Electronic Supplementary Information for:

Ligand Non-Innocence Allows Isolation of a Neutral and Terminal Niobium Nitride

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Experimental Section

General Considerations

All operations were performed in a M. Braun Lab Master glove box or using standard Schlenk techniques under a nitrogen atmosphere. Anhydrous solvents (toluene, Et_2O, THF, pentane) were purchased from Fisher Scientific or Aldrich. All anhydrous solvents were purified and dried by passage through two columns of activated alumina and Q-5 drying agent in a Grubbs-type solvent system. All bulk solvents were stored over sodium and 4 Å molecular sieves (Acros Organics) prior to use. Benzene-d_6 (Cambridge Isotope Laboratories) was dried over a potassium mirror, sublimed, and degassed using freeze-pump-thaw cycles prior to use. Celite and 4 Å molecular sieves were dried under vacuum overnight at 200 °C prior to use. NaN_3 was dried under vacuum overnight and brought into the box. For further purification, it was stirred in dry THF overnight, filtered and washed with copious amount of THF, and dried under vacuum overnight. (*Warning: Caution is advised while handling NaN_3 due to its explosive nature*). (PNP)$NbCl_2$(N[^{t}Bu]Ar),[1] Na/NaCl,[2] and $PhICl_2$[3] were prepared according to literature procedures. ^{1}H, ^{31}P, NMR spectra were recorded on a Bruker AV-II 500 MHz or AVIII 400 MHz spectrometers. ^{13}C, HSQC, COSY, and HMQC, and ^{15}N NMR spectra were recorded on a Bruker AV-II 500 MHz spectrometer. ^{1}H, ^{13}C NMR chemical shifts are referenced to the internal residual proton or carbon resonances of C_6D_6 (δ = 7.16 ppm or 128.06 ppm). ^{31}P NMR chemical shifts are reported with respect to external H_3PO_4 (δ 0.0 ppm). ^{15}N NMR shifts are referenced to AdCN (242 ppm vs. NH_3(l) at 0 ppm). Elemental analyses were performed by Midwest Microlab, Inc (Indiana, USA).

Synthesis of (PNPN)$NbCl_2$(N[^{t}Bu]Ar) (2) and (PNP)Nb≡N(N[^{t}Bu]Ar) (3)

To a solution of (PNP)$NbCl_2$(N[^{t}Bu]Ar) (**1**) (100mg, 130 µmol) in THF (5 mL) was added NaN_3 (6.7 mg, 130 µmol) in THF (2 mL) at room temperature. After stirring for 16 hours, the reaction mixture changed color from purple to maroon. The solvent was removed under vacuum and the dark residue was extracted into pentane, filtered through Celite and washed twice with pentane. The red-orange filtrate was concentrated to ~2 mL and cooled to -35 °C overnight. Dark red crystals of (PNPN)$NbCl_2$(N[^{t}Bu]Ar) (**2**) deposited on the bottom of the vial from which the mother liquor was decanted off and stored in a separate vial. The dark red crystals were washed with pentane to afford pure **2** (28 mg, 36.7 µmol, 28% yield based on **1**). The mother liquor was then filtered through a glass fiber pad, concentrated, and stored at -35 °C overnight from which blocks of orange crystals deposit on the vial. Decantation followed by pentane washes of the crystals gives pure (PNP)Nb≡N(N[^{t}Bu]Ar) **3** (26.4 mg, 37.1 µmol, 28% yield based on **1**). The ^{15}N-

isotopomers, (PNP^{15}N)NbCl$_2$(N[^{t}Bu]Ar) and (PNP)Nb≡^{15}N(N[^{t}Bu]Ar), were prepared following the same procedure using 50% enriched Na^{15}N$_3$.

2: ^{1}H NMR (500 MHz, C_6D_6) δ 7.55 (s, 1H, p-Xyl-C*H*), 7.24 (d, $^3J_{HP}$ = 7.5 Hz, 1H, PNPAr), 7.21 (s, 1H, o-Xyl-C*H*), 7.19 (s, 1H, PNPAr), 7.03 (dd, $^3J_{HH}$ = 8.3, $^4J_{HP}$ = 4.5 Hz, 1H, PNPAr), 6.93 (d, $^3J_{HH}$ = 8.4 Hz, 1H, PNPAr), 6.84 (d, $^3J_{HH}$ = 11.0 Hz, 1H), 6.65 (s, 1H, o-Xyl-C*H*), 6.63 (s, 1H, PNPAr), 2.68 – 2.59 (m, 1H, PC*H*(CH$_3$)$_2$), 2.18 (s, 3H, PNP C*H*$_3$), 2.16 (s, 3H, NAr Xyl C*H*$_3$), 2.15 (s, 3H, NAr Xyl C*H*$_3$), 2.07 (s, 3H, PNP C*H*$_3$), 1.96 – 1.86 (m, 1H, PC*H*(CH$_3$)$_2$), 1.77 (s, 9H, NC(C*H*$_3$)$_3$), 1.42 – 1.31 (m, 13H, overlapped, PC*H*(CH$_3$)+ PCH(C*H*$_3$)$_2$), 1.28 – 1.20 (m, 4H, overlapped, PC*H*(CH$_3$)+PCH(C*H*$_3$)$_2$), 1.18 – 1.10 (m, 3H, PCH(C*H*$_3$)$_2$), 1.01 (dd, $^3J_{HH}$ = 16.1, $^3J_{HP}$ = 7.1 Hz, 3H, PCH(C*H*$_3$)$_2$), 0.91 – 0.83 (m, 3H, overlapped, PCH(C*H*$_3$)$_2$). **^{13}C{^{1}H} NMR** (126 MHz, C_6D_6) δ 165.09 (d, $^2J_{CP}$ = 2.5 Hz, PNPAr), 163.33 (d, $^2J_{CP}$ = 19.2 Hz, PNPAr), 146.54 (i-NXyl), 138.22 (m-NXyl), 137.78 (m-NXyl), 134.54 (d, $^4J_{CP}$ = 2.3 Hz, PNPAr), 132.25 (d, $^4J_{CP}$ = 2.3 Hz, PNPAr), 131.23 (PNPAr), 129.71 (d, $^2J_{CP}$ = 11.0 Hz, PNPAr), 127.64 (overlapped with C_6D_5H, PNPAr), 127.48 (d, $^3J_{CP}$ = 4.1 Hz, PNPAr), 127.27 (d, $^1J_{CP}$ = 30.9 Hz, PNPAr), 127.03 (d, $^2J_{CP}$ = 8.4 Hz, PNPAr), 126.72 (p-NXyl), 124.60 (d, $^3J_{CP}$ = 12.4 Hz, PNPAr), 122.69 (d, $^3J_{CP}$ = 6.0 Hz, PNPAr), 112.39 (d, $^1J_{CP}$ = 89.0 Hz, PNPAr), 63.97 (N*C*(CH$_3$)$_3$), 33.50 (NC(*C*H$_3$)$_3$), 28.65 (Xyl *C*H$_3$), 28.12 (d, $^1J_{CP}$ = 8.2 Hz, P*C*H(CH$_3$)$_3$), 23.87 (P*C*H(CH$_3$)$_3$), 23.40 (P*C*H(CH$_3$)$_3$), 21.44 (Xyl *C*H$_3$), 21.24 (PNP tolyl CH$_3$), 21.09 – 20.96 (multiple peaks overlapped, P*C*H(CH$_3$)$_3$ and PCH(*C*H$_3$)$_3$), 20.89 (d, $^3J_{CP}$ = 6.9 Hz, PCH(*C*H$_3$)$_3$), 20.56 (PNP tolyl CH$_3$), 20.51 (d, $^3J_{CP}$ = 1.9 Hz, PCH(*C*H$_3$)$_3$) 18.73 (d, $^3J_{CP}$ = 2.1 Hz, PCH(*C*H$_3$)$_3$), 18.65 (d, $^3J_{CP}$ = 3.7 Hz, PCH(*C*H$_3$)$_3$), 16.91 (d, $^3J_{CP}$ = 3.4 Hz, PCH(*C*H$_3$)$_3$), 16.65 (d, $^3J_{CP}$ = 2.3 Hz, PCH(*C*H$_3$)$_3$), 14.85 (d, $^3J_{CP}$ = 2.5 Hz, PCH(*C*H$_3$)$_3$). **^{31}P{^{1}H} NMR** (162 MHz, C_6D_6) δ 41.57 (d, $^3J_{PP}$ = 44 Hz, *P*NP=N), 11.83 (d, $^3J_{PP}$ = 40 Hz, PN*P*=N). **^{15}N NMR** (51 MHz, C_6D_6) δ 350.88 ($\Delta\nu_{1/2}$ = 11 Hz). Multiple attempts to obtain a satisfactory elemental analysis failed. The data is provided here for transparency: Elemental analysis calcd (%) for $C_{38}H_{58}ClN_2NbP_3$: C, 58.32; H, 7.47; N, 5.37. Found: C, 56.25 H, 6.99 N, 5.68.

3: ^{1}H NMR (500 MHz, C_6D_6) δ 7.27 (dd, $^3J_{HH}$ = 8.4, $^4J_{HP}$ = 4.2 Hz, 1H, PNPAr), 7.02 (dd, $^3J_{HH}$ = 8.3, $^4J_{HP}$ = 3.9 Hz, 1H, PNPAr), 6.95 (dd, $^3J_{HP}$ = 6.1, $^4J_{HH}$ = 2.3 Hz, 1H, PNPAr), 6.88 (dd, $^3J_{HH}$ = 8.5, $^4J_{HH}$ = 2.2 Hz, 1H, PNPAr), 6.84 (dd, $^3J_{HP}$ = 6.2, $^4J_{HH}$ = 2.1 Hz, 1H, PNPAr), 6.79 (dd, $^3J_{HH}$ = 8.3, $^4J_{HH}$ = 2.1 Hz, 1H, PNPAr), 6.58 (s, 2H, Xyl-C*H*), 6.40 (s, 1H, Xyl-C*H*), 2.56-2.49 (m, 1H, PNP PC*H*(CH$_3$)$_2$), 2.43 – 2.34 (m, 1H, PNP PC*H*(CH$_3$)$_2$), 2.34 – 2.25 (m, 1H, PNP PC*H*(CH$_3$)$_2$), 2.17 (s, 3H, PNP tolyl CH$_3$), 2.14 (s, 3H, PNP tolyl CH$_3$), 2.01 (s, 9H, NC(C*H*$_3$)$_3$), 1.87 (s, 6H, NAr Xyl C*H*$_3$), 1.67 (dd, $^3J_{HH}$ = 7.0, $^3J_{HP}$ = 3.6 Hz, 3H, PCH(C*H*$_3$)$_2$), 1.64 (dd, $^3J_{HH}$ = 7.0, $^3J_{HP}$ = 4.2 Hz, 3H, PCH(C*H*$_3$)$_2$), 1.38 – 1.27 (m, 13H, overlapped with residual pentane, PCH(C*H*$_3$)$_2$ + PC*H*(CH$_3$)$_2$), 0.73 (dd, $^3J_{HH}$ = 9.9, $^3J_{HP}$ = 6.9 Hz, 3H, PCH(C*H*$_3$)$_2$), 0.28 (dd, $^3J_{HH}$ = 15.5, $^3J_{HP}$ = 6.9 Hz, 3H, PCH(C*H*$_3$)$_2$). **^{13}C{^{1}H} NMR** (126 MHz, C_6D_6) δ 161.98 (dd, $^2J_{CP}$ =

19.1, PNPAr), 161.42 (dd, $^{2}J_{CP}$ = 20.4, PNPAr), 148.18 (i-NXyl), 138.56 (m-NXyl), 132.55 (d, $^{4}J_{CP}$ = 2.2 Hz, PNPAr), 132.52 (d, $^{4}J_{CP}$ = 1.5 Hz, PNPAr), 132.01 (PNPAr), 131.22 (PNPAr), 128.35 (PNPAr), 126.59 (d, $^{3}J_{CP}$ = 4.9 Hz, PNPAr), 126.50 (d, $^{3}J_{CP}$ = 5.1 Hz, PNPAr), 125.25 (p-NXyl), 121.30 (d, $^{1}J_{CP}$ = 31.4 Hz, PNPAr), 121.09 (o-NXyl), 119.68 (d, $^{3}J_{CP}$ = 7.4 Hz, PNPAr), 118.18 (d, $^{1}J_{CP}$ = 34.3 Hz, PNPAr), 117.88 (d, $^{3}J_{CP}$ J = 7.5 Hz, PNPAr), 59.03 (N*C*(CH$_3$)$_3$), 35.81 (NC(*C*H$_3$)$_3$), 27.27 (d, $^{1}J_{CP}$ = 14.1 Hz, P*C*H(CH$_3$)$_2$), 23.56 (d, $^{3}J_{CP}$ = 9.1, PCH(*C*H$_3$)$_2$), 20.98 (Xyl *C*H$_3$), 20.80 (PNP tolyl CH$_3$), 20.77 (d, $^{1}J_{CP}$ = 11.3 Hz, P*C*H(CH$_3$)$_2$), 20.77 (PNP tolyl CH$_3$), 20.70 (d, $^{3}J_{CP}$ =2.8 Hz, PCH(*C*H$_3$)$_2$), 19.39 (d, $^{3}J_{CP}$ = 2.2 Hz, PCH(*C*H$_3$)$_2$), 19.37 (d, $^{1}J_{CP}$ = 20.1 Hz, P*C*H(CH$_3$)$_2$), 19.08 (d, $^{3}J_{CP}$ = 4.2 Hz, PCH(*C*H$_3$)$_2$), 18.72 (d, $^{3}J_{CP}$ = 6.4 Hz, PCH(*C*H$_3$)$_2$), 18.60 (d, $^{3}J_{CP}$ = 5.7 Hz, PCH(*C*H$_3$)$_2$), 18.45 (d, $^{1}J_{CP}$ = 10.0 Hz, P*C*H(CH$_3$)$_2$), 17.74 (d, $^{3}J_{CP}$ = 2.2 Hz, PCH(*C*H$_3$)$_2$), 15.21 (d, $^{3}J_{CP}$ = 6.4 Hz, PCH(*C*H$_3$)$_2$). **^{31}P{^{1}H} NMR** (203 MHz, C_6D_6) δ 35.36 (br, $\Delta\nu_{1/2}$ = 190 Hz, PNP), 36.58 (br, $\Delta\nu_{1/2}$ = 221 Hz, PNP). **^{15}N NMR** (51 MHz, C_6D_6) δ 823.84 ($\Delta\nu_{1/2}$ = 10 Hz). Multiple attempts to obtain a satisfactory elemental analysis failed. The data is provided here for transparency: Elemental analysis calcd (%) for $C_{38}H_{58}ClN_2NbP_3$: C, 64.13; H, 8.21; N, 5.90. Found: C, 61.36 H, 8.66 N, 4.64.

Reduction of 2 with 2 Na/NaCl:

To a red solution of **2** (11 mg, 14 μmol) in THF was added Na/NaCl (13.5 mg, 28 μmol) in THF. After stirring for 12 hours, the reaction mixture was evaporated to dryness. The residue was extracted into pentane and filtered through Celite and the filtrate was evaporated to dryness. The resulting solid was dissolved in 0.5 mL C_6D_6 and transferred to a J-Young NMR tube. ^{31}P revealed the formation of **3** along with NaPNP and PNPH (Figure S18).

Oxidation of 3 with Iodobenzene dichloride ($PhICl_2$):

In a J-Young valve NMR tube, a C_6D_6 (0.5 mL) solution of **3** (14 mg, 21 μmol) was treated with $PhICl_2$ (6.1 mg, 22 μmol) at room temperature resulting in a color change from orange to dark red. After 1 day at room temperature, ^{31}P NMR revealed the formation of **2** and other unknown side products (Figure S19).

Statement on Elemental Analysis

Elemental analysis (EA) for compounds **2** and **3** always resulted in low carbon values despite multiple attempts in sending pure crystalline samples. This error could be due to partial degradation of the sample during shipment and handling of these extremely air-sensitive compounds in a glove box with suboptimal H_2O and O_2 content in the third party laboratory (Midwest Microlab, Inc. (Indiana, USA). However, thorough NMR characterization and complete single crystal X-ray diffraction (sc-XRD) data provides

confirmation of bulk purity of **2** and **3** and in lieu of EA. We refer to the reader to an interesting discussion on the controversy behind EA.[4]

NMR Spectroscopy

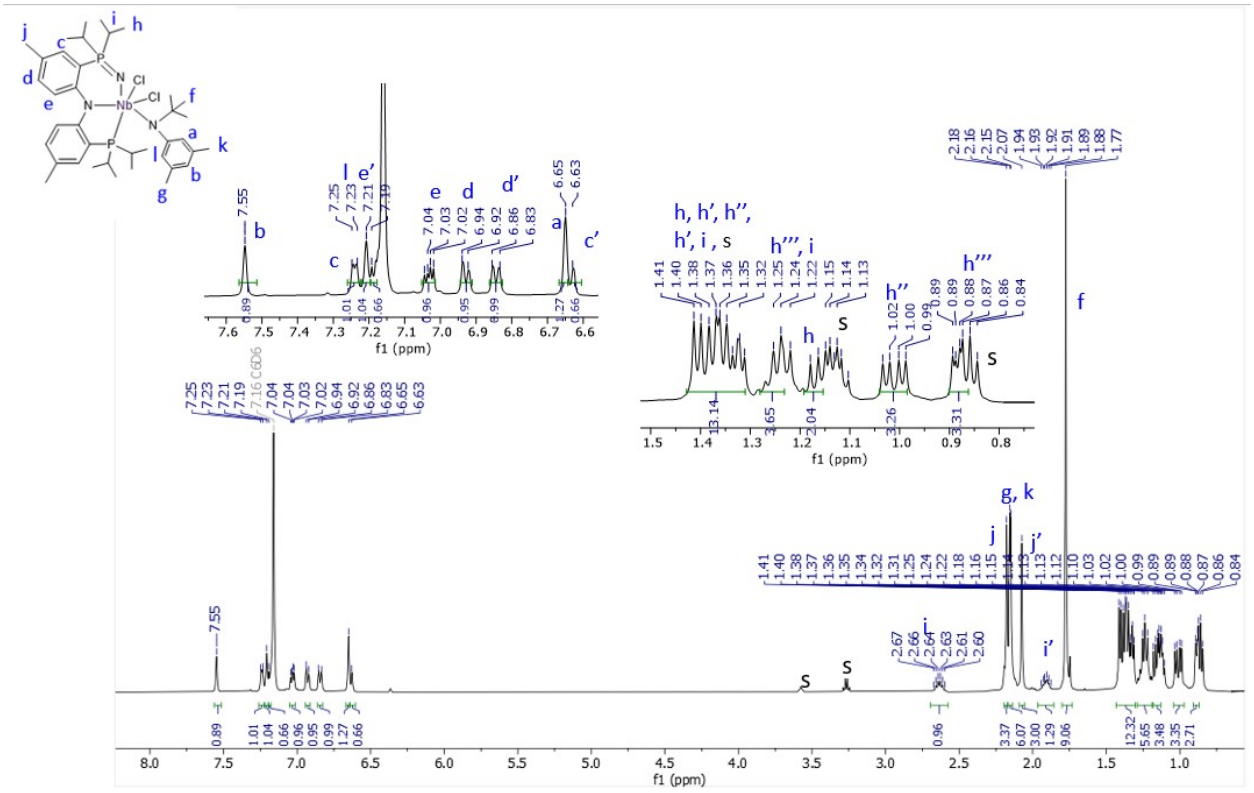

Figure S1. ^{1}H NMR (500 MHz, C_6D_6, 300 K) spectrum of **2**. Residual solvent peaks (THF, Et_2O) are marked as 's'.

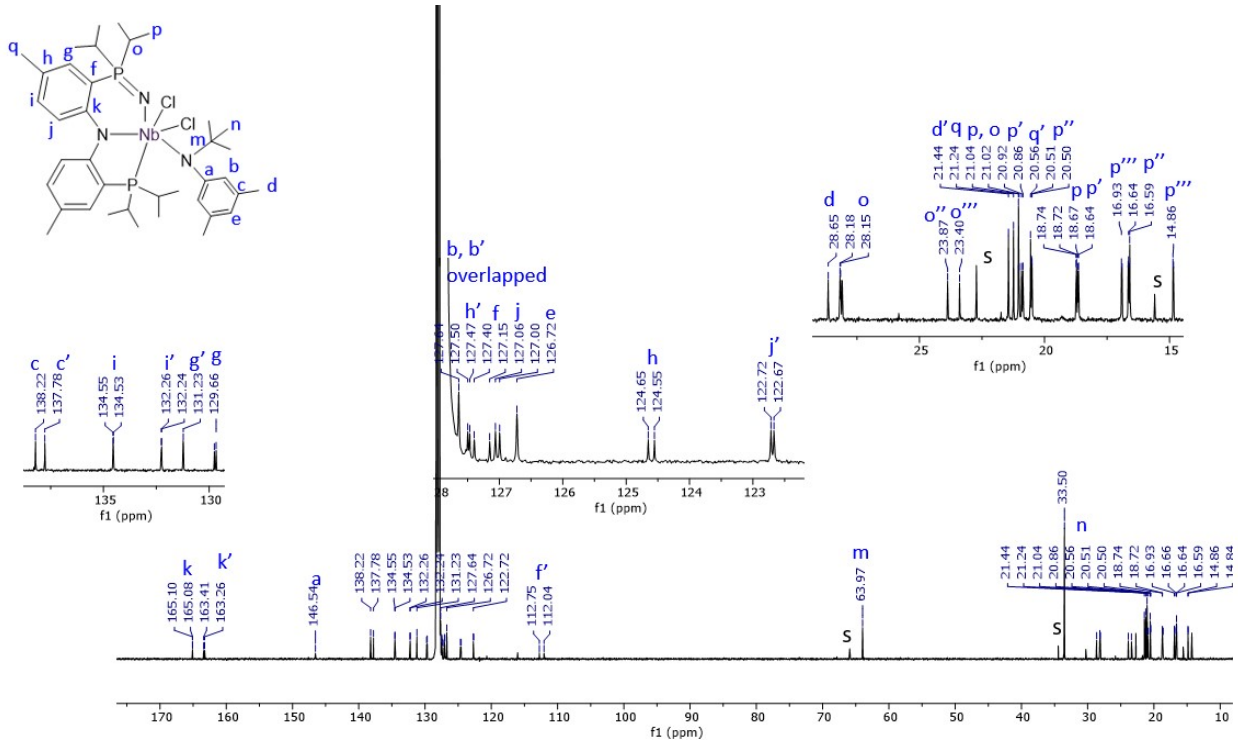

Figure S2. $^{13}C\{^{1}H\}$ (126 MHz, C_6D_6, 300K) NMR of **2**. Residual solvent peaks (THF, Et_2O) are marked as 's'.

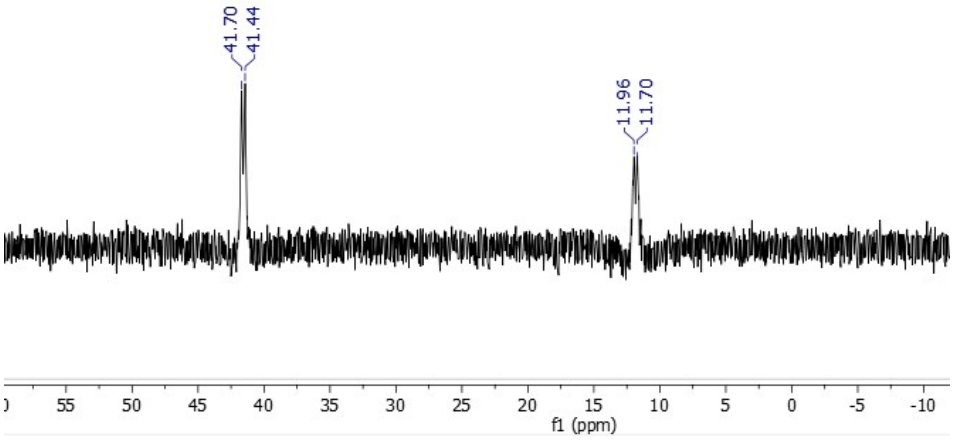

Figure S3. $^{31}P\{^{1}H\}$ (162 MHz, C_6D_6, 300K) NMR of **2**.

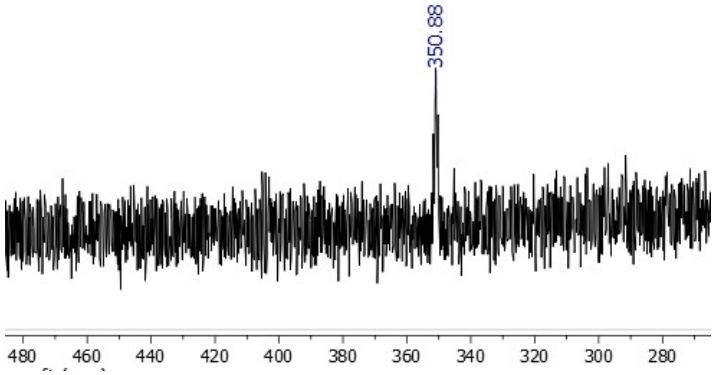

Figure S4. ^{15}N (51 MHz,C_6D_6, 300K) NMR of **2**-^{15}N.

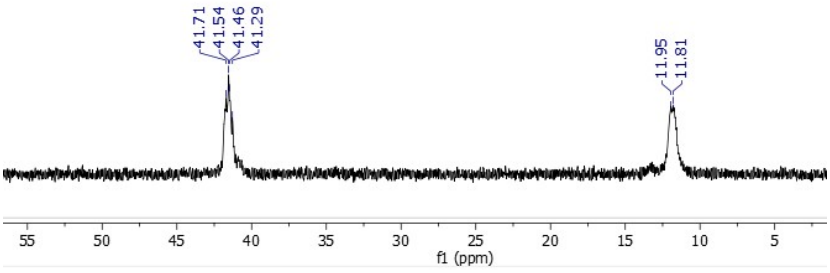

Figure S5. $^{31}P\{^{1}H\}$ NMR (162 MHz, C_6D_6, 300K) of **2**-^{15}N.

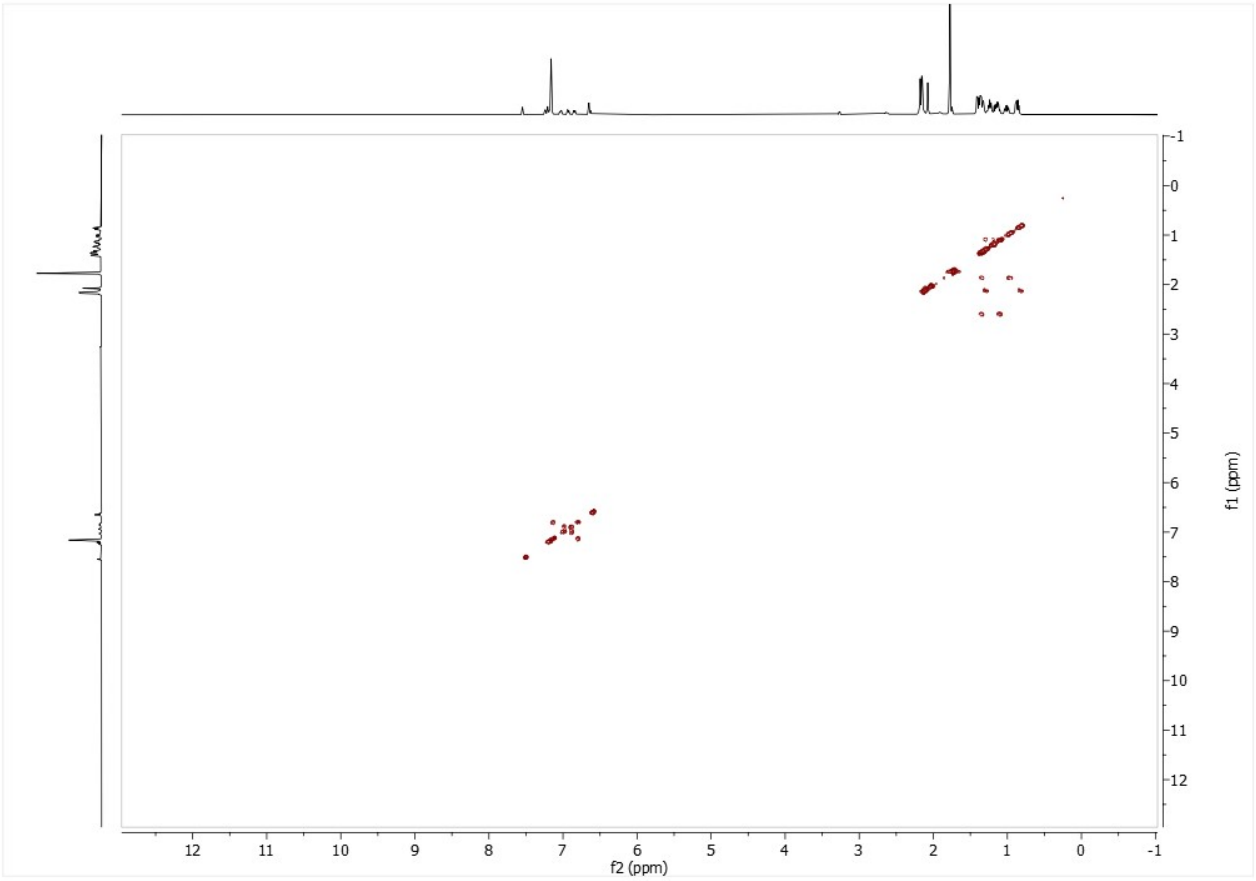

Figure S6. ^{1}H-^{1}H COSY spectrum (C_6D_6, 300K) of **2**.

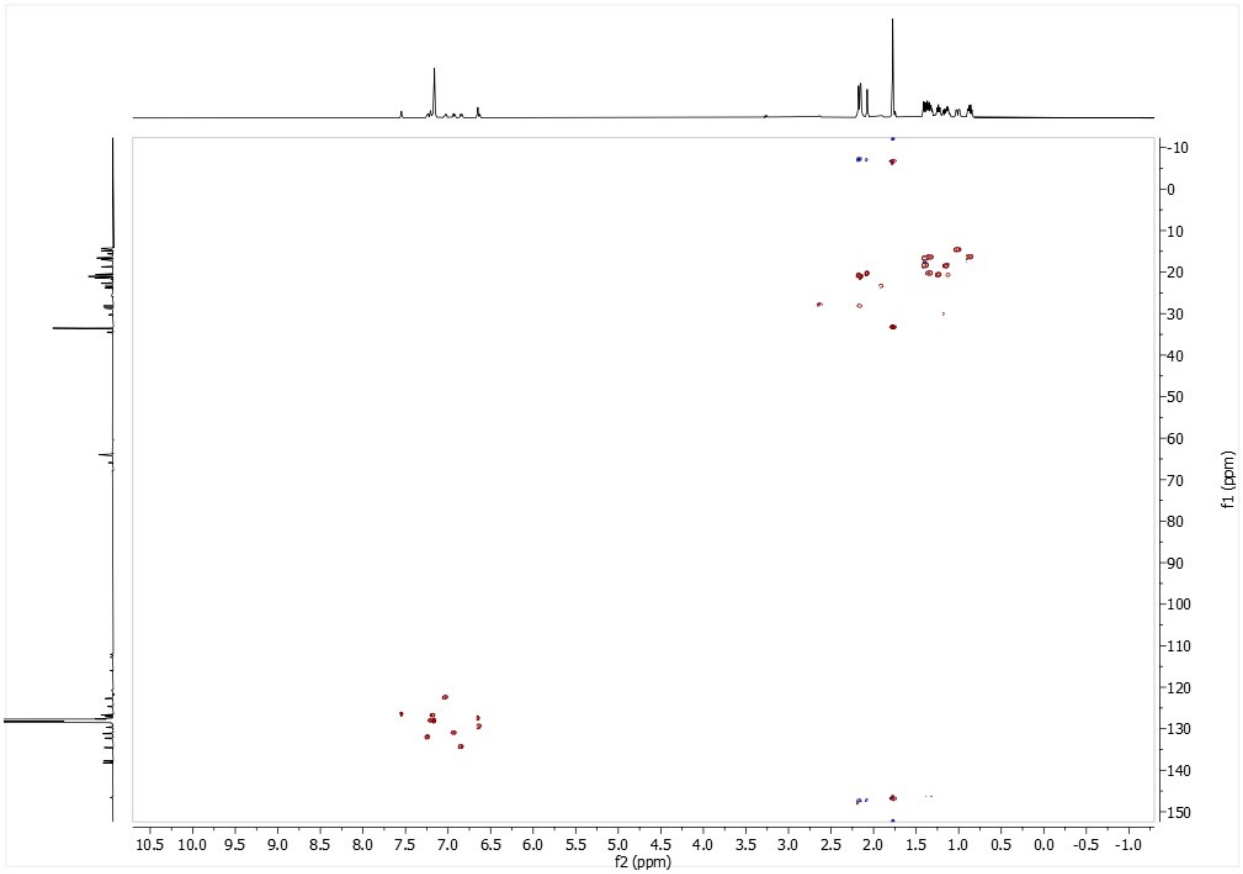

Figure S7. ^{1}H-^{13}C HSQC spectrum (C_6D_6, 300K) of **2**.

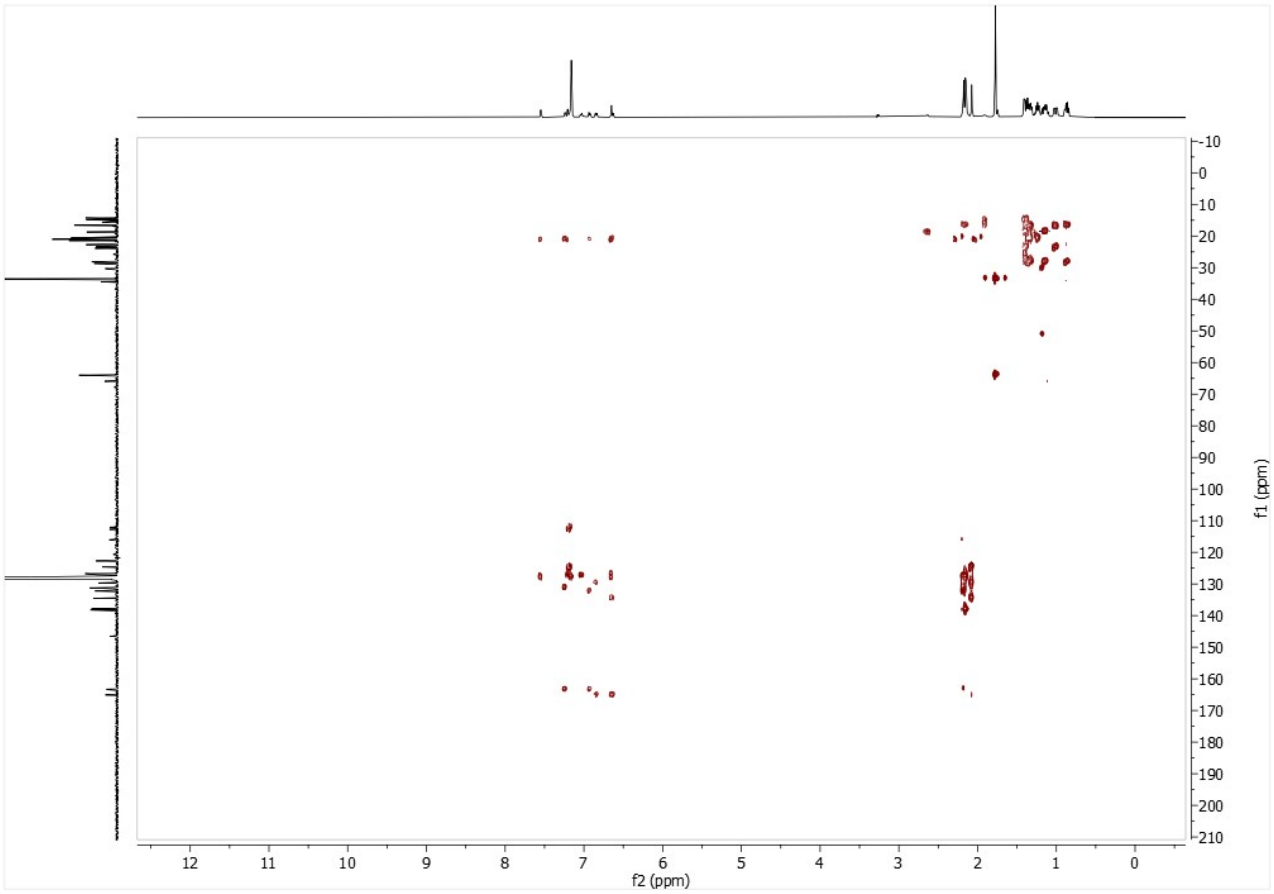

Figure S8. ^{1}H-^{13}C HMBC spectrum (C_6D_6, 300K) of **2**.

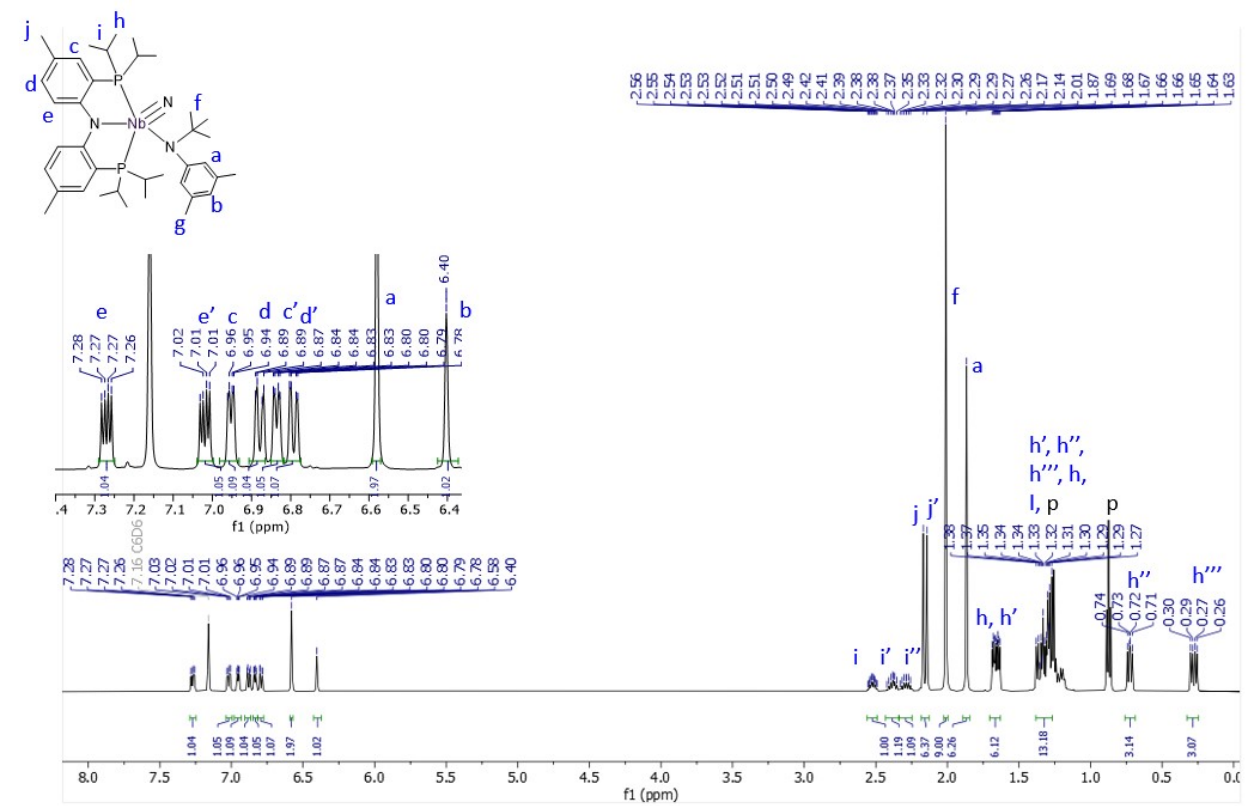

Figure S9. ^{1}H NMR (500 MHz, C_6D_6, 300K) of **3**. Residual solvent peak (pentane) is marked as 'p'.

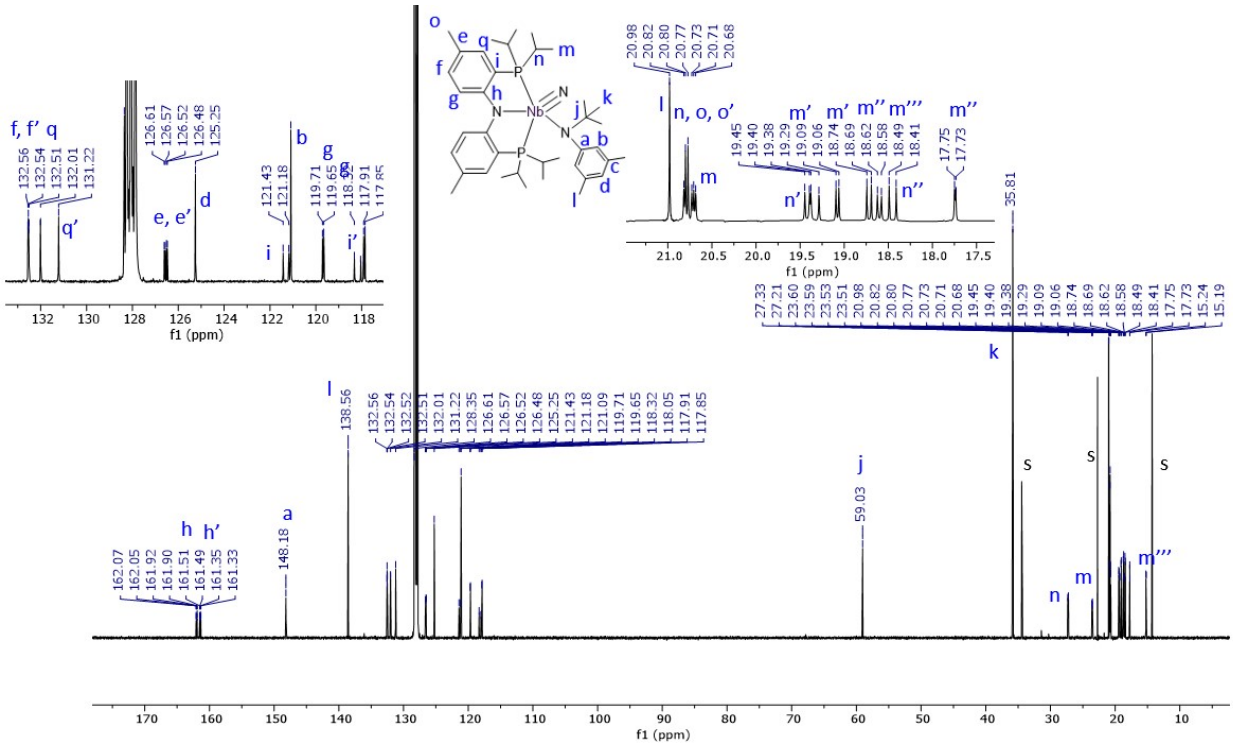

Figure S10. $^{13}C\{^{1}H\}$ (126 MHz, C_6D_6, 300K) NMR of **3**. Residual solvent peak (pentane) is marked as 's'.

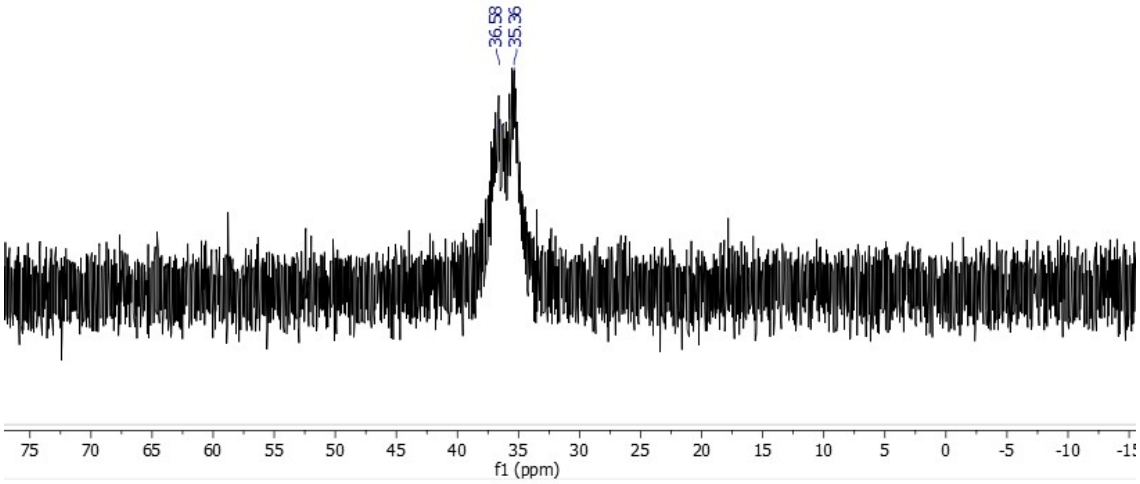

Figure S11. $^{31}P\{^{1}H\}$ (203 MHz, C_6D_6, 300K) NMR of **3**.

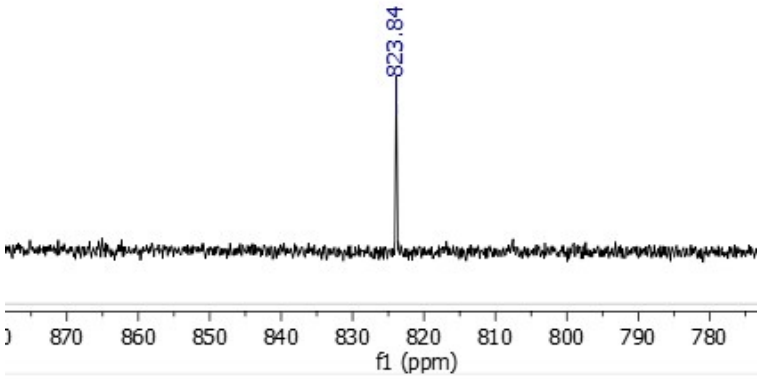

Figure S12. ^{15}N (51 MHz,C_6D_6, 300K) NMR of **3-**^{15}N.

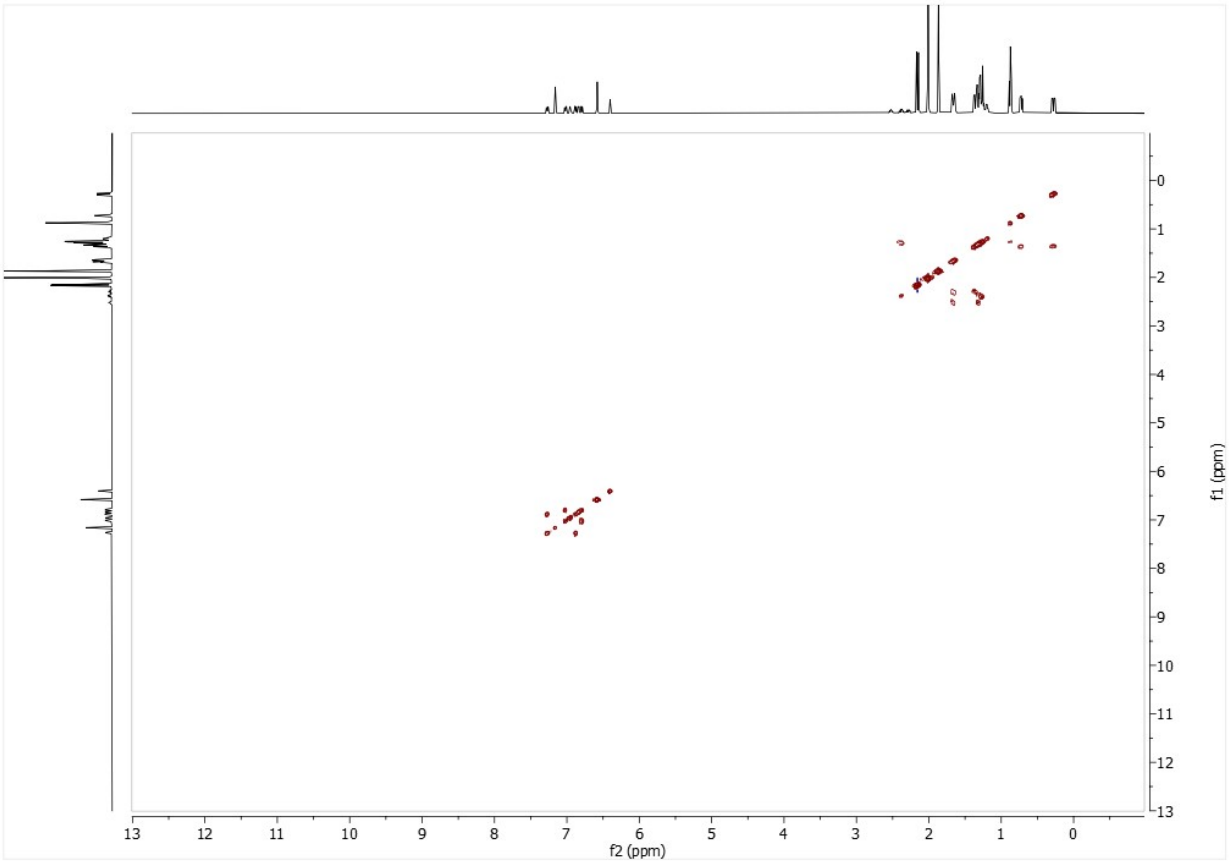

Figure S13. ^{1}H-^{1}H COSY spectrum (C_6D_6, 300K) of **3**.

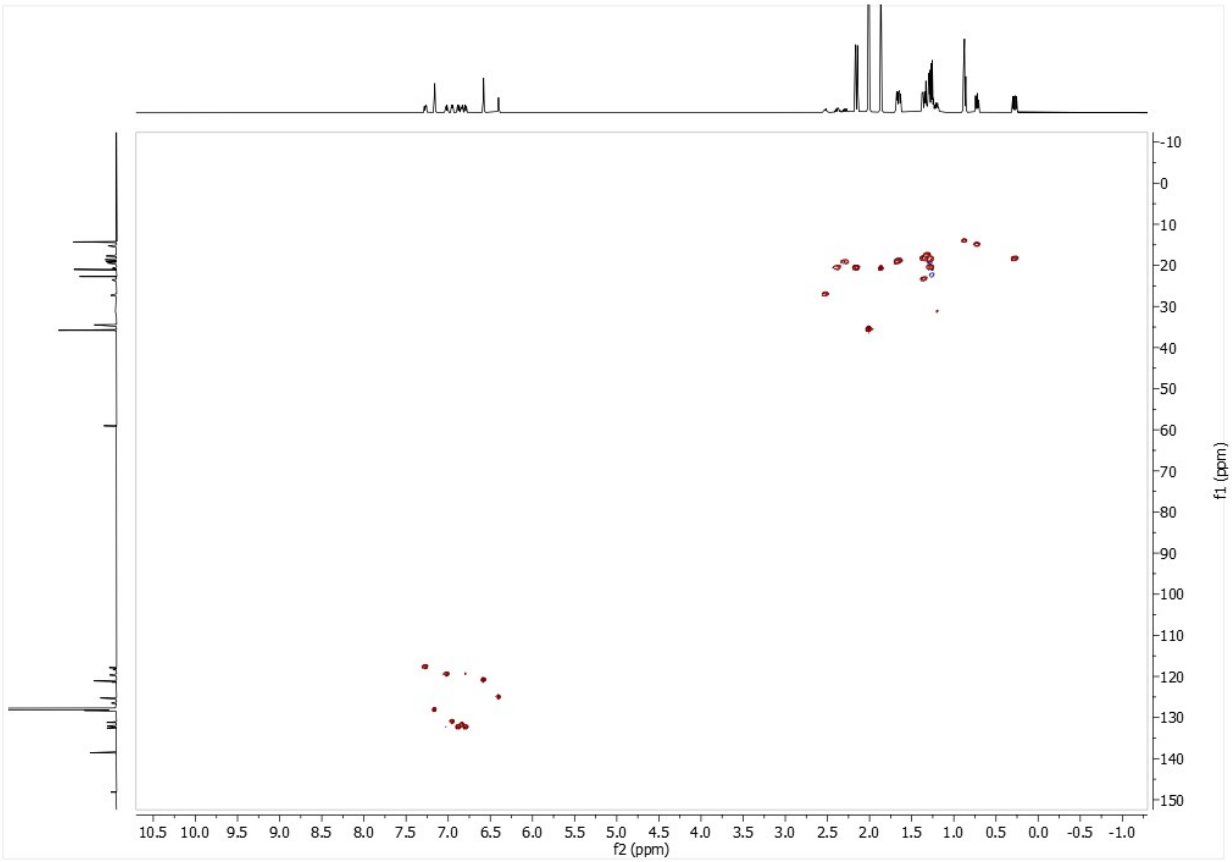

Figure S14. ^{1}H-^{13}C HSQC spectrum (C_6D_6, 300K) of **3**.

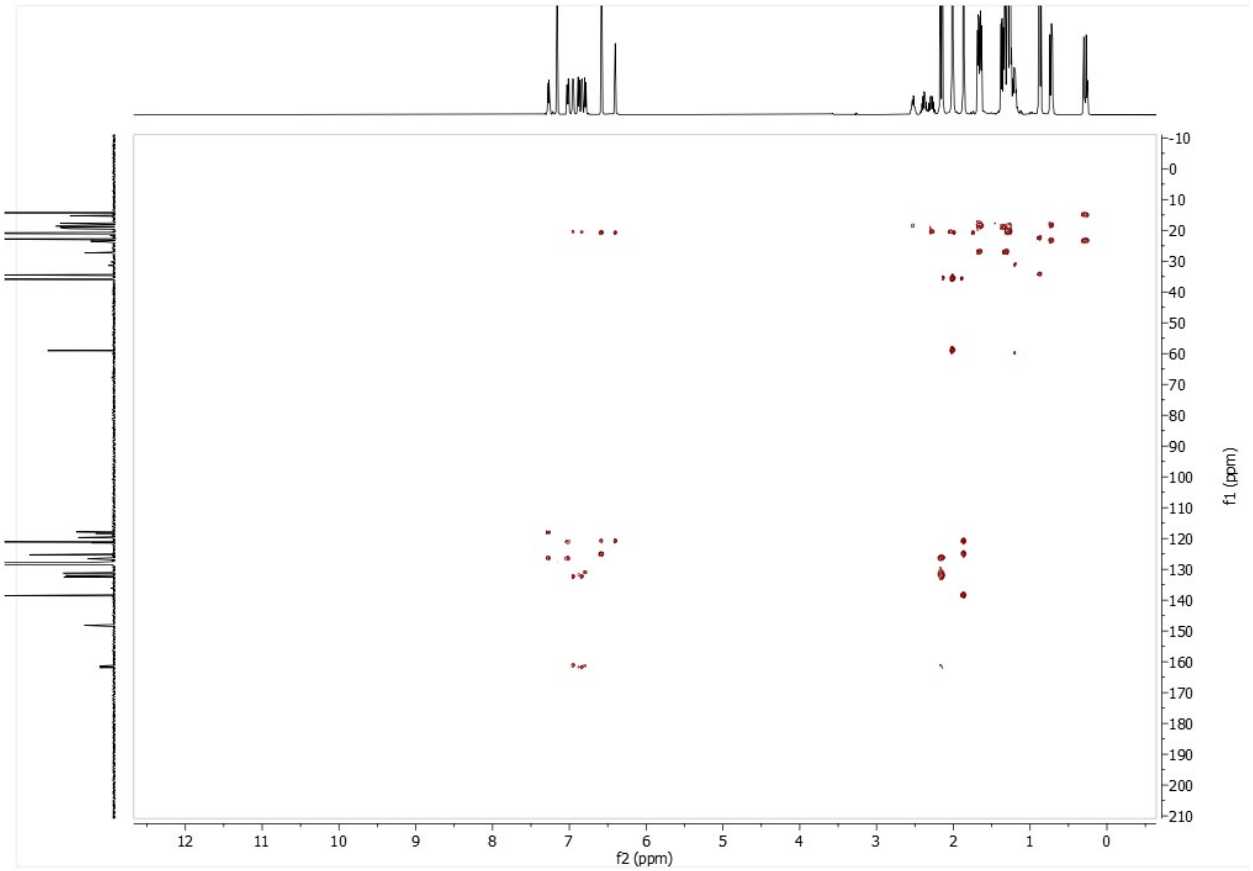

Figure S15. ^{1}H-^{13}C HMBC spectrum (C_6D_6, 300K) of **3**.

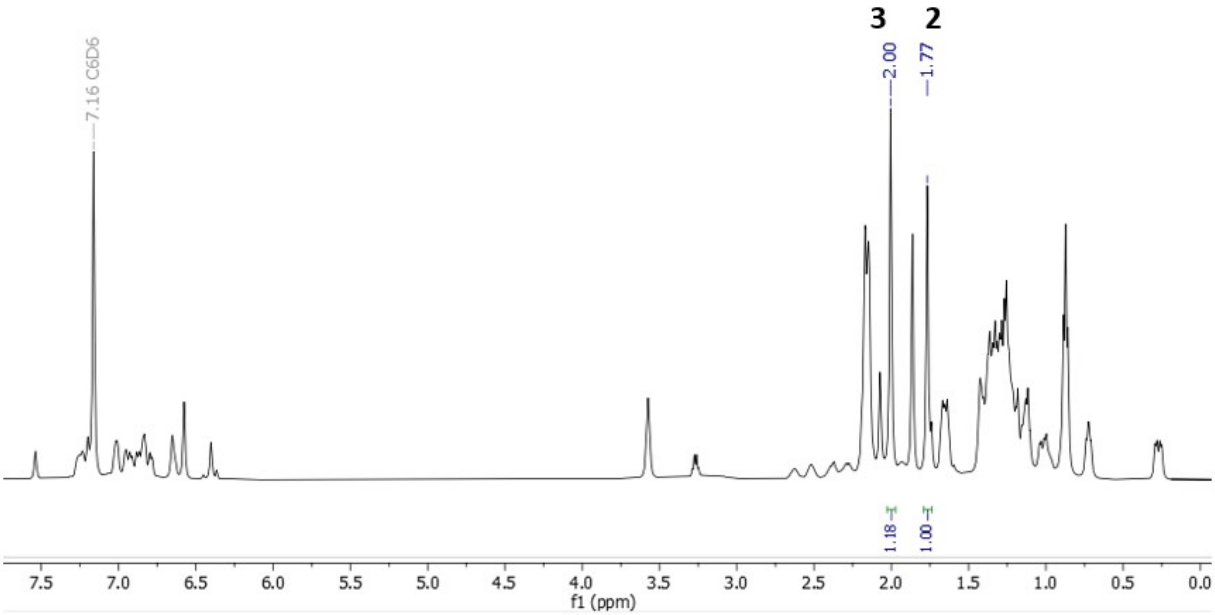

Figure S16. ^{1}H NMR (400 MHz, C_6D_6, 300K) of the crude reaction mixture between **1** and NaN_3 showing products **2** and **3** in a 1:1 ratio. The labeled peaks correspond to the -^{t}Bu group in (PNPN)$NbCl_2$(N[^{t}Bu]Ar) (**2**) and (PNP)Nb≡N(N[^{t}Bu]Ar) (**3**)

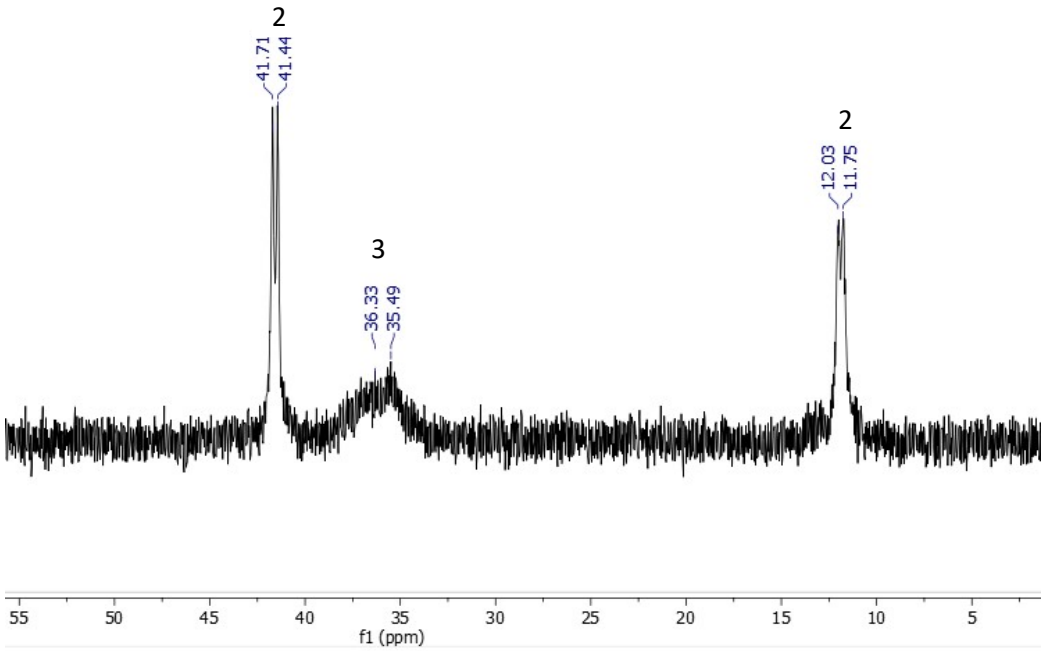

Figure S17. ^{31}P NMR (162 MHz, C_6D_6, 300K) of the crude reaction mixture between **1** and NaN_3 showing both products **2** and **3**

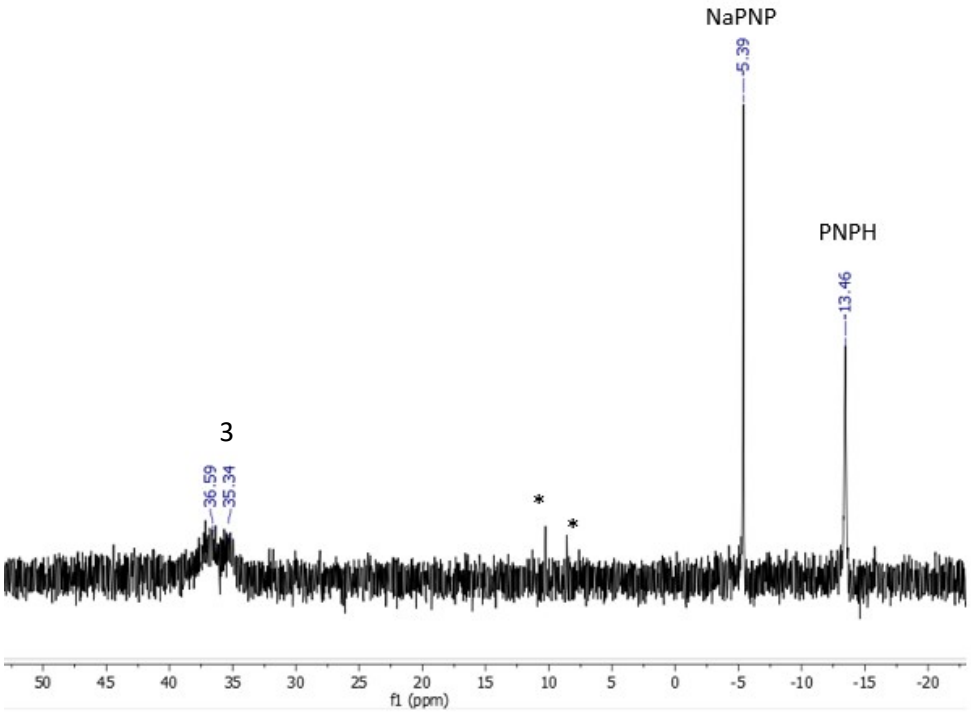

Figure S18. ^{31}P (162 MHz, C_6D_6, 300K) NMR of the crude reaction mixture from the reduction of (PNP=N)$NbCl_2$(N[^{t}Bu](Xyl)) (**2**) with 2 Na/NaCl. Impurities/unidentified products are marked as '*'.

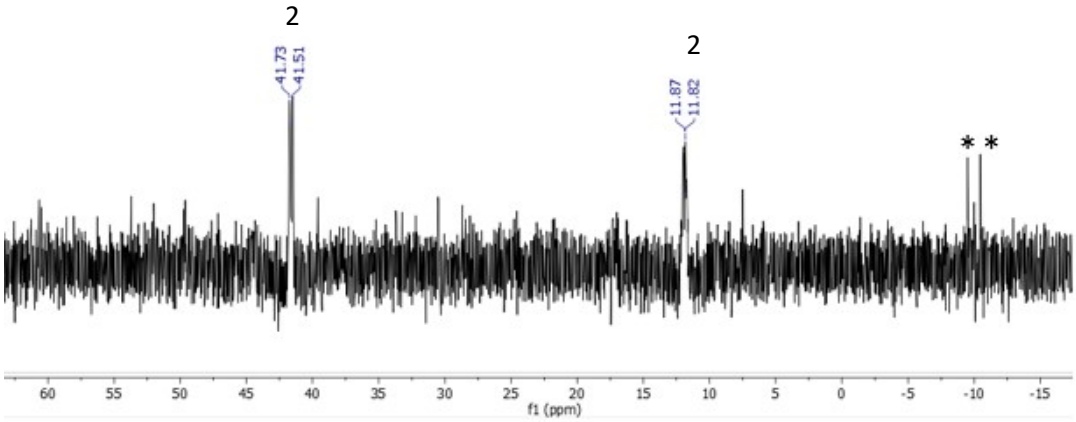

Figure S19. ^{31}P (203 MHz, C_6D_6, 300K) NMR of the crude reaction mixture from the oxidation of (PNP)Nb≡N[^{t}Bu](Xyl) (**3**) with $PhICl_2$. Impurities/unidentified products are marked as '*'.

NMR Spectroscopic yields for the conversion of 2 to 3 by reduction and 3 to 2 by oxidation

To determine the yields for the NMR reactions involving the reduction of complex **2** to **3** using two equiv Na/NaCl and oxidation of complex **3** to **2** using one equiv $PhICl_2$, an internal standard, 9,10-dihydroanthracene (9,10-DHA) was chosen as the internal reference peak did not overlap with any of the product peaks and the internal standard remained unreactive during the course of the reaction. This was confirmed by the presence of internal standard both before and after the reaction, and no new product formation in the NMR besides the expected impurities and unidentified products from the reaction that was conducted without the internal standard (Figures S18 and S19). The -^{t}Bu groups integrating to 9H's in the product were compared relative to the 9,10-DHA (4 H's).

$$c_{product} = \frac{int_{product}}{int_{standard}} \times \frac{4}{9} \times c_{standard}$$

Reduction of **2** to **3**: A solution of **2** (14 mg, 18 μmol) and 9,10-DHA (3.4 mg, 19 μmol) in 0.5 mL C_6D_6 was prepared and transferred to a J-Young NMR tube. ^{1}H and ^{31}P NMR (Figure S20) were collected after which the contents were transferred into a vial. Additional THF was added (2 mL) followed by Na/NaCl (17.4 mg, 36 μmol) and the reaction was stirred overnight. The solvent was evacuated under vacuum, and the residue was dissolved in pentane (4 mL), filtered through Celite, and the filtrate was evacuated under vacuum leaving behind an orange residue. To this was added 0.5 mL C_6D_6, and the contents were transferred into a J-Young NMR tube to quantify the formation of **3** (5.6 mg, 8 μmol, 43%).

Oxidation of **3** to **2**: A solution of **3** (9.4 mg, 13 μmol) and 9,10-DHA (5.8 mg, 32 μmol) in 0.5 mL C_6D_6 was prepared and transferred to a J-Young NMR tube. ^{1}H and ^{31}P NMR spectra (Figure S22) were collected before the reaction. To the NMR tube, $PhICl_2$ was added as a solid and ^{1}H and ^{31}P NMR spectra were collected after one day to quantify the formation of **2** (3.6 mg, 5 μmol, 36%).

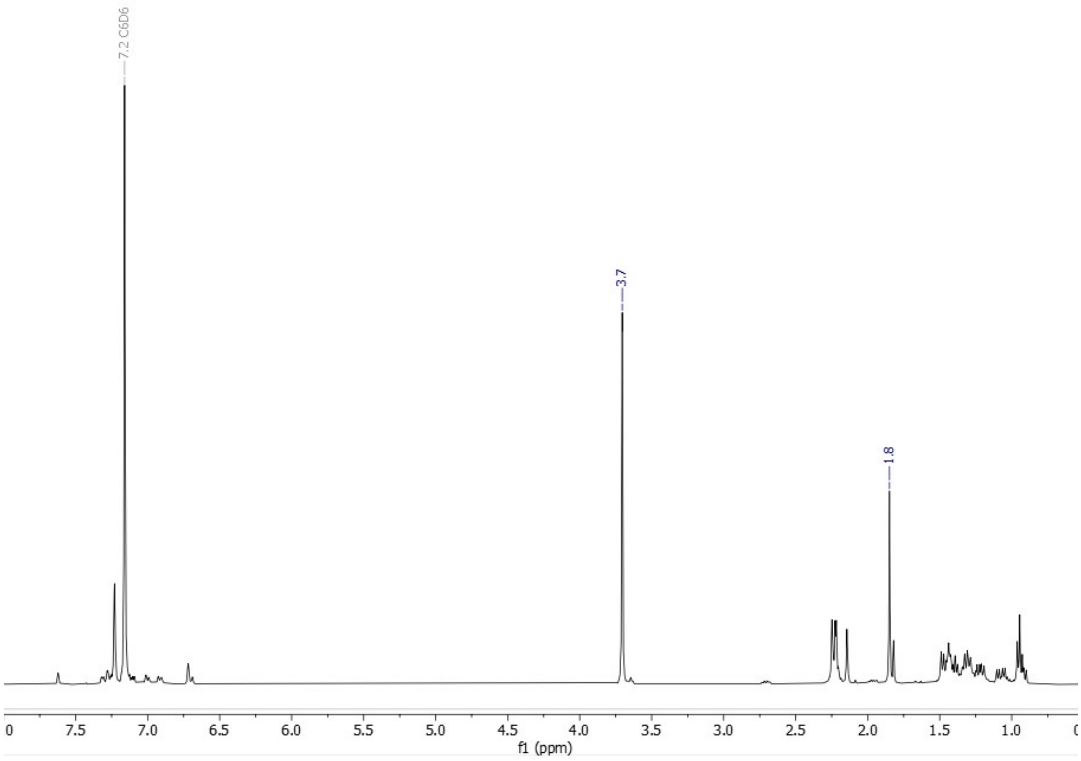

Figure S20. ^{1}H NMR (400 MHz, C_6D_6) of (PNP=N)$NbCl_2$(N[^{t}Bu](Xyl)) (**2**) before the addition of 2 equiv. Na/NaCl in the presence of internal standard (δ 3.7 ppm) with the -^{t}Bu group in **2** labeled for comparison.

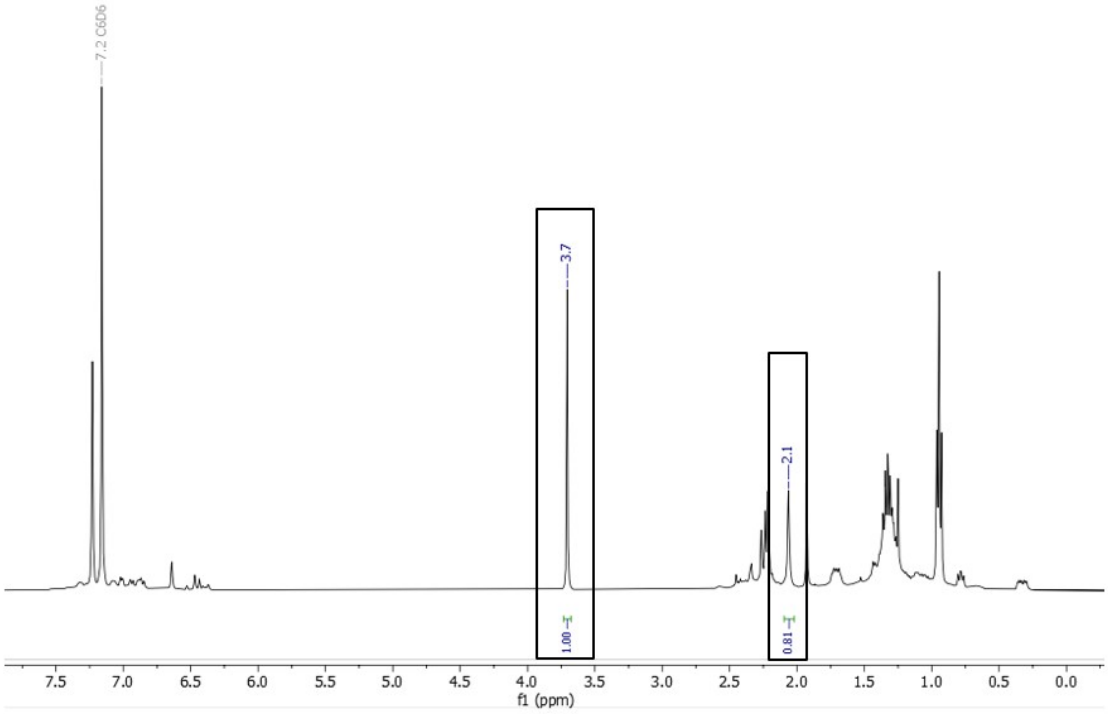

Figure S21. ^{1}H NMR (400 MHz, C_6D_6) of the conversion of (PNP=N)$NbCl_2$(N[^{t}Bu](Xyl)) (**2**) to (PNP)Nb≡N[^{t}Bu](Xyl) (**3**) in the presence of internal standard (δ 3.7 ppm) with the -^{t}Bu group in **3** labeled for comparison.

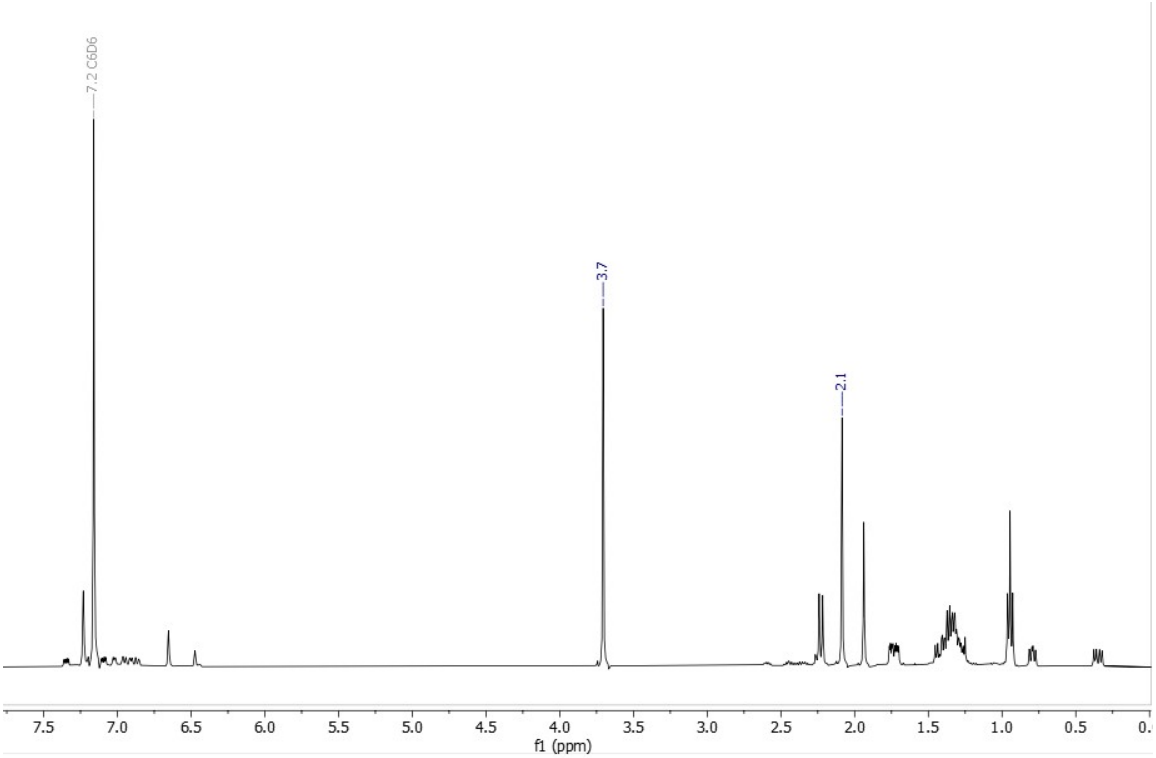

Figure S22. ^{1}H NMR (400 MHz, C_6D_6) of (PNP)Nb≡N[^{t}Bu](Xyl) (**3**) before the addition of 1 equiv. $PhICl_2$ in the presence of internal standard (δ 3.7 ppm) with the -^{t}Bu group in **3** labeled for comparison.

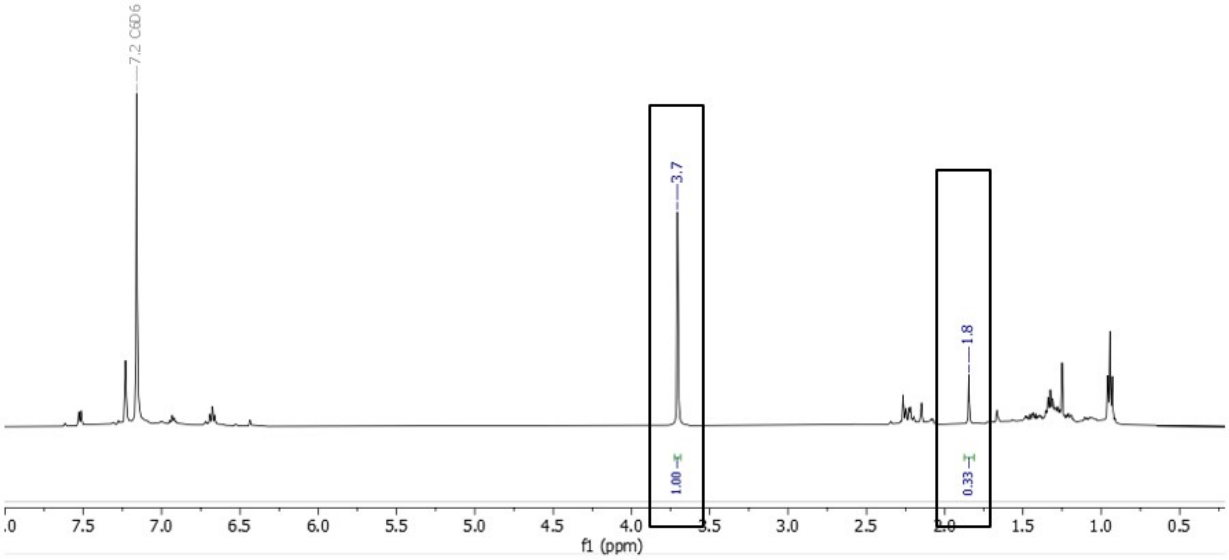

Figure S23. ^{1}H NMR (500 MHz, C_6D_6) of the conversion of (PNP)Nb≡N[^{t}Bu](Xyl) (**3**) to (PNP=N)$NbCl_2$(N[^{t}Bu](Xyl)) (**2**) in the presence of internal standard (δ 3.7 ppm) with the -^{t}Bu group in **2** labeled for comparison.

X-ray Crystallography

Crystallographic data for are summarized in **Tables S1-S2**. Suitable crystals for X-ray analysis of **2** and **3** were placed on the end of a Cryoloop coated in NVH oil. X-ray intensity data were collected on a Rigaku XtaLAB Synergy-S diffractometer[5] equipped with an HPC area detector (Dectris Pilatus3 R 200K or HyPix 3000HE) and employing confocal multilayer optic-monochromated Mo-Kα radiation (λ=0.71073 Å) at a temperature of 100K. Rotation frames were integrated using CrysAlisPro,[6] producing a listing of unaveraged F^2 and $\sigma(F^2)$ values. The intensity data were corrected for Lorentz and polarization effects and for absorption using SCALE3 ABSPACK[7] (minimum and maximum transmission 0.6143, 1.0000). The structure was solved by direct methods – SHELXT.[8] Refinement was by full-matrix least squares based on F^2 using SHELXL.[9] All reflections were used during refinement. The weighting scheme used was $w=1/[\sigma^2(F_o^2)+ (0.0772P)^2 + 11.2345P]$ where $P = (F_o^2 + 2F_c^2)/3$. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a riding model.

These results were checked using the IUCR's CheckCIF routine.

Table S1. Summary of Structure Determination of Compound 2•(1/2 pentane)

Empirical formula	$C_{40.5}H_{64}Cl_2N_3NbP_2$
Formula weight	818.69
Diffractometer	Rigaku XtaLAB Synergy-S (Dectris Pilatus3 R 200K)
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
A	15.9677(4)Å
B	12.7824(4)Å
C	21.3828(8)Å
β	103.243(3)°
Volume	4248.3(2)Å^3
Z	4
d_{calc}	1.280 g/cm^3
μ	0.515 mm^{-1}
F(000)	1732.0
Crystal size, mm	0.2 × 0.11 × 0.05
2θ range for data collection	4.816 - 56.564°
Index ranges	$-20 \leq h \leq 21$, $-17 \leq k \leq 17$, $-28 \leq l \leq 28$
Reflections collected	123109
Independent reflections	10530[R(int) = 0.0921]
Data/restraints/parameters	10530/24/468
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	$R_1 = 0.0669$, $wR_2 = 0.1577$
Final R indexes [all data]	$R_1 = 0.1035$, $wR_2 = 0.1812$
Largest diff. peak/hole	2.07/-0.62 eÅ^{-3}

Table S2. Summary of Structure Determination of Compound 3

Empirical formula	$C_{38}H_{58}N_3NbP_2$
Formula weight	711.72
Diffractometer	Rigaku XtaLAB Synergy-i (HyPix 3000HE)
Temperature/K	100
Crystal system	triclinic
Space group	P**Error!**
a	13.0304(3)Å
b	13.4804(3)Å
c	14.1210(3)Å
α	101.554(2)°
β	111.506(2)°
γ	99.442(2)°
Volume	2182.89(9)Å^3
Z	2
d_{calc}	1.083 g/cm^3
μ	0.374 mm^{-1}
F(000)	756.0
Crystal size, mm	0.26 × 0.15 × 0.11
2θ range for data collection	3.846 - 54.968°
Index ranges	$-16 \leq h \leq 16$, $-17 \leq k \leq 16$, $-18 \leq l \leq 18$
Reflections collected	63386
Independent reflections	9946[R(int) = 0.0768]
Data/restraints/parameters	9946/0/412
Goodness-of-fit on F^2	1.075
Final R indexes [I>=2σ (I)]	R_1 = 0.0474, wR_2 = 0.1294
Final R indexes [all data]	R_1 = 0.0669, wR_2 = 0.1368
Largest diff. peak/hole	0.50/-0.60 eÅ^{-3}

Computational Details

All calculations were carried out using density functional theory[10] (DFT) implemented in the Jaguar 9.1 suite of ab initio quantum chemistry programs.[11] The Becke's three-parameter exchange functional B3LYP[12] with Grimme's D3 dispersion correction[13] was employed. Geometry optimizations were performed with the 6-31G** basis set, where Nb was represented with the Los Alamos LACVP basis set,[14-16] which contains the relativistic effective core potentials. The energies of the optimized structures were reevaluated with high quality triple-ζ basis set cc-pVTZ(–f).[17] Nb was treated with LACV3P** basis set, in which the exponents were decontracted to match the triple-ζ functions of the main group elements. Vibrational frequencies within the harmonic approximation were computed with the optimized geometries at the same level of theory to confirm proper convergence to well-defined minima or saddle points on the potential energy surface. Calculated vibrational zero-point energies and vibrational entropy corrections were used for the proper approximations of thermodynamics. Solvation free energies were evaluated by a self-consistent reaction field (SCRF) approach[18–20] based on accurate numerical solutions of the Poisson–Boltzmann equation. In the results reported, solvation calculations were carried out with the 6-31G**/LACVP basis set employing the dielectric constant of ε = 7.6 for THF on the gas-phase optimized structures. We employed the standard set of optimized radii in Jaguar for H (1.150 Å), C (1.900 Å), N (1.600 Å), P (2.074 Å), Cl (1.974 Å) and Nb (1.583 Å).[21] The solution-phase Gibbs free energies were computed as follows:

$$G(Sol) = G(gas) + G^{solv} \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(Gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta G(Sol) = \Sigma G(Sol) \text{ for products} - \Sigma G(Sol) \text{ for reactants} \quad (4)$$

G(Sol) is the solvation-corrected Gibbs free energy from gas phase free energy G(gas); H(gas) is the enthalpy in gas phase; T is the temperature (298.15 K); S(gas) is the entropy in the gas phase; E(SCF) is the self-consistent field converged electronic energy; and ZPE is the vibrational zero-point energy. Note that entropy here refers specifically to the vibrational/rotational/translational entropy of the solute(s). The solvent entropies are implicitly included in the continuum model.

The Xylyl group of anilide ligand was replaced with the phenyl group to reduce computational cost without any perturbation of electronic and steric properties.

Intrinsic Bond Orbital (IBO) Analysis of N_2 Release

N_2 release is the key step in generating the transient nitride intermediate **D** (Fig. 3; manuscript) followed by ligand-assisted N–P bond formation. We conducted detailed electronic structure analysis with respect to the spin density and IBO of key atoms to elucidate the driving force of this process. Figure S24 shows the Mulliken spin density of the metal center, three nitrogen atoms of the azide bound to niobium, and the nitrogen atom in the PNP scaffold. The reaction coordinate is defined as the Nα–Nβ distance increasing 0.05 Å from intermediate **A**.

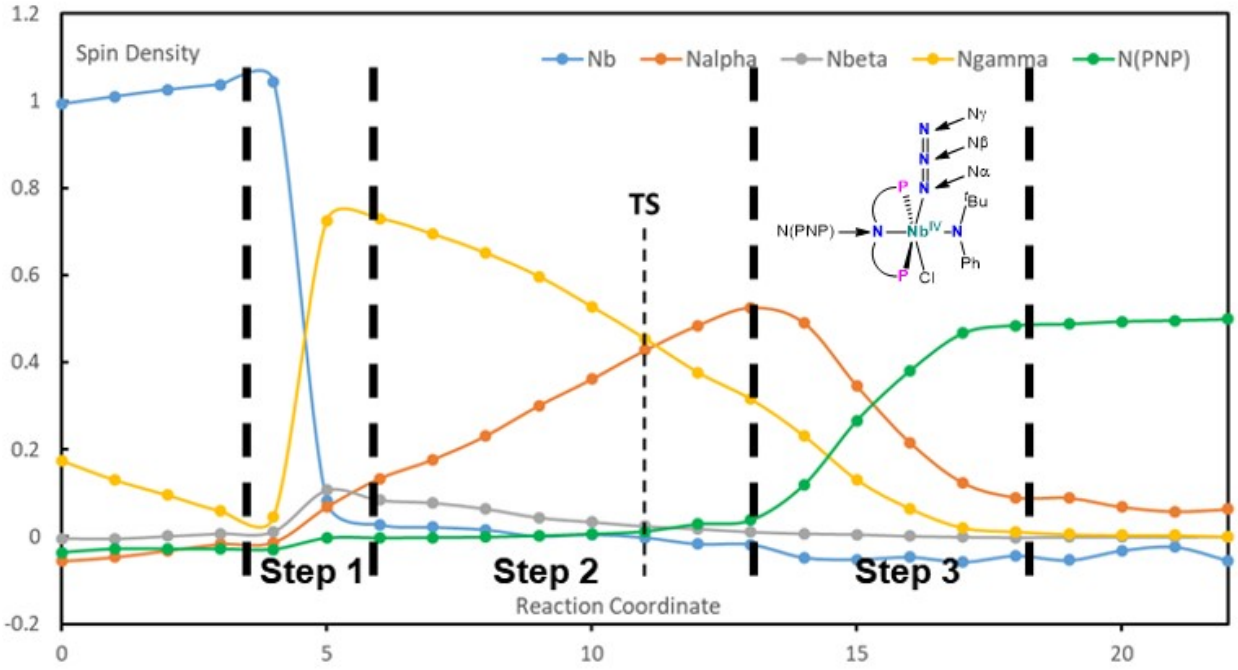

Figure S24. Mulliken spin density of key atoms along the reaction coordinate. Reaction coordinate 0 indicates intermediate **A**. TS indicates the geometry corresponding to the transition state.

Interestingly, we could detect three consecutive steps involving different intramolecular electron transfer. In the first step, the spin density of the metal center becomes zero and it moves to the azide moiety. IBO suggests that this reaction corresponds to an electron transfer from π*(Nb–N_3) to π(Nβ–Nγ), making the Nb(V) intermediate, and the geometry of azide changes from linear to bent simultaneously.

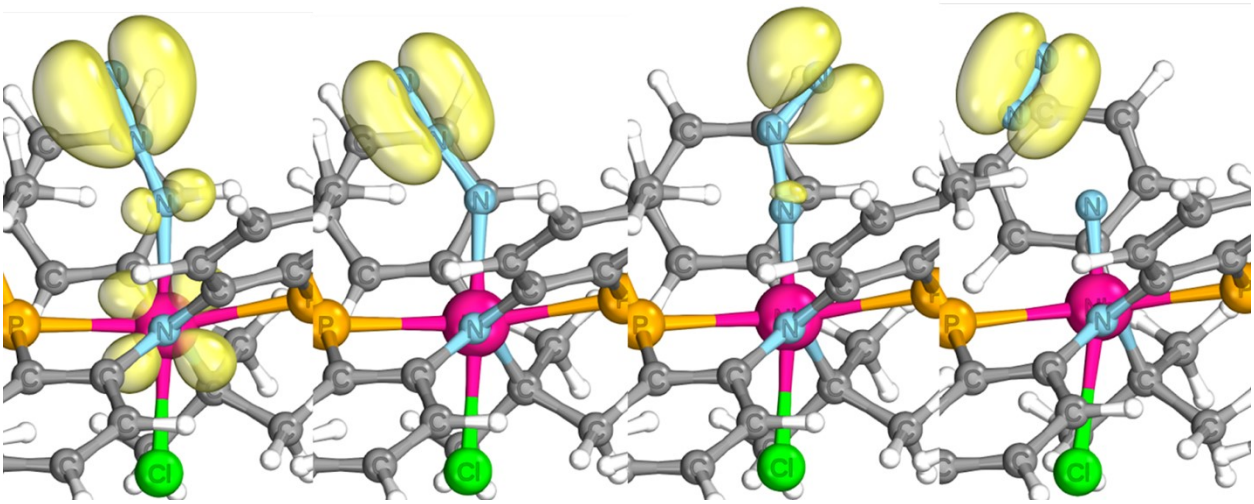

Figure S25. IBO #183 (yellow, α) obtained from reaction coordinate 0, 2, 4 and 20.

The second step occurs with the Nα–Nβ sigma bond cleavage, rendering α- and β-spin electrons on the Nb–Nα bond and the Nβ lone pair, respectively. Therefore, the spin density of Nα continuously increases while the spin density of Nγ diminishes.

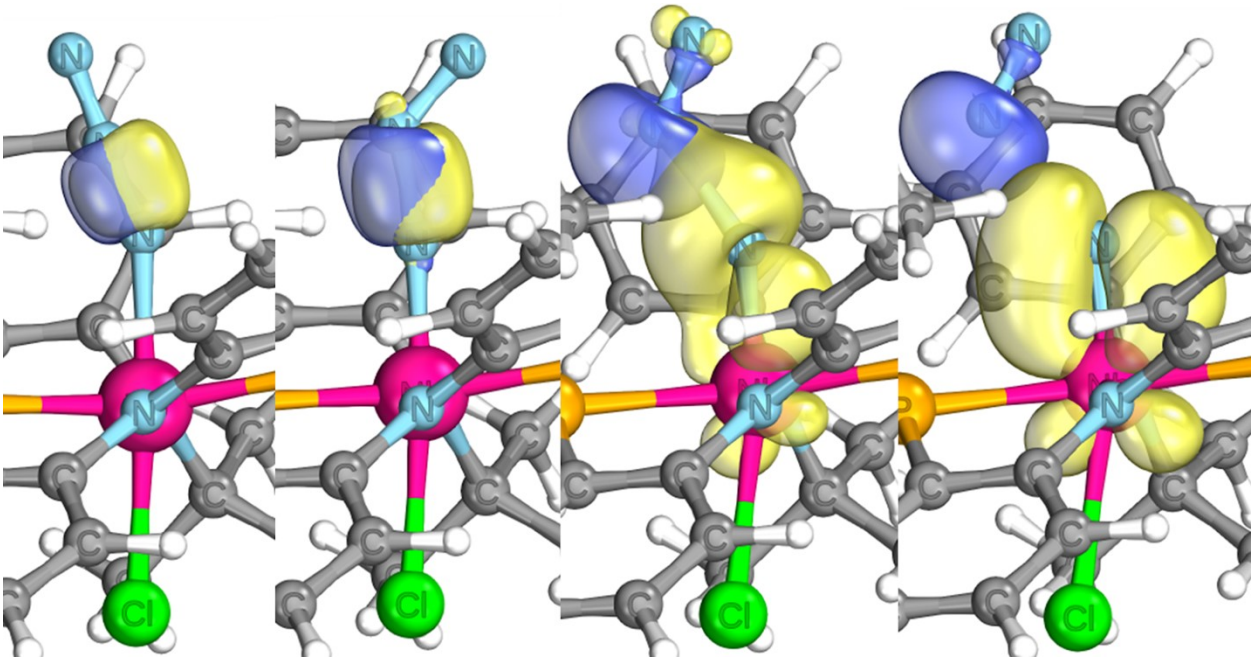

Figure S26. IBO #62 (yellow, α) and #244 (blue, β) obtained from reaction coordinate 0, 4, 15 and 20.

Finally, the redox-active PNP ligand donates an electron in the last step. It is notable that only the α-spin electron moves from the HOMO of PNP to the Nb–Nα bond. Combined with the β-spin electron on the Nb–Nα bond derived in the second step, Nb–Nα becomes a triple bond. From this analysis, we can understand that the spin distribution along the conjugate pincer scaffold and the formation of triple bond are the driving force of nitride formation.

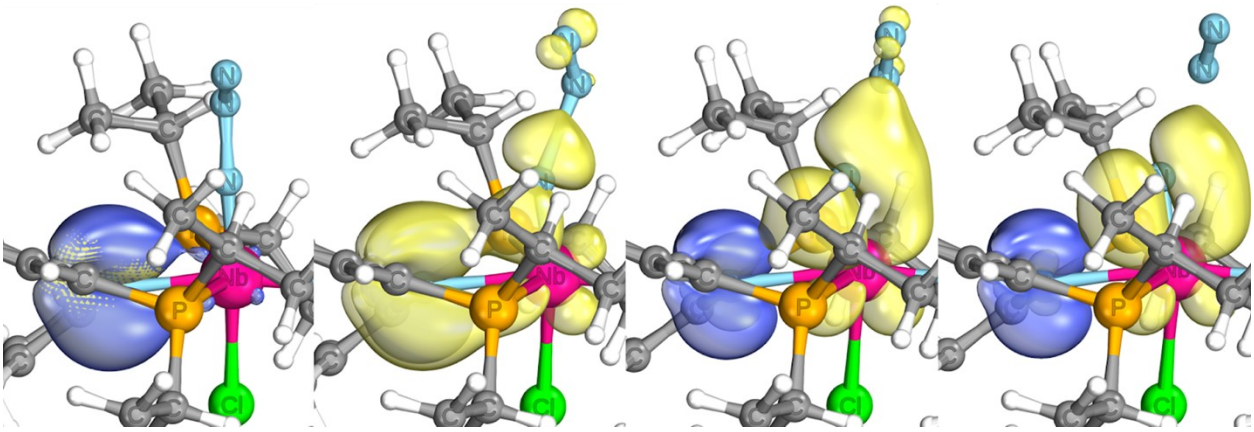

Figure S27. IBO #179 (yellow, α) and #360 (blue, β) obtained from reaction coordinate 5, 14, 16 and 20.

Detailed Mechanisms of the Formation of B

Once the nitride intermediate **D** is generated by N_2 release, it can undergo direct N–P bond formation with 18.0 kcal/mol of barrier (**D-TS2**). The alternative approach involves several isomerizations with respect to the coordination site of the anilide and chloride ligands. Triggered by an intramolecular electron transfer from anilide to PNP moiety, the elongation of Nb–anilide bond relieves steric congestion of the metal center enabling chloride ligand to take the equatorial position. Following this process, isomers **E** and **F** are reversibly formed from **D**, and the following N–P bond formation from **F** is much more facile than from **D**.

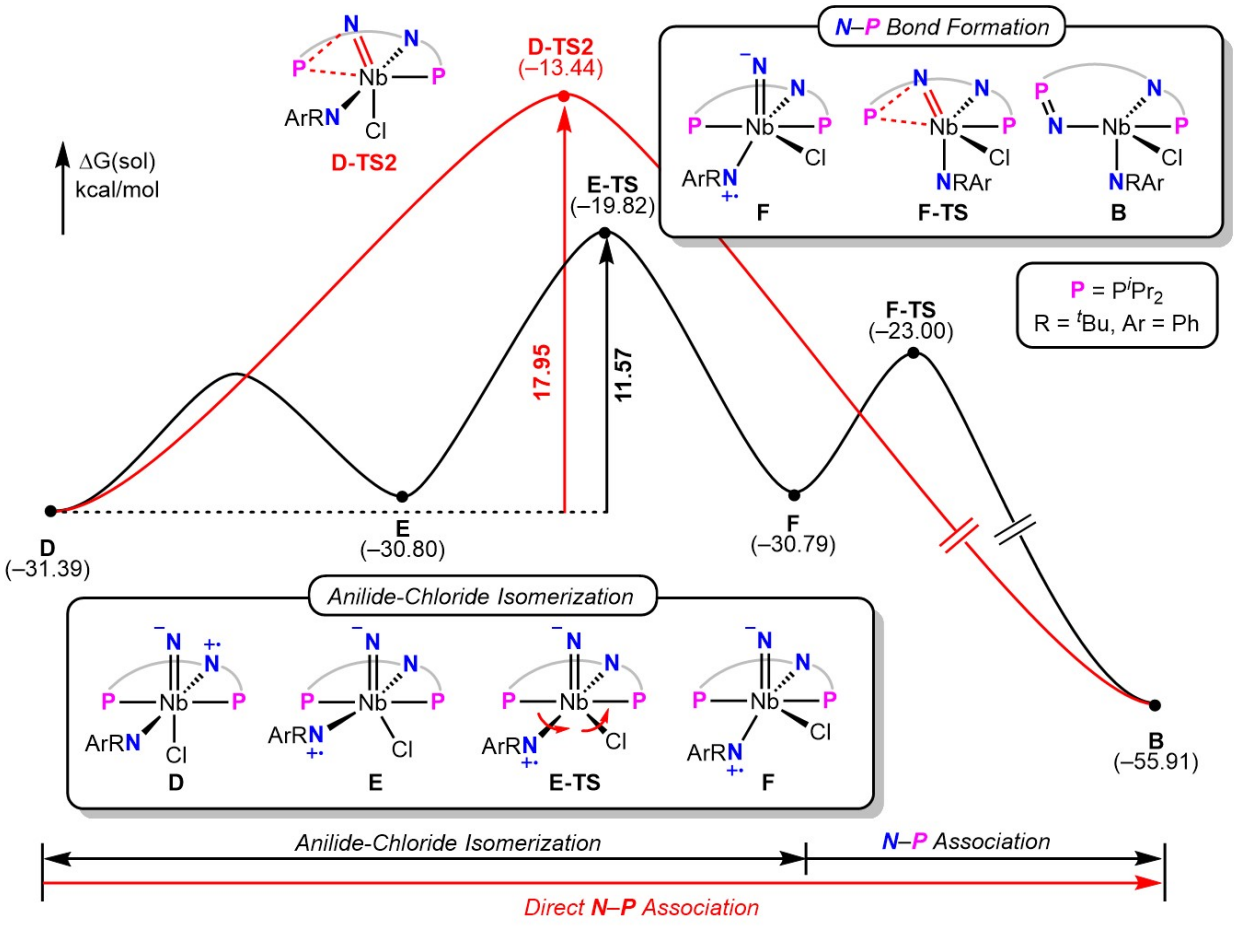

Figure S28. Gibbs energy profile of the formation of **B**. Numbers indicated in the parenthesis are relative to the azide-bound complex **A**.

Relationship between the Stability of the Nitride Intermediate and the Pincer Redox Non-Innocence

It is surprising that the analogous reaction forming the phosphide instead of nitride shows a different reactivity relative to this case.[1] One can immediately recognize that the liberation of N_2 and CO are highly exothermic and endothermic when X = N and P, respectively (Figure S29a). Electronic structure analysis shows that the radical character is distributed through the conjugated PNP scaffold in **D** while localized on the terminal phosphide in **D_P**. Figure S29b illustrates the conceptual MO diagram between the metal center, nitride (or phosphide) and PNP moiety. The low-lying orbitals of nitrogen make the Nb–N bonds more electronegative, resulting in the donation of an electron from the HOMO of the PNP scaffold. This intramolecular electron transfer supports the Nb nitride formation in **D** and distributes the spin density throughout the conjugated system simultaneously. In contrast, the high-lying orbitals of phosphorus prevent the electron transfer, rendering the spin density localized on the terminal phosphide resulting in the phosphidyl radical complex **D_P**.

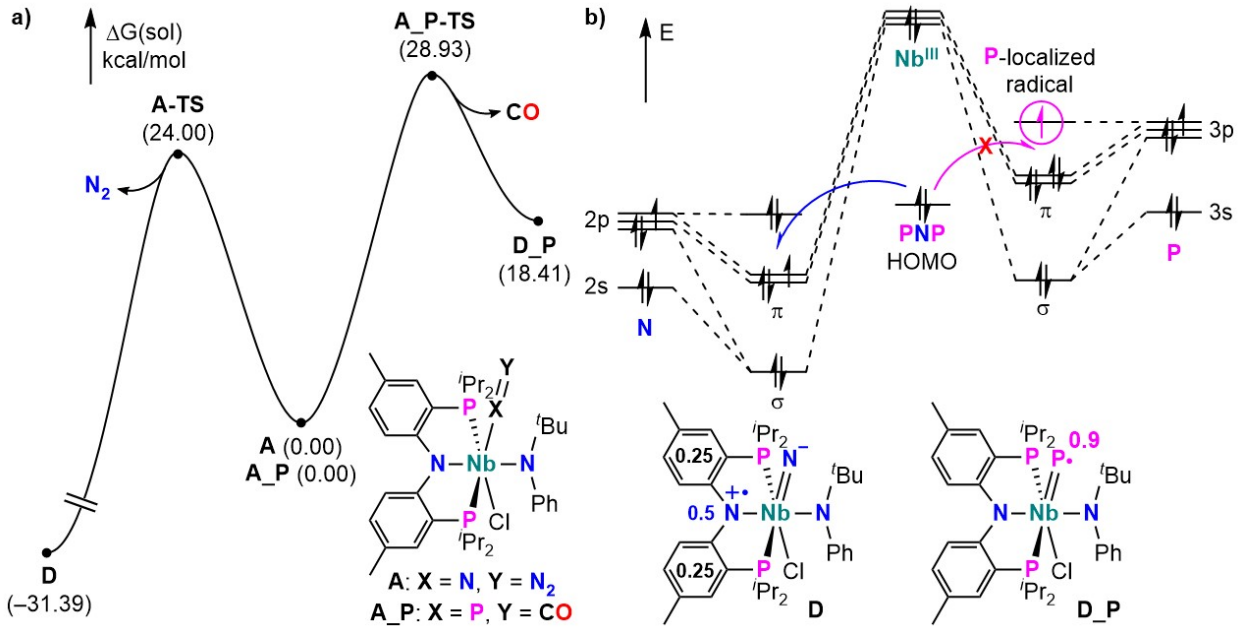

Figure S29. (a) N_2 and CO release process making nitride and phosphide intermediate, respectively. (b) Conceptual MO diagrams of **D** and **D_P**. Numbers indicate the sum of spin density on each moiety.

Theoretical Investigation on the Role of Anilide

We conducted molecular orbital analysis to understand the precise role of anilide in the stabilization of **C** and in the formation of the nitride. Figure S30a illustrates the disproportionation step that the Nb(IV) intermediate **B** generates Nb(V) and Nb(III) products, while the anilide aryl makes an additional coordination to the Nb(III) center. The strong π-donation from the anilide was identified in the HOMO–1 of **2** while the pseudo-octahedral structure maximizes the interaction (Figure S30b). In contrast, the metal center of **C** plays a role of π-base, donating an electron to the LUMO of anilide. Finally, to indirectly estimate the effect of orbital interactions, we examined the disproportionation of hypothetical intermediate **B'** where the anilide is substituted with a chloride ligand (Figure S30c). Surprisingly, the process starting from **B'** requires 21.8 kcal/mol of energy to proceed, and this result strongly corroborates the stabilization afforded by the anilide in the preparation of nitrides.

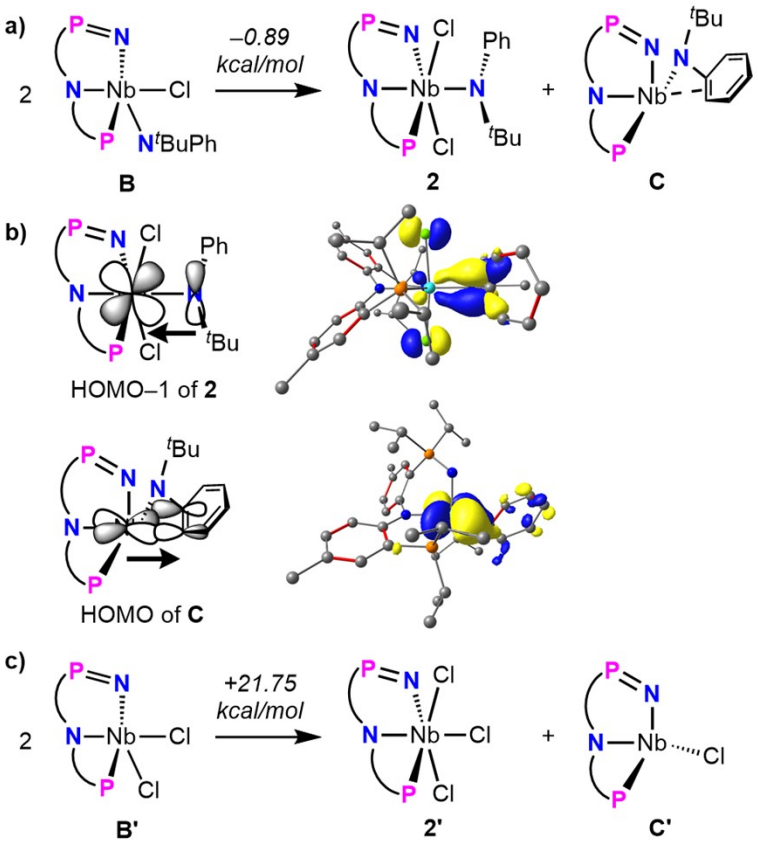

Figure S30. (a) The disproportionation scheme of intermediate **B**. (b) Favorable orbital interactions between anilides and metal centers. (c) The disproportionation scheme of hypothetical intermediate **B'**.

Energy Components for the DFT-Optimized Structures

Table S3. Computed Energy Components for Optimized Structures

	E(SCF) (eV)	**ZPE (kcal/mol)**	**S(gas) (cal/mol K)**	**G^{solv} (kcal/mol)**
	B3LYP-D3 /cc-pVTZ(-f)	B3LYP-D3 /6-31G**/LACVP	B3LYP-D3 /6-31G**/LACVP	B3LYP-D3 /6-31G**/LACVP
N_2	–2981.407	3.52	45.78	0.00
CO	–3084.528	3.16	47.24	0.00
A	–78320.836	528.96	285.72	–12.59
A-TS	–78319.812	526.46	285.96	–9.63
D	–75339.751	521.15	275.02	–17.10
D-TS2	–75339.447	521.42	273.45	–11.61
E	–75339.943	522.01	276.58	–11.74
E-TS	–75339.713	521.62	274.90	–11.62
F	–75339.924	521.89	275.87	–14.71
F-TS	–75339.767	521.63	274.16	–13.74
B	–75341.349	522.37	276.94	–10.12
2	–87867.289	523.39	284.68	–11.46
C	–62815.391	520.28	265.96	–9.70
C-TS	–62814.460	520.23	267.34	–10.01
3	–62816.477	520.95	268.86	–11.65
A_P	–86224.898	526.89	288.51	–13.10
A_P-TS	–86223.602	524.93	292.56	–10.82
D_P	–83139.047	521.30	278.17	–11.77
B'	–75773.063	384.99	237.26	–17.70
2'	–88298.547	385.98	243.09	–14.85
C'	–63246.793	383.67	232.60	–16.25

Cartesian Coordinates of the Optimized Geometries

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N_2

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N	1.088109255	0.000000000	-2.631234407
N	1.088109255	0.000000000	-3.736182213

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CO

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C	-0.147268862	-0.018646235	-2.334356070
O	-0.147268862	-0.018646235	-3.472287416

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A

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Nb	0.142612278	0.061449915	0.192831993
N	-0.681051135	-0.073356509	2.208122969
C	-0.466497332	-1.209551215	3.008783102
C	-1.511386871	0.939632833	2.712790251
C	-1.304294825	2.284367323	2.312010765
C	-2.142829180	3.293269157	2.806314707
C	-3.218548536	3.022104502	3.653217077
C	-3.433338165	1.685004115	4.015539169
C	-2.601945400	0.669816017	3.567209005
C	-0.276530623	-1.118582368	4.398833752
C	-0.108283646	-2.258242846	5.177736759
C	-0.127917290	-3.536524534	4.607324600
C	-0.287488252	-3.628489494	3.219472647
C	-0.420669645	-2.496009827	2.409400225
N	0.769789457	0.064260937	-1.769486070
Cl	2.325251579	-0.616685271	1.163548470
C	-4.123903751	4.119166374	4.159599304
C	0.048633296	-4.781200409	5.444667816
P	-0.624659836	-2.458859682	0.587461233
C	0.304029346	-3.850295305	-0.307816356
C	0.536832690	-5.168272495	0.448319227
C	1.631590486	-3.361666441	-0.904655635
C	-2.448083401	-2.862807512	0.304982871
C	-3.337317467	-2.013026953	1.226765275
C	-2.808447838	-4.348455906	0.451263189
P	0.092853710	2.558384895	1.157686353
C	1.406848669	3.356557608	2.240554333
C	0.937726557	4.631408691	2.960953474
C	1.912453413	2.323016644	3.261516809
C	-0.402360171	3.792014599	-0.208669916
C	-1.752226233	4.514803410	-0.086637944
C	0.721684098	4.794866085	-0.524738312
C	0.062200241	-0.207738727	-3.073472023
C	-0.585541189	1.096764326	-3.583154917
C	-1.037800670	-1.260974407	-2.863637447
C	1.038742423	-0.742414236	-4.141047001
C	2.080390692	0.641936183	-1.914128423
C	2.216883898	2.033321381	-2.022961140
C	3.473860979	2.629694462	-2.131982803
C	4.621387959	1.838848591	-2.133293867
C	4.497107029	0.449606985	-2.037744999
C	3.243310213	-0.144531205	-1.931097269
H	-1.962575316	4.322154522	2.520702600
H	-4.279648304	1.432913303	4.651242256
H	-2.802954197	-0.355580896	3.855872393
H	-0.274302095	-0.138254702	4.863481998
H	0.035499632	-2.151675463	6.250577927
H	-0.310888797	-4.615097523	2.775683165
H	-3.966730356	4.310363770	5.228791714
H	-3.953146219	5.059242249	3.626445770
H	-5.178819180	3.850746393	4.031888962
H	-0.218983188	-4.602222443	6.490610123
H	-0.571826160	-5.605097294	5.075007439
H	1.089674473	-5.128005981	5.428606033
H	-0.380928546	-4.050508976	-1.143918037
H	-0.374624342	-5.598036289	0.867851913
H	0.959432304	-5.904673576	-0.245671138
H	1.260651350	-5.027274132	1.255794883
H	1.485068202	-2.480801821	-1.529837012
H	2.069233179	-4.156966209	-1.520495534
H	2.344143867	-3.092066526	-0.121413894
H	-2.619607449	-2.552891731	-0.733082712
H	-3.238081217	-2.345762730	2.265246868
H	-3.091694355	-0.952927291	1.191252947
H	-4.387134075	-2.128258467	0.935134292
H	-2.584383965	-4.707986355	1.461980462
H	-2.290212154	-4.987437248	-0.268520474
H	-3.884977818	-4.480456829	0.289693177
H	2.225856543	3.600702763	1.553439856
H	0.507418931	5.378137112	2.288361311
H	1.787342072	5.095394135	3.475412846
H	0.186109126	4.388849258	3.717781782
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C	0.132902175	-0.816475868	4.264251232

C	0.573974788	-1.890178442	5.025737286
C	0.563051462	-3.199007750	4.523798943
C	0.132480428	-3.377489090	3.207293272
C	-0.299018472	-2.308814764	2.414613724
N	0.680651784	0.375258714	-1.805072546
Cl	2.095780373	-0.263175786	1.073330283
C	-3.597478151	4.326165199	4.918293476
C	1.020324349	-4.362519741	5.370438099
P	-0.718384385	-2.440169334	0.642749667
C	0.280589104	-3.817893982	-0.165679201
C	-0.057034962	-5.273643970	0.201742366
C	1.788589954	-3.560159922	-0.040078882
C	-2.519741058	-2.983297348	0.569053233
C	-2.962332964	-3.999330759	1.632061601
C	-2.919566154	-3.395849466	-0.857064605
P	-0.510474503	2.686220169	0.817308724
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C	0.700800776	5.187311172	1.671223998
C	1.615843296	3.017174482	2.597529888
C	-1.544296622	3.703197479	-0.400976151
C	-2.381666660	4.886330128	0.108338922
C	-0.674433708	4.090492725	-1.606887579
C	2.002939701	0.887422800	-2.332323074
C	3.028714418	-0.263506234	-2.357448816
C	2.521406651	2.017691374	-1.433275223
C	1.846827865	1.454764009	-3.759742498
C	-0.096825182	-0.309142530	-2.802562952
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C	-0.666706681	-2.359545708	-3.984023333
C	-1.633821487	-1.679106951	-4.724161625
C	-1.820039749	-0.308008552	-4.519483566
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D_P

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P	-0.576977432	-2.533060074	0.662689209

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C	-0.328665227	4.321465492	-1.386748433
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H	2.766795158	1.484451532	-0.327395290
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H	-2.604610682	1.064552546	-4.920635223
H	-1.037703514	1.864555001	-3.170788050
P	-2.409349442	0.218334794	-0.590576768

Vibrational Frequencies (in cm^{-1}) of the Optimized Structures

N_2

2460.69

CO

2209.07

A

22.76 34.29 41.39 44.60 46.26 48.60
53.46 58.26 61.17 65.64 70.71 74.65
76.14 82.86 88.18 91.81 94.83 98.71
102.10 110.17 116.10 126.97 129.39 133.76
137.03 143.56 151.10 154.37 160.47 162.52
171.37 175.94 186.60 194.85 205.20 217.30
221.75 229.21 233.19 243.99 257.74 262.52
267.15 269.41 270.45 271.14 279.32 282.50
285.40 288.35 296.77 301.11 305.61 307.40
311.66 312.60 314.21 323.64 337.16 340.05
342.46 344.94 349.47 355.28 371.25 378.37
382.36 394.31 406.78 414.27 415.71 425.49
430.91 433.41 442.91 451.98 462.30 484.41
492.33 502.49 504.96 515.39 516.77 535.70
545.72 554.48 569.92 571.39 574.27 598.45
611.84 618.10 621.93 629.00 638.15 642.08
646.80 702.98 708.78 715.39 736.34 756.01
756.81 802.74 827.63 834.73 852.63 855.59
868.26 871.66 893.36 894.43 898.73 900.26
906.42 908.41 911.47 924.98 927.61 928.52
937.94 950.37 952.70 954.10 958.46 963.48
967.53 975.14 976.99 977.92 979.71 980.03
983.94 985.16 994.74 1020.34 1024.49 1026.65
1058.71 1060.29 1063.20 1064.94 1066.89 1068.18
1071.54 1078.31 1083.21 1086.76 1088.41 1105.46
1106.94 1112.22 1122.61 1131.52 1183.18 1190.23
1192.81 1193.75 1193.92 1195.89 1200.25 1210.41
1215.84 1225.15 1234.62 1244.96 1246.14 1248.47
1272.48 1283.62 1285.21 1299.37 1302.92 1306.78
1311.57 1319.51 1321.45 1326.29 1327.05 1334.06
1335.74 1337.90 1355.73 1360.70 1405.69 1411.35
1416.72 1417.61 1418.11 1422.86 1424.51 1427.21
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1501.94 1502.07 1502.35 1502.91 1504.69 1505.10
1506.92 1507.62 1508.21 1509.04 1510.91 1512.23
1513.23 1518.17 1518.99 1520.23 1521.25 1522.03
1524.71 1525.32 1527.69 1530.80 1531.62 1534.89
1537.15 1544.01 1596.37 1604.50 1629.74 1648.53
1649.58 1656.02 2223.44 3021.23 3030.60 3031.29
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3058.44 3069.22 3087.70 3088.82 3098.65 3100.89
3101.65 3111.88 3112.08 3112.79 3115.76 3116.87
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A-TS

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53.04 59.02 64.77 68.70 70.12 72.26
74.74 79.69 84.32 88.43 91.38 94.31
103.43 105.28 107.76 115.12 119.54 125.46
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426.36 431.65 432.15 439.51 450.22 459.98
466.98 483.50 495.53 501.57 509.65 513.17
519.46 541.18 547.93 551.50 568.98 571.41
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D

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187.96 193.37 197.98 214.40 225.15 230.88
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287.37 294.89 300.12 302.92 307.71 312.61
314.17 317.80 327.13 329.57 345.69 346.07
359.67 367.13 377.13 384.55 397.68 402.21
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746.60 753.83 807.91 814.14 827.48 849.32
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1328.92 1331.43 1336.53 1342.29 1344.44 1352.55
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1508.07 1509.46 1512.30 1514.77 1516.69 1519.93
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D-TS2

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E-TS

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