_2$PCl, ^1J(^{31}P,^{1}H) = 174 Hz, ^2J(^{31}P,^{31}P) = 49 Hz), 246.2 (dd, HP(μ-NTer)$_2$*P*Cl, ^2J(^{31}P,^{31}P) = 49 Hz, ^3J(^{31}P,^{1}H) = 18 Hz). **IR** (ATR-IR, 32 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 2999 (w), 2970 (w), 2943 (w), 2914 (w), 2853 (w), 2193 (w), 1610 (w), 1581 (w), 1484 (w), 1455 (w), 1430 (m), 1410 (s), 1375 (m), 1294 (w), 1235 (vs), 1187 (w), 1078 (m), 1031 (w), 1006 (w), 973 (w), 938 (w), 909 (m), 897 (m), 880 (s), 845 (s), 816 (w), 796 (m), 777 (w), 763 (w), 750 (m), 738 (w), 695 (m), 651 (w), 592 (w), 575 (w), 559 (w), 548 (w), 536 (w), 497 (w), 435 (w), 404 (m). **Raman** (633 nm, 8 mW, 20 s, 20 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 3068 (1), 3039 (0), 3036 (1), 2952 (3), 2895 (7), 2839 (1), 2824 (1), 1594 (1), 1466 (1), 1441 (1), 1406 (1), 1377 (1), 1335 (1),

1332 (1), 1263 (1), 1241 (2), 1197 (10), 1164 (1), 1101 (1), 1017 (4), 913 (3), 862 (1), 828 (1), 794 (4), 780 (1), 748 (1), 738 (1), 726 (1), 713 (3), 690 (2), 632 (9), 623 (5), 556 (4), 544 (3), 530 (1), 455 (1), 440 (1), 415 (3). **MS** (CI^+, m/z (%)): 330 (8) $[TerNH_3]^+$, 687 (21) $(\mu\text{-NTer})_2PH^+$, 716 (100) $[P(\mu\text{-NTer})]_2^+$, 754 (18) $HP(\mu\text{-NTer})_2PClH^+$.

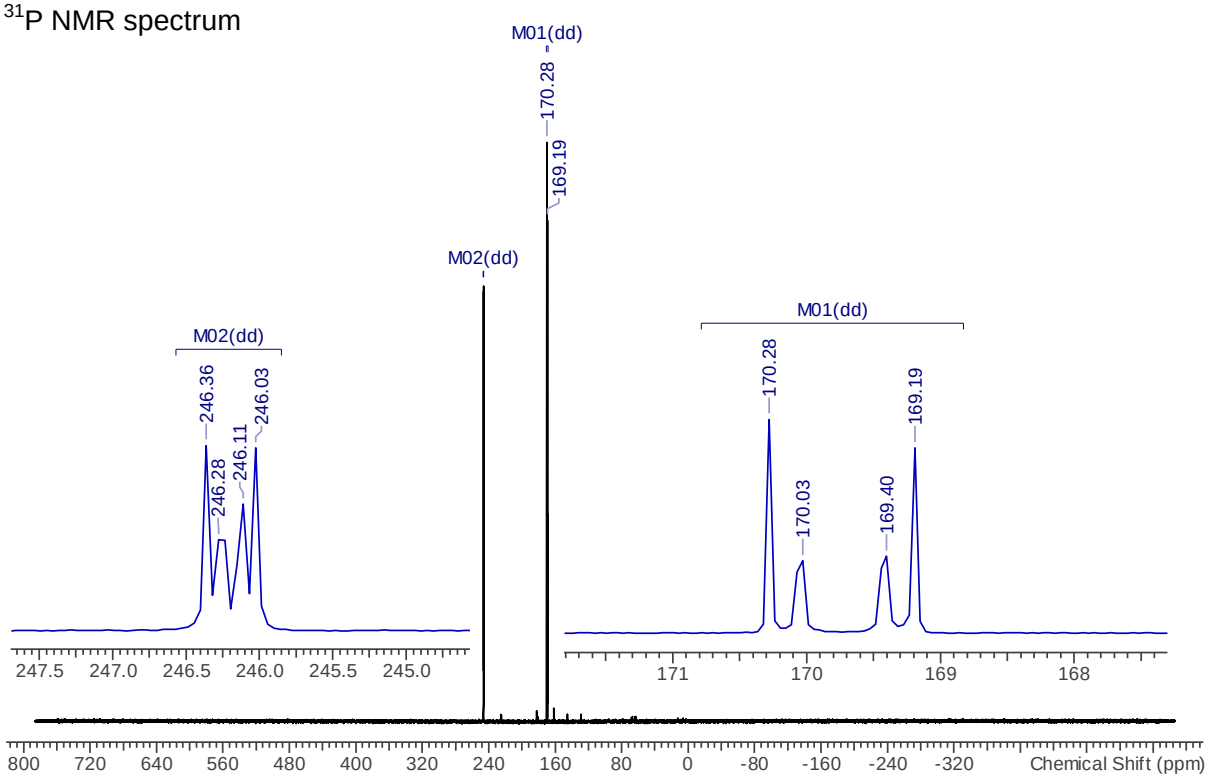
Figure S17: Raman, IR and NMR spectra of **3Cl** in C_6D_6.

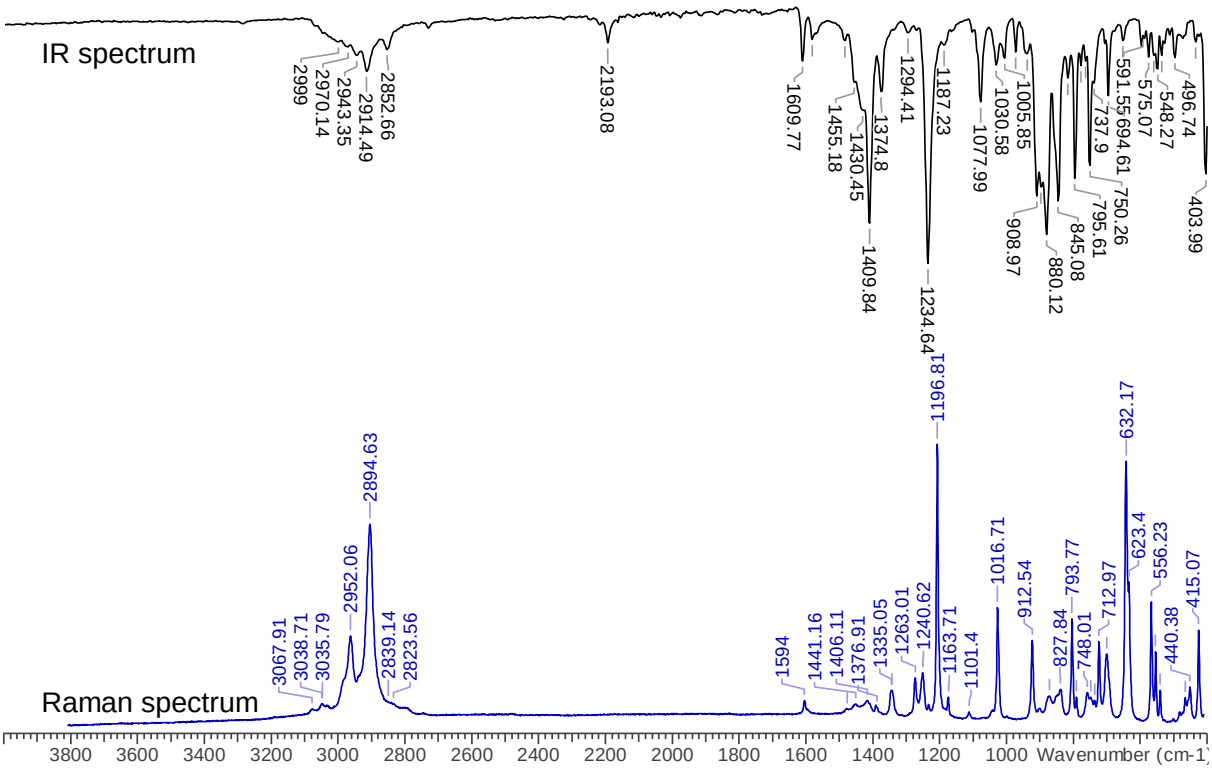


$^{13}C\{^{1}H\}$ NMR spectrum

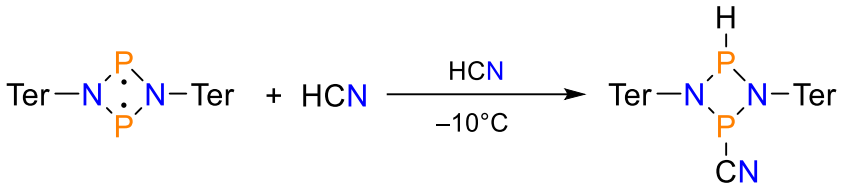


^{31}P NMR spectrum




IR spectrum
2999
2970.14
2943.35
2914.49
2852.66
2193.08
1609.77
1455.18
1430.45
1374.8
1409.84
1294.41
1234.64
1187.23
1196.81
1077.99
1030.58
1005.85
908.97
880.12
845.08
795.61
750.26
737.9
694.61
591.55
575.07
548.27
496.74
403.99
Raman spectrum
3067.91
3038.71
3035.79
2952.06
2894.63
2839.14
2823.56
1594
1441.16
1406.11
1376.91
1335.05
1263.01
1240.62
1163.71
1101.4
1016.71
912.54
827.84
793.77
748.01
712.97
632.17
623.4
556.23
440.38
415.07
3800 3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 Wavenumber (cm-1)

3.3 Synthesis of [HP(μ-NTer)$_2$PCN] (3CN)



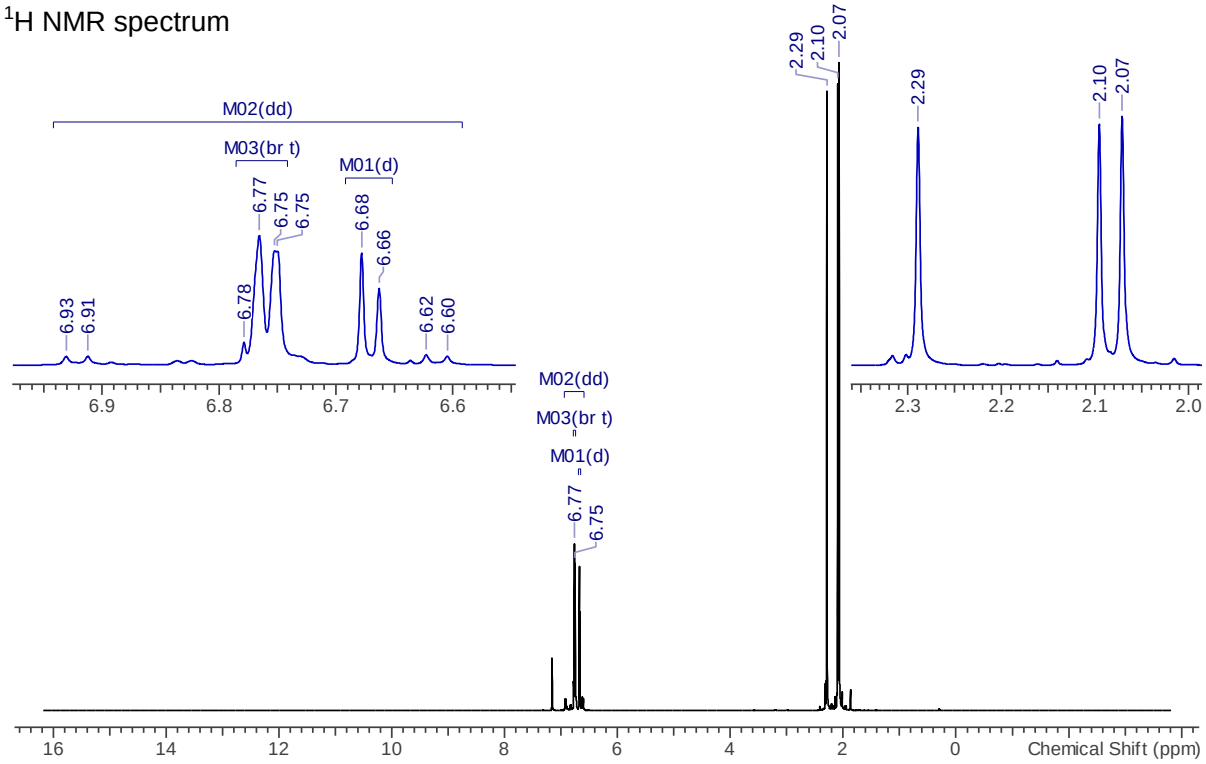
3.3.1 Method A

[P(μ-NTer)]$_2$ (154 mg, 0.21 mmol) is cooled to −10 °C (isopropanol bath) and pure HCN (0.5 mL, 725 g, 27 mmol) is added *via* syringe. Upon addition of HCN the reaction mixture turns colourless. All volatile components are removed (1·10^{-3} mbar, 25 °C, 1 h). Single crystals suitable for X-ray structure elucidation can be grown from a benzene solution overnight by cooling slowly from 40 °C (oil bath) to ambient temperature. The structure elucidation identified the crystals as [HP(μ-NTer)$_2$PCN] (**3CN**). The supernatant is removed by syringe and discarded. The remaining crystals are dried (1·10^{-3} mbar, 40 °C (water bath), 2 h), yielding 112 mg (0.15 mmol, 70 %) of **3CN**.

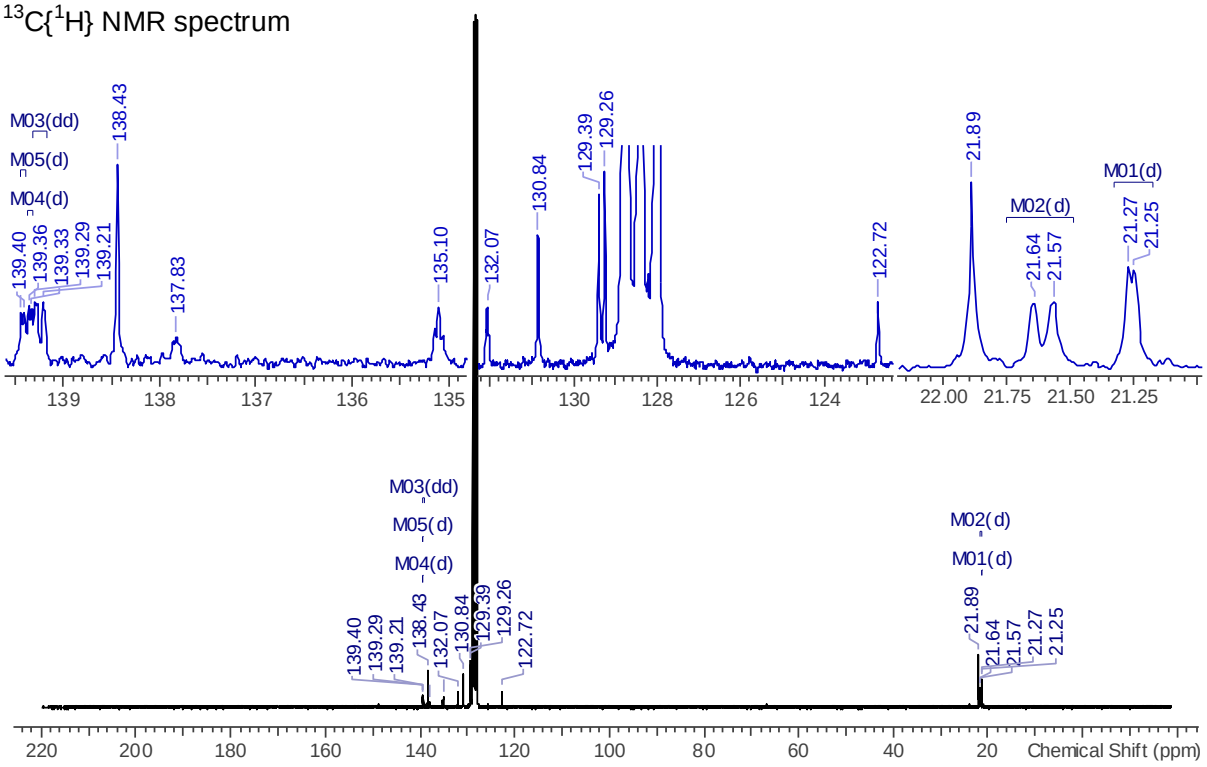
[HP(μ-NTer)$_2$PCN] (743.91 g·mol^{-1}): **mp**. 45 °C (dec.). **EA** calc. (found), %: C, 79.11 (79.72); H, 6.91 (6.78); N, 5.65 (5.48). **^{1}H NMR** (298 K, C_6D_6, 500.13 MHz): *δ* = 2.07 (s, 6H, Mes, *o*-C*H*$_3$), 2.10 (s, 6H, Mes, *o*-C*H*$_3$), 2.29 (s, 6H, Mes, *p*-CH$_3$), 6.67 (d, 2H, *m*-C*H*, ^3J(^{1}H,^{1}H) = 7.5 Hz), 6.75 (s, 2H, Mes, m-C*H*), 6.76 (t, 1H, *p*-C*H*, ^3J(^{1}H,^{1}H) = 7.5 Hz), 6.77 (s, 2H, Mes, m-C*H*), 6.77 (dd, 1H, *H*P(μ-NTer)$_2$PCl, ^1J(^{1}H,^{31}P) = 152.0 Hz, ^3J(^{1}H,^{31}P) = 9.5 Hz). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 62.9 MHz): *δ* = 21.3 (d, *o*-*C*H$_3$, J(^{13}C,^{31}P) = 1.4 Hz), 21.6 (d, *o*-*C*H$_3$, J(^{13}C,^{31}P) = 4.6 Hz), 21.9 (s, *p*-*C*H$_3$), 122.7 (s, *C*H), 129.3 (s, *C*H), 129.4 (s, *C*H), 130.8 (s, *C*H), 132.1 (s, *C*), 135.1 (s, *C*), 137.8 (s, *C*), 138.4 (s, *C*), 139.2 (dd, *C*N, ^1J(^{13}C,^{31}P) = 5 Hz, ^3J(^{13}C,^{31}P) = 1 Hz), 139.3 (d, *C,* J(^{13}C,^{31}P) = 2 Hz), 139.4 (d, *C, J*(^{13}C,^{31}P) = 2 Hz). **^{14}N{^{1}H} NMR** (298 K, C_6D_6, 36.1 MHz): *δ* = not observed. **^{31}P{^{1}H} NMR** (298 K, C_7D_8, 101.3 MHz): *δ* = 163.9 (d, HP(μ-NTer)$_2$*P*CN, ^2J(^{31}P,^{31}P) = 33 Hz), 185.0 (d, H*P*(μ-NTer)$_2$PCN, ^2J(^{31}P,^{31}P) = 33 Hz). **^{31}P NMR** (298 K, C_6D_6, 202.5 MHz): *δ* = 163.9 (d, HP(μ-NTer)$_2$*P*CN, ^2J(^{31}P,^{31}P) = 33 Hz), 185.0 (dd, H*P*(μ-NTer)$_2$PCN, ^1J(^{31}P,^{1}H) = 152 Hz, ^2J(^{31}P,^{31}P) = 33 Hz). **IR** (ATR-IR, 32 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 2943 (w), 2912 (w), 2853 (w), 1610 (w), 1581 (w), 1484 (w), 1453 (w), 1412 (s), 1375 (m), 1292 (w), 1235 (s), 1165 (w), 1078 (m), 1031 (w), 1006 (w), 969 (w), 946 (w), 903 (m), 876 (vs), 845 (s), 818 (m), 796 (m), 765 (w), 752 (m),

738 (m), 705 (w), 693 (m), 649 (w), 589 (w), 573 (w), 557 (m), 548 (m), 493 (s), 435 (m), 404 (m). **Raman** (633 nm, 8 mW, 20 s, 20 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 2950 (3), 2893 (8), 2783 (1), 1443 (1), 1405 (1), 1265 (1), 1244 (1), 1052 (1), 869 (1), 837 (1), 746 (1), 690 (2), 628 (10), 601 (2), 497 (1), 464 (1), 424 (2), 401 (1). **MS** (CI^+, m/z (%)): 330 (23) $[TerNH_3]^+$, 687 (77) $(\mu\text{-NTer})_2PH^+$, 716 (100) $[P(\mu\text{-NTer})]_2^+$, 743 (18) $HP(\mu\text{-NTer})_2PCN^+$.

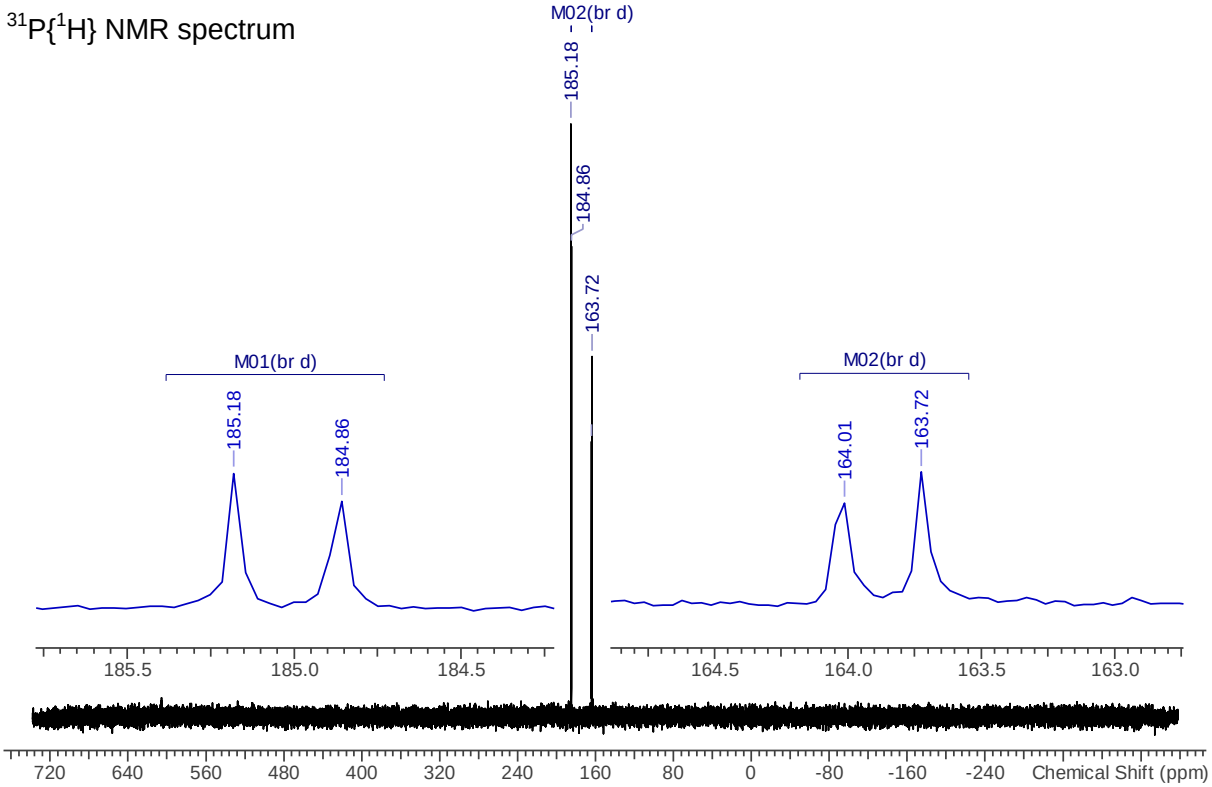
Figure S18: Raman, IR and NMR spectra of **3CN** in C_6D_6.

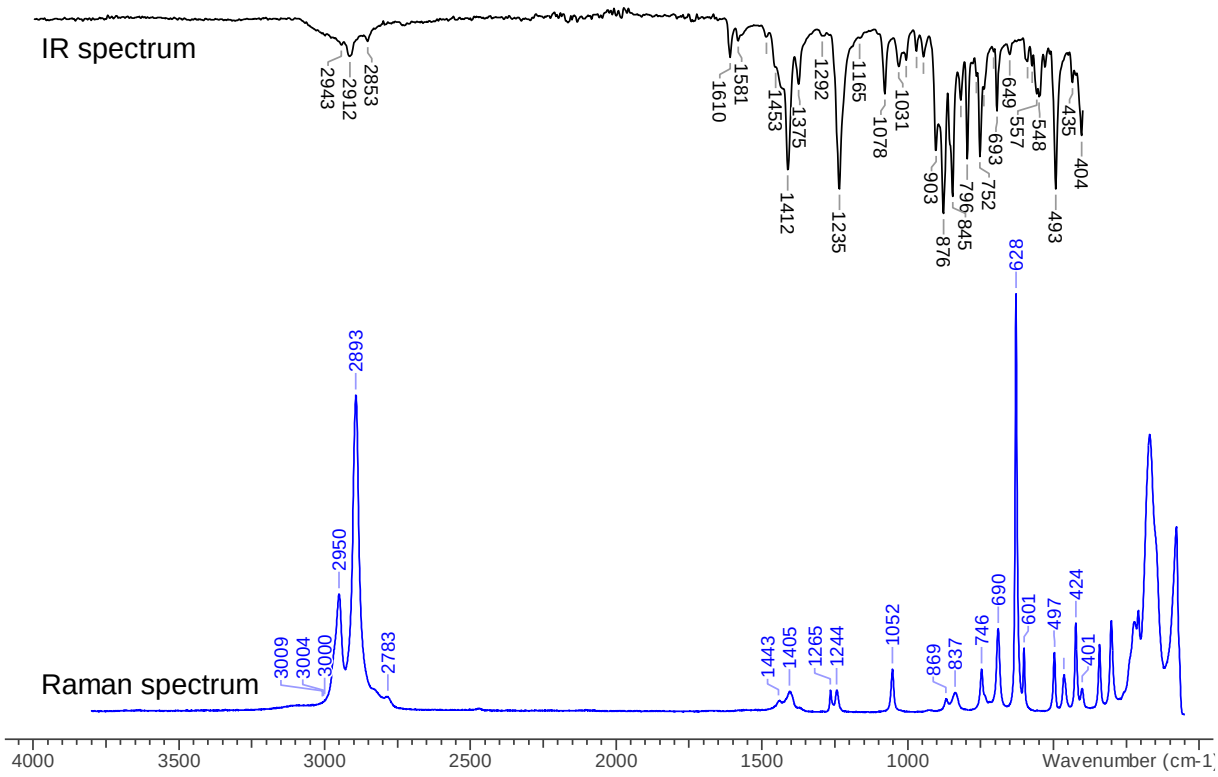


$^{13}C\{^{1}H\}$ NMR spectrum

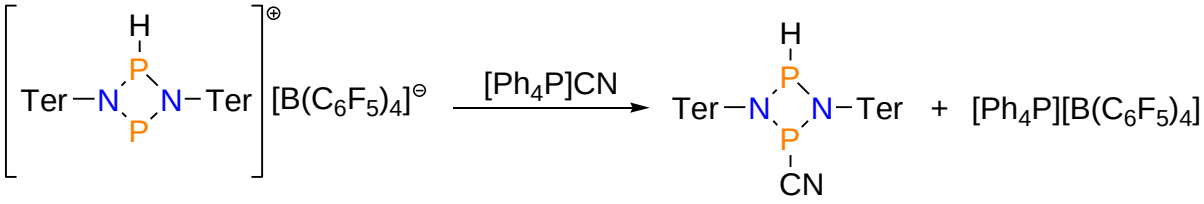


$^{31}P\{^{1}H\}$ NMR spectrum





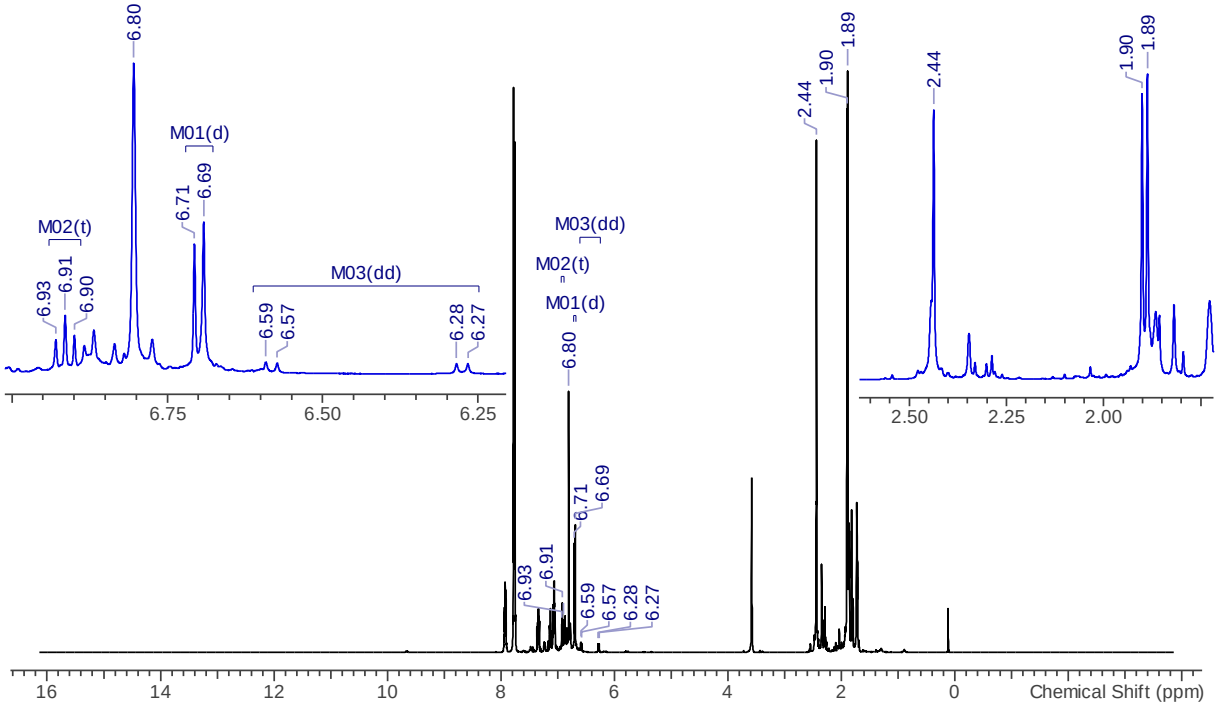
3.3.2 Method B



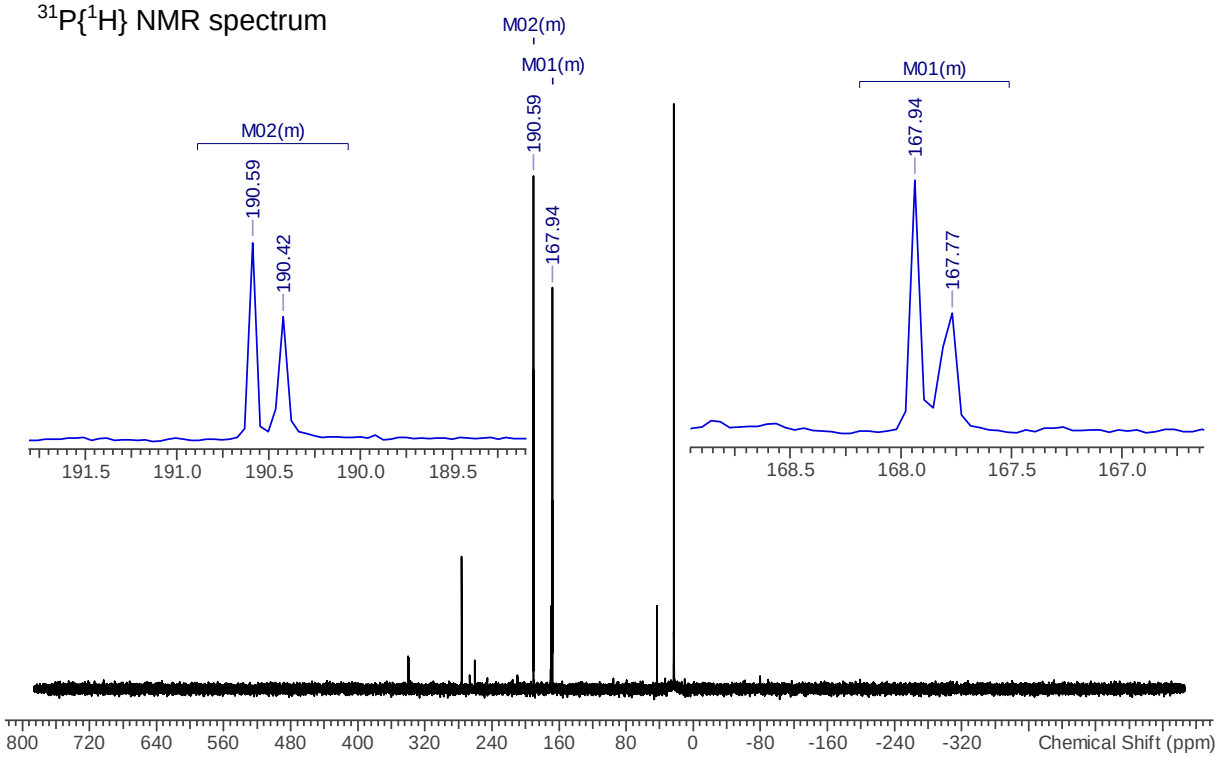
[HP(μ-NTer)$_2$P][B(C$_6$F$_5$)$_4$] (15 mg, 0.01 mmol) and (Ph$_4$P)CN (4 mg, 0.01 mmol) are placed in a NMR tube and dissolved in THF-d_8 (0.5 mL), resulting in a colourless solution. Quantitative NMR spectra indicate the formation of **3CN**.

^{1}H NMR (298 K, THF-d$_8$, 500.13 MHz): δ = 1.89 (s, 6H, Mes, *o*-C*H*$_3$), 1.90 (s, 6H, Mes, *o*-C*H*$_3$), 2.44 (s, 6H, Mes, *p*-CH$_3$), 6.43 (dd, 1H, *H*P(μ-NTer)$_2$PCl, ^1J(^{1}H,^{31}P) = 152 Hz, ^3J(^{1}H,^{31}P) = 9.5 Hz), 6.70 (d, 2H, *m*-C*H*, ^3J(^{1}H,^{1}H) = 7.5 Hz), 6.80 (s, 2H, Mes, m-C*H*), 6.91 (t, 1H, *p*-C*H*, ^3J(^{1}H,^{1}H) = 7.5 Hz). **^{31}P{^{1}H} NMR** (298 K, THF-d$_8$, 101.3 MHz): δ = 167.9 (d, HP(μ-NTer)$_2$*P*CN, ^2J(^{31}P,^{31}P) = 33 Hz), 190.5 (d, H*P*(μ-NTer)$_2$PCN, ^2J(^{31}P,^{31}P) = 33 Hz). **^{31}P NMR** (298 K, THF-d$_8$, 202.5 MHz): δ = 167.9 (d, HP(μ-NTer)$_2$*P*CN, ^2J(^{31}P,^{31}P) = 33 Hz), 190.5 (dd, H*P*(μ-NTer)$_2$PCN, ^1J(^{31}P,^{1}H) = 152 Hz, ^2J(^{31}P,^{31}P) = 33 Hz).

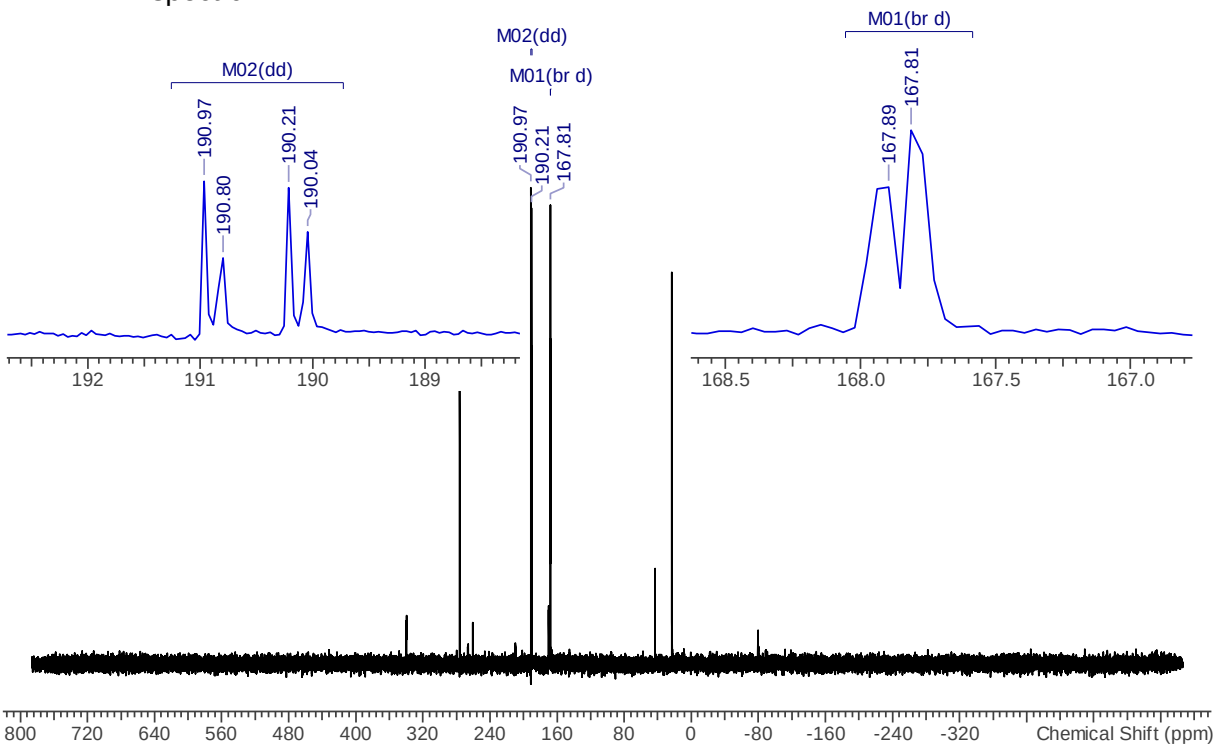
^{1}H NMR spectrum



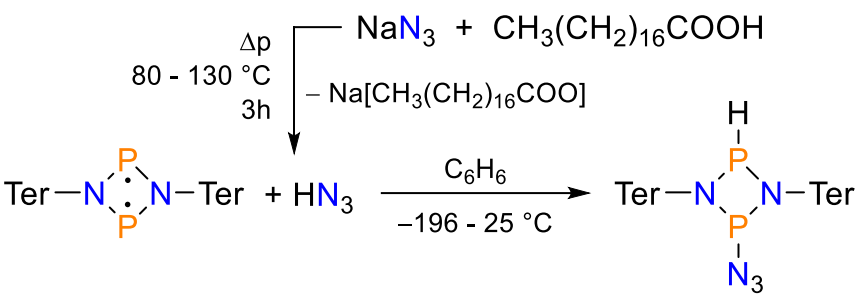
^{31}P{^{1}H} NMR spectrum



^{31}P NMR spectrum



3.4 Synthesis of [HP(μ-NTer)$_2$PN$_3$] (3N$_3$)



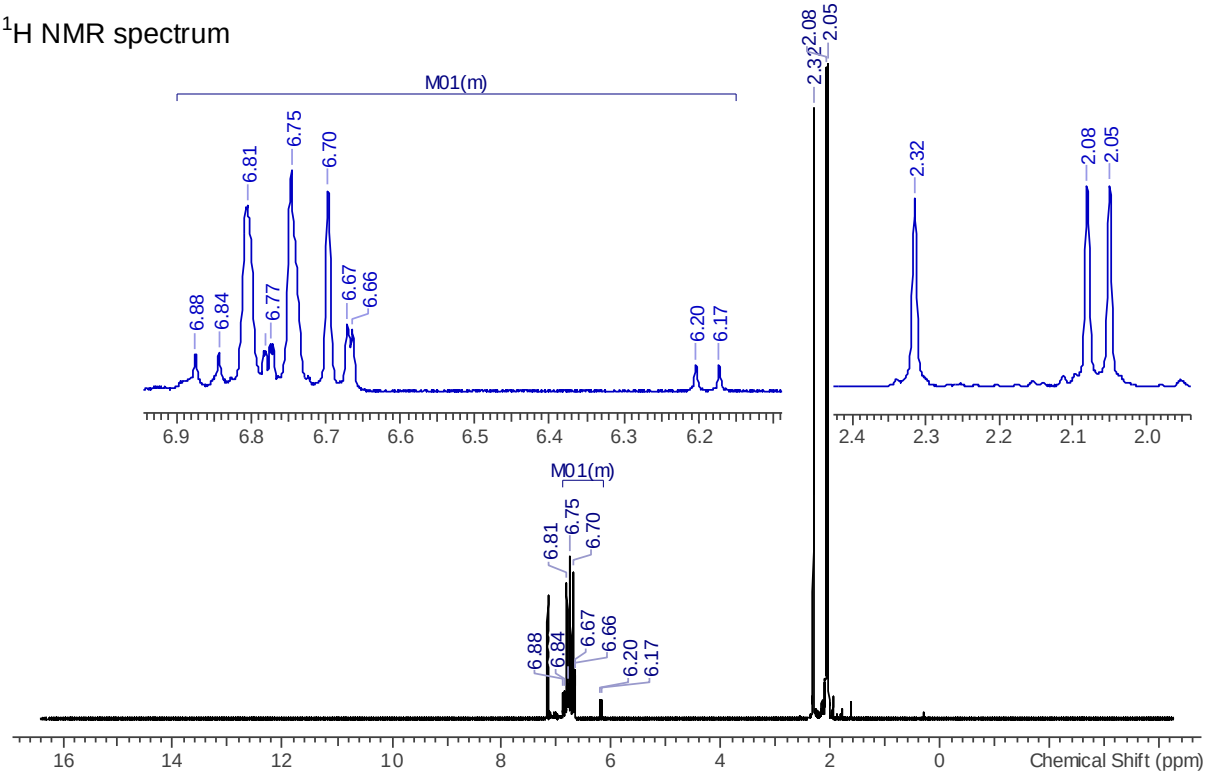
[P(μ-NTer)]$_2$ (155 mg, 0.22 mmol) is suspended in C_6H_6 (10 mL) and the mixture is degassed *in vacuo*. HN_3 is added as described in *section 2.5* (NaN_3 400 mg, 6.15 mmol; stearic acid 4.00 g, 14.06 mmol). After addition of HN_3, the reaction vessel is separated and warmed to ambient temperature, whereupon the reaction mixture turns colourless. All volatile components are removed ($1\cdot10^{-3}$ mbar, 50 °C, 2 h). Single crystals suitable for X-ray structure elucidation can be grown from a benzene solution overnight by cooling from 50 °C to ambient temperature. The structure elucidation identified the crystals as [HP(μ-NTer)$_2$PN$_3$] (**3N$_3$**). The supernatant is discarded by syringe and the remaining crystals are dried ($1\cdot10^{-3}$ mbar, 60 °C, 2 h), yielding 75 mg (0.10 mmol, 46 %) of **3N$_3$**.

[HP(μ-NTer)$_2$PN$_3$] (759.91 g·mol^{-1}): **mp**. >85 °C (dec.). **EA** calc. (found), %: C, C 75.87 (75.18), H 6.76 (6.78), N 9.22 (9.26). **^{1}H NMR** (298 K, C_6D_6, 250.13 MHz): δ = 2.04 (s, 6H, Mes, *o*-C*H*$_3$), 2.06 (s, 6H, Mes, *o*-C*H*$_3$), 2.31 (s, 6H, Mes, *p*-CH$_3$), 6.52 (dd, 1H, *H*P(μ-NTer)$_2$PCl, $^1J(^1H,^{31}P)$ = 168 Hz, $^3J(^1H,^{31}P)$ = 8.0 Hz), 6.67 (m, 1H, *p*-C*H*), 6.70 (m, 1H, *p*-C*H*), 6.75 (br, 2H, *m*-C*H*), 6.81 (br, 2H, Mes, m-C*H*). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 125.8 MHz): δ = 20.9 (s, *C*H$_3$), 21.3 (d, *o*-*C*H$_3$, $J(^{13}C,^{31}P)$ = 5.5 Hz), 21.9 (s, *C*H$_3$), 122.5 (s, *C*H), 129.1 (s, *C*H), 129.1 (s, *C*H), 130.9 (s, *C*H), 132.1 (s, *C*), 135.6 (s, *C*), 137.9 (s, *C*), 138.7 (d, *C*, $J(^{13}C,^{31}P)$ = 4.6 Hz), 138.7 (d, *C*, $J(^{13}C,^{31}P)$ = 1.8 Hz). **^{14}N{^{1}H} NMR** (298 K, C_6D_6, 36.1 MHz): δ = not observed. **^{31}P{^{1}H} NMR** (298 K, C_6D_6, 101.3 MHz): δ = 173.3 (d, H*P*(μ-NTer)$_2$PN$_3$, $^2J(^{31}P,^{31}P)$ = 33 Hz), 225.4 (d, HP(μ-NTer)$_2$*P*N$_3$, $^2J(^{31}P,^{31}P)$ = 33 Hz). **^{31}P NMR** (298 K, C_6D_6, 101.3 MHz): δ = 173.3 (dd, H*P*(μ-NTer)$_2$PN$_3$, $^1J(^{31}P,^1H)$ = 168 Hz, $^2J(^{31}P,^{31}P)$ = 31 Hz), 225.4 (dd, HP(μ-NTer)$_2$*P*N$_3$, $^2J(^{31}P,^{31}P)$ = 31 Hz, $^3J(^{31}P,^1H)$ = 7 Hz). **IR** (ATR-IR, 32 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 3000 (w), 2943 (w), 2912 (w), 2852 (w), 2205 (w), 2145 (w), 2083 (m), 1609 (w), 1583 (w), 1486 (w), 1414 (m), 1374 (m), 1304 (w), 1238 (vs), 1189 (m), 1152 (m), 1127 (m), 1102

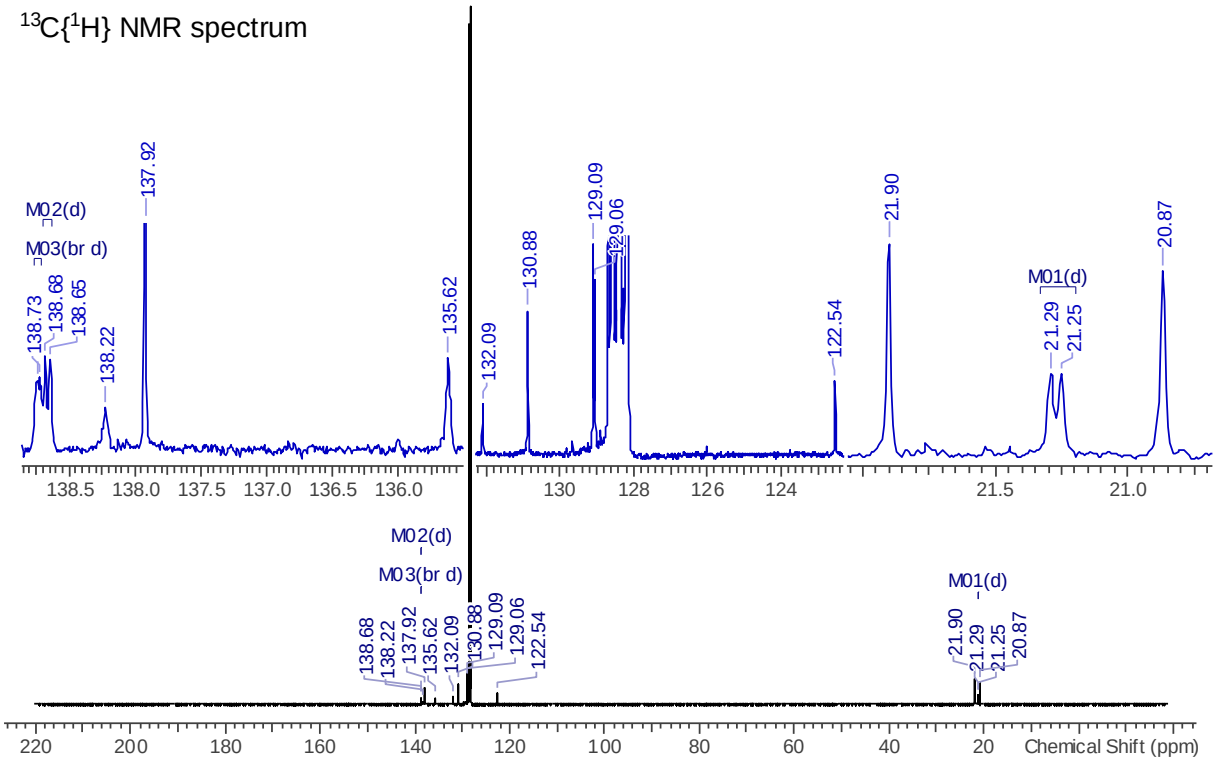
(m), 1078 (m), 1032 (w), 1006 (w), 983 (m), 975 (m), 946 (w), 903 (m), 888 (s), 847 (m), 822 (m), 793 (m), 764 (w), 750 (m), 696 (m), 674 (m), 649 (w), 596 (w), 587 (w), 573 (w), 558 (m), 550 (m), 538 (m), 528 (w), 486 (m), 468 (s), 437 (m), 422 (m). **Raman** (633 nm, 8 mW, 20 s, 20 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 3073 (1), 3057 (1), 3048 (1), 3014 (2), 2985 (1), 2947 (1), 2916 (5), 2856 (1), 2730 (1), 2206 (1), 2086 (2), 1613 (4), 1585 (2), 1485 (1), 1443 (2), 1419 (1), 1386 (2), 1377 (1), 1308 (8), 1277 (1), 1256 (2), 1242 (1), 1192 (1), 1165 (1), 1158 (1), 1104 (1), 1092 (1), 1028 (1), 1007 (2), 974 (1), 961 (1), 945 (1), 914 (1), 907 (1), 891 (1), 851 (1), 824 (1), 759 (1), 737 (3), 708 (1), 676 (1), 653 (1), 597 (1), 588 (3), 578 (10), 563 (5), 541 (3), 530 (2), 523 (3), 513 (1), 500 (1), 488 (3), 476 (1), 469 (5), 436 (1), 424 (3). **MS** (CI^+, m/z (%)): 330 (68) $[TerNH_3]^+$, 386 (26), 687 (100) $(\mu\text{-NTer})_2PH^+$, 716 (4) $[P(\mu\text{-NTer})]_2^+$, 743 (30) $P(\mu\text{-NTer})_2PN2^+$, 762 (10) $H[P(\mu\text{-NTer})]_2N_3H^+$.

Figure S19: Raman, IR and NMR spectra of **$3N_3$** in C_6D_6.

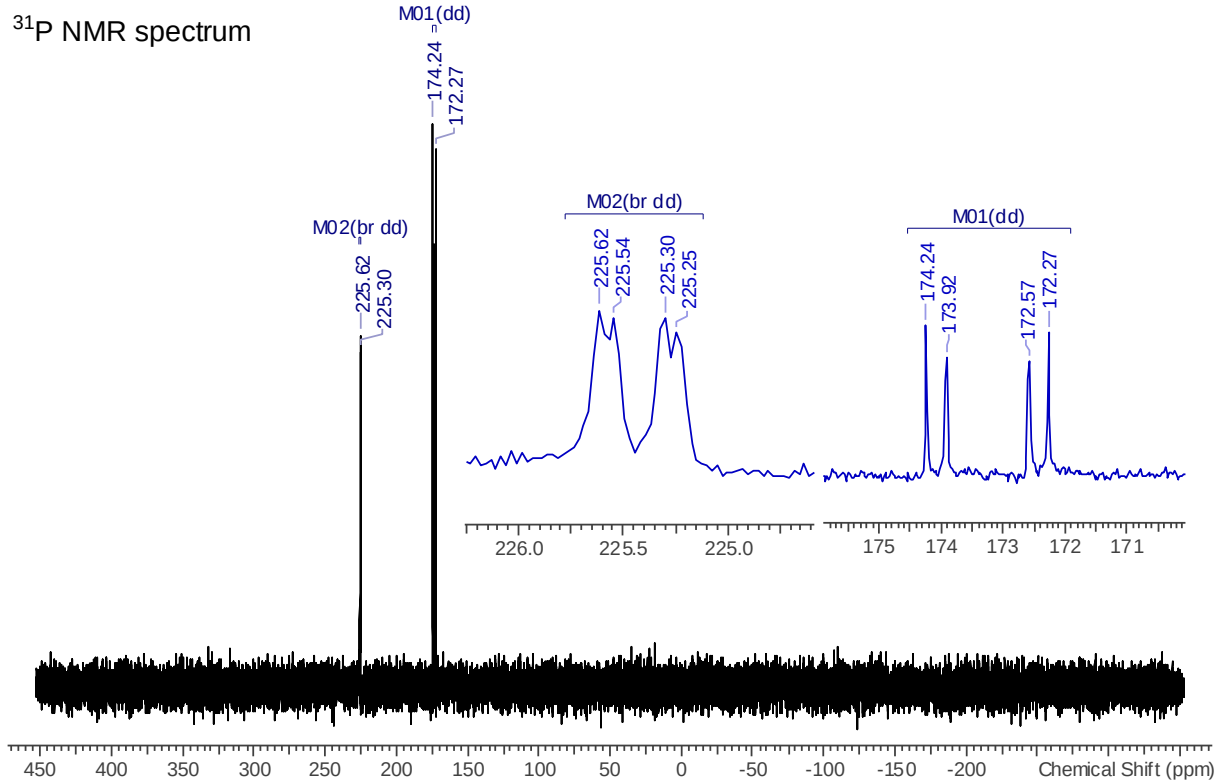
^{1}H NMR spectrum

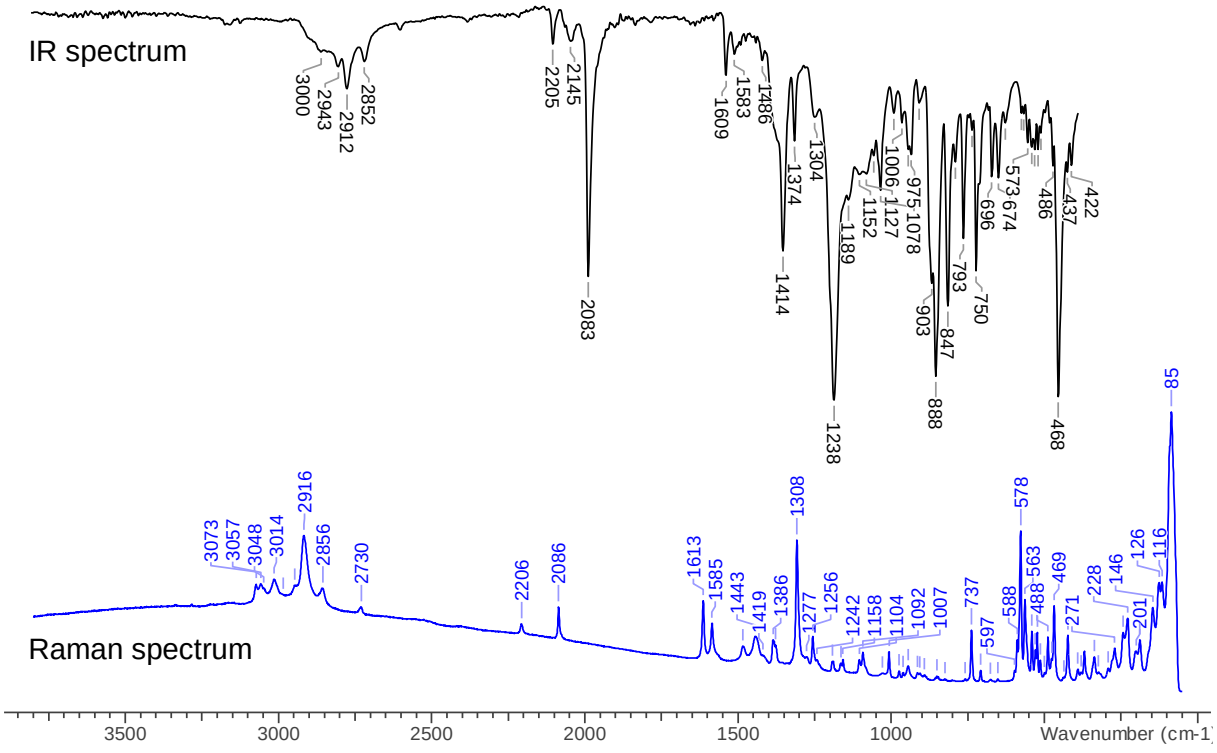


$^{13}C\{^{1}H\}$ NMR spectrum

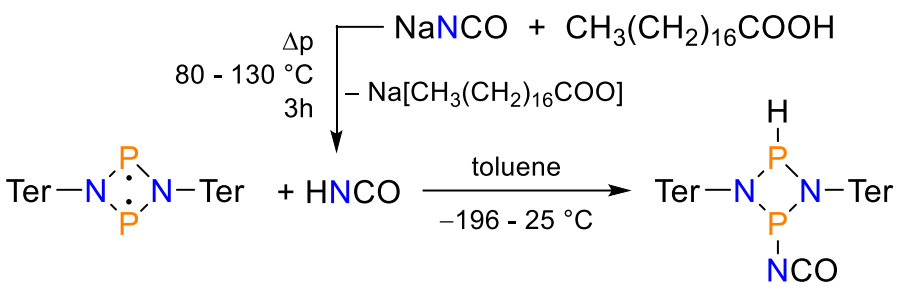


^{31}P NMR spectrum




IR spectrum
3000
2943
2912
2852
2205
2145
2083
1609
1583
1486
1414
1374
1304
1238
1189
1152
1127
1006
975
1078
903
888
847
793
750
696
674
573
486
468
437
422
Raman spectrum
3073
3057
3048
3014
2916
2856
2730
2206
2086
1613
1585
1443
1419
1386
1308
1277
1256
1242
1158
1104
1092
1007
737
597
588
578
563
488
469
271
228
201
146
126
116
85
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)

3.5 Synthesis of [HP(μ-NTer)2PNCO] (3NCO)



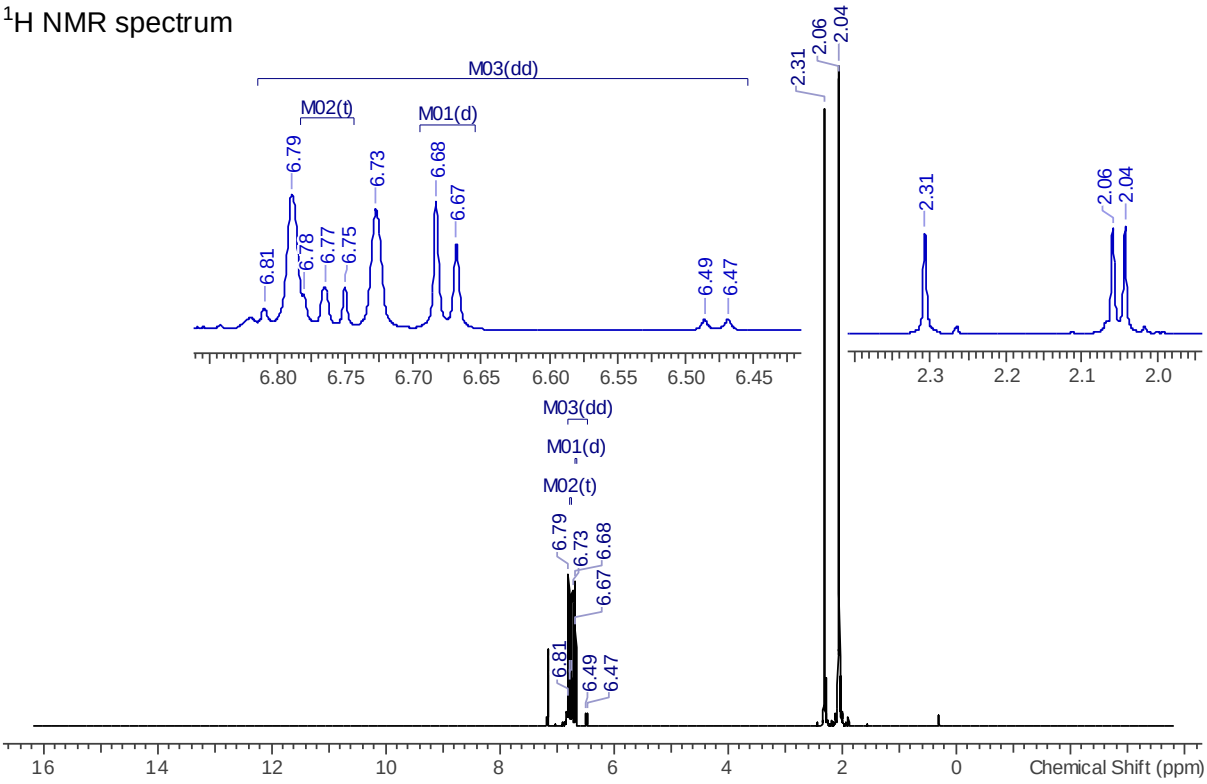
[P(μ-NTer)]$_2$ (209 mg, 0.29 mmol) is suspended in toluene (5 mL) and the mixture is degassed *in vacuo*. HNCO is added as described in *section 2.6* (NaNCO 206 mg, 3.17 mmol; stearic acid 1.95 g, 6.85 mmol). After addition of HNCO, the reaction vessel is separated and warmed up to ambient temperature, whereupon the reaction mixture turns colourless. All volatile components are removed ($1\cdot10^{-3}$ mbar, 50 °C (water bath), 2 h). Single crystals suitable for X-ray structure elucidation can be grown from a benzene solution overnight by cooling from 50 °C to ambient temperature. The structure elucidation identified the crystals as [HP(μ-NTer)$_2$PNCO] (**3NCO**). The supernatant is discarded by syringe and the remaining crystals are dried ($1\cdot10^{-3}$ mbar, 50 °C (water bath), 2 h), yielding 157 mg (0.21 mmol, 72 %) of **3NCO**.

[HP(μ-NTer)$_2$PNCO] (759.91 g·mol^{-1}): **mp**. >118 °C (dec.). **EA** calc. (found), %: C, 77.45 (77.28); H, 6.76 (6.73); N, 5.53 (5.53). **^{1}H NMR** (298 K, C_6D_6, 500.13 MHz): δ = 2.04 (s, 6H, Mes, *o*-C*H*$_3$), 2.06 (s, 6H, Mes, *o*-C*H*$_3$), 2.31 (s, 6H, Mes, *p*-CH$_3$), 6.64 (dd, 1H, *H*P(μ-NTer)$_2$PCl, $^1J(^1H,^{31}P)$ = 160 Hz, $^3J(^1H,^{31}P)$ = 8.7 Hz), 6.68 (d, 2H, *m*-C*H*, $^3J(^1H,^1H)$ = 7.5 Hz), 6.73 (s, 2H, Mes, m-C*H*), 6.76 (t, 1H, *p*-C*H*, $^3J(^1H,^1H)$ = 7.5 Hz), 6.79 (s, 2H, Mes, m-C*H*). **^{13}C{^{1}H} NMR** (298 K, C_6D_6, 125.8 MHz): δ = 20.9 (d, *o*-*C*H$_3$, $J(^{13}C,^{31}P)$ = 1.6 Hz), 21.4 (d, *o*-*C*H$_3$, $J(^{13}C,^{31}P)$ = 5.0 Hz), 21.9 (s, *p*-*C*H$_3$), 122.4 (s, *C*H), 128.9 (s, *C*H), 129.0 (s, *C*H), 130.9 (s, *C*H), 131.8 (s, *C*), 135.7 (s, *C*), 138.1 (s, *C*), 138.3 (t, N*C*O, $^1J(^{13}C,^{17}O)$ = 3.7 Hz), 138.8 (d, *C*, $J(^{13}C,^{31}P)$ = 4.6 Hz), 139.1 (d, *C*, $J(^{13}C,^{31}P)$ = 4.2 Hz). **^{14}N{^{1}H} NMR** (298 K, C_6D_6, 36.1 MHz): δ = not observed. **^{31}P{^{1}H} NMR** (298 K, C_6D_6, 202.5 MHz): δ = 170.7 (d, H*P*(μ-NTer)$_2$PNCO, $^2J(^{31}P,^{31}P)$ = 30 Hz), 195.7 (d, HP(μ-NTer)$_2$*P*NCO, $^2J(^{31}P,^{31}P)$ = 30 Hz). **^{31}P NMR** (298 K, C_6D_6, 202.5 MHz): δ = 170.7 (d, H*P*(μ-NTer)$_2$PNCO, $^1J(^{31}P,^1H)$ = 160 Hz, $^2J(^{31}P,^{31}P)$ = 30 Hz), 195.7 (d, HP(μ-NTer)$_2$*P*NCO, $^2J(^{31}P,^{31}P)$ = 30 Hz). **IR** (ATR-IR, 32 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 2999 (w), 2943 (w), 2914 (w), 2855 (w), 2729 (w), 2226 (w), 2205 (m), 2148 (w), 1694 (w), 1610 (w), 1581 (w), 1484 (w), 1433 (m), 1412 (s), 1375 (m), 1239 (m), 1222 (m), 1080

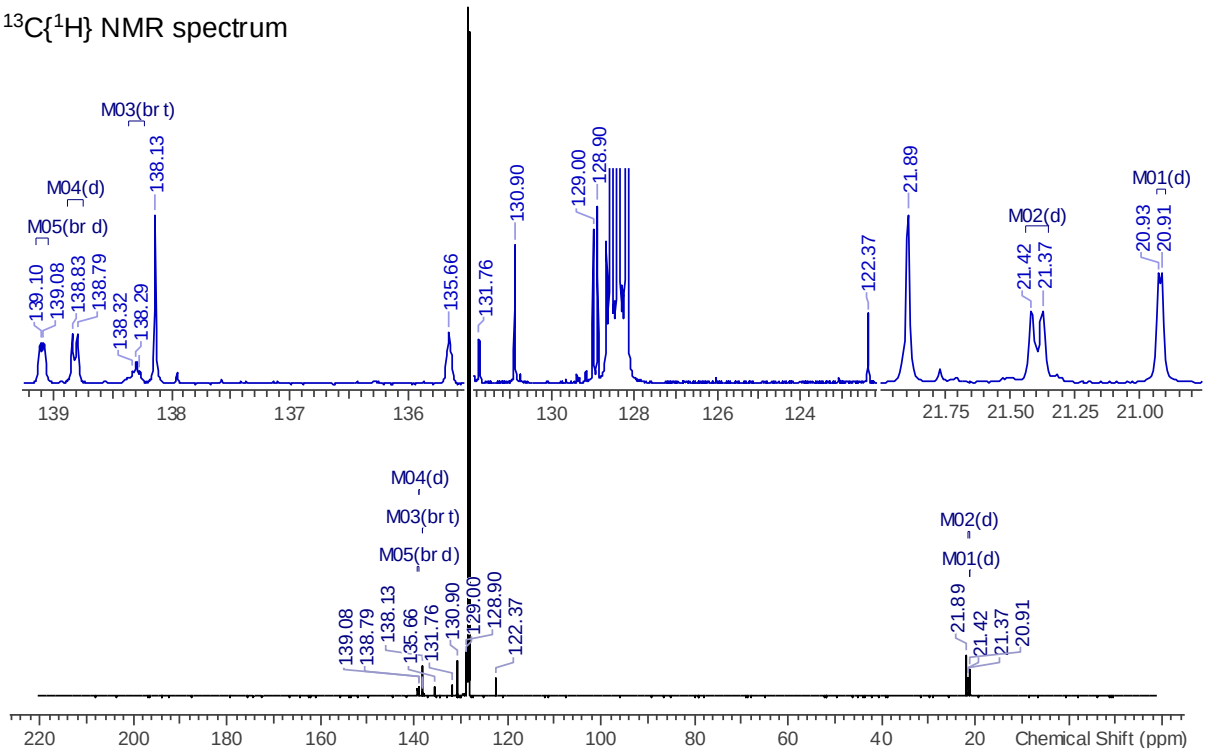
(m), 1031 (w), 1006 (w), 971 (w), 888 (vs), 847 (s), 822 (m), 794 (m), 750 (m), 738 (m), 730 (m), 697 (m), 653 (m), 606 (m), 600 (m), 573 (m), 559 (m), 550 (m), 497 (s), 466 (m), 437 (m), 423 (m). **Raman** (633 nm, 8 mW, 20 s, 20 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 3073 (1), 3043 (1), 3019 (1), 2952 (4), 2895 (9), 2117 (1), 1684 (1), 1666 (1), 1593 (3), 1469 (1), 1444 (1), 1405 (1), 1379 (1), 1328 (1), 1258 (2), 1241 (1), 1195 (4), 1163 (1), 1098 (1), 1015 (1), 912 (1), 885 (1), 862 (1), 832 (1), 792 (1), 747 (1), 711 (1), 689 (4), 630 (10), 604 (1), 554 (2), 542 (1), 525 (1), 503 (1), 459 (1), 445 (1), 428 (1), 412 (2), 404 (2). **MS** (CI^+, m/z (%)): 330 (23) $[TerNH_3]^+$, 687 (100) $(\mu\text{-NTer})_2PH^+$, 716 (63) $[P(\mu\text{-NTer})]_2^+$, 717 (63) $[P(\mu\text{-NTer})]_2H^+$, 760 (36) $[H_2P(\mu\text{-NTer})_2PNCO]^+$.

Figure S20: Raman, IR and NMR spectra of **3NCO** in C_6D_6.

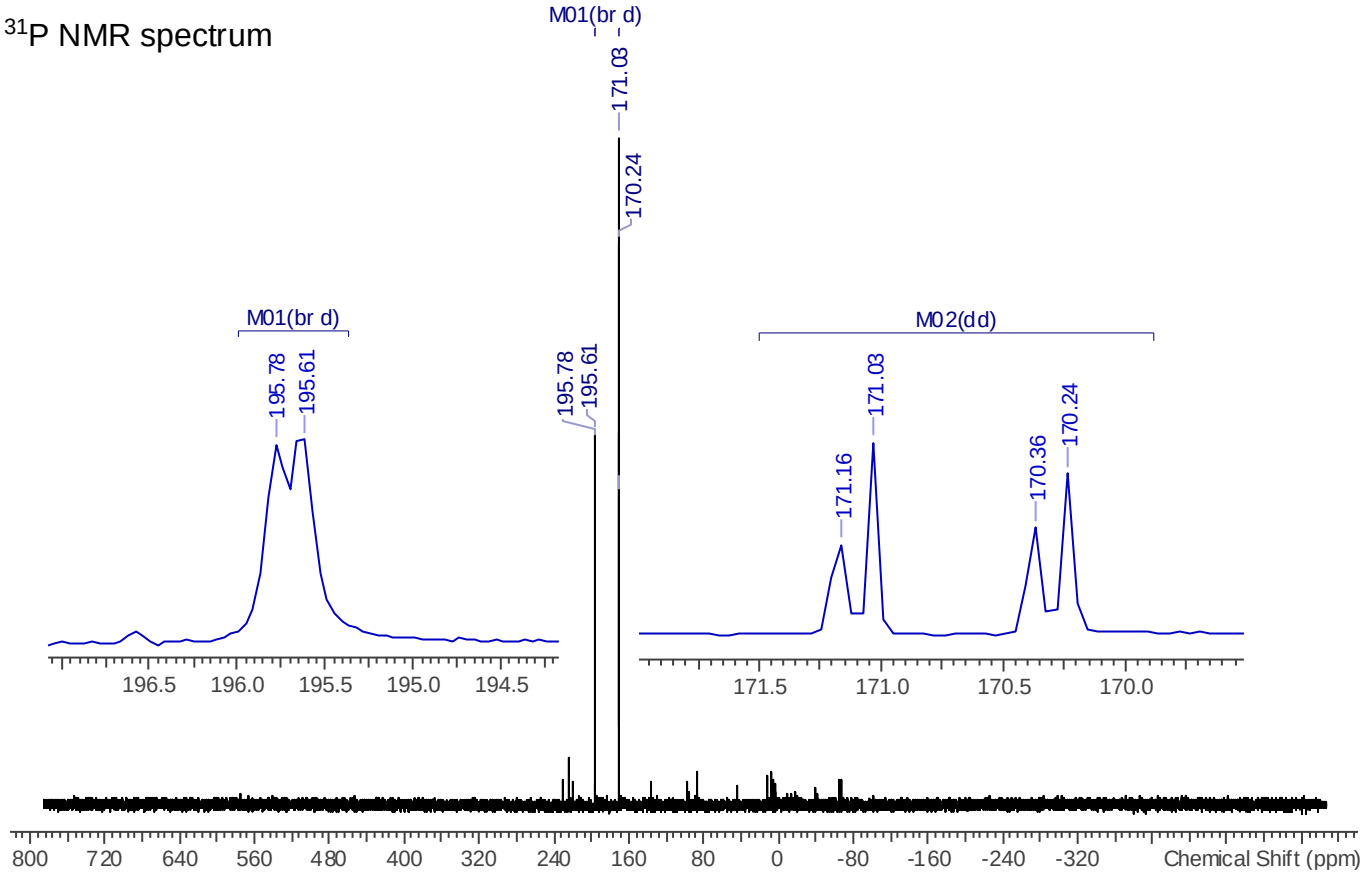
^{1}H NMR spectrum

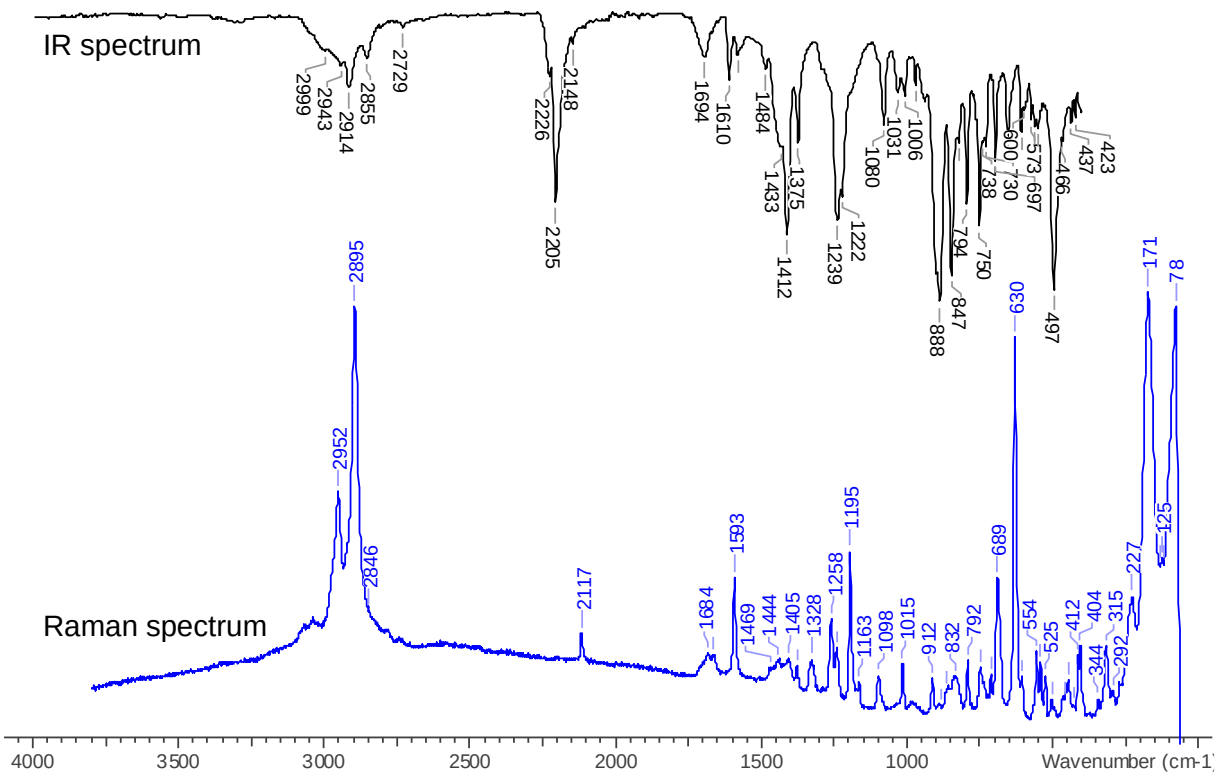


$^{13}C\{^{1}H\}$ NMR spectrum

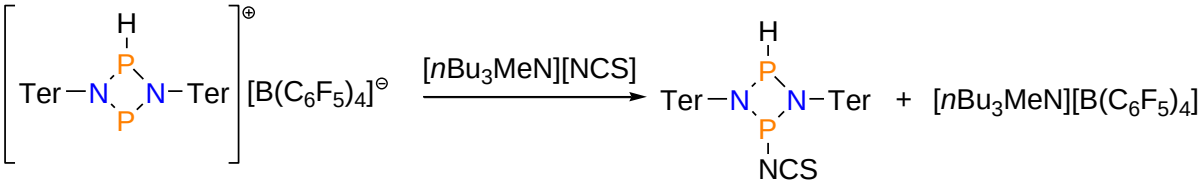


^{31}P NMR spectrum




IR spectrum
2999
2943
2914
2855
2729
2226
2148
2205
1694
1610
1484
1433
1375
1412
1239
1222
1080
1031
1006
888
847
794
750
738
730
697
600
573
497
466
437
423
Raman spectrum
2952
2895
2846
2117
1684
1593
1469
1444
1405
1328
1258
1195
1163
1098
1015
912
832
792
689
630
554
525
412
404
344
315
292
227
171
125
78
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)

3.6 Synthesis of [HP(μ-NTer)2PNCS] (3NCS)

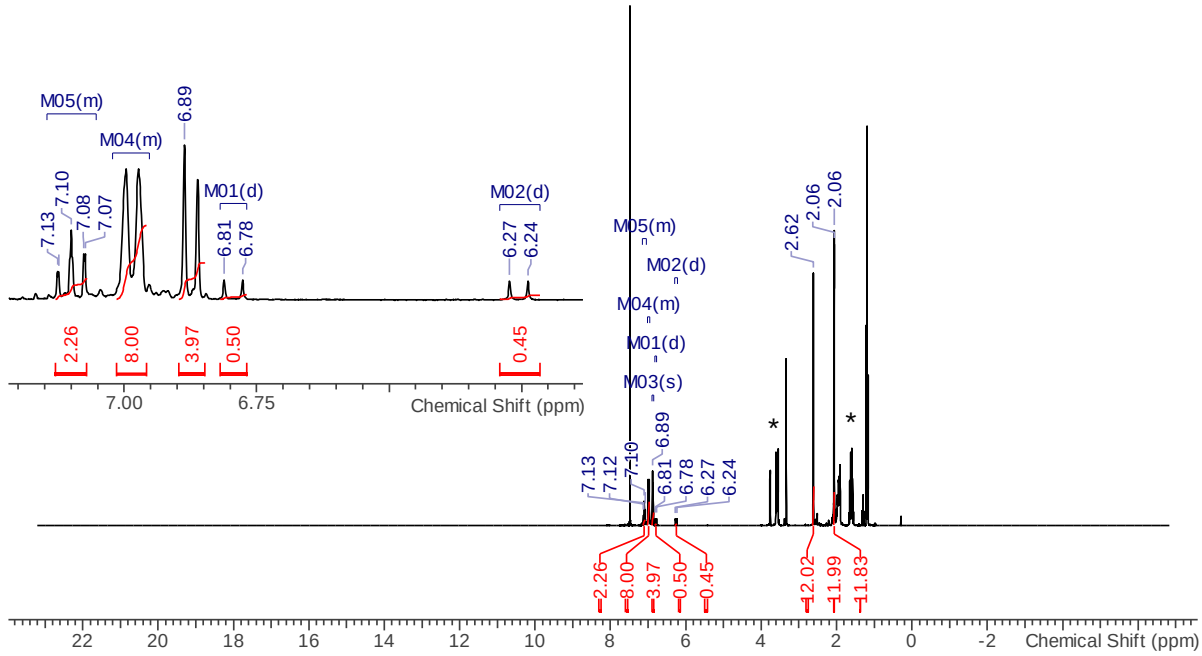


$[HP(\mu\text{-NTer})_2P][B(C_6F_5)_4]$ (15 mg, 0.01 mmol) and $(n\text{Bu}_3\text{MeN})$NCS (4 mg, 0.01 mmol) are combined in an NMR tube and dissolved in THF-d_8 (0.5 mL), resulting in a colourless solution. Quantitative NMR spectra indicate the formation of **3NCS**. However, it is not possible to isolate the pure product from the reaction mixture.

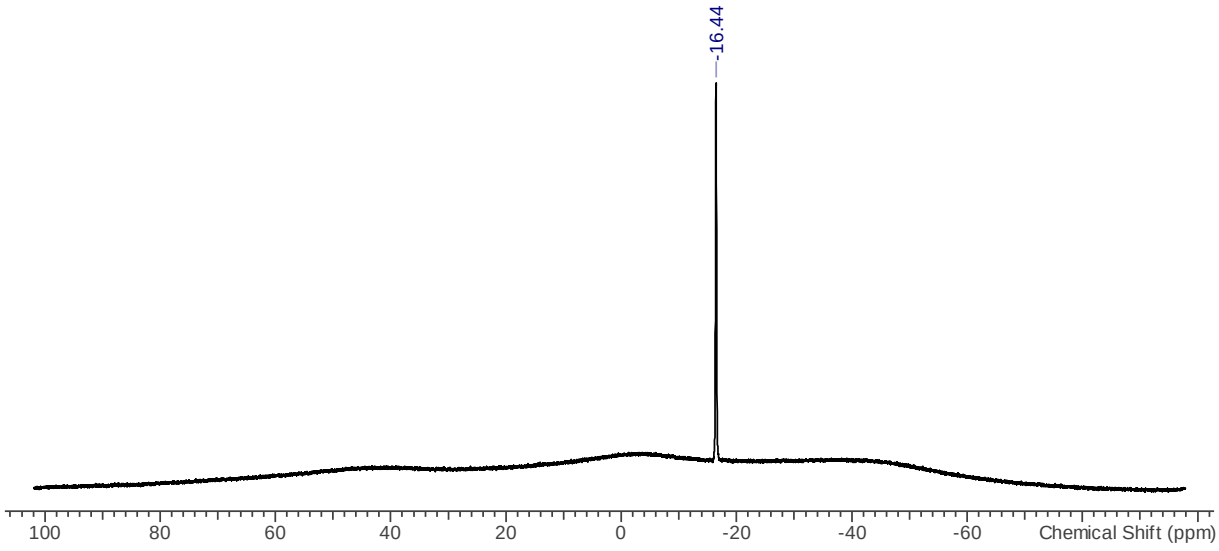
$[HP(\mu\text{-NTer})_2PNCS]$ (775.98 g·mol^{-1}): **^{1}H NMR** (298 K, THF-d_8, 300.1 MHz): δ = 2.06 (s, 12H, Mes, *o*-CH_3), 2.06 (s, 12H, Mes, *o*-CH_3), 2.62 (s, 12H, Mes, *p*-CH_3), 6.52 (dd, 1H, *H*P(μ-NTer)$_2$PNCS, $^{1}J(^{1}H,^{31}P)$ = 161.7 Hz, $^{3}J(^{1}H,^{31}P)$ = 10.5 Hz), 6.87 (d, 4H, *m*-C*H*, $^{3}J(^{1}H,^{1}H)$ = 7.4 Hz), 6.99 (d, 8H, Mes, m-C*H,* $^{3}J(^{1}H,^{1}H)$ = 7.2 Hz), 6.76 (m, 2H, *p*-C*H*). **^{11}B NMR** (298 K, THF-d_8, 96.3 MHz): δ = −16.4 (s, 1B, $[B(C_6F_5)_4]^-$). **^{19}F NMR** (298 K, THF-d_8, 282.4 MHz): δ = −132.6 (m), −164.3 (t, J = 40 Hz), −168.4 (t, J = 36 Hz).**^{13}C{^{1}H} NMR** (298 K, THF-d_8, 75.5 MHz): δ = 20.8 (s, *o*-CH_3), 21.3 (d, *o*-CH_3, $J(^{13}C,^{31}P)$ = 6 Hz), 21.8 (s, *p*-CH_3), 122.9 (s, *C*H), 129.5 (s, *C*H), 129.7 (s, *C*H), 130.1 (s, *C*H), 130.7 (s, *C*H), 131.2 (s, *C*), 132.1 (s, *C*), 135.4 (s, *C*), 138.7 (s, *C*), 138.9 (s, *C*), 139.5 (s, *C*). **^{14}N{^{1}H} NMR** (298 K, THF-d_8, 36.1 MHz): δ = No signals observed. **^{31}P NMR** (298 K, C_6D_6, 121.5 MHz): δ = 176.2 (dd, 1P, H*P*(μ-NTer)$_2$PNCS, $^{1}J(^{31}P,^{1}H)$ = 162 Hz, $^{2}J(^{31}P,^{31}P)$ = 36 Hz), 199.9 (m, 1P, HP(μ-NTer)$_2$*P*NCS).

Figure S21: NMR spectra of **3NCS** in THF-d_8 (solvent signals indicated by asterisk).

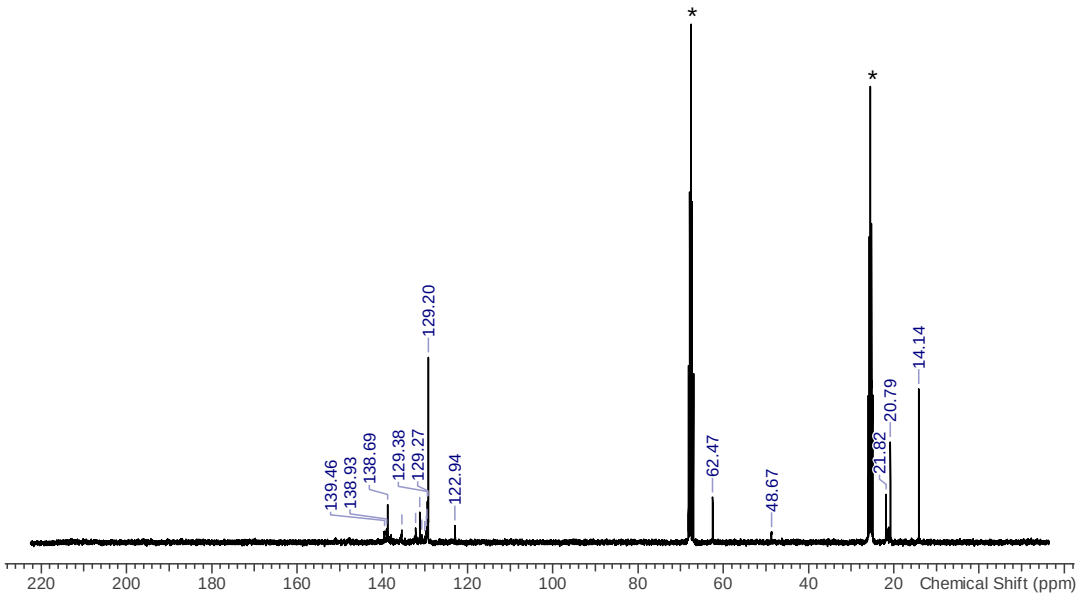
^{1}H NMR spectrum



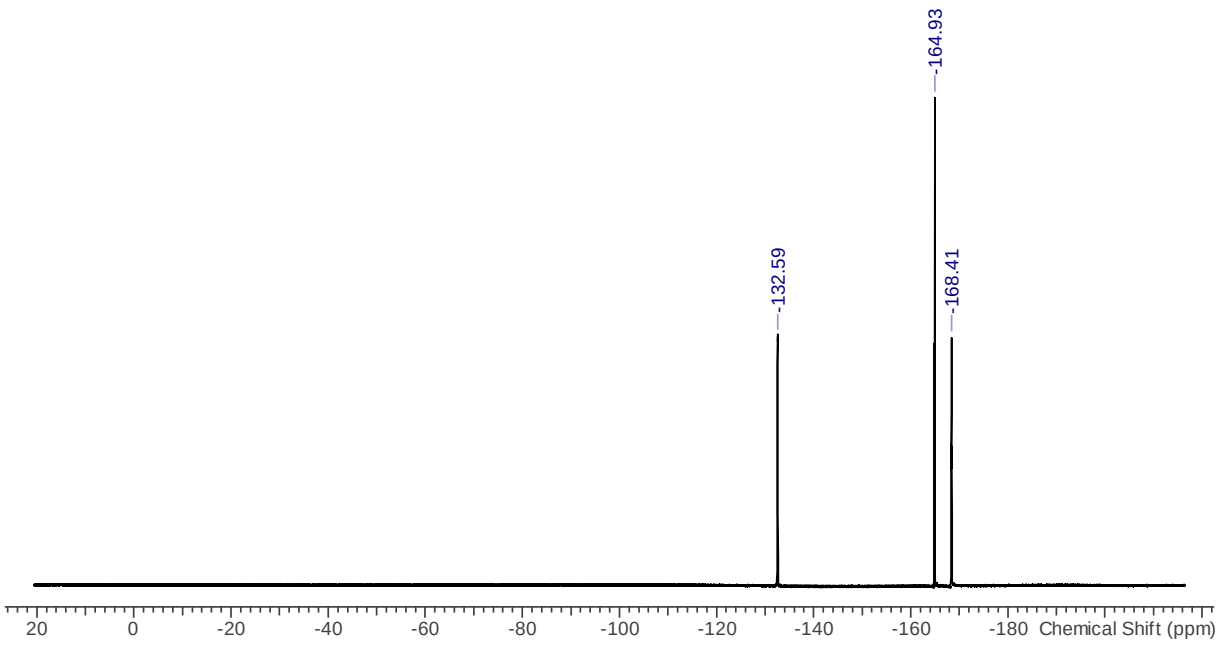
^{11}B NMR spectrum



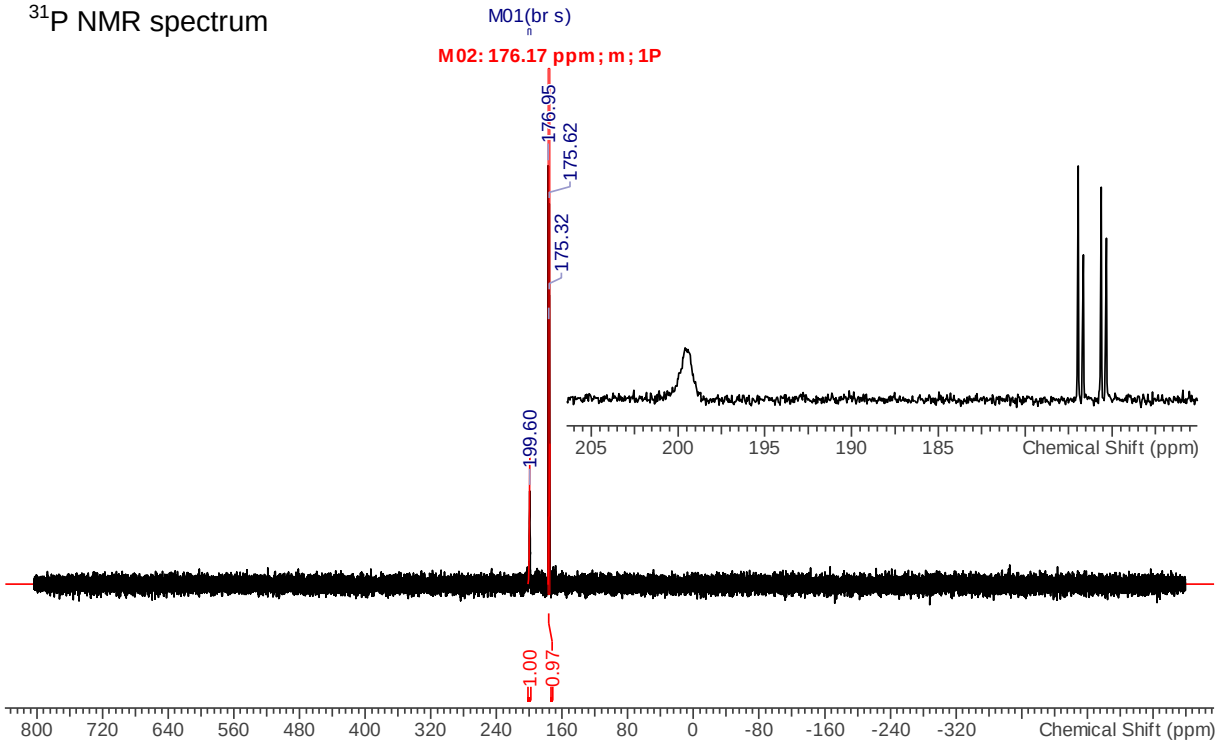
^{13}C NMR spectrum



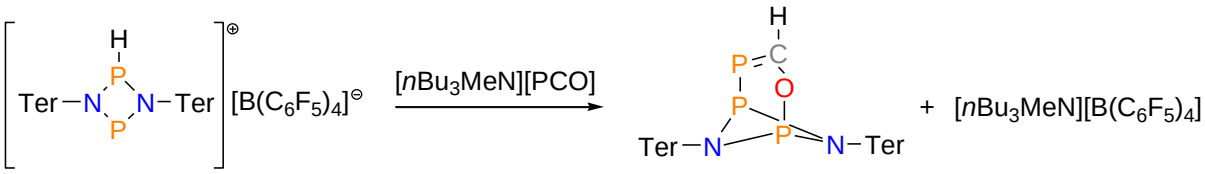
^{19}F NMR spectrum



^{31}P NMR spectrum



3.7 Synthesis of [(μ-PNTer)PC(H)O] (3PCO)



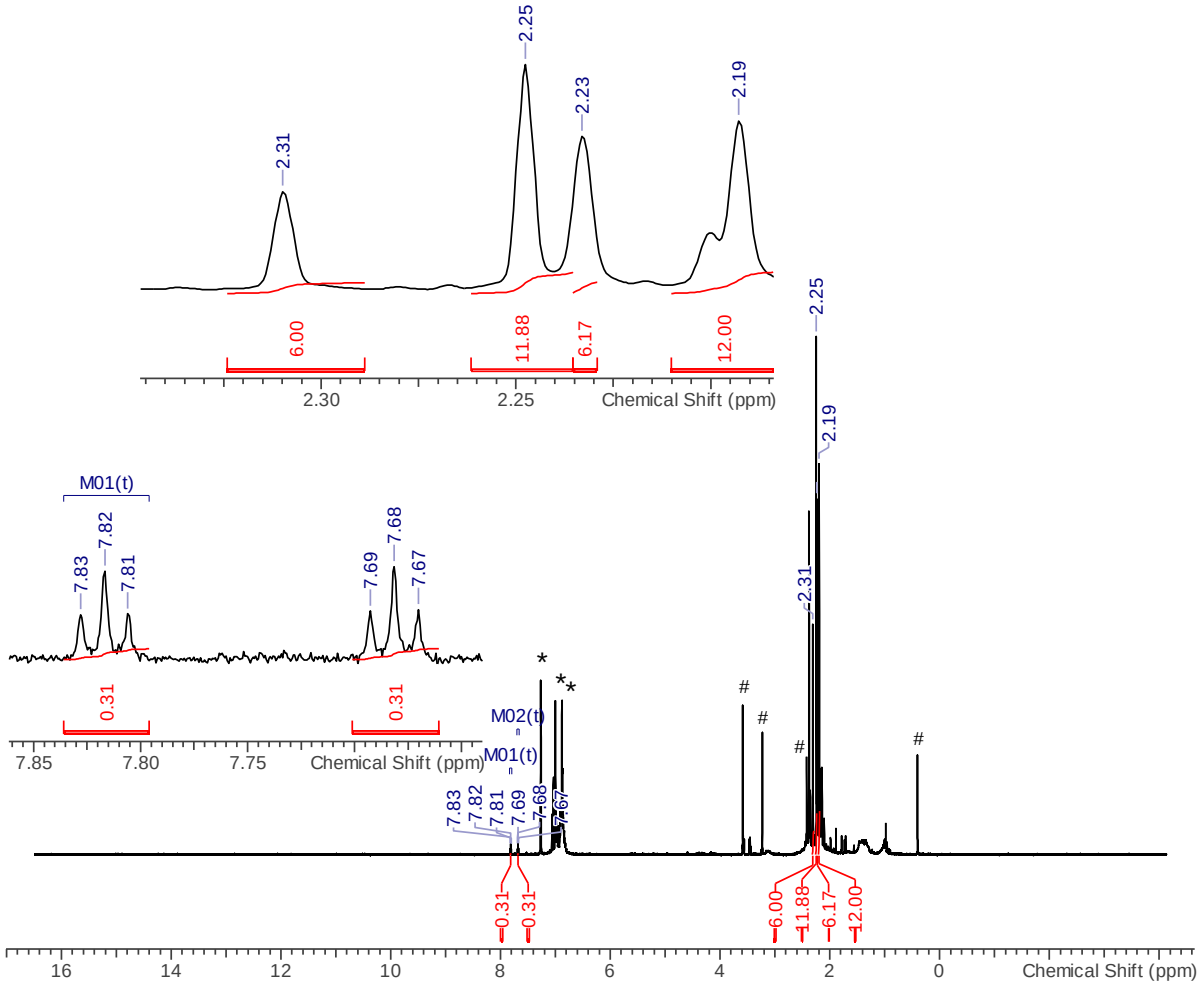
[HP(μ-NTer)$_2$P][B(C$_6$F$_5$)$_4$] (606 mg, 0.43 mmol) and (*n*Bu$_3$MeN)PCO (127 mg, 0.49 mmol) are combined in a flask and suspended in benzene (22 mL). After 10 min of stirring, the solids dissolve and a clear red solution is obtained. After further 20 min of stirring and 5 min of ultrasonic bath the solution discolours to pale yellow. All volatile components are removed (1·10^{-3} mbar, 40 °C, 1 h). The residue is transferred into an extraction thimble, which is sealed with glass wool and filter paper. The loaded thimble is extracted with *n*-pentane (50 mL, 16 h, 60 °C oil bath temp.) using a Soxhlet extractor. During the extraction process, the extract becomes cloudy and formation of a white precipitate can be observed. At the end, all volatile components are removed (1·10^{-3} mbar, 40 °C, 2 h). Single crystals suitable for X-ray structure elucidation can be grown from a toluene (~ 5 mL) solution over two days by cooling from 50 °C to −40 °C. The structure elucidation identified the crystals as [(μ-PNTer)PC(H)O] (**3PCO**). The supernatant is discarded by syringe and the remaining crystals are dried (1·10^{-3} mbar, 50 °C, 2 h), yielding 70 mg (0.09 mmol, 21 %) of **3PCO**.

[(μ-PNTer)$_2$PC(H)O] (776.88 g·mol^{-1}): **mp**. 170 °C (dec.). **EA** calc. (found), %: C, 75.76 (75.60); H, 6.62 (6.98); N, 3.61 (3.26). **^{1}H NMR** (298 K, C$_6$D$_6$, 300.1 MHz): δ = 2.09 (s, 12H, Mes, *o*-C*H*$_3$), 2.13 (s, 6H, Mes, *p*-C*H*$_3$), 2.14 (s, 12H, Mes, *o*-C*H*$_3$), 2.20 (s, 6H, Mes, *p*-CH$_3$), 6.72-6.96 (m, 13H, p/*m*-C*H*), 7.71 (ddd, 1H, P(μ-NTer)$_2$PPC(*H*)O, ^3J(^{1}H,^{31}P) = 3.4 Hz, ^3J(^{1}H,^{31}P) = 3.4 Hz, ^2J(^{1}H,^{31}P) = 40.6 Hz). **^{13}C{^{1}H} NMR** (298 K, Tol-*d*$_8$, 125.8 MHz): δ = 21.5 (s, *C*H$_3$), 21.7 (d, *C*H$_3$, J(^{13}C,^{31}P) = 4 Hz), 21.8 (s, *C*H$_3$), 21.9 (d, *C*H$_3$, J(^{13}C,^{31}P) = 3 Hz), 118.9 (s, *C*H), 122.2 (s, *C*H), 125.8 (s, *C*H), 126.6 (s, *C*H), 126.6 (s, *C*), 128.6 (s, P*C*H), 129.1 (s, *C*H), 129.4 (s, *C*H), 129.6 (s, *C*H), 130.8 (s, *C*H), 131.2 (s, *C*H), 133.1 (s, *C*H), 136.3 (s, *C*), 137.2 (s, *C*), 137.4 (s, *C*), 141.6 (s, *C*). **^{14}N{^{1}H} NMR** (298 K, Tol-*d*$_8$, 36.1 MHz): δ = No signals observed. **^{31}P NMR** (298 K, Tol-*d*$_8$, 202.5 MHz): δ = 158.0 (dd, 1P, P*P*C, ^1J(^{31}P,^{31}P) = 203 Hz, ^2J(^{1}H,^{31}P) = 42 Hz), 216.0 (br. dd, 1P, N*P*P, ^1J(^{31}P,^{31}P) = 203 Hz, ^2J(^{31}P,^{31}P) = 17 Hz), 226.4 (d, 1P, N*P*O, ^2J(^{31}P,^{31}P) = 17 Hz). **IR** (ATR-IR, 32 Scans, 298 K, cm^{-1}): $\tilde{\nu}$ = 2998 (w), 2943

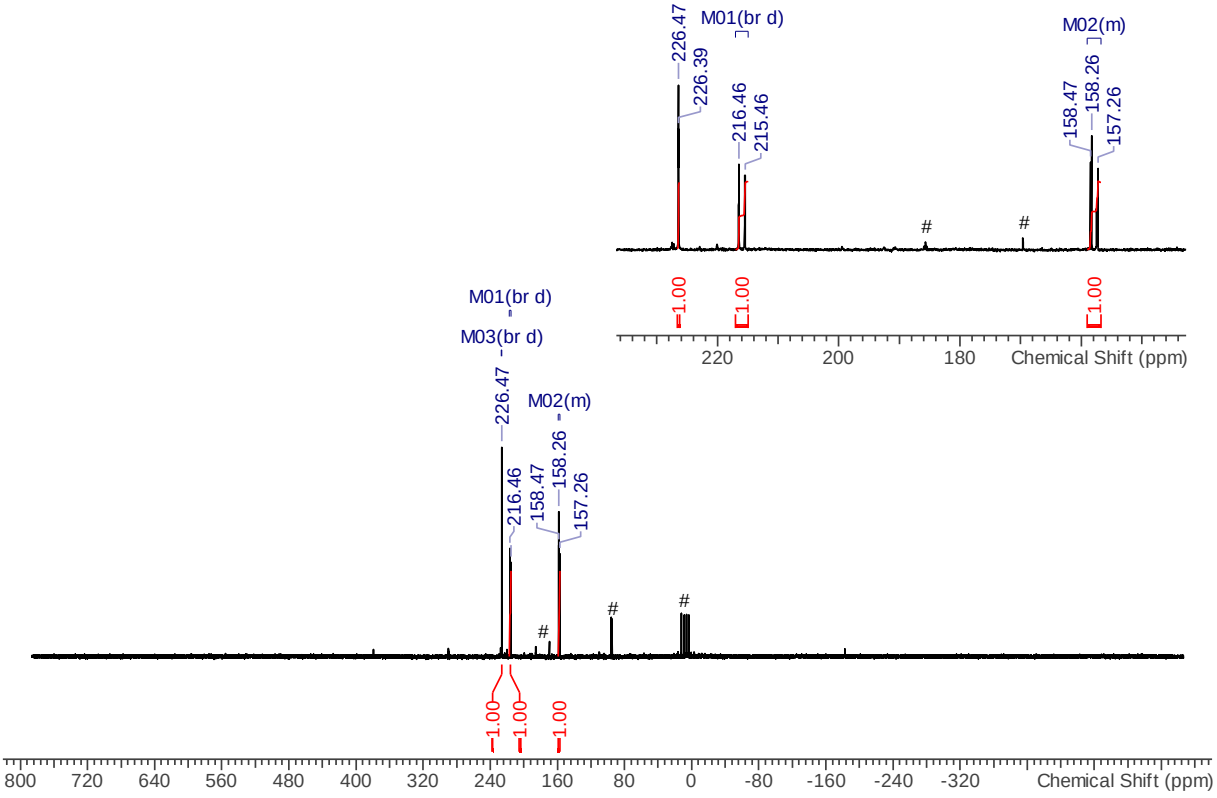
(m), 2914 (m), 2852 (m), 2728 (w), 1731 (w), 1609 (m), 1578 (w), 1484 (w), 1434 (m), 1405 (s), 1372 (m), 1350 (m), 1226 (vs), 1158 (m), 1148 (s), 1080 (m), 1028 (m), 1006 (m), 946 (m), 898 (s), 884 (m), 870 (s), 845 (s), 793 (s), 775 (m), 752 (s), 692 (m), 647 (m), 631 (m), 593 (m), 560 (s), 532 (m), 511 (m), 497 (m), 488 (m), 474 (m), 466 (m), 441 (m), 408 (m). **Raman** (633 nm, 8 mW, 10 s, 10 acc., 298 K, cm^{-1}): $\tilde{\nu}$ = 3065 (1), 3043 (1), 3009 (1), 2972 (1), 2953 (1), 2915 (2), 2855 (1), 2728 (1), 1611 (3), 1581 (2), 1480 (1), 1422 (1), 1405 (1), 1380 (2), 1350 (1), 1303 (5), 1285 (2), 1270 (1), 1245 (1), 1227 (1), 1187 (1), 1158 (1), 1102 (1), 1087 (1), 1029 (1), 1005 (1), 956 (1), 943 (1), 931 (1), 909 (1), 899 (1), 870 (1), 831 (1), 820 (1), 797 (1), 787 (1), 755 (1), 734 (2), 704 (1), 632 (2), 589 (1), 576 (6), 560 (2), 523 (1), 512 (4), 499 (1), 487 (2), 470 (1), 432 (1), 421 (2), 410 (1), 391 (1), 369 (1), 336 (1), 301 (1), 272 (2), 256 (1), 237 (2), 191 (1), 154 (4), 135 (3), 92 (10), 78 (8). **MS** (CI^+, m/z (%)): 330 (14) $[TerNH_3]^+$, 687 (100) $(\mu\text{-NTer})_2PH^+$, 716 (6) $[P(\mu\text{-NTer})]_2^+$, 743 (20), 777 (9) $P(\mu\text{-NTer})_2PPC(H)O^+$.

Figure S22. Raman, IR and NMR spectra of **3PC(H)O** (solvent signals indicated by asterisk, unknown impurities indicated by rhomb).

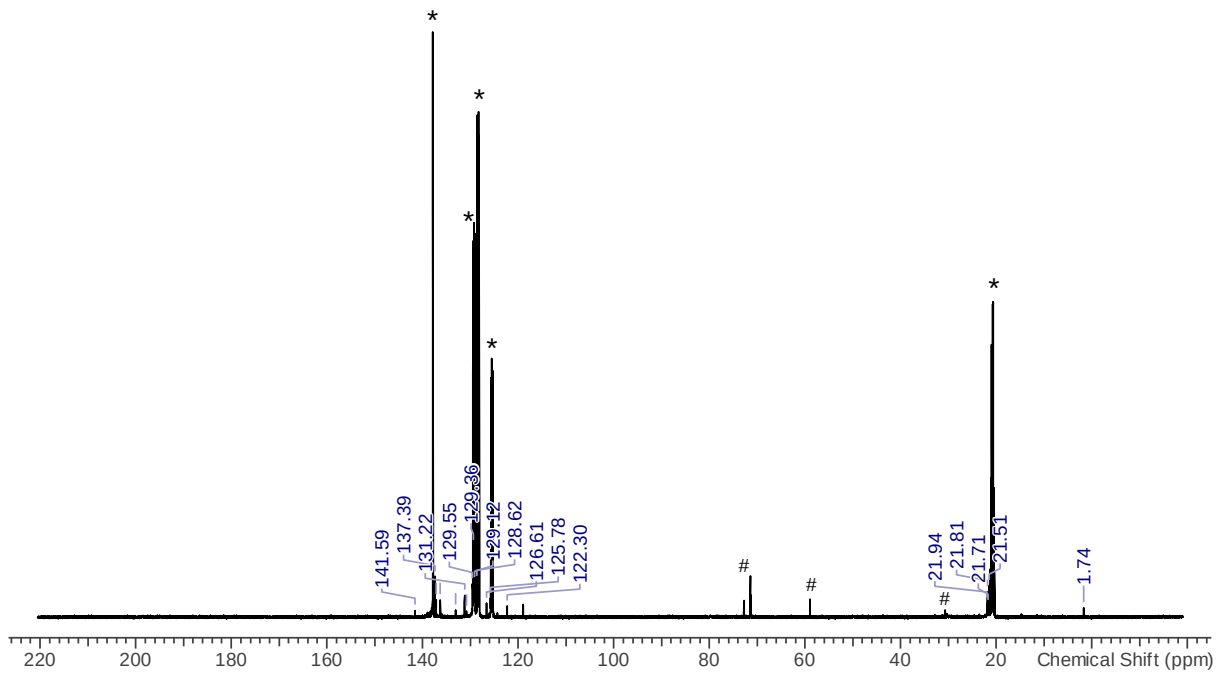
^{1}H NMR spectrum

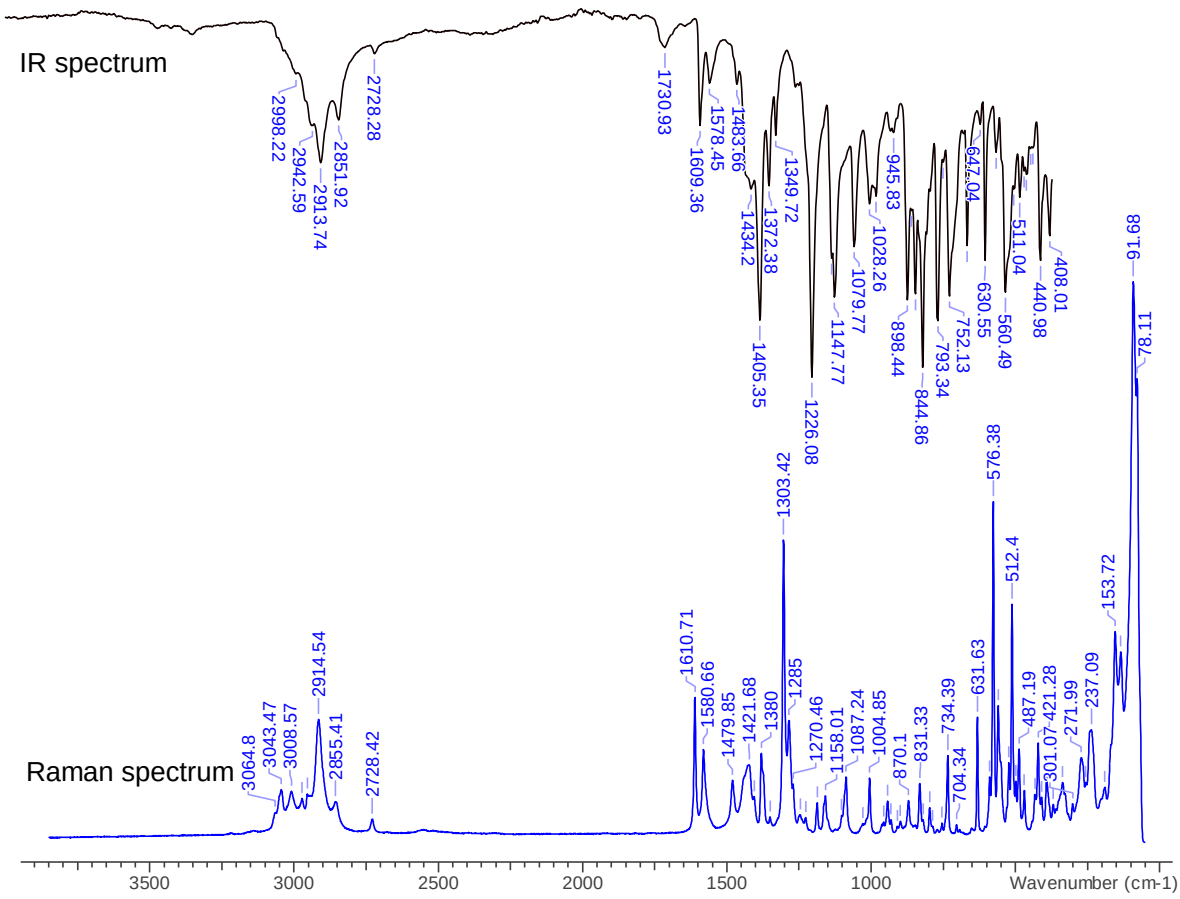


^{31}P NMR spectrum



^{13}C NMR spectrum



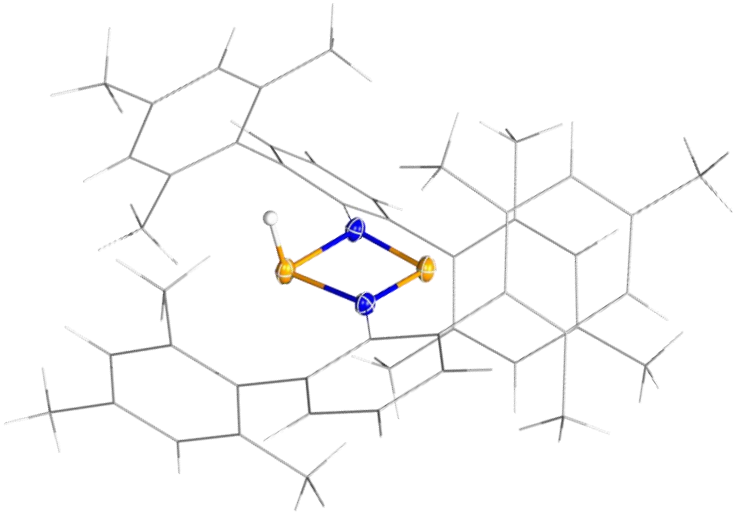

IR spectrum
2998.22
2942.59
2913.74
2851.92
2728.28
1730.93
1609.36
1578.45
1483.66
1434.2
1372.38
1349.72
1405.35
1226.08
1147.77
1079.77
1028.26
945.83
898.44
844.86
793.34
752.13
647.04
630.55
560.49
511.04
440.98
408.01
91.68
78.11
Raman spectrum
3064.8
3043.47
3008.57
2914.54
2855.41
2728.42
1610.71
1580.66
1479.85
1421.68
1380
1303.1
1285
1270.46
1158.01
1087.24
1004.85
870.1
831.33
734.39
704.34
631.63
576.38
512.4
487.19
421.28
301.07
271.99
237.09
153.72
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)

4 Structure elucidation

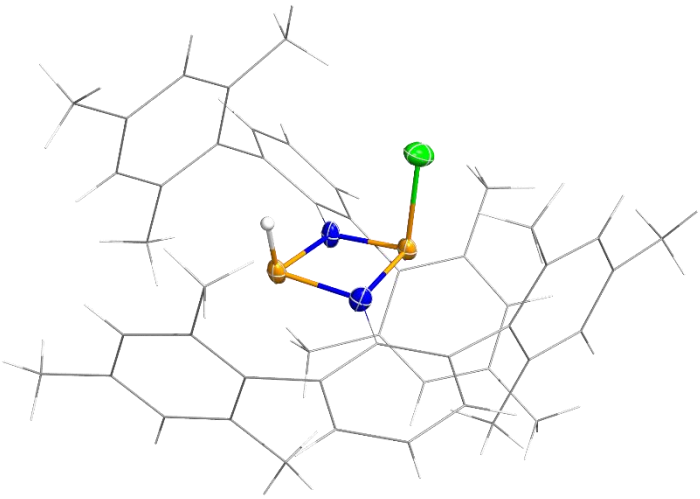
X-ray Structure Determination: X-ray quality crystals were selected in Fomblin YR-1800 perfluoroether (Alfa Aesar) at ambient temperature. The samples were cooled to 123(2) K during measurement. The data were collected on a Bruker D8 Quest diffractometer or a Bruker Kappa Apex II diffractometer using Mo K_α radiation (λ = 0.71073 Å). The structures were solved by iterative methods (SHELXT)[18] and refined by full matrix least squares procedures (SHELXL).[19] Semi-empirical absorption corrections were applied (SADABS).[20] All non-hydrogen atoms were refined anisotropically, hydrogen atoms were included in the refinement at calculated positions using a riding model.

Table S2: Crystallographic details.

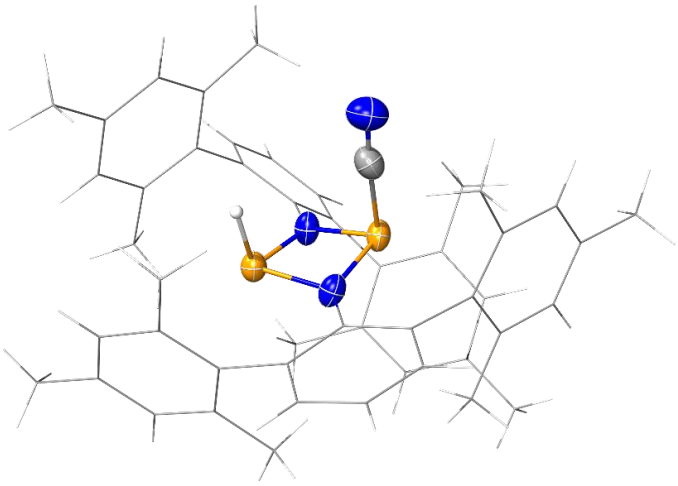
Compound	**2**
Chem. Formula	$[C_{48}H_{51}N_2P_2][B(C_6F_5)_4]$
Formula weight [g/mol]	1589.09
Colour	colourless
Crystal system	triclinic
Space group	P_1
a [Å]	12.756(2)
b [Å]	15.269(2)
c [Å]	19.312(2)
α [°]	87.366(4)
β [°]	79.437(4)
γ [°]	84.981(4)
V [Å^3]	3681.7(7)
Z	2
$\rho_{calcd.}$ [g/cm^3]	1.433
μ [mm^{-1}]	0.71073
T [K]	123
Measured reflections	201587
Independent reflections	26620
Reflections with $I > 2\sigma(I)$	18931
R_{int}	0.059
F(000)	1624
$R_1(R[F^2>2\sigma(F^2)])$	0.056
$wR_2(F^2)$	0.139
GooF	1.03
No. of Parameters	1000
CCDC #	1976818



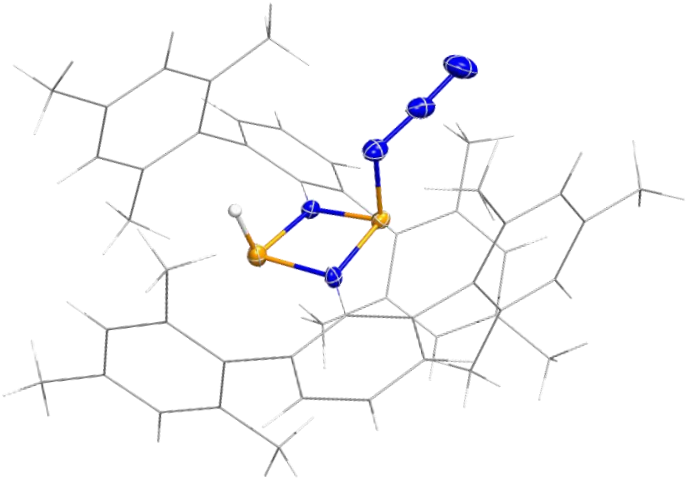
Compound	**3Cl**
Chem. Formula	$C_{48}H_{51}ClN_2P_2$
Formula weight [g/mol]	753.35
Colour	colourless
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	12.423(2)
b [Å]	20.972(2)
c [Å]	16.397(2)
α [°]	90
β [°]	108.795(2)
γ [°]	90
V [Å^3]	4044.1(8)
Z	4
$\rho_{calcd.}$ [g/cm^3]	1.237
μ [mm^{-1}]	0.71073
T [K]	123
Measured reflections	70308
Independent reflections	10732
Reflections with $I > 2\sigma(I)$	7775
R_{int}	0.080
F(000)	1600
$R_1(R[F^2>2\sigma(F^2)])$	0.058
$wR_2(F^2)$	0.142
GooF	1.06
No. of Parameters	526
CCDC #	1976821



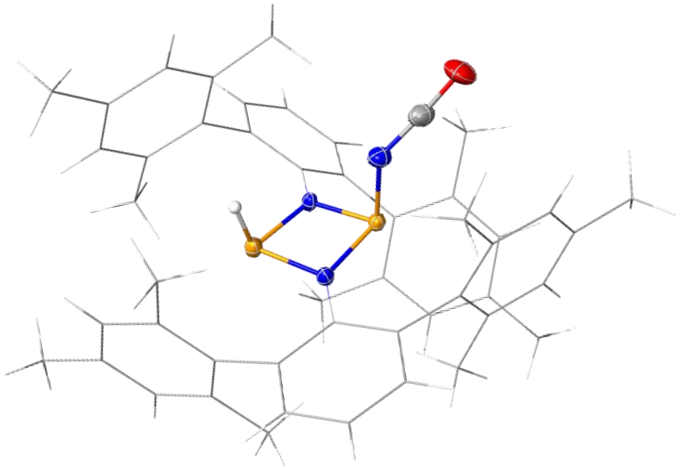
Compound	**3CN**
Chem. Formula	$C_{49}H_{51}N_3P_2$
Formula weight [g/mol]	743.91
Colour	colourless
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	12.7266(6)
b [Å]	20.713(1)
c [Å]	16.2878(8)
α [°]	90
β [°]	105.289(2)
γ [°]	90
V [Å^3]	4141.6(3)
Z	4
$\rho_{calcd.}$ [g/cm^3]	1.193
μ [mm^{-1}]	0.71073
T [K]	123
Measured reflections	111194
Independent reflections	8138
Reflections with $I > 2\sigma(I)$	5894
R_{int}	0.093
F(000)	1584
$R_1(R[F^2>2\sigma(F^2)])$	0.067
$wR_2(F^2)$	0.148
GooF	1.13
No. of Parameters	545
CCDC #	1976819



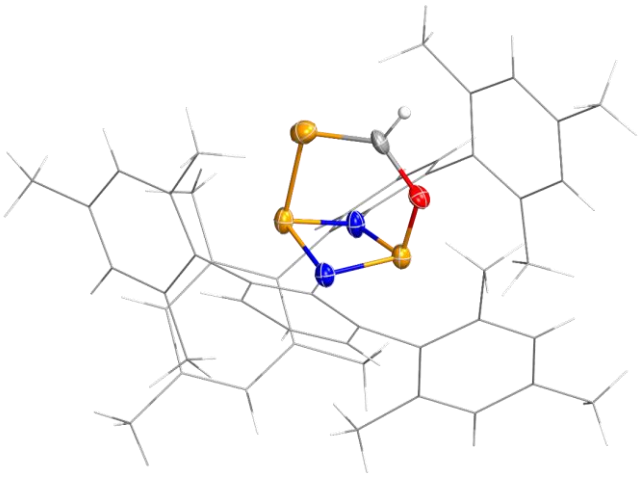
Compound	**3N$_3$**
Chem. Formula	$C_{48}H_{51}N_5P_2$
Formula weight [g/mol]	759.91
Colour	colourless
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	16.478(2)
b [Å]	15.443(2)
c [Å]	16.5828(9)
α [°]	90
β [°]	91.484(2)
γ [°]	90
V [Å^3]	4218.0(4)
Z	4
$\rho_{calcd.}$ [g/cm^3]	1.197
μ [mm^{-1}]	0.71073
T [K]	123
Measured reflections	245131
Independent reflections	13435
Reflections with $I > 2\sigma(I)$	10942
R_{int}	0.048
F(000)	1616
$R_1(R[F^2>2\sigma(F^2)])$	0.046
$wR_2(F^2)$	0.143
GooF	1.08
No. of Parameters	512
CCDC #	1976822



Compound	**3NCO**
Chem. Formula	$C_{49}H_{51}N_3OP_2$
Formula weight [g/mol]	759.91
Colour	colourless
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	16.513(2)
b [Å]	15.4285(8)
c [Å]	16.5927(9)
α [°]	90
β [°]	91.549
γ [°]	90
V [Å^3]	4225.7(4)
Z	4
$\rho_{calcd.}$ [g/cm^3]	1.194
μ [mm^{-1}]	0.71073
T [K]	123
Measured reflections	141261
Independent reflections	12307
Reflections with $I > 2\sigma(I)$	9088
R_{int}	0.061
F(000)	1616
$R_1(R[F^2>2\sigma(F^2)])$	0.047
$wR_2(F^2)$	0.135
GooF	1.08
No. of Parameters	512
CCDC #	1976820



Compound	**3PCO**
Chem. Formula	$C_{49}H_{51}N_2OP_3$
Formula weight [g/mol]	776.82
Colour	yellow
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	12.673(2)
b [Å]	20.949(2)
c [Å]	16.019(2)
α [°]	90
β [°]	105.781(3)
γ [°]	90
V [Å^3]	4092.2(6)
Z	4
$\rho_{calcd.}$ [g/cm^3]	1.261
μ [mm^{-1}]	0.71073
T [K]	123
Measured reflections	69830
Independent reflections	10351
Reflections with $I > 2\sigma(I)$	6777
R_{int}	0.094
F(000)	1648
$R_1(R[F^2>2\sigma(F^2)])$	0.053
$wR_2(F^2)$	0.135
GooF	1.01
No. of Parameters	595
CCDC #	2014417



5 Comparison of experimental spectroscopic data

5.1 Comparison of ^{31}P NMR data

The following table contains experimental ^{31}P NMR data.

Table S3: Experimental NMR data.

	Chemical shift [ppm]			**Coupling constant [Hz]**		
	^{1}H	**^{31}P(H)**	**^{31}P(X)**	**$^{1}J(^{31}P,^{1}H)$**	**$^{2}J(^{31}P,^{31}P)$**	**$^{3}J(^{31}P,^{1}H)$**
2	5.97	168.9	339.6	195	51	17
3Cl	6.77	169.7	246.2	174	49	18
3CN	6.77	185.0	163.9	152	33	-
3N$_3$	6.52	173.3	225.4	168	31	7
3NCO	6.64	170.7	195.7	160	30	-
3NCS	6.52	176.2	199.9	162	36	10
	^{1}H	**^{31}P(H)**	**^{31}P(X)**	**$^{1}J(^{31}P,^{31}P)$**	**$^{2}J(^{31}P,^{31}P)$**	**$^{2}J(^{1}H,^{31}P)$**
3PCO	7.71	158.0	216.0	203	42 / 17	41 / 4 (^{2}J)

5.2 Comparison of structural data

Table S4: Experimental structural data (in Å).

	P1−X	**P2−H**	**P1−P2**	**P1−N1**	**P1−N2**	**P2−N1**	**P2−N2**
2	-	1.38(2)	2.607(3)	1.774(3)	1.773(3)	1.663(2)	1.667(2)
3Cl	2.174(1)	1.35(3)	2.6153(9)	1.695(2)	1.680(2)	1.724(2)	1.803(2)
3CN	1.863(5)	1.56(4)	2.613(2)	1.700(2)	1.717(2)	1.788(2)	1.717(2)
3N$_3$	1.810(2)	1.36(2)	2.6109(5)	1.696(2)	1.714(2)	1.723(2)	1.780(2)
3NCO	1.773(2)	1.32(2)	2.6260(5)	1.697(2)	1.717(2)	1.730(2)	1.774(2)

Table S5: Experimental structural data of **3PCO** (in Å).

P1−O	P2−P	P-C	C-O	P1−P2	P1−N1	P1−N2	P2−N1	P2−N2
1.612(4)	2.192(2)	1.678(7)	1.426(8)	2.597(1)	1.714(2)	1.762(2)	1.732(2)	1.750(2)

Table S6: Experimental structural data (in °).

	P2−P1−X1	P1−X1−X2	P2−P1−H	P1−N1−P2−N2
2	-	-	103(2)	−5.82(9)
3Cl	97.62(4)	-	97(2)	−9.4(8)
3CN	91.2(2)	175.0(6)	94(2)	12.4(2)
$3N_3$	96.61(5)	115.3(2)	97.5(9)	−7.90(6)
3NCO	99.10(5)	130.8(2)	97.3(9)	6.47(6)

6 Computational Details

All computations were carried out using Gaussian09[21] or ORCA 4[22] as well as the standalone version of NBO 6.0.[23–26]

Methods. DFT calculations were carried out using the pure DFT functional PBE[27–30] including Grimme's dispersion model D3(BJ)[31,32] in conjunction with the def2−SVP[33] basis set. All structures were fully optimized and confirmed as minima by frequency analyses. Calculated frequencies were scaled by 0.984 (as derived from Truhlar's Reduced Scale Factor Optimization model).[34] Partial charges were determined by Natural Population analysis using the NBO program. Chemical shifts and coupling constants were derived by the GIAO method.[35–39] The calculated absolute shifts ($\sigma_{calc,X}$) were referenced to the calculated absolute shifts of $BF_3{\cdot}Et_2O$ (^{11}B, σ_{ref} = 104.65 ppm), Me_4Si (^{1}H, σ_{ref} = 30.96 ppm; ^{13}C, σ_{ref} = 187.90 ppm, ^{29}Si, σ_{ref} = 391.81 ppm), CH_3NO_2 (^{14}N, σ_{ref} = −95.69 ppm), $CFCl_3$ (^{19}F, σ_{ref} = 172.67 ppm),H_2O (^{17}O, σ_{ref} = 333.91 ppm) or to the experimental absolute shift of 85 % H_3PO_4 in the gas phase (^{31}P, $\sigma_{ref,1}$ = 328.35 ppm),[40] using PH_3 ($\sigma_{ref,2}$ = 594.45 ppm) as a secondary standard:[41]

$$\delta_{calc,X} = (\sigma_{ref,1} - \sigma_{ref,2}) - (\sigma_{calc,X} - \sigma_{calc,PH3})$$

$$= \sigma_{calc,PH3} - \sigma_{calc,X} - 266.1 \text{ ppm}$$

At the PBE-D3/def2-SVP level of theory, $\sigma_{calc,PH3}$ amounts to +617.22 ppm.

Accurate electronic energies for optimized structures were computed by single-point DLPNO-CCSD(T)[42–44] calculations employing the def2-TZVP basis set[45] and def2-TZVP/C correlation fitting basis[46] (notation: DLPNO-CCSD(T)/def2-TZVP//PBE-D3/def2-SVP). Thermodynamic quantities at this level of theory were calculated using the DLPNO-CCSD(T) single point energy and the thermal corrections at the PBE-D3/def2-SVP level of theory. The T_1 diagnostic was evaluated to ensure reliable results (empirically, CCSD(T) results are considered reliable if $T_1 < 0.02$).[47]

Please note that all computations were carried out for single, isolated molecules in the gas phase (ideal gas approximation). There may well be significant differences between gas phase and condensed phase.

6.1 Thermodynamic data (in a.u.)

Table S7. Absolute energies (DLPNO-CCSD(T)/def2-TZVP//PBE-D3/def2-SVP).

Compound	E^{tot}	H^{298}	G^{298}	T_1
[P(*μ*-NTer)]$_2$	−2646.8588	−2645.9804	−2646.1139	0.010
HCl	−460.3310	−460.3211	−460.3423	0.006
HCN	−93.2765	−93.2571	−93.2800	0.015
HN$_3$	−164.5400	−164.5147	−164.5419	0.020
HNCO	−168.4361	−168.4111	−168.4383	0.018
HNCS	−491.0216	−490.9988	−491.0273	0.019
HNSO	−528.0926	−528.0708	−528.1001	0.021
HPCO	−454.6393	−454.6195	−454.6489	0.020
3Cl (cis)	−3107.2273	−3106.3363	−3106.4736	0.010
3Cl (trans)	−3107.2235	−3106.3325	−3106.4689	0.010
3CN (cis)	−2740.1618	−2739.2635	−2739.4034	0.010
3CN (trans)	−2740.1563	−2739.2580	−2739.3966	0.011
3CN (bridged)	−2740.1558	−2739.2556	−2739.3910	0.011
3N$_3$ (cis)	−2811.4374	−2810.5331	−2810.6729	0.011
3N$_3$ (trans)	−2811.4330	−2810.5288	−2810.6680	0.011
3NCO (cis)	−2815.3334	−2814.4289	−2814.5688	0.011
3NCO (trans)	−2815.3296	−2814.4252	−2814.5645	0.011
3NCS (cis)	−3137.9244	−3137.0220	−3137.1634	0.011
3NCS (trans)	−3137.9204	−3137.0181	−3137.1588	0.011
3NSO (cis)	−3174.9817	−3174.0813	−3174.2208	0.011
3NSO (trans)	−3174.9780	−3174.0779	−3174.2188	0.011
3PCO (cis) exo	−3101.5320	−3100.6307	−3100.7715	0.011
3PCO (trans) exo	−3101.5274	−3100.6258	−3100.7663	0.011
3PCO (cis) endo	−3101.5292	−3100.6277	−3100.7684	0.011
3PCO (trans) endo	−3101.5261	−3100.6246	−3100.7652	0.011
3OCP (cis) exo	−3101.5154	−3100.6138	−3100.7550	0.011
3OCP (trans) exo	−3101.5104	−3100.6089	−3100.7497	0.011

Compound	E^{tot}	H^{298}	G^{298}	T_1
3OCP (cis) endo	−3101.5110	−3100.6096	−3100.7502	0.011
3OCP (trans) endo	−3101.5062	−3100.6050	−3100.7461	0.011
3P(H)CO	−3101.4550	−3100.5558	−3100.6967	0.012
3PC(H)O	−3101.5447	−3100.6417	−3100.7811	0.011
3PCO(H)	−3101.4258	−3100.5238	−3100.6639	0.012
3NN(H)N	−2811.4231	−2810.5164	−2810.6535	0.011
3NC(H)O	−2815.3360	−2814.4299	−2814.5671	0.011
3NC(H)S	−3137.9251	−3137.0214	−3137.1599	0.011

6.2 Different Isomers of 3HPCO

Table S 8: Isomerisation energy of different isomers of **3H(PCO/OCP)** relative to "**3HPCO** *cis* exo" (DLPNO-CCSD(T)/def2-TZVP//PBE-D3/def2-SVP, in kcal·mol^{-1}).

Compound	ΔE^{tot}	ΔH^{298}	ΔG^{298}
3PCO *cis* exo	0.00	+0.00	+0.00
3PCO *trans* exo	+2.93	+3.04	+3.28
3PCO *cis* endo	+1.75	+1.90	+1.99
3PCO *trans* endo	+3.70	+3.80	+3.95
3OCP *cis* exo	+10.43	+10.58	+10.36
3OCP *trans* exo	+13.60	+13.70	+13.73
3OCP *cis* endo	+13.17	+13.25	+13.39
3OCP *trans* endo	+16.19	+16.11	+15.98

6.3 Isomerisation energy

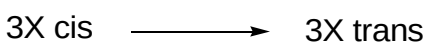


Table S9. Isomerisation energy from the *cis*- into *trans*-isomer (DLPNO-CCSD(T)/def2-TZVP//PBE-D3/def2-SVP, in kcal·mol^{-1}).

Compound	ΔE^{tot}	ΔH^{298}	ΔG^{298}
3Cl	+2.37	+2.41	+2.99
3CN	+3.43	+3.45	+4.27
3N$_3$	+2.78	+2.71	+3.03
3NCO	+2.39	+2.35	+2.69
3NCS	+2.46	+2.43	+2.86
3NSO	+2.31	+2.16	+1.26
3PCO	+2.93	+3.04	+3.28

6.4 Reaction energy

Table S10. Reaction energy (DLPNO-CCSD(T)/def2-TZVP//PBE-D3/def2-SVP, in kcal·mol^{-1}).

Reaction	ΔE^{tot}	$\Delta_R H^{298}$	$\Delta_R G^{298}$
[P(*μ*−NTer)]$_2$ + HCl → 3Cl (cis)	−23.52	−21.88	−10.93
[P(*μ*−NTer)]$_2$ + HCl → 3Cl (trans)	−21.15	−19.47	−7.94
[P(*μ*−NTer)]$_2$ + HCN → 3CN (cis)	−16.62	−16.34	−5.96
[P(*μ*−NTer)]$_2$ + HCN → 3CN (trans)	−13.19	−12.89	−1.70
[P(*μ*−NTer)]$_2$ + HCN → 3CN (bridged)	−12.86	−11.37	1.85
[P(*μ*−NTer)]$_2$ + HN$_3$ → 3N$_3$ (cis)	−24.24	−23.88	−10.72
[P(*μ*−NTer)]$_2$ + HN$_3$ → 3N$_3$ (trans)	−21.46	−21.17	−7.69
[P(*μ*−NTer)]$_2$ + HNCO → 3NCO (cis)	−24.12	−23.52	−10.44
[P(*μ*−NTer)]$_2$ + HNCO → 3NCO (trans)	−21.73	−21.17	−7.75
[P(*μ*−NTer)]$_2$ + HNCS → 3NCS (cis)	−27.58	−26.88	−13.94
[P(*μ*−NTer)]$_2$ + HNCS → 3NCS (trans)	−25.12	−24.45	−11.07
[P(*μ*−NTer)]$_2$ + HNSO → 3NSO (cis)	−19.04	−18.93	−4.26
[P(*μ*−NTer)]$_2$ + HNSO → 3NSO (trans)	−16.74	−16.77	−3.00
[P(*μ*−NTer)]$_2$ + HPCO → 3PCO (cis)	−21.27	−19.37	−5.50

Reaction	ΔE^{tot}	$\Delta_R H^{298}$	$\Delta_R G^{298}$
[P(*μ*−NTer)]$_2$ + HPCO → 3PCO (trans)	−18.35	−16.32	−2.22
[P(*μ*−NTer)]$_2$ + HPCO → 3P(H)CO	+27.09	+27.61	+41.43
[P(*μ*−NTer)]$_2$ + HPCO → 3PC(H)O	−29.24	−26.25	−11.48
[P(*μ*−NTer)]$_2$ + HPCO → 3PCO(H)	+45.38	+47.72	+62.02

6.5 Comparison of computed NMR shifts

Table S11. Calculated NMR shifts (PBE-D3/def2-SVP, in ppm).

compound	^{1}H	^{31}P(H)	^{31}P(X)	^{31}P
3Cl (cis)	6.93	139.39	231.53	−
3Cl (trans)	6.63	149.13	210.22	−
3CN (cis)	6.87	173.86	132.94	−
3CN (trans)	6.39	171.56	98.13	−
3N$_3$ (cis)	6.79	140.16	201.92	−
3N$_3$ (trans)	6.77	158.63	190.55	−
3NCO (cis)	6.95	136.61	166.87	−
3NCO (trans)	6.82	164.55	162.24	−
3NCS (cis)	6.94	147.72	178.25	−
3NCS (trans)	6.74	165.44	161.25	−
3NSO (cis)	6.71	129.50	144.23	−
3NSO (trans)	6.82	179.48	153.83	−
3PCO (cis)	6.58	125.64	235.57	−197.65
3PCO (trans)	6.73	141.11	213.01	−186.13
3P(H)CO	2.57	245.78	286.58	−289.39
3PC(H)O	7.80	195.59	202.98	131.22
3PCO(H)	2.21	299.43	330.80	−94.70

6.6 Theoretical structural data

Table S12: Theoretical structural data (PBE-D3/def2-SVP, in Å).

	P1−X	P2−H	P1−P2	P1−N1	P1−N2	P2−N1	P2−N2
3Cl (cis)	2.250	1.450	2.711	1.745	1.752	1.782	1.812
3Cl (trans)	2.271	1.446	2.692	1.752	1.747	1.812	1.801
3CN (cis)	1.866	1.458	2.706	1.774	1.757	1.818	1.777
3CN (trans)	1.866	1.447	2.710	1.767	1.777	1.808	1.802
3N$_3$ (cis)	1.850	1.451	2.718	1.756	1.756	1.811	1.780
3N$_3$ (trans)	1.855	1.450	2.705	1.755	1.760	1.799	1.806
3NCO (cis)	1.796	1.454	2.722	1.761	1.760	1.780	1.808
3NCO (trans)	1.796	1.450	2.713	1.761	1.765	1.800	1.802
3NCS (cis)	1.811	1.454	2.714	1.754	1.754	1.780	1.813
3NCS (trans)	1.810	1.449	2.704	1.756	1.759	1.799	1.806
3NSO (cis)	1.790	1.449	2.717	1.765	1.765	1.787	1.804
3NSO (trans)	1.794	1.452	2.716	1.766	1.768	1.803	1.807
3PCO (cis)	2.382	1.459	2.719	1.769	1.770	1.774	1.805
3PCO (trans)	2.400	1.446	2.705	1.766	1.774	1.794	1.805

Table S13: Theoretical structural data of **3CN** (bridged) (PBE-D3/def2-SVP, in Å).

P1−C	P2−N	C-N	P1−P2	P1−N1	P1−N2	P2−N1	P2−N2
1.978	1.930	1.271	2.606	1.773	1.830	1.764	1.797

Table S14: Theoretical structural data of **3PCO** (bridged) (PBE-D3/def2-SVP, in Å).

	P1−P2	P2−P3	P3-C	P1−O	O/P/C−H	C−O	P1−N4	P2−N4
3P(H)CO	2.721	2.220	1.938	2.207	1.437	1.235	1.758	1.838
3PC(H)O	2.679	2.277	1.726	1.776	1.111	1.337	1.785	1.808
3PCO(H)	2.707	2.251	1.737	2.328	0.993	1.367	1.725	1.857

Table S15: Theoretical structural data (PBE-D3/def2-SVP, in Å).

	P2−P1−X1	P1−X1−X2	P2−P1−H	P1−N1−P2−N2
3Cl (cis)	100.05	-	96.40	−6.07
3Cl (trans)	93.35	-	109.81	14.74
3CN (cis)	92.80	171.59	92.36	−11.08
3CN (trans)	91.30	167.80	110.09	−13.89
3N_3 (cis)	97.54	119.53	97.55	−5.07
3N_3 (trans)	91.42	120.43	109.16	−13.27
3NCO (cis)	100.11	133.85	98.26	−4.27
3NCO (trans)	94.73	135.18	108.23	−11.87
3NCS (cis)	98.52	136.95	96.59	−6.13
3NCS (trans)	93.43	139.14	109.07	−13.27
3NSO (cis)	99.47	115.37	101.92	0.41
3NSO (trans)	91.11	118.26	107.58	11.61
3PCO (cis)	96.26	91.69	95.97	6.25
3PCO (trans)	91.04	93.33	110.40	14.45

6.7 NBO

Table S 16: NBO partial charges in e, polarization in % and orbital occupation in e, R = terphenyl; method: PBE-D3/def2-SVP level of theory.

	H	P-H	P-X	X	P2N2	pol.P-H	occ(P-H)
2+	0.03	0.93	1.18	0.00	0.23	52/48	1.95
3HCl	0.00	0.89	1.16	-0.38	0.09	51/49	1.98
3HCN	-0.01	0.89	1.17	-0.40	0.11	51/49	1.98
3HN3	-0.01	0.89	1.30	-0.49	0.23	51/49	1.98
3NCS	-0.01	0.89	1.34	-0.54	0.27	51/49	1.98
3NCO	-0.01	0.89	1.33	-0.50	0.27	51/49	1.98
	H	**P-P**	**P-O**	**X**	**P2N2**	**C-H**	**occ(C-H)**
3PC(H)O	0.22	0.87	1.39	-0.77	0.27	62/38	1.98

6.8 Reaction mechanism

Table S 17: Minima: Absolute (a.u.) and relative (kcal/mol) energies of for the model system (all considered isomers of) **3HPCO_Ph** at the PBE0-D3/def2-SVP level of theory (phenyl substituent instead of terphenyl). Structures can be found in Figure S23.

			E	H	G	Nimag	DE	DH	DG
I1	P-PCO	cis_exo	−1708.8452	−1708.6110	−1708.6803	0	**0.00**	**0.00**	**0.00**
I2	P-PCO	cis_endo	−1708.8434	−1708.6092	−1708.6768	0	1.12	1.16	2.20
I3	P-PCO	trans_exo	−1708.8413	−1708.6071	−1708.6758	0	2.46	2.45	2.85
I4	P-PCO	trans_endo	−1708.8429	−1708.6087	−1708.6766	0	1.46	1.43	2.33
I5	P-OCP	cis_exo	−1708.8129	−1708.5785	−1708.6460	0	20.28	20.40	21.52
I6	P-OCP	cis_endo	−1708.8148	−1708.5804	−1708.6478	0	19.08	19.20	20.41
I7	P-OCP	trans_exo	−1708.8113	−1708.5769	−1708.6443	0	21.29	21.37	22.62
I8	P-OCP	trans_endo	−1708.8156	−1708.5812	−1708.6479	0	18.59	18.68	20.33
I9	PC(H)O	1,3_bridge	−1708.8572	−1708.6205	−1708.6848	0	**−7.50**	**−5.99**	**−2.80**
I10	HPCO	1,3_bridge	−1708.7789	−1708.5464	−1708.6114	0	41.61	40.55	43.23
I11	HOCP	1,3_bridge	decomp in HOPC + birad						
I12	HPCO	CO 1,2 bridge	−1708.8375	−1708.6032	−1708.6671	0	4.84	4.92	8.30
I13	HOCP	PC 1,2 bridge	−1708.8347	−1708.5975	−1708.6612	0	6.58	8.46	12.00
I14	HPCO	PC 1,2 bridge	−1708.8508	−1708.6170	−1708.6826	0	−3.49	−3.78	−1.41
I15	H-P-OCP	endo	−1708.7267	−1708.4928	−1708.5580	0	74.41	74.18	76.75
I16	H-P-OCP	exo	−1708.7937	−1708.5591	−1708.6261	0	32.32	32.60	34.02
I17	H-P-PCO	endo	−1708.8165	−1708.5821	−1708.6460	0	18.00	18.12	21.52
I18	H-P-PCO	exo	−1708.8290	−1708.5949	−1708.6645	0	10.19	10.08	9.95

I19	PC(H)_rot		−1708.8221	−1708.5860	−1708.6532	0	14.53	15.66	17.02
I20	P-P open		−1708.8290	−1708.5949	−1708.6645	0	10.19	10.08	9.95
I21	P-P open		−1708.8308	−1708.5967	−1708.6655	0	9.07	8.98	9.31
I22	inversionP	release of CO	−1708.7998	−1708.5659	−1708.6401	0	28.52	28.31	25.21

Table S 18: Transition states: Absolute (a.u.) and relative (kcal/mol) energies of for the model system (all considered isomers of) 3HPCO_Ph at the PBE0-D3/def2-SVP level of theory (phenyl substituent instead of terphenyl). Structures can be found in Figure S24.

			E	**H**	**G**	**Nimag**	**DE**	**DH**	**DG**
I1	P-PCO	cis_exo	−1708.8452	−1708.6110	−1708.6803	0	**0.00**	**0.00**	**0.00**
TS1	rot cis		−1708.8402	−1708.6069	−1708.6721	1	3.14	2.57	5.16
TS2	intermediate_CH		−1708.8198	−1708.5867	−1708.6485	1	15.94	15.24	19.96
TS3	intermediate_rot		−1708.8185	−1708.5833	−1708.6478	1	16.79	17.35	20.41
TS4	rot_trans		−1708.8362	−1708.6029	−1708.6680	1	5.69	5.07	7.74
TS5	inversion	trans->cis PH rotation	−1708.7765	−1708.5448	−1708.6117	1	43.15	41.52	43.03
TS6	inversion	P-H	−1708.7343	−1708.5019	−1708.5723	1	69.59	68.47	67.78

Table S 18: Transition states: Absolute (a.u.) and relative (kcal/mol) energies of for the model system (all considered isomers of) 3HPCO_Ph at the PBE0-D3/def2-SVP level of theory (phenyl substituent instead of terphenyl). Structures can be found in Figure S24.

		DE	**DH**	**DG**
TS1: I1->I2	PCO cis: exo -> endo barrier	3.14	2.57	5.16
TS2: I2->I19	cis_endo -> 3PCHO_int	14.82	14.09	17.76
TS3: I19->I9	3PCHO_int->3PCHO	2.26	1.69	3.38
TS4: I3->I4	PCO trans: exo -> endo barrier	3.23	2.63	4.89
TS5: I4->I2	trans_endo->cis_endo rotation	41.69	40.09	40.70
TS6: I3->I1	inversion	67.14	66.02	64.92

Table S 19: Absolute (a.u.) and relative (kcal/mol) energies of 3HPCO at the DLPNO-CCSD(T)/def2-TZVP//PBE-D3/def2-SVP level of theory.

	E	H	G	Nimag	DE	DH	DG	T_1
3HPCO_exo	−3101.5320	−3100.6307	−3100.7715	0	**0.0**	**0.0**	**0.0**	0.011
TS1	−3101.5159	−3100.6153	−3100.7546	1	10.1	9.7	10.6	0.011
3HPCO_endo	−3101.5292	−3100.6277	−-3100.7684	0	1.8	1.9	2.0	0.011
TS2	−3101.4971	−3100.5955	−3100.7349	1	21.9	22.1	23.0	0.012
3PC(H)O	−3101.5447	−3100.6417	−3100.7811	0	**−8.0**	**−6.9**	**−6.0**	0.011

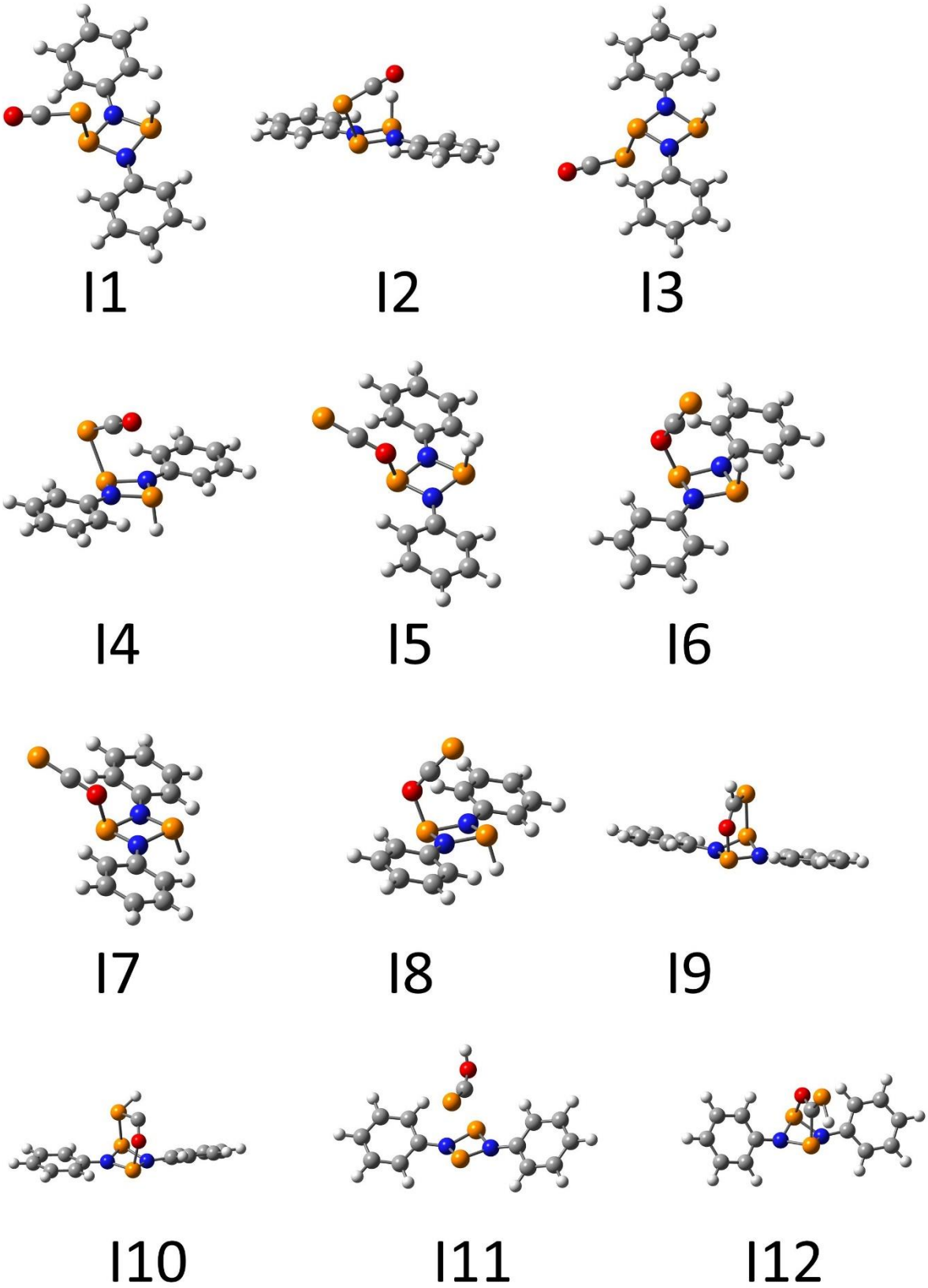
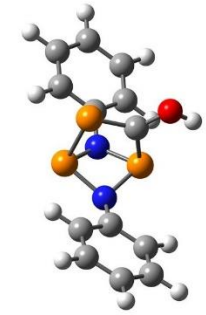
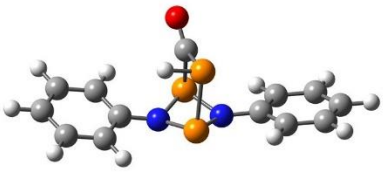


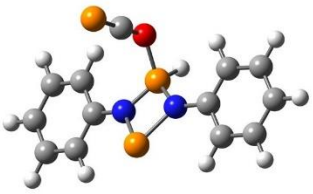
Figure S23. Optimized minimum structures (NImag = 0) for the model system with **3**HPCO_Ph at the PBE0-D3/def2-SVP level of theory (phenyl substituent instead of terphenyl). Energies can be found in Table S18.



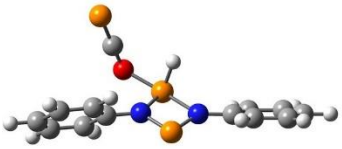
I13



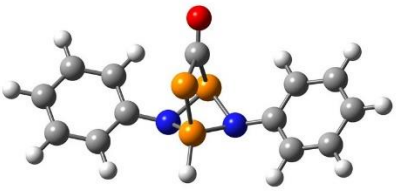
I14



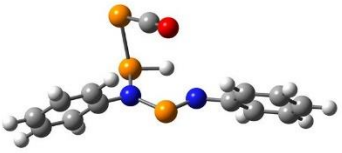
I15



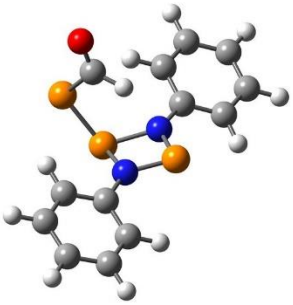
I16



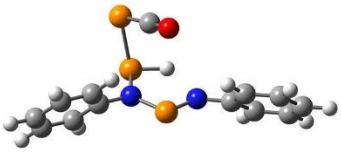
I17



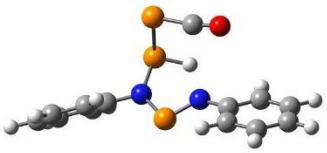
I18



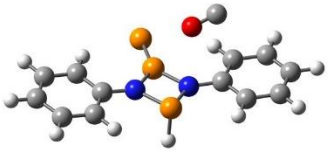
I19



I20



I21



I22

Continued. Optimized minimum structures (NImag = 0) for the model system with **3**HPCO_Ph at the PBE0-D3/def2-SVP level of theory (phenyl substituent instead of terphenyl). Energies can be found in Table S18.

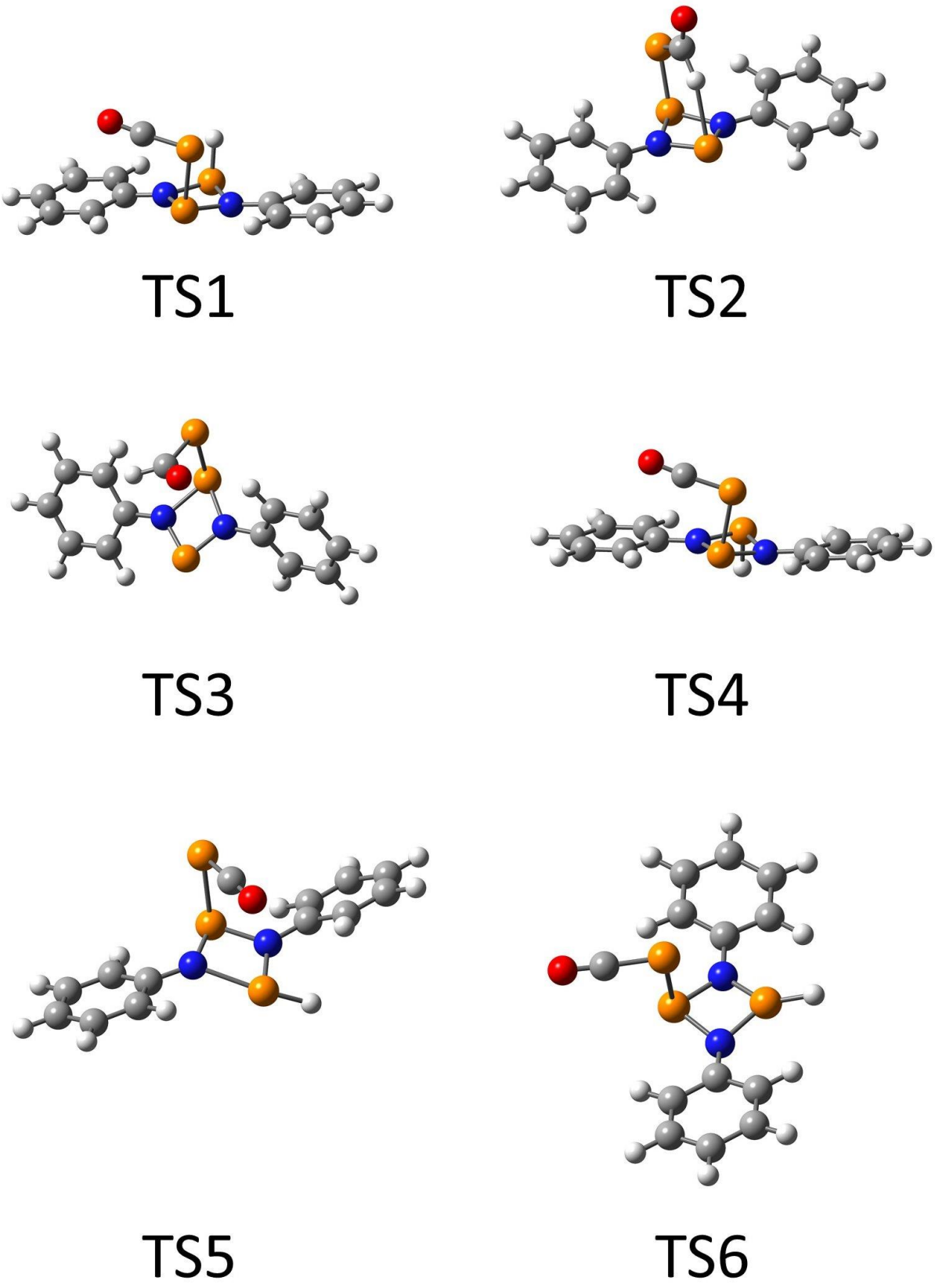


Figure S24. Optimized transition state structures (NImag = 1) for the model system with **3**HPCO_Ph at the PBE0-D3/def2-SVP level of theory (phenyl substituent instead of terphenyl). Energies can be found in Table S18. Description of the mechanism see next page.

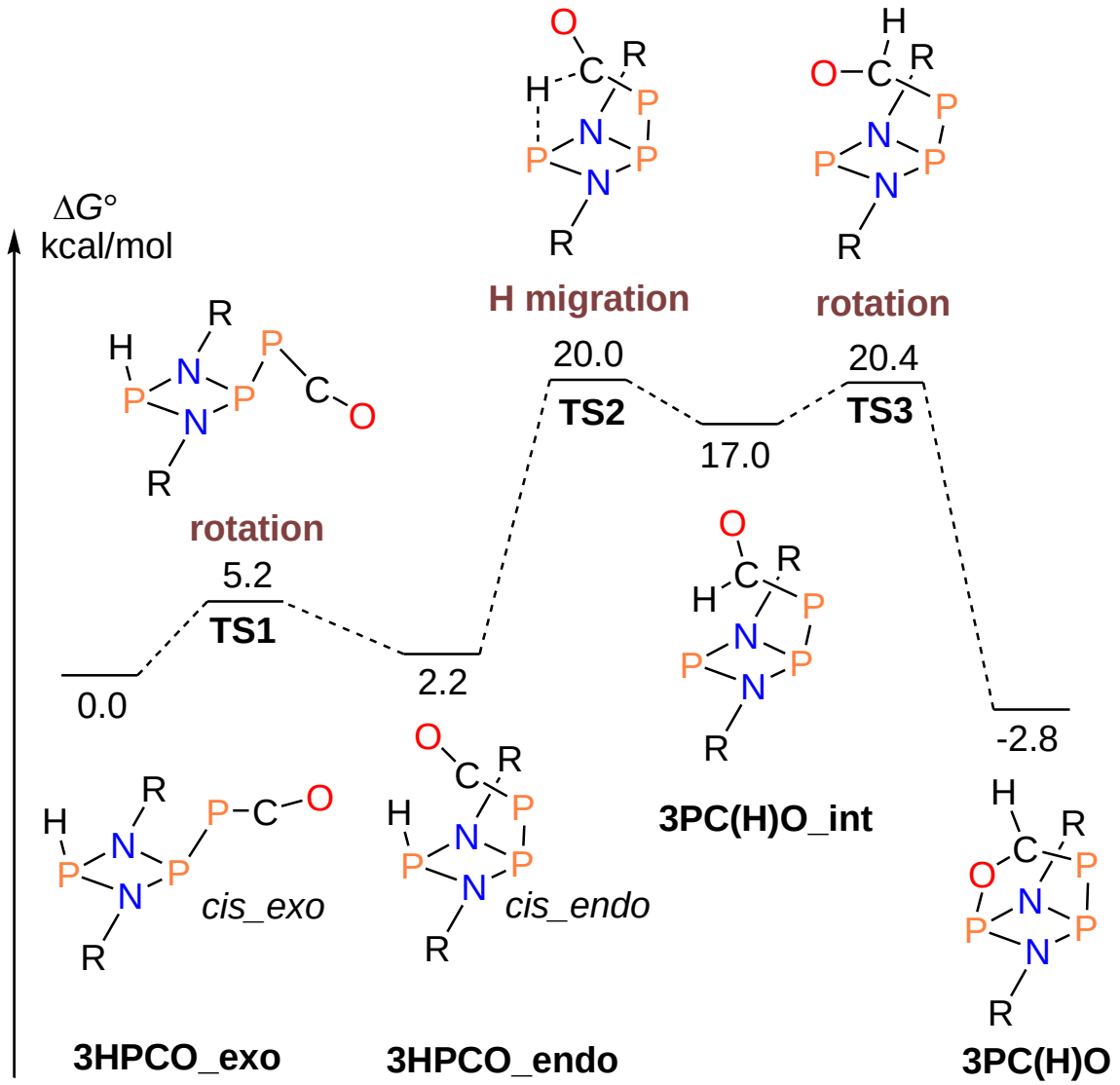


Figure S25. The 2-step isomerization process starting from the *cis*-endo isomer starts with an H-migration of the proton, which is attached to the ring phosphorus atom, to the C-atom of the PCO-unit, resulting in the formation of a labile intermediate **3PC(H)O_int**. The activation barrier for this proton migration is 17.8 kcal/mol and the intermediate is 14.8 kcal/mol energetically less favourable than the *cis*-endo isomer. Finally, the intermediate **3PC(H)O_int** lacks the P-O bond, which is spatially enabled by a simple rotation around the C-P axis. The barrier for this rotation is very small with 3.4 kcal/mol and now leads in an exergonic process directly to the experimentally observed product **3PC(H)O**.

*Note: For R = Terphenyl it was impossible to localize an intermediate **3PC(H)O_int** as it does not represent a true minimum structure!*

6.9 Molecular orbitals

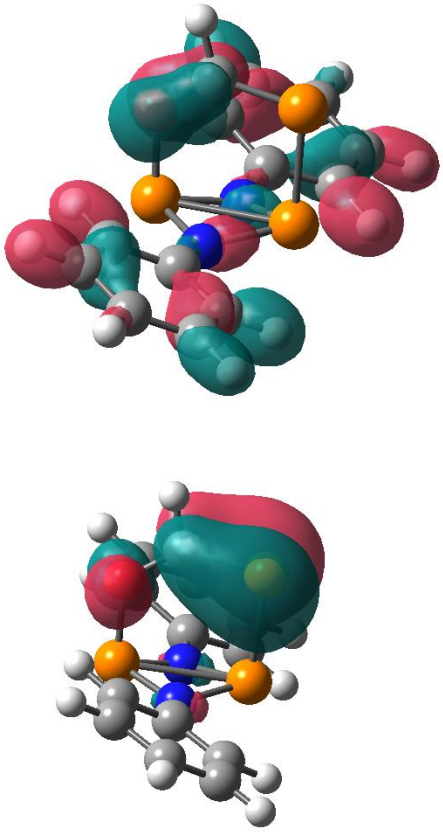


Figure S26. Molecular orbitals of **3PC(H)O** displaying π bonding along the PCO unit.

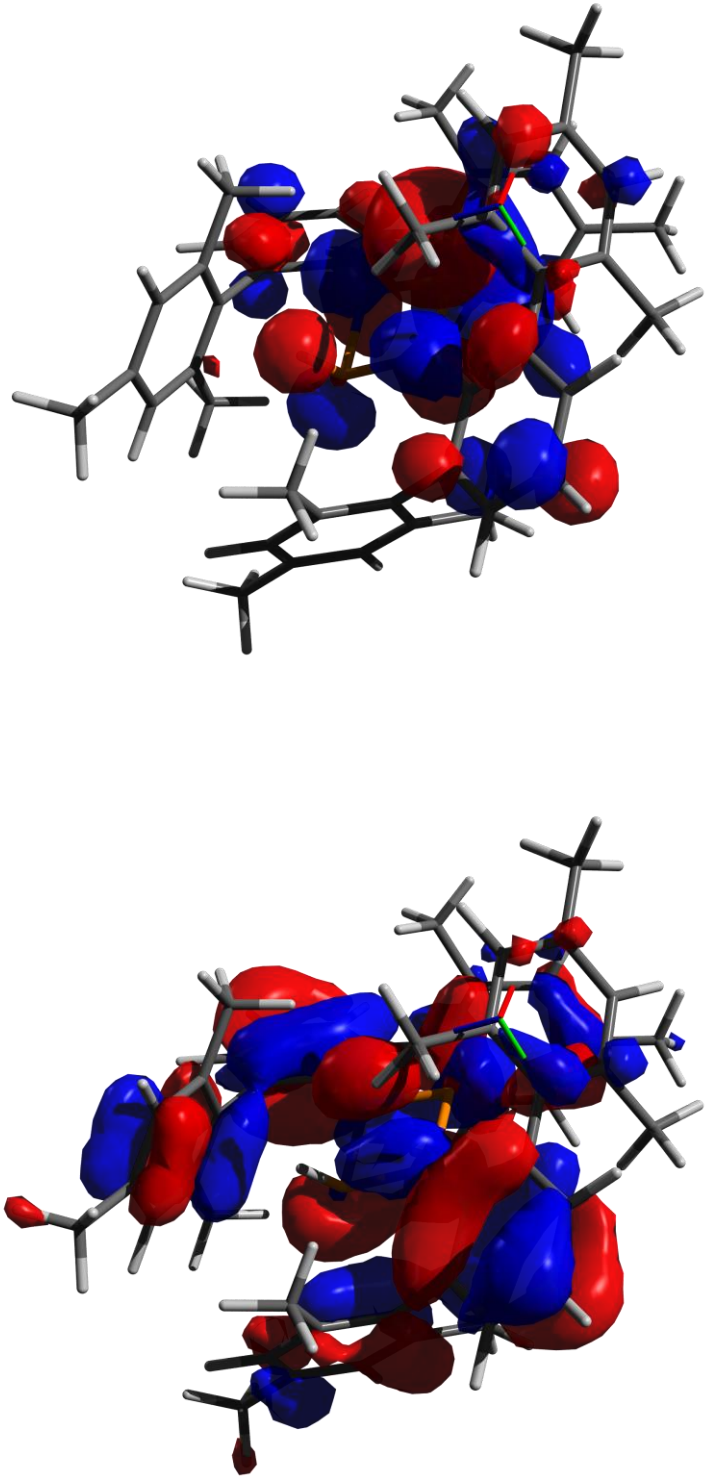
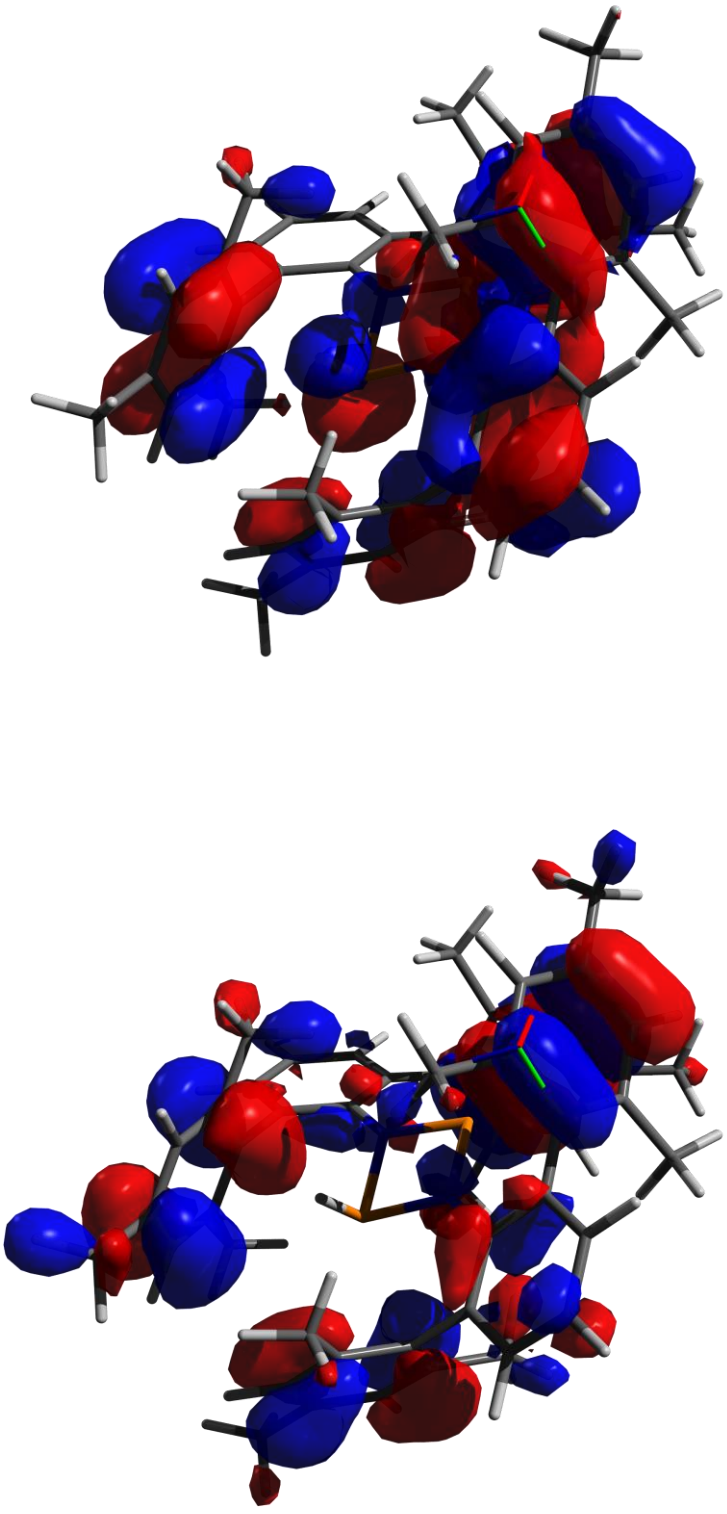


Figure S27. Molecular orbitals of **2.** Top LUMO, bottom HOMO.



Continued. Molecular orbitals of **2**. Top HOMO−1, bottom HOMO−2.

6.10 Optimized structures (.xyz files)

6.10.1 $B(C_6F_5)_3$

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
B	0.00003	−0.01603	−0.00079
C	−0.00003	1.54500	−0.00043
C	−1.35518	−0.78747	0.02033
C	1.35528	−0.78740	−0.02111
C	0.89138	2.28316	0.77412
C	0.89466	3.66469	0.80013
C	−0.00018	4.35810	0.00027
C	−0.89150	2.28344	−0.77462
C	−0.89494	3.66499	−0.79994
C	1.54301	−1.97043	0.69257
C	2.45973	−0.33139	−0.74073
C	3.66798	−1.00197	−0.76384
C	3.81220	−2.16461	−0.02342
C	2.74481	−2.65194	0.71502
C	−1.54326	−1.97062	−0.69306
C	−2.74507	−2.65213	−0.71480
C	−3.81209	−2.16469	0.02410
C	−3.66750	−1.00192	0.76424
C	−2.45926	−0.33135	0.74043
F	−2.37569	0.77500	1.47204
F	−4.68531	−0.54750	1.47687
F	−4.96390	−2.80470	0.02448
F	−2.88605	−3.75807	−1.42715
F	−0.55255	−2.47910	−1.41827
F	−1.76809	1.66370	−1.55933
F	−1.73865	4.32936	−1.57294
F	−0.00025	5.67597	0.00061
F	1.73828	4.32878	1.57347
F	1.76808	1.66311	1.55846
F	2.37652	0.77484	−1.47257
F	4.68615	−0.54767	−1.47602
F	4.96401	−2.80460	−0.02311
F	2.88544	−3.75775	1.42763
F	0.55193	−2.47882	1.41732

6.10.2 $[P(\mu-NTer)]_2$

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
N	1.12205	−0.00034	0.00428
N	−1.12209	0.00049	0.00394
P	−0.00055	−1.36161	0.00437
P	0.00049	1.36177	0.00455
C	−2.52556	0.00060	0.00208
C	−3.24482	−1.15228	0.43111
C	−3.24382	1.15331	−0.42929
C	−4.65149	−1.13105	0.42078
C	−4.65050	1.13167	−0.42346
C	−5.36120	0.00019	−0.00250
H	−5.18683	−2.02924	0.76536
H	−5.18502	2.02969	−0.76975
H	−6.46126	0.00000	−0.00427
C	2.52552	−0.00045	0.00274
C	3.24392	−1.15316	−0.42840
C	3.24466	1.15244	0.43197
C	4.65060	−1.13146	−0.42223
C	4.65133	1.13128	0.42193
C	5.36117	0.00006	−0.00119
H	5.18524	−2.02948	−0.76836
H	5.18654	2.02949	0.76665
H	6.46123	0.00028	−0.00273
C	2.53620	2.37249	0.92240
C	2.38503	3.50176	0.07741
C	2.01828	2.39384	2.24716
C	1.71367	4.63405	0.57421
C	1.35790	3.54656	2.69949
C	1.18805	4.67593	1.87610
H	1.58308	5.50530	−0.08695
H	0.95058	3.55778	3.72382
C	2.53469	−2.37384	−0.91604
C	2.38683	−3.50220	−0.06931
C	2.01283	−2.39692	−2.23917
C	1.71460	−4.63547	−0.56263

C	1.35191	−3.55065	−2.68820
C	1.18537	−4.67924	−1.86303
H	1.58620	−5.50590	0.10006
H	0.94137	−3.56327	−3.71122
C	−2.53443	2.37393	−0.91688
C	−2.38687	3.50246	−0.07033
C	−2.01211	2.39674	−2.23983
C	−1.71445	4.63562	−0.56366
C	−1.35103	3.55036	−2.68889
C	−1.18477	4.67912	−1.86389
H	−1.58627	5.50620	0.09888
H	−0.94011	3.56275	−3.71175
C	−2.53651	−2.37244	0.92149
C	−2.01844	−2.39387	2.24620
C	−2.38559	−3.50172	0.07648
C	−1.35821	−3.54671	2.69845
C	−1.71440	−4.63414	0.57321
C	−1.18867	−4.67612	1.87506
H	−0.95080	−3.55801	3.72274
H	−1.58405	−5.50541	−0.08797
C	−2.87176	3.46569	1.35726
H	−2.75076	4.45126	1.84663
H	−3.93553	3.16525	1.43159
H	−2.28908	2.72105	1.94090
C	−2.12516	1.18026	−3.12203
H	−3.17037	0.81536	−3.18508
H	−1.76133	1.38913	−4.14621
H	−1.52305	0.34222	−2.70862
C	−0.44440	5.89247	−2.36708
H	0.60680	5.64048	−2.62126
H	−0.90759	6.29748	−3.29089
H	−0.42509	6.70263	−1.61254
C	−2.86291	−3.46642	−1.35370
H	−2.75786	−4.45764	−1.83534
H	−3.92010	−3.14609	−1.43619
H	−2.26208	−2.73762	−1.93922
C	−2.13466	−1.17673	3.12709
H	−1.52659	−0.34084	2.71797
H	−3.17911	−0.80844	3.18199
H	−1.77921	−1.38627	4.15408
C	−0.44810	−5.88811	2.38119
H	0.60500	−5.63653	2.62810
H	−0.90681	−6.28698	3.30983
H	−0.43410	−6.70248	1.63106
C	0.44526	−5.89273	−2.36626
H	−0.60567	−5.64072	−2.62153
H	0.90924	−6.29831	−3.28943
H	0.42516	−6.70250	−1.61130
C	0.44724	5.88776	2.38229
H	−0.60589	5.63601	2.62890
H	0.90569	6.28651	3.31111
H	0.43331	6.70226	1.63230
C	2.13488	1.17674	3.12805
H	3.17962	0.80935	3.18369
H	1.77852	1.38590	4.15480
H	1.52784	0.34034	2.71844
C	2.12615	−1.18064	−3.12159
H	3.17116	−0.81498	−3.18342
H	1.76376	−1.39007	−4.14617
H	1.52287	−0.34293	−2.70920
C	2.87128	−3.46512	1.35842
H	2.74951	−4.45040	1.84818
H	3.93522	−3.16533	1.43297
H	2.28891	−2.71985	1.94157
C	2.86227	3.46654	−1.35279
H	2.75691	4.45771	−1.83448
H	3.91956	3.14652	−1.43530

6.10.3 HCl

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
Cl	0.00000	0.00000	−0.38504
H	0.00000	0.00000	−1.68104

6.10.4 HCN

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
C	0.00000	0.00000	−0.49978
H	0.00000	0.00000	−1.58691
N	0.00000	0.00000	0.66742

6.10.5 HN_3

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
H	−1.10113	1.40920	0.00000
N	−0.11099	1.12051	0.00000
N	−0.00125	−0.11179	0.00000
N	0.27659	−1.22769	0.00000

6.10.6 HNCO

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
N	−0.45538	1.07717	0.00000
H	−1.44077	1.33246	0.00000
C	0.00000	−0.05944	0.00000
O	0.58933	−1.08109	0.00000

6.10.7 HNCS

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
N	−0.53235	1.13464	0.00000
H	−1.49888	1.45502	0.00000
C	−0.03638	0.02237	0.00000
S	0.76078	−1.34293	0.00000

6.10.8 HNSO

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
N	−0.39248	1.18245	0.00000
H	−1.38826	1.48191	0.00000
S	−0.43624	−0.38002	0.00000
O	0.91015	−1.01525	0.00000

6.10.9 HPCO

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	−0.25100	1.51649	0.00000
H	−1.64300	1.13635	0.00000
C	0.11459	−0.13494	0.00000
O	0.47259	−1.24881	0.00000

6.10.10 3Cl (cis)

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	−0.16544	3.72811	2.32678
P	−1.66154	5.74493	3.34847
Cl	−1.35951	3.24968	0.48111
N	−1.49893	3.97221	3.42483
N	−0.16497	5.47955	2.36188
H	−2.56241	5.86642	2.21846
C	−2.22717	3.04751	4.18433
C	0.57813	6.41129	1.62511
C	−3.59569	3.29383	4.49024
C	−1.59859	1.87122	4.68250
C	1.65684	6.00780	0.78179
C	0.27501	7.80166	1.72692
C	−4.31541	2.35232	5.24874
C	−4.29328	4.52669	4.01054
C	−2.36240	0.94331	5.41603
C	−0.13042	1.62892	4.54428
C	2.35338	6.97759	0.03703
C	2.11002	4.58871	0.67673
C	0.99561	8.73570	0.96033
C	−0.74961	8.32432	2.68131
H	−5.37387	2.56067	5.46911
C	−3.71505	1.16997	5.70028
C	−4.88885	4.53765	2.71842
C	−4.41914	5.65417	4.86505
H	−1.85778	0.04115	5.79511
C	0.76985	2.36486	5.36202
C	0.35952	0.62148	3.67344
H	3.18310	6.63563	−0.60061
C	2.02938	8.33753	0.10538
C	1.81786	3.83740	−0.49496
C	2.92027	4.02726	1.70089
H	0.73544	9.80047	1.06514
C	−2.03434	8.71435	2.21862

C	−0.39024	8.52112	4.04628
H	−4.29280	0.43740	6.28297
C	−5.56706	5.69304	2.29573
C	−4.78142	3.33714	1.81759
C	−5.11751	6.78458	4.40003
C	−3.80079	5.65293	6.24068
C	2.13889	2.05095	5.31908
C	0.27252	3.47267	6.25637
C	1.73559	0.33192	3.67769
C	−0.56449	−0.08445	2.71235
H	2.58825	9.07864	−0.48442
C	2.28555	2.51628	−0.58538
C	1.02153	4.44239	−1.62218
C	3.39312	2.71380	1.54848
C	3.23535	4.80432	2.95288
C	−2.94313	9.27305	3.13576
C	−2.42551	8.51427	0.77605
C	−1.32732	9.08897	4.92117
C	0.95708	8.07229	4.54743
H	−6.02022	5.70200	1.29085
C	−5.69231	6.82812	3.11941
H	−5.42266	3.44852	0.92226
H	−3.73601	3.19402	1.47041
H	−5.07012	2.40700	2.34703
H	−5.20875	7.65980	5.06136
H	−2.69604	5.55940	6.17515
H	−4.03017	6.58996	6.78355
H	−4.15512	4.79670	6.84894
H	2.83321	2.61777	5.96110
C	2.64049	1.02037	4.50360
H	−0.08975	4.33433	5.65518
H	−0.58665	3.14364	6.87529
H	1.07241	3.83811	6.92833
H	2.11282	−0.45631	3.00656
H	−0.02851	−0.87123	2.14728
H	−1.42954	−0.54996	3.22476
H	−0.98348	0.63539	1.97640
H	2.02999	1.92530	−1.47983
C	3.07013	1.93301	0.42553
H	0.74931	3.67518	−2.37171
H	0.08606	4.90197	−1.24763
H	1.59267	5.24223	−2.13779
H	4.02513	2.28401	2.33886
H	3.50060	5.85745	2.73273
H	2.35169	4.82958	3.62853
H	4.06322	4.33557	3.51835
H	−3.94468	9.56158	2.78153
C	−2.61159	9.46951	4.48696
H	−2.24010	7.47086	0.44862
H	−3.49650	8.74342	0.61567
H	−1.82737	9.15938	0.09994
H	−1.05032	9.22997	5.97871
H	1.78068	8.46306	3.91672
H	1.12647	8.39043	5.59361
H	1.03623	6.96380	4.51040
C	−6.43799	8.04576	2.63414
C	4.10215	0.65082	4.54098
C	3.52730	0.50093	0.31366
C	−3.59819	10.07000	5.45588
H	−5.99505	8.44285	1.69654
H	−7.49771	7.80536	2.40676
H	−6.43025	8.85852	3.38611
H	4.74977	1.54609	4.63585
H	4.32583	0.00002	5.41375
H	4.40898	0.09604	3.63266
H	3.86172	0.25547	−0.71447
H	4.35938	0.28061	1.01065
H	2.69670	−0.19621	0.55735
H	−4.56713	10.29336	4.96905
H	−3.79301	9.38399	6.30684
H	−3.21126	11.01501	5.89136

6.10.11 3Cl (trans)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	−1.24810	4.79744	2.22057
P	−1.98063	3.57692	−0.06450
Cl	−2.82078	6.42249	2.01285
N	−2.08512	3.33847	1.72861
N	−0.77628	4.77157	0.53911
H	−1.00188	2.57283	−0.41947

C	−3.00950	2.53425	2.41292
C	0.03512	5.67430	−0.15589
C	−3.57871	1.41239	1.73884
C	−3.36474	2.77304	3.77393
C	1.10892	6.32673	0.51902
C	−0.15751	5.91079	−1.54647
C	−4.53709	0.61620	2.39229
C	−3.11004	0.98357	0.38514
C	−4.31939	1.94166	4.39038
C	−2.74114	3.85014	4.60095
C	1.90907	7.24387	−0.18657
C	1.47114	5.98273	1.92705
C	0.67734	6.82258	−2.21785
C	−1.22197	5.19561	−2.31330
H	−4.95615	−0.24354	1.84679
C	−4.92437	0.87757	3.71160
C	−1.86755	0.29252	0.28252
C	−3.92100	1.16081	−0.76866
H	−4.57255	2.14366	5.44250
C	−3.49768	5.00955	4.93234
C	−1.43870	3.67363	5.14087
H	2.73628	7.73149	0.35216
C	1.69879	7.50643	−1.54654
C	2.08980	4.72880	2.19178
C	1.25043	6.90490	2.98388
H	0.50410	6.99150	−3.29201
C	−0.91244	3.98041	−2.98088
C	−2.52381	5.76206	−2.41986
H	−5.66741	0.24176	4.21481
C	−1.45377	−0.18560	−0.97128
C	−0.99937	0.09951	1.49891
C	−3.46661	0.65738	−2.00135
C	−5.20851	1.93927	−0.69645
C	−2.91104	5.99340	5.74251
C	−4.89775	5.19141	4.40620
C	−0.90577	4.67491	5.97179
C	−0.59911	2.47133	4.79469
H	2.33945	8.22164	−2.08294
C	2.48256	4.42793	3.50625
C	2.29932	3.71855	1.09171
C	1.67274	6.56226	4.28160

C	0.51931	8.20185	2.74256
C	−1.92392	3.33234	−3.71467
C	0.47691	3.39451	−2.91410
C	−3.49575	5.08246	−3.16940
C	−2.85621	7.04370	−1.70562
H	−0.48814	−0.71203	−1.04636
C	−2.23800	−0.01211	−2.12782
H	−0.11391	−0.52264	1.26773
H	−0.64459	1.07598	1.89139
H	−1.56261	−0.37888	2.32587
H	−4.09064	0.80713	−2.89572
H	−4.98651	3.01655	−0.53312
H	−5.78725	1.84883	−1.63562
H	−5.84849	1.61549	0.14678
H	−3.48734	6.90549	5.96710
C	−1.61350	5.85017	6.26817
H	−4.92146	5.07421	3.30475
H	−5.59430	4.43813	4.82818
H	−5.28621	6.19803	4.65171
H	0.10200	4.53416	6.38913
H	0.13900	2.25482	5.59144
H	−1.21180	1.56636	4.61868
H	−0.01758	2.66579	3.86492
H	2.96492	3.45691	3.70675
C	2.29696	5.33624	4.56504
H	2.96630	2.89839	1.41966
H	1.33023	3.26963	0.78291
H	2.73171	4.18544	0.18400
H	1.49909	7.27843	5.10068
H	0.99140	8.80771	1.94430
H	−0.52405	8.00352	2.41656
H	0.47723	8.81217	3.66520
H	−1.68838	2.38347	−4.22141
C	−3.21985	3.86393	−3.81942
H	0.85189	3.33840	−1.87233
H	0.50307	2.37636	−3.34807
H	1.20447	4.02516	−3.46651
H	−4.50606	5.51691	−3.24409
H	−2.11264	7.83618	−1.92412
H	−3.86095	7.41238	−1.98765
H	−2.84228	6.89648	−0.60387

C	−1.75990	−0.52643	−3.46194
C	−0.99551	6.94516	7.09959
C	2.78343	5.00548	5.95356
C	−4.29432	3.16163	−4.61036
H	−0.80575	−0.04184	−3.75921
H	−1.56449	−1.61848	−3.42933
H	−2.49988	−0.33678	−4.26337
H	−0.69128	7.80008	6.45767
H	−1.70891	7.34527	7.84839
H	−0.09213	6.59355	7.63542
H	3.88839	5.10073	6.02281
H	2.34590	5.68167	6.71377
H	2.53532	3.96149	6.23520
H	−3.91624	2.23497	−5.08391
H	−5.15413	2.88851	−3.96314
H	−4.69568	3.81468	−5.41303

6.10.12 3CN (cis)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
N	5.23818	6.43852	4.16876
P	5.82881	5.13271	5.21373
P	3.56945	6.58217	4.87563
C	5.96531	7.40912	3.47030
N	4.12458	5.07468	5.63509
C	6.37706	6.15753	6.67328
H	3.94349	7.52241	5.92565
C	7.37135	7.27580	3.26199
C	5.30061	8.54964	2.92864
C	3.35561	4.08431	6.26100
N	6.78085	6.65561	7.66067
C	8.07111	8.27812	2.56681
C	8.11607	6.07742	3.74817
C	6.03948	9.52695	2.23702
C	3.82052	8.71718	3.04249
C	2.25752	4.46709	7.08495
C	3.63287	2.70433	6.05428
H	9.15492	8.14651	2.42543
C	7.42236	9.40819	2.05439
C	8.03737	4.85947	3.01336
C	8.96044	6.16875	4.88984
H	5.49504	10.39203	1.82736
C	3.27095	9.62152	3.99151
C	2.96428	8.01109	2.14924
C	1.49156	3.47392	7.72071
C	1.93151	5.91253	7.28660
C	2.85722	1.74279	6.73161
C	4.64854	2.23536	5.06401
H	7.98514	10.17995	1.50946
C	8.76120	3.74643	3.46455
C	7.16152	4.75842	1.79180
C	9.62775	5.01056	5.32936
C	9.17058	7.47554	5.61159
C	1.87343	9.77053	4.05393
C	4.16316	10.38514	4.93759
C	1.57790	8.20344	2.24091
C	3.53866	7.03050	1.16079
H	0.65134	3.78919	8.35859
C	1.79431	2.11424	7.56473
C	0.89983	6.53341	6.53413
C	2.65125	6.65544	8.26318
H	3.08118	0.67868	6.55841
C	5.85371	1.62721	5.49876
C	4.36085	2.33228	3.67537
H	8.70234	2.80876	2.89411
C	9.53442	3.78976	4.63913
H	6.08818	4.79926	2.07600
H	7.33710	5.59911	1.09096
H	7.32677	3.80390	1.25764
H	10.24657	5.07113	6.23933
H	10.00630	8.04386	5.14892
H	8.27658	8.12417	5.56909
H	9.41956	7.30679	6.67630
H	1.44665	10.45510	4.80356
C	1.01025	9.07079	3.19361
H	4.87397	11.03739	4.39123
H	3.56938	11.01697	5.62554
H	4.78450	9.69835	5.54897
H	0.91759	7.64869	1.55439
H	2.77257	6.68805	0.43937
H	4.39070	7.46387	0.60018

H	3.93374	6.13511	1.68821
H	1.19389	1.34730	8.07596
C	0.63534	7.90051	6.74678
C	0.12858	5.76724	5.48889
C	2.36243	8.01964	8.42776
C	3.69093	5.97835	9.11632
C	6.72684	1.08276	4.54095
C	6.22250	1.61081	6.96148
C	5.26993	1.78450	2.75369
C	3.10763	3.01447	3.18603
C	10.21890	2.55245	5.16084
C	−0.48588	9.22894	3.28808
H	−0.15957	8.38336	6.15730
C	1.36331	8.66477	7.67291
H	0.76086	5.60418	4.58879
H	−0.18194	4.76728	5.84866
H	−0.77391	6.32368	5.17021
H	2.93513	8.59544	9.17285
H	4.44877	5.46104	8.49839
H	4.22471	6.70310	9.75896
H	3.22685	5.20376	9.76203
H	7.66120	0.60861	4.88242
C	6.44876	1.13656	3.16450
H	7.20282	1.12231	7.12301
H	6.28778	2.64488	7.36249
H	5.46740	1.08658	7.58057
H	5.03832	1.85267	1.67798
H	2.93469	2.81654	2.11085
H	2.21375	2.68856	3.75463
H	3.17789	4.11503	3.32117
H	11.20281	2.78543	5.61467
H	9.60292	2.07162	5.95157
H	10.37161	1.80079	4.36163
H	−0.96557	8.28036	3.60997
H	−0.77093	10.01482	4.01396
H	−0.92891	9.49249	2.30559
C	1.09687	10.13786	7.85311
C	7.37582	0.50952	2.15337
H	0.19887	10.46376	7.29294
H	0.94860	10.39830	8.92119
H	1.95637	10.74378	7.49453
H	7.55768	1.18367	1.29095
H	8.35587	0.25149	2.60051
H	6.94388	−0.42667	1.73942

6.10.13 3CN (trans)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
N	5.21443	5.94107	4.63294
P	5.84941	4.75559	5.77862
P	3.78816	6.50414	5.59028
C	5.85711	6.64057	3.60639
N	4.24140	5.01065	6.49104
C	6.70892	5.83831	7.03177
H	2.69375	5.90533	4.85725
C	7.25192	6.49730	3.34507
C	5.08656	7.51233	2.77851
C	3.71383	4.47977	7.67082
N	7.18075	6.34469	7.98489
C	7.84516	7.26201	2.32326
C	8.11767	5.54238	4.10177
C	5.72430	8.26393	1.77463
C	3.59747	7.57967	2.89078
C	2.70758	5.17545	8.40223
C	4.14714	3.20238	8.13981
H	8.92394	7.13379	2.14474
C	7.10102	8.15590	1.54361
C	8.13057	4.16265	3.75397
C	9.01436	6.03486	5.09168
H	5.10439	8.92464	1.14882
C	2.94661	8.72729	3.41985
C	2.82328	6.49522	2.38444
C	2.19057	4.61333	9.58346
C	2.18120	6.49492	7.93880
C	3.61720	2.68657	9.33606
C	5.09499	2.37290	7.34062
H	7.58433	8.74358	0.74958
C	9.01785	3.30132	4.42137
C	7.18054	3.61546	2.72125
C	9.86160	5.12949	5.75094

C	9.05901	7.50160	5.43650
C	1.53980	8.76178	3.43944
C	3.73224	9.85784	4.03311
C	1.42189	6.57391	2.43261
C	3.49555	5.26333	1.83626
H	1.41600	5.17541	10.12817
C	2.64511	3.38014	10.06775
C	1.05148	6.53946	7.07814
C	2.76633	7.70152	8.41949
H	3.96370	1.69685	9.67165
C	6.42355	2.15137	7.79351
C	4.64938	1.78428	6.12339
H	9.02638	2.23542	4.14966
C	9.87743	3.75881	5.43409
H	6.16384	3.49527	3.15808
H	7.07860	4.29123	1.84950
H	7.50269	2.61744	2.36687
H	10.52529	5.50853	6.54464
H	9.67584	8.06407	4.70334
H	8.05081	7.95742	5.41829
H	9.48944	7.65839	6.44355
H	1.03886	9.64743	3.85978
C	0.75827	7.69859	2.95834
H	4.60487	10.15038	3.41902
H	3.09548	10.74955	4.19101
H	4.12884	9.54246	5.02331
H	0.82964	5.72824	2.04601
H	2.76474	4.58411	1.35749
H	4.28013	5.52099	1.09666
H	4.00673	4.70465	2.64939
H	2.23441	2.95662	10.99582
C	0.55208	7.79293	6.67744
C	0.39149	5.26625	6.60901
C	2.22811	8.92606	7.99741
C	3.96579	7.65969	9.32755
C	7.28109	1.35193	7.01467
C	6.92778	2.77280	9.07290
C	5.54359	0.99634	5.38145
C	3.25328	2.02580	5.60624
C	10.77382	2.80834	6.18577
C	−0.74781	7.74769	3.00835
H	−0.31468	7.82769	5.99916
C	1.12728	8.99531	7.12097
H	1.12663	4.55225	6.18598
H	−0.09807	4.73626	7.45264
H	−0.37536	5.47280	5.83772
H	2.68822	9.85995	8.35953
H	4.85724	7.25391	8.80349
H	4.22497	8.66982	9.69792
H	3.79489	6.99628	10.19882
H	8.31368	1.18857	7.36243
C	6.86345	0.76215	5.81050
H	8.01462	2.60091	9.19429
H	6.74998	3.86649	9.09617
H	6.41523	2.35301	9.96244
H	5.19441	0.54173	4.43952
H	2.99159	1.30739	4.80593
H	2.49783	1.95025	6.41350
H	3.16412	3.05199	5.18779
H	11.80744	3.20110	6.27094
H	10.40292	2.65659	7.22227
H	10.82016	1.81518	5.69804
H	−1.15616	6.91536	3.61994
H	−1.11215	8.69832	3.44361
H	−1.19128	7.64481	1.99599
C	0.58789	10.33232	6.68016
C	7.78290	−0.12603	5.01102
H	−0.31790	10.22370	6.05273
H	0.32611	10.96865	7.55075
H	1.34443	10.89314	6.09185
H	7.74369	0.11530	3.92888
H	8.83407	−0.03666	5.34747
H	7.49211	−1.19378	5.11026

6.10.14 3CN (bridged)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
N	1.14676	0.07966	−0.10085
N	−1.11377	−0.03784	0.14388
P	0.04378	−1.37577	0.02063
P	0.02931	1.08235	0.88602

C	−2.51205	−0.01146	0.12210
C	−3.28571	−1.14594	0.49836
C	−3.16755	1.17178	−0.32618
C	−4.69019	−1.07399	0.44121
C	−4.57489	1.20829	−0.34543
C	−5.34087	0.09823	0.03435
H	−5.27175	−1.96200	0.73381
H	−5.06700	2.12623	−0.70260
H	−6.43949	0.14163	−0.00140
C	2.54782	0.05178	−0.00167
C	3.27883	−1.08975	−0.45170
C	3.27509	1.17029	0.50346
C	4.68360	−1.09477	−0.38336
C	4.68100	1.12627	0.54812
C	5.39587	0.00451	0.11122
H	5.21652	−1.98941	−0.74113
H	5.21199	2.00928	0.93620
H	6.49487	−0.01063	0.15054
C	2.57375	2.40646	0.95855
C	2.11860	3.33903	−0.01520
C	2.40332	2.67778	2.34475
C	1.46494	4.50403	0.41265
C	1.71733	3.84757	2.72091
C	1.23008	4.76551	1.77472
H	1.11875	5.22507	−0.34204
H	1.56428	4.04741	3.79408
C	2.57293	−2.28758	−0.99263
C	2.43723	−3.45271	−0.19215
C	2.03081	−2.25757	−2.30787
C	1.73387	−4.55629	−0.71141
C	1.34707	−3.38550	−2.78610
C	1.18081	−4.54405	−2.00208
H	1.60979	−5.45202	−0.08150
H	0.92149	−3.35679	−3.80270
C	−2.40771	2.34756	−0.85081
C	−2.37942	3.56615	−0.12579
C	−1.77956	2.26419	−2.12385
C	−1.76806	4.69174	−0.70653
C	−1.16718	3.41128	−2.65663
C	−1.16541	4.64146	−1.97419
H	−1.75109	5.63696	−0.14018
H	−0.68738	3.34262	−3.64693
C	−2.63057	−2.40949	0.95410
C	−2.37425	−2.61232	2.33812
C	−2.31474	−3.42473	0.01170
C	−1.75264	−3.80830	2.74288
C	−1.69594	−4.60359	0.46518
C	−1.38841	−4.80788	1.82125
H	−1.54601	−3.96068	3.81511
H	−1.43690	−5.38170	−0.26940
C	−2.93153	3.64650	1.27581
H	−2.88980	4.68232	1.66466
H	−3.97823	3.29121	1.34393
H	−2.33551	3.00362	1.95960
C	−1.76023	0.96936	−2.89533
H	−2.76456	0.50145	−2.93700
H	−1.39798	1.12126	−3.93014
H	−1.09035	0.23665	−2.39728
C	−0.53297	5.86375	−2.59136
H	0.50732	5.66123	−2.92202
H	−1.09221	6.19720	−3.49113
H	−0.50541	6.71356	−1.88160
C	−2.61327	−3.23066	−1.45329
H	−2.44736	−4.16483	−2.02294
H	−3.65571	−2.89377	−1.61839
H	−1.95145	−2.45061	−1.88722
C	−2.74827	−1.55951	3.34901
H	−2.09804	−0.66457	3.24678
H	−3.79176	−1.21441	3.20925
H	−2.63505	−1.93844	4.38288
C	−0.65873	−6.04767	2.27320
H	0.42856	−5.84417	2.38870
H	−1.02448	−6.40629	3.25612
H	−0.76110	−6.87323	1.54194
C	0.43486	−5.73605	−2.54617
H	−0.59057	−5.45747	−2.86683
H	0.94370	−6.15683	−3.43874
H	0.34995	−6.54477	−1.79459
C	0.45295	5.98324	2.20542
H	−0.62672	5.73933	2.30906
H	0.79547	6.36489	3.18771
H	0.53226	6.80358	1.46498

C	2.88144	1.71566	3.40218
H	3.87114	1.28395	3.15969
H	2.94165	2.21145	4.39035
H	2.16298	0.87130	3.48857
C	2.14754	−1.01447	−3.15108
H	3.19136	−0.64311	−3.18676
H	1.79789	−1.19344	−4.18579
H	1.53728	−0.19397	−2.71635
C	3.01284	−3.51070	1.20187
H	2.57122	−4.34484	1.78146
H	4.11274	−3.66068	1.17975
H	2.84590	−2.56584	1.75623
C	2.30091	3.05957	−1.48455
H	2.04707	3.94584	−2.09612
H	3.33850	2.74747	−1.71786
H	1.63589	2.23006	−1.80626
C	0.32716	−1.24624	1.97428
N	0.30062	−0.05595	2.42047
H	0.47821	−2.13584	2.61769

6.10.15 3N3 (cis)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	7.82099	10.99650	5.87548
P	10.12647	9.55727	5.82516
N	9.16002	10.56742	6.92696
N	8.66271	9.88319	4.81017
N	8.52299	12.60059	5.27838
H	10.96438	10.56152	5.19597
C	9.39499	10.81627	8.28375
C	8.43710	9.54398	3.47153
N	7.85906	13.62701	5.38164
C	10.73509	10.85866	8.76735
C	8.31899	11.00982	9.19623
C	7.29280	10.01612	2.76098
C	9.35736	8.69277	2.78682
N	7.28281	14.62648	5.45823
C	10.97193	11.08815	10.13535
C	11.90443	10.71884	7.84464
C	8.60213	11.26448	10.55134
C	6.88932	10.90420	8.77864
C	7.12686	9.67623	1.40522
C	6.22502	10.84287	3.39902
C	9.15294	8.38223	1.43016
C	10.52013	8.05772	3.47942
H	12.01586	11.12307	10.48371
C	9.91716	11.30049	11.03198
C	12.30768	11.83574	7.05893
C	12.65484	9.51271	7.80444
H	7.75463	11.41105	11.23873
C	6.31492	9.62448	8.55368
C	6.09249	12.07260	8.67095
H	6.23162	10.05538	0.88839
C	8.04846	8.87268	0.72444
C	6.14846	12.23438	3.11990
C	5.22047	10.21724	4.18570
H	9.88292	7.72191	0.93650
C	10.31472	6.86783	4.23608
C	11.83149	8.57596	3.30919
H	10.11791	11.49179	12.09637
C	13.44162	11.71490	6.23791
C	11.51181	13.11346	7.07767
C	13.78733	9.44348	6.97269
C	12.21553	8.30325	8.58949
C	4.94274	9.53837	8.26492
C	7.16458	8.38002	8.60623
C	4.72298	11.93725	8.38063
C	6.69887	13.44293	8.85253
H	7.89855	8.61802	−0.33480
C	5.09159	12.98037	3.66966
C	7.18598	12.90527	2.25510
C	4.17043	10.99894	4.69341
C	5.29548	8.74434	4.49402
C	11.41985	6.23591	4.82393
C	8.92242	6.33234	4.44164
C	12.90781	7.91321	3.92687
C	12.06561	9.82637	2.49966
H	13.74604	12.57992	5.62609
C	14.19646	10.52840	6.17933
H	12.06340	13.93899	6.58843
H	11.25522	13.41963	8.11153

H	10.55143	12.97750	6.53403
H	14.36195	8.50505	6.93773
H	11.24850	7.92355	8.19399
H	12.05091	8.53555	9.65986
H	12.95850	7.48572	8.51730
H	4.49660	8.54372	8.10005
C	4.12274	10.67987	8.19592
H	6.54606	7.46523	8.53128
H	7.75854	8.33008	9.54126
H	7.89870	8.36697	7.77190
H	4.10533	12.84689	8.30218
H	7.71585	13.49980	8.41602
H	6.81018	13.70138	9.92694
H	6.07453	14.22335	8.37717
H	5.05007	14.06387	3.47579
C	4.09314	12.38321	4.45961
H	7.11531	12.56793	1.20049
H	8.21068	12.65412	2.59578
H	7.06963	14.00570	2.27364
H	3.39033	10.50936	5.29477
H	5.45774	8.14007	3.57877
H	4.37537	8.39132	4.99740
H	6.15015	8.52886	5.17185
H	11.25615	5.32188	5.41785
C	12.72533	6.74570	4.68729
H	8.37915	6.22510	3.48138
H	8.32325	7.03430	5.06169
H	8.93672	5.35237	4.95541
H	13.92179	8.32649	3.81165
H	11.82952	9.66584	1.42751
H	13.11745	10.16240	2.57670
H	11.40987	10.65463	2.83764
C	15.40856	10.43420	5.28719
C	2.63696	10.55334	7.97204
C	2.99244	13.21540	5.06555
C	13.88812	6.05163	5.34963
H	15.87768	9.43241	5.33729
H	16.17782	11.18327	5.56923
H	15.14464	10.63456	4.22730
H	2.22330	11.43999	7.45327
H	2.09842	10.46141	8.94009
H	2.38554	9.65267	7.37702
H	2.75292	14.09768	4.43997
H	3.29912	13.59834	6.06305
H	2.06418	12.62780	5.20914
H	14.85051	6.54534	5.11355
H	13.96061	4.99091	5.03152
H	13.77151	6.04544	6.45400

6.10.16 $3N_3$ (trans)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	11.88906	11.64887	4.47400
P	10.23909	9.88415	5.69090
N	11.12662	11.41022	6.03669
N	10.71874	10.41103	4.03159
N	13.36341	10.57536	4.81431
H	8.91815	10.47124	5.80953
C	11.29443	12.09036	7.24471
C	10.57733	9.65943	2.85758
N	14.49833	11.01230	4.66050
C	11.01593	11.44129	8.48308
C	11.70651	13.45600	7.25911
C	11.37051	9.90504	1.69788
C	9.58080	8.63754	2.80339
N	15.59159	11.36951	4.53730
C	11.17071	12.14641	9.69048
C	10.57651	10.01379	8.52916
C	11.87236	14.11579	8.49068
C	11.91255	14.22899	5.99916
C	11.20420	9.08962	0.56210
C	12.35345	11.02617	1.60308
C	9.45678	7.84250	1.64910
C	8.58464	8.43761	3.90192
H	10.95353	11.61736	10.63146
C	11.60951	13.47628	9.70866
C	11.54435	8.97290	8.44325
C	9.20307	9.69917	8.70989
H	12.19169	15.16931	8.47337
C	10.78682	14.63665	5.23184
C	13.22203	14.59514	5.59270

H	11.82785	9.30440	−0.31941
C	10.26913	8.04880	0.52825
C	13.74734	10.74467	1.62825
C	11.90060	12.35199	1.36489
H	8.67786	7.06431	1.63822
C	7.49628	9.35220	4.01155
C	8.63946	7.29719	4.75046
H	11.73674	14.01152	10.66097
C	11.11423	7.64017	8.53075
C	12.99328	9.29845	8.19986
C	8.81944	8.34735	8.78141
C	8.16746	10.79208	8.81030
C	10.99510	15.42207	4.08620
C	9.39272	14.21116	5.61846
C	13.38050	15.38311	4.43815
C	14.43374	14.14821	6.37391
H	10.15499	7.42565	−0.37071
C	14.65823	11.79987	1.45375
C	14.24545	9.33943	1.85534
C	12.84970	13.37050	1.17391
C	10.42990	12.67878	1.35076
C	6.50719	9.12434	4.98267
C	7.41949	10.55709	3.11017
C	7.61983	7.10679	5.69956
C	9.81453	6.35702	4.70672
H	11.86426	6.83567	8.45780
C	9.75695	7.30440	8.69655
H	13.63661	8.40944	8.34396
H	13.34911	10.10914	8.86653
H	13.13789	9.65625	7.15615
H	7.75272	8.10306	8.90532
H	8.28285	11.53836	7.99819
H	8.26413	11.35688	9.76078
H	7.14221	10.37737	8.75962
H	10.12059	15.74181	3.49587
C	12.28186	15.82283	3.68052
H	8.62763	14.75419	5.03134
H	9.19847	14.37927	6.69696
H	9.25146	13.12248	5.44210
H	14.39914	15.66418	4.12427
H	14.29478	13.13630	6.80241
H	14.63422	14.82358	7.23277
H	15.33801	14.13341	5.73611
H	15.73688	11.58229	1.50307
C	14.23126	13.12091	1.22674
H	14.01499	8.68034	0.99314
H	13.75381	8.88317	2.73819
H	15.34034	9.32628	2.01592
H	12.49391	14.39359	0.98161
H	9.84009	11.91743	0.80295
H	10.24334	13.67170	0.89863
H	10.02930	12.71130	2.38834
H	5.67399	9.84086	5.06983
C	6.55091	8.00857	5.83953
H	7.50072	10.26862	2.04247
H	8.26286	11.25298	3.30570
H	6.47325	11.11173	3.25696
H	7.67312	6.23022	6.36354
H	10.09617	6.07851	3.67339
H	9.61390	5.43327	5.28279
H	10.70140	6.85581	5.15706
C	9.33255	5.86026	8.78126
C	12.47070	16.73403	2.49417
C	15.23281	14.23800	1.08397
C	5.48178	7.79879	6.88154
H	8.23649	5.76094	8.90286
H	9.81658	5.34813	9.63900
H	9.62802	5.30112	7.86892
H	13.44653	16.56441	1.99890
H	12.44452	17.80028	2.80726
H	11.66914	16.59945	1.74072
H	16.17112	13.89010	0.60858
H	15.50687	14.64393	2.08197
H	14.82977	15.07809	0.48467
H	5.64254	6.86297	7.45106
H	4.47207	7.75000	6.42326
H	5.46014	8.63856	7.60815

6.10.17 3NCO (cis)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z

P	10.05351	5.26259	5.60600
P	7.93433	3.56132	5.45853
N	9.09773	4.16738	6.63345
N	8.77454	4.72946	4.44451
H	11.08040	4.36026	5.11162
N	8.78761	2.02724	5.07746
C	9.21296	3.97835	8.01350
C	8.63144	5.04874	3.09071
C	8.44300	0.85468	5.03227
C	8.09557	3.58575	8.80520
C	10.47243	4.18815	8.64897
C	9.46538	6.04959	2.50273
C	7.66132	4.40704	2.26205
O	8.18469	−0.30011	4.97859
C	8.25560	3.41596	10.19286
C	6.74039	3.37292	8.21563
C	10.58123	4.03432	10.04367
C	11.70746	4.48925	7.85996
C	9.34890	6.35131	1.13391
C	10.43841	6.84940	3.30813
C	7.57625	4.74639	0.89830
C	6.70022	3.37888	2.76516
H	7.37601	3.11192	10.78126
C	9.48456	3.64731	10.82381
C	5.91925	4.49293	7.91647
C	6.25501	2.05625	8.00847
H	11.56614	4.19691	10.50847
C	12.36220	3.42525	7.17514
C	12.27638	5.79159	7.85756
H	10.00794	7.13045	0.72004
C	8.41345	5.70562	0.31780
C	9.97193	7.97999	4.03853
C	11.82525	6.54600	3.27448
H	6.81516	4.23248	0.29072
C	6.93487	2.00607	2.48525
C	5.49698	3.77933	3.40538
H	9.58840	3.51877	11.91118
C	4.61242	4.27161	7.45348
C	6.45330	5.89418	8.06911
C	4.94029	1.88299	7.53722
C	7.12621	0.85529	8.28761

C	13.55635	3.69288	6.48492
C	11.76862	2.04113	7.16631
C	13.47857	6.00733	7.16013
C	11.57107	6.94470	8.52326
H	8.32859	5.95543	−0.74975
C	10.89790	8.77130	4.73285
C	8.49786	8.28054	4.10606
C	12.71572	7.36326	3.99509
C	12.33520	5.35802	2.49791
C	5.97908	1.05641	2.88486
C	8.19793	1.57007	1.78619
C	4.56040	2.79767	3.76834
C	5.24724	5.23038	3.72263
H	3.97290	5.14177	7.23130
C	4.09430	2.97467	7.27722
H	7.27637	6.08237	7.34628
H	6.88432	6.05942	9.07727
H	5.66399	6.64989	7.89343
H	4.56381	0.85878	7.37961
H	6.79916	−0.02357	7.69915
H	7.09597	0.57434	9.36198
H	8.18933	1.05787	8.05161
H	14.05434	2.86802	5.94932
C	14.13147	4.97725	6.46254
H	10.83996	2.01729	6.55668
H	11.48619	1.71386	8.18720
H	12.47437	1.30316	6.73940
H	13.91103	7.01966	7.15229
H	12.21151	7.84738	8.54811
H	11.25568	6.70583	9.55731
H	10.64758	7.19670	7.95710
H	10.53227	9.63941	5.30540
C	12.27546	8.47841	4.72753
H	8.04381	8.33203	3.09606
H	8.30195	9.23290	4.63447
H	7.96081	7.47143	4.64751
H	13.78919	7.11782	3.98383
H	11.80452	4.42832	2.78832
H	13.41881	5.20496	2.66479
H	12.16494	5.48131	1.40866
H	6.17713	−0.01014	2.69322

C	4.78592	1.43043	3.52919
H	8.21475	1.90711	0.72916
H	8.30215	0.46822	1.79979
H	9.09284	2.01237	2.26850
H	3.62755	3.11322	4.25872
H	5.40525	5.87931	2.83785
H	5.95363	5.58344	4.50602
H	4.22118	5.38938	4.10543
C	2.65835	2.76613	6.86731
C	15.40857	5.23275	5.70267
C	13.24326	9.34696	5.49013
C	3.79763	0.38660	3.98250
H	2.27980	3.60695	6.25242
H	2.00036	2.69793	7.76060
H	2.52580	1.82830	6.29405
H	15.28012	5.02020	4.62006
H	16.23106	4.57819	6.05906
H	15.74228	6.28368	5.80393
H	14.28502	8.98558	5.39089
H	12.99205	9.37347	6.57114
H	13.21216	10.39661	5.13019
H	3.84188	−0.52200	3.35054
H	2.75834	0.77044	3.96877
H	4.01803	0.06862	5.02477

6.10.18 3NCO (trans)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.26233	5.46924	5.65403
P	11.81036	3.55226	4.51866
N	11.08259	3.92453	6.07850
N	10.72607	4.85401	4.02456
H	8.91795	4.94444	5.79065
N	13.35545	4.42469	4.79807
C	11.23889	3.31023	7.32128
C	10.59812	5.54245	2.81268
C	14.54053	4.14526	4.69065
C	11.65468	1.94825	7.41822
C	10.95460	4.02596	8.52230
C	9.61572	6.57497	2.70253
C	11.39375	5.23325	1.66869
O	15.70614	3.94419	4.62041
C	11.80054	1.35417	8.68501
C	11.89840	1.11252	6.20583
C	11.08914	3.38519	9.76735
C	10.55162	5.46447	8.49193
C	9.50669	7.31527	1.51107
C	8.61528	6.83964	3.78322
C	11.24070	5.99472	0.49386
C	12.37732	4.10857	1.62843
H	12.12348	0.30237	8.72718
C	11.51853	2.05576	9.86389
C	10.79387	0.62267	5.45583
C	13.22336	0.77220	5.82793
H	10.86666	3.96693	10.67551
C	11.55175	6.47080	8.36904
C	9.18711	5.82893	8.64086
H	8.73785	8.10185	1.45978
C	10.31942	7.04426	0.40438
C	7.52010	5.93881	3.93230
C	8.67377	8.01926	4.57535
H	11.86648	5.73065	−0.37268
C	13.76980	4.39704	1.64986
C	11.93305	2.77153	1.44649
H	11.62928	1.57147	10.84503
C	11.03792	−0.21273	4.35435
C	9.38535	1.02537	5.81173
C	13.41865	−0.06432	4.71319
C	14.41158	1.29149	6.60043
C	11.16269	7.81860	8.38522
C	12.99304	6.08844	8.16337
C	8.84444	7.19355	8.63942
C	8.11850	4.77362	8.78368
H	10.21657	7.62395	−0.52449
C	6.52643	6.22151	4.88379
C	7.44130	4.69034	3.09232
C	7.64909	8.26391	5.50720
C	9.85616	8.94871	4.49797
C	14.68748	3.34144	1.52549
C	14.25926	5.81186	1.83229
C	12.88885	1.74955	1.30678

C	10.46537	2.43258	1.44489
H	10.17992	−0.59498	3.77709
C	12.34208	−0.58188	3.97350
H	9.22324	2.10563	5.60385
H	9.18021	0.88286	6.89193
H	8.64075	0.44933	5.22975
H	14.44894	−0.32390	4.41900
H	15.31857	1.32647	5.96686
H	14.63605	0.64610	7.47638
H	14.22611	2.30604	7.00344
H	11.93782	8.59572	8.28331
C	9.81406	8.20252	8.51384
H	13.13499	5.64278	7.15442
H	13.32217	5.32368	8.89506
H	13.65988	6.96820	8.24217
H	7.78435	7.47547	8.73761
H	7.10643	5.21952	8.73418
H	8.21024	4.23090	9.74723
H	8.19867	4.00278	7.99019
H	5.68768	5.51579	5.00099
C	6.57244	7.37852	5.68433
H	7.51969	4.92608	2.01143
H	6.49502	4.14435	3.26846
H	8.28560	4.00517	3.31958
H	7.70427	9.17215	6.12730
H	10.72105	8.48566	5.02348
H	9.63990	9.91783	4.98750
H	10.17888	9.13979	3.45710
H	15.76484	3.56609	1.57392
C	14.26844	2.00855	1.35507
H	14.04560	6.43696	0.94085
H	15.35030	5.83528	2.01680
H	13.74790	6.30170	2.68527
H	12.53913	0.71664	1.16010
H	9.85934	3.20680	0.93507
H	10.08823	2.35896	2.48994
H	10.27844	1.45370	0.96286
C	12.57184	−1.54241	2.83427
C	9.43102	9.66056	8.50824
C	5.49878	7.64680	6.70821
C	15.27658	0.89147	1.26756
H	11.78061	−1.46156	2.06233
H	12.56280	−2.59319	3.19674
H	13.55189	−1.37422	2.34724
H	9.68830	10.13638	7.53853
H	9.97481	10.22461	9.29413
H	8.34579	9.80025	8.67776
H	5.65120	8.61853	7.21657
H	5.48299	6.85563	7.48777
H	4.48981	7.65714	6.24615
H	16.22436	1.22934	0.80405
H	14.89022	0.03284	0.68376
H	15.52885	0.51456	2.28261

6.10.19 3NCS (cis)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.03832	5.24201	5.59075
P	8.00099	3.45761	5.40962
N	9.12054	4.09745	6.59881
N	8.75523	4.70175	4.42975
H	11.07350	4.36755	5.06321
N	8.96624	1.99294	4.96022
C	9.23994	3.85563	7.97212
C	8.61821	5.00757	3.07044
C	8.83027	0.78513	5.02110
C	8.10348	3.49641	8.75237
C	10.50890	3.98883	8.60556
C	9.42009	6.03662	2.48958
C	7.68302	4.32294	2.23662
S	8.70438	−0.79836	5.08788
C	8.26783	3.22859	10.12427
C	6.72708	3.46759	8.17389
C	10.62289	3.73972	9.98582
C	11.73323	4.35648	7.82788
C	9.31322	6.32165	1.11641
C	10.34247	6.87361	3.31503
C	7.60729	4.64429	0.86855
C	6.75501	3.27570	2.75963
H	7.37704	2.95229	10.70933
C	9.51600	3.34636	10.74906

C	6.06601	4.69382	7.88902
C	6.06217	2.23319	7.96029
H	11.61459	3.84265	10.45304
C	12.43204	3.34543	7.11014
C	12.23460	5.68528	7.85598
H	9.94583	7.12330	0.70442
C	8.41746	5.62996	0.29301
C	9.81067	7.96866	4.05536
C	11.74179	6.63098	3.30707
H	6.87502	4.09798	0.25408
C	7.02879	1.90261	2.50747
C	5.55813	3.65292	3.42517
H	9.62337	3.14197	11.82449
C	4.74202	4.65787	7.42177
C	6.77254	6.01411	8.06816
C	4.73603	2.24732	7.49011
C	6.76308	0.92098	8.21365
C	13.60366	3.69019	6.41624
C	11.90351	1.93628	7.07482
C	13.41663	5.98054	7.15149
C	11.48913	6.77796	8.57863
H	8.34043	5.86624	−0.77825
C	10.68533	8.78188	4.78976
C	8.32426	8.20905	4.08834
C	12.57862	7.46730	4.06898
C	12.32124	5.48559	2.51548
C	6.13100	0.93280	2.98120
C	8.27506	1.49027	1.76601
C	4.67763	2.64761	3.86004
C	5.26270	5.10040	3.71980
H	4.22829	5.61028	7.21068
C	4.05117	3.44641	7.23204
H	7.57348	6.14154	7.30839
H	7.26984	6.08068	9.05671
H	6.07028	6.86367	7.96753
H	4.22447	1.28672	7.31615
H	6.24104	0.08442	7.71084
H	6.81473	0.68690	9.29793
H	7.80997	0.93659	7.85116
H	14.13696	2.90555	5.85491
C	14.11261	5.00306	6.42139

H	10.94361	1.89632	6.52025
H	11.69512	1.55461	8.09454
H	12.61299	1.24861	6.57659
H	13.79849	7.01301	7.16858
H	12.08384	7.71084	8.61881
H	11.21937	6.48574	9.61224
H	10.53668	7.00361	8.05131
H	10.26976	9.62151	5.37061
C	12.07317	8.54381	4.81698
H	7.89555	8.25784	3.06717
H	8.07705	9.14530	4.62398
H	7.80479	7.37192	4.60309
H	13.66135	7.26702	4.07981
H	11.79827	4.53350	2.73843
H	13.39772	5.35062	2.73545
H	12.20921	5.64951	1.42383
H	6.36751	−0.13133	2.82304
C	4.95529	1.28393	3.67082
H	8.20964	1.74926	0.68867
H	8.44675	0.40039	1.85096
H	9.16789	2.01465	2.16073
H	3.75419	2.94128	4.37923
H	5.49430	5.75632	2.85749
H	5.88386	5.45494	4.57253
H	4.20366	5.24493	4.00729
C	2.60769	3.44676	6.79517
C	15.36675	5.34252	5.65612
C	12.98305	9.42481	5.63462
C	4.04438	0.21501	4.21786
H	2.41731	4.20375	6.00709
H	1.93560	3.69465	7.64478
H	2.29483	2.45751	6.40762
H	15.22539	5.18631	4.56543
H	16.21604	4.69670	5.96123
H	15.66789	6.39688	5.81000
H	14.04500	9.13146	5.52540
H	12.72470	9.37369	6.71331
H	12.89073	10.48956	5.33534
H	3.80715	−0.55302	3.45352
H	3.09127	0.63758	4.59104
H	4.53356	−0.31569	5.06286

6.10.20 3NCS (trans)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.28302	5.47395	5.64271
P	11.87380	3.59998	4.51625
N	11.12972	3.94464	6.06866
N	10.74207	4.84811	4.01145
H	8.94900	4.92986	5.80040
N	13.38420	4.55780	4.79576
C	11.29730	3.32369	7.30862
C	10.59468	5.52149	2.79106
C	14.58356	4.37827	4.88668
C	11.66438	1.94707	7.38555
C	11.06432	4.04507	8.51558
C	9.57296	6.51170	2.66808
C	11.41010	5.23332	1.65622
S	16.15939	4.20561	5.02007
C	11.84416	1.34941	8.64630
C	11.79544	1.10660	6.15908
C	11.23061	3.40130	9.75512
C	10.65487	5.48158	8.48472
C	9.43568	7.23056	1.46640
C	8.57215	6.75345	3.75342
C	11.22949	5.97166	0.47107
C	12.44517	4.15606	1.65331
H	12.12859	0.28635	8.67906
C	11.63407	2.06220	9.83374
C	10.62426	0.72032	5.44891
C	13.07125	0.66621	5.72134
H	11.04952	3.98443	10.67146
C	11.64453	6.49581	8.34988
C	9.28592	5.83290	8.62731
H	8.63671	7.98558	1.40323
C	10.26229	6.97792	0.36547
C	7.50919	5.81814	3.92241
C	8.60616	7.93684	4.54114
H	11.87208	5.72644	−0.38860
C	13.82286	4.50704	1.71951
C	12.06487	2.79778	1.48986
H	11.77137	1.57526	10.81025
C	10.75574	−0.10895	4.32391
C	9.26321	1.21421	5.87117
C	13.15291	−0.15914	4.58381
C	14.32904	1.07245	6.44884
C	11.24068	7.83939	8.34271
C	13.08976	6.12328	8.15598
C	8.92844	7.19374	8.60238
C	8.22899	4.76873	8.79160
H	10.13798	7.54083	−0.57111
C	6.52094	6.07333	4.88696
C	7.46356	4.55917	3.09567
C	7.58970	8.15071	5.49019
C	9.75400	8.90682	4.43942
C	14.78696	3.48890	1.67522
C	14.24234	5.94674	1.87483
C	13.06800	1.81305	1.43664
C	10.61349	2.39780	1.43146
H	9.84638	−0.41225	3.77922
C	12.00966	−0.57095	3.88008
H	9.15067	2.29726	5.64674
H	9.10869	1.10418	6.96340
H	8.45628	0.67164	5.34238
H	14.14639	−0.48721	4.23710
H	15.21252	1.01422	5.78466
H	14.52029	0.41478	7.32353
H	14.26447	2.10477	6.84334
H	12.00781	8.62297	8.23068
C	9.88726	8.21067	8.45963
H	13.23432	5.65027	7.16123
H	13.42746	5.38296	8.90840
H	13.74868	7.01075	8.20777
H	7.86527	7.46575	8.69543
H	7.21218	5.20297	8.73650
H	8.32924	4.24592	9.76532
H	8.31434	3.98320	8.01334
H	5.70657	5.34217	5.01905
C	6.54393	7.23302	5.68522
H	7.54747	4.78236	2.01280
H	6.52804	3.99463	3.27091
H	8.31983	3.89502	3.34096
H	7.62676	9.06146	6.10809

H	10.63941	8.48685	4.96677
H	9.50494	9.87632	4.91228
H	10.06208	9.09020	3.39281
H	15.85023	3.76067	1.76856
C	14.42995	2.13262	1.54848
H	14.04655	6.53105	0.95187
H	15.32023	6.02377	2.11293
H	13.67097	6.44168	2.68540
H	12.77050	0.76130	1.31687
H	10.00423	3.12292	0.85715
H	10.18423	2.34987	2.45750
H	10.49174	1.39231	0.98446
C	12.10867	−1.51052	2.70480
C	9.48675	9.66347	8.41938
C	5.47898	7.46952	6.72582
C	15.48910	1.06086	1.57274
H	11.41450	−1.22241	1.88923
H	11.83962	−2.54705	3.00193
H	13.13539	−1.54421	2.29086
H	9.69396	10.10545	7.42189
H	10.05821	10.26214	9.15826
H	8.40830	9.79772	8.63144
H	5.60513	8.44907	7.22624
H	5.50438	6.68304	7.50985
H	4.46273	7.44116	6.28089
H	16.30411	1.27253	0.85049
H	15.07052	0.06276	1.33848
H	15.95978	1.00555	2.57789

6.10.21 3NSO (cis)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.01876	5.31707	5.63654
P	7.82478	3.72062	5.49036
N	9.00706	4.27497	6.67824
N	8.79604	4.75210	4.43697
H	11.07716	4.40792	5.24487
N	8.62420	2.14925	5.18155
C	9.02253	4.25897	8.07219
C	8.42847	5.35696	3.23616
S	7.67199	0.89778	5.17885
C	7.88046	3.89770	8.84489
C	10.23083	4.61203	8.74628
C	9.19600	6.44470	2.71918
C	7.30984	4.89265	2.47879
O	8.40756	−0.38653	4.95465
C	7.93900	3.99279	10.24725
C	6.62895	3.36910	8.22233
C	10.23860	4.71050	10.14986
C	11.52143	4.74635	8.00261
C	8.77516	7.10394	1.54977
C	10.49228	6.87594	3.33042
C	6.92368	5.58648	1.31633
C	6.57143	3.62899	2.79364
H	7.04069	3.71613	10.82101
C	9.09765	4.42203	10.90854
C	5.59850	4.25066	7.80714
C	6.45463	1.96430	8.11180
H	11.18355	4.97922	10.64709
C	12.13290	3.56929	7.47810
C	12.19773	5.99625	7.91253
H	9.38801	7.94151	1.18153
C	7.62949	6.70295	0.85220
C	10.57305	8.08437	4.07917
C	11.67340	6.13656	3.04275
H	6.05570	5.20615	0.75530
C	7.11660	2.38711	2.37064
C	5.27354	3.67272	3.37409
H	9.12102	4.49494	12.00566
C	4.40328	3.71110	7.30238
C	5.81339	5.74035	7.86088
C	5.24978	1.46835	7.58150
C	7.54346	1.01968	8.55772
C	13.40079	3.67284	6.87832
C	11.44436	2.23074	7.54091
C	13.46555	6.04411	7.30967
C	11.53993	7.26521	8.38961
H	7.31356	7.22798	−0.06088
C	11.82721	8.52860	4.52098
C	9.31817	8.82159	4.46180
C	12.90920	6.62168	3.51028

C	11.60136	4.86277	2.23874
C	6.36071	1.21247	2.55468
C	8.51368	2.29927	1.82254
C	4.55453	2.47641	3.53855
C	4.70135	4.97919	3.85414
H	3.60313	4.39812	6.98264
C	4.20452	2.32339	7.18703
H	6.64238	6.03672	7.18138
H	6.11030	6.07637	8.87476
H	4.90599	6.29498	7.55449
H	5.11925	0.37771	7.48755
H	7.35223	−0.01380	8.20891
H	7.62839	0.99972	9.66439
H	8.53668	1.33584	8.18121
H	13.87104	2.75907	6.47974
C	14.08819	4.89517	6.78820
H	10.64605	2.15822	6.76888
H	10.95939	2.06687	8.52381
H	12.15954	1.40629	7.35741
H	13.98275	7.01371	7.24226
H	12.20092	8.13986	8.23736
H	11.25629	7.22050	9.45948
H	10.60152	7.44038	7.82001
H	11.88419	9.45692	5.11265
C	13.01138	7.82075	4.23568
H	8.68729	9.05932	3.58279
H	9.54650	9.76108	5.00044
H	8.69631	8.18503	5.12946
H	13.82250	6.04836	3.28255
H	10.97865	4.09765	2.74677
H	12.60755	4.43221	2.07563
H	11.12830	5.03984	1.25090
H	6.79085	0.24911	2.23616
C	5.07841	1.23437	3.14156
H	8.76032	3.15744	1.16831
H	8.67323	1.35729	1.26412
H	9.23764	2.31373	2.66984
H	3.55594	2.51778	3.99904
H	4.66914	5.73910	3.04838
H	5.34211	5.39929	4.65915
H	3.68143	4.84841	4.26241
C	2.89614	1.75877	6.69443
C	15.44097	4.96943	6.12721
C	14.35121	8.36615	4.65914
C	4.33073	−0.04811	3.39308
H	2.29215	2.52220	6.16598
H	2.28295	1.38305	7.54161
H	3.05355	0.90349	6.00741
H	15.33829	5.05492	5.02357
H	16.04173	4.05916	6.32375
H	16.01980	5.84794	6.47328
H	15.10711	7.56498	4.76537
H	14.28454	8.91140	5.62187
H	14.73860	9.08709	3.90699
H	4.49917	−0.78782	2.58549
H	3.24089	0.12140	3.49179
H	4.68172	−0.51970	4.33783

6.10.22 3NSO (trans)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.27985	5.45371	5.64094
P	11.80187	3.51225	4.50468
N	11.10479	3.91137	6.07729
N	10.71223	4.81235	4.00761
H	8.94321	4.91594	5.81745
N	13.29443	4.46481	4.79299
C	11.25446	3.29671	7.31747
C	10.56750	5.48526	2.79081
S	14.67604	3.73108	4.68397
C	11.57281	1.90637	7.41548
C	11.05417	4.04122	8.51840
C	9.52544	6.45656	2.66218
C	11.40328	5.23401	1.65963
O	15.83883	4.64982	4.90763
C	11.72510	1.31823	8.68412
C	11.69304	1.05468	6.19650
C	11.19247	3.40664	9.76532
C	10.70486	5.49248	8.46749
C	9.37173	7.17150	1.46120
C	8.53061	6.69248	3.75408

C	11.20283	5.96559	0.47250
C	12.49540	4.21433	1.65487
H	11.96682	0.24515	8.73190
C	11.53953	2.05273	9.86242
C	10.52604	0.72375	5.45212
C	12.96047	0.56654	5.78391
H	11.03748	4.00910	10.67392
C	11.72669	6.46499	8.27483
C	9.35367	5.89787	8.64110
H	8.55577	7.90822	1.39857
C	10.20455	6.93957	0.36014
C	7.48101	5.74698	3.94382
C	8.56528	7.87969	4.53607
H	11.86170	5.74546	−0.38181
C	13.85175	4.63527	1.73336
C	12.18809	2.83810	1.47490
H	11.65444	1.57270	10.84519
C	10.65617	−0.07332	4.30438
C	9.17377	1.25663	5.85262
C	13.04355	−0.21252	4.61393
C	14.20962	0.86463	6.57621
C	11.36922	7.82260	8.24911
C	13.15191	6.04564	8.03275
C	9.04416	7.26893	8.59110
C	8.26277	4.87726	8.85340
H	10.06606	7.49662	−0.57785
C	6.50514	5.99629	4.92257
C	7.44120	4.48152	3.12669
C	7.56410	8.08542	5.50300
C	9.70075	8.86188	4.41226
C	14.86843	3.66542	1.68891
C	14.20009	6.07450	1.99971
C	13.23907	1.90176	1.43630
C	10.76066	2.37073	1.36965
H	9.74990	−0.32912	3.73089
C	11.90571	−0.54963	3.86332
H	9.08966	2.33740	5.60413
H	9.00742	1.17395	6.94514
H	8.35884	0.72353	5.32641
H	14.03237	−0.57021	4.28259
H	15.11789	0.74372	5.95448
H	14.30735	0.17936	7.44509
H	14.20162	1.88973	6.99585
H	12.16018	8.57477	8.09520
C	10.03491	8.24632	8.39573
H	13.27546	5.67491	6.99045
H	13.45878	5.22084	8.70587
H	13.85028	6.89380	8.16682
H	7.99412	7.58115	8.70669
H	7.26376	5.35413	8.85135
H	8.38838	4.34041	9.81607
H	8.27645	4.09754	8.06449
H	5.70102	5.25701	5.07134
C	6.53104	7.15786	5.71821
H	7.50886	4.69757	2.04118
H	6.51582	3.90545	3.31789
H	8.31046	3.83238	3.36766
H	7.60467	8.99699	6.11986
H	10.59414	8.46085	4.94102
H	9.44195	9.83534	4.87154
H	10.00094	9.03302	3.36148
H	15.91679	3.99183	1.78229
C	14.58144	2.28830	1.56031
H	13.65482	6.77231	1.33598
H	15.28707	6.25294	1.89697
H	13.91130	6.33152	3.04329
H	12.99511	0.83646	1.31192
H	10.13289	3.08314	0.80002
H	10.31516	2.27804	2.38527
H	10.69819	1.37288	0.89431
C	12.00498	−1.42561	2.64000
C	9.68306	9.71062	8.32483
C	5.48395	7.38620	6.77858
C	15.68611	1.26588	1.60577
H	11.37417	−1.04296	1.81185
H	11.65383	−2.45701	2.85810
H	13.04753	−1.50302	2.27410
H	9.82208	10.10241	7.29494
H	10.33322	10.31753	8.98763
H	8.63027	9.89385	8.61514
H	5.60918	8.36896	7.27296
H	5.53393	6.60321	7.56476

H	4.45945	7.34517	6.35398
H	16.58231	1.60083	1.04610
H	15.36034	0.29017	1.19554
H	16.00850	1.09353	2.65619

6.10.23 3PCO (cis endo)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.08753	5.18845	5.58597
P	7.98358	3.47443	5.42135
N	9.13339	4.09986	6.61132
N	8.79531	4.69288	4.42693
H	11.08729	4.24960	5.08862
P	9.26223	1.54738	4.85228
C	9.22762	3.95212	7.99907
C	8.66021	5.03829	3.07751
C	7.95711	0.54116	5.12056
C	8.10076	3.56927	8.78164
C	10.46883	4.21385	8.65340
C	9.51176	6.03913	2.51336
C	7.67460	4.43874	2.23459
O	7.07336	−0.21679	5.31371
C	8.23540	3.45788	10.17841
C	6.75530	3.31337	8.18714
C	10.55185	4.11144	10.05411
C	11.71359	4.53099	7.88643
C	9.40237	6.37504	1.15197
C	10.48596	6.82653	3.32938
C	7.59607	4.81609	0.88013
C	6.68714	3.42395	2.70871
H	7.34755	3.16638	10.76067
C	9.44609	3.73314	10.82551
C	5.92757	4.40606	7.81510
C	6.27403	1.98232	8.08071
H	11.52252	4.31482	10.53249
C	12.44839	3.46107	7.29930
C	12.22095	5.85732	7.82975
H	10.07462	7.15315	0.75814
C	8.45391	5.76889	0.32133
C	10.01637	7.94629	4.07493
C	11.87551	6.54094	3.27149
H	6.81928	4.33965	0.26246
C	6.82423	2.07168	2.28910
C	5.54593	3.82622	3.45321
H	9.52793	3.64974	11.91915
C	4.61755	4.14639	7.37954
C	6.44877	5.81912	7.88078
C	4.96058	1.77033	7.62473
C	7.15109	0.81413	8.45802
C	13.64380	3.74929	6.61996
C	11.95157	2.04535	7.41150
C	13.43330	6.09215	7.15627
C	11.44847	7.00659	8.42299
H	8.37242	6.04763	−0.73931
C	10.94398	8.74835	4.75439
C	8.54026	8.22958	4.16779
C	12.76784	7.37113	3.97482
C	12.38820	5.36309	2.48124
C	5.84633	1.14132	2.67201
C	7.99772	1.63418	1.44956
C	4.58736	2.85928	3.80376
C	5.37084	5.25895	3.88629
H	3.97044	4.99620	7.10695
C	4.10614	2.83822	7.29801
H	7.28516	5.96743	7.16405
H	6.85810	6.05596	8.88401
H	5.65720	6.55392	7.63941
H	4.59039	0.73580	7.53868
H	6.71744	−0.14043	8.10663
H	7.29130	0.75084	9.55718
H	8.16550	0.91576	8.02120
H	14.20231	2.91973	6.15625
C	14.15243	5.05891	6.53237
H	10.99884	1.90537	6.85521
H	11.73777	1.77632	8.46579
H	12.68579	1.32539	7.00254
H	13.82016	7.12119	7.10845
H	12.04591	7.93845	8.41608
H	11.12306	6.80116	9.46134
H	10.52669	7.18945	7.82825
H	10.57697	9.60949	5.33647

C	12.32613	8.48047	4.71494
H	8.07131	8.28731	3.16480
H	8.34239	9.17455	4.70849
H	8.01754	7.41002	4.70763
H	13.84460	7.14260	3.94119
H	11.84102	4.43335	2.73774
H	13.46650	5.19455	2.66691
H	12.24448	5.51257	1.39116
H	5.97034	0.08776	2.37445
C	4.72773	1.50927	3.44143
H	7.93155	2.03237	0.41561
H	8.05250	0.53039	1.38916
H	8.95305	2.00341	1.87276
H	3.70823	3.17372	4.38514
H	5.64347	5.97020	3.08149
H	6.02767	5.48795	4.75479
H	4.32965	5.45835	4.20391
C	2.66692	2.59013	6.92315
C	15.43209	5.33511	5.78420
C	13.29784	9.37498	5.44175
C	3.74674	0.46528	3.90540
H	2.24661	3.42183	6.32345
H	2.03533	2.49519	7.83284
H	2.54869	1.65154	6.34792
H	15.31670	5.11458	4.70144
H	16.26332	4.69792	6.15069
H	15.74432	6.39302	5.88107
H	14.33341	8.98732	5.38622
H	13.02667	9.48058	6.51278
H	13.29804	10.39878	5.01167
H	3.65611	−0.36521	3.17770
H	2.73861	0.89041	4.07747
H	4.09536	0.02032	4.86285

6.10.24 3PCO (trans exo)

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.33229	5.50591	5.66155
P	11.90949	3.62497	4.52510
N	11.14779	3.96468	6.08153
N	10.75879	4.87843	4.02347
H	8.98587	5.00433	5.82247
P	13.86705	4.94726	4.94956
C	11.26025	3.32719	7.31773
C	10.59748	5.56457	2.81245
C	14.90946	3.71464	4.52931
C	11.66009	1.95967	7.39962
C	10.92718	4.01804	8.52158
C	9.60752	6.59282	2.72952
C	11.35005	5.24727	1.64095
O	15.68892	2.86959	4.25921
C	11.74420	1.33726	8.65879
C	11.94507	1.13649	6.18748
C	11.00841	3.35077	9.75676
C	10.50906	5.45250	8.51034
C	9.45092	7.32345	1.53751
C	8.63005	6.85960	3.83000
C	11.14525	5.99674	0.46596
C	12.33772	4.12982	1.56840
H	12.04829	0.27965	8.69156
C	11.42245	2.01577	9.84043
C	10.87375	0.69092	5.36548
C	13.27770	0.73499	5.90310
H	10.74822	3.91298	10.66711
C	11.50247	6.47314	8.52543
C	9.13194	5.79498	8.56870
H	8.67703	8.10614	1.50911
C	10.21986	7.04367	0.40262
C	7.53937	5.95705	4.00187
C	8.69164	8.05103	4.60390
H	11.73331	5.72393	−0.42360
C	13.72244	4.43118	1.43504
C	11.89505	2.78141	1.49718
H	11.48602	1.50777	10.81377
C	11.15636	−0.16475	4.28754
C	9.45886	1.14138	5.62789
C	13.51247	−0.10874	4.80292
C	14.42594	1.19492	6.76687
C	11.09388	7.81502	8.55122
C	12.96169	6.11112	8.49113
C	8.77156	7.15477	8.59552

C	8.07109	4.72264	8.60099
H	10.07844	7.61339	−0.52738
C	6.54812	6.25530	4.95085
C	7.45920	4.69273	3.18611
C	7.66622	8.31295	5.53046
C	9.87232	8.98092	4.50524
C	14.63546	3.37624	1.29054
C	14.21585	5.85609	1.45664
C	12.84902	1.75893	1.34361
C	10.43335	2.43018	1.60578
H	10.32325	−0.51912	3.65853
C	12.46557	−0.58912	3.99659
H	9.33644	2.21981	5.38508
H	9.18680	1.03130	6.69721
H	8.73380	0.57084	5.01664
H	14.54884	−0.40945	4.57862
H	15.39519	1.02617	6.26244
H	14.44236	0.65839	7.73846
H	14.34179	2.27395	7.00713
H	11.86392	8.60366	8.55040
C	9.73364	8.17850	8.57854
H	13.23116	5.61985	7.53011
H	13.21823	5.38543	9.28912
H	13.60368	7.00553	8.60299
H	7.70393	7.42056	8.62904
H	7.06593	5.14757	8.41507
H	8.05099	4.20564	9.58329
H	8.26272	3.93523	7.84449
H	5.71163	5.54975	5.08400
C	6.58819	7.43250	5.72194
H	7.52966	4.90843	2.10052
H	6.51567	4.14768	3.37870
H	8.30668	4.01363	3.41965
H	7.72049	9.23344	6.13220
H	10.74754	8.52179	5.01635
H	9.66317	9.95162	4.99462
H	10.17703	9.16872	3.45819
H	15.70996	3.61006	1.22277
C	14.22366	2.03124	1.25937
H	13.97352	6.38835	0.51312
H	15.31342	5.89198	1.59492
H	13.74580	6.43131	2.27844
H	12.50145	0.71650	1.29472
H	9.78826	3.17185	1.09530
H	10.11616	2.40055	2.67223
H	10.23092	1.42758	1.18254
C	12.73524	−1.57186	2.88537
C	9.33200	9.63150	8.58310
C	5.49882	7.73395	6.71965
C	15.24182	0.92344	1.19941
H	11.93192	−1.56269	2.12223
H	12.79535	−2.60836	3.28223
H	13.69845	−1.36335	2.38023
H	9.59679	10.11928	7.62102
H	9.85749	10.19514	9.38116
H	8.24251	9.75642	8.73618
H	5.70881	8.66043	7.28840
H	5.37695	6.90533	7.44840
H	4.51662	7.86115	6.21767
H	16.14157	1.22299	0.62643
H	14.82819	0.00282	0.74301
H	15.58245	0.66986	2.22703

6.10.25 3P(H)CO

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	3.40992	6.60296	4.99547
P	5.60132	5.15911	5.71462
N	3.78359	5.17349	5.87487
N	5.10940	6.49941	4.55727
P	6.20079	6.73804	7.15531
C	4.62277	7.79267	7.54575
C	2.96890	4.19082	6.47228
C	5.92441	7.41517	3.88205
C	3.24934	2.81523	6.22759
C	1.85704	4.54503	7.28940
C	5.34666	8.57520	3.27717
C	7.33251	7.19833	3.75462
C	2.49053	1.83125	6.89169
C	4.20826	2.35365	5.17748
C	1.11108	3.52786	7.91478

C	1.44802	5.96763	7.48897
C	6.17537	9.52002	2.65022
C	3.86666	8.77241	3.25939
C	8.12045	8.17797	3.11986
C	7.99367	5.93180	4.19398
H	2.71727	0.77345	6.68688
C	1.43468	2.17625	7.74406
C	3.82572	2.46859	3.81182
C	5.40449	1.67560	5.52440
H	0.25859	3.82293	8.54563
C	1.88380	6.66067	8.64932
C	0.58952	6.60351	6.55631
H	5.70213	10.40471	2.19709
C	7.56339	9.34273	2.58053
C	3.08011	8.03093	2.32881
C	3.24656	9.70655	4.13192
H	9.20095	7.99034	3.02944
C	7.73244	4.72818	3.47634
C	8.96961	5.93391	5.23279
H	0.84612	1.39391	8.24605
C	4.64210	1.88701	2.82658
C	2.55651	3.17965	3.41553
C	6.18017	1.09714	4.50453
C	5.87874	1.62609	6.95419
C	1.49650	7.99610	8.82895
C	2.79389	5.98297	9.64059
C	0.23829	7.95072	6.77273
C	0.05151	5.87948	5.34451
H	8.19997	10.08983	2.08460
C	1.68704	8.20079	2.32934
C	3.73109	7.05803	1.37943
C	1.84371	9.82206	4.11138
C	4.06286	10.57091	5.05718
C	8.39900	3.54920	3.85156
C	6.76298	4.70440	2.32359
C	9.56812	4.71785	5.60356
C	9.39429	7.20723	5.91995
H	4.33756	1.97162	1.77033
C	5.81595	1.18338	3.15017
H	2.62880	4.27407	3.60093
H	1.68718	2.82364	4.00456

H	2.33487	3.03558	2.34073
H	7.10696	0.56784	4.77942
H	5.09130	1.28376	7.65347
H	6.17833	2.64394	7.28912
H	6.75919	0.96407	7.06501
H	1.86385	8.53960	9.71394
C	0.69590	8.66916	7.88713
H	3.05857	6.66138	10.47305
H	3.73766	5.66305	9.15184
H	2.33433	5.06462	10.06077
H	-0.41535	8.45121	6.04122
H	0.67138	6.09532	4.44554
H	-0.98171	6.20838	5.11519
H	0.04424	4.78184	5.48371
H	1.08117	7.62442	1.61104
C	1.04597	9.07826	3.22563
H	4.15569	6.18933	1.92568
H	4.57655	7.52499	0.83540
H	3.00375	6.67022	0.64103
H	1.36031	10.51876	4.81475
H	4.46340	11.45489	4.51610
H	4.93301	10.02709	5.46887
H	3.45096	10.93770	5.90305
H	8.20244	2.62946	3.28346
C	9.28984	3.51089	4.93520
H	6.91233	3.80593	1.69585
H	6.85713	5.60777	1.68926
H	5.71456	4.67059	2.68898
H	10.29022	4.71749	6.43654
H	9.78600	6.99850	6.93462
H	8.56016	7.92757	6.01119
H	10.20482	7.71103	5.35036
C	6.66393	0.56241	2.06871
C	0.38182	10.13421	8.05042
C	-0.45603	9.20729	3.22414
C	9.90704	2.21040	5.38171
H	7.06923	1.33468	1.37989
H	6.07625	-0.14135	1.44349
H	7.52304	0.00620	2.49144
H	1.24646	10.75323	7.72499
H	0.17853	10.39838	9.10769

H	-0.49217	10.43916	7.44163
H	-0.84310	9.41770	2.20592
H	-0.79897	10.01774	3.89574
H	-0.93586	8.26394	3.56004
H	9.25653	1.70600	6.12949
H	10.89501	2.36293	5.85939
H	10.03337	1.50624	4.53539
O	3.76937	7.98834	6.67540
H	6.19106	5.99788	8.38712

6.10.26 3PC(H)O

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	3.43592	6.71197	5.17797
P	5.52765	5.07931	5.54621
O	4.00034	7.81164	6.45303
N	3.74422	5.14075	5.82674
N	5.04315	6.43459	4.45274
P	6.08648	6.21017	7.44191
C	4.94963	7.50474	7.34384
H	4.97303	8.25939	8.15916
C	2.90362	4.18006	6.41209
C	5.85067	7.37670	3.80406
C	3.08729	2.80678	6.08094
C	1.86208	4.55126	7.31121
C	5.24940	8.49035	3.13773
C	7.26937	7.23047	3.74598
C	2.28482	1.83438	6.70781
C	4.03577	2.37345	5.01053
C	1.06642	3.54881	7.89601
C	1.60412	5.98687	7.62927
C	6.06044	9.44467	2.50031
C	3.76419	8.62003	3.07578
C	8.04215	8.21075	3.09522
C	7.95275	6.02920	4.31026
H	2.43832	0.77837	6.43623
C	1.28101	2.19272	7.61668
C	3.69587	2.60339	3.65169
C	5.23085	1.67967	5.33706
H	0.26639	3.85572	8.58740
C	2.18670	6.56622	8.78634
C	0.76170	6.75969	6.78778
H	5.56795	10.28785	1.99160
C	7.45596	9.32353	2.48127
C	3.02495	7.74901	2.22626
C	3.08802	9.58942	3.86617
H	9.13354	8.07045	3.06260
C	7.88039	4.78978	3.61023
C	8.74659	6.13370	5.48857
H	0.65487	1.42057	8.08779
C	4.54910	2.11303	2.64551
C	2.44856	3.36470	3.27795
C	6.04772	1.20277	4.29914
C	5.65728	1.51887	6.77441
C	1.98876	7.93604	9.02958
C	3.00522	5.72397	9.73146
C	0.60028	8.13010	7.06764
C	0.04867	6.13321	5.61437
H	8.07724	10.07552	1.97335
C	1.62309	7.82725	2.22760
C	3.73035	6.72683	1.37242
C	1.68178	9.62510	3.83596
C	3.85190	10.54142	4.75089
C	8.53910	3.66913	4.14066
C	7.08535	4.66661	2.33767
C	9.34747	4.97140	6.00435
C	8.97653	7.46533	6.15785
H	4.28029	2.28801	1.59078
C	5.72239	1.40008	2.94450
H	2.55901	4.44439	3.51523
H	1.56442	3.00934	3.84415
H	2.23375	3.27943	2.19547
H	6.97534	0.66717	4.55988
H	4.87466	1.04314	7.39752
H	5.85930	2.51214	7.23179
H	6.58274	0.91644	6.85473
H	2.45593	8.39009	9.91904
C	1.22768	8.74370	8.16387
H	3.39675	6.32822	10.57235
H	3.87009	5.26502	9.21035
H	2.40616	4.88965	10.15050

H	-0.03430	8.73480	6.40032
H	0.74314	5.97559	4.76096
H	-0.76787	6.78603	5.25195
H	-0.37539	5.14368	5.87474
H	1.05191	7.14131	1.58061
C	0.92974	8.75098	3.03264
H	4.20554	5.94597	2.00258
H	4.54638	7.18719	0.77995
H	3.02668	6.22731	0.67943
H	1.15843	10.35816	4.47099
H	4.44124	11.26756	4.15426
H	4.56888	9.99571	5.39414
H	3.16435	11.11194	5.40470
H	8.47535	2.71346	3.59877
C	9.24349	3.72734	5.35558
H	7.40480	3.78494	1.75110
H	7.17240	5.57258	1.70702
H	6.00707	4.52712	2.56735
H	9.92287	5.04469	6.94129
H	9.31737	7.33260	7.20220
H	8.05881	8.08385	6.16642
H	9.75421	8.04624	5.61685
C	6.60452	0.85138	1.85137
C	1.11801	10.23070	8.38413
C	-0.57558	8.82780	3.00049
C	9.84461	2.48179	5.95484
H	7.67727	1.05665	2.04871
H	6.35022	1.28370	0.86401
H	6.50312	-0.25190	1.76846
H	1.92924	10.76230	7.83970
H	1.21396	10.49864	9.45494
H	0.15597	10.63323	8.00935
H	-0.92194	9.51521	2.19861
H	-0.98616	9.21124	3.95562
H	-1.03134	7.83817	2.79955
H	9.07791	1.91793	6.52986
H	10.67166	2.71617	6.65321
H	10.23038	1.79709	5.17326

6.10.27 3PCO(H)

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	3.35987	6.51272	4.91798
P	5.55828	5.08228	5.58641
N	3.70140	5.11197	5.78973
N	5.02045	6.45184	4.45371
P	5.97583	6.17199	7.51109
C	4.85374	7.48760	7.67195
C	2.85855	4.15029	6.38175
C	5.81108	7.39359	3.79542
C	3.03857	2.77815	6.05203
C	1.82272	4.53384	7.28208
C	5.20981	8.49784	3.11401
C	7.23196	7.25302	3.75808
C	2.21765	1.81388	6.66808
C	4.00246	2.34204	4.99665
C	1.00586	3.54128	7.85226
C	1.62811	5.97165	7.63341
C	6.02148	9.45696	2.48641
C	3.72543	8.61066	3.02355
C	8.00440	8.23867	3.11646
C	7.91787	6.05230	4.32316
H	2.36490	0.75603	6.40082
C	1.20599	2.18437	7.56339
C	3.66578	2.53189	3.63176
C	5.21296	1.68937	5.34933
H	0.20915	3.85227	8.54543
C	2.23894	6.49278	8.80162
C	0.85645	6.81127	6.78589
H	5.53069	10.29561	1.96867
C	7.41848	9.34629	2.49160
C	3.01653	7.75616	2.13117
C	3.02005	9.55123	3.82108
H	9.09690	8.10573	3.09627
C	7.85711	4.81638	3.61602
C	8.71104	6.15991	5.50263
H	0.56553	1.41810	8.02495
C	4.54558	2.05257	2.64271
C	2.39398	3.23609	3.22926

C	6.05439	1.22004	4.32813
C	5.62465	1.56358	6.79401
C	2.16039	7.87752	9.04582
C	2.99318	5.59247	9.74215
C	0.81361	8.19172	7.05992
C	0.06957	6.23168	5.63646
H	8.04197	10.10189	1.99194
C	1.61424	7.83024	2.08802
C	3.75639	6.76290	1.27198
C	1.61513	9.58683	3.74211
C	3.75325	10.49213	4.74382
C	8.53298	3.70065	4.13838
C	7.05740	4.68638	2.34683
C	9.32980	5.00393	6.00657
C	8.88700	7.48389	6.19884
H	4.28127	2.19719	1.58223
C	5.73841	1.38511	2.96661
H	2.47191	4.33442	3.39407
H	1.52478	2.89086	3.82384
H	2.17065	3.08028	2.15622
H	6.99524	0.71857	4.60804
H	4.84294	1.08322	7.41515
H	5.80161	2.56889	7.23580
H	6.56061	0.98128	6.89659
H	2.67239	8.28577	9.92988
C	1.48340	8.75143	8.16878
H	3.37636	6.15715	10.61234
H	3.86659	5.14124	9.22789
H	2.35599	4.76044	10.10468
H	0.24483	8.84962	6.38445
H	0.71785	5.70689	4.90340
H	-0.47825	7.02063	5.08886
H	-0.66139	5.47990	5.99870
H	1.06766	7.15907	1.40546
C	0.89192	8.73352	2.89078
H	4.24233	5.98070	1.89274
H	4.57027	7.25206	0.69995
H	3.07420	6.25980	0.56062
H	1.06830	10.30822	4.37110
H	4.24465	11.30874	4.17450
H	4.55346	9.97055	5.30290
H	3.05983	10.96024	5.46993
H	8.47874	2.74709	3.59182
C	9.24169	3.76180	5.34894
H	7.39737	3.82031	1.74824
H	7.11527	5.60082	1.72480
H	5.98533	4.51172	2.58351
H	9.90168	5.07824	6.94533
H	9.34920	7.35050	7.19499
H	7.91415	7.99552	6.33984
H	9.53232	8.16589	5.60604
C	6.64933	0.84585	1.89264
C	1.44622	10.23613	8.44097
C	-0.61176	8.80906	2.80774
C	9.86060	2.52267	5.94319
H	7.71223	1.09256	2.09538
H	6.38971	1.24922	0.89448
H	6.58744	-0.26175	1.83166
H	2.46288	10.63651	8.63459
H	0.83651	10.46529	9.34042
H	1.01101	10.79652	7.59037
H	-0.93141	9.44978	1.95770
H	-1.05206	9.24389	3.72671
H	-1.06279	7.80980	2.64587
H	9.13165	2.00290	6.60290
H	10.74776	2.75992	6.56285
H	10.16394	1.79985	5.15985
O	4.06463	7.91237	6.63986
H	3.29404	8.41170	7.01723

6.10.28 3HOCP cis endo

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	10.06523	5.32365	5.63048
P	8.25353	3.33314	5.33909
N	9.28402	3.99676	6.55641
N	8.90800	4.63473	4.40260
H	11.22933	4.62916	5.14229
C	9.31799	3.79183	7.94704
C	8.72810	5.00682	3.05939

C	10.52813	1.93311	4.20551
C	8.13959	3.46600	8.67081
C	10.55179	3.95348	8.63850
C	9.45241	6.11207	2.52847
C	7.80908	4.31382	2.21846
C	8.23524	3.23609	10.05809
C	6.78182	3.46377	8.04627
C	10.59958	3.73838	10.02663
C	11.78218	4.33061	7.88179
C	9.30200	6.45267	1.17126
C	10.33073	6.97143	3.38119
C	7.69293	4.68577	0.86759
C	6.92284	3.23736	2.75100
H	7.31447	2.98637	10.60758
C	9.45248	3.36282	10.73909
C	6.14935	4.70673	7.76969
C	6.08728	2.24683	7.82746
H	11.56453	3.85865	10.54268
C	12.50359	3.31946	7.19082
C	12.22542	5.67949	7.85245
H	9.87528	7.31053	0.78711
C	8.44087	5.74010	0.32905
C	9.74746	8.03243	4.13472
C	11.74238	6.80453	3.35794
H	6.97927	4.13089	0.23946
C	7.21916	1.86933	2.50579
C	5.73842	3.60000	3.44919
H	9.50302	3.18641	11.82373
C	4.81718	4.70540	7.32182
C	6.88928	6.00850	7.95059
C	4.75032	2.29620	7.39566
C	6.78759	0.92194	7.99842
C	13.62854	3.68714	6.43608
C	12.05941	1.88332	7.27159
C	13.36795	5.99707	7.09251
C	11.48116	6.75800	8.60135
H	8.33780	6.01653	-0.73039
C	10.58274	8.87924	4.87738
C	8.25149	8.19868	4.18049
C	12.53702	7.67191	4.13022
C	12.37168	5.70799	2.54177

C	6.36426	0.88860	3.03880
C	8.40408	1.47130	1.66678
C	4.89527	2.58450	3.92686
C	5.40688	5.04887	3.70133
H	4.32599	5.67106	7.11792
C	4.08992	3.51315	7.15417
H	7.69742	6.12040	7.19539
H	7.38465	6.06368	8.94104
H	6.20993	6.87603	7.84654
H	4.20973	1.34996	7.23411
H	6.09233	0.07544	7.83888
H	7.24585	0.81381	9.00135
H	7.61594	0.82194	7.26348
H	14.16565	2.90623	5.87513
C	14.07287	5.02216	6.36694
H	11.02191	1.76438	6.90169
H	12.06438	1.52611	8.32238
H	12.70804	1.22627	6.66411
H	13.70760	7.04385	7.06007
H	11.98333	7.73828	8.49078
H	11.40147	6.52682	9.68258
H	10.44297	6.86447	8.22254
H	10.12774	9.68942	5.47012
C	11.98053	8.70865	4.89832
H	7.80245	8.17449	3.16772
H	7.96436	9.14488	4.67730
H	7.78531	7.36429	4.74952
H	13.62898	7.53022	4.12838
H	12.01787	4.70284	2.86211
H	13.47466	5.72283	2.63010
H	12.10542	5.79522	1.46920
H	6.61325	-0.17264	2.87641
C	5.20411	1.22304	3.75901
H	8.19540	1.64290	0.58908
H	8.64648	0.39974	1.79788
H	9.31211	2.05606	1.91032
H	3.97487	2.86614	4.45703
H	5.45558	5.65026	2.77122
H	6.13143	5.50397	4.41053
H	4.39973	5.15738	4.14632
C	2.63996	3.54805	6.74057

C	15.26646	5.38426	5.52037
C	12.84906	9.61450	5.73341
C	4.32870	0.14794	4.35067
H	2.46132	4.28896	5.93441
H	1.98851	3.83985	7.59211
H	2.29087	2.55935	6.38339
H	15.04699	5.22715	4.44292
H	16.14347	4.74924	5.76148
H	15.56178	6.44283	5.65642
H	13.92566	9.40704	5.57986
H	12.63076	9.48864	6.81516
H	12.66806	10.68294	5.49493
H	4.18190	-0.69586	3.64659
H	3.33264	0.54029	4.63460
H	4.79294	-0.27518	5.26760
O	9.43321	1.80008	4.81380
P	11.90947	2.03086	3.41409

6.10.29 3HOCP trans endo

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.29655	5.05638	5.50069
P	8.10912	3.46254	5.39405
N	9.26328	4.00100	6.55918
N	8.88709	4.65635	4.41320
H	9.78441	6.28874	6.07472
C	9.34044	3.77543	7.94179
C	8.75515	4.97299	3.04861
C	10.25718	1.87959	4.32189
C	8.17856	3.42732	8.68626
C	10.57969	3.94550	8.62281
C	9.53006	6.04009	2.51045
C	7.83834	4.28321	2.20294
C	8.29657	3.18296	10.06816
C	6.81178	3.42310	8.08263
C	10.65000	3.71363	10.00723
C	11.79740	4.35785	7.86673
C	9.44439	6.33443	1.13702
C	10.37944	6.92307	3.36968
C	7.78435	4.61383	0.83644
C	6.88643	3.25706	2.72481
H	7.38544	2.91549	10.62537
C	9.52139	3.31406	10.73465
C	6.16053	4.66715	7.85784
C	6.13764	2.20529	7.81106
H	11.62153	3.84439	10.50821
C	12.55899	3.36500	7.19036
C	12.19674	5.72049	7.83537
H	10.05475	7.16260	0.74505
C	8.59034	5.61950	0.28957
C	9.75291	7.95551	4.12643
C	11.79829	6.82227	3.34045
H	7.07103	4.06647	0.20154
C	7.10749	1.87590	2.46431
C	5.70889	3.67404	3.40405
H	9.59095	3.12480	11.81590
C	4.83122	4.66514	7.40342
C	6.88740	5.96890	8.08676
C	4.80162	2.25311	7.37436
C	6.86083	0.88651	7.92379
C	13.67543	3.76611	6.44271
C	12.16322	1.91628	7.28982
C	13.33076	6.07228	7.07901
C	11.42726	6.77413	8.59500
H	8.53269	5.86228	-0.78156
C	10.55478	8.84567	4.86024
C	8.25089	8.07772	4.15134
C	12.55774	7.74177	4.08503
C	12.47083	5.71142	2.58085
C	6.18482	0.93906	2.95802
C	8.29029	1.41757	1.65334
C	4.79831	2.69983	3.84726
C	5.44739	5.13036	3.69265
H	4.32534	5.63049	7.23731
C	4.12396	3.46906	7.18071
H	7.71254	6.09923	7.35320
H	7.35784	6.00296	9.09038
H	6.20532	6.83470	7.98669
H	4.27589	1.30645	7.17155
H	6.17337	0.03492	7.75815

H	7.34856	0.75852	8.91021
H	7.66773	0.82141	7.16160
H	14.24698	3.00028	5.89488
C	14.07261	5.11533	6.36598
H	11.12101	1.76116	6.94754
H	12.20716	1.56794	8.34300
H	12.81563	1.27530	6.66948
H	13.63626	7.12941	7.03997
H	11.70560	7.79155	8.25870
H	11.62525	6.70878	9.68581
H	10.33196	6.65572	8.47347
H	10.06580	9.63667	5.45213
C	11.95949	8.75453	4.85514
H	7.83233	8.12967	3.12569
H	7.92808	8.97579	4.71158
H	7.78611	7.18876	4.62848
H	13.65518	7.65346	4.07202
H	12.22013	4.72715	3.03593
H	13.57163	5.82431	2.59065
H	12.13111	5.65965	1.52810
H	6.37613	-0.13198	2.78224
C	5.02845	1.32726	3.65826
H	8.13549	1.63143	0.57435
H	8.44951	0.32796	1.76190
H	9.22745	1.92944	1.94713
H	3.88487	3.02631	4.36456
H	5.74569	5.78359	2.84954
H	6.02609	5.46352	4.58310
H	4.37905	5.30649	3.92288
C	2.67300	3.50065	6.77095
C	15.26021	5.51182	5.52670
C	12.79352	9.71415	5.66556
C	4.07668	0.29272	4.20277
H	2.47727	4.28903	6.01569
H	2.01901	3.72309	7.64142
H	2.34249	2.53027	6.35184
H	15.04770	5.35984	4.44734
H	16.15028	4.89451	5.76571
H	15.53083	6.57562	5.67263
H	13.87681	9.55131	5.50532
H	12.59222	9.60117	6.75217
H	12.56389	10.76898	5.40869
H	3.85819	-0.49697	3.45550
H	3.11629	0.74434	4.51928
H	4.51434	-0.21660	5.08828
O	9.12768	1.75740	4.85449
P	11.68258	2.03414	3.61915

6.10.30 3HPCO cis endo

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	10.12363	5.26585	5.62254
P	8.16733	3.39297	5.40128
N	9.25325	4.06285	6.60809
N	8.92044	4.64303	4.42064
H	11.23775	4.46234	5.16169
P	9.22864	1.26947	4.96841
C	9.33314	3.86722	7.99081
C	8.78766	4.96352	3.06469
C	10.41358	1.92684	4.00271
C	8.19736	3.45137	8.74337
C	10.56494	4.11190	8.66690
C	9.59231	5.99940	2.50025
C	7.85172	4.29061	2.22162
O	11.23076	2.35008	3.25610
C	8.32712	3.25304	10.13157
C	6.83929	3.29838	8.13984
C	10.64299	3.92432	10.05848
C	11.79386	4.52016	7.91923
C	9.50626	6.28428	1.12597
C	10.48425	6.86192	3.33466
C	7.80187	4.61038	0.85144
C	6.87423	3.28198	2.73038
H	7.43494	2.93862	10.69501
C	9.53666	3.48559	10.79747
C	6.08416	4.45857	7.81821
C	6.26447	2.00962	7.98542
H	11.60690	4.11388	10.55572
C	12.58544	3.51502	7.29454
C	12.21227	5.87738	7.89116

H	10.14076	7.08995	0.72514
C	8.62807	5.58832	0.28732
C	9.91599	7.95717	4.04921
C	11.89178	6.66822	3.32839
H	7.07181	4.07365	0.22659
C	7.01168	1.91290	2.37407
C	5.72914	3.71392	3.45975
H	9.61402	3.33444	11.88420
C	4.75690	4.30641	7.38208
C	6.69428	5.83239	7.93354
C	4.93218	1.90767	7.54820
C	7.06968	0.76590	8.27166
C	13.75143	3.89619	6.61092
C	12.17509	2.06954	7.36784
C	13.39838	6.20709	7.20828
C	11.38450	6.95888	8.53788
H	8.57084	5.82192	-0.78574
C	10.76248	8.81830	4.76169
C	8.42316	8.15191	4.08018
C	12.69879	7.55532	4.06462
C	12.51101	5.52896	2.56019
C	6.04201	0.99513	2.81578
C	8.14888	1.43082	1.50899
C	4.77144	2.76472	3.84829
C	5.54533	5.16198	3.83398
H	4.17017	5.20894	7.14445
C	4.15276	3.04220	7.26111
H	7.49835	5.97552	7.17960
H	7.17047	5.98563	8.92316
H	5.93732	6.62480	7.77902
H	4.48667	0.90532	7.43780
H	6.51513	-0.14576	7.97759
H	7.32844	0.67916	9.34677
H	8.03496	0.77416	7.72362
H	14.35340	3.11670	6.11608
C	14.17464	5.23792	6.55211
H	11.21754	1.89404	6.83163
H	12.00855	1.75181	8.41718
H	12.93933	1.40966	6.91479
H	13.71824	7.25983	7.18297
H	11.93066	7.92155	8.56087
H	11.08905	6.69452	9.57203
H	10.44438	7.11602	7.96568
H	10.31864	9.65756	5.32175
C	12.15806	8.63270	4.78616
H	7.98409	8.11882	3.06299
H	8.15015	9.11274	4.55648
H	7.93499	7.33608	4.65689
H	13.78846	7.39786	4.07128
H	12.06377	4.55244	2.83523
H	13.60191	5.47310	2.73988
H	12.34694	5.64212	1.46884
H	6.16993	-0.07059	2.56570
C	4.91824	1.39654	3.55645
H	7.87487	1.49035	0.43325
H	8.39342	0.37441	1.73175
H	9.06394	2.03759	1.63585
H	3.88405	3.10619	4.40057
H	5.85113	5.84408	3.01647
H	6.16746	5.41830	4.72013
H	4.49372	5.37423	4.10568
C	2.70097	2.90880	6.87575
C	15.42916	5.61137	5.80384
C	13.03992	9.57368	5.56696
C	3.90982	0.38972	4.04756
H	2.35456	3.77154	6.27250
H	2.05446	2.86395	7.77878
H	2.51349	1.98290	6.29744
H	15.32373	5.40104	4.71825
H	16.30199	5.02440	6.15723
H	15.67139	6.68569	5.91853
H	14.10845	9.29467	5.48860
H	12.76642	9.57999	6.64304
H	12.93403	10.61813	5.20623
H	3.95435	-0.55368	3.46929
H	2.87544	0.78450	3.98936
H	4.10064	0.13447	5.11243

6.10.31 3HPCO trans endo

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	10.29270	5.02719	5.50308
P	8.07835	3.47376	5.42377
N	9.21479	4.09821	6.60670
N	8.88355	4.67670	4.41943
H	9.91954	6.32792	6.01841
P	9.04179	1.28584	5.01691
C	9.36019	3.79262	7.96051
C	8.79529	4.93756	3.04569
C	10.30069	1.89349	4.11459
C	8.24447	3.33010	8.72128
C	10.61255	3.97962	8.61702
C	9.63444	5.94404	2.47869
C	7.86747	4.25979	2.19824
O	11.17641	2.29939	3.42713
C	8.41892	3.01973	10.08293
C	6.86703	3.24776	8.14910
C	10.73627	3.67525	9.98403
C	11.80904	4.48332	7.87806
C	9.60047	6.18515	1.09381
C	10.49441	6.83303	3.31943
C	7.86502	4.54211	0.81830
C	6.85266	3.28679	2.70337
H	7.54149	2.67288	10.65035
C	9.65332	3.18280	10.72343
C	6.14455	4.44545	7.88857
C	6.24651	1.98605	7.94736
H	11.71700	3.82498	10.46172
C	12.65572	3.55907	7.20270
C	12.13498	5.86498	7.90564
H	10.26036	6.96763	0.68812
C	8.73225	5.48161	0.25093
C	9.88220	7.90968	4.02463
C	11.91016	6.69785	3.31667
H	7.13945	4.00691	0.18706
C	6.95859	1.91042	2.36052
C	5.71100	3.75301	3.41558
H	9.76590	2.94352	11.79096
C	4.81383	4.35515	7.44706
C	6.79321	5.79544	8.06128
C	4.91123	1.94749	7.50769
C	7.00054	0.70216	8.19227
C	13.79279	4.04349	6.54006
C	12.31904	2.09323	7.19231
C	13.28845	6.30283	7.22787
C	11.26805	6.84925	8.65220
H	8.71066	5.68465	-0.82968
C	10.69450	8.81440	4.72790
C	8.38333	8.06507	4.02606
C	12.68099	7.63676	4.02451
C	12.56890	5.53822	2.61725
C	5.95927	1.02252	2.79436
C	8.10250	1.39027	1.52670
C	4.72535	2.83045	3.80262
C	5.55074	5.20761	3.77572
H	4.25579	5.28567	7.25179
C	4.17054	3.11735	7.26632
H	7.55372	5.97168	7.26966
H	7.32914	5.87003	9.02904
H	6.04730	6.61104	8.00485
H	4.43268	0.96605	7.35611
H	6.44743	-0.16759	7.78855
H	7.17000	0.52512	9.27455
H	8.00481	0.72441	7.72159
H	14.43885	3.32861	6.00506
C	14.12766	5.41137	6.53928
H	11.32366	1.91010	6.73390
H	12.26061	1.68719	8.22306
H	13.06897	1.51023	6.62483
H	13.53675	7.37534	7.23948
H	11.53083	7.89249	8.39059
H	11.38013	6.73053	9.75045
H	10.19150	6.69657	8.43624
H	10.21576	9.64016	5.27943
C	12.09716	8.69786	4.73827
H	7.98091	8.09807	2.99301
H	8.07311	8.98563	4.55608
H	7.89309	7.19893	4.51892
H	13.77602	7.52582	4.02803

H	12.22990	4.57479	3.05338
H	13.67089	5.58988	2.70685
H	12.30692	5.50028	1.54129
H	6.06293	-0.04813	2.55441
C	4.83788	1.45803	3.52061
H	7.87622	1.48458	0.44258
H	8.28735	0.31922	1.73620
H	9.03988	1.94932	1.70307
H	3.84222	3.19961	4.34438
H	5.92996	5.87803	2.97998
H	6.11917	5.44594	4.70256
H	4.49058	5.45344	3.97803
C	2.71723	3.04908	6.87009
C	15.36411	5.89151	5.82275
C	12.94187	9.68987	5.49715
C	3.80004	0.47985	4.00823
H	2.41268	3.93033	6.27092
H	2.06305	3.02705	7.76850
H	2.49413	2.13615	6.28405
H	15.32444	5.64006	4.74218
H	16.27690	5.40719	6.22822
H	15.49287	6.98732	5.91453
H	14.01900	9.44059	5.43876
H	12.65723	9.72439	6.56988
H	12.81039	10.71860	5.10085
H	3.80059	-0.45318	3.41152
H	2.78027	0.91321	3.97465
H	3.99833	0.19562	5.06450

6.10.32 3HOCP trans exo

	PBE−D3BJ/def2−SVP		
Atom	x	y	z
P	10.20189	4.97966	5.46758
P	8.02637	3.41532	5.36844
N	9.14835	3.99399	6.54778
N	8.74441	4.68460	4.42190
H	9.84847	6.24596	6.07413
C	9.25865	3.72842	7.92018
C	8.62933	4.99012	3.05328
C	9.08209	0.79207	5.02593
C	8.09521	3.44194	8.68947
C	10.52594	3.81140	8.56157
C	9.42127	6.04215	2.51070
C	7.71174	4.30173	2.20879
C	8.23937	3.16828	10.06293
C	6.72115	3.52658	8.10789
C	10.62247	3.54358	9.93862
C	11.73863	4.21601	7.78921
C	9.33385	6.33595	1.13664
C	10.28814	6.90246	3.37425
C	7.65295	4.63127	0.84309
C	6.79683	3.25635	2.75285
H	7.33116	2.95496	10.64736
C	9.49110	3.20275	10.69110
C	6.17881	4.80651	7.80052
C	5.93446	2.35831	7.93060
H	11.61336	3.60511	10.41430
C	12.46801	3.24609	7.04576
C	12.16891	5.57022	7.81954
H	9.95470	7.15413	0.74009
C	8.46455	5.63264	0.29451
C	9.67678	7.92771	4.15405
C	11.70482	6.77661	3.35131
H	6.93959	4.08210	0.20974
C	7.11049	1.87966	2.58266
C	5.59540	3.64341	3.40634
H	9.58023	2.98731	11.76600
C	4.85663	4.89098	7.33309
C	7.00394	6.05961	7.95889
C	4.61227	2.49654	7.46990
C	6.50934	0.98776	8.17879
C	13.59566	3.66135	6.32077
C	12.00787	1.81442	7.00788
C	13.30332	5.93778	7.07156
C	11.42640	6.60201	8.63347
H	8.40456	5.87702	-0.77616
C	10.49094	8.78686	4.90994
C	8.17680	8.06856	4.18769
C	12.47736	7.66470	4.12154
C	12.37038	5.66194	2.58856

C	6.25564	0.91826	3.14638
C	8.33857	1.45336	1.82044
C	4.75458	2.64318	3.92301
C	5.25078	5.09963	3.59155
H	4.43851	5.88450	7.10156
C	4.04950	3.74932	7.17488
H	7.79769	6.11302	7.18314
H	7.52249	6.08786	8.93855
H	6.37772	6.96737	7.86478
H	4.00533	1.58778	7.33034
H	5.73810	0.20339	8.05593
H	6.94642	0.89026	9.19172
H	7.32812	0.76035	7.46009
H	14.15465	2.91142	5.73765
C	14.02532	5.00257	6.31157
H	11.05813	1.72138	6.44365
H	11.80649	1.42114	8.02406
H	12.75194	1.16066	6.51512
H	13.62881	6.98970	7.08320
H	11.77732	7.62492	8.39696
H	11.56560	6.43361	9.72168
H	10.33279	6.55922	8.45557
H	10.01315	9.57288	5.51735
C	11.89435	8.67095	4.91037
H	7.75112	8.12375	3.16552
H	7.86873	8.97047	4.74994
H	7.70746	7.18495	4.67111
H	13.57310	7.55597	4.11339
H	12.21397	4.69892	3.12327
H	13.46109	5.82857	2.50149
H	11.94863	5.53453	1.57348
H	6.52781	-0.14517	3.06229
C	5.08119	1.27953	3.83231
H	8.18583	1.56313	0.72570
H	8.58609	0.39607	2.03285
H	9.21527	2.07269	2.08927
H	3.82569	2.94205	4.42972
H	5.41362	5.68619	2.66561
H	5.88776	5.55922	4.37859
H	4.19855	5.22425	3.91133
C	2.61531	3.87704	6.72656
C	15.22364	5.41560	5.49534
C	12.74049	9.59834	5.74501
C	4.22472	0.22265	4.47943
H	2.50953	4.60364	5.89503
H	1.96908	4.24189	7.55359
H	2.20276	2.90551	6.39072
H	15.01469	5.32053	4.40872
H	16.10120	4.77141	5.70846
H	15.51337	6.46589	5.69299
H	13.82158	9.41093	5.59739
H	12.52026	9.47652	6.82682
H	12.54085	10.66174	5.49852
H	4.00360	-0.61016	3.78119
H	3.26383	0.63556	4.84349
H	4.75733	-0.22183	5.34770
O	9.26895	1.99439	4.69777
P	8.86815	-0.73003	5.44158

6.10.33 3HOCP cis exo

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	9.97773	5.30125	5.62137
P	8.12004	3.36281	5.33208
N	9.16004	4.01298	6.55212
N	8.75431	4.69526	4.41858
H	11.08956	4.54890	5.08303
C	9.22725	3.78068	7.93699
C	8.59272	5.05557	3.07116
C	9.24847	0.82882	4.95865
C	8.05545	3.48080	8.68355
C	10.48239	3.89253	8.59777
C	9.34928	6.13145	2.52522
C	7.66345	4.37175	2.23397
C	8.17716	3.23483	10.06556
C	6.68898	3.51296	8.07914
C	10.55621	3.65727	9.98210
C	11.71051	4.25514	7.82736
C	9.19539	6.47222	1.16805
C	10.28273	6.94716	3.36027

C	7.54083	4.74402	0.88422
C	6.80409	3.27974	2.77486
H	7.26278	3.00891	10.63544
C	9.41433	3.31277	10.71764
C	6.10012	4.76980	7.76618
C	5.94676	2.31543	7.90779
H	11.53641	3.73935	10.47651
C	12.40930	3.24547	7.10970
C	12.18556	5.59332	7.82830
H	9.79255	7.30931	0.77433
C	8.30283	5.78466	0.33780
C	9.77012	8.03555	4.12402
C	11.68106	6.69747	3.32215
H	6.81680	4.19581	0.26210
C	7.16791	1.92039	2.57365
C	5.60380	3.60991	3.46022
H	9.48513	3.12157	11.79861
C	4.77036	4.80347	7.31273
C	6.87891	6.05280	7.91694
C	4.61527	2.40258	7.46314
C	6.57932	0.96854	8.14766
C	13.54847	3.60590	6.37155
C	11.92497	1.82142	7.13943
C	13.33815	5.90338	7.08052
C	11.46304	6.67248	8.59634
H	8.19350	6.06406	-0.72024
C	10.66346	8.83638	4.85029
C	8.28570	8.27955	4.19428
C	12.53634	7.52203	4.07539
C	12.23407	5.55422	2.50968
C	6.36070	0.91665	3.13543
C	8.39529	1.55676	1.77829
C	4.81089	2.57008	3.97200
C	5.21395	5.05115	3.66991
H	4.31470	5.78006	7.08029
C	4.00237	3.63326	7.17372
H	7.67048	6.13591	7.14101
H	7.39857	6.10459	8.89493
H	6.22007	6.93686	7.82005
H	4.04079	1.47160	7.33256
H	5.83856	0.15353	8.03695

H	7.03573	0.88945	9.15377
H	7.39577	0.77457	7.41667
H	14.08177	2.82364	5.80711
C	14.02736	4.93050	6.33854
H	10.90670	1.73382	6.71467
H	11.86175	1.43960	8.17873
H	12.58697	1.15214	6.55863
H	13.70099	6.94274	7.07488
H	11.98230	7.64543	8.50118
H	11.37945	6.42409	9.67331
H	10.42649	6.80209	8.22006
H	10.26322	9.67011	5.44987
C	12.05034	8.59243	4.84562
H	7.82389	8.30077	3.18711
H	8.05537	9.22909	4.71367
H	7.78328	7.45843	4.75127
H	13.61825	7.31821	4.06085
H	11.77035	4.58944	2.80258
H	13.32959	5.46311	2.63728
H	12.01796	5.68233	1.42952
H	6.67003	-0.13416	3.02510
C	5.18667	1.22100	3.84835
H	8.21864	1.69327	0.69026
H	8.68181	0.50280	1.95509
H	9.25664	2.19727	2.04801
H	3.88216	2.82366	4.50215
H	5.20573	5.61828	2.71713
H	5.93921	5.56463	4.33718
H	4.21656	5.13173	4.14190
C	2.55784	3.70618	6.74626
C	15.24565	5.28381	5.52336
C	12.98116	9.45712	5.65695
C	4.38119	0.12187	4.49066
H	2.41311	4.41896	5.90854
H	1.91184	4.05783	7.57912
H	2.17401	2.71731	6.42723
H	15.05808	5.13345	4.43888
H	16.11096	4.64154	5.78742
H	15.54629	6.33919	5.67120
H	14.04036	9.17057	5.50987
H	12.75514	9.37844	6.74141

H	12.87608	10.52846	5.38749
H	4.20836	-0.72181	3.79207
H	3.39793	0.48536	4.84752
H	4.92845	-0.29335	5.36428
O	9.41526	2.04622	4.66126
P	9.05114	-0.70142	5.34423

6.10.34 3NC(H)O

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	3.41729	6.70658	5.12390
P	5.52197	5.19636	5.67201
O	4.07487	7.78926	6.38952
N	3.72651	5.15431	5.81540
N	5.01466	6.39332	4.38012
N	5.81119	6.29501	7.01303
C	5.09485	7.35772	7.15421
H	5.26902	8.04945	8.00801
C	2.88922	4.19697	6.40814
C	5.82286	7.36171	3.76474
C	3.05710	2.82999	6.05123
C	1.87504	4.57030	7.33350
C	5.22550	8.46393	3.07784
C	7.24470	7.24588	3.76913
C	2.24705	1.85803	6.66895
C	4.00965	2.42062	4.97485
C	1.07133	3.57040	7.91164
C	1.67462	6.00802	7.68321
C	6.04306	9.43266	2.47004
C	3.73978	8.56307	2.98357
C	8.02552	8.24160	3.15395
C	7.90799	6.05108	4.36876
H	2.38161	0.80394	6.38058
C	1.26012	2.21745	7.59702
C	3.68054	2.68934	3.61955
C	5.20351	1.71987	5.28983
H	0.29056	3.87342	8.62633
C	2.37748	6.56638	8.78173
C	0.79446	6.81082	6.91231
H	5.55668	10.26659	1.94059
C	7.44044	9.33953	2.51090
C	3.03233	7.65421	2.14551
C	3.02786	9.52448	3.75252
H	9.12034	8.12757	3.17482
C	7.90408	4.82271	3.64508
C	8.57985	6.13925	5.61925
H	0.62801	1.44582	8.06118
C	4.54122	2.22837	2.60607
C	2.43455	3.45678	3.25596
C	6.02618	1.26989	4.24356
C	5.62969	1.52392	6.72275
C	2.22576	7.93629	9.05689
C	3.29775	5.70867	9.61389
C	0.69037	8.18193	7.21346
C	-0.00638	6.21493	5.78068
H	8.06643	10.10461	2.02883
C	1.62868	7.68384	2.14333
C	3.77377	6.64284	1.30967
C	1.62076	9.51275	3.71653
C	3.75296	10.51087	4.63278
C	8.51659	3.69779	4.21456
C	7.21121	4.71620	2.31272
C	9.14597	4.97216	6.16501
C	8.70487	7.45036	6.35050
H	4.27917	2.43277	1.55492
C	5.71138	1.50496	2.89318
H	2.55672	4.53772	3.48360
H	1.55388	3.11176	3.83345
H	2.20774	3.36862	2.17610
H	6.94993	0.72380	4.49568
H	4.81728	1.12043	7.35750
H	5.92545	2.49995	7.16675
H	6.50086	0.84426	6.79392
H	2.77905	8.37216	9.90517
C	1.41120	8.76828	8.26699
H	3.68970	6.26783	10.48536
H	4.16622	5.36062	9.01658
H	2.78379	4.79843	9.98300
H	0.02603	8.80964	6.59767
H	0.64118	6.00138	4.90284
H	-0.79710	6.91108	5.44263

H	-0.47806	5.25620	6.07295
H	1.08355	6.96765	1.50658
C	0.90116	8.59688	2.93110
H	4.24905	5.87412	1.95454
H	4.59306	7.11620	0.73252
H	3.09328	6.12775	0.60502
H	1.07059	10.23890	4.33670
H	4.37174	11.21303	4.03827
H	4.43653	9.98732	5.32935
H	3.03739	11.10493	5.23338
H	8.50725	2.75007	3.65473
C	9.11298	3.74122	5.48872
H	7.55501	3.82667	1.75236
H	7.37006	5.61836	1.69034
H	6.11512	4.60789	2.45809
H	9.62880	5.03115	7.15383
H	8.84752	7.28678	7.43538
H	7.81214	8.08664	6.20738
H	9.57651	8.02830	5.97387
C	6.59545	0.97893	1.79049
C	1.34860	10.25405	8.51334
C	-0.60604	8.61156	2.89916
C	9.67169	2.48968	6.11610
H	7.67098	1.10359	2.03272
H	6.39924	1.49147	0.82843
H	6.42974	-0.10767	1.62701
H	2.12988	10.77686	7.91898
H	1.52624	10.50469	9.57790
H	0.37076	10.68074	8.21393
H	-0.98078	9.14939	2.00168
H	-1.02905	9.12007	3.78769
H	-1.02191	7.58503	2.85748
H	8.85879	1.89457	6.58591
H	10.41126	2.71891	6.90796
H	10.15707	1.83622	5.36362

6.10.35 3NC(H)S

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	3.61897	6.83361	5.51207
P	5.44032	4.89579	5.12752
S	4.85666	7.55966	7.31000
N	3.69183	5.09235	5.64990
N	5.04903	6.53536	4.51259
N	6.07223	5.11144	6.74833
C	5.84840	6.10273	7.53714
H	6.28147	6.07212	8.56218
C	2.92522	4.18424	6.39554
C	5.83512	7.45517	3.81276
C	3.16631	2.78462	6.23927
C	1.88632	4.60903	7.27570
C	5.22958	8.62406	3.26105
C	7.22726	7.23275	3.59941
C	2.42718	1.86258	7.00186
C	4.13802	2.26727	5.23053
C	1.16780	3.64933	8.01382
C	1.49705	6.04368	7.41837
C	6.02523	9.56450	2.58188
C	3.75264	8.83414	3.32170
C	7.98293	8.19501	2.90416
C	7.91348	5.98943	4.06867
H	2.63091	0.79046	6.85640
C	1.43564	2.28058	7.89782
C	3.80103	2.33372	3.84899
C	5.36877	1.68465	5.63668
H	0.37081	4.00576	8.68458
C	1.90033	6.77987	8.56596
C	0.64928	6.64489	6.44880
H	5.53210	10.45448	2.16097
C	7.40027	9.36694	2.40507
C	2.90134	8.03312	2.50989
C	3.19968	9.84563	4.15023
H	9.05616	7.99954	2.75475
C	7.92998	4.83129	3.24381
C	8.62802	5.99730	5.29852
H	0.86183	1.54584	8.48143
C	4.70744	1.83121	2.90265
C	2.50892	2.96479	3.39553
C	6.23954	1.18697	4.64936
C	5.79423	1.67772	7.08336

C	1.51327	8.12558	8.67971
C	2.72439	6.12874	9.64639
C	0.26351	7.98486	6.62110
C	0.20307	5.87890	5.23066
H	8.00760	10.10789	1.86486
C	1.51641	8.26519	2.54255
C	3.46816	6.94091	1.63865
C	1.80731	10.04655	4.14149
C	4.07815	10.66590	5.06244
C	8.62844	3.69454	3.68376
C	7.14528	4.78651	1.95976
C	9.29140	4.82883	5.70739
C	8.67324	7.24272	6.14371
H	4.44361	1.88665	1.83350
C	5.93223	1.24900	3.28091
H	2.54879	4.06835	3.51738
H	1.64709	2.61539	3.99845
H	2.30734	2.74651	2.32931
H	7.19874	0.74553	4.96437
H	4.99784	1.30932	7.75810
H	6.04068	2.71408	7.40308
H	6.69612	1.05189	7.22879
H	1.85890	8.70408	9.55176
C	0.70569	8.75127	7.71246
H	3.15938	6.88432	10.32784
H	3.54848	5.52433	9.21948
H	2.10831	5.43172	10.25315
H	-0.39118	8.44785	5.86835
H	1.02455	5.82304	4.48252
H	-0.65265	6.37634	4.73535
H	-0.08034	4.83677	5.47652
H	0.85997	7.64464	1.91043
C	0.94822	9.27537	3.34122
H	3.88320	6.11874	2.25943
H	4.30704	7.31220	1.01593
H	2.69428	6.51439	0.97231
H	1.37982	10.82764	4.79089
H	4.78417	11.30583	4.49512
H	4.70375	10.01432	5.70780
H	3.47115	11.32090	5.71706
H	8.63166	2.79610	3.04812
C	9.29513	3.66345	4.92064
H	7.50505	3.97645	1.29631
H	7.18440	5.74596	1.40854
H	6.07415	4.57753	2.18042
H	9.81497	4.82843	6.67707
H	9.10488	7.03575	7.14175
H	7.66502	7.68155	6.28073
H	9.28769	8.03078	5.65936
C	6.87066	0.69388	2.23947
C	0.35613	10.21310	7.82672
C	-0.53810	9.52865	3.31518
C	9.95428	2.40146	5.41518
H	7.83503	0.37853	2.68314
H	7.08453	1.44148	1.44763
H	6.42996	-0.19015	1.73165
H	1.20171	10.84480	7.47700
H	0.14755	10.50691	8.87503
H	-0.52639	10.47359	7.21003
H	-0.85179	9.96915	2.34482
H	-0.84897	10.22985	4.11405
H	-1.11455	8.58846	3.43775
H	9.29427	1.87886	6.14150
H	10.90789	2.61162	5.93988
H	10.16019	1.69425	4.58786

6.10.36 3NN(H)N

	PBE-D3BJ/def2-SVP		
Atom	x	y	z
P	3.40313	6.77515	5.12851
P	5.48123	5.22755	5.68192
N	4.04477	7.87223	6.35518
N	3.71424	5.18916	5.82135
N	5.03573	6.39579	4.38364
N	5.73182	6.33363	7.05729
N	5.01166	7.41373	7.09257
H	5.23377	8.03051	7.90031
C	2.87369	4.22434	6.39196

C	5.85314	7.31907	3.71866
C	3.00072	2.87263	5.96454
C	1.89238	4.57499	7.35982
C	5.25513	8.35945	2.94083
C	7.27614	7.22440	3.75812
C	2.18135	1.89008	6.55091
C	3.91449	2.50707	4.83977
C	1.07578	3.56653	7.90500
C	1.75097	5.99529	7.79914
C	6.07278	9.28668	2.27221
C	3.76954	8.42919	2.82576
C	8.05749	8.17695	3.07948
C	7.93302	6.09058	4.47159
H	2.28268	0.84870	6.20775
C	1.22381	2.22720	7.51829
C	3.53450	2.83922	3.51064
C	5.11716	1.79365	5.07646
H	0.32073	3.85018	8.65449
C	2.51484	6.46604	8.89701
C	0.86621	6.86907	7.11475
H	5.58642	10.07166	1.67241
C	7.47073	9.21304	2.34136
C	3.08615	7.44543	2.05343
C	3.03301	9.43378	3.51265
H	9.15315	8.07980	3.12933
C	8.01136	4.82126	3.82803
C	8.49546	6.27028	5.76398
H	0.58306	1.44865	7.95856
C	4.35479	2.42805	2.44542
C	2.27245	3.61654	3.23551
C	5.90022	1.39393	3.97815
C	5.59052	1.51973	6.48144
C	2.41153	7.82002	9.26429
C	3.45397	5.54056	9.63063
C	0.81551	8.22076	7.50210
C	-0.00013	6.36421	5.98689
H	8.09617	9.94537	1.81019
C	1.68309	7.44418	2.04250
C	3.85440	6.39178	1.29763
C	1.62605	9.38842	3.46963
C	3.72727	10.48514	4.34134

C	8.59188	3.74670	4.51565
C	7.43737	4.62539	2.45023
C	9.04061	5.15337	6.42571
C	8.52954	7.62700	6.41992
H	4.05230	2.68169	1.41599
C	5.53462	1.69045	2.65426
H	2.38703	4.68045	3.53466
H	1.41221	3.21953	3.81055
H	2.01664	3.60086	2.15876
H	6.82984	0.83294	4.16789
H	4.79601	1.08600	7.11913
H	5.90686	2.46914	6.96685
H	6.45921	0.83313	6.48624
H	3.00365	8.18584	10.12021
C	1.59110	8.72066	8.56182
H	3.83291	6.00723	10.56082
H	4.33148	5.28855	8.99749
H	2.96449	4.58175	9.89285
H	0.15014	8.90450	6.95003
H	0.61310	6.10119	5.09894
H	-0.72919	7.13393	5.66952
H	-0.55392	5.44918	6.27719
H	1.15778	6.66918	1.46025
C	0.93157	8.39632	2.75884
H	4.33099	5.67565	1.99948
H	4.67277	6.83793	0.69799
H	3.19055	5.81877	0.62229
H	1.05608	10.14859	4.02816
H	4.51360	11.01646	3.77110
H	4.21510	10.00868	5.21742
H	3.00234	11.23126	4.72007
H	8.64300	2.76505	4.01876
C	9.08375	3.88312	5.82859
H	7.82736	3.70220	1.98294
H	7.65600	5.48508	1.78728
H	6.33228	4.52538	2.50145
H	9.44027	5.28365	7.44435
H	8.55026	7.53372	7.52241
H	7.66006	8.24660	6.13050
H	9.43662	8.18943	6.10887
C	6.36449	1.21144	1.48987

C	1.57485	10.18865	8.90282
C	-0.57532	8.35578	2.73796
C	9.62117	2.68588	6.57057
H	7.42026	1.04220	1.78091
H	6.34896	1.93646	0.65175
H	5.97713	0.24826	1.09259
H	2.27375	10.74487	8.24059
H	1.89162	10.37343	9.94825
H	0.56990	10.63386	8.76042
H	-0.97114	8.62809	1.73635
H	-1.01352	9.05764	3.47378
H	-0.95349	7.33852	2.96685
H	8.79150	2.01814	6.88791
H	10.17784	2.98078	7.48113
H	10.29574	2.07945	5.93241

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