Supporting information

Controlling Intramolecular Electronic Communication through the Conformation Changes via Stepwise Oxidations in Dicopper(II) and Dinickel(II) Porphyrin Dimers

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Experimental Section

Materials

All the reagents and solvents were purchased from commercial sources and purified by standard procedures before use. $1 \cdot M$, $2 \cdot M$, and $3 \cdot M$ (M= Ni, Cu) were prepared according to the literature procedures.¹ The preparations of $4 \cdot M$, $[3 \cdot M]SbF_6$, $[3 \cdot M](SbF_6)_2$, $[4 \cdot M]SbF_6$, $[4 \cdot M](SbF_6)_2$, (M= Ni, Cu) reported in the present work, are described below.

Syntheses

Preparation of **4**•Ni and **4**•Cu was carried out using a general procedure; details for one representative case are described below.

Synthesis of **4**•Ni: To a solution of **1**•Ni (50 mg, 0.033 mmol) in CH₂Cl₂ (100 mL) was added DDQ (45 mg, 0.198 mmol) dissolved in acetonitrile, and the reaction mixture was stirred at room temperature for 2 hours. The reaction mixture was evaporated to complete dryness and further redissolved in CH₂Cl₂ (100 mL), washed initially with an aqueous solution of NaHCO₃ (2 × 200 mL) and then with water (3 × 200 mL). The crude solution was then evaporated to complete dryness, and it was further subjected to silica gel column chromatography (CH₃OH/CH₂Cl₂ = 5:95 v/v) to yield the desired product as a light greenish solid. Yield: 41 mg (80%). ¹H NMR (CDCl₃, 295 K, ppm): δ = 10.11 (s, 1H; *meso-H*), 9.75 (s, 1H; *meso-H*), 9.59 (s, 1H; *meso-H*), 9.45 (s, 1H; *meso-H*), 9.22 (s, 2H; *meso-H*),7.15 (d, *J* = , 2H; Ph-*H*), 7.06 (t, *J* = , 1H; Ph-*H*), 5.52 (d, *J* = , 1H; Py-*H*), 5.33 (br, 1H; -NH), 5.28 (d, *J* = , 1H; Py-*H*), 5.09 (d, *J* = , 1H; Py-*H*), 4.15–3.11 (m, 36H; -CH₂(por)), 2.21–0.84 (m, 54H; -CH₃(por)). UV-vis-NIR (CH₂Cl₂) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 403 (1.2 ×10⁵), 471 (7.1 ×10⁴), 554 (3.4 ×10⁴), 640 (3.3 ×10⁴), 1018 (2.1 ×10⁴).

Synthesis of **4**•Cu: Yield: 42 mg (82%) UV-vis-NIR (CH₂Cl₂) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 405 (1.2 ×10⁵), 475 (6.1 ×10⁴), 560 (3.2 ×10⁴), 640 (3.0 ×10⁴), 994 (2.0 ×10⁴).

The preparation of $[3 \cdot M]$ SbF₆, $[3 \cdot M]$ (SbF₆)₂, $[4 \cdot M]$ SbF₆, and $[4 \cdot M]$ (SbF₆)₂ (M = Ni, Cu) was done by employing a general synthetic method. The procedure for one such compound is given below.

Synthesis of $[3 \cdot Ni]SbF_6$: To a solution of $3 \cdot Ni$ (20 mg, 0.013 mmol) in CH₂Cl₂ (20 mL) was added a solution of one equivalent of silver hexafluoroantimonate (4.46 mg) in methanol. The solution was stirred for 15 minutes in the air and then dried under a vacuum. The solid thus obtained was dissolved in distilled CH₂Cl₂ and carefully layered with *n*-hexane. A light brown crystalline solid was obtained after 48 hours. Yield: 17 mg (85%). UV-vis-NIR (CH₂Cl₂, 295 K) $[\lambda_{max}, nm (\epsilon, M^{-1} cm^{-1})]$: 398 (6.0 ×10⁴), 525 (2.8 ×10⁴), 560 (2.9 × 10⁴), 695 (2.0 × 10⁴), 1095 (5.5 × 10⁴).

Synthesis of [**3**•Cu]SbF₆: Yield: 16 mg (80%). UV-vis-NIR (CH₂Cl₂, 295 K) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 404 (8.2 ×10⁴), 486 (4.8 ×10⁴), 564 (3.6 × 10⁴), 680 (3.1 x 10⁴), 1125 (4.8 × 10⁴).

Synthesis of [4•Cu]SbF₆: Yield: 17 mg (85%). UV-vis-NIR (CH₂Cl₂, 295 K) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 402 (1.0 ×10⁵), 357 (7.1 ×10⁴), 480 (5.6 × 10⁴), 645 (2.2 x 10⁴), 1075 (1.9 × 10⁴).

Synthesis of [**4**•Ni]SbF₆: Yield: 16.5mg (82%). UV-vis-NIR (CH₂Cl₂, 295 K) [λ_{max}, nm (ε, M⁻¹ cm⁻¹)]: 401 (9.7 ×10⁴), 355 (5.8 ×10⁴), 475 (5.7 × 10⁴), 640 (2.1 x 10⁴), 1192 (2.4 × 10⁴).

The general procedures of the dication species: To a solution of $3 \cdot M$ (30 mg, 0.020 mmol) in CH₂Cl₂ (20 mL) was added a solution of two equivalents of silver hexafluoroantimonate (13.8 mg) in methanol, and the solution was stirred for 20 minutes in air. The resulting solution was then dried under a vacuum. The solid thus obtained was dissolved in distilled CH₂Cl₂ and carefully layered with *n*-hexane. The dark brown crystalline solid was obtained after 48 hours.

Synthesis of $[3 \cdot Cu](SbF_6)_2$: Yield: 25 mg (83%). UV-vis-NIR (CH₂Cl₂, 295 K) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 406 (7.2 ×10⁴), 486 (6.3 ×10⁴), 668 (3.1 ×10⁴).

Synthesis of $[3 \cdot Ni](SbF_6)_2$: Yield: 23 mg (77%). UV-vis-NIR (CH₂Cl₂, 295 K) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 404 (6.0 ×10⁴), 479 (3.4 ×10⁴), 522 (3.2 × 10⁴), 855 (3.8 × 10⁴).

Synthesis of $[4 \cdot Cu](SbF_6)_2$: Yield: 25 mg (83%). UV-vis-NIR (CH₂Cl₂, 295 K) [λ_{max} , nm (ϵ , M⁻¹ cm⁻¹)]: 379 (8.2 ×10⁵), 357 (8.0 ×10⁴), 480 (4.9 × 10⁴), 785 (3.2 × 10⁴).

Synthesis of [**4**•Ni](SbF₆)₂: Yield: 24 mg (80%). UV-vis-NIR (CH₂Cl₂, 295 K) [λ_{max}, nm (ε, M⁻¹ cm⁻¹)]: 400 (7.1 ×10⁴), 353 (4.8 ×10⁴), 475 (4.6 × 10⁴), 912 (2.1 × 10⁴).

Instrumentation

UV-vis-NIR absorption spectra were measured on a Perkin Elmer spectrometer. The ESI mass spectra were recorded with a Waters Micromass QuattroMicro triple quadrupole mass spectrometer. ¹H NMR spectra were recorded on a JEOL 500 MHz instrument. The residual ¹H resonances of the solvents were used as a secondary reference. Electron paramagnetic resonance (EPR) spectra were obtained on a Bruker EMX spectrometer. EPR spectral simulations were carried out using the WinEPR SimFonia software.² Cyclic voltammetric studies were performed on a BAS Epsilon electrochemical workstation in dichloromethane with 0.1 M tetrabutylammonium hexafluorophosphate (TBAH) as a supporting electrolyte; the reference electrode was Ag/AgCl, and a platinum wire was used as the auxiliary electrode. The concentration of the compounds was of the order of 10⁻³ M. The ferrocene/ferrocenium couple occurs at $E_{1/2} = +0.45$ (65) V versus Ag/AgCl, under the same experimental conditions.

X-ray Structure Solution and Refinement

Crystals were coated with light hydrocarbon oil and mounted in the 100 K dinitrogen stream of a Bruker SMART APEX CCD diffractometer equipped with CRYO industries low temperature apparatus, and intensity data were collected using graphite-monochromated Mo Ka radiation ($\lambda = 0.71073$ Å). The data integration and reduction were processed with SAINT software.³ An absorption correction was applied. ⁴ Structures were solved by the direct method using SHELXS-97 and were refined on F² by full-matrix least-squares technique using the SHELXL-

2018 program package.⁵ Non-hydrogen atoms were refined anisotropically. In the refinement, the hydrogen atoms were included in geometrically calculated positions and were refined according to the "riding model".

Magnetic measurements

Magnetic susceptibility data were collected with a Quantum Design MPMS SQUID magnetometer over the temperature range of 5–300 K in an applied magnetic field of 0.1 T and corrected for diamagnetism by using Pascal's constants.⁶ The magnetic data were fitted with PHI software.⁷ The presence of a small amount of monomeric impurity and temperature-independent paramagnetism was also taken into account.

Computational details

DFT calculations were carried out by using the *Gaussian 16*, *Revision C.01* program suite.⁸ The method used was Becke's three-parameter hybrid-exchange functional, ⁹ the non-local correlation provided by the Lee, Yang, and Parr expression, and the Vosko, Wilk, and Nuair 1980 correlation functional (III) for local correction.⁹ The basis set was 6-31G** for C, N, Cl, O, and H atoms and LANL2DZ for Ni and Cu atoms. Geometry optimizations were executed in which all the coordinates were taken from the molecular structures wherever possible. The optimized geometry was confirmed to be the potential energy minima by vibrational frequency calculations at the same level of theory as no imaginary frequencies were found. Chloroform and dichloromethane were used for solvent correction in all the calculations. Zero-point energies (ZPEs) and thermal corrections were also included. The orbital surfaces were visualized by the *Chemcraft* software program.¹⁰ The HOMO and LUMO levels for all the molecules were also generated and prepared graphically with this software. Anisotropy of the current-induced density (ACID) plots was obtained by employing the continuous set of gauge transformations (CSGT) method to calculate the current densities, and the results were plotted using POVRAY 3.7 beta for Windows.¹¹ Finally, LOL functions were calculated using Multiwfn 3.8 software.¹²

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Figure S1. (A) A plausible reaction mechanism for the formation of **4**•M with **I**-1 as intermediate, (B) ESI-MS (positive ion mode) of the crude reaction mixture of **4**•Cu, and (C) ESI-MS (positive ion mode) of the crude reaction mixture of **4**•Ni.



Figure S2. ESI-MS and isotopic distribution pattern (positive ion mode) of **4**•Cu. (A) experimental (selected range) (B) experimental spectra (expanded) and (C) simulated spectra of final product **4**•Cu (D) experimental spectra (expanded) of intermediate species; **I**-1 and (E) simulated spectra of intermediate species; **I**-1 of **4**•Cu.



Figure S3. ESI-MS and isotopic distribution pattern (positive ion mode) of **4**•Ni. (A) experimental (selected range) (B) experimental spectra (expanded) and (C) simulated spectra of final product **4**•Ni (D) experimental spectra (expanded) of intermediate species; **I**-1 and (E) simulated spectra of intermediate species; **I**-1 of **4**•Ni.



Figure S4. Isotopic distribution pattern for $4 \cdot Cu^{-16}O$ (Positive ion mode); (A) experimental with $[4 \cdot Cu + H]^+$ peak at m/z = 1533.5803, (B) simulated and for $4 \cdot Cu^{-18}O$ (C) experimental with $[4 \cdot Cu]^+$ peak at m/z = 1536.5873.



Figure S5. Diagram showing the molecular packing of **3**•Ni in the unit cell (H atoms have been omitted for clarity).



Figure S6. Diagram showing the molecular packing of $4 \cdot Cu.C_6H_{14}$ in the unit cell (H atoms have been omitted for clarity).



Figure S7. Diagram showing the molecular packing of **4**•Cu.CH₂Cl₂ in the unit cell (H atoms have been omitted for clarity).



Figure S8. Atom numbering scheme for (A) 3•Ni (B) 4•Cu.



Figure S9. UV-vis-NIR spectra of (A) **2**•Cu (red line) and **2**•Ni (blue line); (B) **3**•Cu (red line) and **3**•Ni (blue line) and (C) **4**•Cu (red line) and **4**•Ni (blue line) in CH₂Cl₂ at 295 K.



Figure S10. Electronic absorption spectrum (curved line, left axis) determined in CH₂Cl₂ and oscillator strengths (vertical line, right axis) obtained from TD-DFT calculations at the uB3LYP/6-31G**/LANL2DZ level of theory for **4**•Cu.



Figure S11. Electronic absorption spectrum (curved line, left axis) determined in CH₂Cl₂ and oscillator strengths (vertical line, right axis) obtained from TD-DFT calculations at the uB3LYP/6-31G**/LANL2DZ level of theory for **4**•Ni.



Figure S12. NICS(0) values of (A) 2•Ni, (B) 3•Ni , and (C) 4•Ni.



Figure S13. AICD plots for (A) 2•Ni, (B) 3•Ni and (C) 4•Ni with isosurface values of 0.05



Figure S14. LOL- π isosurface map of (A) **2**•Ni and (B) **3**•Ni and (C) **4**•Ni with iso-values of 0.45 a.u.



Figure S15. The numbering scheme used for the ¹H NMR assignment for (A) **3**•Ni and (B) **4**•Ni.



Figure S16. UV-Vis-NIR (in CH₂Cl₂ at 295 K) spectral changes of 1.0×10^{-5} M solution of **3**•Cu upon gradual additions of (A) 0 to 1.0 eqv. and (B) 1.0 to 2.0 eqv. of AgSbF₆. (C) UV-Vis-NIR spectra (in CH₂Cl₂ at 295 K) of **3**•Cu (red line), [**3**•Cu]SbF₆ (green line) and [**3**•Cu](SbF₆)₂ (blue line).



Figure S17. UV-vis-NIR (in CH_2Cl_2 at 295 K) spectral changes of 1.0×10^{-5} M solution of **3**•Ni upon gradual additions of (A) 0 to 1.0 eqv. and (B) 1.0 to 2.0 eqv. of AgSbF₆. (C) UV-vis-NIR spectra (in CH_2Cl_2 at 295 K) of **3**•Ni (blue line), [**3**•Ni]SbF₆ (red line) and [**3**•Ni](SbF₆)₂ (green line).



Figure S18. UV-vis-NIR (in CH_2Cl_2 at 295 K) spectra of (A) $[2 \cdot Cu]SbF_6$ (blue line), $[3 \cdot Cu]SbF_6$ (red line), $[4 \cdot Cu]SbF_6$ (green line); (B) $[2 \cdot Cu](SbF_6)_2$ (blue line) and $[3 \cdot Cu](SbF_6)_2$ (red line), $[4 \cdot Cu](SbF_6)_2$ (green line).



Figure S19. Isotopic distribution pattern of the (A) experimental and (B) simulated ESI-MS of $[3 \cdot Cu]^{2+}$.



Figure S20. Isotopic distribution pattern of the (A) experimental and (B) simulated ESI-MS of [**3**•Ni]²⁺.



Figure S21. UV-vis-NIR (in CH₂Cl₂ at 295 K) spectral changes of 1.2×10^{-5} M solution of **4**•Cu upon gradual additions of (A) 0 to 1.0 eqv. and (B) 1.0 to 2.0 eqv. of AgSbF₆. (C) UV-vis-NIR spectra (in CH₂Cl₂ at 295 K) of **4**•Cu (red line), [**4**•Cu]SbF₆ (green line) and [**4**•Cu](SbF₆)₂ (blue line).



Figure S22. UV-vis-NIR (in CH_2Cl_2 at 295 K) spectral changes of 1.2×10^{-5} M solution of $4 \cdot Ni$ upon gradual additions of (A) 0 to 1.0 eqv. and (B) 1.0 to 2.0 eqv. of AgSbF₆. (C) UV-vis-NIR spectra (in CH_2Cl_2 at 295 K) of $4 \cdot Ni$ (blue line), $[4 \cdot Ni]SbF_6$ (red line) and $[4 \cdot Ni](SbF_6)_2$ (green line).



Figure S23. Isotopic distribution pattern of the (A) experimental and (B) simulated ESI-MS of $[4 \cdot Cu]^{2+}$.



Figure S24. Isotopic distribution pattern of the (A) experimental and (B) simulated ESI-MS of [4•Ni]²⁺.



Figure S25. DFT computed bond critical points using AIM analysis showing an interaction between the Cu and O atoms in [4•Cu]²⁺.



Figure S26. Models obtained from the fragmentation and saturating the carbon valency with hydrogen of the optimised geometry of (A) $[3 \cdot Cu](SbF_6)_2$ (B) $[4 \cdot Cu](SbF_6)_2$ to compute the J_{Cu} . r. Colour code: cyan, Cu; blue, N; grey, C. Hydrogen atoms are omitted for clarity.



Figure S27. BS-DFT spin density plot for the model used to calculate the J_{Cu-r} in [**3**•Cu](SbF₆)₂ showing the presence of two unpaired electrons in antiferromagnetic fashion, one in Cu $d_{x^2-y^2}$ orbital and another in the π -SOMO of the porphyrin ring.



Figure S28. (A) Experimental EPR spectrum of $[4 \cdot Cu]^{2+}$ (in the solid state at 120 K) and (B) simulated EPR spectrum of $[4 \cdot Cu]^{2+}$. With the triangle and squares are indicated the parallel and perpendicular components of the zero-field splitting tensor *D*, respectively, while with the circle is shown the forbidden transition $\Delta M_{\rm S} = \pm 2$ at half-field. In the inset and with the asterisks the hyperfine resonances due to the coupling between the two unpaired electrons and the two Cu nuclei are denoted; this region, between 2300 and 2715 G, was amplified 10 and 8 times compared to the traces (A)-(B).



Figure S29. (A) simulated EPR spectrum of $[3 \cdot Ni]^{2+}$; (B) experimental EPR spectrum of $[3 \cdot Ni]^{2+}$ (in CHCl₃/toluene mixture at 120 K); (C) experimental EPR spectrum of $[4 \cdot Ni]^{2+}$ (in CHCl₃/toluene mixture at 120 K); (D) simulated EPR spectrum of $[4 \cdot Ni]^{2+}$.



Figure S30. Optimized geometry for the 2S+1 = 2 state of (A) $[3 \cdot Ni]^+$ and 2S+1 = 2, (2S + 1 = 4) states of (B) $[3 \cdot Cu]^+$, at the uB3LYP level of theory. Selected bond lengths are given in Å and angle in degree. ΔG is given relative to the doublet spin state in kcal/mol (including ZPE).



Figure S31. Optimized geometry for the 2S+1 = 1 and (2S+1 = 3) states of (A) $[\mathbf{3} \cdot \text{Ni}]^{2+}$ and 2S+1 = 1, (2S+1 = 5) and [2S+1 = 3] states of (B) $[\mathbf{3} \cdot \text{Cu}]^{2+}$ at the uB3LYP level of theory. Selected bond lengths are given in Å and angle in degrees. ΔG is given relative to the singlet spin state in kcal/mol (including ZPE).



Figure S32. Optimized geometry for the 2S+1 = 2 state of (A) $[4 \cdot Ni]^+$ and 2S+1 = 2, (2S + 1 = 4) states of (B) $[4 \cdot Cu]^+$, at the uB3LYP level of theory. Selected bond lengths are given in Å and angle in degree. ΔG is given relative to the doublet spin state in kcal/mol (including ZPE).



Figure S33. Optimized geometry for the 2S+1 = 1 and (2S+1 = 3) states of (A) $[4 \cdot Ni]^{2+}$ and 2S+1 = 1, (2S+1 = 5) and [2S+1 = 3] states of (B) $[4 \cdot Cu]^{2+}$ at the uB3LYP level of theory. Selected bond lengths are given in Å and angle in degrees. ΔG is given relative to the singlet spin state in kcal/mol (including ZPE).



Figure S34. Calculated spin-density distribution plots of (A) **3**•Cu, (B) [**3**•Cu]⁺ and (C) [**3**•Cu]²⁺. Positive (blue) and negative (green) spin densities are shown at the isodensity level of 0.001 electrons/bohr.



Figure S35. Calculated spin-density distribution plots of (A) $4 \cdot Cu$, (B) $[4 \cdot Cu]^+$, and (C) $[4 \cdot Cu]^{2+}$ Positive (blue) and negative (green) spin densities are shown at the isodensity level of 0.001 electrons/bohr.



Figure S36. Calculated spin-density distribution plots of (A) $[3 \cdot Ni]^+$ and (B) $[3 \cdot Ni]^{2+}$ positive (blue) and negative (green) spin densities are shown at the isodensity level of 0.001 electrons/bohr.



Figure S37. Relative spin-state energies of singlet (1) and triplet (3) states of $[4 \bullet Ni]^{2+}$ as calculated using unrestricted uB3LYP functional in DFT. All the ΔE and $\Delta E+ZPE$ values are relative to singlet (1) state.



Figure S38. Electronic absorption spectra (curved line, left axis) in CH_2Cl_2 and oscillator strength (vertical line, right axis) obtained from TD-DFT calculations at the uB3LYP/6-31G**/LANL2DZ level of theory for (A) [**3**•Cu]⁺ and (B) [**3**•Cu]²⁺.



Figure S39. Electronic absorption spectra (curved line, left axis) in CH_2Cl_2 and oscillator strength (vertical line, right axis) obtained from TD-DFT calculations at the uB3LYP/6-31G**/LANL2DZ level of theory for (A) [4•Ni]SbF₆ and (B) [4•Ni](SbF₆)₂.



Figure S40. Electronic absorption spectra (curved line, left axis) in CH_2Cl_2 and oscillator strength (vertical line, right axis) obtained from TD-DFT calculations at the uB3LYP/6-31G**/LANL2DZ level of theory for (A) [4•Cu]SbF₆ and (B) [4•Cu](SbF₆)₂.



Figure S41. Electronic absorption spectra (curved line, left axis) in CH_2Cl_2 and oscillator strength (vertical line, right axis) obtained from TD-DFT calculations at the uB3LYP/6-31G**/LANL2DZ level of theory for (A) [**2**•Ni]SbF₆ and (B) [**2**•Ni](SbF₆)₂. The spectra has been taken from reference 1a.



Figure S42. Electronic absorption spectra (curved line, left axis) in CH_2Cl_2 and oscillator strength (vertical line, right axis) obtained from TD-DFT calculations at the uB3LYP/6-31G**/LANL2DZ level of theory for (A) [**2**•Cu]SbF₆ and (B) [**2**•Cu](SbF₆)₂. The spectra has been taken from reference 1a.



Figure S43. (A) Energy profile of **2**•Ni, **3**•Ni, and **4**•Ni; (B) Kohn-Sham orbital representations of the HOMOs and LUMOs (isovalue = 0.020).



Figure S44. Kohn-Sham orbital representations of the HOMOs and LUMOs (isovalue = 0.020) of 1e-oxidised complexes.



Figure S45. Kohn-Sham orbital representations of the HOMOs and LUMOs (isovalue = 0.020) of 2e-oxidised complexes.

	3 ∙Ni	4 •Cu.C ₆ H ₁₄	4•Cu.CH ₂ Cl ₂
Formula	C ₈₉ H ₉₆ Cl ₂ Ni ₂ N ₁₀	C ₉₅ H ₁₀₈ Cl ₂ N ₁₀ Cu ₂ O ₂	C90H96Cl4 N10Cu2O2
Т (К)	100(2)	100(2)	100(2)
Formula weight	1494.07	1619.89	1618.64
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P-1	P 21/C	P 21/n
<i>a,</i> Å	14.646(6)	13.663(3) Å	14.8325(13) Å
<i>b,</i> Å	15.152(6)	24.416(6) Å	27.771(2) Å
<i>c,</i> Å	21.438(8)	25.603(6) Å	19.6630(16) Å
lpha , deg	74.290(10)	90	90
eta, deg	55.570(10)	104.301(6)	92.232(3)
γ, deg	63.779(7)	90	90
<i>V,</i> Å ³	4084(3)	8276(3)	8093.4(12)
Ζ	2	4	4
dcalcd, g•cm ⁻³	1.215	1.300	1.328
μ , mm ⁻¹	0.577	0.635	0.713
F(000)	1580	3424	3392
Crystal size, mm ³	0.160 x 0.150 x 0.100	0.160 x 0.140 x	0.180 x 0.140 x
		0.100	0.100
No. of unique data	15176	15391	14254
Completeness to theta = 25.00°	99.8 %	99.8 %	99.8 %
No of parameters refined	944	1018	990
GOF on F ²	1.058	1.121	1.044
R1 ^a [/> 2σ(/)]	0.1388	0.1167	0.0566
R1ª (all data)	0.2051	0.1784	0.1784
wR2 ^b (all data)	0.3157	0.2525	0.1484
Largest diff. peak and hole	1.241 and -0.939 e.Å ⁻³	0.876 and -0.911 e.Å ⁻³	1.747 and -1.343 e.Å ⁻³

Table S1. Crystallographic Data and Data Collection Parameters.

$${}^{a}R1 = \frac{\Sigma ||F_{o}| - |F_{c}||}{\Sigma |F_{o}|}; \quad {}^{b}wR2 = \sqrt{\frac{\Sigma [w(F_{o}^{2} - F_{c}^{2})^{2}]}{\Sigma [w(F_{o}^{2})^{2}]}}$$

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