Supporting Information for:
Molecular Titanium Nitrides: Nucleophiles Unleashed

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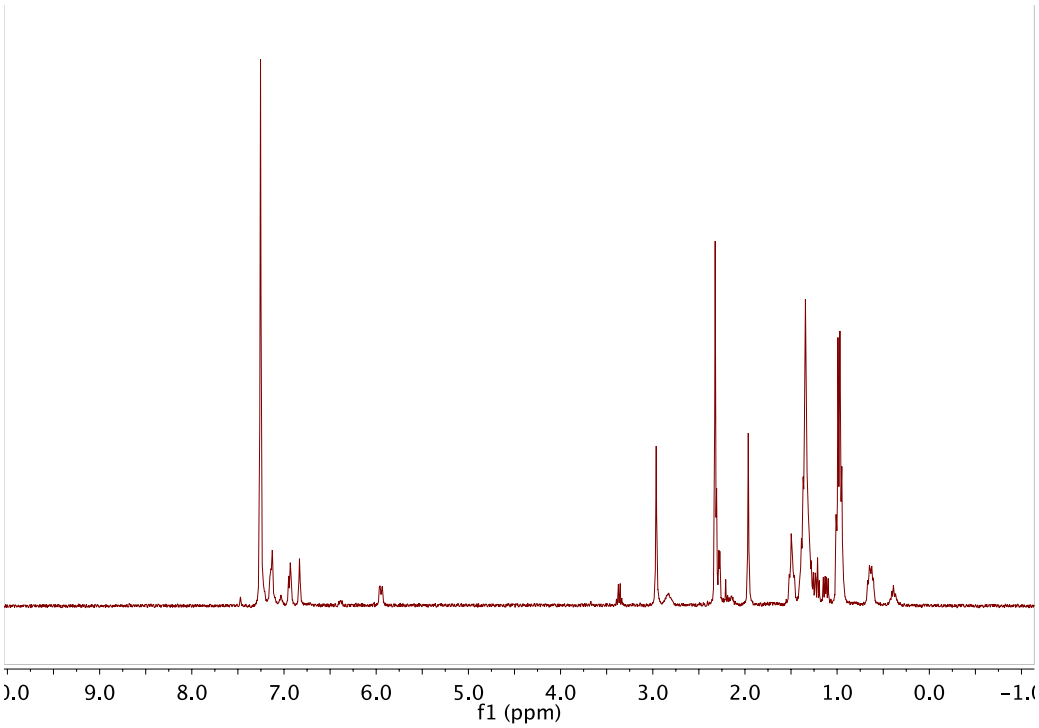

Figure S1: ^{1}H NMR Spectrum of **2** in C_6D_6, 400 MHz, 300K

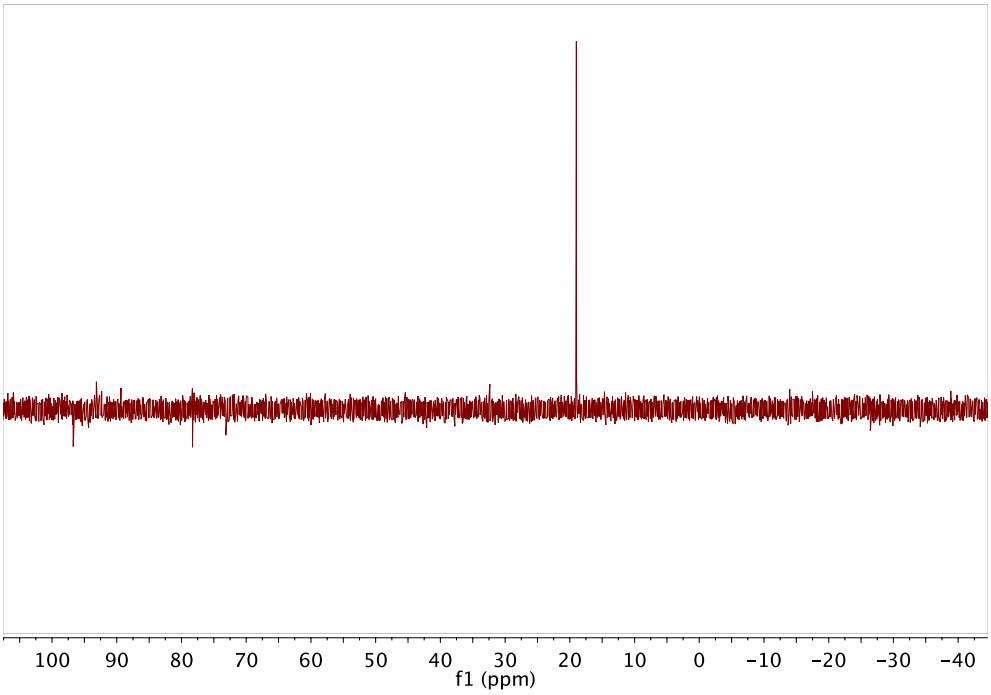

Figure S2: $^{31}P\{^{1}H\}$ NMR Spectrum of **2** in C_6D_6, 162 MHz, 300K

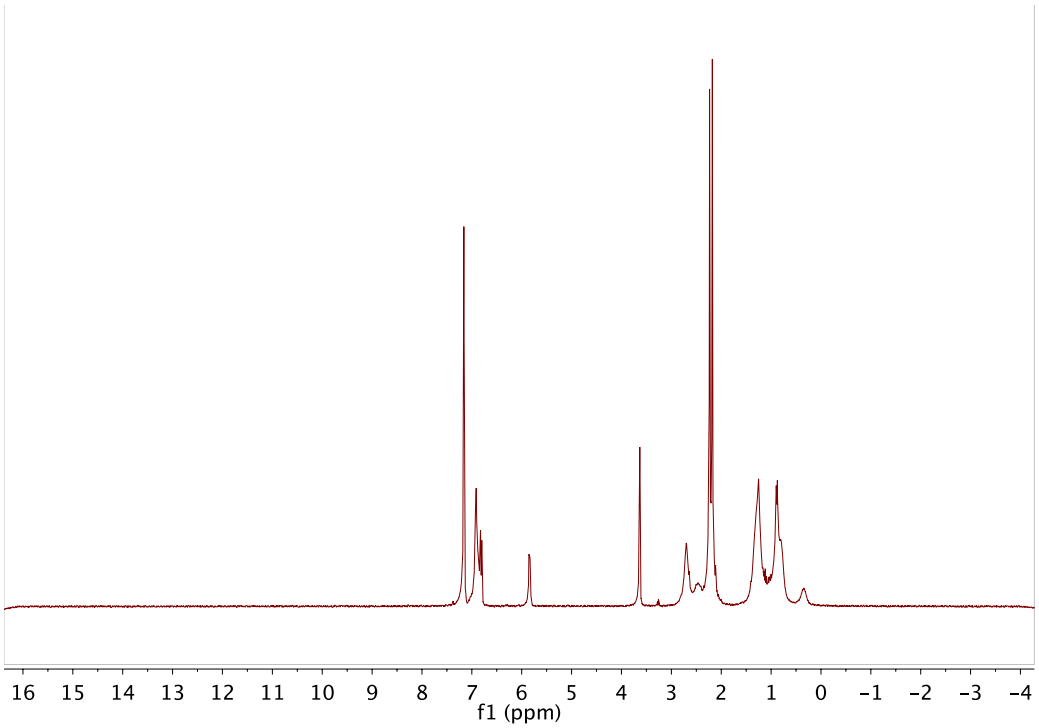

Figure S3: ^{1}H NMR Spectrum of **3** in C_6D_6, 400 MHz, 300K

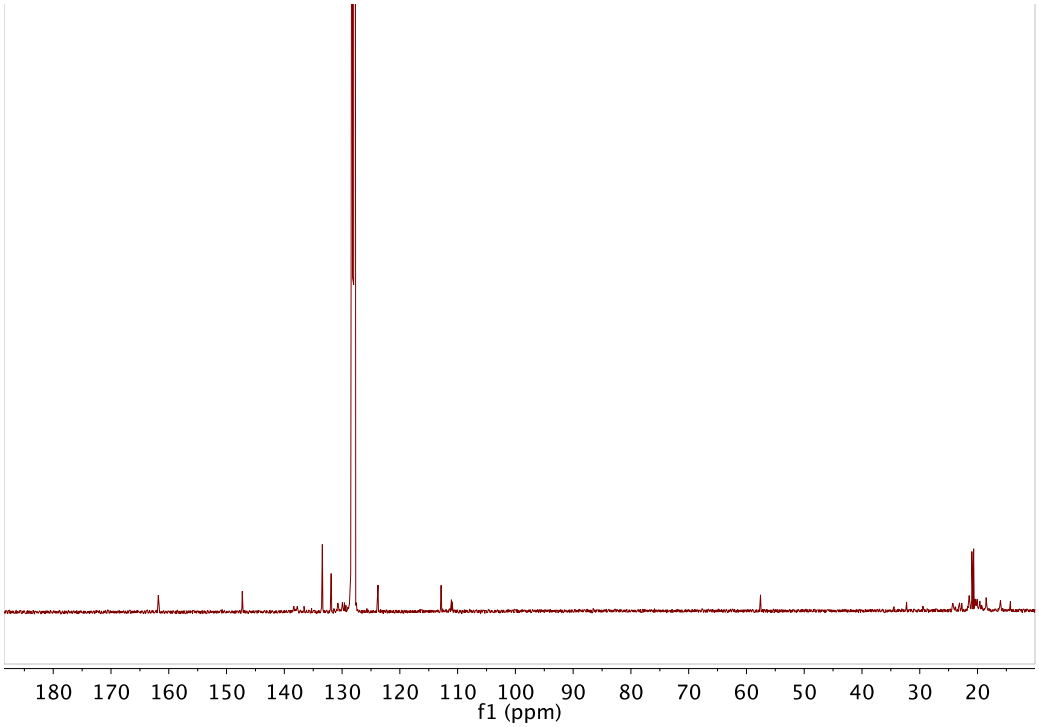

Figure S4: $^{13}C\{^{1}H\}$ NMR Spectrum of **3** in C_6D_6, 125.8 MHz, 300K

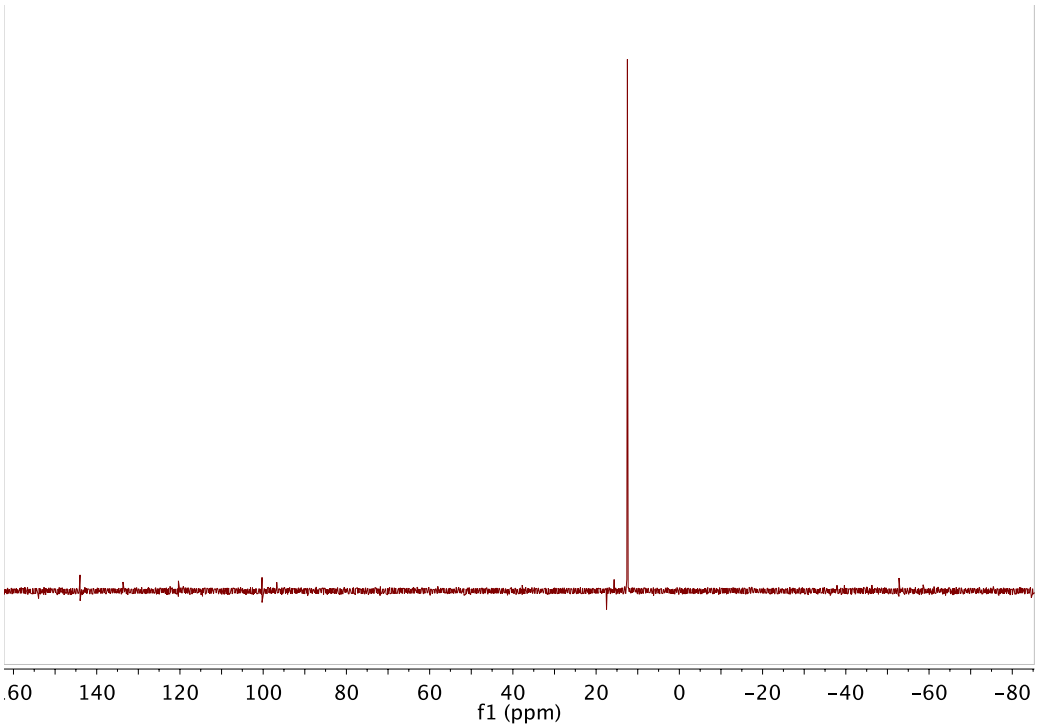

Figure S5: $^{31}P\{^{1}H\}$ NMR Spectrum of **3** in C_6D_6, 162 MHz, 300K

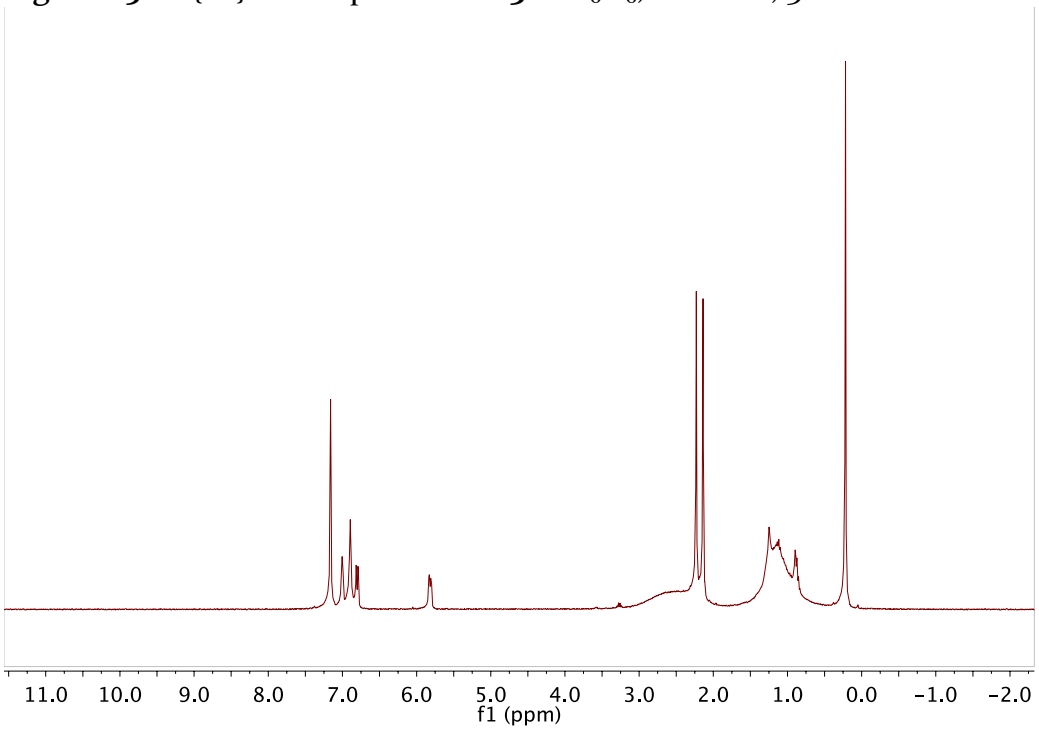

Figure S6: ^{1}H NMR Spectrum of **4** in C_6D_6, 400 MHz, 300K

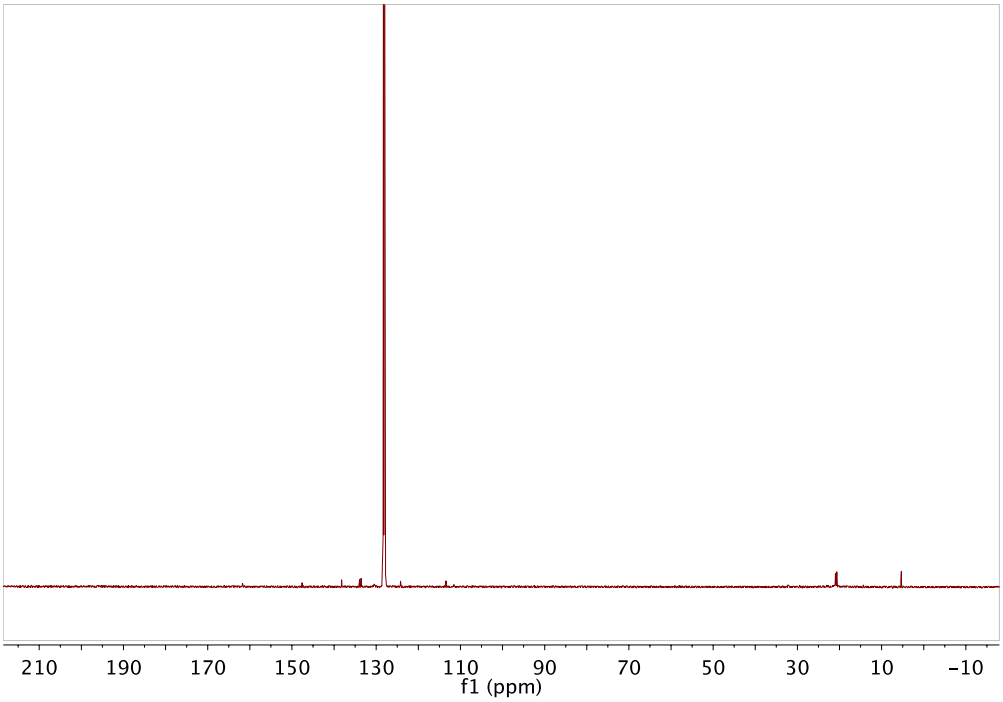

Figure S7: $^{13}C\{^{1}H\}$ NMR Spectrum of **4** in C_6D_6, 125.8 MHz, 300K

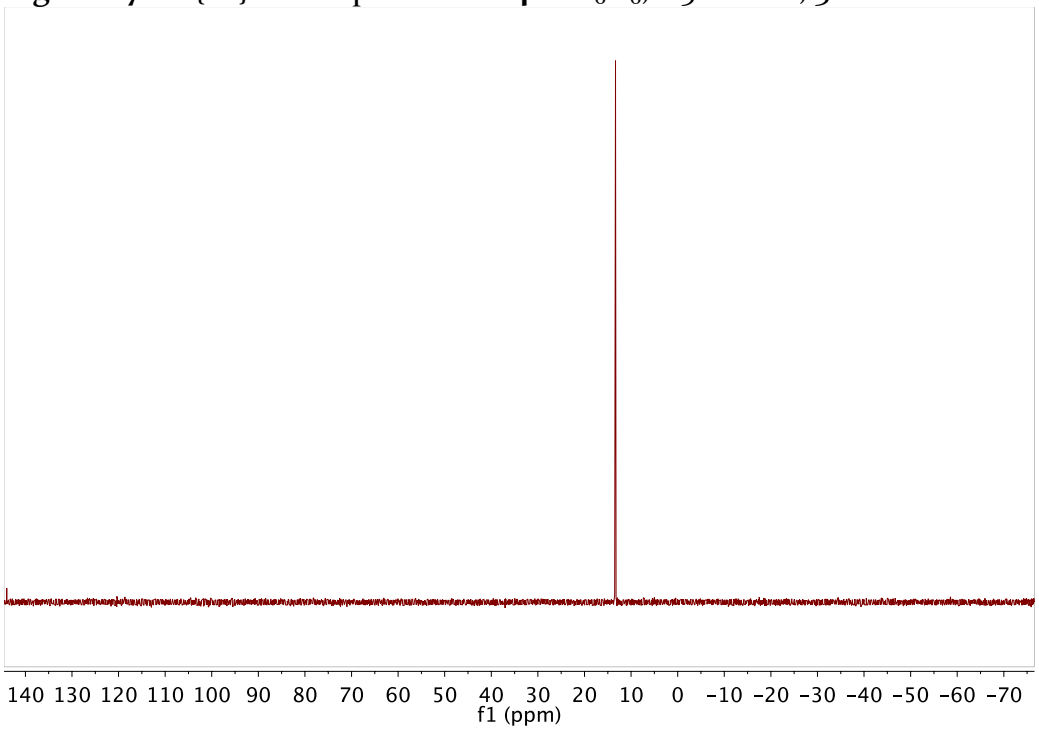

Figure S8: $^{31}P\{^{1}H\}$ NMR Spectrum of **4** in C_6D_6, 162 MHz, 300K

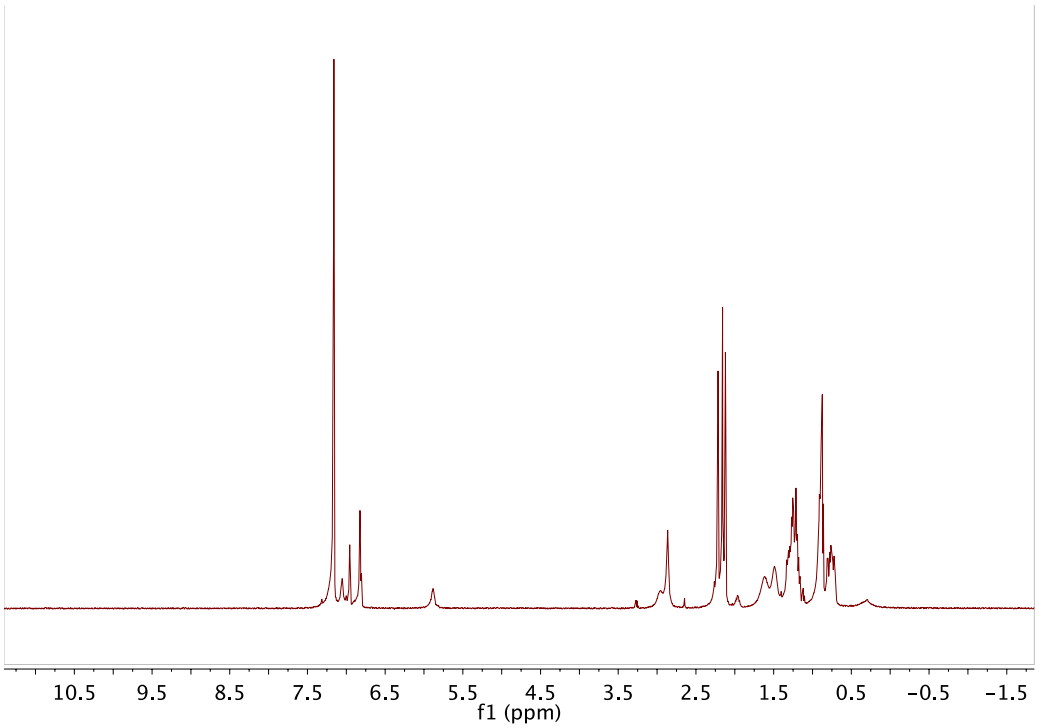

Figure S9: ^{1}H NMR Spectrum of **5** in C_6D_6, 400 MHz, 300K

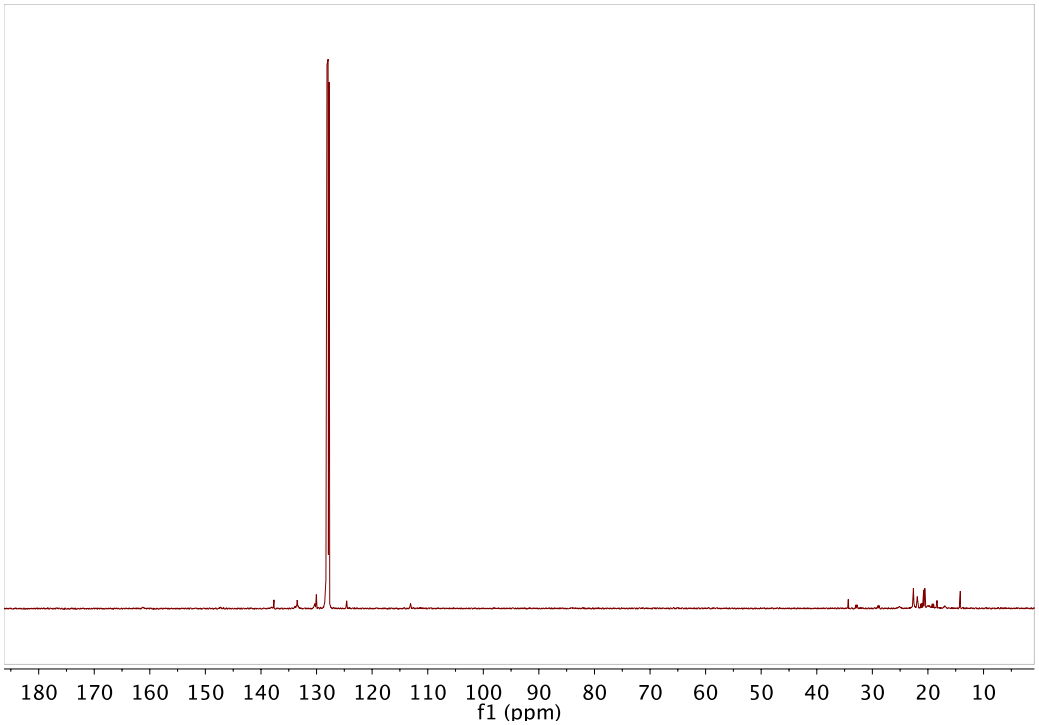

Figure S10: $^{13}C\{^{1}H\}$ NMR Spectrum of **5** in C_6D_6, 125.8 MHz, 300K

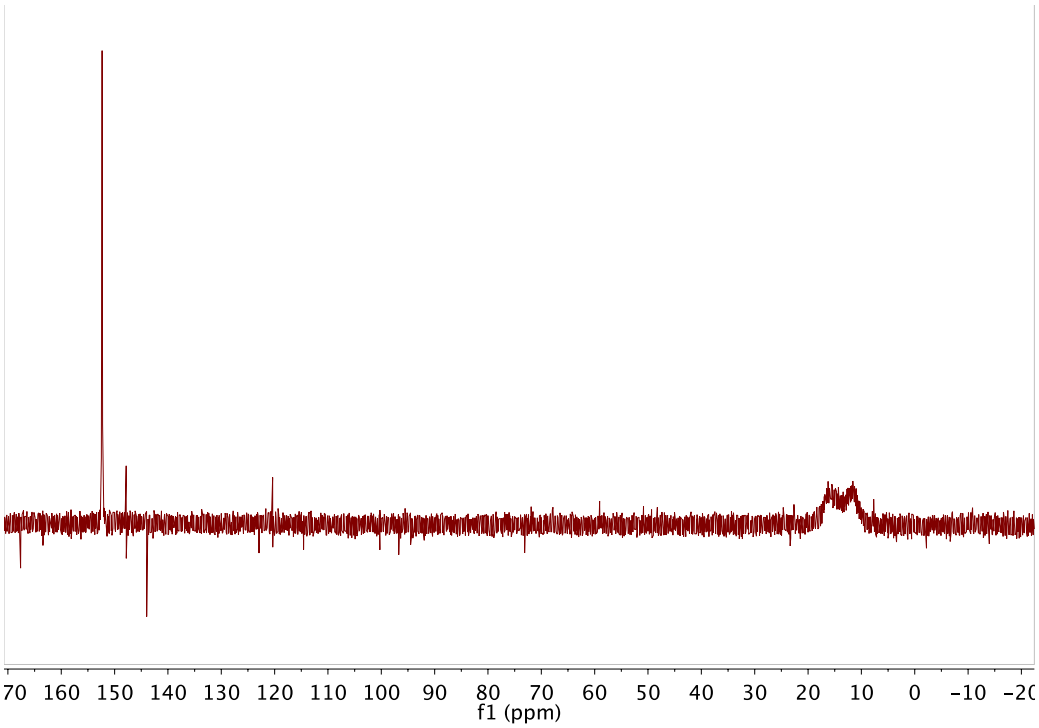

Figure S11: $^{31}P\{^{1}H\}$ NMR Spectrum of **5** in C_6D_6, 162 MHz, 300K

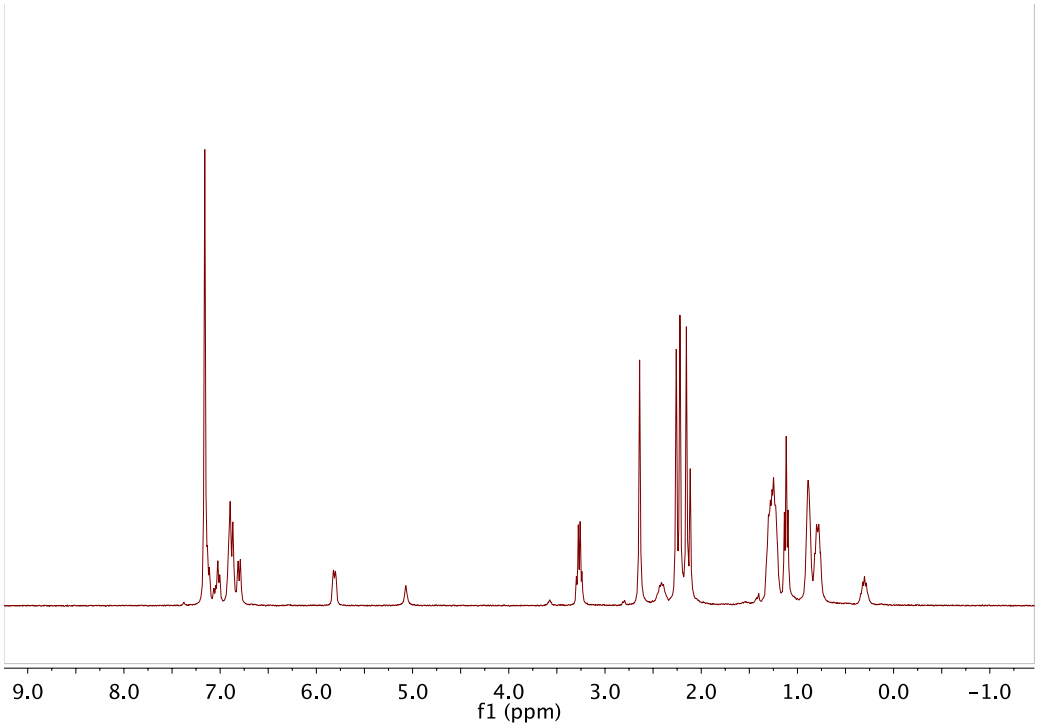

Figure S12: ^{1}H NMR Spectrum of **7** in C_6D_6, 400 MHz, 300K

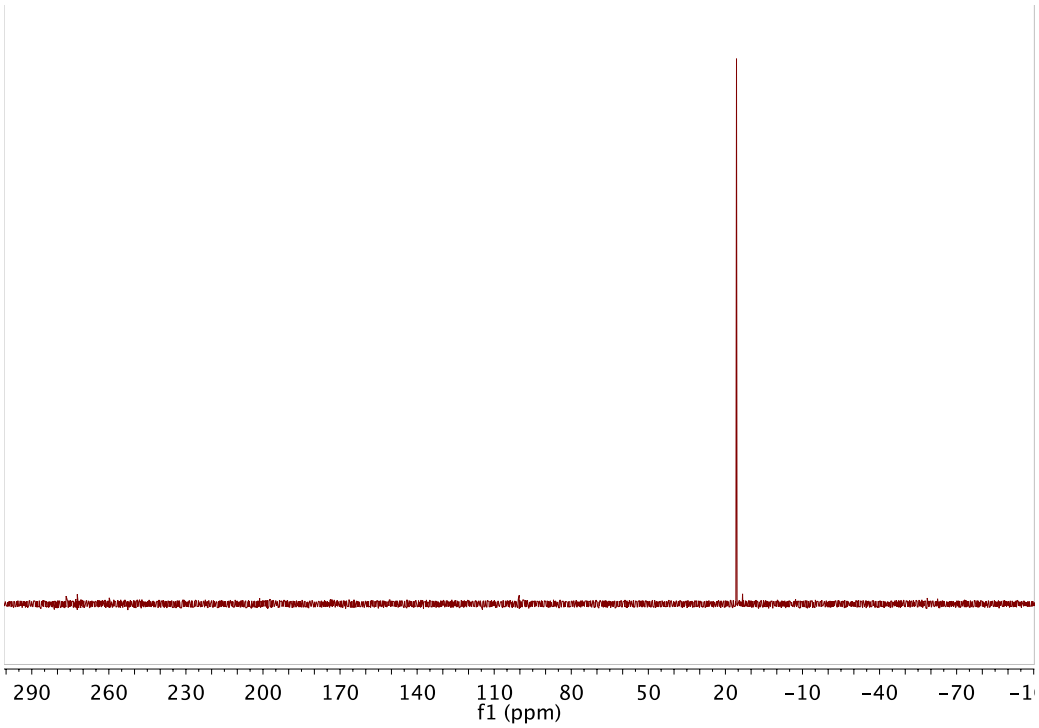

Figure S13: $^{31}P\{^{1}H\}$ NMR Spectrum of **7** in C_6D_6, 162 MHz, 300K

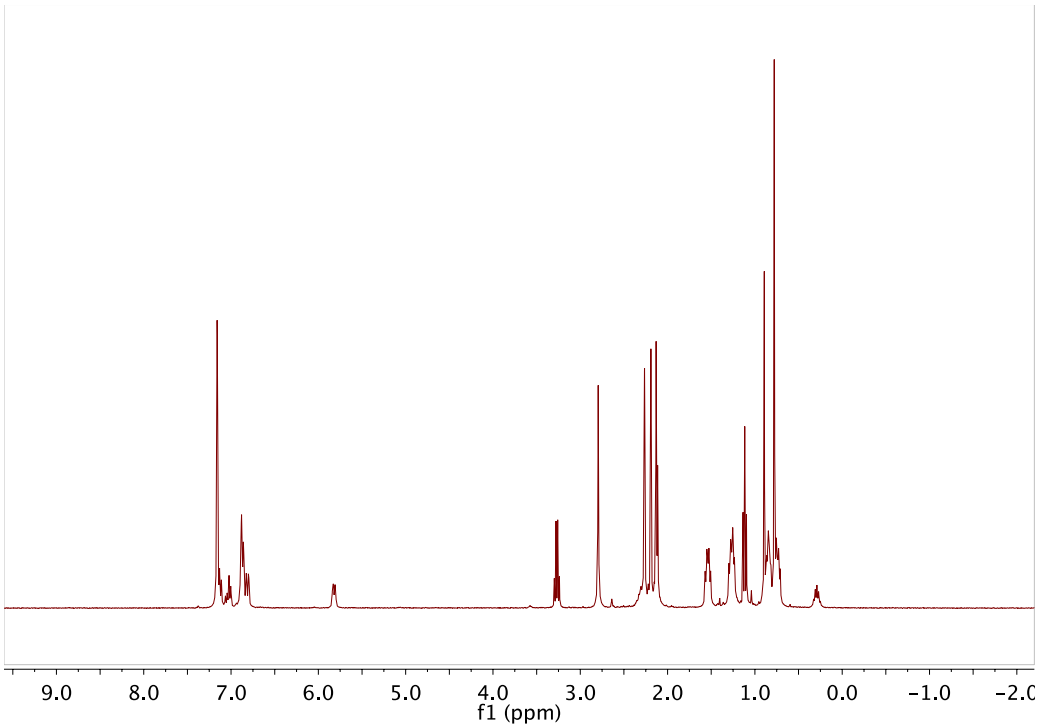

Figure S14: ^{1}H NMR Spectrum of **8** in C_6D_6, 400 MHz, 300K

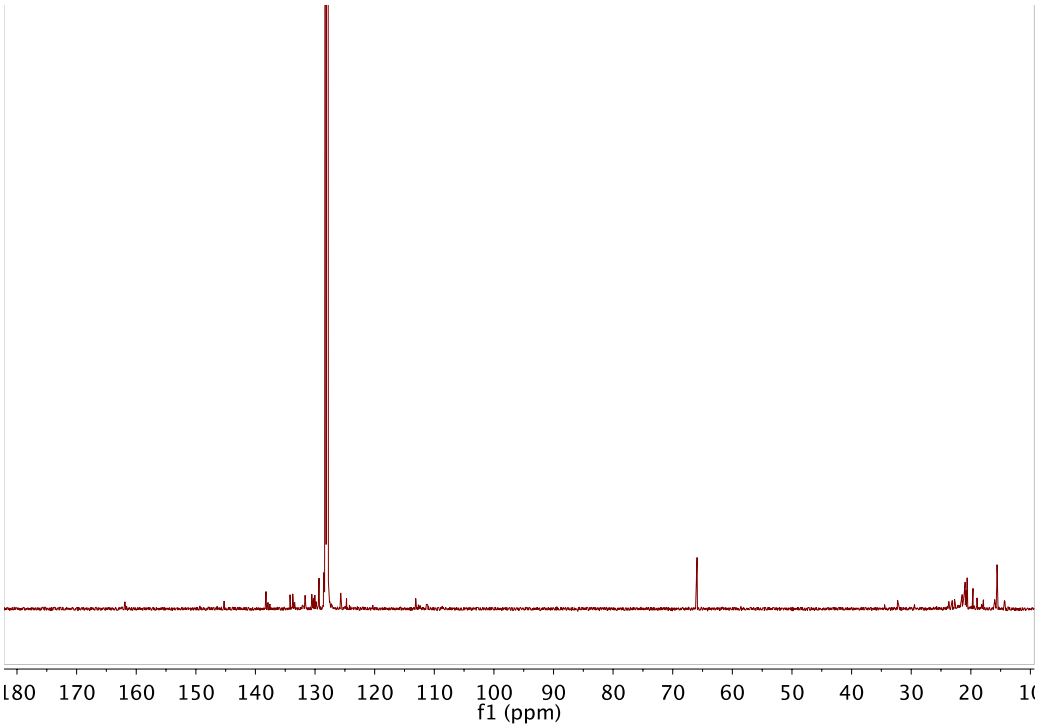

Figure S15: $^{13}C\{^{1}H\}$ NMR Spectrum of **8** in C_6D_6, 125.8 MHz, 300K

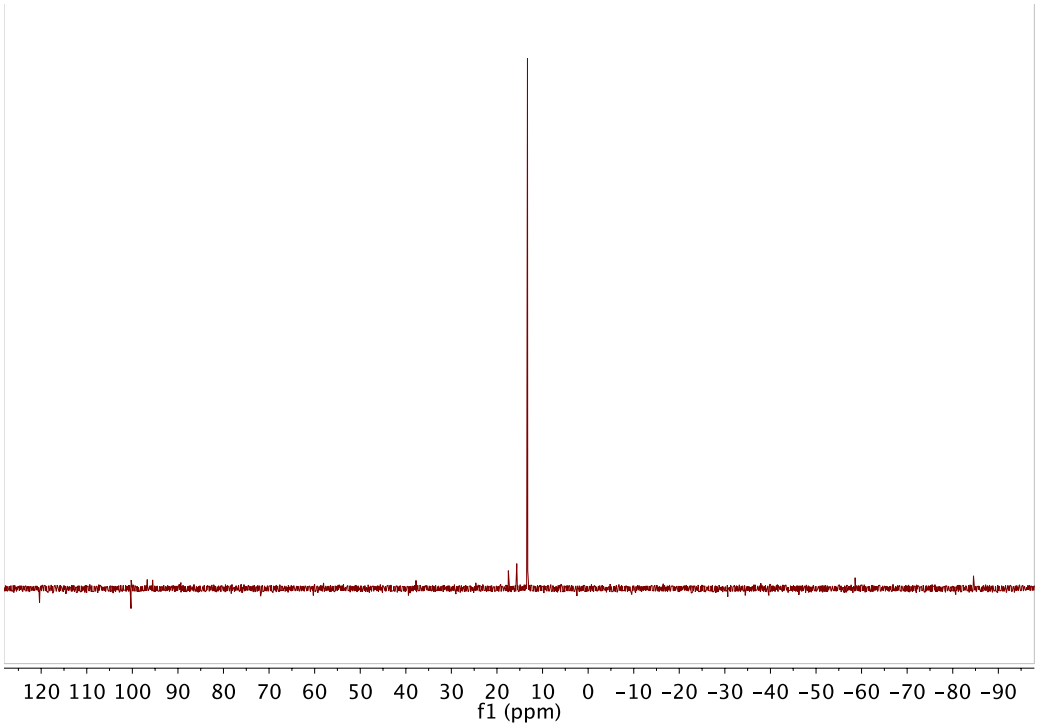

Figure S16: $^{31}P\{^{1}H\}$ NMR Spectrum of **8** in C_6D_6, 162 MHz, 300K

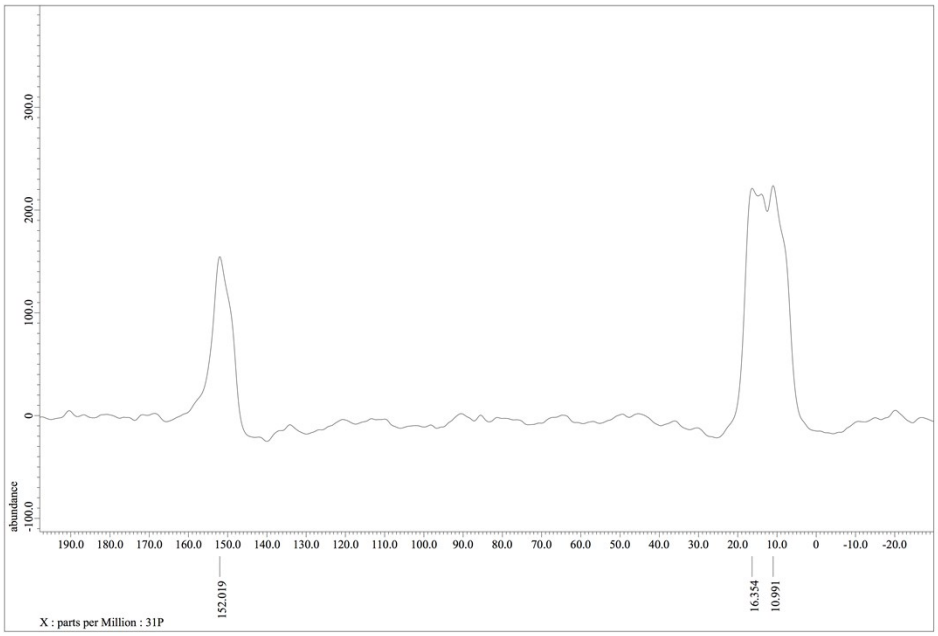

Figure S17: ^{31}P NMR Spectrum of **5** in C_7D_8, 162 MHz, 265K

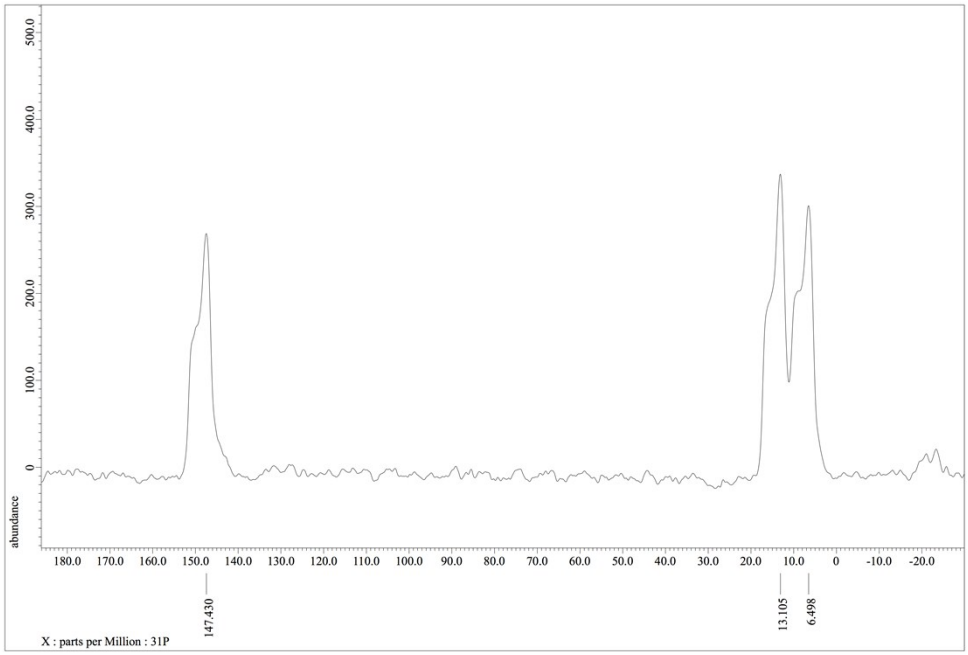

Figure S18: ^{31}P NMR Spectrum of **5** in C_7D_8, 162 MHz, 219K

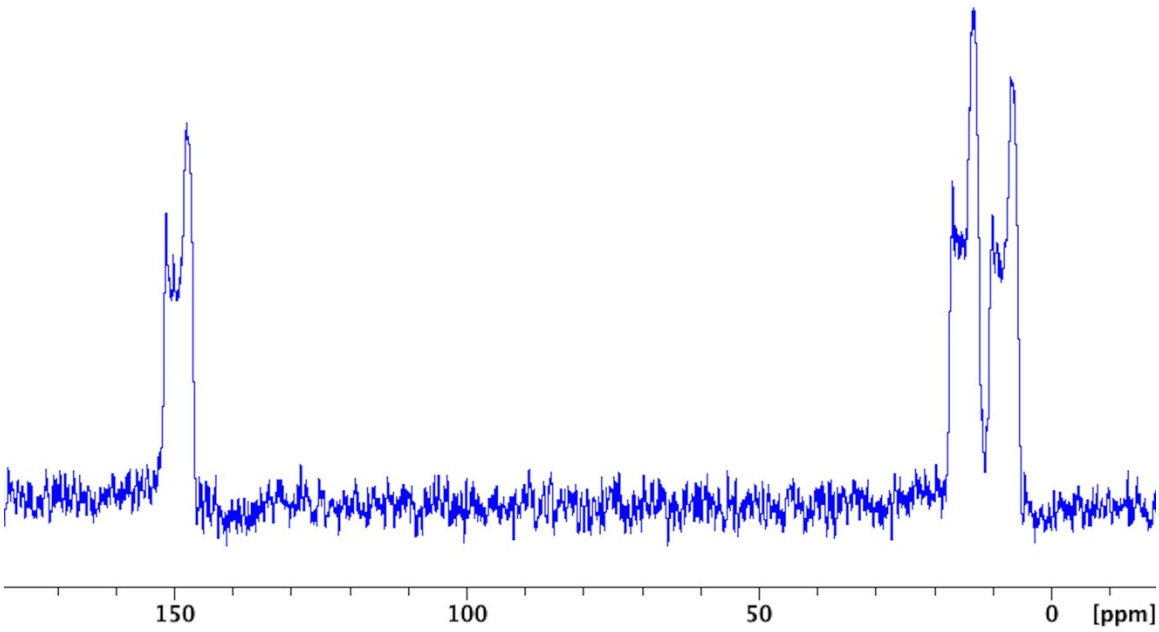

Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum of **5**, taken at 219 K in C_7D_8, 162 MHz.

Computational Details. All calculations were carried out using DFT as implemented in the ORCA program package[1]. Final geometry optimizations were performed using the BLYP[2,3] functional and the all-electron def2-TZVP(-f)-ZORA[4] basis set in combination with the auxiliary basis set def2-TZV/J[5]. To accelerate geometry optimizations we used the resolution of the identity, R[6], approximation. For these optimizations a tight convergence of the wavefuntion was demanded on grid quality of Grid4 (also using SlowConv). The scalar relativistic zero'th order regular approximation (ZORA)[7] was employed to take into account relativistic effects whereas to dispersion was considered using Grimme's D3 method in all ORCA calculations. Our experience with the optimizations of the investigated extended molecules (~ 200 atoms) is that the convergence to the equilibrium structure is much faster when optimizing in Cartesian coordinates (COPT). Finally, the above-described final geometry optimizations were started from pre-optimized structures obtained via a lower level of theory (BLYP/def2-SV(P), def2-SVP/J, ZORA, RI, d3, LooseSCF, Grid3).

We used the NMR module of ADF2013[8] code to compute ^{15}N NMR chemical shifts on the equilibrium structures obtained via the protocol described above. The functional employed consisted of the local density approximation of Vosko, Wilk, and Nusair (LDA VWN)[9] augmented with the nonlocal gradient correction PW91

from Perdew and Wang[10]. This functional has been shown to provide reliable chemical shift values even for heavy atom containing transition metal complexes[11]. The full electron basis set TZVP was utilized in these calculations and relativistic corrections were applied using ZORA. The computed isotropic shielding values of complexes were referenced to that of ammonia modeled in the same way.

Cartesian coordinates of the optimized structures. Values are in Å.

$[(PN)_2Ti{\equiv}N]^-$

Ti	13.626698087600018	3.96420658351770	11.086507931125 11
P	13.38157696391465	2.75197968063771	13.42612122613409
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$(PN)_2Ti{\equiv}NK(18\text{-crown-}6)$

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N	13.21241711108372	5.75388186652770	11.631160888261510
C	11.12259058351467	2.34627965818560	12.012872507203 10
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C	9.15470802214545	1.21710319845795	12.969515312838 06
H	8.15888075112672	0.79870646773375	12.822578818878 96
C	11.02365767231998	1.72836882414282	14.390518893113 51
H	11.48613282417543	1.71172390882038	15.375098453674 50
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H	13.00545145734246	3.04738662324358	15.832365382422 88
C	12.40442503369135	4.95976599336525	15.033817107045 31
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H	11.38516954862470	4.61464833459866	14.829424337426 68
H	12.40407797774127	5.50670786388241	15.988249093287 34
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H	15.52111412891778	3.45584994590617	15.569246974143 52
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C	9.62797111797185	3.82469336107217	8.05448871183538
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C	10.25980340475111	3.90563840307101	9.30361124883222
C	12.14291058644708	0.56474874028774	9.34811231557452
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H	11.62131470504951	0.02238274274228	10.14956200482874
C	9.97639140482797	5.04323144035162	10.25722203191558
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C	7.844502929417 27	19.076176750869 53	13.809486246484 36
H	7.882055611904 04	19.808861630630 02	14.624866161489 43
H	8.849308887310 97	18.981131406780 80	13.385584585620 79
H	7.162945298986 08	19.448127024903 50	13.036139258787 40
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H	5.609081063509 04	16.918011982618 61	15.422581253290 39
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C	6.820220453353 27	14.853630453098 11	13.771521410287 56
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H	8.581495489500 45	14.467898988990 215	15.016152375990 39
H	7.292668207817 76	15.351134692259 97	15.866904740850 38
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C	1.272989075496 22	25.320182418977 40	12.687086837017 50
C	1.572957279800 777	24.860417472842 23	13.977618843589 82
C	2.892237855815 55	24.501049872087 98	14.262773827551 25
H	3.129691481452 96	24.138366080800 39	15.260618771505 96
C	3.913293210088 39	24.598411870789 92	13.305751422272 57
C	5.598081237193 02	22.786145751973 77	14.819551224464 74
H	4.860961273779 76	23.026893458673 41	15.596239141204 90
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H	4.104820592143 86	21.782585254175 01	13.595459141620 26
H	5.791041873161 861	21.320446873204 16	13.236282732392 58
C	6.934917263873 09	22.481381293881 02	15.510177546639 46
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H	7.322541257089 34	23.336061331826 04	16.072609831298 76
H	6.804770786726 98	21.643746390585 25	16.209958547401 72
C	6.112253582508 55	25.702035779007 17	14.895632110952 24
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C	5.850616272447 39	27.038747979376 70	14.185244592914 60
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H	6.297896058917 38	27.057878518985 74	13.189725711509 35
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2

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H	17.830237194113 46	18.916436152066 54	6.239621321787 07
H	8.469310214804 85	27.198516472775 81	10.180447021816 17
H	17.048423496045 27	24.740379705042 57	8.326635890260 49
H	14.069748017424 09	27.203398278384 27	-0.546874369601 93
H	5.501210866489 38	24.679622332109 48	1.310191612770 30

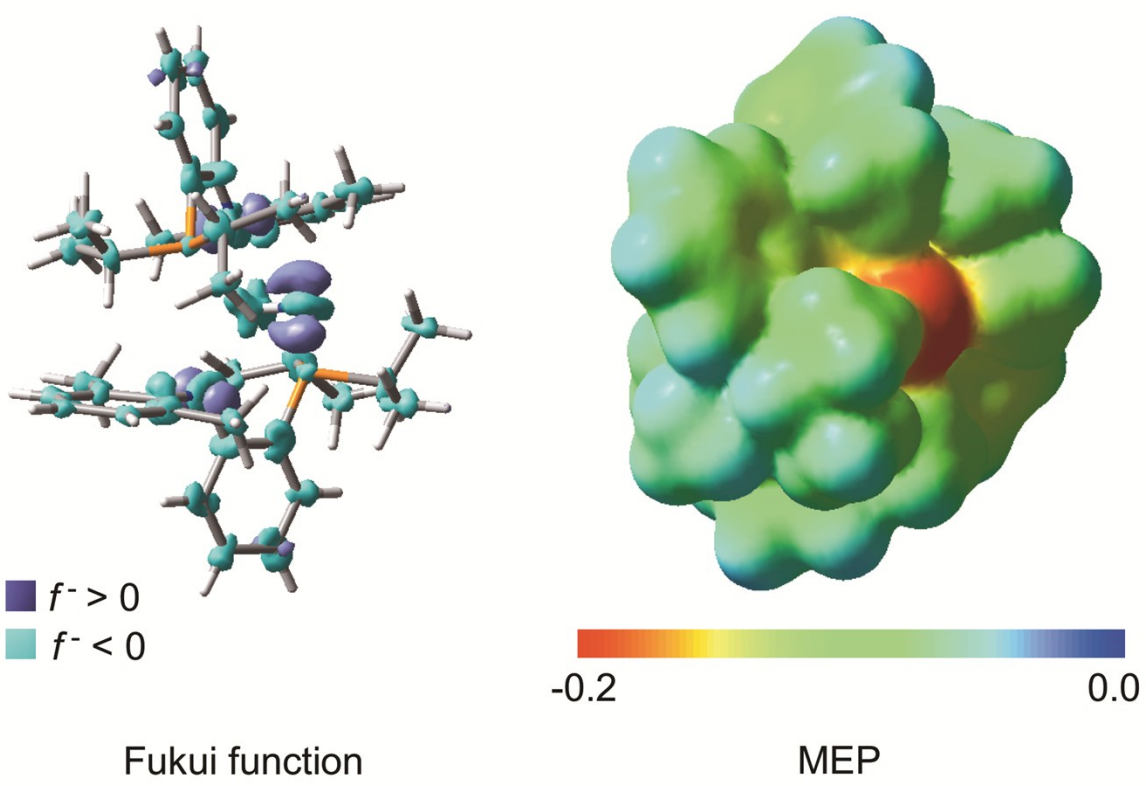

Figure S19. Nucleophilic Fukui function, f, and molecular electrostatic potential, MEP, for $[(PN)_2Ti{\equiv}N]^-$ characterizing soft (purple regions) and hard (red sites) electrophilic reactivity of the titanium-nitride functionality, respectively,.

Crystallography Details. Suitable single crystals for X-ray analysis of **2**-**8** were placed on the end of a Cryoloop coated in NVH oil. The X-ray intensity data collection was carried out on a Bruker APEXII CCD area detector using graphite-monochromated Mo-K radiation (λ = 0.71073 Å) at 100(1) K. Preliminary indexing was performed from a series of thirty-six 0.5° rotation frames with exposures of 10 seconds. Rotation frames were integrated using SAINT,[12] producing a listing of non-averaged F^2 and $\sigma(F^2)$ values which were then passed to the SHELXTL[13] program package for further processing and structure solution. The intensity data were corrected for Lorentz and polarization effects and for absorption using SADABS.[14] All calculations were performed using SHELXS[15] and SHELXL.[16] The structures were solved by Patterson and Fourier transform methods. All reflections were used during refinement. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using riding models with exception for **7**. For **4**, two crystallographically independent, but chemically equivalent molecules are present in the asymmetric unit. For **5**, ^{i}Pr groups of NP^iPr_2 were disordered over two on the crystallographycally special position. The thermal ellipsoids were fixed by SHELXL restraint commands,

DELU and SIMU. Disordered pentane molecule was located with 0.5 occupancies and a negative PART number, and refined with a rigid group model. For **6**, one site occupied by hexane was identified in the asymmetric unit. This site was considerably disordered and was treated by SQUEEZE as a diffuse contribution.[17, 18] In the resulting void space, a contribution of 134 e^- per unit cell was found and taken to represent one hexane in the asymmetric unit, giving one pentane molecule for each Ti complex. For **7**, one site occupied by THF was identified in the asymmetric unit. This site was also treated by SQUEEZE as a diffuse contribution, resulting in a contribution of 186 e^- per unit cell to give one THF molecule for each Ti complex. This data was treated as a two-component crystal data. One component with 0.8 occupancies was refined as a terminally bound parent imide complex **7**. The hydrogen atom of the imide ligand was located from the difference map and refined isotropically. The second component was considerably an insertion product in which the imide ligand has inserted into the arm of the PN ligand. The phosphorus atom and corresponding ^{i}Pr groups were refined with 0.2 occupancies, but the hydrogen atom corresponding to the parent imide hydrogen in **7** could not be located from the difference map due to its low occupancy. These results were checked using the IUCR's CheckCIF routine. The alerts in the output are related to the disordered groups and crystal solvents.

Solid state ^{15}N NMR Details. Solid-state ^{15}N NMR spectra were recorded under the cross polarization (CP) magic-angle spinning (MAS) condition on a Bruker Avance-600 NMR spectrometer (14.1 T) operating at the ^{1}H and ^{15}N Larmor frequencies of 600.17 and 60.81 MHz, respectively. The Hartmann-Hahn matching condition was established with a solid $^{15}NH_4NO_3$ sample. High-power ^{1}H decoupling (70 kHz) was applied during data acquisition. A 4-mm Bruker MAS probe was used with sample spinning frequencies between 5.0 and 14.5 kHz. A relaxation delay of 2 s and a contact time of 2 ms for CP were used. Powder samples were packed into a ZrO_2 rotor (4-mm o.d.) in a glove box. All ^{15}N chemical shifts were referenced to that of NH_3(liq) (δ = 0 ppm) by using solid $^{15}NH_4NO_3$ as a secondary ^{15}N chemical shift reference (δ = 23.8 ppm). Spectral simulations were performed using DMFit.[19]

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