

Supporting Information

Photochemical preparation of pyrrole ring-contracted chlorins by the Wolff rearrangement

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1) Syntheses

Materials and General Procedures. All chemicals and solvents were obtained from Aldrich and Fluka. The products were purified by flash chromatography using silica gel (200-400 mesh) or activated neutral aluminum oxide (~150 mesh). UV-visible spectra were obtained using Perkin Elmer Lambda 19 spectrophotometer using Winlab software. ¹H-NMR spectra were recorded on VXR 400 MHz or Gem 300 MHz NMR spectrometers and referenced to the proton resonances resulting from incomplete deuteration of deuterated solvents. Infrared spectra were measured from KBr pellets on a Nicolet 510P FTIR spectrometer. MALDI-TOF, ESI and EI-HRMS data were obtained on a Bruker Biglex III MALDI-TOF mass spectrometer, a PE-Sciex API III Triple Quadrupole and Thermo-Finnigan MAT 95 XP high resolution mass spectrometers, respectively.

(2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) (4).¹

(2,3-dioxo-5,10,15,20-tetraphenylchlorinato)nickel(II) (**1**) (40 mg, 0.056 mmol) was dissolved in CH₂Cl₂ (25 ml) and *p*-toluenesulfonylhydrazine (183 mg, 20 eq) was added. The reagents were stirred for 9 h under reflux. The reaction mixture was cooled to room temperature and the solvent evaporated under reduced pressure. The purple residue was purified on an Al₂O₃ column with CH₂Cl₂/hexanes (2:1) as the eluent. Yield: 24 mg (60%). ESI *m/z* isotope pattern at 713.2 (M⁺); EI-HRMS Calcd. for C₄₄H₂₆N₄ONi (M-N₂): 684.1455, Found: 684.1426; ¹H NMR (CDCl₃): δ 8.61-8.59 (d, 1H, β-pyrrolic H), 8.52-8.47 (m, 4H, β-pyrrolic H), 8.43-8.41 (d, 1H, β-pyrrolic H), 7.93-7.88 (m, 6H, meso-ArH), 7.68-7.63 (m, 14H, meso-ArH); IR (cm⁻¹): 2103, 1669, 1594, 1553, 1528, 1448, 1390, 1363, 1338, 1175, 1139, 1069, 1010, 1003, 831, 792, 745, 697.

(2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) (5).¹

(2,3-dioxo-5,10,15,20-tetraphenylchlorinato)copper(II) (**2**) (65 mg, 0.09 mmol) was dissolved in CH₂Cl₂ (50 ml) and *p*-toluenesulfonylhydrazine (345 mg, 20 eq) was added. The reaction mixture was stirred for 6 h under reflux and cooled to room temperature. The solvent was subsequently evaporated under reduced pressure. The dark green residue was purified on a silica gel column with CH₂Cl₂/hexanes (2:1) as the eluent. Yield: 51 mg (77%). MALDI-TOF: *m/z* = 689.2 (M – N₂); ESI: *m/z* isotope pattern at 718.2 (M⁺); EI-HRMS: Calcd. for C₄₄H₂₆N₆OCu (M – N₂): 689.1397, Found: 689.1397; IR (cm⁻¹): 2098, 1735, 1669, 1598, 1576, 1510, 1432, 1388, 1342, 1273, 1175, 1133, 1071, 1007, 991, 844, 795, 795, 750, 702.

(2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)zinc(II) (6)

(2,3-dioxo-5,10,15,20-tetraphenylchlorinato)zinc(II) (**3**) (65 mg, 0.09 mmol) was dissolved in CH₂Cl₂ (50ml) and *p*-toluenesulfonylhydrazine (342 mg, 20 equiv.) was added. The reaction mixture was stirred for 3 h under reflux conditions. The resulting mixture was cooled to room temperature and the solvent was evaporated under reduced pressure. The dark green residue was purified on Al₂O₃ column with CH₂Cl₂/Hexanes (2:1) as eluent. Yield: 74%.

UV-Vis (CH₂Cl₂): λ_{max} (log ε) = 616 (4.11), 567 (3.66), 433 (4.94); IR (cm⁻¹): 3053, 2130, 2095, 1668, 1485, 1441, 1417, 1363, 1321, 1237, 1175, 1130, 1071, 1007, 987, 797, 756, 740, 702; ¹H NMR (DMSO-*d*₆): δ 8.65-8.64 (d, 1H, β-pyrrolic H), 8.57-8.50 (m, 3H, β-pyrrolic H), 8.46-8.45 (d, 1H, β-pyrrolic H), 8.31-8.30 (d, 1H, β-pyrrolic H), 8.13-8.11 (m, 6H, meso-ArH), 7.84-7.70 (m, 11H, meso-ArH), 7.65-7.61 (m, 3H, meso-ArH); ESI *m/z* isotope pattern at 720 (MH⁺); EI-HRMS Calcd. for C₄₄H₂₆N₄OZn (M-N₂): 690.1393, Found: 690.1390.

2) Physical Measurements

Photolyses were performed using a linear optical path photochemistry apparatus. A 1000-W XeHg lamp (Oriel model 66021) was collimated through a cooled filter bath and subsequently focused on a stirring sample contained within a second cooled chamber. The lamp-sample distance measures 30 inches. For the $\lambda \geq 395$ nm experiments, the cutoff wavelength was selected using a series of long-wavelength pass Schott filters (Oriel 51872). Samples were contained in Pyrex vessels and maintained at 10 °C using a temperature-controlled recirculating bath.

Quantum yield measurements for the photochemical reaction of **5** are reported relative to $K_3[Fe(C_2O_4)_3] \cdot 3 H_2O$. The quantum yield for **5** was performed via photolysis at 365 nm with 1000-W HgXe source utilizing a 365 nm notch filter. From a total of 8 measurements, the quantum yield for the bleaching of the electronic spectra at 430 nm of **5** (Φ_{365}) was determined to be 0.13 (± 0.04).

Photochemistry

Broadband Photolysis of (2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) (**4**).

A solution of **4** (20 mg, 0.028 mmol) in 25 ml degassed dichloromethane and 15 ml dried and degassed methanol was irradiated with a HgXe lamp (200 W) for 6 h at 10 °C in a pyrex vessel under a nitrogen atmosphere. The solvent was evaporated under reduced pressure and the residue purified on silica gel with hexanes/ CH_2Cl_2 (2:1) as the eluent. Analytically pure compounds were obtained by chromatography on a silica gel plate using hexanes/ CH_2Cl_2 (2:1) as the eluent. Yields: 1.8 mg unreacted starting material **4**, black residue (4 mg), (2-hydroxy-5,10,15,20-tetraphenylchlorinato)nickel(II) **4a** (0.5 mg, 3%), (2-methoxy-3-oxo-5,10,15,20-tetra-

phenylchlorinato)nickel(II) **4b** (0.9 mg, 5%), (2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) **4c** (6.0 mg, 32%), (5,10,15,20-tetraphenylazeteoporphyrinato)nickel(II) **4d** (3.0 mg, 16%), dimer **4e** (traces). Crystals suitable for X-ray diffraction studies were obtained from slow vapor diffusion of diethylether into CH₂Cl₂ for **4d** and slow diffusion of methanol into CH₂Cl₂ for **4e**.

Photolysis ($\lambda \geq 395$ nm) of (2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) (4**).**

A solution of **4** (10 mg, 0.014 mmol) in 13 ml degassed dichloromethane and 8 ml dried and degassed methanol was irradiated with a HgXe lamp (200 W) for 48 h at 10 °C in a pyrex vessel under a nitrogen. The solvent was evaporated under reduced pressure and the residue purified on a silica gel column with hexanes/CH₂Cl₂ (2:1) as the eluent. Analytically pure compounds were obtained by chromatography on a silica gel plate using hexanes/CH₂Cl₂ (2:1) as the eluent. Yields: 1.4 mg unreacted starting material **4**, black residue (1.5 mg), (2-hydroxy-5,10,15,20-tetraphenyl-porphyrinato)nickel(II) **4a** (traces), (2-methoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) **4b** (0.2 mg, 2%), (2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) **4c** (0.6 mg, 7%), (5,10,15,20-tetraphenylazeteoporphyrinato)nickel(II) **4d** (0.5 mg, 6%).

(2-hydroxy-5,10,15,20-tetraphenylporphyrinato)nickel(II) 4a:

MALDI-TOF *m/z* isotope pattern at 686; EI-HRMS Calcd. for C₄₄H₂₈N₄ONi: 686.1611, Found: 686.1578.

(2-methoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) 4b:

MALDI-TOF m/z isotope pattern at 716.5 (M); EI-HRMS Calcd. for $C_{45}H_{30}N_4O_2Ni$: 717.1717, Found: 717.1741; IR (cm^{-1}): 2921, 1729, 1652, 1639, 1597, 1558, 1440, 1383, 1349, 1243, 1154, 1069, 1004, 793, 751, 698, 555, 503.

(2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)nickel(II) 4c:

MALDI-TOF m/z isotope pattern at 746.5 (M); EI-HRMS Calcd. for $C_{46}H_{32}N_4O_3Ni$: 746.1822, Found: 746.1833; 1H NMR ($CDCl_3$): δ 8.44-8.37 (m, 3H, β -pyrrolic H), 8.29-8.27 (m, 2H, β -pyrrolic H), 8.07-8.06 (d, 1H, β -pyrrolic H, $J = 4$ Hz), 7.88-7.86 (m, 4H, meso-ArH), 7.72-7.50 (m, 16H, meso-ArH), 3.34 (s, 6H, CH_3); IR (cm^{-1}): 2920, 1727, 1597, 1549, 1440, 1347, 1240, 1154, 1066, 1007, 793, 750, 715, 698, 502.

(5,10,15,20-tetraphenylazeteoporphyrinato)nickel(II) 4d:

MALDI-TOF m/z isotope pattern at 717 (M^+); EI-HRMS Calcd. for $C_{45}H_{30}N_4O_2Ni$: 716.1717, Found: 716.1723; 1H NMR ($CDCl_3$): δ 8.52-8.47 (m, 4H, β -pyrrolic H), 8.30 (s, 2H, β -pyrrolic H), 7.99-7.97 (m, 3H, meso-ArH), 7.90-7.88 (m, 3H, meso-ArH), 7.68-7.58 (m, 14H, meso-ArH), 5.97 (s, 1H, t -CH), 3.40 (s, 3H, CH_3); IR (cm^{-1}): 1742, 1674, 1599, 1567, 1511, 1440, 1361, 1344, 1260, 1155, 1066, 1019, 1005, 796, 752, 700; X-ray structure: Figure 1S.

Dinickel Chlorin Dimer 4e:

MALDI-TOF m/z isotope pattern at 1370 (M^+); X-ray structure: Figure 2S.

Broadband Photolysis of (2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) (5).

A solution of 15 mg (0.0209 mmol) **5** in 15 ml degassed dichloromethane and 8 ml dried and degassed methanol was irradiated with a HgXe lamp (200 W) for 6 h at 10 °C in a pyrex vessel under a nitrogen atmosphere. The solvent was evaporated under reduced pressure and the residue

purified on a silica gel column with hexanes/CH₂Cl₂ (2:1) as the eluent. Analytically pure compounds were obtained by chromatography on a silica gel plate using hexanes/CH₂Cl₂ (2:1) as the eluent. Yields: Black residue (2 mg), (2-hydroxy-5,10,15,20-tetraphenylporphyrinato)copper(II) **5a** (3.2 mg, 22%), (2-methoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) **5b** (0.6 mg, 4%), (2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) **5c** (1.6 mg, 10%), (5,10,15,20-tetraphenylazeteoporphyrinato)copper(II) **5d** (1.1 mg, 7%). Crystals suitable for X-ray diffraction studies were obtained from slow vapor diffusion of diethylether into CH₂Cl₂ for **5d**.

Photolysis ($\lambda \geq 395$ nm) of (2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) (5**).**

15.0 mg (0.0209 mmol) of **5** in 15 ml degassed dichloromethane and 10 ml dried and degassed methanol were irradiated with a HgXe lamp (200 W, $\lambda \geq 395$ nm) for 48 h at 10 °C in a pyrex vessel under a nitrogen atmosphere. The solvent was evaporated under reduced pressure and the residue purified on silica gel with hexanes/CH₂Cl₂ (2:1). Analytically pure compound were obtained by chromatography on a silica gel plate using hexanes/CH₂Cl₂ (2:1) as the eluent. Yields: 1.2 mg unreacted starting material **5**, black residue (2 mg), (2-hydroxy-5,10,15,20-tetraphenylporphyrinato)copper(II) **5a** (1.3 mg, 10%), (2-methoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) **5b** (0.5 mg, 4%), (2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) **5c** (1.1 mg, 8%), (5,10,15,20-tetraphenylazeteoporphyrinato)copper(II) **5d** (1.1 mg, 8%).

(2-hydroxy-5,10,15,20-tetraphenylporphyrinato)copper(II) 5a:

MALDI-TOF m/z isotope pattern at 691(M); EI-HRMS Calcd. for $C_{44}H_{28}N_4OCu$: 691.1554, Found: 691.1550.

(2-methoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) 5b:

MALDI-TOF m/z isotope pattern at 721.3 (M); EI-HRMS Calcd. for $C_{45}H_{30}N_4O_2Cu$: 721.1659, Found: 721.1658; IR (cm^{-1}): 2921, 1729, 1597, 1539, 1489, 1440, 1343, 1240, 1155, 1066, 1004, 993, 833, 795, 750, 718, 699, 661, 571, 446.

(2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)copper(II) 5c:

MALDI-TOF m/z isotope pattern at 751.8 (M); EI-HRMS Calcd. for $C_{46}H_{32}N_4O_3Cu$: 751.1765, Found: 751.1772; IR (cm^{-1}): 2921, 1733, 1597, 1540, 1540, 1488, 1440, 1384, 1344, 1211, 1154, 1092, 1070, 1008, 888, 833, 796, 752, 739, 700, 620, 555, 502, 446.

(5,10,15,20-tetraphenylazeteoporphyrinato)copper(II) 5d:

MALDI-TOF m/z isotope pattern at 722 (M^+); EI-HRMS Calcd. for $C_{45}H_{30}N_4O_2Cu$: 721.1665, Found: 721.1666; IR (cm^{-1}): 1741, 1648, 1597, 1543, 1499, 1433, 1336, 1212, 1154, 1065, 1024, 1003, 994, 833, 795, 753, 725, 702, 639, 555, 503; X-ray structure: Figure 3S.

Broadband Photolysis of (2-diazo-3-oxo-5,10,15,20-tetraphenylchlorinato)zinc(II) (6).

A solution of **6** (10 mg, 0.014 mmol) in 13 ml degassed dichloromethane and 8 ml dried and degassed methanol was irradiated with a HgXe lamp (200 W) for 6 h at 10 °C in a pyrex vessel under a nitrogen. The solvent was evaporated under reduced pressure and the residue purified on a Al_2O_3 column with CH_2Cl_2 /Hexanes (4:1) as eluent.

Yields: 1.0 mg unreacted starting material **6**, black residue (1.5 mg), (2-hydroxy-5,10,15,20-tetraphenylporphyrinato)zinc(II) **6a** (traces), (2-methoxy-3-oxo-5,10,15,20-tetraphenyl-

chlorinato)zinc(II) **6b** (0.4 mg, 4%), (2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)zinc(II) **6c** (0.7 mg, 7%), (5,10,15,20-tetraphenylazeteoporphyinato)zinc(II) **6d** (0.6 mg, 6%).

(2-hydroxy-5,10,15,20-tetraphenylporphyrinato)zinc(II) 6a:

MALDI-TOF *m/z* isotope pattern at 692.

(2-methoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)zinc(II) 6b:

MALDI-TOF *m/z* isotope pattern at 723 (M) and 695(M-CO).

(2,2-dimethoxy-3-oxo-5,10,15,20-tetraphenylchlorinato)zinc(II) 6c:

MALDI-TOF *m/z* isotope pattern at 752 (M) and 724 (M-CO); EI-HRMS Calcd. for $C_{46}H_{33}N_4O_3Zn(MH^+)$:753.1839, Found: 753.1815.

(5,10,15,20-tetraphenylazeteoporphyinato)zinc(II) 6d:

MALDI-TOF *m/z* isotope pattern at 722 (M^+); EI-HRMS Calcd. for $C_{45}H_{30}N_4O_2Zn(M^+)$: 722.1655, Found: 722.1659.

3) Crystallographic Data Information for 4d

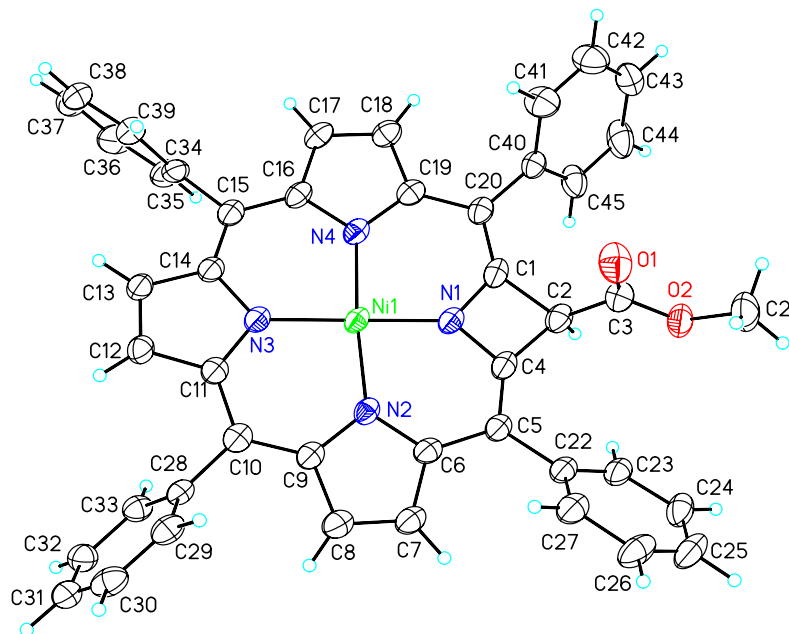


Figure 1S. ORTEP plot of **4d** at 50% probability.

A dark crystal (approximate dimensions $0.25 \times 0.23 \times 0.18 \text{ mm}^3$) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a SMART6000 (Bruker) at 130(2) K.

Data collection

The data collection was carried out using Mo $K\alpha$ radiation (graphite monochromator) with a frame time of 20 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to the extent of a sphere. Four major sections of frames were collected with 0.30° steps in ω at different ϕ settings and a detector position of -43° in 2θ . An additional set of 50 frames was collected in order to model decay. Data to a resolution of 0.84 \AA were considered in the reduction. Final cell constants were calculated from the xyz centroids of 6982 strong reflections from the actual data collection after integration (SAINT).² The intensity data were corrected for absorption (SADABS).³

Structure solution and refinement

The space group Pbcn was determined based on intensity statistics and systematic absences. The structure was solved using SIR-92⁴ and refined with SHELXL-97⁵. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms with individual isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0441$ and $wR2 = 0.1073$ (F^2 , all data). The remaining electron density is located near the metal.

4) Crystallographic Data Information for 4e

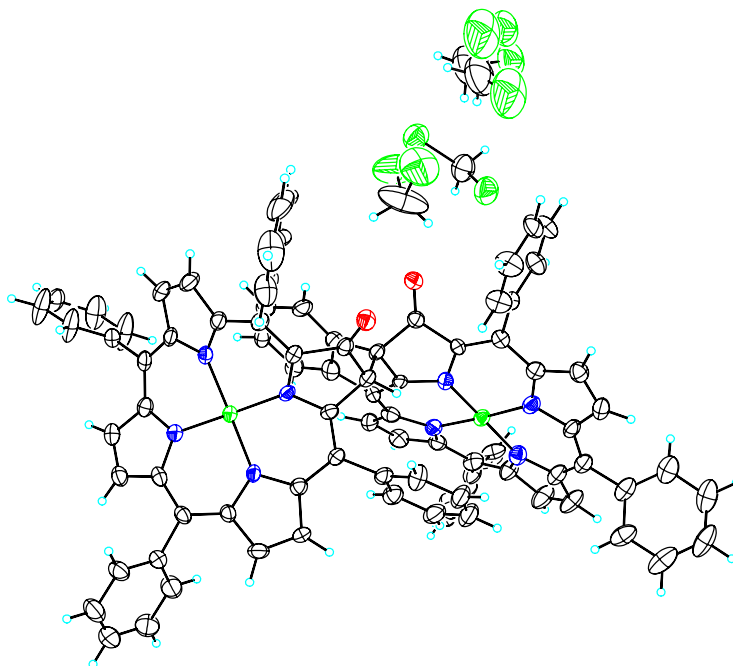


Figure 2Sa. ORTEP plot of 4e at 50% probability.

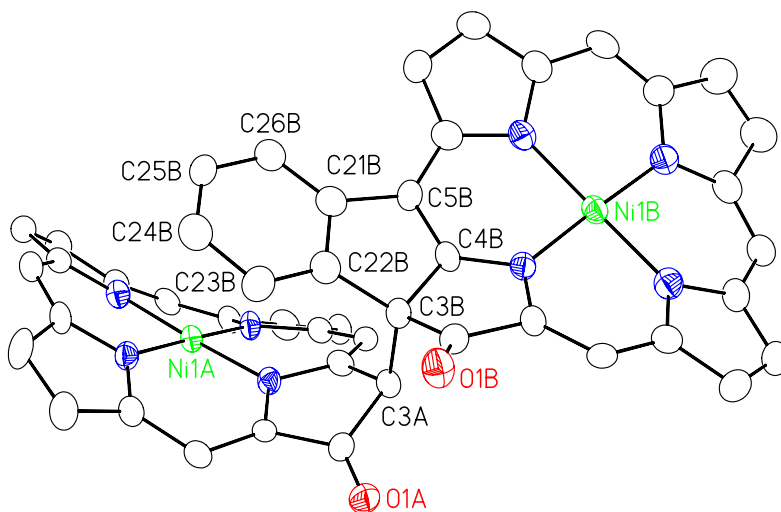


Figure 2Sb. ORTEP plot of 4e at 50% probability, hydrogen atoms and solvent omitted for clarity. Phenyl rings have also been simplified to minimize congestion. Only connectivity related atoms and metal centers are labeled.

Data Collection

The data collection was carried out using Mo K α radiation (graphite monochromator) with a frame time of 50 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to the extent of 1.3 hemispheres. Three major sections of frames were collected with 0.30° steps in ω at different ϕ settings and a detector position of -43° in 2θ . Data to a resolution of 0.84 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 2367 strong reflections from the actual data collection after integration (SAINT)². The intensity data were corrected for absorption (SADABS)³.

Structure solution and refinement

The space group P2₁/n was determined based on intensity statistics and systematic absences. The structure was solved using SIR-92⁴ and refined with SHELXL-97⁵. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to R1 = 0.0715 and wR2 = 0.2276 (F², all data). The remaining electron density is located near the disordered solvent. The data to parameter ratio is low due to the weak diffraction of the very small crystal.

5) Crystallographic Data Information for 5d

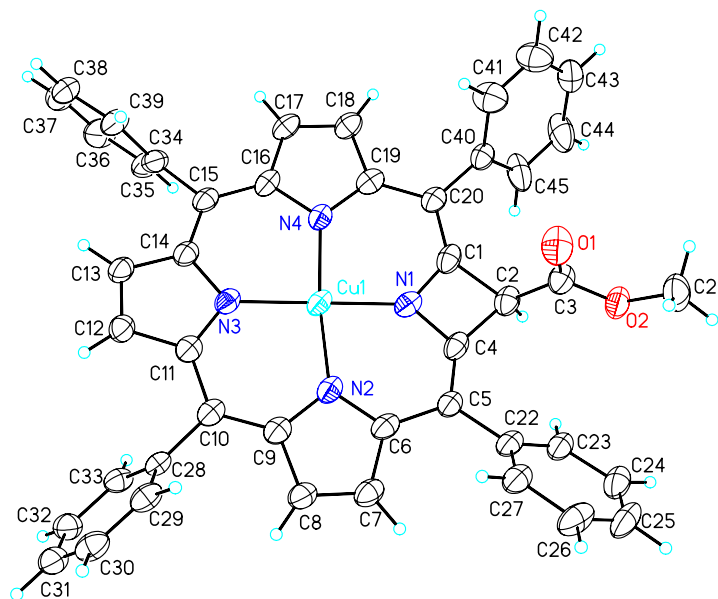


Figure 3S. ORTEP plot of **5d** at 50% probability.

A dark blue crystal (approximate dimensions $0.15 \times 0.11 \times 0.10 \text{ mm}^3$) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a SMART6000 (Bruker) at 130(2) K.

Data collection

The data collection was carried out using Mo $K\alpha$ radiation (graphite monochromator) with a frame time of 60 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to the extent of a sphere. Four major sections of frames were collected with 0.30° steps in ω at different ϕ settings and a detector position of -43° in 2θ . Data to a resolution of 0.80 \AA were considered in the reduction. Final cell constants were calculated from the xyz centroids of 4312 strong reflections from the actual data collection after integration (SAINT)². The intensity data were corrected for absorption (SADABS)³.

Structure solution and refinement

The space group Pbcn was determined based on intensity statistics and systematic absences. The structure was solved using SIR-92⁴ and refined with SHELXL-97⁵. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to R1 = 0.0522 and wR2 = 0.1233 (F², all data). The remaining electron density is located near the metal.

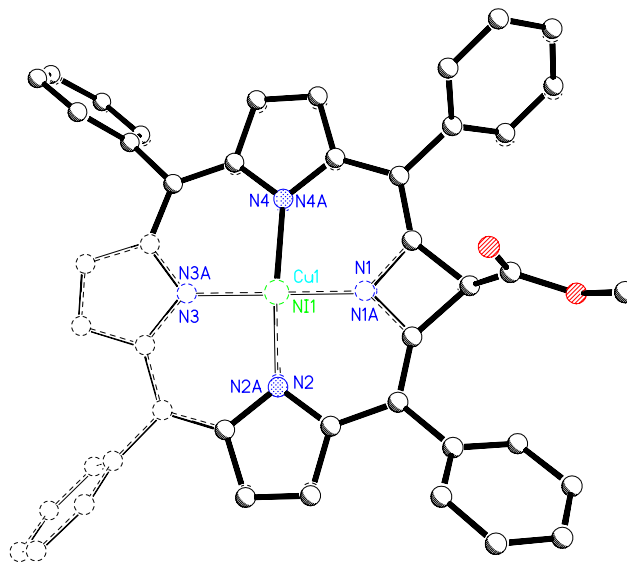
6) Model fitting for 4d and 5d

Orthogonal coordinates from **4d** fit onto fractional coordinates of **5d**

Atom model deviation for atoms fitted

Cu1	Ni1	0.019
N1	N1	0.049
N2	N2	0.063
N3	N3	0.043
N4	N4	0.062

Weighted R.M.S. Deviation = 0.0496 Å



Idealized Crystal Coordinates for all model atoms

NAME	SFAC	X	Y	Z	NEAREST ATOM	DEVIATION
Ni1	3	0.88142	0.20300	0.20408	CU1	0.019
O1	4	0.78851	0.33657	0.36438	O1	0.056

O2	4	0.89337	0.34296	0.41269	O2	0.085
N1	3	0.90121	0.25262	0.26329	N1	0.049
N2	3	0.88797	0.07944	0.23349	N2	0.063
N3	3	0.86180	0.15224	0.14219	N3	0.043
N4	3	0.87318	0.33110	0.18063	N4	0.062
C1	1	0.90021	0.34260	0.28094	C1	0.043
C2	1	0.91750	0.31069	0.33203	C2	0.071
C3	1	0.85774	0.33202	0.37033	C3	0.063
C4	1	0.91121	0.21394	0.30801	C4	0.037
C5	1	0.90874	0.12031	0.31930	C5	0.019
C6	1	0.90142	0.05539	0.28064	C6	0.038
C7	1	0.90957	-0.04354	0.28556	C7	0.055
C8	1	0.90077	-0.08198	0.24197	C8	0.049
C9	1	0.88625	-0.00607	0.20930	C9	0.044
C10	1	0.87192	-0.01776	0.16080	C10	0.024
C11	1	0.85582	0.05863	0.13027	C11	0.039
C12	1	0.83535	0.04807	0.08088	C12	0.045
C13	1	0.83343	0.13595	0.06195	C13	0.041
C14	1	0.85044	0.20015	0.09965	C14	0.035
C15	1	0.85717	0.29730	0.09454	C15	0.045
C16	1	0.86615	0.35884	0.13267	C16	0.063
C17	1	0.86207	0.45847	0.12957	C17	0.095
C18	1	0.86556	0.49260	0.17459	C18	0.087
C19	1	0.87342	0.41476	0.20621	C19	0.055
C20	1	0.88432	0.42283	0.25644	C20	0.039
C21	1	0.84228	0.35067	0.45393	C21	0.093
C22	1	0.91125	0.08860	0.36993	C22	0.031
C23	1	0.96079	0.13273	0.40268	C23	0.057
C24	1	0.96279	0.10504	0.45030	C24	0.062
C25	1	0.91673	0.03057	0.46566	C25	0.040
C26	1	0.86705	-0.01327	0.43379	C26	0.042
C27	1	0.86286	0.01630	0.38650	C27	0.030
C28	1	0.87861	-0.11203	0.13836	C28	0.033
C29	1	0.82743	-0.18569	0.14925	C29	0.048
C30	1	0.83489	-0.27186	0.12657	C30	0.051
C31	1	0.89395	-0.28606	0.09315	C31	0.057
C32	1	0.94570	-0.21494	0.08287	C32	0.044
C33	1	0.93824	-0.12840	0.10519	C33	0.031
C34	1	0.85490	0.33681	0.04484	C34	0.046
C39	1	0.78626	0.33684	0.01772	C39	0.044
C38	1	0.78704	0.36841	-0.02935	C38	0.052
C37	1	0.85541	0.40158	-0.04943	C37	0.061
C36	1	0.92348	0.40469	-0.02279	C36	0.059

C35	1	0.92367	0.37249	0.02453	C35	0.064
C40	1	0.88045	0.51529	0.28053	C40	0.072
C41	1	0.81397	0.57145	0.27689	C41	0.094
C42	1	0.81073	0.65895	0.29869	C42	0.132
C43	1	0.87429	0.69199	0.32426	C43	0.139
C44	1	0.94063	0.63786	0.32770	C44	0.124
C45	1	0.94349	0.54951	0.30625	C45	0.096

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