Supporting Information

Facilitated carbon dioxide reduction using a Zn(II) complex

Elizabeth S. Donovan, Brian M. Barry, Christopher A. Larsen, Melissa N. Wirtz, William E. Geiger, and Richard A. Kemp*

Corresponding author: Richard A. Kemp, email: rakemp@unm.edu

Contents

General synthetic procedures. Reactions were performed using an Ar (g) atmosphere glove box and standard Schlenk techniques. Solvents were purchased from Aldrich and subjected to an LC Technology solvent purification system prior to use. Reagents were purchased from Aldrich without further purification. Bis(2-pyridyl)phenylphosphine was prepared according to the method reported by Saucedo, *et. al.*[1] Despite repeated attempts, and even when employing added oxidant, combustion analyses consistently produced lower than expected C values. We attribute this to incomplete combustion upon metal carbide formation as has been reported for other transition metals.[2] Because we are unable to report EA values as an indication of sample purity, we have included all NMR spectra for compounds **1** and **2** (Figures S1-S6).

Synthesis of (1), Dichloro[phenyldi(2-pyridyl)phosphine-κ^2-*N*,*N*']zinc(II)·0.5THF. Solid $ZnCl_2$ (1.54 g, 11.3 mmol) was added to a gold, translucent stirred solution of phenyldi(2-pyridyl)phosphine (2.99 g, 11.3 mmol) in ca. 30 mL of THF. Within minutes a reaction occurred resulting in a white precipitate and loss of gold color in the supernatant. The reaction was allowed to stir for 2h at room temperature. The resulting white powder was then isolated by filtration and washed with fresh THF (3 × 10 mL), and dried under vacuum for 1h. Yield = 3.90 g (79%). Colorless single crystals were grown from a CH_2Cl_2/pentane mixture. ^{1}H NMR (CD_2Cl_2, 300 MHz): δ 1.82 (m, 2H, THF), 3.68 (m, 2H, THF), 7.19 (d, $^3J_{H\text{-}H}$ = 8.2 Hz, 2H, 6-C_6H_4N), 7.52 (m, 2H, 5-C_6H_4N), 7.67 (m, 2H, 4-C_6H_4N), 7.72-7.87 (overlapping multiplets, 5H, C_6H_5), 9.00 (d, $^3J_{H\text{-}H}$ = 5.3 Hz, 2H, 3-C_6H_4N). ^{13}C{^{1}H} (CD_2Cl_2, 75 MHz): δ 25.9 (s, THF), 68.2 (s, THF), all aromatic *C*: 124.5 (d, $J_{P\text{-}C}$ = 1.6 Hz), 128.7 (d, $J_{P\text{-}C}$ = 11 Hz), 129.9 (d, $J_{P\text{-}C}$ = 4.7 Hz), 130.8 (d, $J_{P\text{-}C}$ = 9.9 Hz), 133.2 (d, $J_{P\text{-}C}$ = 1.6 Hz), 138.6 (d, $J_{P\text{-}C}$ = 25 Hz), 139.7, 150.7 (d, $J_{P\text{-}C}$ = 4.6 Hz), 162.0 (d, $J_{P\text{-}C}$ = 18 Hz). ^{31}P{^{1}H} (CD_2Cl_2, 121 MHz) δ -5.22 ppm. Mp 269-271 °C.

Synthesis of (2), **Dichloro[diphenyl-(2-pyridyl)phosphine-κ^1-*N*]zinc(II).** Solid $ZnCl_2$ (65 mg, 0.47 mmol) was added to a colorless, translucent stirred solution of diphenyl-2-pyridylphosphine (250 mg, 0.95 mmol) in ca. 10 mL of THF. The reaction mixture was allowed to stir for 2h at room temperature followed by removal of solvent *in vacuo* permitting collection of a white powder. Yield = 141 mg (45%). Colorless crystals suitable for single-crystal x-ray diffraction were grown from slow evaporation of CH_2Cl_2. ^{1}H ^{1}H NMR (CD_2Cl_2, 300 MHz): δ 7.19 (m, 8H, *m*-C_6H_5), 7.24-7.40 (overlapping multiplets, 14H, *o*,*p*-C_6H_5 and 6-C_6H_4N), 7.45 (m, 2H, 4-C_6H_4N), 7.77 (m, 2H, 5-C_6H_4N) , 9.19(d, $^3J_{H\text{-}H}$ = 5.0 Hz, 2H, 3-C_6H_4N). ^{13}C{1H} (CD_2Cl_2, 75 MHz): δ all aromatic C: 124.8 (s), 129.1 (d, $J_{P\text{-}C}$ = 7.3 Hz), 129.8 (s), 131.2 (d, $J_{P\text{-}C}$ = 7.8 Hz), 134.1 (d, $J_{P\text{-}C}$ = 19 Hz), 134.8 (d, $J_{P\text{-}C}$ = 5.2 Hz),138.5 (s), 151.7 (d, $J_{P\text{-}C}$ = 13 Hz), 163.2 (s). ^{31}P{1H} (CD_2Cl_2, 121 MHz) δ -5.77 ppm. Mp 176-178 °C.

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[1] Saucedo, A.S.A.; Hagenbach, A.; Abram, U., *Polyhedron*, **2008**, 27, 3587 – 3592.

[2] Stephan, D. W.; Stewart, J. C.; Guérin, F.; Courtenay, S.; Kickham, J.; Hollink, E.; Beddie, C.; Hoskin, A.; Graham, T.; Wei, P.; Spence, R. E. v. H.; Xu, W.; Koch, L.; Gao, X.; Harrison, D. G., *Organometallics* **2003,** *22* (9), 1937-1947.

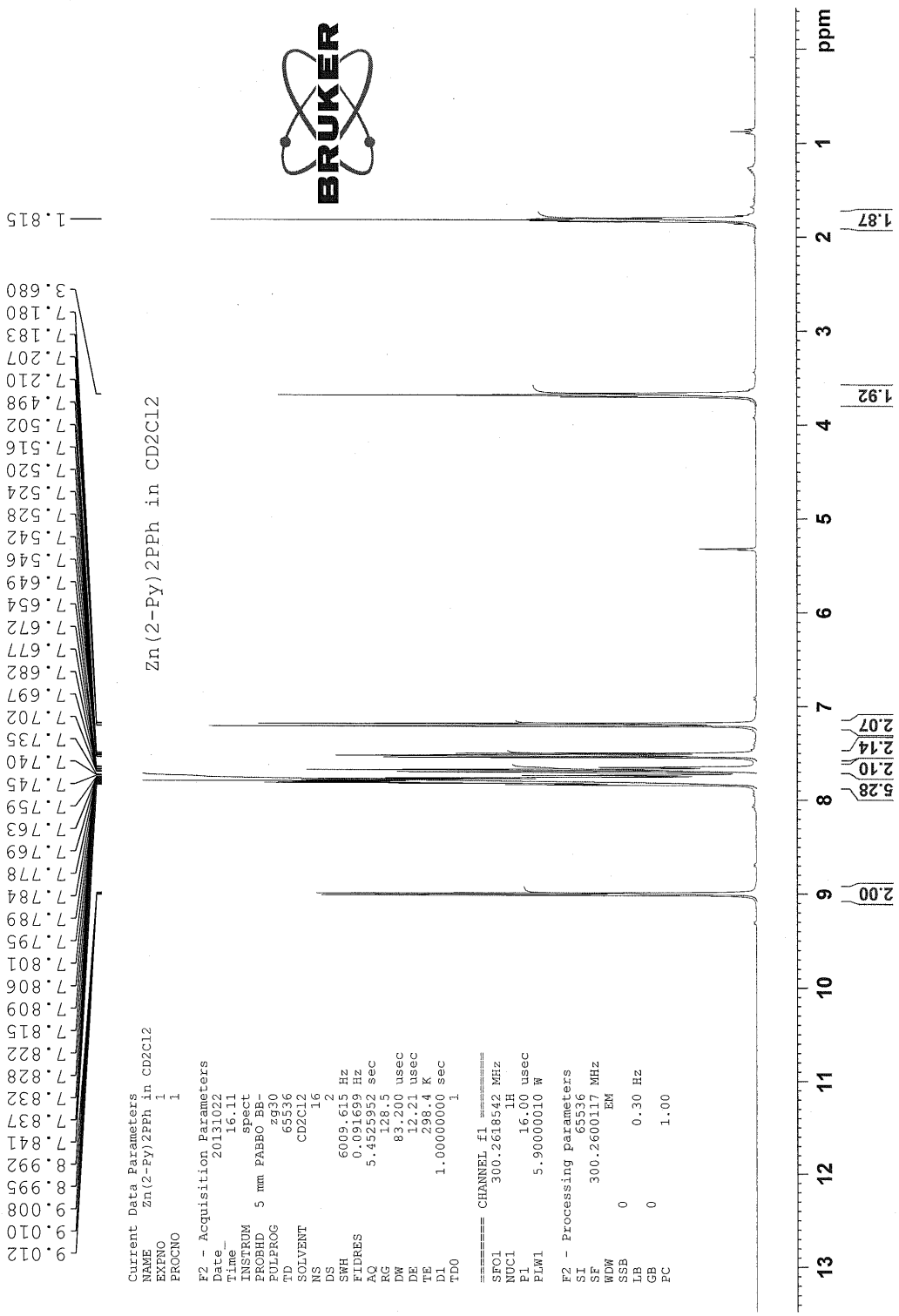

Figure S1. ^{1}H NMR of compound **1** in CD_2Cl_2

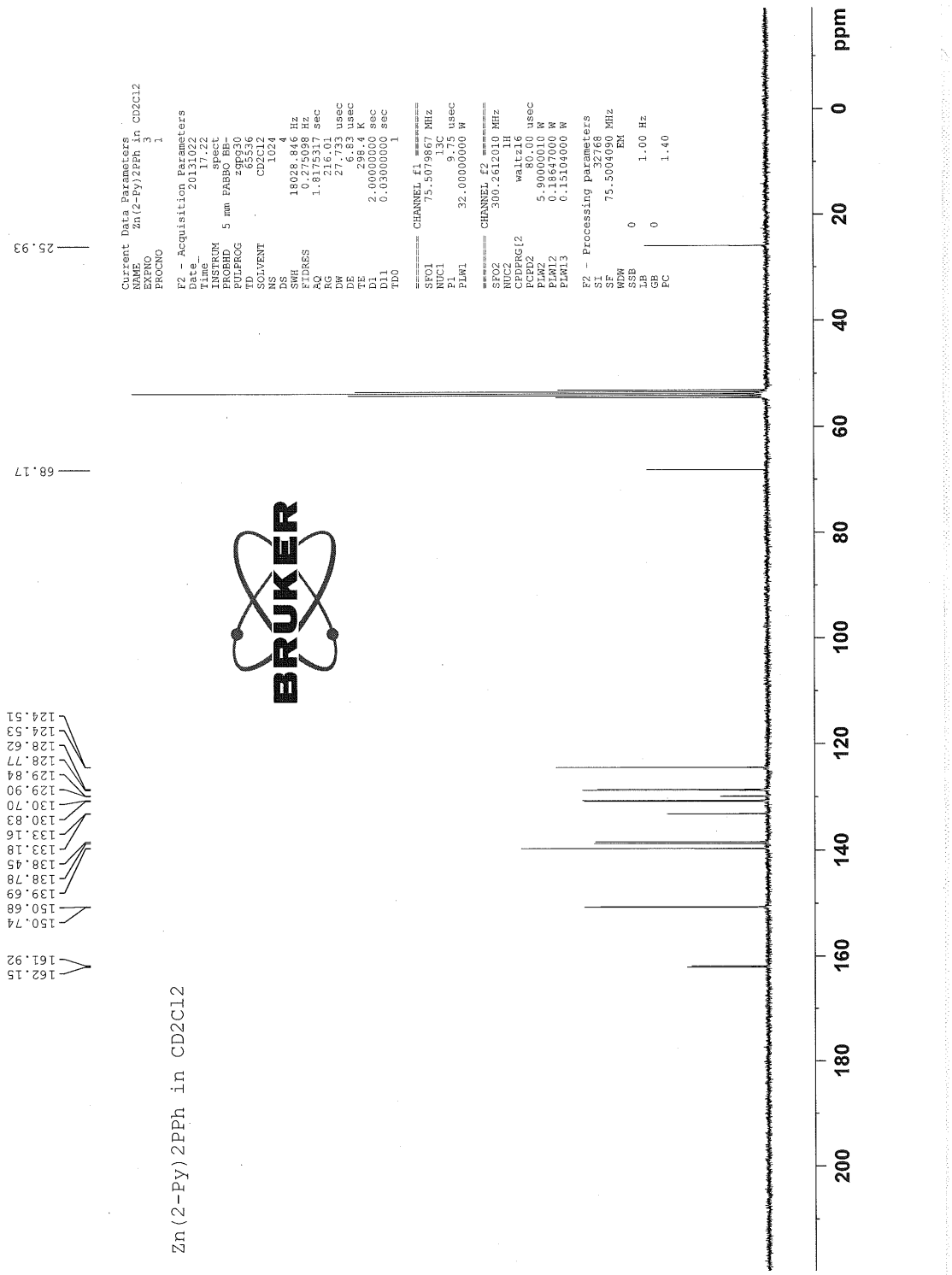

Figure S2. $^{13}C\{^{1}H\}$ NMR of compound **1** in CD_2Cl_2.

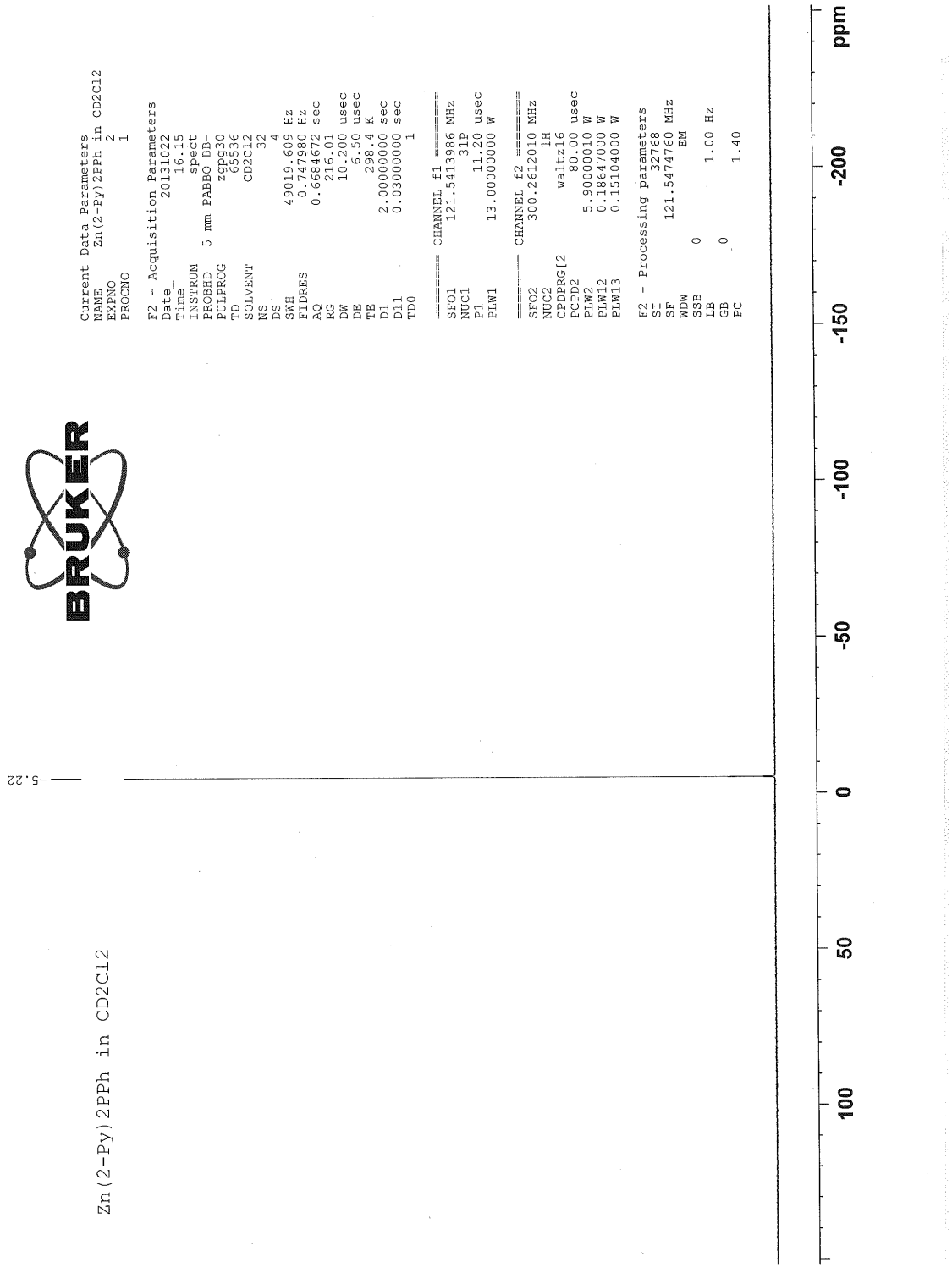

Figure S3. $^{31}P\{^{1}H\}$ NMR of compound **1** in CD_2Cl_2.

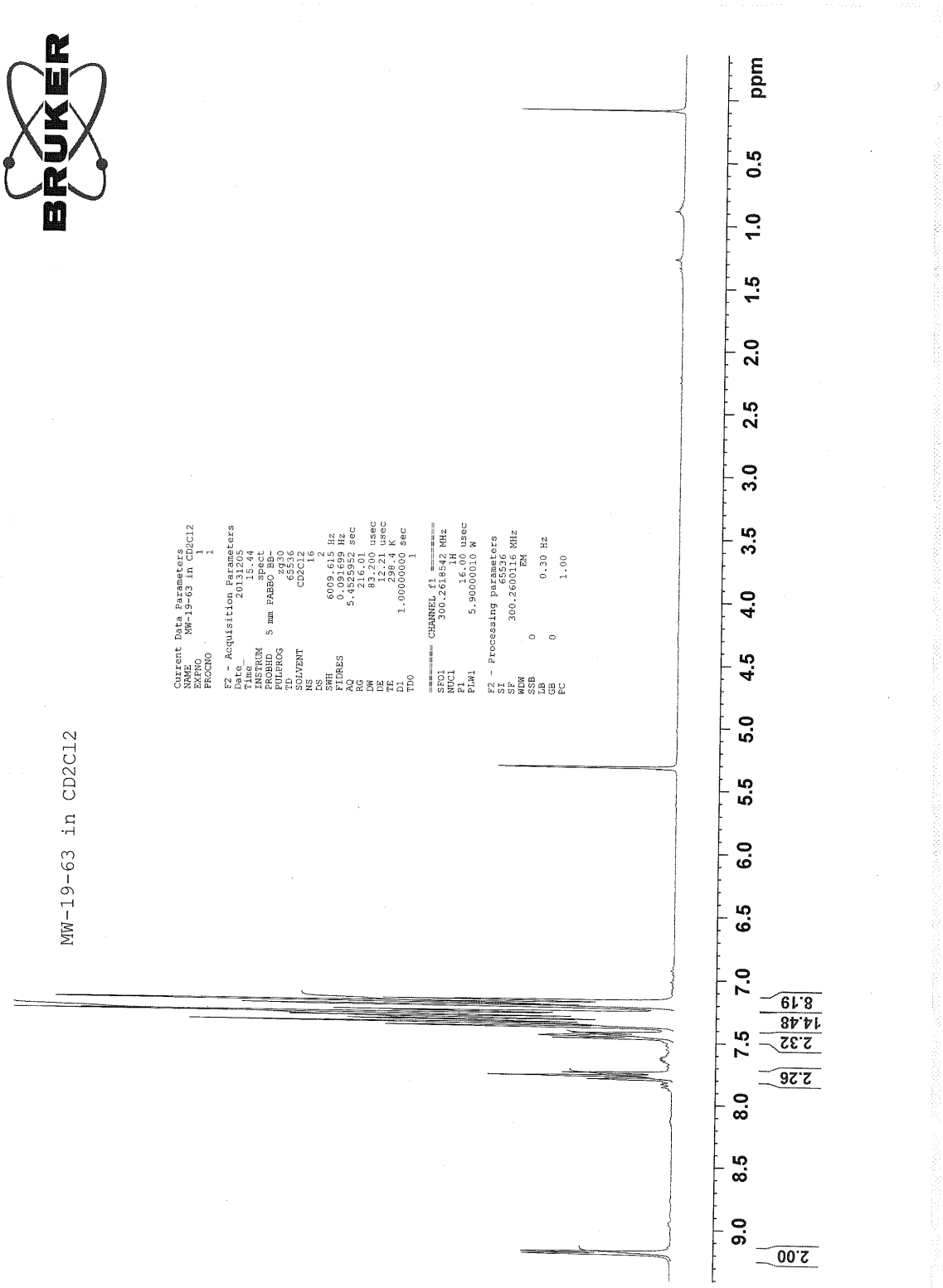

Figure S4. ^{1}H NMR of compound **2** in CD_2Cl_2. Signal at 0.09 ppm attributed to silicone grease.

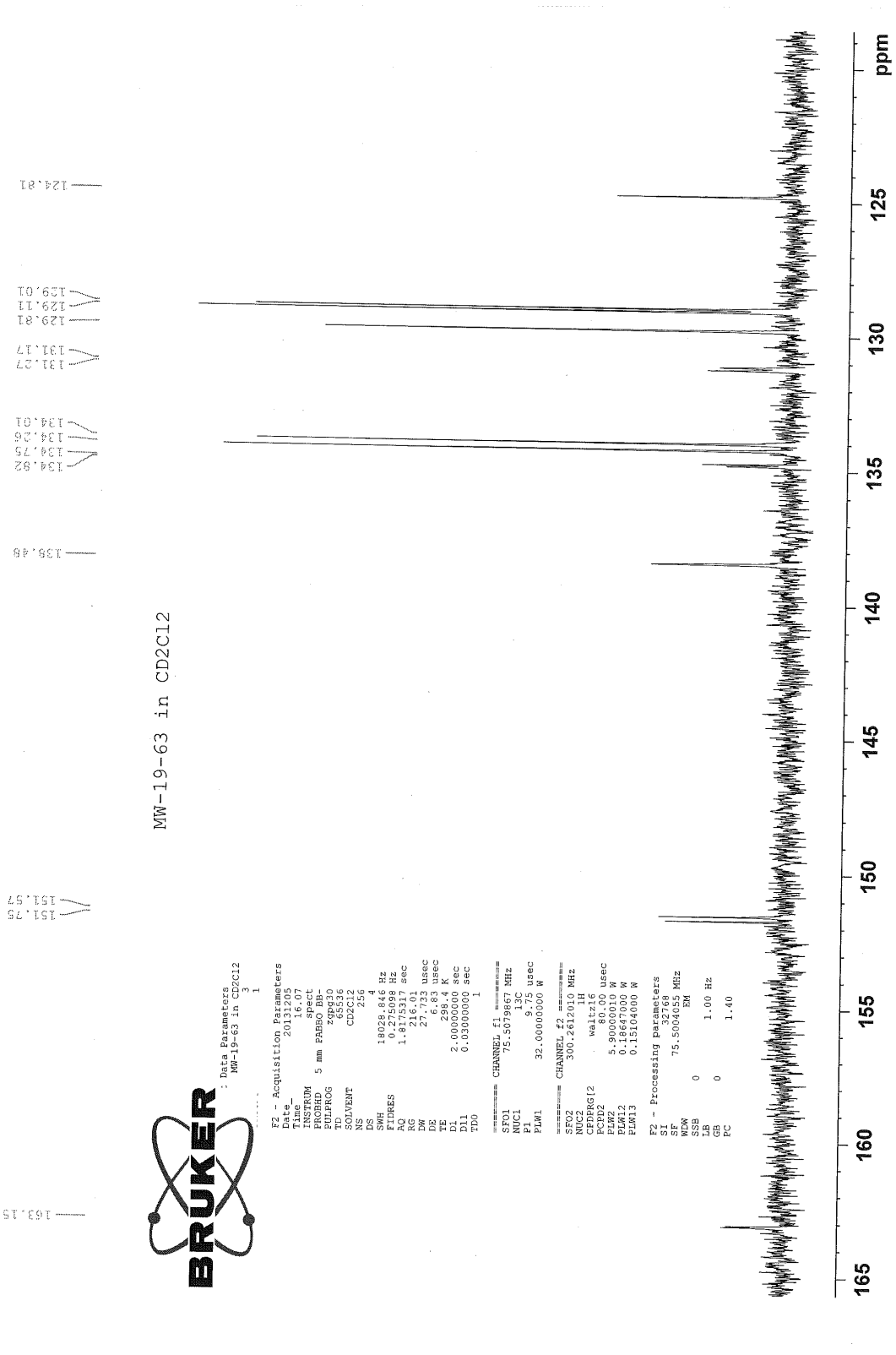

Figure S5. $^{13}C\{^{1}H\}$ NMR of compound **2** in CD_2Cl_2.

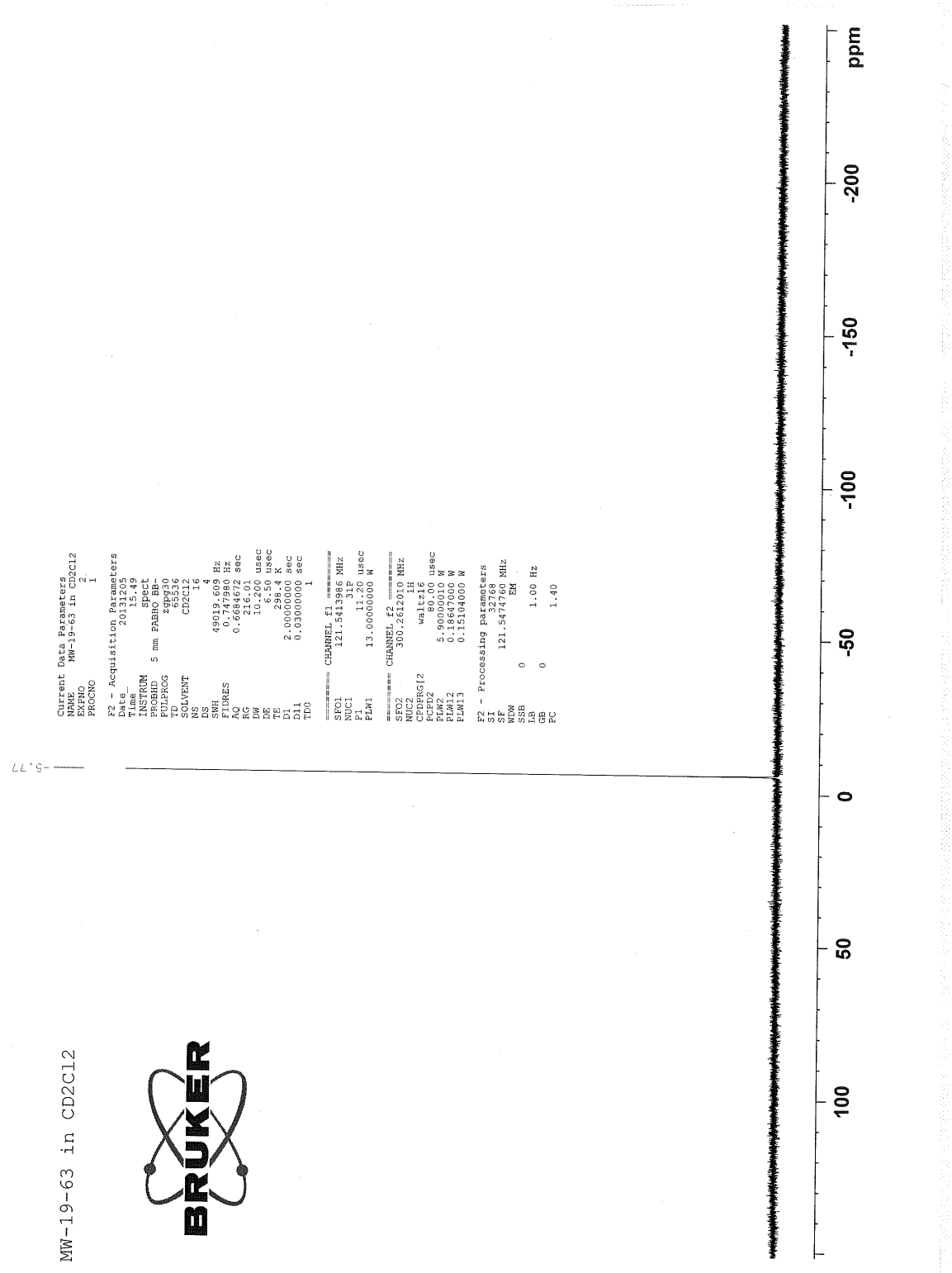

Figure S6. $^{31}P\{^{1}H\}$ NMR of compound **2** in CD_2Cl_2.

Detail of electrochemical conditions and analytical methods. A 3-electrode cell was used for all CV measurements with a 3 mm diameter glassy carbon working electrode. The auxiliary electrode was a coiled Pt wire and the reference electrode was a silver wire in 10 mM $AgNO_3$ in electrolyte solution contained in a fritted half-cell obtained from CH Instruments. Reported potentials are referenced to the ferrocene/ferrocenium redox couple that was measured at the conclusion of each experiment. Electrolyte solution was 0.10 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) in 99.9% anhydrous inhibitor-free THF using electrochemical grade Bu_4NPF_6 from Sigma-Aldrich without further purification. The cell was purged of O_2 prior to each experiment with the gas noted in the figures (CO_2 or Ar). The CO_2 (g) used in experiments was of research purity at 99.999% purchased from Matheson TriGas and passed through anhydrous $CaSO_4$ Drierite prior to use in all experiments.

The CPE experiments were conducted under pseudo-airtight conditions saturated with CO_2 (g) with vigorous stirring using a reticulated vitreous carbon working electrode, a coiled Pt wire contained in a fritted chamber (obtained from BAS Inc.), and the same reference electrode as used for CV measurements. An airtight syringe was used to measure the composition of the CPE headspace *via* mass spectrometry before applying a potential and after holding a potential of -1.80 V for 4 hours that lead to a plateau of residual current, indicating 99% completion of electrolysis. Faradaic efficiency was not calculated nor investigated for this publication since the CPE cell is not quantitatively air-tight. GC/MS measurements were obtained using a Hewlett Packard 5890 Series II Plus Gas Chromatograph using He carrier gas on a Agilent J&W 20 m x 0.180 mm x 1.00 μm DB-624 column observing the mass spectra of the eluent at 1.76 minutes with a Hewlett Packard 5972 Series Mass Selective Detector.

Infrared spectra were recorded on a Nicolet 6700 FT-IR with samples between KBr salt plates. NMR spectra were recorded on a Bruker 300 MHz spectrometer. Crystal structures were determined using a full-matrix least-squares on F^2 refinement method on Apex II software, with R-values for **1** and **2** of 6.33% and 6.40%, respectively.

Calculation of turnover frequency. The following equation was employed to report the TOF of 96 s^{-1} for **2**, noting that the peak potential for catalytic current (i_c) is not equivalent to the peak potential for the catalyst (i_p), and therefore this TOF value should be interpreted as a gross approximation. Here, n is the number of electrons involved in each catalytic turnover, R is the universal gas constant, T is temperature, F is the Faraday constant, v is the scan rate, and k_{obs} is the observed rate constant reported as the turnover frequency, TOF.

$$\frac{i_c}{i_p} = \frac{n}{0.4463}\sqrt{\frac{RTk_{obs}}{Fv}}$$

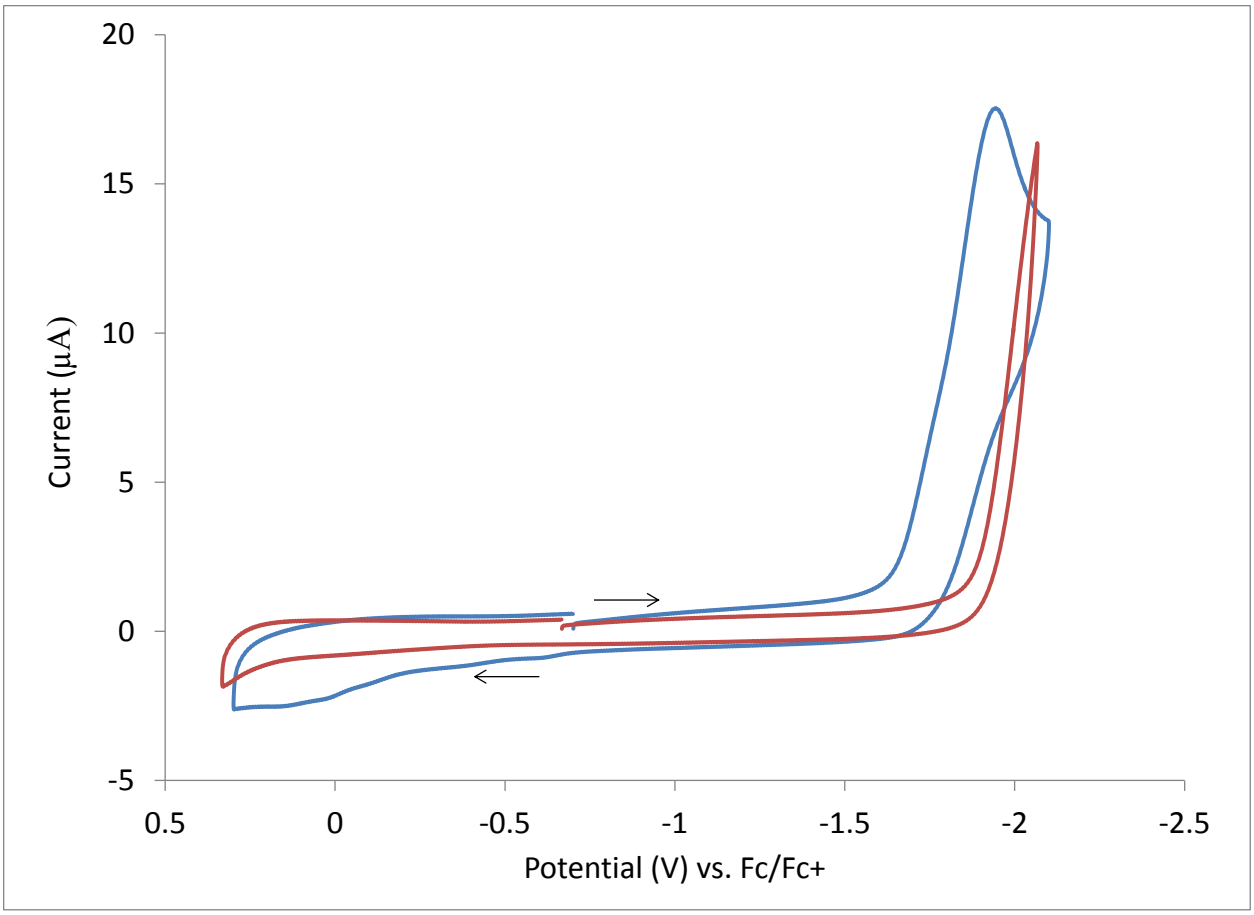

Figure S7. CV of **1** (blue) and **2** (red) at concentrations of 1.0 mM at 0.5 Vs^{-1} in THF under Ar(g) at GC WE.

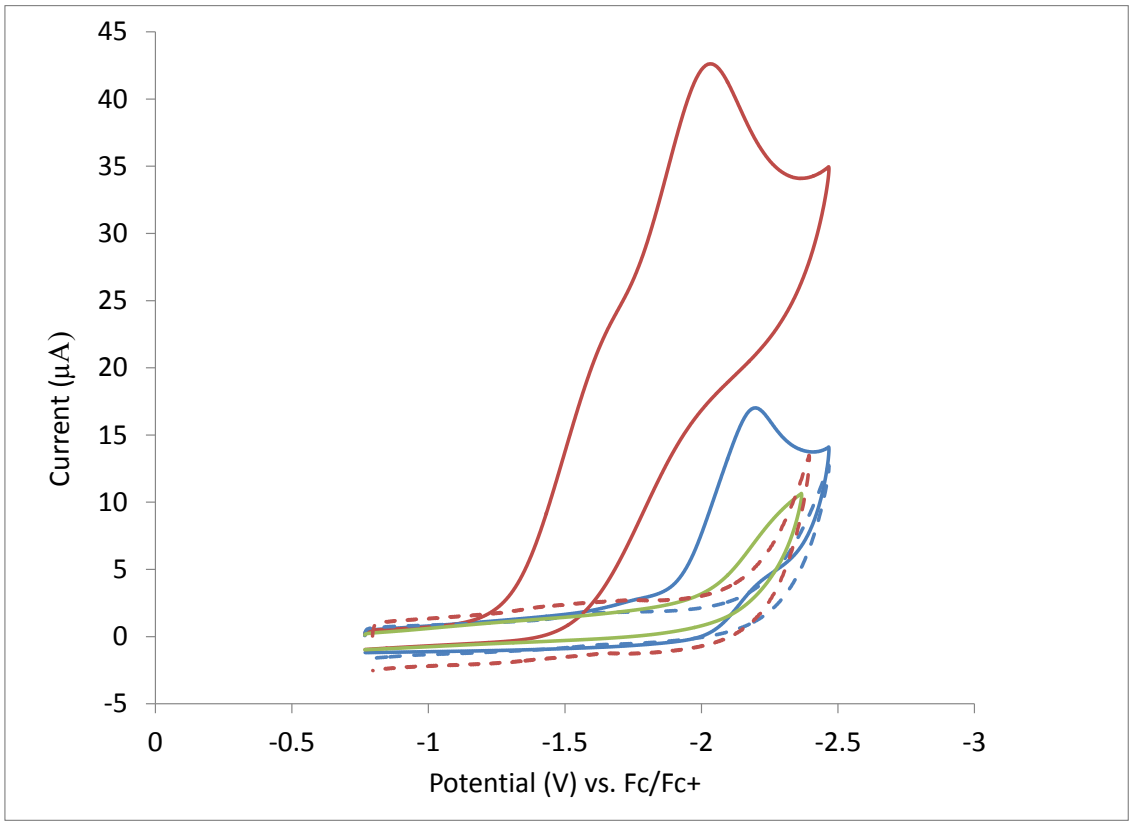

Figure S8. Control experiments for cyclic voltammograms shown in Figure 5 (main paper) (shown as solid red and solid blue lines); 1.98 mM $pyPPh_2$ purged with CO_2 (g) atmosphere (solid green line); electrolyte solution without analyte purged with Ar (g) atmosphere (dashed blue line); electrolyte solution without analyte purged with CO_2 (g) atmosphere (dashed red line). Scan rate is 0.5 Vs^{-1}.

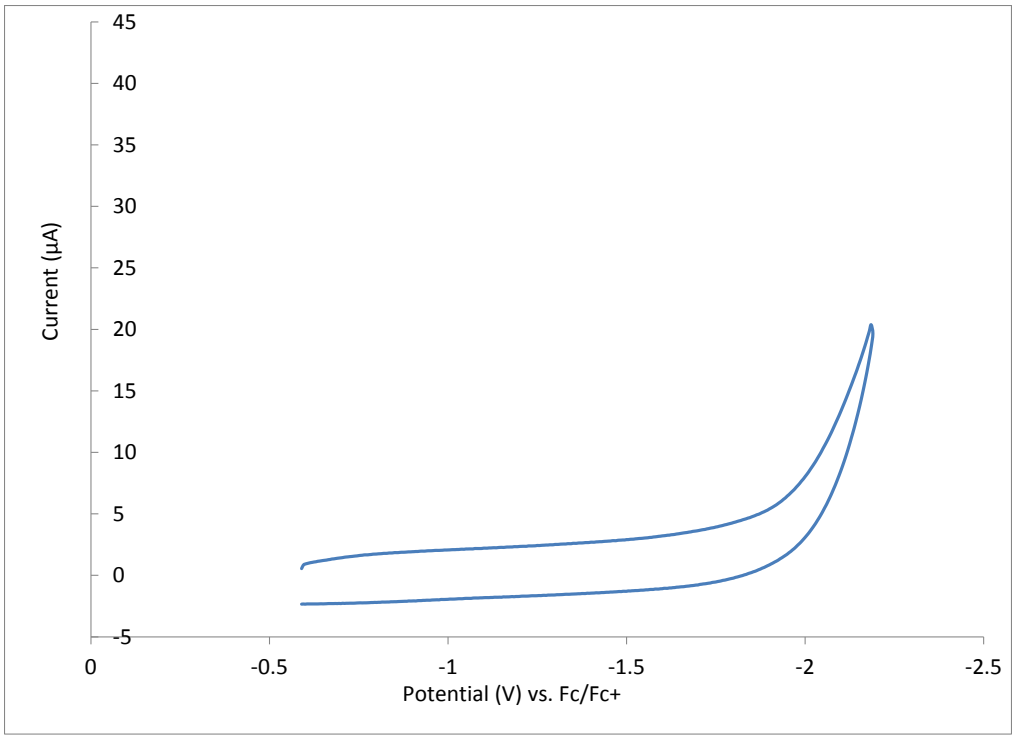

Figure S9. Cyclic voltammogram of 1.99 mM $PhPpy_2$ purged with CO_2 (g) atmosphere using a 0.5 Vs^{-1} scan rate, illustrating no electroactivity in the observed potential range until the solvent (THF) front is reached. Scanning from -0.5 to -2.1 to -0.5 V.

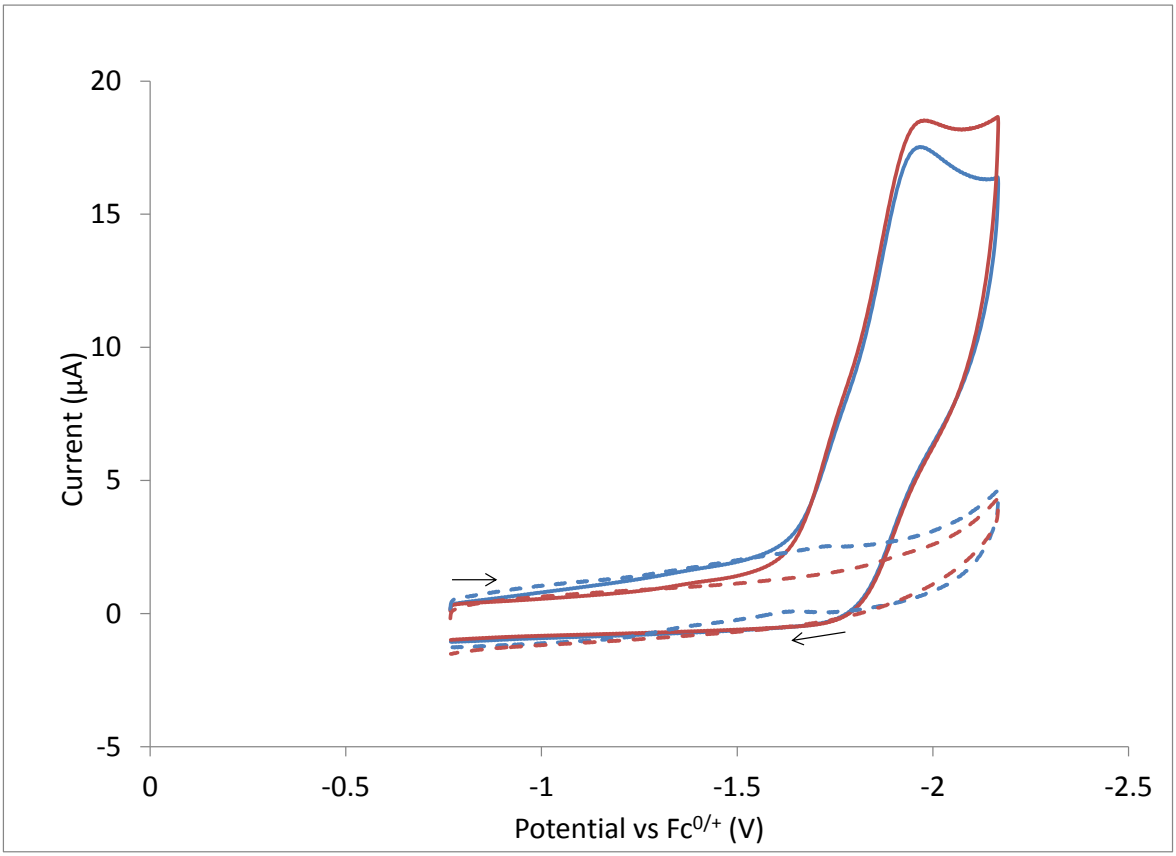

Figure S10. CV of 1.13 mM **1** at 0.5 Vs^{-1} under an Ar (g) atmosphere (solid blue line) and under a CO_2 (g) atmosphere (solid red line). Background scans at 0.5 Vs^{-1} of solely electrolyte under Ar (g) (dashed blue line) and under CO_2 (g) (dashed red line) are also shown.

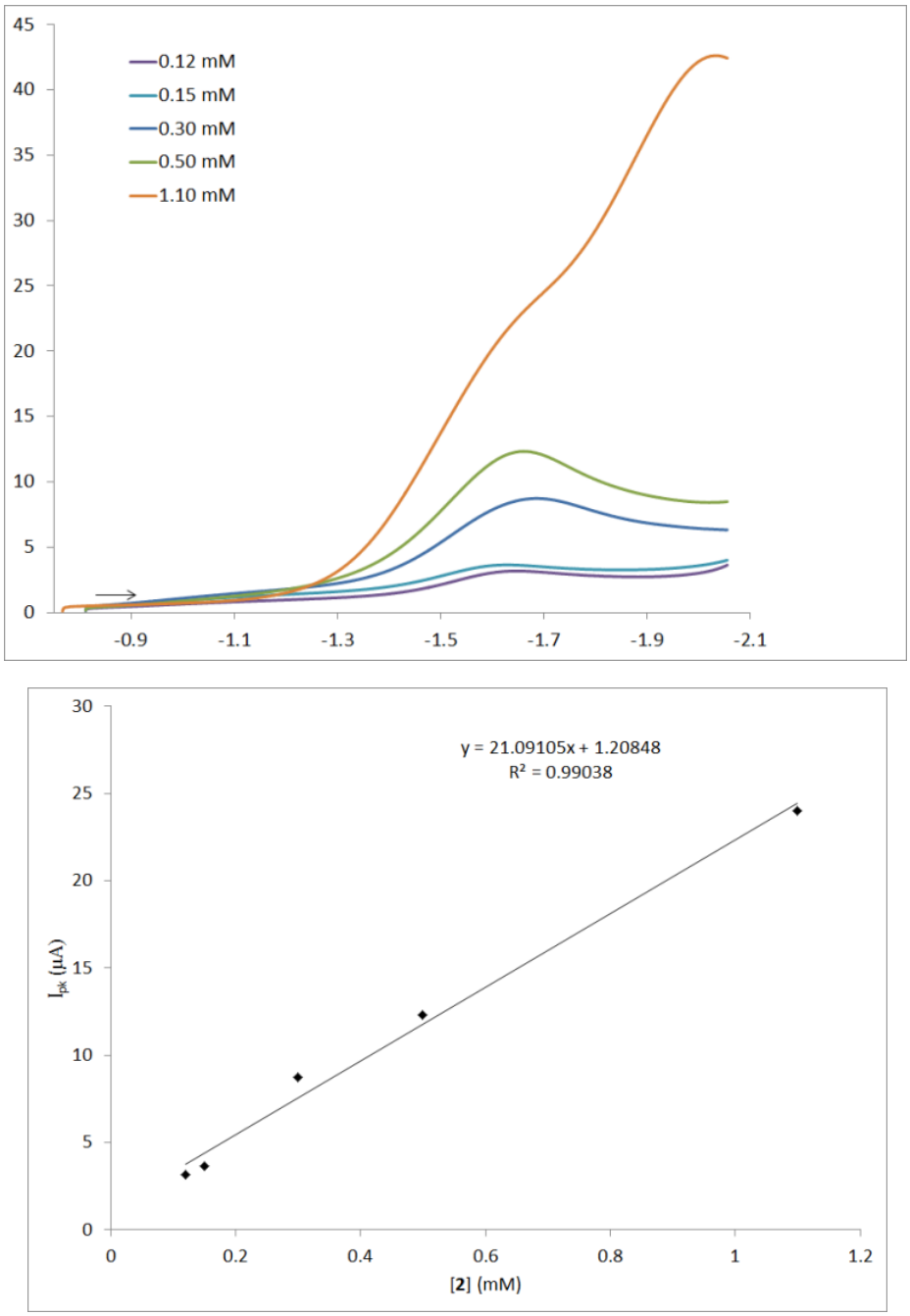

Figure S11. LSV of **2** at the concentrations indicated at 0.5 Vs^{-1} under a CO_2 (g) atmosphere (top); plot of current at the catalytic peak potential of -1.66 V, I_{pk}, versus the concentration of **2** (bottom).

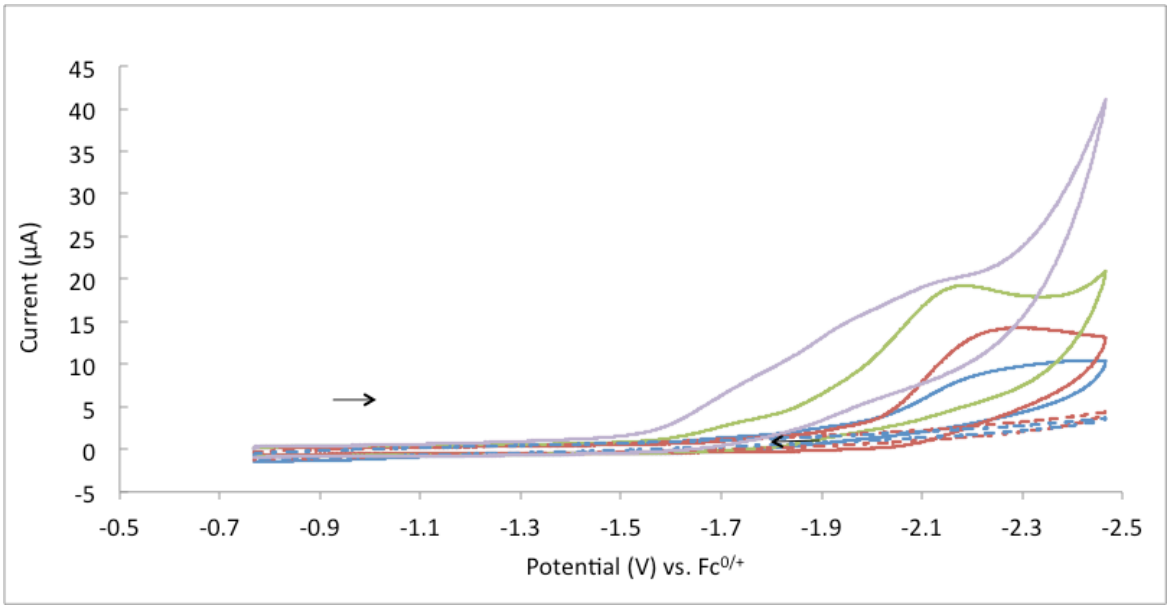

Figure S12. CV of *ca*. 1.0 mM **2** at 0.5 Vs^{-1} under an Ar (g) atmosphere (solid red line); under a CO_2 (g) atmosphere (solid blue line); under CO_2 (g) atmosphere with 1 mM acetic acid (solid green line); under CO_2 (g) atmosphere with 5 mM acetic acid (solid purple line). Scans at 0.5 Vs^{-1} of solely electrolyte with 1 mM acetic acid under Ar (g) (dashed red line) and under CO_2 (g) (dashed blue line) are also shown.

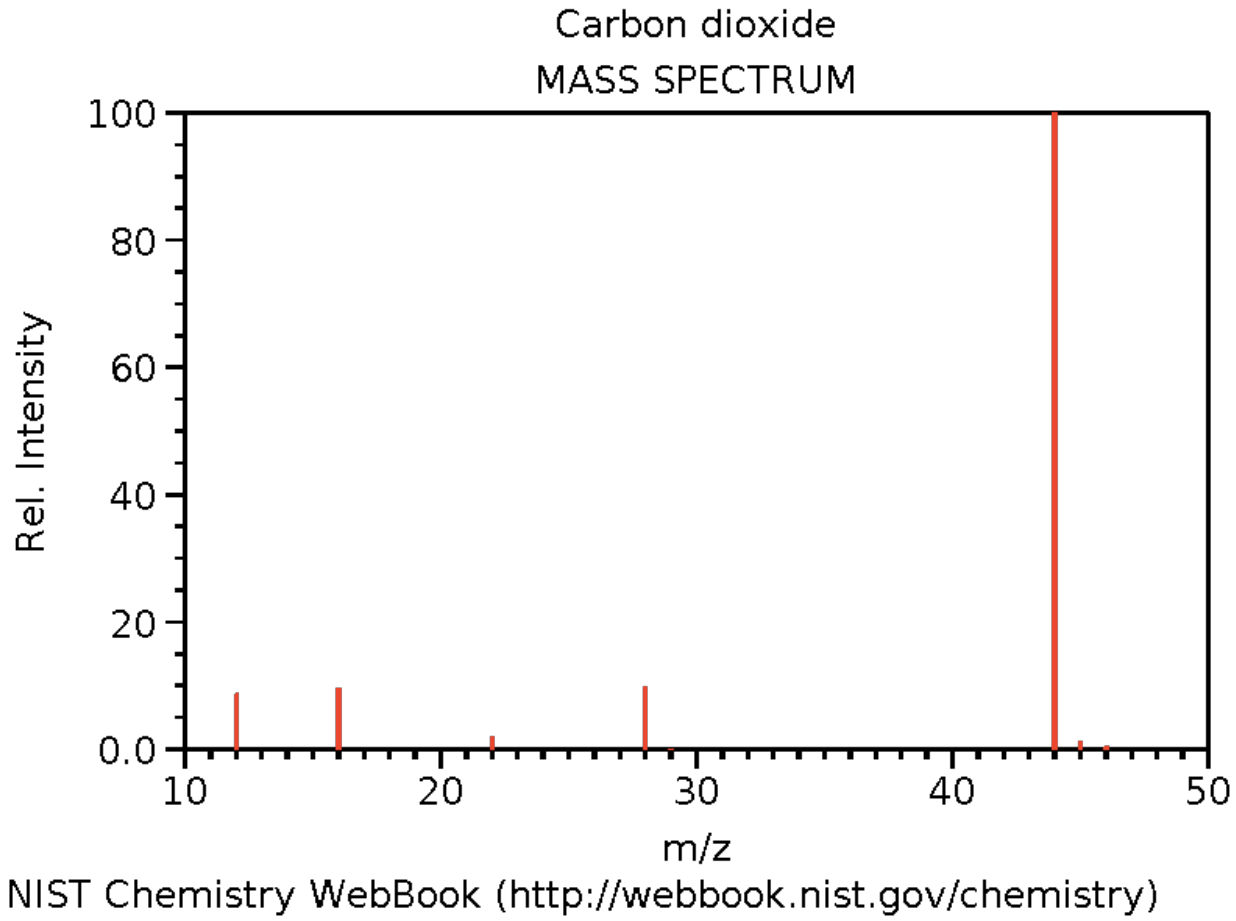

Figure S13. EI mass spectrum of CO_2 reported in the NIST database.

http://webbook.nist.gov/cgi/cbook.cgi?ID=C124389&Mask=200#Mass-Spec

Crystallographic details for compound 1.

Table 1. Crystal data and structure refinement for rkbb10_0m. (CCDC 1029655)

Identification code	rkbb10_0m	
Empirical formula	C18 H17 Cl2 N2 O0.50 P Zn	
Formula weight	436.58	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 16.0669(5) Å	α= 90°.
	b = 12.2540(4) Å	β= 98.966(2)°.
	c = 19.5763(7) Å	γ = 90°.
Volume	3807.2(2) $Å^3$	
Z	8	
Density (calculated)	1.523 Mg/m^3	
Absorption coefficient	1.660 mm^{-1}	
F(000)	1776	
Crystal size	0.64 x 0.14 x 0.13 mm^3	
Theta range for data collection	1.28 to 30.60°.	
Index ranges	-22<=h<=22, -17<=k<=17, -27<=l<=27	
Reflections collected	58745	
Independent reflections	11629 [R(int) = 0.0820]	
Completeness to theta = 30.60°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8119 and 0.4150	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11629 / 0 / 442	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0633, wR2 = 0.1562	
R indices (all data)	R1 = 0.1173, wR2 = 0.1779	
Largest diff. peak and hole	1.089 and -0.787 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for rkbb10_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	8653(1)	2342(1)	6701(1)	29(1)
Zn(2)	4447(1)	2169(1)	1133(1)	26(1)
P(1)	10282(1)	1750(1)	7889(1)	26(1)
P(2)	5410(1)	2630(1)	2711(1)	23(1)
Cl(1)	9516(1)	2429(1)	5929(1)	39(1)
Cl(2)	7295(1)	2687(1)	6395(1)	41(1)
Cl(3)	4381(1)	1929(1)	4(1)	36(1)
Cl(4)	3265(1)	2067(1)	1589(1)	39(1)
O(1)	1763(9)	4254(12)	10141(7)	273(9)
N(1)	9041(3)	3275(3)	7572(2)	26(1)
N(2)	8786(2)	900(3)	7249(2)	26(1)
N(3)	5067(2)	3591(3)	1434(2)	24(1)
N(4)	5345(2)	1160(3)	1648(2)	24(1)
C(1)	10836(3)	1409(4)	8746(2)	28(1)
C(2)	10465(3)	1366(4)	9346(3)	34(1)
C(3)	10941(4)	1104(5)	9972(3)	43(1)
C(4)	11792(4)	869(5)	10015(3)	42(1)
C(5)	12160(4)	894(5)	9426(3)	41(1)
C(6)	11694(3)	1165(4)	8792(3)	35(1)
C(7)	8628(3)	4213(4)	7654(3)	35(1)
C(8)	8867(4)	4924(4)	8186(3)	40(1)
C(9)	9567(4)	4671(5)	8659(3)	42(1)
C(10)	9988(3)	3698(4)	8603(3)	36(1)
C(11)	9706(3)	2996(4)	8053(2)	28(1)
C(12)	8173(3)	142(4)	7109(3)	32(1)
C(13)	8188(3)	-825(4)	7468(3)	36(1)
C(14)	8849(3)	-1018(4)	7992(3)	33(1)
C(15)	9478(3)	-244(4)	8149(2)	28(1)
C(16)	9428(3)	724(4)	7772(2)	24(1)
C(17)	6315(3)	2896(4)	3375(2)	24(1)
C(18)	6161(3)	3063(4)	4044(2)	33(1)

C(19)	6805(4)	3264(5)	4579(3)	44(1)
C(20)	7627(4)	3282(5)	4458(3)	42(1)
C(21)	7800(3)	3103(4)	3792(3)	38(1)
C(22)	7143(3)	2918(4)	3246(2)	28(1)
C(23)	5059(4)	4413(4)	978(3)	35(1)
C(24)	5446(4)	5391(4)	1139(3)	37(1)
C(25)	5887(3)	5536(4)	1802(3)	32(1)
C(26)	5922(3)	4691(4)	2270(3)	27(1)
C(27)	5512(3)	3710(4)	2076(2)	23(1)
C(28)	5537(3)	220(4)	1350(2)	28(1)
C(29)	6061(3)	-561(4)	1688(3)	32(1)
C(30)	6418(3)	-367(4)	2367(3)	32(1)
C(31)	6266(3)	624(4)	2668(3)	28(1)
C(32)	5730(3)	1379(4)	2299(2)	23(1)
C(33)	2251(11)	5244(13)	10371(9)	240(13)
C(34)	2856(7)	5446(8)	10005(6)	101(3)
C(35)	2945(7)	4566(8)	9586(7)	124(5)
C(36)	2397(8)	3790(8)	9704(6)	110(4)

Table 3. Bond lengths [Å] and angles [°] for rkbb10_0m.

Zn(1)-N(2)	2.061(4)
Zn(1)-N(1)	2.067(4)
Zn(1)-Cl(1)	2.2069(14)
Zn(1)-Cl(2)	2.2107(14)
Zn(2)-N(4)	2.043(4)
Zn(2)-N(3)	2.047(4)
Zn(2)-Cl(3)	2.2159(13)
Zn(2)-Cl(4)	2.2245(14)
P(1)-C(1)	1.821(5)
P(1)-C(11)	1.839(5)
P(1)-C(16)	1.848(5)
P(2)-C(17)	1.822(5)
P(2)-C(27)	1.841(5)
P(2)-C(32)	1.843(5)
O(1)-C(33)	1.476(14)
O(1)-C(36)	1.538(15)
N(1)-C(7)	1.349(6)
N(1)-C(11)	1.354(6)
N(2)-C(12)	1.350(6)
N(2)-C(16)	1.353(6)
N(3)-C(23)	1.344(6)
N(3)-C(27)	1.354(5)
N(4)-C(28)	1.349(6)
N(4)-C(32)	1.353(6)
C(1)-C(2)	1.397(7)
C(1)-C(6)	1.400(7)
C(2)-C(3)	1.378(7)
C(3)-C(4)	1.387(8)
C(4)-C(5)	1.377(9)
C(5)-C(6)	1.386(7)
C(7)-C(8)	1.366(8)
C(8)-C(9)	1.376(8)
C(9)-C(10)	1.383(8)
C(10)-C(11)	1.397(7)

C(12)-C(13)	1.377(7)
C(13)-C(14)	1.376(7)
C(14)-C(15)	1.385(7)
C(15)-C(16)	1.392(6)
C(17)-C(18)	1.385(6)
C(17)-C(22)	1.392(7)
C(18)-C(19)	1.375(7)
C(19)-C(20)	1.378(9)
C(20)-C(21)	1.391(8)
C(21)-C(22)	1.400(7)
C(23)-C(24)	1.365(7)
C(24)-C(25)	1.389(7)
C(25)-C(26)	1.378(7)
C(26)-C(27)	1.394(6)
C(28)-C(29)	1.374(7)
C(29)-C(30)	1.385(7)
C(30)-C(31)	1.388(7)
C(31)-C(32)	1.387(6)
C(33)-C(34)	1.317(14)
C(34)-C(35)	1.377(13)
C(35)-C(36)	1.341(13)

N(2)-Zn(1)-N(1)	92.92(15)
N(2)-Zn(1)-Cl(1)	111.89(12)
N(1)-Zn(1)-Cl(1)	113.38(12)
N(2)-Zn(1)-Cl(2)	108.86(12)
N(1)-Zn(1)-Cl(2)	106.01(12)
Cl(1)-Zn(1)-Cl(2)	120.25(5)
N(4)-Zn(2)-N(3)	95.63(15)
N(4)-Zn(2)-Cl(3)	109.45(11)
N(3)-Zn(2)-Cl(3)	110.19(11)
N(4)-Zn(2)-Cl(4)	110.43(12)
N(3)-Zn(2)-Cl(4)	109.87(12)
Cl(3)-Zn(2)-Cl(4)	118.82(5)
C(1)-P(1)-C(11)	102.5(2)
C(1)-P(1)-C(16)	101.8(2)

C(11)-P(1)-C(16)	101.7(2)
C(17)-P(2)-C(27)	102.0(2)
C(17)-P(2)-C(32)	102.4(2)
C(27)-P(2)-C(32)	104.0(2)
C(33)-O(1)-C(36)	96.2(9)
C(7)-N(1)-C(11)	118.8(4)
C(7)-N(1)-Zn(1)	118.6(3)
C(11)-N(1)-Zn(1)	122.6(3)
C(12)-N(2)-C(16)	119.4(4)
C(12)-N(2)-Zn(1)	118.0(3)
C(16)-N(2)-Zn(1)	122.4(3)
C(23)-N(3)-C(27)	119.0(4)
C(23)-N(3)-Zn(2)	119.5(3)
C(27)-N(3)-Zn(2)	121.5(3)
C(28)-N(4)-C(32)	118.4(4)
C(28)-N(4)-Zn(2)	119.6(3)
C(32)-N(4)-Zn(2)	122.0(3)
C(2)-C(1)-C(6)	118.9(5)
C(2)-C(1)-P(1)	124.8(4)
C(6)-C(1)-P(1)	116.3(4)
C(3)-C(2)-C(1)	120.4(5)
C(2)-C(3)-C(4)	120.5(6)
C(5)-C(4)-C(3)	119.5(5)
C(4)-C(5)-C(6)	120.9(5)
C(5)-C(6)-C(1)	119.8(5)
N(1)-C(7)-C(8)	123.4(5)
C(7)-C(8)-C(9)	118.1(5)
C(8)-C(9)-C(10)	120.0(5)
C(9)-C(10)-C(11)	119.2(5)
N(1)-C(11)-C(10)	120.4(4)
N(1)-C(11)-P(1)	116.9(3)
C(10)-C(11)-P(1)	122.3(4)
N(2)-C(12)-C(13)	122.2(5)
C(14)-C(13)-C(12)	118.6(5)
C(13)-C(14)-C(15)	119.9(5)
C(14)-C(15)-C(16)	119.1(4)

N(2)-C(16)-C(15)	120.7(4)
N(2)-C(16)-P(1)	116.7(3)
C(15)-C(16)-P(1)	122.2(4)
C(18)-C(17)-C(22)	119.0(4)
C(18)-C(17)-P(2)	117.4(4)
C(22)-C(17)-P(2)	123.6(3)
C(19)-C(18)-C(17)	121.5(5)
C(18)-C(19)-C(20)	119.9(5)
C(19)-C(20)-C(21)	119.7(5)
C(20)-C(21)-C(22)	120.3(5)
C(17)-C(22)-C(21)	119.5(5)
N(3)-C(23)-C(24)	123.2(5)
C(23)-C(24)-C(25)	118.4(5)
C(26)-C(25)-C(24)	119.1(5)
C(25)-C(26)-C(27)	119.9(4)
N(3)-C(27)-C(26)	120.3(4)
N(3)-C(27)-P(2)	117.4(3)
C(26)-C(27)-P(2)	121.6(3)
N(4)-C(28)-C(29)	123.4(4)
C(28)-C(29)-C(30)	118.3(5)
C(29)-C(30)-C(31)	118.9(5)
C(32)-C(31)-C(30)	119.9(4)
N(4)-C(32)-C(31)	120.9(4)
N(4)-C(32)-P(2)	117.3(3)
C(31)-C(32)-P(2)	121.3(3)
C(34)-C(33)-O(1)	113.0(10)
C(33)-C(34)-C(35)	109.3(10)
C(36)-C(35)-C(34)	108.7(10)
C(35)-C(36)-O(1)	110.1(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for rkbb10_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	28(1)	35(1)	24(1)	6(1)	4(1)	3(1)
Zn(2)	25(1)	31(1)	20(1)	-2(1)	1(1)	-3(1)
P(1)	23(1)	30(1)	26(1)	1(1)	5(1)	1(1)
P(2)	23(1)	28(1)	20(1)	-1(1)	4(1)	-1(1)
Cl(1)	41(1)	48(1)	31(1)	4(1)	14(1)	-2(1)
Cl(2)	32(1)	66(1)	25(1)	6(1)	2(1)	12(1)
Cl(3)	35(1)	51(1)	22(1)	-6(1)	4(1)	-3(1)
Cl(4)	30(1)	55(1)	32(1)	-4(1)	9(1)	-7(1)
O(1)	287(15)	321(17)	254(14)	-195(13)	176(13)	-209(14)
N(1)	29(2)	26(2)	23(2)	4(2)	7(2)	6(2)
N(2)	23(2)	32(2)	23(2)	1(2)	4(2)	3(2)
N(3)	26(2)	28(2)	20(2)	-1(2)	4(2)	-3(2)
N(4)	26(2)	27(2)	20(2)	-1(2)	2(2)	-4(2)
C(1)	22(2)	32(2)	30(2)	-4(2)	-1(2)	-1(2)
C(2)	29(3)	41(3)	30(3)	-3(2)	3(2)	7(2)
C(3)	53(4)	45(3)	30(3)	2(2)	4(3)	3(3)
C(4)	43(3)	39(3)	40(3)	-5(2)	-14(3)	7(2)
C(5)	29(3)	47(3)	45(3)	-1(3)	-6(2)	5(2)
C(6)	31(3)	39(3)	35(3)	-5(2)	3(2)	2(2)
C(7)	38(3)	31(3)	37(3)	12(2)	12(2)	6(2)
C(8)	47(3)	31(3)	45(3)	4(2)	19(3)	4(2)
C(9)	51(4)	34(3)	42(3)	-7(2)	8(3)	-4(3)
C(10)	35(3)	37(3)	37(3)	1(2)	6(2)	0(2)
C(11)	31(2)	26(2)	28(2)	2(2)	10(2)	-1(2)
C(12)	24(2)	39(3)	30(2)	3(2)	0(2)	-5(2)
C(13)	31(3)	39(3)	37(3)	4(2)	7(2)	-4(2)
C(14)	38(3)	30(3)	33(3)	4(2)	11(2)	1(2)
C(15)	30(3)	31(2)	25(2)	0(2)	8(2)	3(2)
C(16)	21(2)	27(2)	24(2)	0(2)	5(2)	2(2)
C(17)	28(2)	26(2)	20(2)	-2(2)	2(2)	0(2)
C(18)	38(3)	42(3)	19(2)	2(2)	6(2)	5(2)

C(19)	61(4)	52(3)	17(2)	-5(2)	-1(2)	6(3)
C(20)	51(4)	42(3)	28(3)	-3(2)	-13(2)	1(3)
C(21)	30(3)	38(3)	41(3)	-4(2)	-5(2)	-1(2)
C(22)	28(2)	32(2)	23(2)	-3(2)	4(2)	-2(2)
C(23)	48(3)	36(3)	22(2)	5(2)	8(2)	0(2)
C(24)	47(3)	29(3)	37(3)	8(2)	12(2)	0(2)
C(25)	31(3)	22(2)	45(3)	-1(2)	11(2)	0(2)
C(26)	24(2)	26(2)	31(2)	-8(2)	4(2)	-1(2)
C(27)	21(2)	26(2)	22(2)	-5(2)	5(2)	0(2)
C(28)	33(3)	29(2)	23(2)	-4(2)	5(2)	-5(2)
C(29)	34(3)	26(2)	36(3)	-4(2)	8(2)	-1(2)
C(30)	31(3)	24(2)	39(3)	5(2)	3(2)	3(2)
C(31)	24(2)	29(2)	31(2)	1(2)	3(2)	-2(2)
C(32)	20(2)	27(2)	23(2)	-2(2)	6(2)	-2(2)
C(33)	300(20)	195(15)	290(20)	-181(16)	250(20)	-181(16)
C(34)	101(8)	67(6)	132(9)	-11(6)	5(7)	13(5)
C(35)	125(9)	66(6)	206(14)	-29(7)	105(10)	-12(6)
C(36)	167(12)	69(6)	92(7)	-29(6)	17(8)	-10(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rkbb10_0m.

	x	y	z	U(eq)
H(2A)	9894	1516	9322	41
H(3A)	10689	1085	10369	51
H(4A)	12111	696	10439	51
H(5A)	12729	726	9453	50
H(6A)	11951	1184	8398	42
H(7A)	8158	4385	7332	42
H(8A)	8564	5561	8228	48
H(9A)	9757	5153	9016	51
H(10A)	10454	3515	8927	44
H(12A)	7724	279	6758	38
H(13A)	7761	-1338	7360	43
H(14A)	8873	-1667	8240	40
H(15A)	9927	-368	8501	34
H(18A)	5610	3039	4133	40
H(19A)	6686	3388	5023	53
H(20A)	8064	3413	4819	51
H(21A)	8355	3107	3710	45
H(22A)	7258	2810	2800	33
H(23A)	4775	4310	531	42
H(24A)	5416	5948	813	45
H(25A)	6154	6195	1928	38
H(26A)	6219	4774	2714	32
H(28A)	5302	94	892	34
H(29A)	6172	-1204	1466	38
H(30A)	6755	-892	2618	38
H(31A)	6523	782	3116	34
H(33A)	1872	5864	10338	288
H(33B)	2497	5159	10853	288
H(34A)	3381	5578	10312	122
H(34B)	2719	6093	9725	122

H(35A)	2836	4787	9104	149
H(35B)	3516	4285	9685	149
H(36A)	2698	3182	9945	132
H(36B)	2098	3523	9267	132

Table 6. Torsion angles [°] for rkbb10_0m.

N(2)-Zn(1)-N(1)-C(7)	-138.5(4)
Cl(1)-Zn(1)-N(1)-C(7)	106.1(4)
Cl(2)-Zn(1)-N(1)-C(7)	-28.0(4)
N(2)-Zn(1)-N(1)-C(11)	43.2(4)
Cl(1)-Zn(1)-N(1)-C(11)	-72.2(4)
Cl(2)-Zn(1)-N(1)-C(11)	153.8(3)
N(1)-Zn(1)-N(2)-C(12)	136.6(4)
Cl(1)-Zn(1)-N(2)-C(12)	-106.7(4)
Cl(2)-Zn(1)-N(2)-C(12)	28.6(4)
N(1)-Zn(1)-N(2)-C(16)	-38.5(4)
Cl(1)-Zn(1)-N(2)-C(16)	78.2(4)
Cl(2)-Zn(1)-N(2)-C(16)	-146.5(3)
N(4)-Zn(2)-N(3)-C(23)	140.2(4)
Cl(3)-Zn(2)-N(3)-C(23)	27.1(4)
Cl(4)-Zn(2)-N(3)-C(23)	-105.6(4)
N(4)-Zn(2)-N(3)-C(27)	-37.4(4)
Cl(3)-Zn(2)-N(3)-C(27)	-150.5(3)
Cl(4)-Zn(2)-N(3)-C(27)	76.7(4)
N(3)-Zn(2)-N(4)-C(28)	-140.7(4)
Cl(3)-Zn(2)-N(4)-C(28)	-26.9(4)
Cl(4)-Zn(2)-N(4)-C(28)	105.7(3)
N(3)-Zn(2)-N(4)-C(32)	42.6(4)
Cl(3)-Zn(2)-N(4)-C(32)	156.3(3)
Cl(4)-Zn(2)-N(4)-C(32)	-71.0(4)
C(11)-P(1)-C(1)-C(2)	48.4(5)
C(16)-P(1)-C(1)-C(2)	-56.6(5)
C(11)-P(1)-C(1)-C(6)	-132.2(4)
C(16)-P(1)-C(1)-C(6)	122.8(4)
C(6)-C(1)-C(2)-C(3)	0.9(8)
P(1)-C(1)-C(2)-C(3)	-179.7(4)
C(1)-C(2)-C(3)-C(4)	-0.6(9)
C(2)-C(3)-C(4)-C(5)	-0.3(9)
C(3)-C(4)-C(5)-C(6)	0.9(9)
C(4)-C(5)-C(6)-C(1)	-0.5(9)

C(2)-C(1)-C(6)-C(5)	-0.4(8)
P(1)-C(1)-C(6)-C(5)	-179.8(4)
C(11)-N(1)-C(7)-C(8)	2.7(8)
Zn(1)-N(1)-C(7)-C(8)	-175.6(4)
N(1)-C(7)-C(8)-C(9)	0.4(8)
C(7)-C(8)-C(9)-C(10)	-2.6(9)
C(8)-C(9)-C(10)-C(11)	1.6(9)
C(7)-N(1)-C(11)-C(10)	-3.7(7)
Zn(1)-N(1)-C(11)-C(10)	174.5(4)
C(7)-N(1)-C(11)-P(1)	-176.6(4)
Zn(1)-N(1)-C(11)-P(1)	1.7(5)
C(9)-C(10)-C(11)-N(1)	1.6(8)
C(9)-C(10)-C(11)-P(1)	174.1(4)
C(1)-P(1)-C(11)-N(1)	-160.5(4)
C(16)-P(1)-C(11)-N(1)	-55.4(4)
C(1)-P(1)-C(11)-C(10)	26.8(5)
C(16)-P(1)-C(11)-C(10)	131.9(4)
C(16)-N(2)-C(12)-C(13)	-1.9(8)
Zn(1)-N(2)-C(12)-C(13)	-177.2(4)
N(2)-C(12)-C(13)-C(14)	0.6(8)
C(12)-C(13)-C(14)-C(15)	0.3(8)
C(13)-C(14)-C(15)-C(16)	0.1(8)
C(12)-N(2)-C(16)-C(15)	2.3(7)
Zn(1)-N(2)-C(16)-C(15)	177.4(3)
C(12)-N(2)-C(16)-P(1)	175.6(4)
Zn(1)-N(2)-C(16)-P(1)	-9.3(5)
C(14)-C(15)-C(16)-N(2)	-1.4(7)
C(14)-C(15)-C(16)-P(1)	-174.4(4)
C(1)-P(1)-C(16)-N(2)	165.7(4)
C(11)-P(1)-C(16)-N(2)	60.1(4)
C(1)-P(1)-C(16)-C(15)	-21.0(4)
C(11)-P(1)-C(16)-C(15)	-126.7(4)
C(27)-P(2)-C(17)-C(18)	123.9(4)
C(32)-P(2)-C(17)-C(18)	-128.6(4)
C(27)-P(2)-C(17)-C(22)	-57.4(4)
C(32)-P(2)-C(17)-C(22)	50.1(4)

C(22)-C(17)-C(18)-C(19)	0.9(8)
P(2)-C(17)-C(18)-C(19)	179.7(4)
C(17)-C(18)-C(19)-C(20)	-1.2(9)
C(18)-C(19)-C(20)-C(21)	0.4(9)
C(19)-C(20)-C(21)-C(22)	0.7(9)
C(18)-C(17)-C(22)-C(21)	0.2(7)
P(2)-C(17)-C(22)-C(21)	-178.5(4)
C(20)-C(21)-C(22)-C(17)	-1.0(8)
C(27)-N(3)-C(23)-C(24)	-3.2(8)
Zn(2)-N(3)-C(23)-C(24)	179.1(4)
N(3)-C(23)-C(24)-C(25)	1.5(9)
C(23)-C(24)-C(25)-C(26)	0.4(8)
C(24)-C(25)-C(26)-C(27)	-0.6(7)
C(23)-N(3)-C(27)-C(26)	2.9(7)
Zn(2)-N(3)-C(27)-C(26)	-179.4(3)
C(23)-N(3)-C(27)-P(2)	173.4(4)
Zn(2)-N(3)-C(27)-P(2)	-9.0(5)
C(25)-C(26)-C(27)-N(3)	-1.1(7)
C(25)-C(26)-C(27)-P(2)	-171.2(4)
C(17)-P(2)-C(27)-N(3)	163.6(4)
C(32)-P(2)-C(27)-N(3)	57.3(4)
C(17)-P(2)-C(27)-C(26)	-26.1(4)
C(32)-P(2)-C(27)-C(26)	-132.4(4)
C(32)-N(4)-C(28)-C(29)	4.4(7)
Zn(2)-N(4)-C(28)-C(29)	-172.4(4)
N(4)-C(28)-C(29)-C(30)	-0.8(8)
C(28)-C(29)-C(30)-C(31)	-3.0(8)
C(29)-C(30)-C(31)-C(32)	3.1(8)
C(28)-N(4)-C(32)-C(31)	-4.2(7)
Zn(2)-N(4)-C(32)-C(31)	172.5(3)
C(28)-N(4)-C(32)-P(2)	-176.5(3)
Zn(2)-N(4)-C(32)-P(2)	0.2(5)
C(30)-C(31)-C(32)-N(4)	0.5(7)
C(30)-C(31)-C(32)-P(2)	172.6(4)
C(17)-P(2)-C(32)-N(4)	-158.1(4)
C(27)-P(2)-C(32)-N(4)	-52.1(4)

C(17)-P(2)-C(32)-C(31)	29.6(4)
C(27)-P(2)-C(32)-C(31)	135.6(4)
C(36)-O(1)-C(33)-C(34)	15(2)
O(1)-C(33)-C(34)-C(35)	-10(2)
C(33)-C(34)-C(35)-C(36)	-1.4(19)
C(34)-C(35)-C(36)-O(1)	11.5(17)
C(33)-O(1)-C(36)-C(35)	-15.6(18)

Crystallographic details for compound 2.

Table 1. Crystal data and structure refinement for rkbb11_0m. (CCDC 1029656)

Identification code	rkbb11_0m	
Empirical formula	C17 H14 Cl N P Zn0.50	
Formula weight	331.40	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 21.6754(6) Å	α= 90°.
	b = 11.3153(3) Å	β= 102.895(2)°.
	c = 12.8588(3) Å	γ = 90°.
Volume	3074.26(14) Å^3	
Z	8	
Density (calculated)	1.432 Mg/m^3	
Absorption coefficient	1.104 mm^{-1}	
F(000)	1360	
Crystal size	0.24 x 0.11 x 0.11 mm^3	
Theta range for data collection	2.04 to 28.33°.	
Index ranges	-28<=h<=28, -15<=k<=15, -17<=l<=16	
Reflections collected	24258	
Independent reflections	3821 [R(int) = 0.0645]	
Completeness to theta = 28.33°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8929 and 0.7752	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3821 / 0 / 186	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0359, wR2 = 0.0661	
R indices (all data)	R1 = 0.0640, wR2 = 0.0750	
Largest diff. peak and hole	0.355 and -0.343 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for rkbb11_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	10000	8269(1)	2500	22(1)
P(1)	9119(1)	5852(1)	2372(1)	23(1)
Cl(1)	10648(1)	9293(1)	1676(1)	31(1)
N(1)	9310(1)	7722(2)	1178(1)	23(1)
C(1)	8909(1)	6810(2)	1187(2)	23(1)
C(2)	8381(1)	6645(2)	361(2)	30(1)
C(3)	8255(1)	7432(2)	-481(2)	32(1)
C(4)	8666(1)	8361(2)	-486(2)	30(1)
C(5)	9186(1)	8472(2)	344(2)	29(1)
C(6)	9221(1)	4431(2)	1758(2)	22(1)
C(7)	9174(1)	3402(2)	2328(2)	26(1)
C(8)	9278(1)	2311(2)	1925(2)	32(1)
C(9)	9445(1)	2224(2)	949(2)	36(1)
C(10)	9513(1)	3238(2)	392(2)	34(1)
C(11)	9399(1)	4335(2)	785(2)	28(1)
C(12)	8339(1)	5714(2)	2702(2)	26(1)
C(13)	7902(1)	4821(2)	2335(2)	35(1)
C(14)	7331(1)	4773(3)	2657(2)	47(1)
C(15)	7189(1)	5616(3)	3327(2)	51(1)
C(16)	7607(1)	6518(3)	3675(2)	53(1)
C(17)	8184(1)	6571(2)	3374(2)	39(1)

Table 3. Bond lengths [Å] and angles [°] for rkbb11_0m.

Zn(1)-N(1)#1	2.0921(17)
Zn(1)-N(1)	2.0921(17)
Zn(1)-Cl(1)	2.2585(6)
Zn(1)-Cl(1)#1	2.2586(6)
P(1)-C(6)	1.827(2)
P(1)-C(12)	1.839(2)
P(1)-C(1)	1.842(2)
N(1)-C(5)	1.346(3)
N(1)-C(1)	1.351(3)
C(1)-C(2)	1.390(3)
C(2)-C(3)	1.380(3)
C(3)-C(4)	1.380(3)
C(4)-C(5)	1.375(3)
C(6)-C(7)	1.392(3)
C(6)-C(11)	1.394(3)
C(7)-C(8)	1.377(3)
C(8)-C(9)	1.385(3)
C(9)-C(10)	1.377(3)
C(10)-C(11)	1.383(3)
C(12)-C(17)	1.389(3)
C(12)-C(13)	1.394(3)
C(13)-C(14)	1.390(3)
C(14)-C(15)	1.366(4)
C(15)-C(16)	1.371(4)
C(16)-C(17)	1.391(4)
N(1)#1-Zn(1)-N(1)	145.58(10)
N(1)#1-Zn(1)-Cl(1)	97.27(5)
N(1)-Zn(1)-Cl(1)	100.20(5)
N(1)#1-Zn(1)-Cl(1)#1	100.20(5)
N(1)-Zn(1)-Cl(1)#1	97.27(5)
Cl(1)-Zn(1)-Cl(1)#1	118.24(3)
C(6)-P(1)-C(12)	103.34(10)
C(6)-P(1)-C(1)	101.02(9)

C(12)-P(1)-C(1)	99.80(10)
C(5)-N(1)-C(1)	118.33(18)
C(5)-N(1)-Zn(1)	116.08(14)
C(1)-N(1)-Zn(1)	124.29(14)
N(1)-C(1)-C(2)	121.2(2)
N(1)-C(1)-P(1)	114.57(15)
C(2)-C(1)-P(1)	124.27(17)
C(3)-C(2)-C(1)	119.9(2)
C(4)-C(3)-C(2)	118.7(2)
C(5)-C(4)-C(3)	119.0(2)
N(1)-C(5)-C(4)	122.9(2)
C(7)-C(6)-C(11)	118.4(2)
C(7)-C(6)-P(1)	118.59(16)
C(11)-C(6)-P(1)	122.79(17)
C(8)-C(7)-C(6)	121.0(2)
C(7)-C(8)-C(9)	120.2(2)
C(10)-C(9)-C(8)	119.4(2)
C(9)-C(10)-C(11)	120.6(2)
C(10)-C(11)-C(6)	120.3(2)
C(17)-C(12)-C(13)	118.4(2)
C(17)-C(12)-P(1)	116.51(18)
C(13)-C(12)-P(1)	125.06(18)
C(14)-C(13)-C(12)	120.7(2)
C(15)-C(14)-C(13)	120.1(3)
C(14)-C(15)-C(16)	120.1(3)
C(15)-C(16)-C(17)	120.7(3)
C(12)-C(17)-C(16)	120.1(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for rkbb11_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	21(1)	20(1)	25(1)	0	5(1)	0
P(1)	23(1)	22(1)	24(1)	0(1)	5(1)	-2(1)
Cl(1)	30(1)	30(1)	34(1)	3(1)	10(1)	-8(1)
N(1)	22(1)	22(1)	26(1)	1(1)	7(1)	0(1)
C(1)	23(1)	20(1)	27(1)	-2(1)	8(1)	-1(1)
C(2)	30(1)	28(1)	31(1)	2(1)	3(1)	-6(1)
C(3)	28(1)	39(1)	28(1)	0(1)	2(1)	0(1)
C(4)	32(1)	34(1)	26(1)	8(1)	6(1)	4(1)
C(5)	29(1)	26(1)	31(1)	5(1)	7(1)	-3(1)
C(6)	17(1)	24(1)	24(1)	0(1)	2(1)	-1(1)
C(7)	21(1)	28(1)	29(1)	4(1)	8(1)	-3(1)
C(8)	27(1)	24(1)	43(1)	6(1)	4(1)	-1(1)
C(9)	35(2)	27(1)	41(1)	-8(1)	0(1)	4(1)
C(10)	38(1)	38(1)	25(1)	-6(1)	5(1)	8(1)
C(11)	30(1)	27(1)	26(1)	3(1)	5(1)	1(1)
C(12)	24(1)	29(1)	24(1)	5(1)	6(1)	3(1)
C(13)	25(1)	31(1)	49(2)	3(1)	10(1)	3(1)
C(14)	23(1)	47(2)	70(2)	18(2)	11(1)	4(1)
C(15)	29(2)	75(2)	53(2)	23(2)	19(1)	17(2)
C(16)	45(2)	75(2)	42(2)	-4(2)	19(1)	21(2)
C(17)	36(2)	45(2)	35(1)	-2(1)	8(1)	8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rkbb11_0m.

	x	y	z	U(eq)
H(2A)	8112	6007	375	37
H(3A)	7899	7337	-1033	39
H(4A)	8592	8904	-1044	36
H(5A)	9465	9093	330	34
H(7A)	9071	3452	2991	31
H(8A)	9235	1631	2309	38
H(9A)	9511	1487	673	43
H(10A)	9636	3183	-254	40
H(11A)	9442	5013	398	33
H(13A)	7993	4251	1870	42
H(14A)	7046	4166	2417	56
H(15A)	6809	5579	3548	61
H(16A)	7503	7100	4118	63
H(17A)	8466	7181	3622	46

Table 6. Torsion angles [°] for rkbb11_0m.

N(1)#1-Zn(1)-N(1)-C(5)	-152.43(17)
Cl(1)-Zn(1)-N(1)-C(5)	-33.07(16)
Cl(1)#1-Zn(1)-N(1)-C(5)	87.43(16)
N(1)#1-Zn(1)-N(1)-C(1)	40.82(16)
Cl(1)-Zn(1)-N(1)-C(1)	160.18(16)
Cl(1)#1-Zn(1)-N(1)-C(1)	-79.32(17)
C(5)-N(1)-C(1)-C(2)	-0.1(3)
Zn(1)-N(1)-C(1)-C(2)	166.37(16)
C(5)-N(1)-C(1)-P(1)	-179.28(16)
Zn(1)-N(1)-C(1)-P(1)	-12.8(2)
C(6)-P(1)-C(1)-N(1)	-120.20(16)
C(12)-P(1)-C(1)-N(1)	134.01(16)
C(6)-P(1)-C(1)-C(2)	60.6(2)
C(12)-P(1)-C(1)-C(2)	-45.1(2)
N(1)-C(1)-C(2)-C(3)	-0.9(3)
P(1)-C(1)-C(2)-C(3)	178.25(18)
C(1)-C(2)-C(3)-C(4)	0.9(4)
C(2)-C(3)-C(4)-C(5)	0.0(4)
C(1)-N(1)-C(5)-C(4)	1.0(3)
Zn(1)-N(1)-C(5)-C(4)	-166.52(18)
C(3)-C(4)-C(5)-N(1)	-1.0(4)
C(12)-P(1)-C(6)-C(7)	-55.67(19)
C(1)-P(1)-C(6)-C(7)	-158.64(17)
C(12)-P(1)-C(6)-C(11)	130.25(19)
C(1)-P(1)-C(6)-C(11)	27.3(2)
C(11)-C(6)-C(7)-C(8)	-2.4(3)
P(1)-C(6)-C(7)-C(8)	-176.75(17)
C(6)-C(7)-C(8)-C(9)	1.4(3)
C(7)-C(8)-C(9)-C(10)	0.6(4)
C(8)-C(9)-C(10)-C(11)	-1.7(4)
C(9)-C(10)-C(11)-C(6)	0.7(4)
C(7)-C(6)-C(11)-C(10)	1.4(3)
P(1)-C(6)-C(11)-C(10)	175.44(17)
C(6)-P(1)-C(12)-C(17)	167.47(17)

C(1)-P(1)-C(12)-C(17)	-88.62(18)
C(6)-P(1)-C(12)-C(13)	-12.1(2)
C(1)-P(1)-C(12)-C(13)	91.8(2)
C(17)-C(12)-C(13)-C(14)	-1.6(3)
P(1)-C(12)-C(13)-C(14)	177.96(18)
C(12)-C(13)-C(14)-C(15)	1.0(4)
C(13)-C(14)-C(15)-C(16)	0.6(4)
C(14)-C(15)-C(16)-C(17)	-1.5(4)
C(13)-C(12)-C(17)-C(16)	0.7(3)
P(1)-C(12)-C(17)-C(16)	-178.9(2)
C(15)-C(16)-C(17)-C(12)	0.9(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+1/2