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SUPPLEMENTARY MATERIAL

Iminoacyl alkyl complexes of zirconium supported by a ferrocene-linked diphosphinoamide ligand scaffold

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Contents

SI-1 General Experimental Considerations

Unless otherwise noted all experiments were carried out using oven-dried glassware cooled under vacuum, and all compounds were handled under an atmosphere of dry N_2 in a glovebox (Innovative Technology) equipped with a freezer (- 35°C), or using standard Schlenk technique. Hexanes, Et_2O, toluene and THF were purchased anhydrous from Aldrich, were passed over alumina under a nitrogen atmosphere and were collected over activated 4 Å molecular sieves under vacuum. Pentane was degassed by sparging with N_2 and was dried by distillation from potassium benzophenone-ketyl. C_6D_6, THF-d_8 and toluene-d_8 were distilled from sodium benzophenone-ketyl, and were degassed *via* 3 freeze-pump-thaw cycles. $Zr(NMe_2)_4$, MeLi and ^{t}BuLi was all purchased from commercial sources and used as received, TMSCl was purchased and distilled prior to use. KCH_2Ph[1] and ^{t}BuCH$_2$Li[2] were synthesized according to literature procedures. $LiN(SiMe_3)_2$ was purchased and purified by sublimation. Proligand fc(NHP^{i}Pr$_2$)$_2$ (fc = 1,1'-ferrocene) was prepared according to a previously published procedure.[3]

SI-2 Characterization Techniques

^{1}H, ^{13}C and ^{31}P NMR spectra were recorded on a Bruker Avance 300 or 400 MHz spectrometer. ^{1}H and ^{13}C NMR chemical shifts were referenced to residual solvents signals from the deuterated solvents. ^{31}P NMR chemical shifts were referenced to external samples of phosphoric acid (85 % in aqueous solution) at δ = 0 ppm. FT-IR spectra were recorded on a Perkin Elmer Frontier Spectrometer with Attenuated total reflectance. Samples (typically crystalline) were coated in nujol to prevent oxidation, and nujol backgrounds were subtracted from the FT-IR spectra.

Elemental analyses (EA) determinations were performed using a Carlo Erba Elemental Analyzer 1108, and were performed in the Department of Chemistry at the University of British Columbia by Mr. David Wong or Mr. Derek Smith.

Single crystal X-ray data was collected on a Bruker X8 Apex II diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) integrated using the Bruker SAINT software package.[4] Suitable single crystals were selected, coated in Fomblin oil and mounted on a nylon loop. All absorption corrections were performed using the multi-scan technique (SADABS).[5] Structures were solved by direct methods and refined using all reflections with the SHELX-97 program package.[6] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms (unless specified) were placed in calculated positions and assigned to an isotropic displacement parameter, other specified hydrogen atoms were located in the difference map and were refined isotropically. Structures were solved and refined using the WinGX (version 1.80.05) software package.[7]

SI-3 Syntheses of Compounds

Complex 1

Solid samples of fc(NHP^{i}Pr$_2$)$_2$ (0.335 mmol, 150 mg) and Zr(NMe$_2$)$_4$ (0.335 mmol, 90 mg) were weighed to the same Schlenk flask. At room temperature 5 mL of hexanes was added *via* cannula and the mixture was allowed to stir for 6 hours. The volatiles were removed *in vacuo* to give 200 mg (yield: 91%) of orange powder. The product can be recrystallized from hexanes at -35°C and X-ray quality crystals were obtained in this manner. $^{31}P\{^1H\}$ NMR (δ in ppm, C_6D_6, 293 K, 162 MHz): 29.4 (s); ^1H NMR (δ in ppm, C_6D_6, 293 K, 400 MHz); 4.09 (s, 4H, Cp-*H*), 3.90 (s, 4H, Cp-H), 3.27 (s, 12H, N-C*H*$_3$), 2.00 (septet of d, 4H, $^2J_{HP}$: 1.9 Hz,

$^{3}J_{HH}$: 7.2 Hz, P-C*H*), 1.09 (dd, 12H, $^{2}J_{HP}$: 13.2 Hz, $^{3}J_{HH}$: 7.2 Hz, CH_3-^{i}Pr), 1.04 (dd, 12H, $^{2}J_{HP}$: 15.0 Hz, $^{3}J_{HH}$: 7.2 Hz, CH_3-^{i}Pr), ^{13}C{^{1}H} NMR (δ in ppm, C_6D_6, 100.6 MHz): 112.1 (s, (Cp)*C*-N), 67.4 (s, (Cp)*C*), 65.1 (s, (Cp)*C*), 46.7 (t, $^{3}J_{CP}$: 5.4 Hz, N-CH_3), 25.4 (t, $^{2,4}J_{CP}$: 4.6 Hz, P-*C*H), 19.1 (t, $^{2,4}J_{CP}$: 3.6 Hz, *C*H$_3$-^{i}Pr), 18.8 (t, $^{2,4}J_{CP}$: 3.6 Hz, *C*H$_3$-^{i}Pr). For $C_{28}H_{54}N_4P_2Fe_1Zr_1$ EA (%, calc.): C, 51.28; H, 8.30; N, 8.54. EA (%, found): C, 50.17; H, 7.96; N, 8.78; repeated analyses were low in carbon.

Complex 2

fc(NHP^{i}Pr$_2$)$_2$ (5.35 mmol, 2.400 g) and Zr(NMe$_2$)$_4$ (5.35 mmol, 1.432 g) were weighed to the same Schlenk flask. At room temperature 80 mL of hexanes was added *via* cannula and the mixture was allowed to stir for 4 hours. The volatiles were removed *in vacuo* and the residue was dissolved in 30 mL toluene, and TMSCl (42.8 mmol, 5.4 mL) was added *via* syringe. After the addition the reaction mixture was heated at 65 °C for 17 hours, and the volatiles were removed *in vacuo*. The yellow solids were washed onto a glass frit with 25 mL hexanes and the solids were dried *in vacuo*, yield: 2.950 g (91 %). ^{31}P{^{1}H} NMR (δ in ppm, C_6D_6, 293 K, 162 MHz): 19.2 (s); ^{1}H NMR (δ in ppm, C_6D_6, 293 K, 400 MHz); 4.21 (s, 4H, Cp-*H*), 3.79 (s, 4H, Cp-H), 2.15 (br, 4H, P-C*H*), 1.21 (br m, 12H, CH_3-^{i}Pr), 1.06 (br m, 12H, CH_3-^{i}Pr). The solubility of the complex in C_6D_6 or toluene-d_8 was too low to obtain suitable ^{13}C NMR data. Repeated attempts to obtain acceptable elemental analysis were unsuccessful, a typical result is: for $C_{24}H_{42}N_2P_2Cl_2Fe_1Zr_1$ EA (%, calc.): C, 45.14; H, 6.63; N, 4.39. EA (%, found): C, 43.57; H, 6.00; N, 5.17.

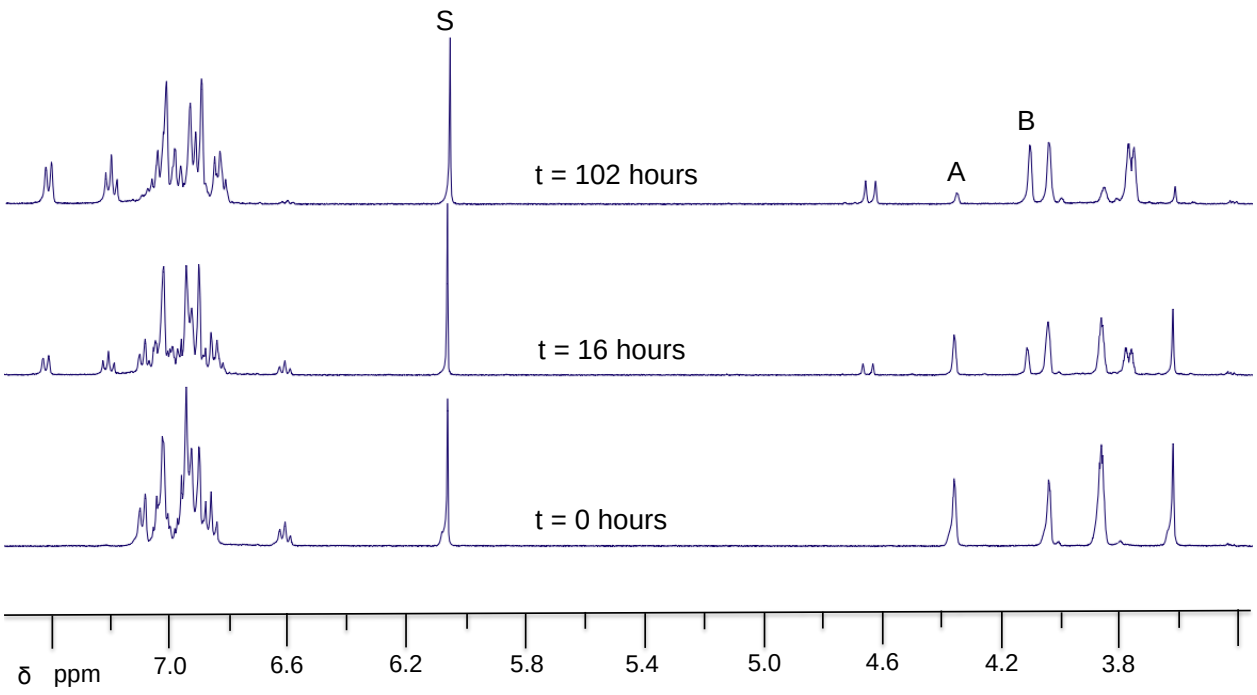
Complex 3

Complex **2** was dissolved in THF and the volatiles were then removed in vacuo to give a yellow powder in quantitative yield. ^{31}P{^{1}H} NMR (δ in ppm, C_6D_6, 293 K, 162 MHz): 20.5 (s); ^{1}H NMR (δ in ppm, C_6D_6, 293 K, 400 MHz); 4.50 (s, 4H, Cp-*H*), 4.10 (br, 4H, THF),

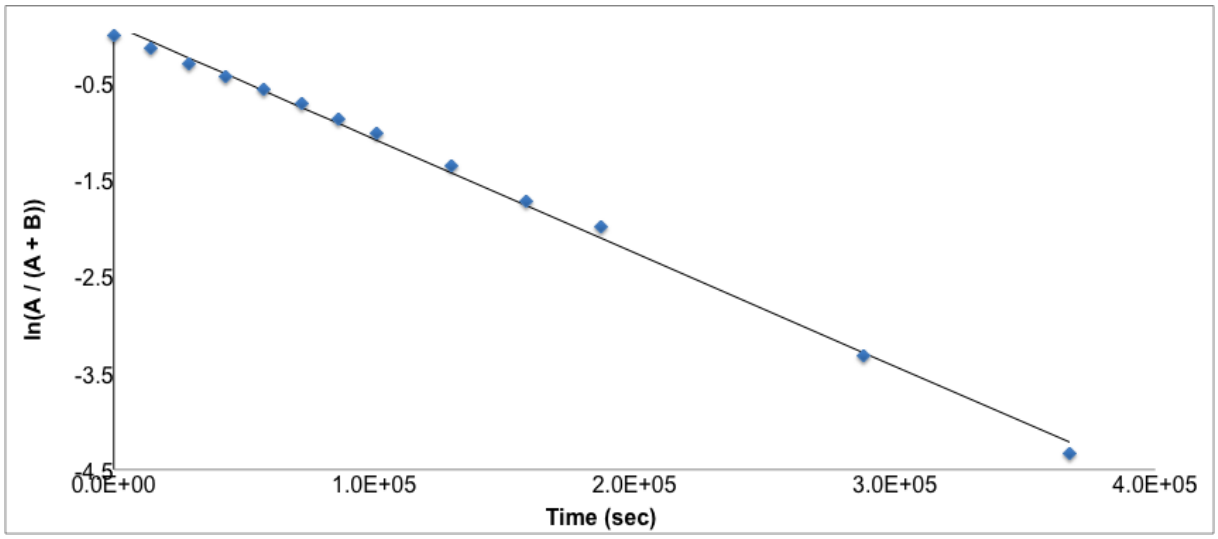
3.93 (s, 4H, Cp-H), 2.39 (septet of d, 4H, $^{2}J_{HP}$: 3.6 Hz, $^{3}J_{HH}$: 7.2 Hz, P-C*H*), 1.42 (br, 4H, THF), 1.33 (dd, 12H, $^{2}J_{HP}$: 16.8 Hz, $^{3}J_{HH}$: 7.2 Hz, C*H*$_3$-^{i}Pr), 1.08 (dd, 12H, $^{2}J_{HP}$: 14.8 Hz, $^{3}J_{HH}$: 7.2 Hz, C*H*$_3$-^{i}Pr). ^{13}C{^{1}H} NMR (δ in ppm, C_6D_6, 75.5 MHz): 115.0 (s, (Cp)*C*-N), 73.0 (s, THF), 67.6 (s, (Cp)*C*), 65.2 (s, (Cp)*C*), 26.7 (s P-*C*H), 25.8 (s, THF), 20.8 (t, $^{2,4}J_{CP}$: 4.7 Hz, *C*H$_3$-^{i}Pr), 19.3 (t, $^{2,4}J_{CP}$: 2.5 Hz, *C*H$_3$-^{i}Pr). Repeated attempts to obtain acceptable elemental analysis were unsuccessful, a typical result is: for $C_{48}H_{84}N_4P_4Cl_4Fe_2Zr_2$ EA (%, calc.): C, 45.14; H, 6.63; N, 4.39. EA (%, found): C, 43.80; H, 5.84; N, 4.64.

SI-4 Details of Kinetics Experiments

In a sealed J-Young NMR tube 20 mM solutions of **5b** in toluene-d_8 containing an internal standard of trimethoxybenzene were lowered into a preheated NMR spectrometer (95, 101 or 110 °C), or alternatively were lowered into an oil bath (80 °C) and removed and cooled to room temperature for spectroscopic analysis. The samples were allowed to equilibrate during routine shimming and ^{1}H NMR spectra were recorded at regular intervals. The rate of consumption of **5b** was obtained as a ratio of the integrals of 2 resonances (A / (A+B)), both normalized against the internal standard, is shown below: a portion of the ^{1}H NMR spectra taken during a kinetic run at 80 °C: S = arene resonance for trimethoxybenzene standard, A = Cp resonance for **5b**, B = Cp resonance for **6**.



The decay of **4.10** was found to follow first order kinetics using the integrated rate law method, a representative plot (80 °C) of ln(A / (A+B)) against time is shown below.



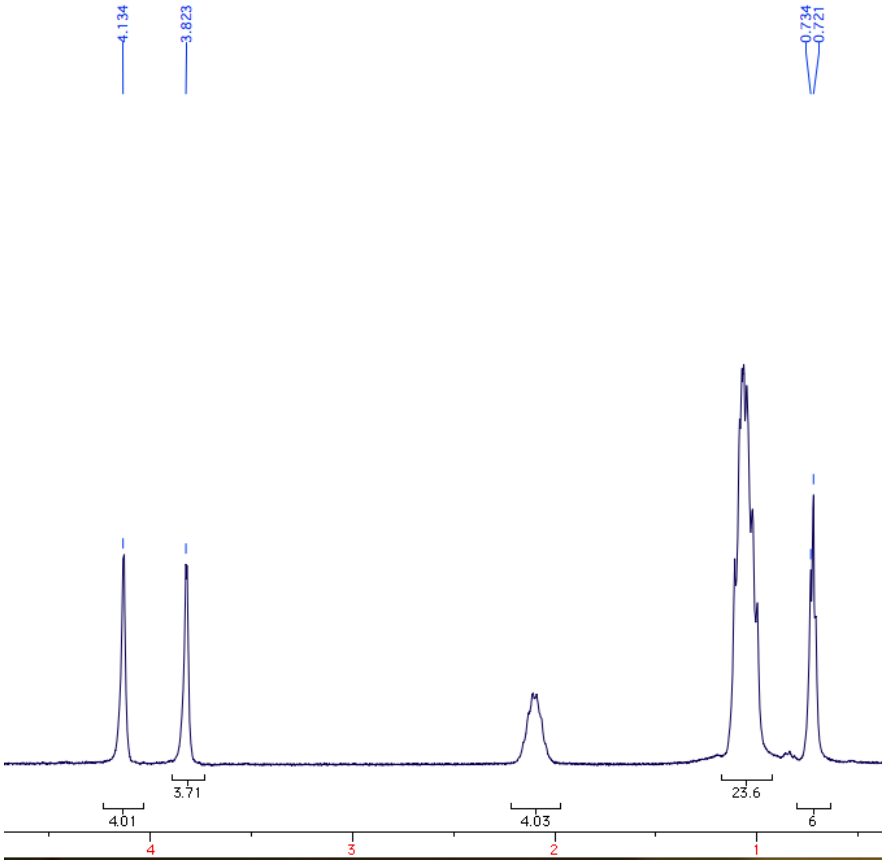
The temperature dependent rate constants were obtained using linear regression and the error for each value was taken from the least-squares analysis. The rate constants obtained are as follows: k_{80} = 1.18(2) x 10^{-5} s^{-1}, k_{95} = 5.61(9) x 10^{-5} s^{-1}, k_{101} = 1.21(4) x 10^{-4} s^{-1}, k_{110} =

2.11(11) x 10^{-4} s^{-1}. For the benzyl-group deuterated analog **6**-d_{14} a rate constant k_{110} = 4.75(11) x 10^{-5} s^{-1} was obtained.

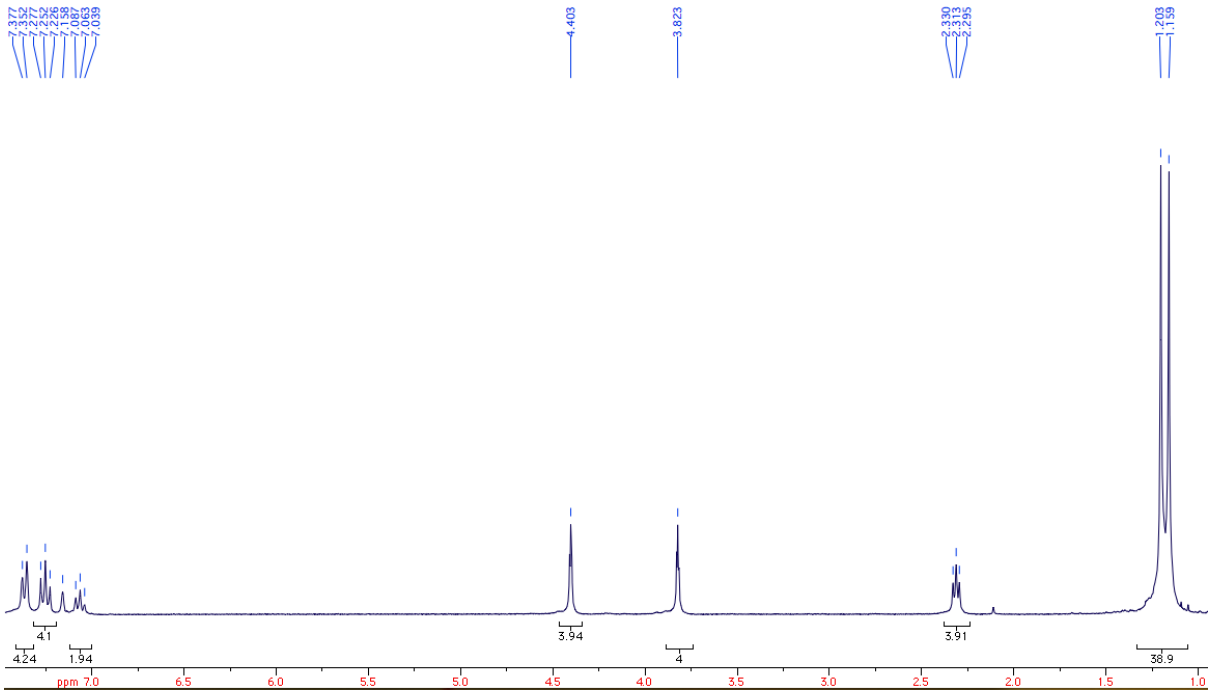
The plotting the ln(k / T) *vs* (1 / T), where T is in Kelvin, allows us to obtain thermodynamic data of the transition state of the transformation from the Eyring equation:

$\ln(k / T) = (-\Delta H^{\ddagger} / R)(1 / T) + \ln(K_B / h) + (\Delta S^{\ddagger} / R)$. The Eyring plot (shown in the main article) was analyzed by regression analysis and the resulting slope of the line is -1.34(11) x 10^4 and the intercept is 21(3). Temperature error values were estimated to be ± 1 K, and the error in the ln(k / T) values were determined statistically. Rearrangement of the Eyring plot gives values of $\Delta H^{\ddagger}$ = 26.7 ± 2.1 (kcal / mol) and $\Delta S^{\ddagger}$ = -5.7 ± 0.7 (cal / K mol).

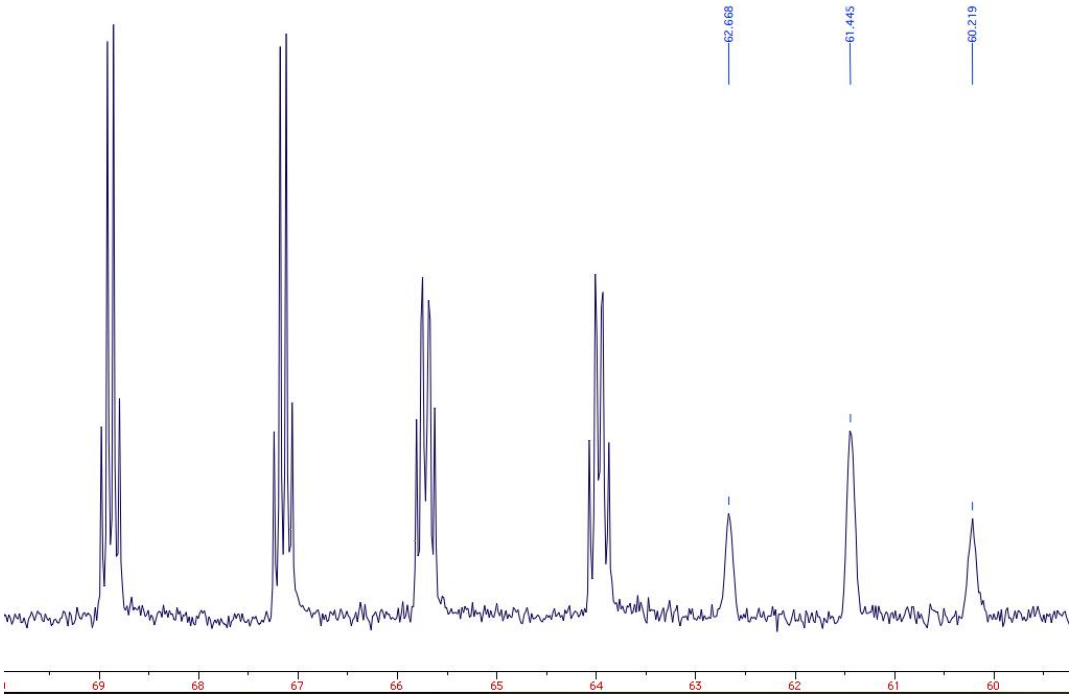
SI-5 Selected NMR spectra



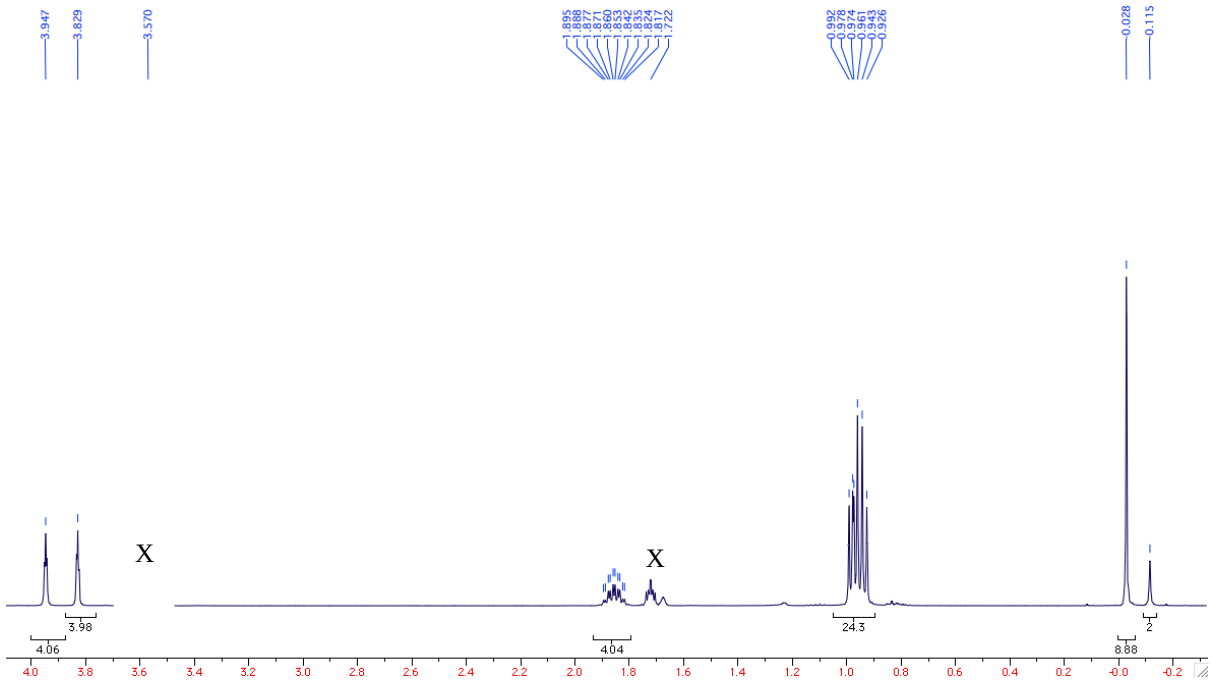
^{1}H NMR spectrum of **4a** in C_6D_6



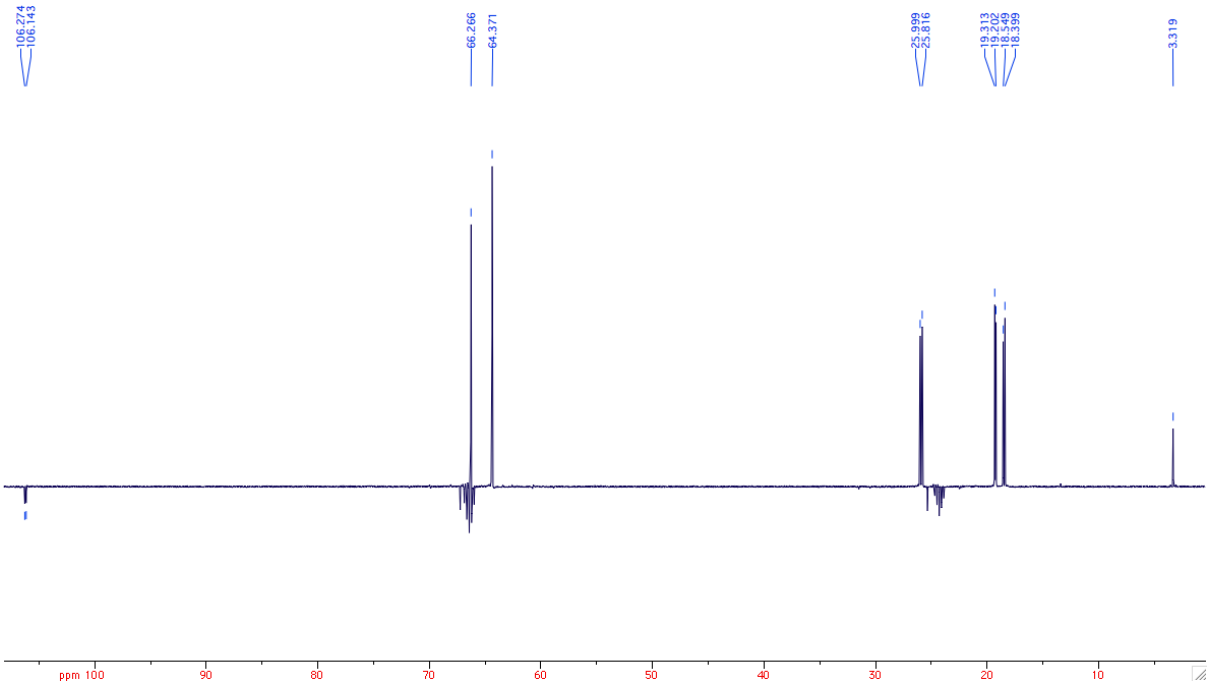
^{1}H NMR spectrum of **4b** in C_6D_6



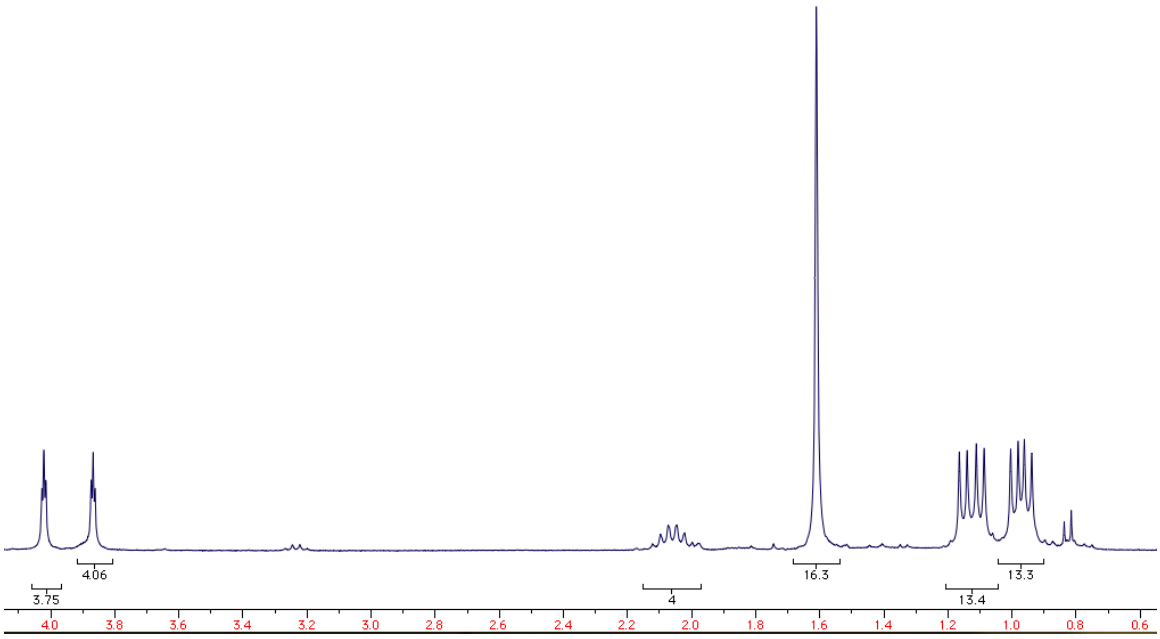
Selection of a ^{13}C-gated spectrum of **4b** showing 123 Hz $^{1}J_{CH}$ coupling for the benzylic carbons at δ 61.5 ppm



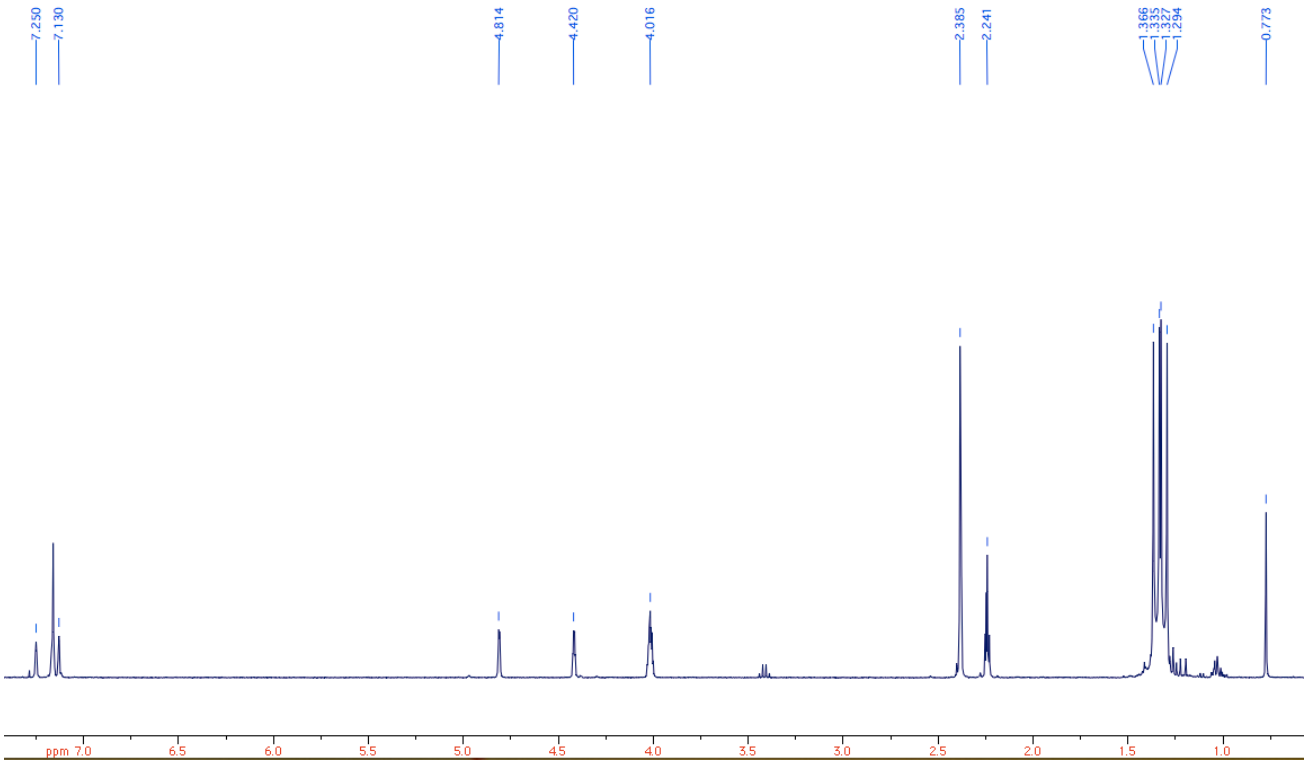
^{1}H NMR spectrum of **4c** in C_6D_6 (X marks THF impurity)



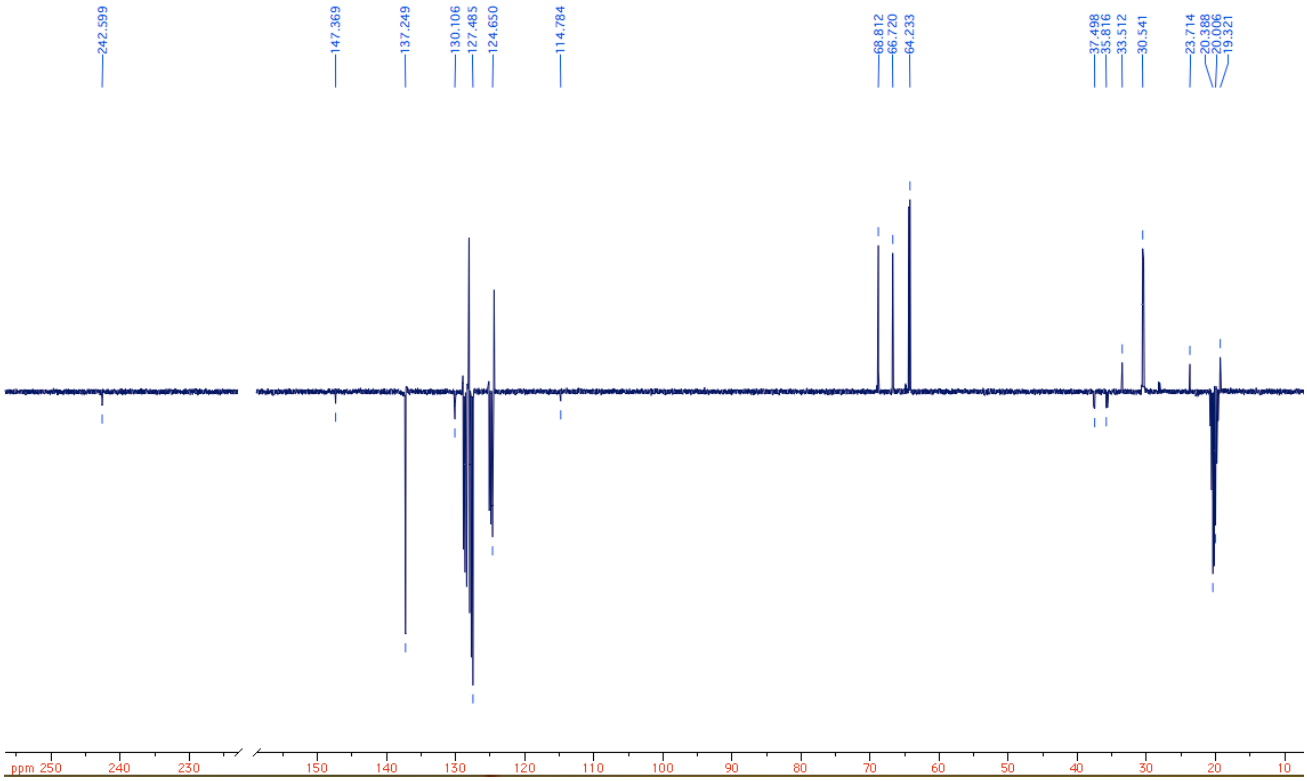
^{13}C-{^{1}H}APT NMR spectrum of **4c** in C_6D_6



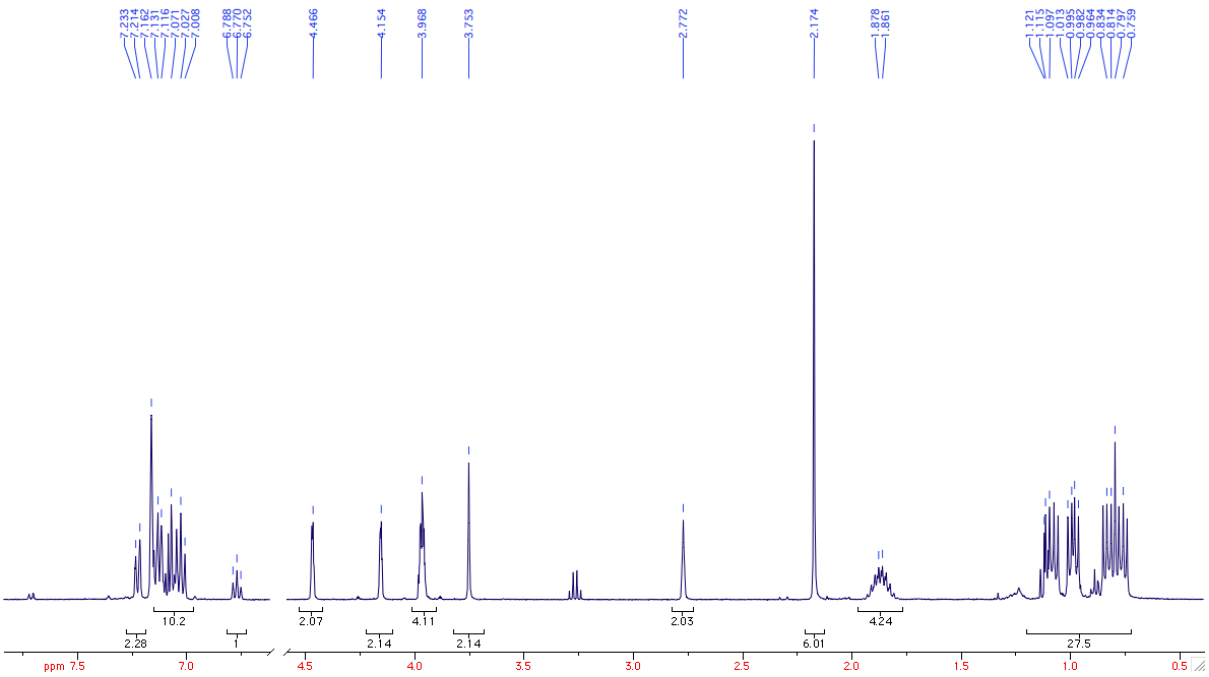
^{1}H NMR of **4d** in C_6D_6



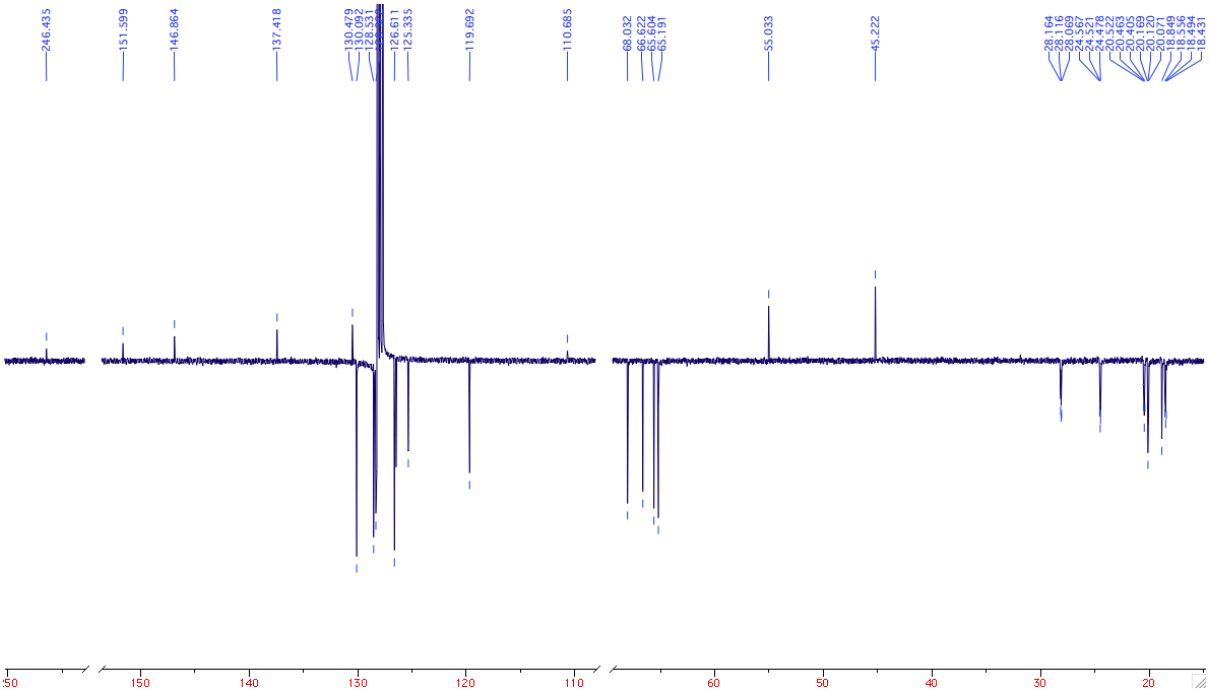
^{1}H NMR spectrum of **5a** in C_6D_6



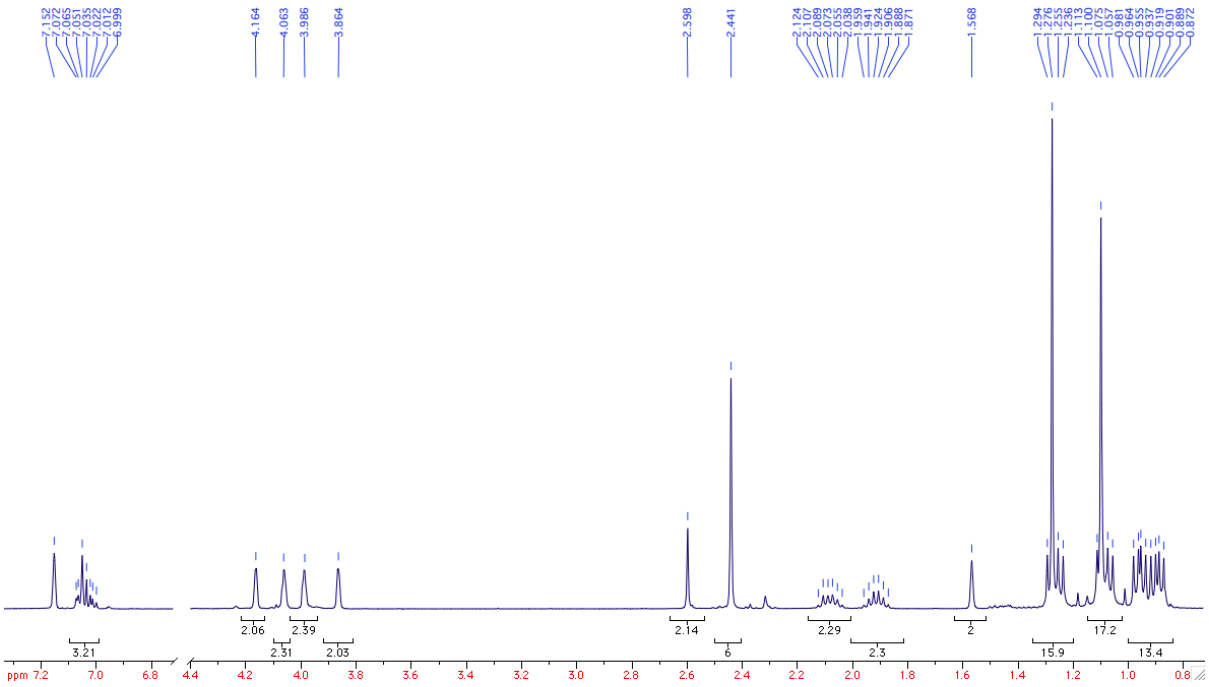
^{13}C{^{1}H}-APT NMR spectrum of **5a** in C_6D_6



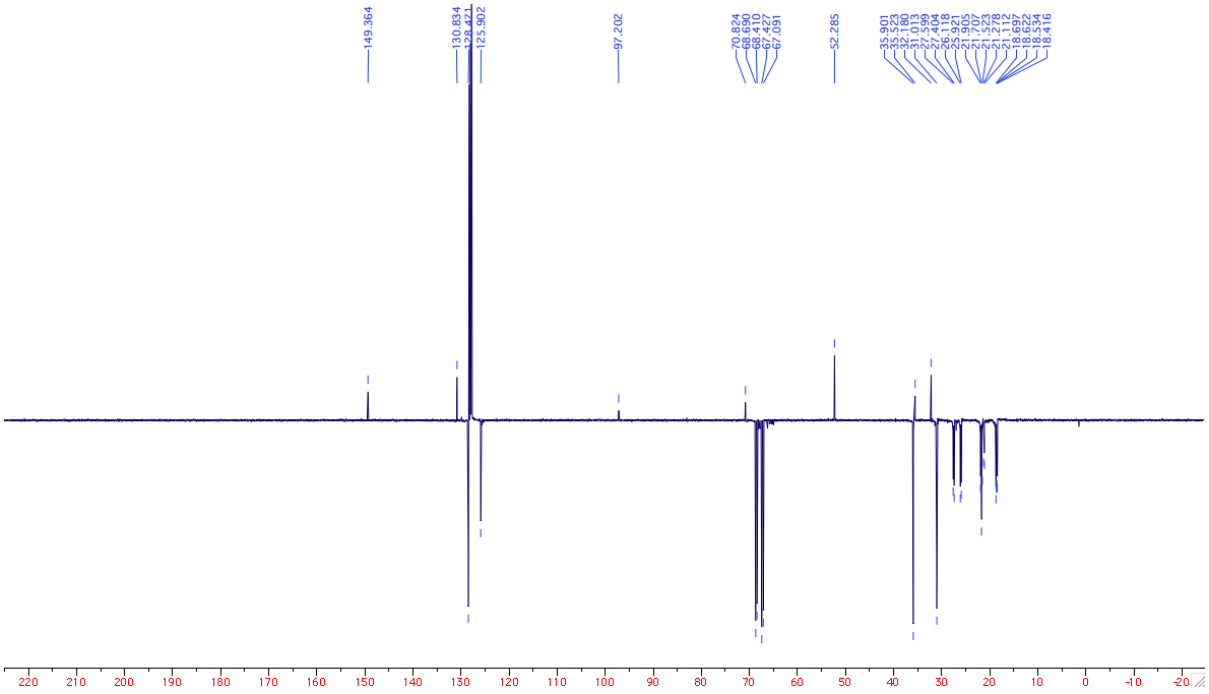
^{1}H NMR spectrum of **5b** in C_6D_6



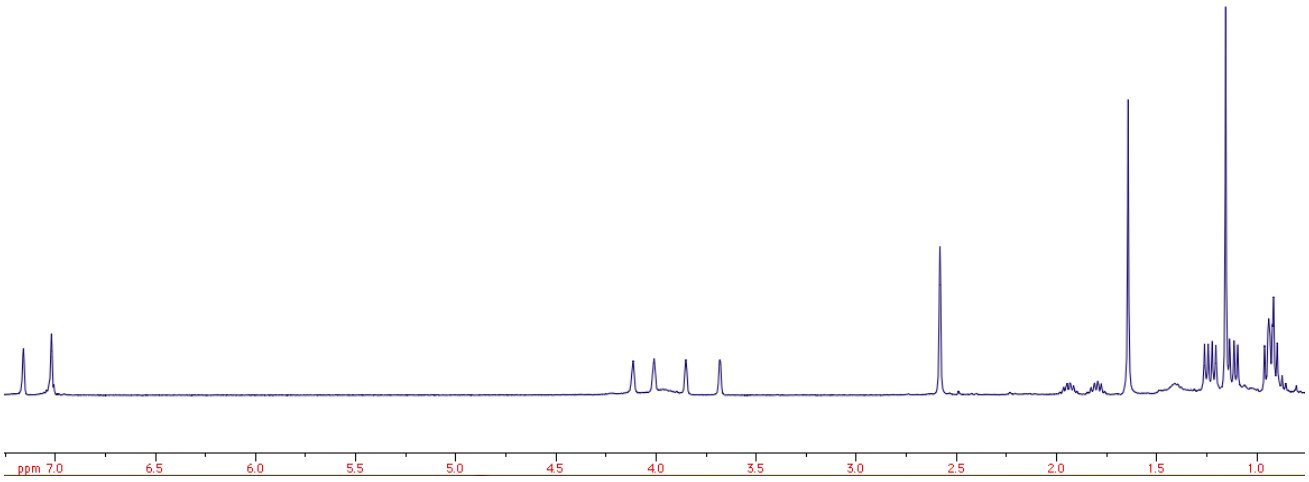
^{13}C-{^{1}H}APT NMR spectrum of **5b** in C_6D_6



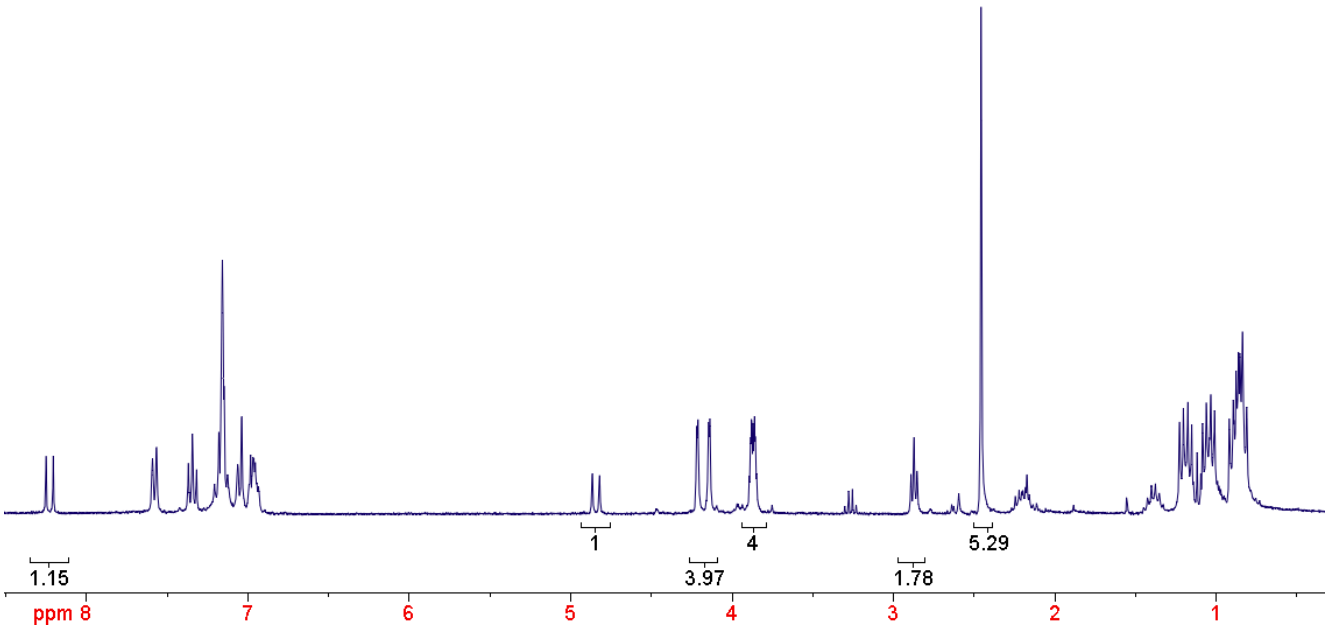
^{1}H NMR spectrum of **5c** in C_6D_6



^{13}C-{^{1}H}APT NMR spectrum of **5c** in C_6D_6



^{1}H NMR spectrum of **5d** in C_6D_6



^{1}H NMR spectrum of **6** in C_6D_6

SI-6: Crystal structure and refinement data				
	1	**2**	**3**	**4b**
CCDC number	1438943	1438944	1438945	1438946
Chemical formula	$C_{26}H_{48}Fe_1N_4P_2Zr_1$	$C_{44}H_{72}Cl_4Fe_2N_4P_4Zr_2$	$C_{26}H_{44}Cl_2Fe_1N_2O_1P_2Zr_1$	$C_{36}H_{50}Fe_1N_2P_2Zr_1 \cdot C_6H_6$
M_r	625.69	1216.88	680.54	797.90
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	P -1	P -1	C 2/c	P 2(1)/n
a / Å	8.6763(8)	9.7543(5)	12.7839(7)	10.671(3)
b / Å	10.6088(10)	12.6740(8)	19.2894(10)	22.035(5)
c / Å	16.8357(15)	12.8007(7)	12.8641(7)	16.918(4)
α / °	86.213(4)	113.771(2)	90.00	90.00
β / °	84.125(4)	104.526(2)	104.6010(10)	100.116(8)
γ / °	88.942(4)	103.544(2)	90.00	90.00
Volume / $Å^3$	1538.0(2)	1297.66(13)	3069.8(3)	3916.1(2)
T / K	100(2)	100(2)	100(2)	100(2)
Z	2	1	4	4
μ / mm^{-1}	0.935	1.302	1.112	0.749
ρ (calcd) / g/cm^3	1.351	1.557	1.473	1.353
F(000)	656	624	1408	1672
Absorption Correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Crystal size / mm^3	0.10 x 0.18 x 0.20	0.22 x 0.24 x 0.28	0.12 x 0.16 x 0.18	0.10 x 0.18 x 0.20
Wavelength / Å	0.71073	0.71073	0.71073	0.71073
Reflections collected	19322	16012	9716	23988
Independent reflections	5208 [R_{int} = 0.0305]	4439 [R_{int} = 0.0286]	2695 [R_{int} = 0.0197]	6827 [R_{int} = 0.0373]
Data / restraints / parameters	5208 / 0 / 319	4431 / 0 / 327	2695 / 0 / 240	6827 / 0 / 441
Goodness-of-fit on F^2	1.049	1.052	1.092	1.033
R indices [I>2σ(I)] (R1, *w*R2)	0.0253, 0.0664	0.0170, 0.0441	0.0210, 0.0545	0.0276, 0.0621
R indices [all data] (R1, *w*R2)	0.0312, 0.0688	0.0179, 0.0445	0.0224, 0.0551	0.0373, 0.0651
Completeness to theta max	0.969	0.964	1.000	0.985
Min. and max. transmission	0.7209 and 0.9107	0.5865 and 0.7509	0.8221 and 0.8751	0.8130 and 0.8735
Theta range for data collection	1.22 - 24.92	1.89 - 25.05	1.96 - 24.95	1.85 - 25.05
$R1 = \Sigma \lvert\lvert Fo\rvert - \lvert Fc\rvert\rvert / \Sigma \lvert Fo\rvert$; $wR2 = [\Sigma (w(Fo^2 - Fc^2)^2) / \Sigma w(Fo^2)^2]^{1/2}$				

Crystallographic data is available free of charge from http://ccdc.cam.ac.uk/

SI-6: Crystal structure and refinement data				
	4c	**4d**	**5b**	**5d**
CCDC number	1438947	1438948	1438949	1438950
Chemical formula	$C_{32}H_{58}Fe_1N_2P_2Zr_1$	$C_{30}H_{54}Fe_1N_2P_2Zr_1$	$C_{45}H_{59}Fe_1N_3P_2Zr_1$	$C_{39}H_{63}Fe_1N_3P_2Zr_1$
M_r	679.81	651.76	850.96	782.93
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	P -1	C 2/c	P -1	P -1
a / Å	10.7135(13)	15.1713(14)	11.999(5)	10.7355(7)
b / Å	10.7916(13)	10.6687(10)	21.756(5)	12.0266(9)
c / Å	17.012(2)	20.3050(19)	25.177(5)	17.0117(12)
α / °	82.547(6)	90.00	85.715(5)	94.0343(33)
β / °	80.239(6)	102.182(2)	77.313(5)	96.3112(34)
γ / °	65.230(5)	90.00	79.964(5)	112.1908(33)
Volume / $Å^3$	1756.2(4)	3212.5(5)	6309(3)	2006.40(31)
T / K	100(2)	90(2)	100(2)	100(2)
Z	2	4	6	2
μ / mm^{-1}	0.823	0.896	0.703	0.730
ρ (calcd) / g/cm^3	1.286	1.348	1.344	1.296
F(000)	720	1376	2676	828
Absorption Correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Crystal size / mm^3	0.16 x 0.20 x 0.22	0.02 x 0.10 x 0.27	0.20 x 0.26 x 0.28	0.08 x 0.16 x 0.22
Wavelength / Å	0.71073	0.71073	0.71073	0.71069
Reflections collected	21658	28284	89844	33587
Independent reflections	6041 [R_{int} = 0.0319]	4919 [R_{int} = 0.0490]	22236 [R_{int} = 0.0422]	9076 [R_{int} = 0.0381]
Data / restraints / parameters	6041 / 0 / 421	4919 / 0 / 171	22236 / 219 / 1427	9076 / 0 / 431
Goodness-of-fit on F^2	1.086	1.015	1.046	1.123
R indices [I>2σ(I)] (R1, *w*R2)	0.0258, 0.0675	0.0312, 0.0680	0.0461, 0.1072	0.0448, 0.1089
R indices [all data] (R1, *w*R2)	0.0312, 0.0704	0.0610, 0.0752	0.0762, 0.1298	0.0529, 0.1117
Completeness to theta max	0.976	0.999	0.998	0.984
Min. and max. transmission	0.8368 and 0.8766	0.7942 and 0.9822	0.5994 and 0.8688	0.4988 and 0.9432
Theta range for data collection	2.08 – 25.02	2.05 – 30.52	1.24 – 25.03	1.21 – 27.50
$R1 = \Sigma \lvert\lvert Fo\rvert - \lvert Fc\rvert\rvert / \Sigma \lvert Fo\rvert$; $wR2 = [\Sigma (w(Fo^2 - Fc^2)^2) / \Sigma w(Fo^2)^2]^{1/2}$				

Crystallographic data is available free of charge from http://ccdc.cam.ac.uk/

SI-7 Solid-state bond distances and angles

Bond lengths for **1**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	N1	1.418(3)	C11	C13	1.536(3)
C1	C2	1.429(3)	C11	P1	1.852(2)
C1	C5	1.435(3)	C14	C16	1.527(4)
C1	Fe1	2.047(2)	C14	C15	1.532(3)
C2	C3	1.421(3)	C14	P1	1.855(2)
C2	Fe1	2.043(2)	C17	C18	1.535(3)
C3	C4	1.421(3)	C17	C19	1.536(3)
C3	Fe1	2.046(2)	C17	P2	1.858(2)
C4	C5	1.429(3)	C20	C22	1.528(3)
C4	Fe1	2.044(2)	C20	C21	1.541(3)
C5	Fe1	2.039(2)	C20	P2	1.856(2)
C6	N2	1.414(3)	C23	N3	1.453(3)
C6	C7	1.427(3)	C24	N3	1.450(3)
C6	C10	1.433(3)	C25	N4	1.459(3)
C6	Fe1	2.033(2)	C26	N4	1.463(3)
C7	C8	1.430(3)	N1	P1	1.6721(17)
C7	Fe1	2.037(2)	N1	Zr1	2.1616(17)
C8	C9	1.421(3)	N2	P2	1.6681(17)
C8	Fe1	2.056(2)	N2	Zr1	2.1299(17)
C9	C10	1.419(3)	N3	Zr1	2.0349(18)
C9	Fe1	2.058(2)	N4	Zr1	2.0930(17)
C10	Fe1	2.042(2)	P1	Zr1	2.8005(6)
C11	C12	1.534(3)	P2	Zr1	2.7405(6)

Bond Angles for **1**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	125.10(19)	N2	P2	C20	109.43(10)
N1	C1	C5	127.91(19)	N2	P2	C17	108.66(10)
C2	C1	C5	106.93(18)	C20	P2	C17	105.10(10)
N1	C1	Fe1	124.23(13)	N2	P2	Zr1	50.98(6)
C2	C1	Fe1	69.40(11)	C20	P2	Zr1	131.44(8)
C5	C1	Fe1	69.12(11)	C17	P2	Zr1	122.86(7)
C3	C2	C1	108.83(19)	C6	Fe1	C7	41.06(8)
C3	C2	Fe1	69.75(12)	C6	Fe1	C5	117.19(9)
C1	C2	Fe1	69.69(12)	C7	Fe1	C5	104.90(9)
C4	C3	C2	107.95(19)	C6	Fe1	C10	41.18(8)
C4	C3	Fe1	69.60(12)	C7	Fe1	C10	68.76(9)
C2	C3	Fe1	69.58(12)	C5	Fe1	C10	153.54(9)
C3	C4	C5	108.1(2)	C6	Fe1	C2	119.36(9)
C3	C4	Fe1	69.74(12)	C7	Fe1	C2	155.63(8)
C5	C4	Fe1	69.33(12)	C5	Fe1	C2	68.64(9)
C4	C5	C1	108.23(19)	C10	Fe1	C2	106.03(9)
C4	C5	Fe1	69.70(12)	C6	Fe1	C4	155.53(9)
C1	C5	Fe1	69.76(11)	C7	Fe1	C4	122.94(10)

N2	C6	C7	127.24(19)	C5	Fe1	C4	40.97(8)
N2	C6	C10	125.46(19)	C10	Fe1	C4	163.20(9)
C7	C6	C10	107.26(18)	C2	Fe1	C4	68.43(9)
N2	C6	Fe1	124.16(13)	C6	Fe1	C3	158.07(9)
C7	C6	Fe1	69.61(12)	C7	Fe1	C3	160.84(9)
C10	C6	Fe1	69.74(11)	C5	Fe1	C3	68.75(9)
C6	C7	C8	108.1(2)	C10	Fe1	C3	125.01(9)
C6	C7	Fe1	69.33(12)	C2	Fe1	C3	40.67(9)
C8	C7	Fe1	70.29(12)	C4	Fe1	C3	40.66(9)
C9	C8	C7	108.2(2)	C6	Fe1	C1	101.02(8)
C9	C8	Fe1	69.87(12)	C7	Fe1	C1	118.86(8)
C7	C8	Fe1	68.82(12)	C5	Fe1	C1	41.12(8)
C10	C9	C8	107.91(19)	C10	Fe1	C1	117.83(8)
C10	C9	Fe1	69.13(11)	C2	Fe1	C1	40.90(8)
C8	C9	Fe1	69.73(12)	C4	Fe1	C1	69.10(9)
C9	C10	C6	108.58(19)	C3	Fe1	C1	69.00(8)
C9	C10	Fe1	70.38(12)	C6	Fe1	C8	68.88(8)
C6	C10	Fe1	69.08(11)	C7	Fe1	C8	40.89(8)
C12	C11	C13	110.9(2)	C5	Fe1	C8	124.70(9)
C12	C11	P1	108.37(16)	C10	Fe1	C8	68.16(9)
C13	C11	P1	112.07(19)	C2	Fe1	C8	161.17(9)
C16	C14	C15	111.1(2)	C4	Fe1	C8	111.69(9)
C16	C14	P1	108.95(16)	C3	Fe1	C8	126.99(9)
C15	C14	P1	115.82(17)	C1	Fe1	C8	157.87(9)
C18	C17	C19	111.1(2)	C6	Fe1	C9	68.95(8)
C18	C17	P2	110.62(17)	C7	Fe1	C9	68.64(9)
C19	C17	P2	109.13(15)	C5	Fe1	C9	163.02(9)
C22	C20	C21	111.6(2)	C10	Fe1	C9	40.50(9)
C22	C20	P2	109.16(15)	C2	Fe1	C9	123.74(9)
C21	C20	P2	114.03(16)	C4	Fe1	C9	128.42(9)
C1	N1	P1	126.17(13)	C3	Fe1	C9	111.95(9)
C1	N1	Zr1	140.86(13)	C1	Fe1	C9	155.84(9)
P1	N1	Zr1	92.97(8)	C8	Fe1	C9	40.41(9)
C6	N2	P2	126.83(14)	N3	Zr1	N4	103.67(7)
C6	N2	Zr1	141.60(13)	N3	Zr1	N2	105.97(7)
P2	N2	Zr1	91.55(8)	N4	Zr1	N2	126.33(7)
C24	N3	C23	111.5(2)	N3	Zr1	N1	105.69(7)
C24	N3	Zr1	129.40(18)	N4	Zr1	N1	127.88(7)
C23	N3	Zr1	119.01(15)	N2	Zr1	N1	84.66(6)
C25	N4	C26	108.33(17)	N3	Zr1	P2	106.25(6)
C25	N4	Zr1	134.47(14)	N4	Zr1	P2	91.48(5)
C26	N4	Zr1	117.15(14)	N2	Zr1	P2	37.48(5)
N1	P1	C11	106.64(10)	N1	Zr1	P2	119.49(5)
N1	P1	C14	110.99(10)	N3	Zr1	P1	104.28(6)
C11	P1	C14	104.49(11)	N4	Zr1	P1	94.66(5)
N1	P1	Zr1	50.43(6)	N2	Zr1	P1	119.32(5)
C11	P1	Zr1	125.78(8)	N1	Zr1	P1	36.60(4)
C14	P1	Zr1	128.92(8)	P2	Zr1	P1	146.413(19)

Bond Lengths for **2**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**

Zr1	N1	2.0680(13)	P2	C20	1.8512(16)
Zr1	N2	2.0741(13)	P2	C17	1.8567(16)
Zr1	Cl2	2.4402(4)	N1	C1	1.420(2)
Zr1	Cl1	2.5475(4)	N2	C6	1.422(2)
Zr1	P1	2.6951(4)	C4	C3	1.422(2)
Zr1	Cl1[1]	2.6963(4)	C4	C5	1.424(2)
Zr1	P2	2.7143(4)	C7	C8	1.423(3)
Fe1	C1	2.0138(15)	C7	C6	1.429(2)
Fe1	C6	2.0168(16)	C18	C17	1.527(2)
Fe1	C7	2.0230(18)	C6	C10	1.427(2)
Fe1	C5	2.0252(17)	C12	C11	1.533(2)
Fe1	C2	2.0336(17)	C16	C14	1.530(2)
Fe1	C10	2.0373(18)	C22	C20	1.532(2)
Fe1	C8	2.0397(19)	C13	C11	1.526(2)
Fe1	C9	2.0472(18)	C14	C15	1.528(2)
Fe1	C4	2.0486(17)	C2	C3	1.426(2)
Fe1	C3	2.0508(17)	C2	C1	1.429(2)
Cl1	Zr1[1]	2.6963(4)	C20	C21	1.524(2)
P1	N1	1.6881(13)	C10	C9	1.426(3)
P1	C11	1.8517(17)	C19	C17	1.532(2)
P1	C14	1.8544(17)	C9	C8	1.410(3)
P2	N2	1.6860(13)	C5	C1	1.431(2)

[1]2-X,-Y,1-Z

Bond Angles for **2**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1	Zr1	N2	86.64(5)	N1	P1	C11	107.82(7)
N1	Zr1	Cl2	94.74(4)	N1	P1	C14	106.17(7)
N2	Zr1	Cl2	103.06(4)	C11	P1	C14	105.92(8)
N1	Zr1	Cl1	97.25(4)	N1	P1	Zr1	50.10(5)
N2	Zr1	Cl1	99.48(4)	C11	P1	Zr1	133.32(6)
Cl2	Zr1	Cl1	154.996(14)	C14	P1	Zr1	119.14(5)
N1	Zr1	P1	38.77(4)	N2	P2	C20	109.00(7)
N2	Zr1	P1	125.38(4)	N2	P2	C17	109.30(7)
Cl2	Zr1	P1	84.364(13)	C20	P2	C17	102.45(7)
Cl1	Zr1	P1	91.376(14)	N2	P2	Zr1	49.80(4)
N1	Zr1	Cl1[1]	140.82(4)	C20	P2	Zr1	126.36(5)
N2	Zr1	Cl1[1]	132.46(4)	C17	P2	Zr1	130.15(5)
Cl2	Zr1	Cl1[1]	80.397(13)	C1	N1	P1	125.41(11)
Cl1	Zr1	Cl1[1]	76.438(13)	C1	N1	Zr1	141.82(10)
P1	Zr1	Cl1[1]	102.160(13)	P1	N1	Zr1	91.12(6)
N1	Zr1	P2	125.01(4)	C6	N2	P2	126.42(11)
N2	Zr1	P2	38.38(4)	C6	N2	Zr1	141.72(10)

Cl2	Zr1	P2	98.249(13)	P2	N2	Zr1	91.83(6)
Cl1	Zr1	P2	92.701(13)	C3	C4	C5	108.19(15)
P1	Zr1	P2	163.744(14)	C3	C4	Fe1	69.78(10)
Cl1[1]	Zr1	P2	94.094(13)	C5	C4	Fe1	68.67(9)
C1	Fe1	C6	101.27(6)	C8	C7	C6	108.04(17)
C1	Fe1	C7	116.05(7)	C8	C7	Fe1	70.12(11)
C6	Fe1	C7	41.42(7)	C6	C7	Fe1	69.06(9)
C1	Fe1	C5	41.49(6)	N2	C6	C10	126.09(15)
C6	Fe1	C5	116.96(7)	N2	C6	C7	126.31(15)
C7	Fe1	C5	152.34(7)	C10	C6	C7	107.56(15)
C1	Fe1	C2	41.35(7)	N2	C6	Fe1	123.88(11)
C6	Fe1	C2	120.27(7)	C10	C6	Fe1	70.16(9)
C7	Fe1	C2	104.54(7)	C7	C6	Fe1	69.52(9)
C5	Fe1	C2	69.23(7)	C15	C14	C16	112.32(14)
C1	Fe1	C10	120.98(7)	C15	C14	P1	114.52(12)
C6	Fe1	C10	41.22(7)	C16	C14	P1	112.77(12)
C7	Fe1	C10	69.14(8)	C3	C2	C1	108.26(15)
C5	Fe1	C10	106.10(8)	C3	C2	Fe1	70.22(10)
C2	Fe1	C10	157.99(7)	C1	C2	Fe1	68.58(9)
C1	Fe1	C8	153.77(8)	C21	C20	C22	110.31(14)
C6	Fe1	C8	69.36(7)	C21	C20	P2	111.45(11)
C7	Fe1	C8	41.02(8)	C22	C20	P2	110.90(11)
C5	Fe1	C8	164.58(8)	C9	C10	C6	107.84(17)
C2	Fe1	C8	121.13(8)	C9	C10	Fe1	69.94(10)
C10	Fe1	C8	68.70(8)	C6	C10	Fe1	68.62(9)
C1	Fe1	C9	160.44(8)	C18	C17	C19	111.10(14)
C6	Fe1	C9	69.15(7)	C18	C17	P2	111.69(11)
C7	Fe1	C9	68.65(8)	C19	C17	P2	113.39(11)
C5	Fe1	C9	126.45(8)	C8	C9	C10	108.36(17)
C2	Fe1	C9	158.19(8)	C8	C9	Fe1	69.53(11)
C10	Fe1	C9	40.88(7)	C10	C9	Fe1	69.18(10)
C8	Fe1	C9	40.37(9)	C13	C11	C12	111.02(14)
C1	Fe1	C4	69.35(7)	C13	C11	P1	110.86(11)
C6	Fe1	C4	154.89(7)	C12	C11	P1	110.65(12)
C7	Fe1	C4	163.66(7)	C4	C5	C1	108.16(14)
C5	Fe1	C4	40.91(7)	C4	C5	Fe1	70.43(10)
C2	Fe1	C4	68.69(7)	C1	C5	Fe1	68.83(9)
C10	Fe1	C4	122.67(7)	C4	C3	C2	107.94(15)
C8	Fe1	C4	128.73(7)	C4	C3	Fe1	69.62(10)
C9	Fe1	C4	111.84(8)	C2	C3	Fe1	68.93(10)
C1	Fe1	C3	69.38(7)	N1	C1	C2	125.95(14)
C6	Fe1	C3	159.30(7)	N1	C1	C5	126.54(14)
C7	Fe1	C3	124.81(7)	C2	C1	C5	107.45(14)

C5	Fe1	C3	68.87(7)	N1	C1	Fe1	123.52(11)
C2	Fe1	C3	40.85(7)	C2	C1	Fe1	70.07(9)
C10	Fe1	C3	159.31(7)	C5	C1	Fe1	69.68(9)
C8	Fe1	C3	110.56(8)	C9	C8	C7	108.19(17)
C9	Fe1	C3	125.08(7)	C9	C8	Fe1	70.10(11)
C4	Fe1	C3	40.60(7)	C7	C8	Fe1	68.86(10)
Zr1	Cl1	Zr1[1]	103.563(13)				

[1]2-X,-Y,1-Z

Bond Lengths for **3**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Zr1	N1	2.0852(15)	P1	N1	1.6763(15)
Zr1	N1[1]	2.0853(15)	P1	C6	1.8454(19)
Zr1	O1	2.2691(18)	P1	C9	1.848(2)
Zr1	Cl1[1]	2.4844(5)	O1	C12	1.448(2)
Zr1	Cl1	2.4845(5)	O1	C12[1]	1.448(2)
Zr1	P1	2.6565(5)	N1	C1	1.408(2)
Zr1	P1[1]	2.6565(5)	C10	C9	1.524(3)
Fe1	C1[1]	2.0326(19)	C1	C5	1.423(3)
Fe1	C1	2.0327(19)	C1	C2	1.426(3)
Fe1	C2[1]	2.036(2)	C9	C11	1.528(3)
Fe1	C2	2.036(2)	C2	C3	1.423(3)
Fe1	C5[1]	2.039(2)	C8	C6	1.514(3)
Fe1	C5	2.039(2)	C6	C7	1.521(3)
Fe1	C3	2.045(2)	C12	C13	1.507(3)
Fe1	C4	2.045(2)	C5	C4	1.420(3)
Fe1	C3[1]	2.046(2)	C4	C3	1.406(4)
Fe1	C4[1]	2.046(2)	C13	C13[1]	1.507(5)

[1]-X,+Y,3/2-Z

Bond Angles for **3**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1	Zr1	N1[1]	87.32(8)	C2	Fe1	C3[1]	158.24(9)
N1	Zr1	O1	136.34(4)	C5[1]	Fe1	C3[1]	68.32(10)
N1[1]	Zr1	O1	136.34(4)	C5	Fe1	C3[1]	126.93(10)
N1	Zr1	Cl1[1]	96.98(4)	C3	Fe1	C3[1]	125.10(13)
N1[1]	Zr1	Cl1[1]	95.81(4)	C4	Fe1	C3[1]	112.15(10)
O1	Zr1	Cl1[1]	81.144(13)	C1[1]	Fe1	C4[1]	68.68(8)
N1	Zr1	Cl1	95.81(4)	C1	Fe1	C4[1]	153.41(9)
N1[1]	Zr1	Cl1	96.98(4)	C2[1]	Fe1	C4[1]	68.22(9)

O1	Zr1	Cl1	81.144(13)	C2	Fe1	C4^{1}	121.83(10)
Cl1^{1}	Zr1	Cl1	162.29(3)	C5^{1}	Fe1	C4^{1}	40.69(9)
N1	Zr1	P1	39.12(4)	C5	Fe1	C4^{1}	165.64(9)
N1^{1}	Zr1	P1	126.08(4)	C3	Fe1	C4^{1}	112.15(10)
O1	Zr1	P1	97.425(11)	C4	Fe1	C4^{1}	130.41(13)
Cl1^{1}	Zr1	P1	96.526(15)	C3^{1}	Fe1	C4^{1}	40.21(11)
Cl1	Zr1	P1	85.764(15)	N1	P1	C6	110.66(8)
N1	Zr1	P1^{1}	126.08(4)	N1	P1	C9	107.66(8)
N1^{1}	Zr1	P1^{1}	39.12(4)	C6	P1	C9	107.12(9)
O1	Zr1	P1^{1}	97.423(11)	N1	P1	Zr1	51.71(5)
Cl1^{1}	Zr1	P1^{1}	85.764(15)	C6	P1	Zr1	133.18(7)
Cl1	Zr1	P1^{1}	96.525(15)	C9	P1	Zr1	119.39(7)
P1	Zr1	P1^{1}	165.15(2)	C12	O1	C12^{1}	110.4(2)
C1^{1}	Fe1	C1	101.51(11)	C12	O1	Zr1	124.80(11)
C1^{1}	Fe1	C2^{1}	41.02(8)	C12^{1}	O1	Zr1	124.80(11)
C1	Fe1	C2^{1}	121.25(8)	C1	N1	P1	128.03(12)
C1^{1}	Fe1	C2	121.25(8)	C1	N1	Zr1	141.57(12)
C1	Fe1	C2	41.02(8)	P1	N1	Zr1	89.17(7)
C2^{1}	Fe1	C2	158.52(11)	N1	C1	C5	126.18(18)
C1^{1}	Fe1	C5^{1}	40.92(8)	N1	C1	C2	126.34(18)
C1	Fe1	C5^{1}	115.98(8)	C5	C1	C2	107.41(18)
C2^{1}	Fe1	C5^{1}	68.58(9)	N1	C1	Fe1	123.58(13)
C2	Fe1	C5^{1}	105.76(9)	C5	C1	Fe1	69.79(12)
C1^{1}	Fe1	C5	115.98(8)	C2	C1	Fe1	69.62(11)
C1	Fe1	C5	40.92(8)	C10	C9	C11	112.80(18)
C2^{1}	Fe1	C5	105.76(9)	C10	C9	P1	115.27(15)
C2	Fe1	C5	68.58(9)	C11	C9	P1	112.18(15)
C5^{1}	Fe1	C5	150.93(12)	C3	C2	C1	108.1(2)
C1^{1}	Fe1	C3	160.70(9)	C3	C2	Fe1	69.95(12)
C1	Fe1	C3	68.87(8)	C1	C2	Fe1	69.36(11)
C2^{1}	Fe1	C3	158.24(9)	C8	C6	C7	111.1(2)
C2	Fe1	C3	40.80(9)	C8	C6	P1	111.08(14)
C5^{1}	Fe1	C3	126.93(10)	C7	C6	P1	109.34(15)
C5	Fe1	C3	68.32(10)	O1	C12	C13	104.66(19)
C1^{1}	Fe1	C4	153.41(9)	C4	C5	C1	108.0(2)
C1	Fe1	C4	68.68(8)	C4	C5	Fe1	69.89(14)
C2^{1}	Fe1	C4	121.83(10)	C1	C5	Fe1	69.29(12)
C2	Fe1	C4	68.22(9)	C3	C4	C5	108.5(2)
C5^{1}	Fe1	C4	165.64(9)	C3	C4	Fe1	69.89(13)
C5	Fe1	C4	40.69(9)	C5	C4	Fe1	69.42(12)
C3	Fe1	C4	40.21(11)	C12	C13	C13^{1}	102.79(16)
C1^{1}	Fe1	C3^{1}	68.87(8)	C4	C3	C2	108.0(2)
C1	Fe1	C3^{1}	160.70(9)	C4	C3	Fe1	69.89(13)

C2[1] Fe1 C3[1] 40.80(9) C2 C3 Fe1 69.25(12)

[1]-X,+Y,3/2-Z

Bond Lengths for **4b**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zr1	N2	2.0745(17)	C5	C4	1.423(3)
Zr1	N1	2.1024(17)	C5	C1	1.428(3)
Zr1	C23	2.277(2)	C36	C35	1.382(3)
Zr1	C30	2.327(2)	C36	C31	1.410(3)
Zr1	C31	2.720(2)	C40	C41	1.377(3)
Zr1	P2	2.7208(8)	C40	C39	1.379(3)
Zr1	P1	2.7576(8)	C31	C32	1.406(3)
Fe1	C6	2.023(2)	C26	C27	1.377(3)
Fe1	C1	2.024(2)	C10	C9	1.421(3)
Fe1	C2	2.028(2)	C10	C6	1.428(3)
Fe1	C10	2.033(2)	C7	C8	1.421(3)
Fe1	C5	2.034(2)	C7	C6	1.425(3)
Fe1	C7	2.037(2)	C33	C32	1.386(3)
Fe1	C9	2.037(2)	C16	C14	1.527(3)
Fe1	C4	2.046(2)	C29	C28	1.381(3)
Fe1	C3	2.048(2)	C22	C20	1.533(3)
Fe1	C8	2.048(2)	C15	C14	1.532(3)
P1	N1	1.6794(17)	C2	C3	1.424(3)
P1	C11	1.850(2)	C2	C1	1.428(3)
P1	C14	1.858(2)	C12	C11	1.529(3)
P2	N2	1.6809(17)	C17	C18	1.527(3)
P2	C17	1.849(2)	C17	C19	1.537(3)
P2	C20	1.852(2)	C41	C42	1.371(3)
C34	C33	1.384(3)	C39	C38	1.378(3)
C34	C35	1.389(3)	C37	C42	1.379(3)
N1	C1	1.422(2)	C37	C38	1.382(4)
N2	C6	1.417(3)	C20	C21	1.528(3)
C23	C24	1.478(3)	C11	C13	1.533(3)
C30	C31	1.469(3)	C27	C28	1.378(3)
C24	C29	1.400(3)	C9	C8	1.419(3)
C24	C25	1.402(3)	C3	C4	1.418(3)
C25	C26	1.381(3)			

Bond Angles for **4b**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Zr1	N1	86.15(6)	C1	N1	Zr1	141.20(13)
N2	Zr1	C23	107.10(7)	P1	N1	Zr1	92.96(7)
N1	Zr1	C23	107.06(7)	C6	N2	P2	124.56(14)
N2	Zr1	C30	116.72(7)	C6	N2	Zr1	143.17(13)
N1	Zr1	C30	117.86(7)	P2	N2	Zr1	92.25(8)
C23	Zr1	C30	117.40(7)	C24	C23	Zr1	121.82(14)
N2	Zr1	C31	130.75(6)	C31	C30	Zr1	88.52(12)
N1	Zr1	C31	136.92(6)	C29	C24	C25	116.5(2)

C23	Zr1	C31	84.80(7)	C29	C24	C23	122.21(19)
C30	Zr1	C31	32.69(7)	C25	C24	C23	121.29(19)
N2	Zr1	P2	38.12(5)	C26	C25	C24	121.9(2)
N1	Zr1	P2	123.80(5)	C4	C5	C1	108.28(18)
C23	Zr1	P2	98.52(6)	C4	C5	Fe1	70.03(12)
C30	Zr1	P2	90.84(6)	C1	C5	Fe1	69.05(11)
C31	Zr1	P2	93.69(5)	C35	C36	C31	121.6(2)
N2	Zr1	P1	122.60(5)	C41	C40	C39	120.4(2)
N1	Zr1	P1	37.46(5)	C32	C31	C36	116.81(19)
C23	Zr1	P1	101.06(6)	C32	C31	C30	121.1(2)
C30	Zr1	P1	91.05(6)	C36	C31	C30	121.7(2)
C31	Zr1	P1	100.28(5)	C32	C31	Zr1	100.24(13)
P2	Zr1	P1	156.833(18)	C36	C31	Zr1	105.51(13)
C6	Fe1	C1	101.16(8)	C30	C31	Zr1	58.79(10)
C6	Fe1	C2	119.71(8)	C27	C26	C25	120.1(2)
C1	Fe1	C2	41.25(8)	C9	C10	C6	107.84(18)
C6	Fe1	C10	41.23(8)	C9	C10	Fe1	69.73(12)
C1	Fe1	C10	118.68(8)	C6	C10	Fe1	69.01(11)
C2	Fe1	C10	155.97(8)	C8	C7	C6	108.18(18)
C6	Fe1	C5	117.27(8)	C8	C7	Fe1	70.07(12)
C1	Fe1	C5	41.19(8)	C6	C7	Fe1	68.93(11)
C2	Fe1	C5	68.91(8)	C34	C33	C32	120.4(2)
C10	Fe1	C5	104.47(9)	N2	C6	C7	125.68(18)
C6	Fe1	C7	41.08(8)	N2	C6	C10	126.54(18)
C1	Fe1	C7	118.06(8)	C7	C6	C10	107.71(18)
C2	Fe1	C7	106.26(8)	N2	C6	Fe1	123.33(14)
C10	Fe1	C7	68.95(8)	C7	C6	Fe1	69.99(11)
C5	Fe1	C7	153.69(8)	C10	C6	Fe1	69.76(11)
C6	Fe1	C9	69.11(8)	C28	C29	C24	121.4(2)
C1	Fe1	C9	157.39(9)	C36	C35	C34	120.2(2)
C2	Fe1	C9	161.21(8)	C3	C2	C1	108.50(18)
C10	Fe1	C9	40.88(8)	C3	C2	Fe1	70.31(11)
C5	Fe1	C9	123.85(9)	C1	C2	Fe1	69.23(11)
C7	Fe1	C9	68.64(8)	C33	C32	C31	121.4(2)
C6	Fe1	C4	155.31(9)	C18	C17	C19	110.04(19)
C1	Fe1	C4	69.17(8)	C18	C17	P2	110.45(15)
C2	Fe1	C4	68.61(8)	C19	C17	P2	112.04(16)
C10	Fe1	C4	122.27(9)	C16	C14	C15	111.21(17)
C5	Fe1	C4	40.84(8)	C16	C14	P1	109.78(14)
C7	Fe1	C4	163.46(8)	C15	C14	P1	114.93(14)
C9	Fe1	C4	110.86(8)	N1	C1	C2	125.71(18)
C6	Fe1	C3	158.71(8)	N1	C1	C5	127.05(18)
C1	Fe1	C3	69.24(8)	C2	C1	C5	107.20(17)

C2	Fe1	C3	40.88(8)	N1	C1	Fe1	124.37(14)
C10	Fe1	C3	160.04(8)	C2	C1	Fe1	69.52(11)
C5	Fe1	C3	68.63(8)	C5	C1	Fe1	69.76(12)
C7	Fe1	C3	125.53(8)	C42	C41	C40	120.1(2)
C9	Fe1	C3	126.45(8)	C38	C39	C40	119.6(2)
C4	Fe1	C3	40.53(8)	C42	C37	C38	120.1(2)
C6	Fe1	C8	68.96(8)	C39	C38	C37	120.0(2)
C1	Fe1	C8	156.36(8)	C21	C20	C22	112.16(18)
C2	Fe1	C8	123.90(9)	C21	C20	P2	111.27(15)
C10	Fe1	C8	68.69(8)	C22	C20	P2	115.83(15)
C5	Fe1	C8	162.43(8)	C12	C11	C13	110.41(18)
C7	Fe1	C8	40.72(8)	C12	C11	P1	111.32(14)
C9	Fe1	C8	40.65(8)	C13	C11	P1	110.99(15)
C4	Fe1	C8	128.15(8)	C26	C27	C28	119.4(2)
C3	Fe1	C8	112.02(9)	C27	C28	C29	120.6(2)
N1	P1	C11	107.93(9)	C8	C9	C10	108.31(18)
N1	P1	C14	109.44(9)	C8	C9	Fe1	70.09(12)
C11	P1	C14	103.02(9)	C10	C9	Fe1	69.39(12)
N1	P1	Zr1	49.58(6)	C41	C42	C37	119.8(2)
C11	P1	Zr1	123.32(7)	C4	C3	C2	107.82(18)
C14	P1	Zr1	132.40(7)	C4	C3	Fe1	69.65(11)
N2	P2	C17	106.10(9)	C2	C3	Fe1	68.81(11)
N2	P2	C20	107.53(9)	C9	C8	C7	107.95(18)
C17	P2	C20	106.66(10)	C9	C8	Fe1	69.26(12)
N2	P2	Zr1	49.63(6)	C7	C8	Fe1	69.21(11)
C17	P2	Zr1	127.38(7)	C3	C4	C5	108.19(18)
C20	P2	Zr1	124.26(7)	C3	C4	Fe1	69.83(11)
C33	C34	C35	119.5(2)	C5	C4	Fe1	69.13(11)
C1	N1	P1	125.53(14)				

Bond Lengths for **4c**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
C1	N1	1.426(3)	C20	C22	1.528(3)
C1	C2	1.437(3)	C20	C21	1.530(3)
C1	C5	1.444(3)	C20	P2	1.866(2)
C1	Fe1	2.048(2)	C23	C24	1.553(3)
C2	C3	1.433(3)	C23	Zr1	2.327(2)
C2	Fe1	2.049(2)	C24	C27	1.532(3)
C3	C4	1.430(3)	C24	C26	1.542(4)
C3	Fe1	2.060(2)	C24	C25	1.547(3)
C4	C5	1.428(3)	C28	C29	1.547(3)
C4	Fe1	2.060(2)	C28	Zr1	2.267(2)

C5	Fe1	2.046(2)	C29	C30	1.539(3)
C6	N2	1.425(3)	C29	C32	1.541(3)
C6	C7	1.437(3)	C29	C31	1.544(3)
C6	C10	1.444(3)	C11	C12	1.534(3)
C6	Fe1	2.047(2)	C11	C13	1.535(3)
C7	C8	1.433(3)	C11	P1	1.872(2)
C7	Fe1	2.050(2)	C14	C15	1.538(3)
C8	C9	1.431(3)	C14	C16	1.540(3)
C8	Fe1	2.061(2)	C14	P1	1.867(2)
C9	C10	1.433(3)	N1	P1	1.6890(17)
C9	Fe1	2.054(2)	N1	Zr1	2.1207(17)
C10	Fe1	2.048(2)	N2	P2	1.7025(17)
C17	C18	1.538(3)	N2	Zr1	2.1104(17)
C17	C19	1.545(3)	P1	Zr1	2.7852(6)
C17	P2	1.875(2)	P2	Zr1	2.7814(6)

Bond Angles for **4c**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1	C1	C2	125.19(18)	C14	P1	C11	103.01(10)
N1	C1	C5	127.73(18)	N1	P1	Zr1	49.48(6)
C2	C1	C5	107.00(18)	C14	P1	Zr1	124.17(8)
N1	C1	Fe1	123.69(13)	C11	P1	Zr1	131.58(7)
C2	C1	Fe1	69.49(11)	N2	P2	C20	107.17(10)
C5	C1	Fe1	69.28(11)	N2	P2	C17	107.96(9)
C3	C2	C1	108.50(19)	C20	P2	C17	104.44(10)
C3	C2	Fe1	70.02(12)	N2	P2	Zr1	49.26(6)
C1	C2	Fe1	69.44(11)	C20	P2	Zr1	127.32(7)
C4	C3	C2	107.93(19)	C17	P2	Zr1	126.54(7)
C4	C3	Fe1	69.67(12)	C5	Fe1	C6	121.35(9)
C2	C3	Fe1	69.16(12)	C5	Fe1	C1	41.30(8)
C5	C4	C3	108.18(19)	C6	Fe1	C1	101.70(8)
C5	C4	Fe1	69.16(12)	C5	Fe1	C10	105.40(9)
C3	C4	Fe1	69.73(12)	C6	Fe1	C10	41.29(8)
C4	C5	C1	108.39(19)	C1	Fe1	C10	116.21(9)
C4	C5	Fe1	70.15(12)	C5	Fe1	C2	68.88(8)
C1	C5	Fe1	69.42(11)	C6	Fe1	C2	116.37(8)
N2	C6	C7	125.52(18)	C1	Fe1	C2	41.06(8)
N2	C6	C10	127.13(18)	C10	Fe1	C2	151.59(9)
C7	C6	C10	107.29(18)	C5	Fe1	C7	158.79(9)
N2	C6	Fe1	124.03(13)	C6	Fe1	C7	41.07(8)
C7	C6	Fe1	69.59(11)	C1	Fe1	C7	121.34(8)
C10	C6	Fe1	69.41(11)	C10	Fe1	C7	68.96(8)

C8	C7	C6	108.45(19)	C2	Fe1	C7	105.85(9)
C8	C7	Fe1	70.00(12)	C5	Fe1	C9	121.18(9)
C6	C7	Fe1	69.34(11)	C6	Fe1	C9	69.22(8)
C9	C8	C7	107.96(19)	C1	Fe1	C9	153.59(9)
C9	C8	Fe1	69.38(12)	C10	Fe1	C9	40.89(9)
C7	C8	Fe1	69.19(11)	C2	Fe1	C9	165.23(9)
C8	C9	C10	108.20(19)	C7	Fe1	C9	68.73(9)
C8	C9	Fe1	69.92(12)	C5	Fe1	C4	40.69(9)
C10	C9	Fe1	69.35(12)	C6	Fe1	C4	160.51(9)
C9	C10	C6	108.10(19)	C1	Fe1	C4	69.07(8)
C9	C10	Fe1	69.76(12)	C10	Fe1	C4	126.07(9)
C6	C10	Fe1	69.30(11)	C2	Fe1	C4	68.58(9)
C18	C17	C19	110.32(17)	C7	Fe1	C4	158.33(9)
C18	C17	P2	116.23(14)	C9	Fe1	C4	111.08(9)
C19	C17	P2	111.97(15)	C5	Fe1	C3	68.59(9)
C22	C20	C21	110.16(19)	C6	Fe1	C3	153.72(9)
C22	C20	P2	111.38(16)	C1	Fe1	C3	69.07(8)
C21	C20	P2	111.67(16)	C10	Fe1	C3	164.92(9)
C24	C23	Zr1	122.46(15)	C2	Fe1	C3	40.81(8)
C27	C24	C26	110.1(2)	C7	Fe1	C3	121.65(9)
C27	C24	C25	108.2(2)	C9	Fe1	C3	129.35(9)
C26	C24	C25	107.47(19)	C4	Fe1	C3	40.60(9)
C27	C24	C23	110.5(2)	C5	Fe1	C8	158.01(9)
C26	C24	C23	109.8(2)	C6	Fe1	C8	69.07(8)
C25	C24	C23	110.72(18)	C1	Fe1	C8	160.61(8)
C29	C28	Zr1	134.46(15)	C10	Fe1	C8	68.74(9)
C30	C29	C32	109.60(18)	C2	Fe1	C8	126.46(9)
C30	C29	C31	108.04(17)	C7	Fe1	C8	40.81(8)
C32	C29	C31	107.85(17)	C9	Fe1	C8	40.70(9)
C30	C29	C28	109.08(17)	C4	Fe1	C8	124.72(9)
C32	C29	C28	110.74(17)	C3	Fe1	C8	111.35(9)
C31	C29	C28	111.48(17)	N2	Zr1	N1	87.31(6)
C12	C11	C13	110.9(2)	N2	Zr1	C28	114.65(7)
C12	C11	P1	109.76(15)	N1	Zr1	C28	106.15(8)
C13	C11	P1	114.40(16)	N2	Zr1	C23	115.24(8)
C15	C14	C16	111.0(2)	N1	Zr1	C23	119.47(7)
C15	C14	P1	110.68(17)	C28	Zr1	C23	111.83(8)
C16	C14	P1	110.45(15)	N2	Zr1	P2	37.68(5)
C1	N1	P1	126.47(13)	N1	Zr1	P2	124.95(5)
C1	N1	Zr1	140.14(13)	C28	Zr1	P2	101.23(6)
P1	N1	Zr1	93.26(8)	C23	Zr1	P2	91.65(6)
C6	N2	P2	125.66(13)	N2	Zr1	P1	121.46(5)
C6	N2	Zr1	141.10(13)	N1	Zr1	P1	37.26(4)

P2	N2	Zr1	93.06(8)	C28	Zr1	P1	101.29(6)
N1	P1	C14	107.58(10)	C23	Zr1	P1	89.30(6)
N1	P1	C11	109.86(10)	P2	Zr1	P1	155.306(18)

Bond Lengths for **4d**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Zr1	N1[1]	2.0838(14)	P1	C6	1.8564(19)
Zr1	N1	2.0838(14)	P1	C9	1.8766(19)
Zr1	C12	2.254(2)	N1	C1	1.412(2)
Zr1	C12[1]	2.254(2)	C6	C7	1.527(3)
Fe1	C4[1]	2.036(2)	C6	C8	1.534(3)
Fe1	C4	2.0362(19)	C1	C2	1.432(3)
Fe1	C3[1]	2.0398(19)	C1	C5	1.438(3)
Fe1	C3	2.0399(19)	C10	C9	1.538(3)
Fe1	C2[1]	2.0500(19)	C3	C2	1.417(3)
Fe1	C2	2.0501(19)	C3	C4	1.420(3)
Fe1	C5[1]	2.0544(19)	C9	C11	1.537(3)
Fe1	C5	2.0544(19)	C12	C14	1.509(3)
Fe1	C1[1]	2.0740(18)	C12	C15	1.528(3)
Fe1	C1	2.0741(18)	C12	C13	1.551(3)
P1	N1	1.7254(15)	C4	C5	1.420(3)

[1]-X,+Y,3/2-Z

Bond Angles for **4d**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1[1]	Zr1	N1	129.19(8)	C3[1]	Fe1	C1	166.43(8)
N1[1]	Zr1	C12	106.40(7)	C3	Fe1	C1	68.32(8)
N1	Zr1	C12	103.15(7)	C2[1]	Fe1	C1	133.56(8)
N1[1]	Zr1	C12[1]	103.15(7)	C2	Fe1	C1	40.62(7)
N1	Zr1	C12[1]	106.41(7)	C5[1]	Fe1	C1	123.41(8)
C12	Zr1	C12[1]	107.07(12)	C5	Fe1	C1	40.77(7)
C4[1]	Fe1	C4	121.94(12)	C1[1]	Fe1	C1	115.39(10)
C4[1]	Fe1	C3[1]	40.76(9)	N1	P1	C6	104.03(8)
C4	Fe1	C3[1]	102.14(8)	N1	P1	C9	103.16(8)
C4[1]	Fe1	C3	102.13(8)	C6	P1	C9	102.49(9)
C4	Fe1	C3	40.76(9)	C1	N1	P1	122.10(12)
C3[1]	Fe1	C3	111.36(12)	C1	N1	Zr1	109.78(11)
C4[1]	Fe1	C2[1]	68.39(8)	P1	N1	Zr1	128.00(8)
C4	Fe1	C2[1]	115.58(8)	C7	C6	C8	108.95(17)
C3[1]	Fe1	C2[1]	40.53(8)	C7	C6	P1	110.20(14)

C3	Fe1	C2[1]	146.48(8)	C8	C6	P1	109.95(15)
C4[1]	Fe1	C2	115.58(8)	N1	C1	C2	126.42(17)
C4	Fe1	C2	68.38(8)	N1	C1	C5	126.41(16)
C3[1]	Fe1	C2	146.48(9)	C2	C1	C5	107.16(17)
C3	Fe1	C2	40.53(8)	N1	C1	Fe1	127.07(12)
C2[1]	Fe1	C2	172.51(11)	C2	C1	Fe1	68.79(10)
C4[1]	Fe1	C5[1]	40.61(8)	C5	C1	Fe1	68.88(10)
C4	Fe1	C5[1]	161.24(9)	C2	C3	C4	108.13(18)
C3[1]	Fe1	C5[1]	68.47(8)	C2	C3	Fe1	70.12(11)
C3	Fe1	C5[1]	125.81(9)	C4	C3	Fe1	69.48(11)
C2[1]	Fe1	C5[1]	68.48(8)	C3	C2	C1	108.39(18)
C2	Fe1	C5[1]	109.97(8)	C3	C2	Fe1	69.35(11)
C4[1]	Fe1	C5	161.24(9)	C1	C2	Fe1	70.59(10)
C4	Fe1	C5	40.61(8)	C11	C9	C10	111.15(16)
C3[1]	Fe1	C5	125.81(9)	C11	C9	P1	109.21(13)
C3	Fe1	C5	68.47(8)	C10	C9	P1	118.42(14)
C2[1]	Fe1	C5	109.97(8)	C14	C12	C15	108.70(19)
C2	Fe1	C5	68.48(8)	C14	C12	C13	108.0(2)
C5[1]	Fe1	C5	157.70(11)	C15	C12	C13	108.26(19)
C4[1]	Fe1	C1[1]	68.38(8)	C14	C12	Zr1	112.75(16)
C4	Fe1	C1[1]	152.50(8)	C15	C12	Zr1	115.63(14)
C3[1]	Fe1	C1[1]	68.32(8)	C13	C12	Zr1	103.06(14)
C3	Fe1	C1[1]	166.43(8)	C3	C4	C5	108.44(18)
C2[1]	Fe1	C1[1]	40.62(7)	C3	C4	Fe1	69.76(11)
C2	Fe1	C1[1]	133.57(8)	C5	C4	Fe1	70.38(11)
C5[1]	Fe1	C1[1]	40.77(7)	C4	C5	C1	107.87(18)
C5	Fe1	C1[1]	123.41(8)	C4	C5	Fe1	69.01(11)
C4[1]	Fe1	C1	152.50(8)	C1	C5	Fe1	70.35(10)
C4	Fe1	C1	68.38(8)				

[1]-X,+Y,3/2-Z

Bond Lengths for **5b**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
C1	N1	1.416(5)	C86	C87	1.381(6)
C1	C5	1.431(5)	C88	C93	1.396(6)
C1	C2	1.437(5)	C88	C89	1.398(6)
C1	Fe1	2.039(4)	C88	N6	1.438(5)
C2	C3	1.428(6)	C93	C92	1.393(6)
C2	Fe1	2.038(4)	C93	C95	1.497(6)
C3	C4	1.433(6)	C92	C91	1.369(7)
C3	Fe1	2.043(4)	C91	C90	1.381(7)
C4	C5	1.425(6)	C90	C89	1.403(6)

C4	Fe1	2.054(4)	C89	C94	1.500(6)
C5	Fe1	2.043(4)	C101	N7	1.416(5)
C6	C10	1.424(5)	C101	C105	1.432(5)
C6	N2	1.426(5)	C101	C102	1.437(5)
C6	C7	1.429(5)	C101	Fe3	2.046(4)
C6	Fe1	2.031(4)	C102	C103	1.430(5)
C7	C8	1.423(6)	C102	Fe3	2.047(4)
C7	Fe1	2.048(4)	C103	C104	1.427(6)
C8	C9	1.419(6)	C103	Fe3	2.055(4)
C8	Fe1	2.060(4)	C104	C105	1.427(6)
C9	C10	1.428(6)	C104	Fe3	2.046(4)
C9	Fe1	2.046(4)	C105	Fe3	2.044(4)
C10	Fe1	2.034(4)	C106	N8	1.423(5)
C11	C12	1.532(6)	C106	C107	1.427(5)
C11	C13	1.534(6)	C106	C110	1.434(5)
C11	P1	1.859(4)	C106	Fe3	2.039(4)
C14	C16	1.524(6)	C107	C108	1.420(5)
C14	C15	1.537(6)	C107	Fe3	2.040(4)
C14	P1	1.847(4)	C108	C109	1.425(6)
C23	C24	1.481(5)	C108	Fe3	2.045(4)
C23	Zr1	2.318(4)	C109	C110	1.419(6)
C24	C29	1.398(6)	C109	Fe3	2.047(4)
C24	C25	1.404(6)	C110	Fe3	2.048(4)
C25	C26	1.383(6)	C111	C112	1.513(7)
C26	C27	1.388(7)	C111	C113	1.538(6)
C27	C28	1.377(7)	C111	P5	1.862(5)
C28	C29	1.410(7)	C114	C115	1.504(7)
C30	N3	1.282(5)	C114	C116	1.529(7)
C30	C31	1.513(5)	C114	P5	1.844(4)
C30	Zr1	2.258(4)	C117	C119	1.527(5)
C31	C32	1.516(5)	C117	C118	1.532(5)
C32	C33	1.381(6)	C117	P6	1.856(4)
C32	C37	1.389(5)	C120	C121	1.528(6)
C33	C34	1.395(6)	C120	C122	1.530(6)
C34	C35	1.381(6)	C120	P6	1.861(4)
C35	C36	1.386(6)	C123	C124	1.478(5)
C36	C37	1.381(6)	C123	Zr3	2.332(4)
C38	C43	1.392(6)	C124	C125	1.399(6)
C38	C39	1.397(6)	C124	C129	1.400(6)
C38	N3	1.445(5)	C125	C126	1.383(6)
C39	C40	1.395(6)	C126	C127	1.373(7)
C39	C44	1.491(7)	C127	C128	1.372(7)
C40	C41	1.372(8)	C128	C129	1.395(6)

C41	C42	1.380(8)	C130	N9	1.287(5)
C42	C43	1.409(6)	C130	C131	1.516(5)
C43	C45	1.501(7)	C130	Zr3	2.258(4)
C51	N4	1.414(5)	C131	C132	1.511(6)
C51	C52	1.432(5)	C132	C137	1.379(6)
C51	C55	1.432(5)	C132	C133	1.401(6)
C51	Fe2	2.033(4)	C137	C136	1.387(6)
C52	C53	1.429(5)	C136	C135	1.384(6)
C52	Fe2	2.044(4)	C135	C134	1.385(6)
C53	C54	1.428(6)	C134	C133	1.382(6)
C53	Fe2	2.056(4)	C138	C139	1.402(6)
C54	C55	1.424(6)	C138	C143	1.403(6)
C54	Fe2	2.052(4)	C138	N9	1.438(5)
C55	Fe2	2.038(4)	C139	C140	1.400(6)
C56	N5	1.417(5)	C139	C144	1.499(6)
C56	C57	1.431(5)	C140	C141	1.377(6)
C56	C60	1.433(5)	C141	C142	1.387(6)
C56	Fe2	2.043(4)	C142	C143	1.402(6)
C57	C58	1.435(5)	C143	C145	1.512(6)
C57	Fe2	2.039(4)	N1	P1	1.685(3)
C58	C59	1.426(6)	N1	Zr1	2.101(3)
C58	Fe2	2.042(4)	N2	P2	1.670(3)
C59	C60	1.433(5)	N2	P2A	1.851(11)
C59	Fe2	2.048(4)	N2	Zr1	2.096(3)
C60	Fe2	2.043(4)	N3	Zr1	2.271(3)
C61	C63	1.506(7)	N4	P3	1.678(3)
C61	C62	1.533(6)	N4	Zr2	2.103(3)
C61	P3	1.851(4)	N5	P4	1.681(3)
C64	C65	1.516(7)	N5	Zr2	2.102(3)
C64	C66	1.541(7)	N6	Zr2	2.281(3)
C64	P3	1.870(5)	N7	P5	1.682(3)
C70	C71	1.531(6)	N7	Zr3	2.116(3)
C70	C72	1.533(6)	N8	P6	1.686(3)
C70	P4	1.856(4)	N8	Zr3	2.098(3)
C67	C68	1.534(6)	N9	Zr3	2.254(3)
C67	C69	1.545(6)	P1	Zr1	2.7696(13)
C67	P4	1.853(4)	P3	Zr2	2.7716(12)
C73	C74	1.481(6)	P4	Zr2	2.7527(13)
C73	Zr2	2.315(4)	P5	Zr3	2.7278(12)
C74	C79	1.394(6)	P6	Zr3	2.7713(12)
C74	C75	1.395(6)	Zr1	P2	2.7560(12)
C79	C78	1.403(7)	Zr1	P2A	2.903(10)
C78	C77	1.367(7)	P2	C17	1.857(5)

C77	C76	1.370(8)	P2	C20	1.867(4)
C76	C75	1.383(7)	C17	C18	1.528(6)
C80	N6	1.284(5)	C17	C19	1.531(6)
C80	C81	1.512(5)	C20	C21	1.529(6)
C80	Zr2	2.258(4)	C20	C22	1.531(6)
C81	C82	1.517(5)	P2A	C17A	1.75(7)
C82	C83	1.387(6)	P2A	C20A	1.83(3)
C82	C87	1.391(6)	C17A	C19A	1.530(16)
C83	C84	1.394(6)	C17A	C18A	1.535(16)
C84	C85	1.386(6)	C20A	C22A	1.526(15)
C85	C86	1.378(6)	C20A	C21A	1.533(16)

Bond Angles for **5b**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1	C1	C5	126.3(3)	P6	N8	Zr3	93.53(14)
N1	C1	C2	126.3(3)	C130	N9	C138	127.7(3)
C5	C1	C2	107.4(3)	C130	N9	Zr3	73.6(2)
N1	C1	Fe1	124.1(3)	C138	N9	Zr3	158.6(3)
C5	C1	Fe1	69.6(2)	N1	P1	C14	108.62(18)
C2	C1	Fe1	69.3(2)	N1	P1	C11	105.77(18)
C3	C2	C1	108.2(3)	C14	P1	C11	105.82(19)
C3	C2	Fe1	69.7(2)	N1	P1	Zr1	49.23(11)
C1	C2	Fe1	69.4(2)	C14	P1	Zr1	128.09(14)
C2	C3	C4	108.0(4)	C11	P1	Zr1	124.39(14)
C2	C3	Fe1	69.3(2)	N4	P3	C61	106.72(18)
C4	C3	Fe1	69.9(2)	N4	P3	C64	106.8(2)
C5	C4	C3	107.9(4)	C61	P3	C64	107.4(2)
C5	C4	Fe1	69.2(2)	N4	P3	Zr2	49.23(11)
C3	C4	Fe1	69.1(2)	C61	P3	Zr2	128.44(16)
C4	C5	C1	108.6(3)	C64	P3	Zr2	122.38(17)
C4	C5	Fe1	70.1(2)	N5	P4	C67	106.80(18)
C1	C5	Fe1	69.4(2)	N5	P4	C70	107.33(17)
C10	C6	N2	126.4(3)	C67	P4	C70	106.42(19)
C10	C6	C7	107.3(3)	N5	P4	Zr2	49.72(10)
N2	C6	C7	126.2(3)	C67	P4	Zr2	123.96(15)
C10	C6	Fe1	69.6(2)	C70	P4	Zr2	128.07(14)
N2	C6	Fe1	123.7(3)	N7	P5	C114	110.3(2)
C7	C6	Fe1	70.1(2)	N7	P5	C111	109.72(18)
C8	C7	C6	108.4(3)	C114	P5	C111	104.0(2)
C8	C7	Fe1	70.2(2)	N7	P5	Zr3	50.86(11)
C6	C7	Fe1	68.9(2)	C114	P5	Zr3	129.15(15)
C9	C8	C7	107.9(3)	C111	P5	Zr3	126.43(15)

C9	C8	Fe1	69.3(2)	N8	P6	C117	105.98(17)
C7	C8	Fe1	69.3(2)	N8	P6	C120	107.50(17)
C8	C9	C10	108.0(3)	C117	P6	C120	106.18(18)
C8	C9	Fe1	70.3(2)	N8	P6	Zr3	49.08(10)
C10	C9	Fe1	69.1(2)	C117	P6	Zr3	122.84(13)
C6	C10	C9	108.3(3)	C120	P6	Zr3	129.02(13)
C6	C10	Fe1	69.4(2)	C6	Fe1	C10	41.02(15)
C9	C10	Fe1	70.0(2)	C6	Fe1	C2	114.49(15)
C12	C11	C13	111.0(3)	C10	Fe1	C2	149.56(16)
C12	C11	P1	113.7(3)	C6	Fe1	C1	101.31(15)
C13	C11	P1	114.7(3)	C10	Fe1	C1	115.19(16)
C16	C14	C15	110.1(4)	C2	Fe1	C1	41.28(15)
C16	C14	P1	110.0(3)	C6	Fe1	C5	122.28(16)
C15	C14	P1	110.5(3)	C10	Fe1	C5	106.22(16)
C24	C23	Zr1	122.3(3)	C2	Fe1	C5	69.01(16)
C29	C24	C25	117.3(4)	C1	Fe1	C5	41.05(15)
C29	C24	C23	122.4(4)	C6	Fe1	C3	151.48(16)
C25	C24	C23	120.3(4)	C10	Fe1	C3	167.40(16)
C26	C25	C24	121.8(4)	C2	Fe1	C3	40.96(16)
C25	C26	C27	120.2(5)	C1	Fe1	C3	69.29(16)
C28	C27	C26	119.5(5)	C5	Fe1	C3	68.87(16)
C27	C28	C29	120.4(5)	C6	Fe1	C9	69.08(15)
C24	C29	C28	120.7(5)	C10	Fe1	C9	40.97(16)
N3	C30	C31	124.4(3)	C2	Fe1	C9	166.17(17)
N3	C30	Zr1	74.2(2)	C1	Fe1	C9	152.55(16)
C31	C30	Zr1	161.4(3)	C5	Fe1	C9	121.41(16)
C30	C31	C32	111.8(3)	C3	Fe1	C9	130.81(16)
C33	C32	C37	118.4(4)	C6	Fe1	C7	41.02(15)
C33	C32	C31	120.7(4)	C10	Fe1	C7	68.55(16)
C37	C32	C31	120.9(4)	C2	Fe1	C7	105.06(16)
C32	C33	C34	120.8(4)	C1	Fe1	C7	121.89(16)
C35	C34	C33	120.0(4)	C5	Fe1	C7	159.73(16)
C34	C35	C36	119.6(4)	C3	Fe1	C7	120.11(16)
C37	C36	C35	119.9(4)	C9	Fe1	C7	68.31(16)
C36	C37	C32	121.3(4)	C6	Fe1	C4	161.96(16)
C43	C38	C39	122.0(4)	C10	Fe1	C4	128.01(16)
C43	C38	N3	118.0(4)	C2	Fe1	C4	68.87(16)
C39	C38	N3	119.8(4)	C1	Fe1	C4	69.01(16)
C40	C39	C38	118.3(5)	C5	Fe1	C4	40.71(15)
C40	C39	C44	120.3(5)	C3	Fe1	C4	40.93(16)
C38	C39	C44	121.3(4)	C9	Fe1	C4	112.21(16)
C41	C40	C39	120.5(5)	C7	Fe1	C4	157.01(16)
C40	C41	C42	121.1(5)	C6	Fe1	C8	68.88(16)

C41	C42	C43	120.1(5)	C10	Fe1	C8	68.48(16)
C38	C43	C42	117.9(5)	C2	Fe1	C8	126.84(17)
C38	C43	C45	121.2(4)	C1	Fe1	C8	161.27(16)
C42	C43	C45	120.8(5)	C5	Fe1	C8	157.63(16)
N4	C51	C52	126.4(3)	C3	Fe1	C8	111.37(16)
N4	C51	C55	126.1(3)	C9	Fe1	C8	40.45(16)
C52	C51	C55	107.4(3)	C7	Fe1	C8	40.53(15)
N4	C51	Fe2	123.6(2)	C4	Fe1	C8	124.57(16)
C52	C51	Fe2	69.9(2)	C51	Fe2	C55	41.20(15)
C55	C51	Fe2	69.6(2)	C51	Fe2	C57	113.65(15)
C53	C52	C51	108.2(3)	C55	Fe2	C57	148.41(16)
C53	C52	Fe2	70.1(2)	C51	Fe2	C58	150.70(16)
C51	C52	Fe2	69.0(2)	C55	Fe2	C58	168.05(16)
C54	C53	C52	107.9(3)	C57	Fe2	C58	41.18(15)
C54	C53	Fe2	69.5(2)	C51	Fe2	C60	122.51(15)
C52	C53	Fe2	69.1(2)	C55	Fe2	C60	105.94(15)
C55	C54	C53	108.1(3)	C57	Fe2	C60	68.90(15)
C55	C54	Fe2	69.1(2)	C58	Fe2	C60	68.89(15)
C53	C54	Fe2	69.8(2)	C51	Fe2	C56	101.05(15)
C54	C55	C51	108.4(3)	C55	Fe2	C56	114.42(15)
C54	C55	Fe2	70.2(2)	C57	Fe2	C56	41.03(14)
C51	C55	Fe2	69.2(2)	C58	Fe2	C56	69.28(15)
N5	C56	C57	126.5(3)	C60	Fe2	C56	41.05(14)
N5	C56	C60	125.9(3)	C51	Fe2	C52	41.14(14)
C57	C56	C60	107.5(3)	C55	Fe2	C52	68.90(15)
N5	C56	Fe2	123.8(2)	C57	Fe2	C52	104.95(15)
C57	C56	Fe2	69.3(2)	C58	Fe2	C52	119.66(16)
C60	C56	Fe2	69.5(2)	C60	Fe2	C52	160.18(15)
C56	C57	C58	108.2(3)	C56	Fe2	C52	122.15(15)
C56	C57	Fe2	69.6(2)	C51	Fe2	C59	162.65(15)
C58	C57	Fe2	69.5(2)	C55	Fe2	C59	128.43(16)
C59	C58	C57	108.0(3)	C57	Fe2	C59	69.01(15)
C59	C58	Fe2	69.8(2)	C58	Fe2	C59	40.82(16)
C57	C58	Fe2	69.3(2)	C60	Fe2	C59	41.00(15)
C58	C59	C60	107.8(3)	C56	Fe2	C59	69.24(15)
C58	C59	Fe2	69.4(2)	C52	Fe2	C59	156.20(15)
C60	C59	Fe2	69.3(2)	C51	Fe2	C54	69.07(15)
C59	C60	C56	108.4(3)	C55	Fe2	C54	40.74(16)
C59	C60	Fe2	69.7(2)	C57	Fe2	C54	167.59(16)
C56	C60	Fe2	69.5(2)	C58	Fe2	C54	131.77(16)
C63	C61	C62	109.7(4)	C60	Fe2	C54	120.71(16)
C63	C61	P3	109.7(3)	C56	Fe2	C54	151.38(16)
C62	C61	P3	111.3(3)	C52	Fe2	C54	68.65(15)

C65	C64	C66	110.1(4)	C59	Fe2	C54	112.28(16)
C65	C64	P3	114.4(4)	C51	Fe2	C53	69.08(15)
C66	C64	P3	115.2(3)	C55	Fe2	C53	68.63(16)
C71	C70	C72	109.9(4)	C57	Fe2	C53	127.74(16)
C71	C70	P4	111.4(3)	C58	Fe2	C53	111.64(16)
C72	C70	P4	109.3(3)	C60	Fe2	C53	156.91(15)
C68	C67	C69	111.5(4)	C56	Fe2	C53	162.01(15)
C68	C67	P4	112.2(3)	C52	Fe2	C53	40.80(15)
C69	C67	P4	115.1(3)	C59	Fe2	C53	123.99(15)
C74	C73	Zr2	121.6(3)	C54	Fe2	C53	40.67(16)
C79	C74	C75	116.4(4)	C106	Fe3	C107	40.94(15)
C79	C74	C73	122.1(4)	C106	Fe3	C105	113.26(15)
C75	C74	C73	121.5(4)	C107	Fe3	C105	146.56(15)
C74	C79	C78	121.1(4)	C106	Fe3	C108	68.74(15)
C77	C78	C79	120.6(5)	C107	Fe3	C108	40.69(15)
C78	C77	C76	119.4(5)	C105	Fe3	C108	170.10(16)
C77	C76	C75	120.3(5)	C106	Fe3	C101	101.62(15)
C76	C75	C74	122.3(4)	C107	Fe3	C101	112.84(15)
N6	C80	C81	124.0(3)	C105	Fe3	C101	41.00(15)
N6	C80	Zr2	74.5(2)	C108	Fe3	C101	148.90(16)
C81	C80	Zr2	161.4(3)	C106	Fe3	C104	149.51(16)
C80	C81	C82	112.3(3)	C107	Fe3	C104	169.55(16)
C83	C82	C87	118.4(4)	C105	Fe3	C104	40.83(16)
C83	C82	C81	121.0(4)	C108	Fe3	C104	133.55(16)
C87	C82	C81	120.6(4)	C101	Fe3	C104	68.97(15)
C82	C83	C84	120.7(4)	C106	Fe3	C102	123.86(15)
C85	C84	C83	119.9(4)	C107	Fe3	C102	105.49(16)
C86	C85	C84	119.8(4)	C105	Fe3	C102	68.85(16)
C85	C86	C87	120.1(4)	C108	Fe3	C102	118.74(16)
C86	C87	C82	121.2(4)	C101	Fe3	C102	41.12(15)
C93	C88	C89	121.8(4)	C104	Fe3	C102	68.70(16)
C93	C88	N6	119.2(4)	C106	Fe3	C109	68.86(15)
C89	C88	N6	118.9(4)	C107	Fe3	C109	68.65(16)
C92	C93	C88	118.7(4)	C105	Fe3	C109	129.94(16)
C92	C93	C95	120.6(4)	C108	Fe3	C109	40.75(16)
C88	C93	C95	120.7(4)	C101	Fe3	C109	164.36(16)
C91	C92	C93	120.6(4)	C104	Fe3	C109	112.60(16)
C92	C91	C90	120.3(4)	C102	Fe3	C109	154.52(16)
C91	C90	C89	121.3(4)	C106	Fe3	C110	41.07(15)
C88	C89	C90	117.2(4)	C107	Fe3	C110	68.68(16)
C88	C89	C94	121.1(4)	C105	Fe3	C110	106.34(16)
C90	C89	C94	121.7(4)	C108	Fe3	C110	68.38(16)
N7	C101	C105	125.1(3)	C101	Fe3	C110	124.34(15)

N7	C101	C102	127.3(3)	C104	Fe3	C110	119.46(16)
C105	C101	C102	107.4(3)	C102	Fe3	C110	162.42(16)
N7	C101	Fe3	122.2(2)	C109	Fe3	C110	40.54(15)
C105	C101	Fe3	69.4(2)	C106	Fe3	C103	164.03(16)
C102	C101	Fe3	69.5(2)	C107	Fe3	C103	129.36(16)
C103	C102	C101	108.2(3)	C105	Fe3	C103	68.69(16)
C103	C102	Fe3	69.9(2)	C108	Fe3	C103	112.27(16)
C101	C102	Fe3	69.4(2)	C101	Fe3	C103	68.99(15)
C104	C103	C102	107.9(3)	C104	Fe3	C103	40.73(16)
C104	C103	Fe3	69.3(2)	C102	Fe3	C103	40.80(15)
C102	C103	Fe3	69.3(2)	C109	Fe3	C103	123.04(16)
C105	C104	C103	108.2(3)	C110	Fe3	C103	154.89(16)
C105	C104	Fe3	69.5(2)	N2	Zr1	N1	87.24(12)
C103	C104	Fe3	70.0(2)	N2	Zr1	C30	108.60(13)
C104	C105	C101	108.2(3)	N1	Zr1	C30	113.96(13)
C104	C105	Fe3	69.6(2)	N2	Zr1	N3	128.68(12)
C101	C105	Fe3	69.6(2)	N1	Zr1	N3	131.62(12)
N8	C106	C107	126.9(3)	C30	Zr1	N3	32.87(12)
N8	C106	C110	125.6(3)	N2	Zr1	C23	112.20(14)
C107	C106	C110	107.5(3)	N1	Zr1	C23	103.16(13)
N8	C106	Fe3	123.7(2)	C30	Zr1	C23	125.17(14)
C107	C106	Fe3	69.6(2)	N3	Zr1	C23	92.32(13)
C110	C106	Fe3	69.8(2)	N2	Zr1	P2	37.22(8)
C108	C107	C106	108.2(3)	N1	Zr1	P2	124.44(9)
C108	C107	Fe3	69.9(2)	C30	Zr1	P2	92.07(10)
C106	C107	Fe3	69.5(2)	N3	Zr1	P2	97.11(9)
C107	C108	C109	108.2(3)	C23	Zr1	P2	98.90(11)
C107	C108	Fe3	69.5(2)	N2	Zr1	P1	124.61(9)
C109	C108	Fe3	69.7(2)	N1	Zr1	P1	37.39(9)
C110	C109	C108	108.0(3)	C30	Zr1	P1	97.10(10)
C110	C109	Fe3	69.8(2)	N3	Zr1	P1	99.11(9)
C108	C109	Fe3	69.5(2)	C23	Zr1	P1	88.61(11)
C109	C110	C106	108.2(3)	P2	Zr1	P1	161.83(3)
C109	C110	Fe3	69.7(2)	N2	Zr1	P2A	39.5(2)
C106	C110	Fe3	69.1(2)	N1	Zr1	P2A	121.1(2)
C112	C111	C113	110.8(4)	C30	Zr1	P2A	107.4(3)
C112	C111	P5	111.7(3)	N3	Zr1	P2A	105.8(2)
C113	C111	P5	109.5(3)	C23	Zr1	P2A	83.9(3)
C115	C114	C116	111.4(4)	P1	Zr1	P2A	154.2(2)
C115	C114	P5	115.1(3)	N5	Zr2	N4	86.66(12)
C116	C114	P5	109.0(3)	N5	Zr2	C80	115.74(13)
C119	C117	C118	111.2(3)	N4	Zr2	C80	108.08(13)
C119	C117	P6	115.6(3)	N5	Zr2	N6	133.67(11)

C118	C117	P6	112.1(3)	N4	Zr2	N6	127.82(11)
C121	C120	C122	109.9(3)	C80	Zr2	N6	32.87(12)
C121	C120	P6	109.4(3)	N5	Zr2	C73	102.71(13)
C122	C120	P6	111.0(3)	N4	Zr2	C73	113.63(14)
C124	C123	Zr3	122.0(3)	C80	Zr2	C73	123.90(14)
C125	C124	C129	115.6(4)	N6	Zr2	C73	91.09(13)
C125	C124	C123	122.1(4)	N5	Zr2	P4	37.60(9)
C129	C124	C123	122.3(4)	N4	Zr2	P4	123.99(9)
C126	C125	C124	122.4(4)	C80	Zr2	P4	96.47(10)
C127	C126	C125	120.4(4)	N6	Zr2	P4	99.74(8)
C128	C127	C126	119.4(4)	C73	Zr2	P4	89.98(12)
C127	C128	C129	120.2(4)	N5	Zr2	P3	123.46(9)
C128	C129	C124	122.0(4)	N4	Zr2	P3	37.18(8)
N9	C130	C131	123.5(3)	C80	Zr2	P3	93.85(10)
N9	C130	Zr3	73.2(2)	N6	Zr2	P3	97.56(9)
C131	C130	Zr3	163.2(3)	C73	Zr2	P3	97.39(12)
C132	C131	C130	113.4(3)	P4	Zr2	P3	161.06(3)
C137	C132	C133	117.7(4)	N8	Zr3	N7	86.82(12)
C137	C132	C131	121.7(4)	N8	Zr3	N9	135.41(12)
C133	C132	C131	120.5(4)	N7	Zr3	N9	125.03(12)
C132	C137	C136	121.6(4)	N8	Zr3	C130	113.29(13)
C135	C136	C137	120.0(4)	N7	Zr3	C130	108.88(13)
C136	C135	C134	119.5(4)	N9	Zr3	C130	33.14(12)
C133	C134	C135	120.0(4)	N8	Zr3	C123	102.11(13)
C134	C133	C132	121.2(4)	N7	Zr3	C123	118.40(13)
C139	C138	C143	122.0(4)	N9	Zr3	C123	89.58(13)
C139	C138	N9	118.5(4)	C130	Zr3	C123	121.52(14)
C143	C138	N9	119.2(3)	N8	Zr3	P5	120.84(9)
C140	C139	C138	117.9(4)	N7	Zr3	P5	38.05(8)
C140	C139	C144	121.2(4)	N9	Zr3	P5	101.07(9)
C138	C139	C144	120.9(4)	C130	Zr3	P5	105.83(10)
C141	C140	C139	121.1(4)	C123	Zr3	P5	92.60(10)
C140	C141	C142	120.4(4)	N8	Zr3	P6	37.39(8)
C141	C142	C143	120.8(4)	N7	Zr3	P6	124.05(9)
C142	C143	C138	117.8(4)	N9	Zr3	P6	102.60(9)
C142	C143	C145	120.5(4)	C130	Zr3	P6	94.92(10)
C138	C143	C145	121.6(4)	C123	Zr3	P6	86.03(10)
C1	N1	P1	125.6(3)	P5	Zr3	P6	156.28(3)
C1	N1	Zr1	141.0(2)	N2	P2	C17	106.24(19)
P1	N1	Zr1	93.38(14)	N2	P2	C20	106.97(18)
C6	N2	P2	125.1(3)	C17	P2	C20	106.5(2)
C6	N2	P2A	122.4(4)	N2	P2	Zr1	49.38(11)
C6	N2	Zr1	141.0(2)	C17	P2	Zr1	130.40(15)

P2	N2	Zr1	93.39(14)	C20	P2	Zr1	121.17(15)
P2A	N2	Zr1	94.5(3)	C18	C17	C19	111.5(4)
C30	N3	C38	128.0(3)	C18	C17	P2	109.6(4)
C30	N3	Zr1	73.0(2)	C19	C17	P2	111.9(3)
C38	N3	Zr1	158.9(3)	C21	C20	C22	112.2(4)
C51	N4	P3	124.9(2)	C21	C20	P2	113.1(3)
C51	N4	Zr2	141.3(2)	C22	C20	P2	115.2(3)
P3	N4	Zr2	93.59(14)	C17A	P2A	C20A	104.7(19)
C56	N5	P4	126.1(2)	C17A	P2A	N2	116.3(16)
C56	N5	Zr2	141.2(2)	C20A	P2A	N2	107.9(15)
P4	N5	Zr2	92.68(14)	C17A	P2A	Zr1	127.0(15)
C80	N6	C88	127.5(3)	C20A	P2A	Zr1	127.8(12)
C80	N6	Zr2	72.6(2)	N2	P2A	Zr1	46.0(3)
C88	N6	Zr2	160.0(2)	C19A	C17A	C18A	111.3(17)
C101	N7	P5	128.2(2)	C19A	C17A	P2A	116(4)
C101	N7	Zr3	140.6(2)	C18A	C17A	P2A	110(4)
P5	N7	Zr3	91.09(14)	C22A	C20A	C21A	112.3(16)
C106	N8	P6	125.7(2)	C22A	C20A	P2A	114(2)
C106	N8	Zr3	140.8(2)	C21A	C20A	P2A	134(2)

Bond Lengths for **5d**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
C1	N1	1.417(4)	C17	C18	1.537(5)
C1	C2	1.434(4)	C17	P2	1.869(3)
C1	C5	1.438(4)	C20	C21	1.531(4)
C1	Fe1	2.076(3)	C20	C22	1.538(5)
C2	C3	1.426(4)	C20	P2	1.880(3)
C2	Fe1	2.051(3)	C27	N3	1.286(4)
C3	C4	1.416(5)	C27	C28	1.521(4)
C3	Fe1	2.044(3)	C27	Zr1	2.230(3)
C4	C5	1.419(5)	C28	C31	1.504(5)
C4	Fe1	2.033(3)	C28	C29	1.540(5)
C5	Fe1	2.033(3)	C28	C30	1.541(5)
C6	N2	1.417(4)	C32	C37	1.401(4)
C6	C10	1.423(5)	C32	C33	1.405(4)
C6	C7	1.431(4)	C32	N3	1.448(4)
C6	Fe1	2.068(3)	C33	C34	1.398(4)
C7	C8	1.414(5)	C33	C38	1.505(4)
C7	Fe1	2.044(3)	C34	C35	1.381(5)
C8	C9	1.406(6)	C35	C36	1.381(5)
C8	Fe1	2.041(4)	C36	C37	1.396(4)
C9	C10	1.426(5)	C37	C39	1.503(4)

C9	Fe1	2.050(3)	C23	C24	1.525(4)
C10	Fe1	2.050(3)	C23	C26	1.534(4)
C11	C13	1.529(5)	C23	C25	1.541(4)
C11	C12	1.542(4)	C23	Zr1	2.300(3)
C11	P1	1.879(3)	N1	P1	1.716(2)
C14	C16	1.532(5)	N1	Zr1	2.096(3)
C14	C15	1.536(4)	N2	P2	1.728(3)
C14	P1	1.859(3)	N2	Zr1	2.083(2)
C17	C19	1.535(4)	N3	Zr1	2.246(2)

Bond Angles for **5d**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1	C1	C2	126.3(3)	C26	C23	Zr1	113.54(19)
N1	C1	C5	126.9(3)	C25	C23	Zr1	101.79(19)
C2	C1	C5	106.8(3)	C1	N1	P1	122.6(2)
N1	C1	Fe1	127.8(2)	C1	N1	Zr1	111.08(17)
C2	C1	Fe1	68.72(16)	P1	N1	Zr1	124.97(13)
C5	C1	Fe1	67.90(17)	C6	N2	P2	120.20(18)
C3	C2	C1	108.5(3)	C6	N2	Zr1	110.95(17)
C3	C2	Fe1	69.37(17)	P2	N2	Zr1	128.82(13)
C1	C2	Fe1	70.63(16)	C27	N3	C32	131.9(2)
C4	C3	C2	108.0(3)	C27	N3	Zr1	72.60(17)
C4	C3	Fe1	69.26(18)	C32	N3	Zr1	155.48(19)
C2	C3	Fe1	69.87(17)	N1	P1	C14	104.42(13)
C3	C4	C5	108.4(3)	N1	P1	C11	104.08(13)
C3	C4	Fe1	70.09(19)	C14	P1	C11	103.51(15)
C5	C4	Fe1	69.55(19)	N2	P2	C17	103.52(13)
C4	C5	C1	108.4(3)	N2	P2	C20	103.30(13)
C4	C5	Fe1	69.6(2)	C17	P2	C20	103.66(14)
C1	C5	Fe1	71.16(18)	C5	Fe1	C4	40.86(13)
N2	C6	C10	126.6(3)	C5	Fe1	C8	158.81(15)
N2	C6	C7	126.3(3)	C4	Fe1	C8	120.51(15)
C10	C6	C7	107.1(3)	C5	Fe1	C7	159.59(13)
N2	C6	Fe1	128.58(19)	C4	Fe1	C7	159.23(14)
C10	C6	Fe1	69.09(18)	C8	Fe1	C7	40.51(15)
C7	C6	Fe1	68.74(17)	C5	Fe1	C3	68.68(14)
C8	C7	C6	108.2(3)	C4	Fe1	C3	40.65(14)
C8	C7	Fe1	69.6(2)	C8	Fe1	C3	103.20(14)
C6	C7	Fe1	70.53(19)	C7	Fe1	C3	124.78(14)
C9	C8	C7	108.5(3)	C5	Fe1	C10	108.47(15)
C9	C8	Fe1	70.3(2)	C4	Fe1	C10	117.16(14)
C7	C8	Fe1	69.88(19)	C8	Fe1	C10	68.16(16)

C8	C9	C10	108.1(3)	C7	Fe1	C10	68.24(15)
C8	C9	Fe1	69.54(19)	C3	Fe1	C10	149.75(13)
C10	C9	Fe1	69.64(18)	C5	Fe1	C9	123.60(17)
C6	C10	C9	108.1(3)	C4	Fe1	C9	102.38(15)
C6	C10	Fe1	70.47(17)	C8	Fe1	C9	40.21(18)
C9	C10	Fe1	69.66(19)	C7	Fe1	C9	67.96(17)
C13	C11	C12	111.3(3)	C3	Fe1	C9	114.07(14)
C13	C11	P1	117.9(2)	C10	Fe1	C9	40.70(14)
C12	C11	P1	109.3(2)	C5	Fe1	C2	68.71(13)
C16	C14	C15	109.0(3)	C4	Fe1	C2	68.51(13)
C16	C14	P1	108.3(2)	C8	Fe1	C2	118.65(15)
C15	C14	P1	111.3(2)	C7	Fe1	C2	110.27(14)
C19	C17	C18	110.0(3)	C3	Fe1	C2	40.76(12)
C19	C17	P2	110.4(2)	C10	Fe1	C2	168.55(12)
C18	C17	P2	108.9(2)	C9	Fe1	C2	150.29(14)
C21	C20	C22	110.6(3)	C5	Fe1	C6	123.70(13)
C21	C20	P2	118.6(2)	C4	Fe1	C6	154.52(14)
C22	C20	P2	109.5(2)	C8	Fe1	C6	68.25(13)
N3	C27	C28	129.6(3)	C7	Fe1	C6	40.74(13)
N3	C27	Zr1	74.00(16)	C3	Fe1	C6	164.77(14)
C28	C27	Zr1	156.4(2)	C10	Fe1	C6	40.44(13)
C31	C28	C27	111.9(3)	C9	Fe1	C6	68.13(13)
C31	C28	C29	109.3(3)	C2	Fe1	C6	131.14(12)
C27	C28	C29	107.4(3)	C5	Fe1	C1	40.94(12)
C31	C28	C30	110.0(3)	C4	Fe1	C1	68.62(13)
C27	C28	C30	109.6(3)	C8	Fe1	C1	156.04(15)
C29	C28	C30	108.5(3)	C7	Fe1	C1	124.91(13)
C37	C32	C33	121.3(3)	C3	Fe1	C1	68.53(12)
C37	C32	N3	118.6(2)	C10	Fe1	C1	130.13(13)
C33	C32	N3	120.0(3)	C9	Fe1	C1	163.73(17)
C34	C33	C32	117.6(3)	C2	Fe1	C1	40.65(11)
C34	C33	C38	119.7(3)	C6	Fe1	C1	113.93(12)
C32	C33	C38	122.7(3)	N2	Zr1	N1	126.87(9)
C35	C34	C33	121.7(3)	N2	Zr1	C27	106.06(10)
C34	C35	C36	119.8(3)	N1	Zr1	C27	100.77(10)
C35	C36	C37	120.7(3)	N2	Zr1	N3	114.11(9)
C36	C37	C32	118.8(3)	N1	Zr1	N3	113.53(9)
C36	C37	C39	119.1(3)	C27	Zr1	N3	33.39(10)
C32	C37	C39	122.1(3)	N2	Zr1	C23	100.15(10)
C24	C23	C26	108.4(2)	N1	Zr1	C23	103.84(10)
C24	C23	C25	108.9(2)	C27	Zr1	C23	121.12(10)
C26	C23	C25	109.3(2)	N3	Zr1	C23	87.77(10)
C24	C23	Zr1	114.65(19)				

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