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Supporting Information

NHCs as Neutral Donors towards Polyphosphorus Complexes

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Supporting Information

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Supporting Information

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1. Experimental details: complex syntheses and characterization

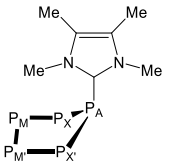
General Procedures: All manipulations were performed with rigorous exclusion of oxygen and moisture in Schlenk-type glassware on a dual manifold Schlenk line in Argon atmosphere or in Argon filled glove box with a high-capacity recirculator (<0.1 ppm O_2). THF, toluene, *n*-hexanes and acetonitrile were dried using conventional techniques, degassed and saturated with Argon. Deuterated solvents were degassed, dried and distilled prior to use. The complexes [Cp*Fe(η^5-P_5)][1] (**1**) and [Cp''Ta(CO)$_2$(η^4-P_4)][2] (**2**) as well as the NHCs (IMe,[3] IMes,[4] IDipp,[5] I^{t}Bu,[6] IDipp=CH_2[7]) were prepared according to published procedure. NMR spectra were recorded on a Bruker Avance 300 MHz and Bruker Avance 400 MHz spectrometers. Chemical shifts are given in ppm; they are referenced to TMS for ^{1}H, and external 85% H_3PO_4 for ^{31}P. Elemental analyses (CHN) were determined using in-house facility. NMR spectrum simulations were performed with the simulation module "daisy", embedded in the software *Bruker Topspin (V. 3.6.1)*. Solid-state ^{31}P NMR: ^{1}H–^{31}P CP/MAS NMR experiments were performed on a Bruker Avance I 400 spectrometer using a 4.0 mm HX MAS probe at 298 K. The sample was packed in a zirconia rotor. A two-pulse phase modulation (TPPM) decoupling scheme was used for 1H decoupling. The spectra were recorded using 3.25 µs proton $\pi/2$ pulse length, a ν_{CP} of 55.0 kHz, a contact time of 5.0 ms, a ν_{dec} of 76.9 kHz and a recycle delay of 6 s.
Due to the dynamic behavior of [Cp*Fe(η^4-P_5IMe)] (**3**), [Cp*Fe(η^4-P_5IMes)] (**4**) and [Cp*Fe(η^4-P_5IDipp)] (**5**) in solutions it was impossible to receive meaningful mass spectra. Due to the low solubility of **1** and NHCs at low temperatures and the dynamic behavior in solutions no ^{13}C{^{1}H} NMR spectra of reasonable quality could be recorded.

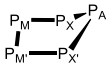
Synthesis of 3, [Cp*Fe(η^4-P_5IMe)]:

A solution of 100 mg (0.289 mmol) [Cp*Fe(η^5-P_5)] and 35 mg (0.281 mmol) IMe in 10 mL toluene was stirred for 1 hour. The solvent was removed in vacuum and the green precipitate dissolved in 3 mL thf, layered with 6 mL *n*-hexanes and stored at 4 °C to give green crystals overnight.

Crystalline yield: 60 mg, 0,123 mmol, 44.2%.

$C_{17}H_{27}FeN_2P_5$ calc: C 43.43, H 5.79, N 5.96. found: C 43.50, H 5.74, N 5.81. ^{1}H NMR (400 MHz, toluene-d_8, 213 K): δ = 2.29 (s, 6H, N(1,3)-*Me*), 1.91 (s, 15H, *Cp**), 0.38 (s, 6H, C(4,5)-*Me*). ^{31}P{^{1}H} NMR (162 MHz, toluene-d_8, 213 K): δ = 34.7 (m, P_M/$P_{M'}$), 31.6 (P_A), -49.1 (m, P_X/$P_{X'}$). For coupling constants see Table S 1.





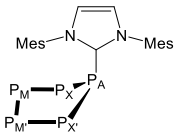
= [Cp*Fe(η^4-P_5)]

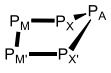
Synthesis of 4, [Cp*Fe(η^4-P$_5$IMes)]:

A solution of 100 mg (0.289 mmol) [Cp*Fe(η^5-P$_5$)] and 88 mg (0.289 mmol) IMes in 10 mL toluene was stirred for 1 hour. The solvent was removed in vacuum and the green precipitate dissolved in 5 mL thf, layered with 10 mL *n*-hexanes and stored at -30 °C to give green crystals within 48 h.

Crystalline yield: 93 mg, 0.143 mmol, 49.5%.

$C_{31}H_{39}FeN_2P_5$ calc: C 57.25, H 6.04, N 4.31. found: C 57.97, H 6.26, N 4.07. ^{1}H NMR (400 MHz, toluene-d$_8$, 213 K): δ = 6.74 (s, 4H, Ar-*H*), 4.82 (s, 2H, NC*H*), 2.19 (s, 6H, 4-*Me*), 1.99 (s, 12H, 2,6-*Me*), 1.67 (s, 15H, *Cp**). ^{31}P{^{1}H} NMR (162 MHz, toluene-d$_8$, 213 K): δ = 44.0 (m, P$_A$), 33.0 (m, P$_M$/P$_{M'}$), -66.0 (m, P$_X$/P$_{X'}$). For coupling constants see Table S 2.





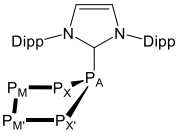
= [Cp*Fe(η^4-P$_5$)]

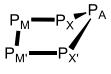
Synthesis of 5, [Cp*Fe(η^4-P$_5$IDipp)]:

A solution of 100 mg (0.289 mmol) [Cp*Fe(η^5-P$_5$)] and 110 mg (0.289 mmol) IDipp in 10 mL toluene was stirred for 1 hour. All volatiles were removed in vacuum, the green precipitate dissolved in 4 mL thf, layered with 20 mL *n*-hexane and stored at -80 °C to give green crystals overnight.

Crystalline yield: 112 mg, 139 mmol, 48.0%.

$C_{37}H_{51}FeN_2P_5$·(thf) Calc: C 61.05, H 7.37, N 3.47. found: C 61.15, H 7.42, N 3.58. ^{31}P{^{1}H} NMR (162 MHz, toluene-d$_8$, 193K): δ = 40.5 (m, 1P), 35.7 (m, 2P), -62.1 (m, 2P).





= [Cp*Fe(η^4-P$_5$)]

SUPPORTING INFORMATION

Synthesis of 6, $[(IMe)_2P][Cp''Ta(CO)_2(\eta^3\text{-}P_3)]$:

100 mg (0.186 mmol) $[Cp''Ta(CO)_2(\eta^4\text{-}P_4)]$ and 100 mg (4.33 eq, 0.805 mmol) IMe were dissolved in 10 mL toluene. The light brownish red solution was stirred for an hour before the solvent was removed. The red precipitate was washed with *n*-hexanes to remove the excess of IMe and then dissolved in 5 mL MeCN. After storage at -30 °C for ten days, red crystals were formed which were suitable for X-ray investigations.

Crystalline yield: 88 mg, 0.112 mmol, 60.2%.

$C_{29}H_{45}N_4O_2P_4Ta$ calc: C 44.28, H 5.77, N 7.12. found: C 44.73, H 5.77, N 7.19. ESI-MS (acetronitrile): anion mode: *m/z* = 507.02 (100 %, $[Cp''Ta(CO)_2(\eta^3\text{-}P_3)]^-$), cation mode: *m/z* = 279.18 (100%, $[(IMe)_2P]^+$). ^{1}H NMR (400 MHz, MeCN-d_3, 25 °C): δ = 5.11 (t, $^4J_{HH}$ = 2.2 Hz, 1H), 4.91 (d, $^4J_{HH}$ = 2.2 Hz, 2H), 3.53 (s, 12H, N(1,3)-*Me*), 2.16 (s, 12H, C(4,5)-*Me*), 1.18 (s, 18H, ^{t}Bu). $^{31}P\{^1H\}$ NMR (162 MHz, MeCN-d_3, 25 °C): δ = -113.1 (s, 1P, IMe-*P*-IMe), -421.9 (s, 3P, cyclo-P_3).

2. Experimental and simulated NMR spectra

Variable temperature $^{31}P\{^{1}H\}$ NMR spectra of **3** in the temperature range of 300 K to 193 K:

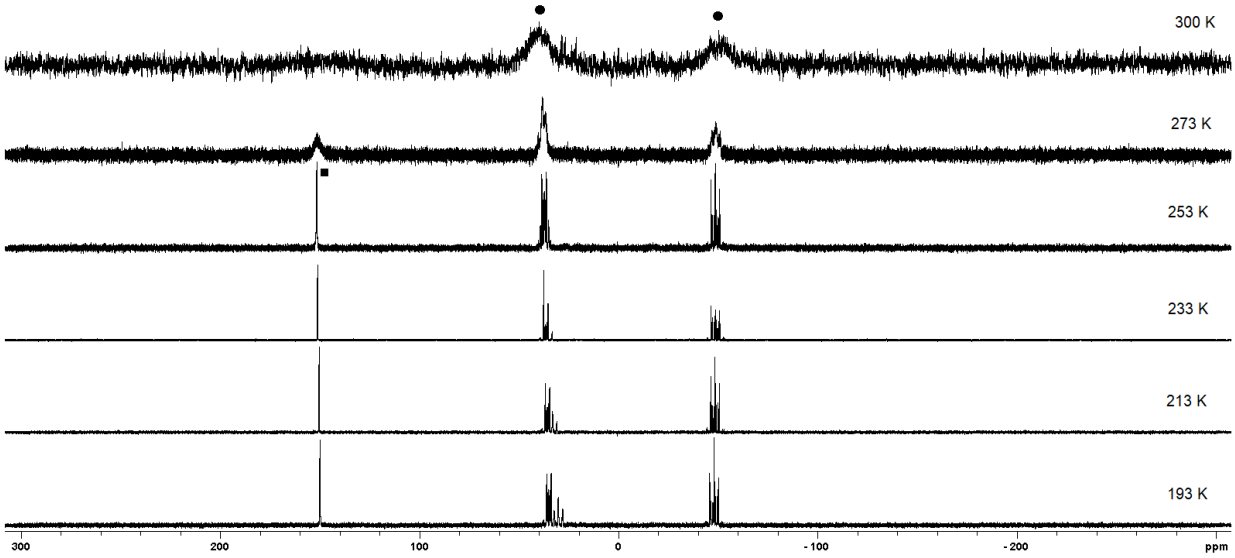


Figure S 1. $^{31}P\{^{1}H\}$ NMR spectra of freshly prepared solution of **1** and IMe in toluene-d_8 in temperature range of 193 K to 300 K. The signal marked with ■ is assigned to **1**. At 300 K first interactions can be detected and is marked with ●. These signals are getting clearer when cooling down and are assigned to compound **3**.

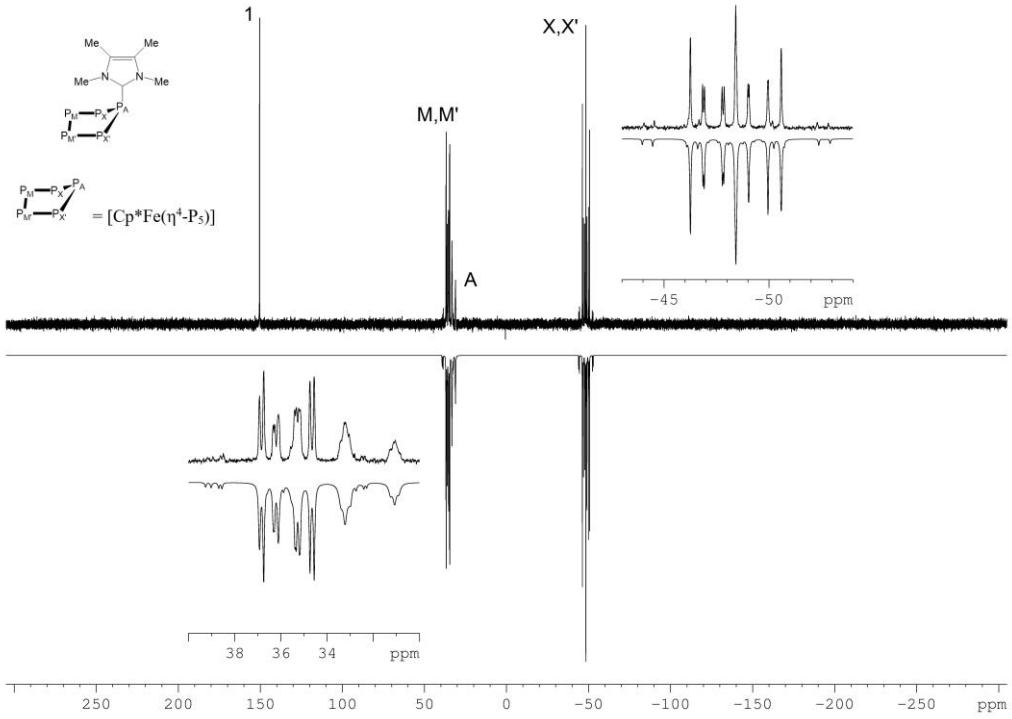


Figure S 2. Experimental (top) and simulated (bottom) $^{31}P\{^{1}H\}$ NMR (162 MHz, toluene-d_8) spectrum of **3** at 213 K.

Table S 1. Chemical shifts and coupling constants obtained from the simulation of the $^{31}P\{^{1}H\}$ NMR spectrum of **3** at 213 K.

***J* (Hz)**				***δ* (ppm)**	
$^{2}J_{P_A,P_M}$	-32.0	$^{1}J_{P_M,P_X}$	365.0	P_A	31.6
$^{2}J_{P_A,P_{M'}}$	-32.0	$^{2}J_{P_M,P_{X'}}$	-8.0	P_M	34.7
$^{1}J_{P_A,P_X}$	355.0	$^{1}J_{P_{M'},P_{X'}}$	365.0	$P_{M'}$	34.7
$^{1}J_{P_A,P_{X'}}$	355.0	$^{2}J_{P_{M'},P_X}$	-8.0	P_X	-49.1
$^{1}J_{P_M,P_{M'}}$	430.0	$^{2}J_{P_X,P_{X'}}$	-50.0	$P_{X'}$	-49.1

Variable temperature $^{31}P\{^{1}H\}$ NMR spectra of **4** in the temperature range of 300 K to 193 K:

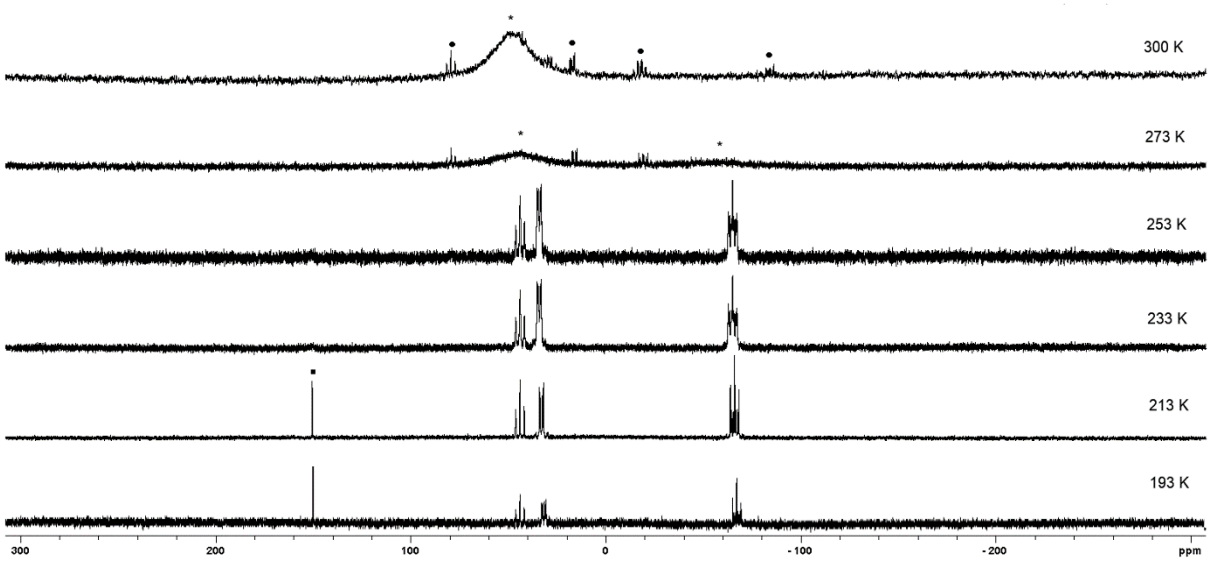


Figure S 3. $^{31}P\{^{1}H\}$ NMR spectra of freshly prepared solution of **1** and IMes in toluene-d_8 in temperature range of 193 K to 300 K. The signals marked with ■ and ● are assigned to **1** and impurities, respectively.

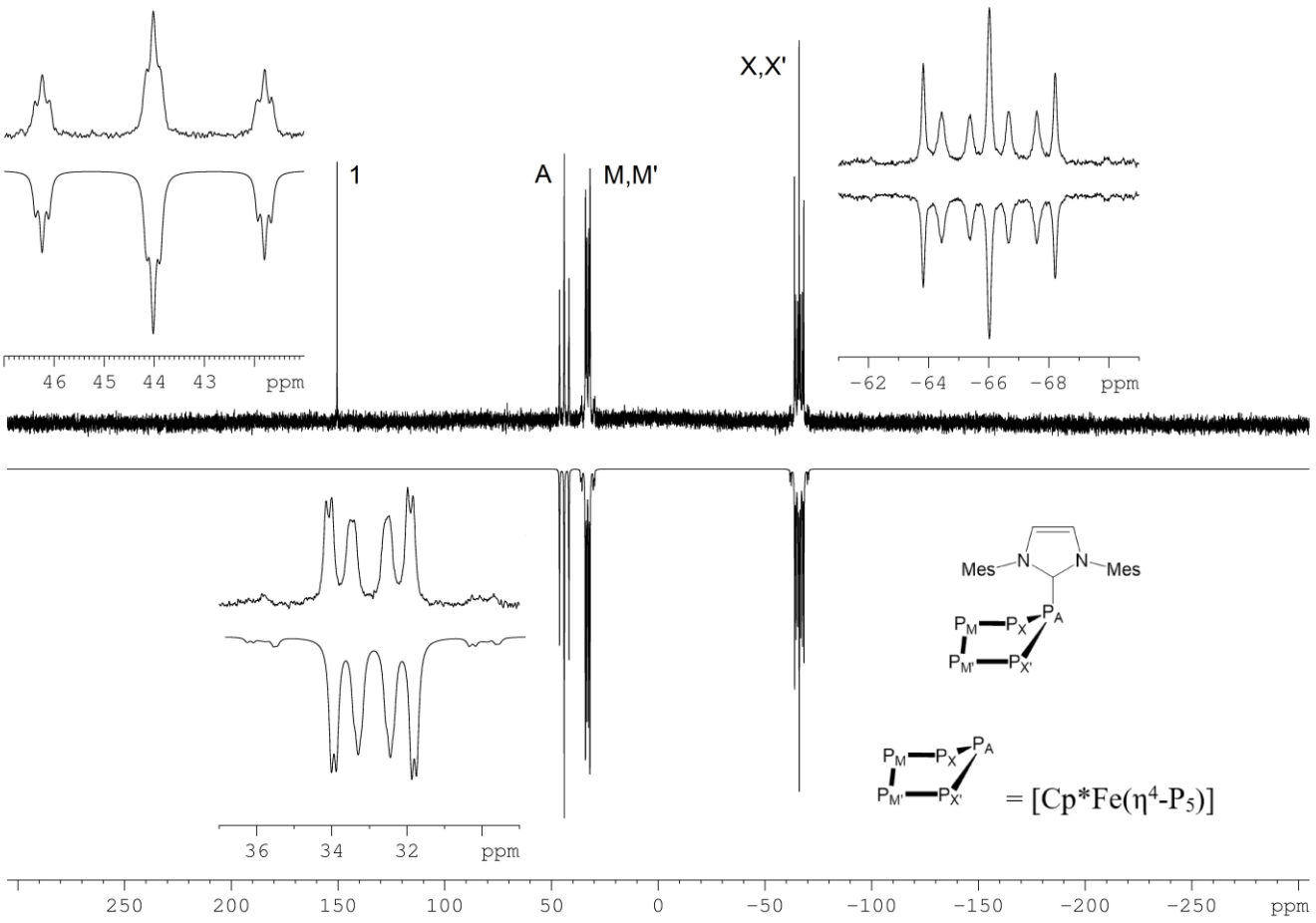


Figure S 4. Experimental (top) and simulated (bottom) $^{31}P\{^{1}H\}$ NMR (162 MHz, toluene-d_8) spectrum of **4** at 213 K.

Table S 2. Chemical shifts and coupling constants obtained from the simulation of the $^{31}P\{^{1}H\}$ NMR spectrum of **4** at 213 K.

***J* (Hz)**				***δ* (ppm)**	
$^{2}J_{P_A,P_M}$	-23.0	$^{1}J_{P_M,P_X}$	354.0	P_A	44.0
$^{2}J_{P_A,P_{M'}}$	-23.0	$^{2}J_{P_M,P_{X'}}$	-8.0	P_M	33.0
$^{1}J_{P_A,P_X}$	354.7	$^{1}J_{P_{M'},P_{X'}}$	354.0	$P_{M'}$	33.0
$^{1}J_{P_A,P_{X'}}$	354.7	$^{2}J_{P_{M'},P_X}$	-8.0	P_X	-66.0
$^{1}J_{P_M,P_{M'}}$	410.0	$^{2}J_{P_X,P_{X'}}$	-55.0	$P_{X'}$	-66.0

Variable temperature $^{31}P\{^{1}H\}$ NMR spectra of **5** in the temperature range of 300 K to 193 K:

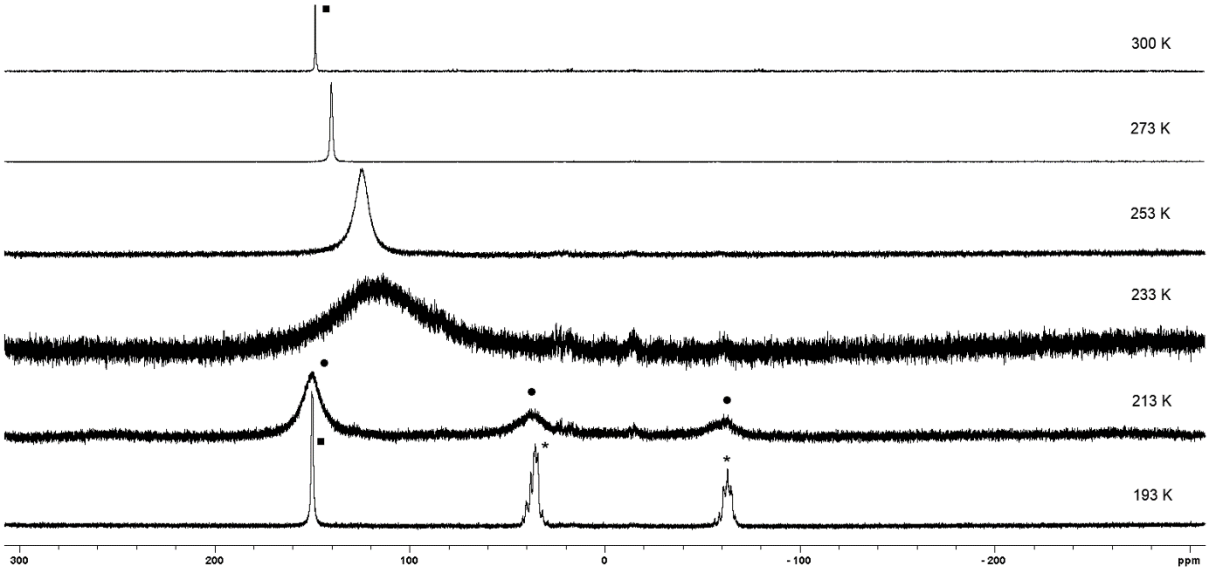


Figure S 5. $^{31}P\{^{1}H\}$ NMR spectra of freshly prepared solution of **1** and IDipp in toluene-d_8 in temperature range of 193 K to 300 K.

Variable temperature $^{31}P\{^{1}H\}$ NMR spectra of **1** and I^{t}Bu in the temperature range of 300 K to 193 K:

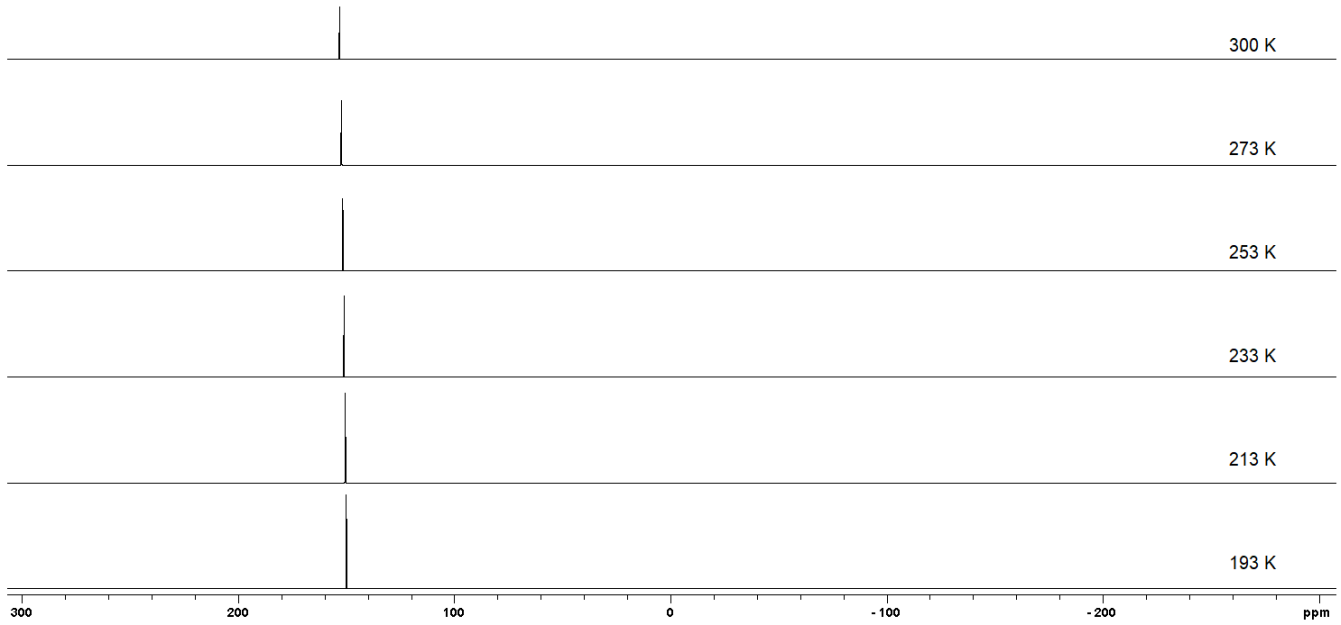


Figure S 6. $^{31}P\{^{1}H\}$ NMR spectra of freshly prepared solution of **1** and I^{t}Bu in toluene-d_8 in temperature range of 193 K to 300 K. Only the signal for **1** is detected.

Variable temperature $^{31}P\{^{1}H\}$ NMR spectra of **1** and IDipp=CH_2 in the temperature range of 300 K to 193 K:

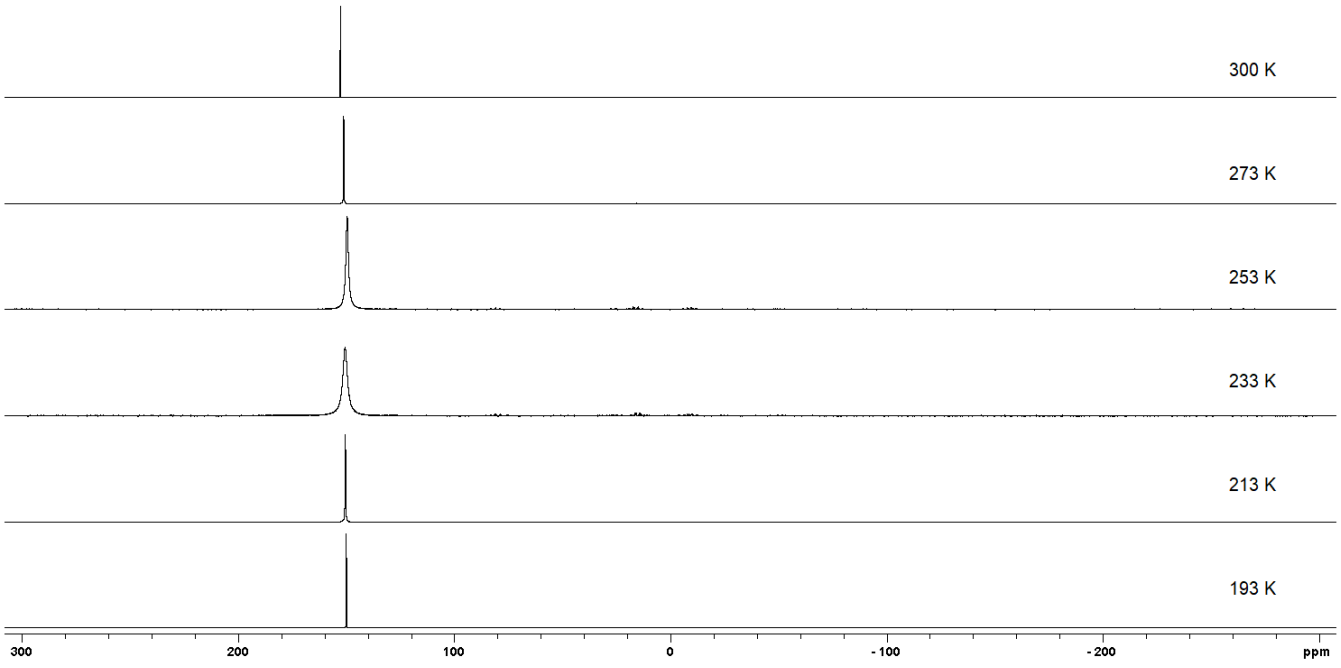


Figure S 7. $^{31}P\{^{1}H\}$ NMR spectra of freshly prepared solution of **1** and IDipp=CH_2 in toluene-d_8 in temperature range of 193 K to 300 K. Only the signal for **1** is detected.

$^{31}P\{^{1}H\}$ NMR spectrum of **6**:

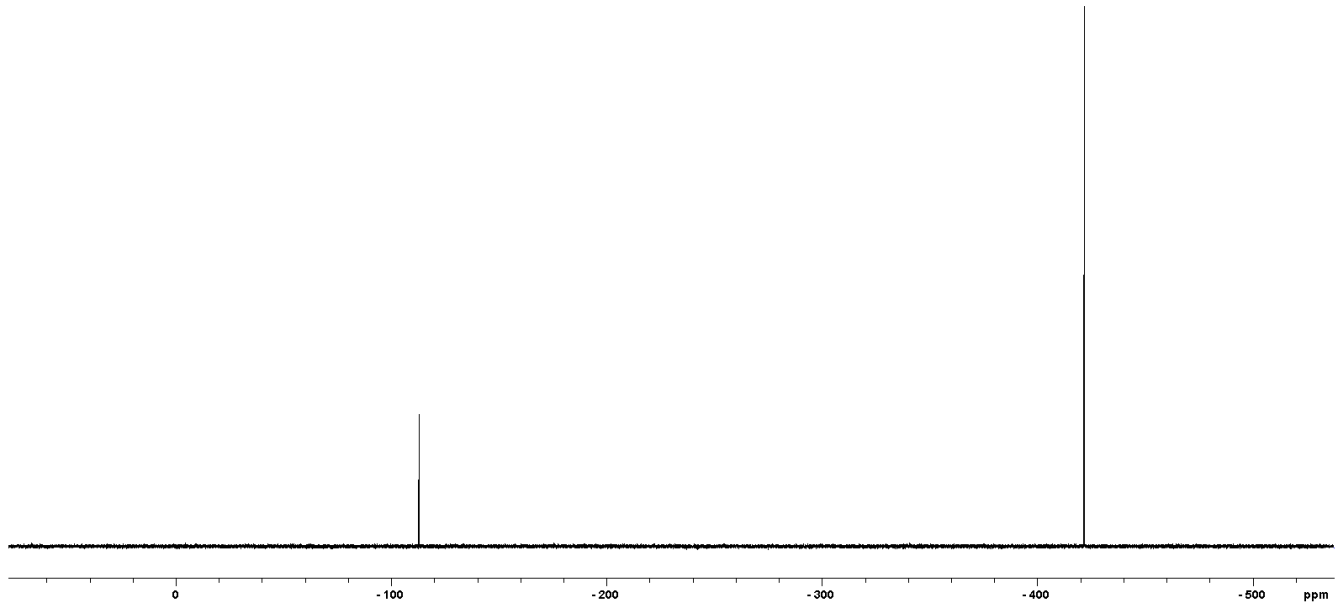


Figure S 8. $^{31}P\{^{1}H\}$ NMR spectrum of compound **6** at 300 K in MeCN-d_3. The singlet at -113.1 ppm is assigned to the cation $[(IMe)_2P]^+$ and the signal at -421.9 ppm is assigned to the anionic complex $[Cp''Ta(CO)_2(\eta^3\text{-}P_3)]^-$.

3. Crystallographic Details

The crystals were selected and mounted on a GV50 diffractometer equipped with a TitanS2 detector. All crystals were kept at T = 123(1) K during data collection. Data collection and reduction were performed with **CrysAlisPro** version 1.171.40.14a.[8] For compound (**3**) an analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid.(Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) was applied. For the compounds (**4**, **5**, **6**) a numerical absorption correction based on gaussian integration over a multifaceted crystal model and an empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm was applied. Using **Olex2**,[9] all structures were solved by **ShelXT**[10] and a least-square refinement on F^2 was carried out with **ShelXL**.[11] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms at the carbon atoms were located in idealized positions and refined isotropically according to the riding model.

The images showing the compounds **3**-**6** were generated using **Olex2**.[9]

CCDC-2015543 (**3**), CCDC-2015544 (**4**), CCDC-2015545 (**5**) and CCDC-2015546 (**6**), contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/contents/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: +44-1223-336-033; e-mail: deposit@ccdc.com.ac.uk).

Compound 3: There is one single molecule of **3** in the asymmetric unit

Compound 4: The asymmetric unit contains one molecule of **4** and two thf solvent molecules. One of these thf molecules was heavily disordered. Therefore, a solvent mask was calculated and 152 electrons were found in a volume of 520 $Å^3$ in one void per unit cell. This is consistent with the presence of one thf molecule per asymmetric unit, which account for 160 electrons per unit cell. Further, the second thf molecule showed a disorder over two positions (67:33). Additionally, both the P_5 and the Cp* ligand are disordered over two position with a distribution of 58:42 and 62:38, respectively. The restraints SADI and SIMU were applied to describe these disorders.

Compound 5: **Compound 5**: Crystals of compound **5** were very sensitive and could only be handled at low temperatures (-70°C). Further, the quality of the crystals was very low, despite several attempts of recrystallization. Additionally, the crystals were weakly diffracting, which is the reason that no reflections above a resolution of 0.89, with an I/σ higher than 3, could be detected. Although, the data quality does not allow the discussion of bond length or angles, the atom connectivity in compound **5** could still be determined unambiguously.

The asymmetric unit contains one molecule of **5** and 4.3 thf solvent molecules. Two of these thf solvent molecules were heavily disordered. Therefore, a solvent mask was calculated and 368 electrons were found in a volume of 1418 $Å^3$ in one void per unit cell. This is consistent with the presence of 2.3 thf molecules per asymmetric unit, which account for 368 electrons per unit cell. Additionally the P_5 ligand shows a disorder over two positions (82:18). To describe this disorder the SADI and SIMU restraint was applied.

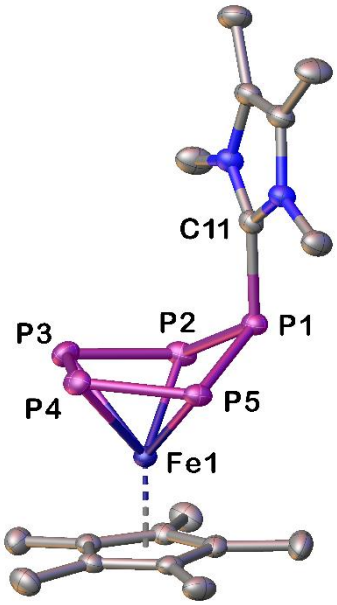
The asymmetric unit contains one molecule of **5** and 4.3 thf solvent molecules. Two of these thf solvent molecules were heavily disordered. Therefore, a solvent mask was calculated and 368 electrons were found in a volume of 1418 $Å^3$ in one void per unit cell. This is consistent with the presence of 2.3 thf molecules per asymmetric unit, which account for 368 electrons per unit cell. Additionally the P_5 ligand shows a disorder over two positions (82:18). To describe this disorder the SADI and SIMU restraint was applied.

Compound 6: The asymmetric unit contains the cation $[(IMe)_2P]^+$ and the anion $[Cp''Ta(CO)_2(\eta^3\text{-}P_3)]^-$.

Table S 3. Crystallographic data and details of the compounds **3**, **4**, **5** and **6**.

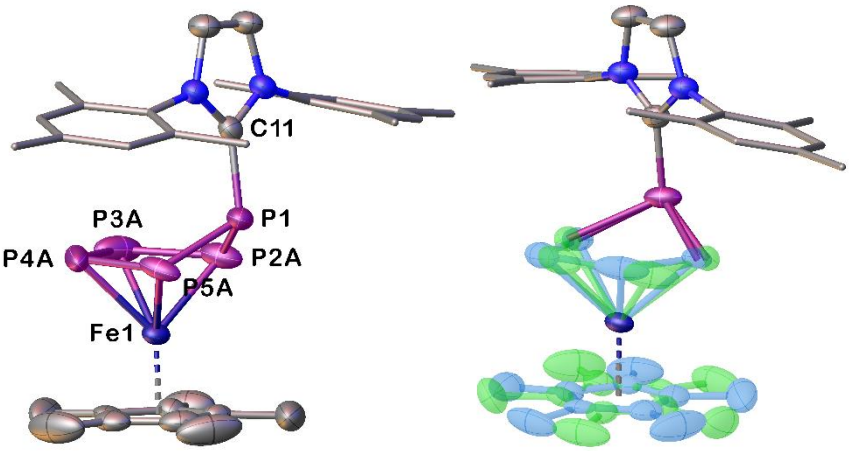
Compound	**3**	**4 · 2 thf**	**5 · 4.3 thf**	**6**
File Name	FR155	FR162	FR313	FR264
CCDC	2015543	2015544	2015545	2015546
Formula	$C_{17}H_{27}FeN_2P_5$	$C_{39}FeH_{55}N_2O_2P_5$	$C_{54.2}FeH_{85.4}N_2O_{4.3}P_5$	$C_{29}H_{45}N_4O_2P_4Ta$
$D_{calc.}$/ g cm^{-3}	1.478	1.305	1.211	1.542
μ/mm^{-1}	9.334	5.132	3.767	8.023
Formula Weight	470.10	794.55	1044.54	786.52
Colour	dark green	dark green	green	red
Shape	block	block	plate	plate
Size/mm^3	0.37×0.15×0.09	0.50×0.30×0.24	0.28×0.15×0.04	0.25×0.13×0.06
T/K	122.99(16)	123.00(10)	122.96(11)	123.0(2)
Crystal System	monoclinic	monoclinic	monoclinic	monoclinic
Space Group	$I2/a$	$P2_1/n$	P21/c	$P2_1/c$
a/Å	13.9605(2)	14.6421(5)	13.6902(11)	13.3561(8)
b/Å	12.4727(2)	18.3526(6)	19.6372(9)	10.5354(6)
c/Å	24.9230(5)	15.9403(6)	22.1012(16)	24.9298(16)
α/°	90	90	90	90
β/°	103.223(2)	109.217(4)	105.284(8)	105.029(6)
γ/°	90	90	90	90
V/Å^3	4224.66(13)	4044.8(3)	5731.5(7)	3387.9(4)
Z	8	4	4	4
Z'	1	1	1	1
Wavelength/Å	1.54184	1.54184	1.54184	1.54184
Radiation type	Cu K_α	Cu K_α	Cu K_α	CuK_α
Θ_{min}/°	3.644	3.558	3.347	3.426
Θ_{max}/°	74.344	74.685	60.002	74.851
Measured Refl's.	18138	38670	20741	17862
Ind't Refl's	4225	8099	8371	6595
Refl's with I > 2(I)	4129	7434	5639	5529
R_{int}	0.0363	0.0810	0.1108	0.0753
Parameters	235	558	555	375
Restraints	0	166	16	0
Largest Peak	0.524	0.665	1.182	4.492
Deepest Hole	-0.661	-0.552	-0.519	-3.513
GooF	1.061	1.031	1.015	1.039
wR_2 (all data)	0.0911	0.1197	0.2740	0.1996
wR_2	0.0904	0.1163	0.2416	0.1869
R_1 (all data)	0.0340	0.0461	0.1169	0.0811
R_1	0.0334	0.0431	0.0911	0.0704

Compound 3:



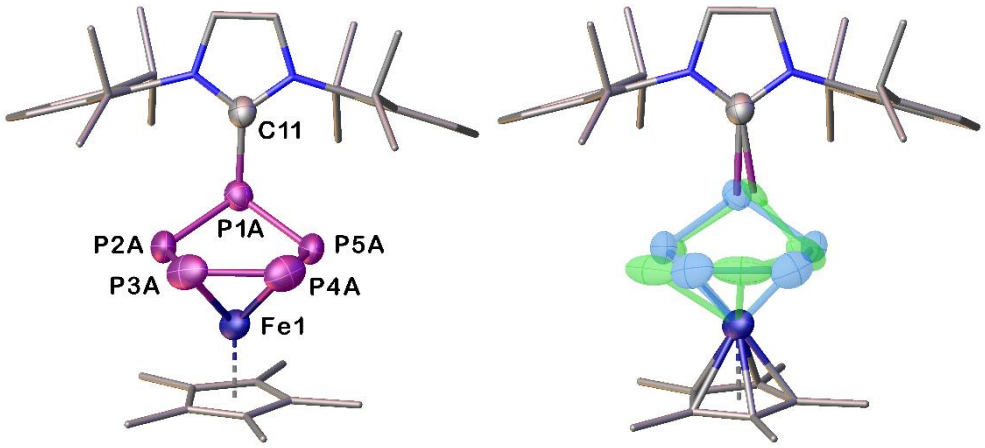
Selected Bond Lengths in Å		Selected Bond Angles in °	
P1–C11	1.860(2)	**C11–P1–P2**	114.99(7)
P1–P2	2.1572(7)	**C11–P1–P5**	111.43(6)
P2–P3	2.1552(8)	**P1–P2–P3**	107.62(3)
P3–P4	2.1302(8)	**P2–P3–P4**	104.18(3)
P4–P5	2.1491(7)	**P3–P4–P5**	104.19(3)
P5–P1	2.1621(7)	**P4–P5–P1**	107.86(3)
Fe1–P2	2.2979(6)	**P5–P1–P2**	95.03(3)
Fe1–P3	2.3415(6)		
Fe1–P4	2.3422(6)		
Fe1–P5	2.3077(5)		

Compound 4:



Selected Bond Lengths in Å		Selected Bond Angles in °	
P1–C11	1.849(2)	**C11–P1–P2A**	112.21(9)
P1–P2A	2.063(3)	**C11–P1–P5A**	112.21(15)
P2A–P3A	2.143(3)	**P1–P2A–P3A**	107.57(11)
P3A–P4A	2.115(3)	**P2A–P3A–P4A**	104.12(12)
P4A–P5A	2.138(5)	**P3A–P4A–P5A**	104.08(16)
P5A–P1	2.184(5)	**P4A–P5A–P1**	105.7(2)
Fe1–P2A	2.339(3)	**P5A–P1–P2A**	96.04(14)
Fe1–P3A	2.353(2)		
Fe1–P4A	2.303(2)		
Fe1–P5A	2.263(5)		

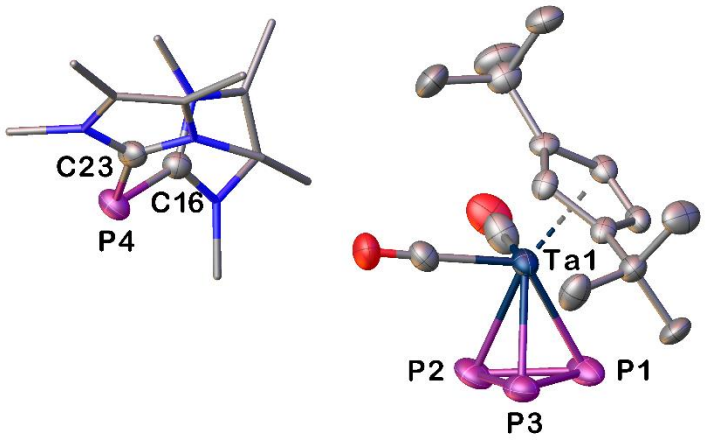
Compound 5:



In the subsequent Table selected bond length and angles of compound **5** are listed. However, it should be kept in mind, that the data quality of the measurement was low. Therefore, the listed bond length and angles are only given to get a rough insight in the connectivity of **5**.

Selected Bond Lengths in Å		Selected Bond Angles in °	
P1A–C11	1.900(7)	**C11–P1A–P2A**	113.8(3)
P1A–P2A	2.146(4)	**C11–P1A–P5A**	110.4(3)
P2A–P3A	2.144(5)	**P1A–P2A–P3A**	109.00(19)
P3A–P4A	2.113(5)	**P2A–P3A–P4A**	105.19(14)
P4A–P5A	2.151(5)	**P3A–P4A–P5A**	104.11(18)
P5A–P1A	2.155(4)	**P4A–P5A–P1A**	109.2(2)
Fe1–P2A	2.295(3)	**P5A–P1A–P2A**	96.1(2)
Fe1–P3A	2.343(2)		
Fe1–P4A	2.387(3)		
Fe1–P5A	2.338(4)		

Compound 6:



Selected Bond Lengths in Å		Selected Bond Angles in °	
P1–P2	2.184(4)	**P1–P2–P3**	60.26(12)
P1–P2	2.186(3)	**P2–P3–P1**	59.53(13)
P1–P2	2.169(4)	**P3–P1–P2**	60.21(12)
P4–C16	1.797(8)	**C16–P4–C23**	97.9(3)
P4–C23	1.796(8)	**P1–Ta1–P2**	49.49(9)
Ta1–P1	2.568(2)	**P2–Ta1–P3**	49.91(9)
Ta1–P2	2.614(2)	**P3–Ta1–P1**	50.43(8)
Ta1–P3	2.563(2)		

4. Details on DFT calculations

The geometries of the compounds have been fully optimized with gradient-corrected density functional theory (DFT) in form of Becke's three-parameter hybrid method B3LYP[12] with all electron 6-31G* basis set as implemented in Gaussian 09 program package.[13] All structures correspond to minima on their respective potential energy surfaces as verified by the subsequent vibrational analysis.

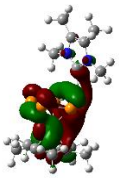
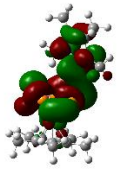
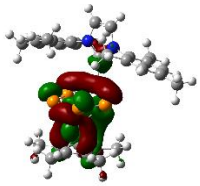
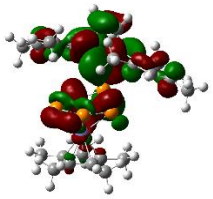
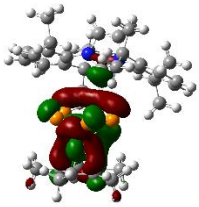
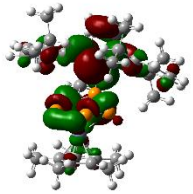
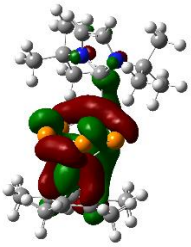
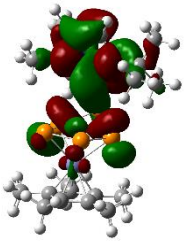
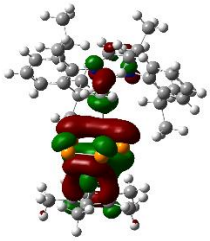
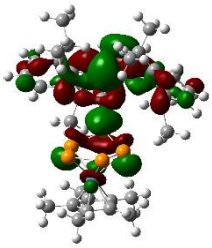
Compound	HOMO	LUMO
1·IMe		
1·IMes		
1·IDipp		
1·I^{t}Bu		
1·IDipp=CH_2		

Figure S 9. HOMO and LUMO of the compounds **1·LB**.

Table S 4. Total energies E^o_0, sum of electronic and thermal enthalpies H^o_{298} (Hartree) and standard entropies S^o_{298} (cal $mol^{-1}K^{-1}$). B3LYP/6-31G* level of theory.

Compound	E^o_0	H^o_{298}	S^o_{298}
1	-3360.581389	-3360.32536	141.236
IMe	-383.4330252	-383.238585	94.543
IMes	-924.1712522	-923.748456	170.758
IDipp	-1160.035165	-1159.431988	201.557
I^{t}Bu	-540.6829029	-540.370817	117.416
IDipp=CH_2	-1199.35876	-1198.726726	206.183
1·IMe	-3744.032328	-3743.578663	198.213
1·IMes	-4284.764922	-4284.084528	259.300
1·IDipp	-4520.622797	-4519.76108	295.303
1·I^{t}Bu	-3901.248443	-3900.678339	208.290
1·IDipp=CH_2	-4559.936175	-4559.044872	304.439

Table S 5. Optimized geometries of theoretically studied compounds. xyz coordinates in angstroms. B3LYP/6-31G* level of theory.

[Cp*Fe(η^5-P_5)] (1)			
26	-0.075360000	0.000085000	0.000031000
15	-1.654218000	1.311178000	-1.258387000
15	-1.653967000	-0.792072000	-1.634911000
15	-1.654322000	-1.799677000	0.248956000
15	-1.651109000	1.603476000	0.858073000
15	-1.654404000	-0.319304000	1.789495000
6	1.623539000	0.216888000	-1.200334000
6	1.623440000	-1.074291000	-0.578033000
6	1.624473000	1.207397000	-0.164594000
6	1.623648000	-0.881921000	0.841844000
6	1.625751000	0.528285000	1.097435000
6	1.711293000	1.179464000	2.447225000
1	1.227445000	2.159900000	2.455420000
1	2.762003000	1.321882000	2.733561000
1	1.234936000	0.571703000	3.220971000
6	1.704000000	-1.965763000	1.877111000
1	1.233057000	-1.663910000	2.816378000
1	2.753255000	-2.209159000	2.091426000
1	1.210114000	-2.882183000	1.542548000
6	1.708089000	-2.394470000	-1.287313000
1	1.221526000	-3.192525000	-0.719243000
1	2.758922000	-2.679740000	-1.431862000
1	1.234302000	-2.356000000	-2.272216000
6	1.708147000	2.692550000	-0.365785000
1	1.236934000	3.000342000	-1.303473000
1	2.758664000	3.011817000	-0.397841000
1	1.217464000	3.240171000	0.444187000
6	1.703711000	0.484536000	-2.674421000
1	1.209782000	-0.299450000	-3.254408000
1	2.752954000	0.530005000	-2.995385000
1	1.231756000	1.434887000	-2.938080000
IMe			
7	-1.060606000	-0.708576000	0.000002000
7	1.060607000	-0.708576000	-0.000002000
6	0.000000000	-1.576803000	-0.000001000

6	0.681925000	0.640154000	-0.000001000
6	-0.681926000	0.640154000	0.000003000
6	-2.434708000	-1.175017000	0.000002000
1	-2.402209000	-2.264931000	-0.000001000
1	-2.974117000	-0.829040000	0.889953000
1	-2.974119000	-0.829036000	-0.889948000
6	-1.662602000	1.766908000	-0.000004000
1	-2.314925000	1.745845000	-0.883278000
1	-2.314949000	1.745838000	0.883251000
1	-1.142686000	2.729490000	0.000007000
6	2.434709000	-1.175015000	-0.000001000
1	2.402211000	-2.264930000	0.000015000
1	2.974115000	-0.829049000	-0.889960000
1	2.974122000	-0.829022000	0.889941000
6	1.662601000	1.766908000	0.000003000
1	2.314937000	1.745837000	0.883267000
1	2.314936000	1.745846000	-0.883262000
1	1.142684000	2.729490000	0.000009000

IMes

7	0.000000000	1.064136000	-0.589575000
7	0.000000000	-1.064136000	-0.589575000
6	-0.000301000	2.435003000	-0.156715000
6	1.191450000	3.174723000	-0.221164000
6	0.000301000	-2.435003000	-0.156715000
6	0.000000000	0.000000000	0.280758000
6	-1.191858000	3.001056000	0.324685000
6	2.481348000	2.541941000	-0.687438000
1	2.683987000	1.615340000	-0.138983000
1	3.323541000	3.223573000	-0.535546000
1	2.451634000	2.279365000	-1.751938000
6	-1.191450000	-3.174723000	-0.221164000
6	1.191858000	-3.001056000	0.324685000
6	0.001144000	-0.677030000	-1.933047000
1	0.007062000	-1.388179000	-2.745420000
6	-0.007670000	5.114980000	0.658439000
6	1.162232000	4.511736000	0.187960000
1	2.082172000	5.091651000	0.147283000
6	-1.169403000	4.339925000	0.726829000
1	-2.086155000	4.787138000	1.105944000
6	-1.162232000	-4.511736000	0.187960000
1	-2.082172000	-5.091651000	0.147283000
6	-0.001144000	0.677030000	-1.933047000
1	-0.007062000	1.388179000	-2.745420000
6	-2.457593000	2.184890000	0.425123000
1	-2.770246000	1.805377000	-0.555613000
1	-3.276167000	2.785436000	0.833072000
1	-2.303995000	1.312685000	1.069289000
6	2.457593000	-2.184890000	0.425123000
1	2.770246000	-1.805377000	-0.555613000
1	3.276167000	-2.785436000	0.833072000
1	2.303995000	-1.312685000	1.069289000
6	0.007670000	-5.114980000	0.658439000
6	-2.481348000	-2.541941000	-0.687438000
1	-2.683987000	-1.615340000	-0.138983000
1	-3.323541000	-3.223573000	-0.535546000
1	-2.451634000	-2.279365000	-1.751938000
6	1.169403000	-4.339925000	0.726829000
1	2.086155000	-4.787138000	1.105944000
6	-0.020219000	6.569980000	1.066665000
1	0.953518000	6.885558000	1.456450000

1	-0.772735000	6.763251000	1.838527000
1	-0.254765000	7.221079000	0.213658000
6	0.020219000	-6.569980000	1.066665000
1	0.772735000	-6.763251000	1.838527000
1	0.254765000	-7.221079000	0.213658000
1	-0.953518000	-6.885558000	1.456450000

IDipp

7	-1.031417000	0.000004000	0.515457000
7	1.098225000	-0.000006000	0.543259000
6	0.693076000	-0.000011000	1.880610000
1	1.394718000	-0.000018000	2.701147000
6	-0.661378000	-0.000005000	1.862568000
1	-1.383590000	-0.000005000	2.665023000
6	3.135487000	1.234505000	-0.047440000
6	-3.057890000	1.232616000	-0.118468000
6	-2.404444000	0.000009000	0.079514000
6	0.044791000	0.000004000	-0.341149000
6	4.482446000	1.206577000	-0.428773000
1	5.014651000	2.139781000	-0.584374000
6	-2.351132000	2.571332000	0.065873000
1	-1.317309000	2.368063000	0.357248000
6	2.482239000	-0.000010000	0.139371000
6	-3.057905000	-1.232593000	-0.118450000
6	3.135471000	-1.234530000	-0.047468000
6	2.388367000	2.557805000	0.088170000
1	1.540101000	2.393154000	0.761386000
6	-2.994938000	3.405054000	1.190279000
1	-4.035765000	3.660215000	0.958268000
1	-2.989823000	2.862211000	2.142326000
1	-2.446441000	4.343895000	1.332092000
6	5.151183000	-0.000019000	-0.615074000
1	6.197408000	-0.000023000	-0.910288000
6	-4.401707000	-1.204823000	-0.511176000
1	-4.928750000	-2.141500000	-0.671492000
6	4.482430000	-1.206611000	-0.428801000
1	5.014623000	-2.139819000	-0.584423000
6	-2.351163000	-2.571314000	0.065916000
1	-1.317328000	-2.368052000	0.357251000
6	-4.401692000	1.204857000	-0.511196000
1	-4.928722000	2.141538000	-0.671528000
6	2.388334000	-2.557823000	0.088117000
1	1.540077000	-2.393176000	0.761346000
6	-2.299451000	3.362002000	-1.255508000
1	-1.803637000	2.779797000	-2.038766000
1	-3.303670000	3.622554000	-1.610725000
1	-1.742130000	4.296552000	-1.118840000
6	-5.071332000	0.000020000	-0.703312000
1	-6.114725000	0.000023000	-1.008080000
6	3.236849000	-3.684244000	0.701359000
1	4.047317000	-4.002347000	0.035256000
1	3.683900000	-3.380968000	1.654918000
1	2.609210000	-4.563850000	0.885168000
6	1.810150000	-2.976221000	-1.280177000
1	1.151704000	-2.194627000	-1.672210000
1	2.614645000	-3.147719000	-2.005985000
1	1.234097000	-3.905423000	-1.187284000
6	3.236892000	3.684199000	0.701447000
1	3.683927000	3.380895000	1.655005000
1	4.047372000	4.002305000	0.035360000
1	2.609265000	4.563811000	0.885268000

6	1.810204000	2.976243000	-1.280121000
1	2.614708000	3.147750000	-2.005915000
1	1.151754000	2.194665000	-1.672180000
1	1.234159000	3.905448000	-1.187212000
6	-2.299538000	-3.362038000	-1.255435000
1	-3.303772000	-3.622593000	-1.610608000
1	-1.803744000	-2.779872000	-2.038735000
1	-1.742224000	-4.296589000	-1.118747000
6	-2.994950000	-3.404982000	1.190374000
1	-2.989795000	-2.862103000	2.142401000
1	-4.035789000	-3.660129000	0.958404000
1	-2.446467000	-4.343829000	1.332206000

I^{t}Bu

7	0.000001000	1.069084000	-0.298844000
7	-0.000001000	-1.069084000	-0.298844000
6	0.000000000	-0.678434000	-1.636250000
1	-0.000004000	-1.364774000	-2.467255000
6	0.000000000	0.678434000	-1.636250000
1	0.000004000	1.364774000	-2.467255000
6	-0.000009000	2.466826000	0.221488000
6	0.000000000	0.000000000	0.554851000
6	0.000009000	-2.466826000	0.221488000
6	0.000001000	3.469145000	-0.940204000
1	0.890696000	3.363388000	-1.569538000
1	-0.890680000	3.363387000	-1.569557000
1	-0.000004000	4.485741000	-0.534352000
6	1.262949000	2.659148000	1.079639000
1	2.166590000	2.542879000	0.470256000
1	1.273362000	3.660519000	1.525405000
1	1.287808000	1.910909000	1.875567000
6	-1.262982000	2.659144000	1.079610000
1	-1.273424000	3.660527000	1.525349000
1	-2.166612000	2.542843000	0.470217000
1	-1.287849000	1.910929000	1.875562000
6	-0.000001000	-3.469145000	-0.940204000
1	0.890680000	-3.363387000	-1.569557000
1	0.000004000	-4.485741000	-0.534352000
1	-0.890696000	-3.363388000	-1.569538000
6	1.262982000	-2.659144000	1.079610000
1	2.166612000	-2.542843000	0.470217000
1	1.287849000	-1.910929000	1.875562000
1	1.273424000	-3.660527000	1.525349000
6	-1.262949000	-2.659148000	1.079639000
1	-1.273362000	-3.660519000	1.525405000
1	-1.287808000	-1.910909000	1.875567000
1	-2.166590000	-2.542879000	0.470256000

IDipp=CH$_2$

7	-1.107513000	0.000000000	-0.580374000
7	1.107513000	0.000000000	-0.580374000
6	0.672941000	0.000000000	-1.916539000
1	1.380385000	0.000000000	-2.730545000
6	-0.672941000	0.000000000	-1.916539000
1	-1.380385000	0.000000000	-2.730545000
6	3.124521000	-1.233148000	0.065021000
6	-3.124521000	-1.233148000	0.065021000
6	-2.470071000	0.000000000	-0.146571000
6	0.000000000	0.000000000	0.280484000
6	4.457603000	-1.205780000	0.492091000
1	4.982399000	-2.141962000	0.663143000
6	-2.419545000	-2.569402000	-0.142542000

1	-1.421768000	-2.359829000	-0.538423000
6	2.470071000	0.000000000	-0.146571000
6	-3.124521000	1.233148000	0.065021000
6	3.124521000	1.233148000	0.065021000
6	2.419545000	-2.569402000	-0.142542000
1	1.421768000	-2.359829000	-0.538423000
6	-3.148488000	-3.448647000	-1.176330000
1	-4.154362000	-3.724727000	-0.838664000
1	-3.249755000	-2.933278000	-2.138153000
1	-2.590908000	-4.377391000	-1.345857000
6	5.120057000	0.000000000	0.704504000
1	6.154870000	0.000000000	1.037567000
6	-4.457603000	1.205780000	0.492091000
1	-4.982399000	2.141962000	0.663143000
6	4.457603000	1.205780000	0.492091000
1	4.982399000	2.141962000	0.663143000
6	-2.419545000	2.569402000	-0.142542000
1	-1.421768000	2.359829000	-0.538423000
6	-4.457603000	-1.205780000	0.492091000
1	-4.982399000	-2.141962000	0.663143000
6	2.419545000	2.569402000	-0.142542000
1	1.421768000	2.359829000	-0.538423000
6	-2.233624000	-3.314824000	1.193533000
1	-1.657312000	-2.706958000	1.898174000
1	-3.198204000	-3.557191000	1.656054000
1	-1.694029000	-4.256189000	1.033323000
6	-5.120057000	0.000000000	0.704504000
1	-6.154870000	0.000000000	1.037567000
6	3.148488000	3.448647000	-1.176330000
1	4.154362000	3.724727000	-0.838664000
1	3.249755000	2.933278000	-2.138153000
1	2.590908000	4.377391000	-1.345857000
6	2.233624000	3.314824000	1.193533000
1	1.657312000	2.706958000	1.898174000
1	3.198204000	3.557191000	1.656054000
1	1.694029000	4.256189000	1.033323000
6	3.148488000	-3.448647000	-1.176330000
1	3.249755000	-2.933278000	-2.138153000
1	4.154362000	-3.724727000	-0.838664000
1	2.590908000	-4.377391000	-1.345857000
6	2.233624000	-3.314824000	1.193533000
1	3.198204000	-3.557191000	1.656054000
1	1.657312000	-2.706958000	1.898174000
1	1.694029000	-4.256189000	1.033323000
6	-2.233624000	3.314824000	1.193533000
1	-3.198204000	3.557191000	1.656054000
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1	-3.249755000	2.933278000	-2.138153000
1	-4.154362000	3.724727000	-0.838664000
1	-2.590908000	4.377391000	-1.345857000
6	0.000000000	0.000000000	1.639328000
1	-0.932042000	0.000000000	2.187351000
1	0.932042000	0.000000000	2.187351000

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26	-1.720096000	-0.040406000	-0.097607000
15	0.072570000	1.499731000	-0.356636000
15	1.154619000	0.337982000	1.186607000
15	-0.143610000	-1.434909000	1.011489000

15	-0.350446000	0.159529000	-2.019846000
15	-0.504500000	-1.790120000	-1.113912000
7	3.730783000	1.131305000	0.297400000
7	3.639268000	-1.032435000	0.301858000
6	-3.096164000	1.288698000	0.768904000
6	-3.180734000	0.011545000	1.404686000
6	-3.363277000	1.111434000	-0.629220000
6	-3.503041000	-0.965370000	0.403690000
6	-3.617141000	-0.283337000	-0.855275000
6	4.917147000	-0.682567000	-0.138455000
6	2.907867000	0.081050000	0.558494000
6	4.971673000	0.681204000	-0.150305000
6	-4.027676000	-0.903502000	-2.159809000
1	-3.579013000	-0.382608000	-3.010813000
1	-5.119441000	-0.867680000	-2.280799000
1	-3.718089000	-1.950825000	-2.221333000
6	3.353516000	2.536110000	0.452633000
1	2.736772000	2.864011000	-0.387788000
1	4.259510000	3.139119000	0.515576000
1	2.776976000	2.651303000	1.373110000
6	-3.772197000	-2.421425000	0.653740000
1	-3.569680000	-3.025563000	-0.235345000
1	-4.821978000	-2.582423000	0.937278000
1	-3.147898000	-2.813117000	1.463213000
6	-3.050650000	-0.247139000	2.878604000
1	-2.671924000	-1.252944000	3.078970000
1	-4.026647000	-0.149453000	3.375482000
1	-2.364852000	0.460281000	3.354537000
6	-3.455991000	2.210248000	-1.648628000
1	-2.726268000	3.002889000	-1.453688000
1	-4.454820000	2.669223000	-1.639332000
1	-3.268570000	1.837217000	-2.659425000
6	3.219525000	-2.419029000	0.502058000
1	3.432025000	-2.997495000	-0.399774000
1	2.148374000	-2.446012000	0.696731000
1	3.758005000	-2.851898000	1.350939000
6	6.076422000	1.604306000	-0.546458000
1	5.771791000	2.279755000	-1.354628000
1	6.934291000	1.029577000	-0.903264000
1	6.420302000	2.221321000	0.292969000
6	-2.868620000	2.602635000	1.460615000
1	-2.224845000	2.493385000	2.338623000
1	-3.823836000	3.029013000	1.799331000
1	-2.394410000	3.330430000	0.796761000
6	5.942381000	-1.704112000	-0.503968000
1	6.168006000	-2.374144000	0.334505000
1	6.874625000	-1.215464000	-0.796591000
1	5.615993000	-2.327107000	-1.345642000

1·IMes

26	-2.482779000	0.000075000	-0.080739000
15	0.493850000	-0.000013000	0.757701000
15	-0.752160000	-1.641975000	0.015138000
15	-0.752063000	1.642020000	0.015133000
15	-1.516084000	-1.077167000	-1.947634000
15	-1.516019000	1.077251000	-1.947638000
7	3.034632000	-1.086698000	-0.183073000
7	3.034699000	1.086515000	-0.183073000
6	2.686262000	-2.485955000	-0.046368000
6	2.387545000	-3.220006000	-1.205084000
6	2.686416000	2.485793000	-0.046368000

6	2.239562000	-0.000067000	0.033190000
6	2.739309000	-3.072110000	1.227648000
6	2.315857000	-2.572156000	-2.566115000
1	1.446293000	-1.906753000	-2.631100000
1	2.210882000	-3.331104000	-3.346214000
1	3.206420000	-1.975321000	-2.793575000
6	2.739498000	3.071944000	1.227649000
6	2.387749000	3.219865000	-1.205083000
6	4.315400000	0.676629000	-0.536969000
1	5.091979000	1.393949000	-0.750276000
6	2.138384000	-5.206669000	0.199112000
6	2.121563000	-4.582945000	-1.052003000
1	1.881303000	-5.168201000	-1.936438000
6	2.455804000	-4.437043000	1.322079000
1	2.485397000	-4.908895000	2.301484000
6	2.456080000	4.436894000	1.322081000
1	2.485702000	4.908744000	2.301487000
6	4.315358000	-0.676891000	-0.536968000
1	5.091894000	-1.394259000	-0.750275000
6	-4.498786000	0.000158000	-0.497824000
6	3.083174000	-2.270386000	2.460061000
1	4.028915000	-1.727107000	2.344404000
1	3.177260000	-2.926388000	3.329917000
1	2.305577000	-1.528945000	2.679777000
6	2.316024000	2.572022000	-2.566116000
1	3.206547000	1.975124000	-2.793572000
1	2.211107000	3.330978000	-3.346215000
1	1.446414000	1.906679000	-2.631106000
6	2.138713000	5.206542000	0.199113000
6	-3.620714000	0.714506000	1.526867000
6	-4.163159000	1.161720000	0.276437000
6	3.083311000	2.270197000	2.460061000
1	2.305675000	1.528793000	2.679767000
1	3.177422000	2.926190000	3.329921000
1	4.029027000	1.726872000	2.344411000
6	2.121856000	4.582821000	-1.052002000
1	1.881637000	5.168093000	-1.936437000
6	-4.163251000	-1.161455000	0.276399000
6	1.797434000	-6.671390000	0.335960000
1	2.103376000	-7.239595000	-0.548769000
1	0.714646000	-6.808998000	0.452980000
1	2.280004000	-7.116797000	1.212121000
6	-3.620772000	-0.714326000	1.526844000
6	1.797857000	6.671286000	0.335963000
1	0.715080000	6.808961000	0.452999000
1	2.103822000	7.239469000	-0.548772000
1	2.280468000	7.116664000	1.212116000
6	-4.427050000	2.591003000	-0.101206000
1	-3.653996000	3.260204000	0.290042000
1	-5.392749000	2.929355000	0.300809000
1	-4.453409000	2.722831000	-1.186595000
6	-3.224411000	1.587910000	2.682822000
1	-2.398635000	1.152102000	3.253573000
1	-4.071159000	1.722412000	3.371534000
1	-2.904667000	2.578762000	2.349783000
6	-5.176194000	0.000208000	-1.838115000
1	-4.902595000	0.880735000	-2.426845000
1	-6.269236000	0.000287000	-1.722281000
1	-4.902723000	-0.880357000	-2.426845000
6	-3.224538000	-1.587800000	2.682769000
1	-2.904839000	-2.578655000	2.349696000

1	-4.071306000	-1.722285000	3.371459000
1	-2.398749000	-1.152058000	3.253554000
6	-4.427253000	-2.590705000	-0.101293000
1	-4.453563000	-2.722505000	-1.186687000
1	-5.393005000	-2.928977000	0.300659000
1	-3.654283000	-3.259985000	0.289982000

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26	-2.922441000	0.000009000	0.167590000
15	0.017436000	0.000229000	-0.638304000
15	-1.191578000	1.649187000	0.122535000
15	-1.191432000	-1.648982000	0.122212000
15	-2.004773000	-1.074580000	2.061233000
15	-2.004936000	1.074372000	2.061409000
7	2.669711000	-1.086519000	-0.060462000
7	2.669852000	1.086560000	-0.060295000
6	3.996356000	0.676512000	0.006058000
1	4.801340000	1.392123000	0.049364000
6	3.996276000	-0.676623000	0.005927000
1	4.801158000	-1.392345000	0.049247000
6	2.234832000	3.166389000	1.166187000
6	2.235184000	-3.166431000	1.166023000
6	2.303978000	-2.491545000	-0.069146000
6	1.844685000	0.000078000	-0.107734000
6	1.968183000	4.539477000	1.127771000
1	1.902274000	5.094058000	2.058391000
6	2.475145000	-2.472244000	2.504381000
1	2.431058000	-1.390189000	2.339560000
6	2.304092000	2.491570000	-0.069014000
6	2.123796000	-3.134394000	-1.308854000
6	2.124232000	3.134452000	-1.308735000
6	2.474572000	2.472084000	2.504527000
1	2.430213000	1.390046000	2.339641000
6	-4.015961000	0.714331000	-1.470069000
6	3.880285000	-2.805636000	3.048926000
1	3.981490000	-3.880859000	3.238019000
1	4.672002000	-2.516481000	2.348224000
1	4.058512000	-2.280142000	3.994366000
6	1.779118000	5.203800000	-0.080264000
1	1.568732000	6.269862000	-0.084302000
6	1.857630000	-4.508181000	-1.282521000
1	1.709579000	-5.038574000	-2.218105000
6	-4.593134000	1.161451000	-0.234973000
6	1.857895000	4.508224000	-1.282415000
1	1.710096000	5.038643000	-2.218024000
6	2.247495000	-2.408557000	-2.645524000
1	2.281089000	-1.332524000	-2.449512000
6	1.968718000	-4.539573000	1.127620000
1	1.903201000	-5.094194000	2.058246000
6	2.248308000	2.408724000	-2.645443000
1	2.282717000	1.332708000	-2.449456000
6	1.396438000	-2.808521000	3.549937000
1	0.393679000	-2.589872000	3.172796000
1	1.430784000	-3.862988000	3.847268000
1	1.558498000	-2.210092000	4.453706000
6	-4.015854000	-0.714189000	-1.470215000
6	1.779335000	-5.203848000	-0.080373000
1	1.569085000	-6.269937000	-0.084422000
6	-4.866206000	2.590937000	0.135583000
1	-4.925614000	2.722017000	1.219763000
1	-4.080158000	3.259191000	-0.230670000

1	-5.818428000	2.931258000	-0.295721000
6	-3.583222000	1.585801000	-2.614117000
1	-3.283268000	2.580335000	-2.273716000
1	-2.733513000	1.152029000	-3.150613000
1	-4.403719000	1.711427000	-3.335459000
6	3.562305000	2.792969000	-3.356105000
1	3.586194000	3.863364000	-3.591952000
1	4.437334000	2.569730000	-2.734637000
1	3.664394000	2.239528000	-4.296910000
6	-4.951610000	-0.000189000	0.528412000
6	1.033159000	2.651916000	-3.559470000
1	0.102530000	2.364324000	-3.061014000
1	0.951807000	3.702864000	-3.859829000
1	1.130611000	2.055649000	-4.474116000
6	3.879830000	2.805089000	3.049050000
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1	3.981321000	3.880288000	3.238117000
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6	1.396023000	2.808595000	3.550142000
1	1.430776000	3.862995000	3.847671000
1	0.393167000	2.590377000	3.173004000
1	1.557885000	2.209959000	4.453809000
6	-4.592973000	-1.161623000	-0.235207000
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1	1.129766000	-2.056059000	-4.474269000
6	-5.665721000	-0.000415000	1.849486000
1	-5.408372000	-0.880839000	2.445590000
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1	-3.284274000	-2.580336000	-2.274518000
1	-4.402991000	-1.709640000	-3.336609000
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1	3.586483000	-3.862298000	-3.591789000
1	3.663624000	-2.238452000	-4.296872000
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1	-4.923896000	-2.722455000	1.219560000
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26	2.046498000	-0.018935000	-0.112880000
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15	0.289853000	1.523982000	-0.134012000
15	0.397634000	-1.595284000	0.412677000
15	0.883995000	0.696237000	-2.052296000
15	0.970490000	-1.424915000	-1.678503000
7	-3.451073000	1.104281000	-0.207119000
7	-3.453249000	-1.093194000	-0.200810000
6	-2.747896000	0.005271000	0.233750000
6	-4.488467000	-0.670185000	-1.018693000
1	-5.152276000	-1.352901000	-1.517791000
6	-4.484631000	0.677596000	-1.025215000
1	-5.142757000	1.359271000	-1.533962000
6	4.022551000	-0.061092000	-0.694815000
6	3.336167000	-0.411243000	1.493914000
6	3.787094000	-1.068360000	0.301385000

6	3.716177000	1.215734000	-0.114654000
6	3.292564000	0.994991000	1.237557000
6	4.056811000	-2.539177000	0.160426000
1	3.341541000	-3.136393000	0.735081000
1	5.064170000	-2.788568000	0.522798000
1	3.986733000	-2.862413000	-0.882116000
6	3.053114000	-1.077436000	2.810032000
1	2.313804000	-0.521252000	3.394216000
1	3.969882000	-1.147588000	3.412948000
1	2.664377000	-2.090329000	2.672905000
6	4.587018000	-0.293582000	-2.066946000
1	4.291447000	-1.269692000	-2.462638000
1	5.685307000	-0.257391000	-2.047084000
1	4.240613000	0.462426000	-2.777762000
6	2.955292000	2.063354000	2.238381000
1	2.500050000	2.934492000	1.758742000
1	3.860523000	2.401860000	2.762548000
1	2.250915000	1.700947000	2.993282000
6	3.901864000	2.555807000	-0.767150000
1	3.809593000	2.490137000	-1.855035000
1	4.895660000	2.966452000	-0.538741000
1	3.157727000	3.279895000	-0.420125000
6	-3.366192000	-2.556154000	0.216955000
6	-3.391875000	2.576926000	0.192124000
6	-4.805190000	-3.118311000	0.281517000
1	-5.268359000	-3.227898000	-0.703271000
1	-4.756563000	-4.119931000	0.718073000
1	-5.454270000	-2.504375000	0.914777000
6	-2.563980000	-3.337505000	-0.832886000
1	-2.535416000	-4.396517000	-0.554336000
1	-3.037941000	-3.257886000	-1.817751000
1	-1.538557000	-2.974743000	-0.908009000
6	-2.776826000	-2.676242000	1.629279000
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1	-1.720081000	-2.416810000	1.672643000
6	-4.845429000	3.041500000	0.448318000
1	-5.456059000	3.074877000	-0.457865000
1	-5.344470000	2.404835000	1.186425000
1	-4.814006000	4.060334000	0.844710000
6	-2.623171000	2.787561000	1.503521000
1	-2.989031000	2.125826000	2.294692000
1	-1.549203000	2.651596000	1.391246000
1	-2.787938000	3.821340000	1.823862000
6	-2.779396000	3.382149000	-0.963539000
1	-2.797574000	4.447899000	-0.710689000
1	-1.742707000	3.088384000	-1.142343000
1	-3.352360000	3.244472000	-1.887371000

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26	-3.483218000	-0.000098000	-0.449051000
15	-0.533729000	0.000059000	0.311609000
15	-1.740801000	-1.648107000	-0.437857000
15	-1.740848000	1.648078000	-0.438241000
15	-2.585421000	1.074736000	-2.361418000
15	-2.585267000	-1.075301000	-2.361269000
7	3.040603000	-1.092345000	0.622478000
7	3.040522000	1.092398000	0.622572000
6	4.107513000	0.676617000	1.413716000
1	4.759273000	1.389382000	1.891220000
6	4.107531000	-0.676551000	1.413704000

1	4.759353000	-1.389309000	1.891129000
6	2.000907000	3.223303000	1.277141000
6	2.001332000	-3.223338000	1.277233000
6	2.742984000	-2.481828000	0.333612000
6	2.394485000	0.000024000	0.122446000
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1	1.198987000	5.175664000	1.683717000
6	1.499874000	-2.625266000	2.589422000
1	1.484275000	-1.535747000	2.480299000
6	2.742825000	2.481860000	0.333667000
6	3.252841000	-3.043516000	-0.855062000
6	3.252874000	3.043604000	-0.854892000
6	1.499298000	2.625209000	2.589263000
1	1.483665000	1.535699000	2.480108000
6	-4.568566000	-0.714492000	1.191496000
6	2.457447000	-2.976504000	3.748439000
1	2.502122000	-4.061268000	3.902033000
1	3.479149000	-2.626075000	3.563373000
1	2.108824000	-2.518636000	4.681276000
6	2.249104000	5.152965000	-0.184618000
1	2.047917000	6.200582000	-0.390573000
6	2.982313000	-4.396122000	-1.092643000
1	3.353771000	-4.861487000	-2.000719000
6	-5.149994000	-1.161653000	-0.041112000
6	2.982218000	4.396177000	-1.092544000
1	3.353826000	4.861579000	-2.000541000
6	4.101663000	-2.259805000	-1.852586000
1	4.121348000	-1.210906000	-1.540261000
6	1.771217000	-4.572963000	0.986286000
1	1.199756000	-5.175798000	1.684003000
6	4.102053000	2.260034000	-1.852225000
1	4.122196000	1.211211000	-1.539664000
6	0.063180000	-3.055538000	2.934626000
1	-0.623785000	-2.850646000	2.108894000
1	0.003041000	-4.122231000	3.180525000
1	-0.283532000	-2.499937000	3.813042000
6	-4.568339000	0.714461000	1.191511000
6	2.249497000	-5.152997000	-0.184540000
1	2.048419000	-6.200647000	-0.390434000
6	-5.421713000	-2.590921000	-0.412896000
1	-5.483656000	-2.719878000	-1.497157000
1	-4.632448000	-3.257659000	-0.050978000
1	-6.372038000	-2.934097000	0.020678000
6	-4.130240000	-1.586881000	2.332560000
1	-3.826648000	-2.578820000	1.987707000
1	-3.280505000	-1.151573000	2.867503000
1	-4.948653000	-1.718519000	3.055512000
6	5.560864000	2.760935000	-1.843945000
1	5.623352000	3.808767000	-2.158991000
1	6.004543000	2.687106000	-0.844610000
1	6.172910000	2.166930000	-2.532631000
6	-5.509785000	0.000167000	-0.804023000
6	3.513657000	2.297595000	-3.275433000
1	2.481548000	1.932995000	-3.294272000
1	3.516302000	3.312549000	-3.688010000
1	4.109858000	1.668133000	-3.946102000
6	2.456774000	2.976400000	3.748380000
1	3.478495000	2.625967000	3.563400000
1	2.501452000	4.061159000	3.902010000
1	2.108061000	2.518510000	4.681173000
6	0.062605000	3.055551000	2.934372000

1	0.002570000	4.122195000	3.180532000
1	-0.624291000	2.850956000	2.108507000
1	-0.284292000	2.499774000	3.812599000
6	-5.149685000	1.161838000	-0.041079000
6	3.513274000	-2.297911000	-3.275782000
1	3.516739000	-3.312880000	-3.688327000
1	2.480876000	-1.934131000	-3.294630000
1	4.108974000	-1.668007000	-3.946478000
6	-6.227784000	0.000120000	-2.122933000
1	-5.972968000	0.881176000	-2.719105000
1	-5.970676000	-0.879443000	-2.720330000
1	-7.316837000	-0.001407000	-1.973492000
6	-4.129632000	1.586746000	2.332499000
1	-3.281196000	1.150203000	2.868505000
1	-3.823878000	2.577927000	1.987343000
1	-4.948514000	1.720295000	3.054574000
6	5.560679000	-2.760098000	-1.844219000
1	6.004395000	-2.685754000	-0.844936000
1	5.623559000	-3.808014000	-2.158912000
1	6.172453000	-2.166081000	-2.533139000
6	-5.420975000	2.591233000	-0.412695000
1	-4.631537000	3.257682000	-0.050641000
1	-5.482818000	2.720374000	-1.496940000
1	-6.371217000	2.934613000	0.020890000
6	1.219804000	-0.000031000	-0.727557000
1	1.178835000	-0.895063000	-1.347598000
1	1.178826000	0.894895000	-1.347764000

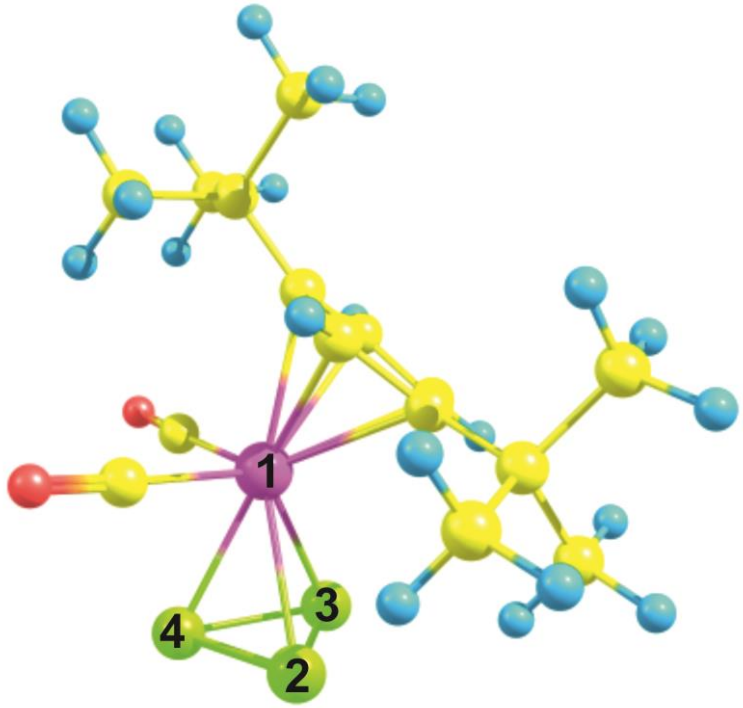


Figure S 10. Molecule model of [Cp''Ta(CO)$_2$(η^3-P$_3$)]$^-$ used for WBI calculations.

Table S 6. Wiberg bond indexes (WBI) for selected bonds in [Cp''Ta(CO)$_2$(η^3-P$_3$)]$^-$. B3LYP/def2-SVPD level of theory.

Bond	Bond distance, Å	WBI
Ta-P2	2.6433	0.8549
Ta-P3	2.6324	0.8705
Ta-P4	2.6802	0.7648
P2-P3	2.2129	1.0064
P2-P4	2.1954	1.0029
P3-P4	2.1951	1.0137

Usually for the single bonds (bond order one) WBI value is slightly less than 1.0. WBI slightly larger than 1.0 may indicate small additional stabilization compared to the single bond.

Wiberg bond index matrix in the NAO basis:

	Atom	1	2	3	4	5	6	7	8	9
1.	Ta	0.0000	0.8549	0.8705	0.7648	0.1125	0.1211	0.2602	0.3323	0.0113
2.	P	0.8549	0.0000	1.0064	1.0029	0.0123	0.0303	0.0378	0.0044	0.0004
3.	P	0.8705	1.0064	0.0000	1.0137	0.0326	0.0085	0.0051	0.0113	0.0009
4.	P	0.7648	1.0029	1.0137	0.0000	0.0299	0.0383	0.0113	0.0110	0.0003
5.	O	0.1125	0.0123	0.0326	0.0299	0.0000	0.0175	0.0015	0.0078	0.0001
6.	O	0.1211	0.0303	0.0085	0.0383	0.0175	0.0000	0.0033	0.0029	0.0003
7.	C	0.2602	0.0378	0.0051	0.0113	0.0015	0.0033	0.0000	1.2641	0.0051
8.	C	0.3323	0.0044	0.0113	0.0110	0.0078	0.0029	1.2641	0.0000	0.8891
9.	H	0.0113	0.0004	0.0009	0.0003	0.0001	0.0003	0.0051	0.8891	0.0000
10.	C	0.3296	0.0103	0.0101	0.0093	0.0088	0.0102	0.0399	1.2286	0.0049
11.	C	1.2928	0.0570	0.0265	0.0928	0.0340	1.9502	0.0106	0.0056	0.0006
12.	C	0.2914	0.0032	0.0390	0.0108	0.0040	0.0010	1.2763	0.0369	0.0101
13.	H	0.0118	0.0002	0.0009	0.0006	0.0003	0.0001	0.0050	0.0101	0.0003
14.	C	0.0120	0.0013	0.0005	0.0009	0.0001	0.0002	0.9825	0.0135	0.0008
15.	C	0.3425	0.0143	0.0059	0.0093	0.0047	0.0097	0.0395	0.0354	0.0100
16.	H	0.0129	0.0009	0.0010	0.0005	0.0005	0.0002	0.0084	0.0098	0.0003
17.	C	0.0137	0.0011	0.0006	0.0007	0.0004	0.0004	0.0072	0.0137	0.0008
18.	C	0.0028	0.0034	0.0013	0.0018	0.0001	0.0002	0.0115	0.0032	0.0006
19.	H	0.0002	0.0002	0.0001	0.0001	0.0000	0.0000	0.0009	0.0006	0.0008
20.	H	0.0023	0.0064	0.0010	0.0009	0.0001	0.0002	0.0008	0.0002	0.0000
21.	H	0.0007	0.0003	0.0001	0.0001	0.0000	0.0000	0.0117	0.0005	0.0001
22.	C	1.2629	0.0320	0.0595	0.0663	1.9784	0.0348	0.0056	0.0190	0.0003

23.	C	0.0016	0.0028	0.0012	0.0042	0.0001	0.0001	0.0111	0.0090	0.0003
24.	H	0.0027	0.0082	0.0011	0.0016	0.0002	0.0003	0.0009	0.0003	0.0000
25.	H	0.0001	0.0002	0.0001	0.0002	0.0000	0.0000	0.0007	0.0003	0.0000
26.	H	0.0005	0.0001	0.0001	0.0002	0.0000	0.0000	0.0115	0.0002	0.0000
27.	C	0.0066	0.0028	0.0002	0.0011	0.0001	0.0001	0.0159	0.0074	0.0002
28.	H	0.0002	0.0001	0.0001	0.0001	0.0000	0.0000	0.0012	0.0003	0.0000
29.	H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0011	0.0005	0.0001
30.	H	0.0005	0.0004	0.0001	0.0002	0.0000	0.0000	0.0117	0.0012	0.0000
31.	C	0.0094	0.0003	0.0003	0.0003	0.0007	0.0007	0.0013	0.0068	0.0002
32.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0006	0.0001
33.	H	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0003	0.0000
34.	H	0.0008	0.0000	0.0000	0.0001	0.0001	0.0001	0.0004	0.0012	0.0000
35.	C	0.0015	0.0004	0.0001	0.0002	0.0001	0.0022	0.0006	0.0086	0.0003
36.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
37.	H	0.0021	0.0015	0.0001	0.0005	0.0000	0.0025	0.0001	0.0003	0.0000
38.	H	0.0004	0.0001	0.0000	0.0000	0.0000	0.0001	0.0004	0.0002	0.0000
39.	C	0.0033	0.0002	0.0012	0.0003	0.0007	0.0003	0.0011	0.0028	0.0005
40.	H	0.0034	0.0003	0.0010	0.0006	0.0005	0.0002	0.0001	0.0003	0.0000
41.	H	0.0003	0.0000	0.0003	0.0000	0.0001	0.0000	0.0002	0.0005	0.0007
42.	H	0.0008	0.0000	0.0001	0.0000	0.0001	0.0000	0.0002	0.0004	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. Ta	0.3296	1.2928	0.2914	0.0118	0.0120	0.3425	0.0129	0.0137	0.0028
2. P	0.0103	0.0570	0.0032	0.0002	0.0013	0.0143	0.0009	0.0011	0.0034
3. P	0.0101	0.0265	0.0390	0.0009	0.0005	0.0059	0.0010	0.0006	0.0013
4. P	0.0093	0.0928	0.0108	0.0006	0.0009	0.0093	0.0005	0.0007	0.0018
5. O	0.0088	0.0340	0.0040	0.0003	0.0001	0.0047	0.0005	0.0004	0.0001
6. O	0.0102	1.9502	0.0010	0.0001	0.0002	0.0097	0.0002	0.0004	0.0002
7. C	0.0399	0.0106	1.2763	0.0050	0.9825	0.0395	0.0084	0.0072	0.0115
8. C	1.2286	0.0056	0.0369	0.0101	0.0135	0.0354	0.0098	0.0137	0.0032
9. H	0.0049	0.0006	0.0101	0.0003	0.0008	0.0100	0.0003	0.0008	0.0006
10. C	0.0000	0.0206	0.0387	0.0084	0.0075	1.2295	0.0050	0.9805	0.0010
11. C	0.0206	0.0000	0.0048	0.0003	0.0008	0.0215	0.0005	0.0011	0.0005
12. C	0.0387	0.0048	0.0000	0.8896	0.0132	1.2645	0.0035	0.0074	0.0094
13. H	0.0084	0.0003	0.8896	0.0000	0.0008	0.0034	0.0008	0.0002	0.0003
14. C	0.0075	0.0008	0.0132	0.0008	0.0000	0.0077	0.0002	0.0002	0.9950
15. C	1.2295	0.0215	1.2645	0.0034	0.0077	0.0000	0.8893	0.0128	0.0007
16. H	0.0050	0.0005	0.0035	0.0008	0.0002	0.8893	0.0000	0.0008	0.0003
17. C	0.9805	0.0011	0.0074	0.0002	0.0002	0.0128	0.0008	0.0000	0.0000
18. C	0.0010	0.0005	0.0094	0.0003	0.9950	0.0007	0.0003	0.0000	0.0000
19. H	0.0002	0.0001	0.0003	0.0000	0.0031	0.0000	0.0000	0.0000	0.9325
20. H	0.0001	0.0008	0.0002	0.0000	0.0041	0.0001	0.0000	0.0000	0.9122
21. H	0.0002	0.0001	0.0003	0.0000	0.0028	0.0005	0.0001	0.0000	0.9340
22. C	0.0178	0.0563	0.0104	0.0007	0.0003	0.0081	0.0011	0.0010	0.0004
23. C	0.0005	0.0003	0.0030	0.0007	0.9965	0.0009	0.0000	0.0002	0.0099
24. H	0.0001	0.0006	0.0002	0.0001	0.0041	0.0001	0.0000	0.0000	0.0006
25. H	0.0000	0.0000	0.0007	0.0006	0.0031	0.0002	0.0000	0.0000	0.0123
26. H	0.0004	0.0000	0.0005	0.0001	0.0028	0.0002	0.0000	0.0001	0.0010
27. C	0.0013	0.0003	0.0077	0.0001	0.9843	0.0015	0.0001	0.0001	0.0097
28. H	0.0001	0.0000	0.0004	0.0001	0.0032	0.0001	0.0000	0.0000	0.0121
29. H	0.0001	0.0000	0.0003	0.0000	0.0032	0.0001	0.0000	0.0000	0.0007
30. H	0.0005	0.0000	0.0010	0.0000	0.0030	0.0006	0.0000	0.0000	0.0007
31. C	0.0153	0.0010	0.0015	0.0001	0.0001	0.0066	0.0002	0.9840	0.0000
32. H	0.0010	0.0001	0.0001	0.0000	0.0000	0.0002	0.0000	0.0032	0.0000
33. H	0.0012	0.0001	0.0001	0.0000	0.0000	0.0004	0.0001	0.0032	0.0000
34. H	0.0117	0.0002	0.0006	0.0000	0.0000	0.0007	0.0000	0.0029	0.0000
35. C	0.0112	0.0011	0.0008	0.0000	0.0003	0.0027	0.0007	0.9974	0.0000
36. H	0.0007	0.0001	0.0002	0.0000	0.0000	0.0007	0.0005	0.0032	0.0000
37. H	0.0008	0.0020	0.0001	0.0000	0.0000	0.0003	0.0001	0.0041	0.0000
38. H	0.0115	0.0001	0.0002	0.0000	0.0001	0.0005	0.0001	0.0029	0.0000
39. C	0.0118	0.0008	0.0006	0.0003	0.0000	0.0094	0.0002	0.9947	0.0000
40. H	0.0007	0.0003	0.0001	0.0000	0.0000	0.0004	0.0000	0.0041	0.0000
41. H	0.0010	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0032	0.0000
42. H	0.0119	0.0001	0.0005	0.0001	0.0000	0.0003	0.0000	0.0027	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. Ta	0.0002	0.0023	0.0007	1.2629	0.0016	0.0027	0.0001	0.0005	0.0066
2. P	0.0002	0.0064	0.0003	0.0320	0.0028	0.0082	0.0002	0.0001	0.0028
3. P	0.0001	0.0010	0.0001	0.0595	0.0012	0.0011	0.0001	0.0001	0.0002
4. P	0.0001	0.0009	0.0001	0.0663	0.0042	0.0016	0.0002	0.0002	0.0011
5. O	0.0000	0.0001	0.0000	1.9784	0.0001	0.0002	0.0000	0.0000	0.0001
6. O	0.0000	0.0002	0.0000	0.0348	0.0001	0.0003	0.0000	0.0000	0.0001
7. C	0.0009	0.0008	0.0117	0.0056	0.0111	0.0009	0.0007	0.0115	0.0159
8. C	0.0006	0.0002	0.0005	0.0190	0.0090	0.0003	0.0003	0.0002	0.0074
9. H	0.0008	0.0000	0.0001	0.0003	0.0003	0.0000	0.0000	0.0000	0.0002

10.	C	0.0002	0.0001	0.0002	0.0178	0.0005	0.0001	0.0000	0.0004	0.0013
11.	C	0.0001	0.0008	0.0001	0.0563	0.0003	0.0006	0.0000	0.0000	0.0003
12.	C	0.0003	0.0002	0.0003	0.0104	0.0030	0.0002	0.0007	0.0005	0.0077
13.	H	0.0000	0.0000	0.0000	0.0007	0.0007	0.0001	0.0006	0.0001	0.0001
14.	C	0.0031	0.0041	0.0028	0.0003	0.9965	0.0041	0.0031	0.0028	0.9843
15.	C	0.0000	0.0001	0.0005	0.0081	0.0009	0.0001	0.0002	0.0002	0.0015
16.	H	0.0000	0.0000	0.0001	0.0011	0.0000	0.0000	0.0000	0.0000	0.0001
17.	C	0.0000	0.0000	0.0000	0.0010	0.0002	0.0000	0.0000	0.0001	0.0001
18.	C	0.9325	0.9122	0.9340	0.0004	0.0099	0.0006	0.0123	0.0010	0.0097
19.	H	0.0000	0.0012	0.0006	0.0000	0.0122	0.0002	0.0011	0.0003	0.0008
20.	H	0.0012	0.0000	0.0010	0.0003	0.0008	0.0002	0.0002	0.0000	0.0110
21.	H	0.0006	0.0010	0.0000	0.0000	0.0009	0.0000	0.0002	0.0005	0.0009
22.	C	0.0000	0.0003	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000	0.0002
23.	C	0.0122	0.0008	0.0009	0.0002	0.0000	0.9116	0.9323	0.9337	0.0097
24.	H	0.0002	0.0002	0.0000	0.0002	0.9116	0.0000	0.0011	0.0010	0.0107
25.	H	0.0011	0.0002	0.0002	0.0000	0.9323	0.0011	0.0000	0.0006	0.0010
26.	H	0.0003	0.0000	0.0005	0.0000	0.9337	0.0010	0.0006	0.0000	0.0008
27.	C	0.0008	0.0110	0.0009	0.0002	0.0097	0.0107	0.0010	0.0008	0.0000
28.	H	0.0002	0.0010	0.0002	0.0000	0.0006	0.0002	0.0004	0.0000	0.9305
29.	H	0.0003	0.0002	0.0000	0.0000	0.0120	0.0010	0.0002	0.0002	0.9311
30.	H	0.0000	0.0002	0.0004	0.0000	0.0008	0.0002	0.0000	0.0004	0.9325
31.	C	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0001
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	C	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		28	29	30	31	32	33	34	35	36
1.	Ta	0.0002	0.0001	0.0005	0.0094	0.0002	0.0003	0.0008	0.0015	0.0001
2.	P	0.0001	0.0001	0.0004	0.0003	0.0000	0.0000	0.0000	0.0004	0.0000
3.	P	0.0001	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0001	0.0000
4.	P	0.0001	0.0001	0.0002	0.0003	0.0000	0.0001	0.0001	0.0002	0.0000
5.	O	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000	0.0001	0.0001	0.0000
6.	O	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000	0.0001	0.0022	0.0000
7.	C	0.0012	0.0011	0.0117	0.0013	0.0001	0.0001	0.0004	0.0006	0.0000
8.	C	0.0003	0.0005	0.0012	0.0068	0.0006	0.0003	0.0012	0.0086	0.0003
9.	H	0.0000	0.0001	0.0000	0.0002	0.0001	0.0000	0.0000	0.0003	0.0000
10.	C	0.0001	0.0001	0.0005	0.0153	0.0010	0.0012	0.0117	0.0112	0.0007
11.	C	0.0000	0.0000	0.0000	0.0010	0.0001	0.0001	0.0002	0.0011	0.0001
12.	C	0.0004	0.0003	0.0010	0.0015	0.0001	0.0001	0.0006	0.0008	0.0002
13.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
14.	C	0.0032	0.0032	0.0030	0.0001	0.0000	0.0000	0.0000	0.0003	0.0000
15.	C	0.0001	0.0001	0.0006	0.0066	0.0002	0.0004	0.0007	0.0027	0.0007
16.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0000	0.0007	0.0005
17.	C	0.0000	0.0000	0.0000	0.9840	0.0032	0.0032	0.0029	0.9974	0.0032
18.	C	0.0121	0.0007	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	H	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0010	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0002	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	C	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0002	0.0002	0.0000
23.	C	0.0006	0.0120	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0002	0.0010	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0004	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0002	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	C	0.9305	0.9311	0.9325	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0006	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0006	0.0000	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
30.	H	0.0005	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	C	0.0000	0.0000	0.0000	0.0000	0.9310	0.9303	0.9331	0.0095	0.0009
32.	H	0.0000	0.0001	0.0000	0.9310	0.0000	0.0006	0.0005	0.0118	0.0002
33.	H	0.0000	0.0000	0.0000	0.9303	0.0006	0.0000	0.0005	0.0007	0.0004
34.	H	0.0000	0.0000	0.0000	0.9331	0.0005	0.0005	0.0000	0.0008	0.0000
35.	C	0.0000	0.0000	0.0000	0.0095	0.0118	0.0007	0.0008	0.0000	0.9318
36.	H	0.0000	0.0000	0.0000	0.0009	0.0002	0.0004	0.0000	0.9318	0.0000
37.	H	0.0000	0.0000	0.0000	0.0111	0.0010	0.0002	0.0002	0.9181	0.0011
38.	H	0.0000	0.0000	0.0000	0.0008	0.0002	0.0000	0.0004	0.9333	0.0006
39.	C	0.0000	0.0000	0.0000	0.0096	0.0007	0.0120	0.0006	0.0100	0.0123
40.	H	0.0000	0.0000	0.0000	0.0114	0.0002	0.0010	0.0002	0.0010	0.0003
41.	H	0.0000	0.0000	0.0000	0.0007	0.0003	0.0001	0.0000	0.0121	0.0011

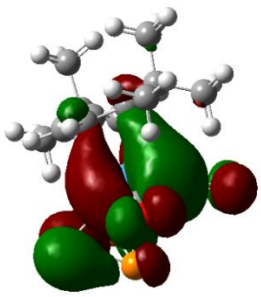
42.	H	0.0000	0.0000	0.0000	0.0010	0.0000	0.0003	0.0004	0.0008	0.0002

Atom		37	38	39	40	41	42
1.	Ta	0.0021	0.0004	0.0033	0.0034	0.0003	0.0008
2.	P	0.0015	0.0001	0.0002	0.0003	0.0000	0.0000
3.	P	0.0001	0.0000	0.0012	0.0010	0.0003	0.0001
4.	P	0.0005	0.0000	0.0003	0.0006	0.0000	0.0000
5.	O	0.0000	0.0000	0.0007	0.0005	0.0001	0.0001
6.	O	0.0025	0.0001	0.0003	0.0002	0.0000	0.0000
7.	C	0.0001	0.0004	0.0011	0.0001	0.0002	0.0002
8.	C	0.0003	0.0002	0.0028	0.0003	0.0005	0.0004
9.	H	0.0000	0.0000	0.0005	0.0000	0.0007	0.0000
10.	C	0.0008	0.0115	0.0118	0.0007	0.0010	0.0119
11.	C	0.0020	0.0001	0.0008	0.0003	0.0000	0.0001
12.	C	0.0001	0.0002	0.0006	0.0001	0.0000	0.0005
13.	H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0001
14.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15.	C	0.0003	0.0005	0.0094	0.0004	0.0003	0.0003
16.	H	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000
17.	C	0.0041	0.0029	0.9947	0.0041	0.0032	0.0027
18.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	C	0.0001	0.0000	0.0013	0.0013	0.0002	0.0002
23.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	C	0.0111	0.0008	0.0096	0.0114	0.0007	0.0010
32.	H	0.0010	0.0002	0.0007	0.0002	0.0003	0.0000
33.	H	0.0002	0.0000	0.0120	0.0010	0.0001	0.0003
34.	H	0.0002	0.0004	0.0006	0.0002	0.0000	0.0004
35.	C	0.9181	0.9333	0.0100	0.0010	0.0121	0.0008
36.	H	0.0011	0.0006	0.0123	0.0003	0.0011	0.0002
37.	H	0.0000	0.0010	0.0006	0.0002	0.0001	0.0000
38.	H	0.0010	0.0000	0.0010	0.0000	0.0003	0.0005
39.	C	0.0006	0.0010	0.0000	0.9205	0.9307	0.9339
40.	H	0.0002	0.0000	0.9205	0.0000	0.0013	0.0009
41.	H	0.0001	0.0003	0.9307	0.0013	0.0000	0.0006
42.	H	0.0000	0.0005	0.9339	0.0009	0.0006	0.0000

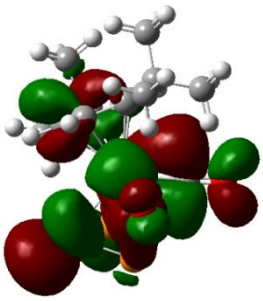
Wiberg bond index, Totals by atom:

Atom		1
1.	Ta	6.9386
2.	P	3.0977
3.	P	3.1015
4.	P	3.0761
5.	O	2.2486
6.	O	2.2365
7.	C	4.0470
8.	C	3.9413
9.	H	0.9398
10.	C	4.0427
11.	C	3.5848
12.	C	3.9334
13.	H	0.9361
14.	C	4.0484
15.	C	3.9353
16.	H	0.9382
17.	C	4.0488
18.	C	3.8584
19.	H	0.9558
20.	H	0.9456
21.	H	0.9561
22.	C	3.5607
23.	C	3.8573
24.	H	0.9476
25.	H	0.9557

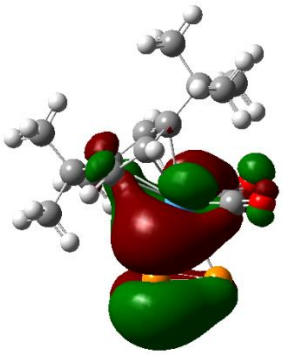
26.	H	0.9553
27.	C	3.8687
28.	H	0.9521
29.	H	0.9527
30.	H	0.9556
31.	C	3.8691
32.	H	0.9526
33.	H	0.9521
34.	H	0.9560
35.	C	3.8583
36.	H	0.9549
37.	H	0.9483
38.	H	0.9547
39.	C	3.8618
40.	H	0.9502
41.	H	0.9544
42.	H	0.9562



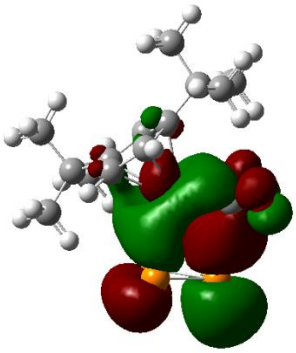
HOMO



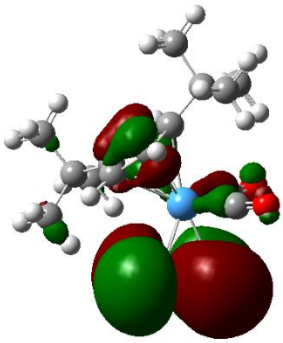
LUMO



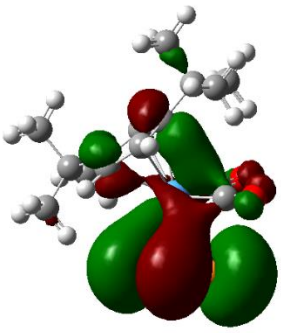
HOMO-1



HOMO-2



HOMO-3



HOMO-4

Figure S 11. HOMO and LUMO and other selected MOs of the anion of **6** (= [Cp''Ta(CO)$_2$(η^3-P$_3$)]$^-$). B3LYP/def2-SVPD level of theory.

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