

Push-Pull Quinoidal Porphyrins

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General Experimental Information

All reagents were used as supplied from the manufacturer unless, in the case of solvents, they were required to be moisture and oxygen-free, in which case they were distilled off calcium hydride (dichloromethane, 1,2-dichloroethane, toluene, dimethylformamide and triethylamine), or sodium/benzophenone (tetrahydrofuran). Phosphorus oxychloride was distilled directly under nitrogen. Air- and moisture-sensitive reactions were carried out using standard Schlenk line techniques.

Flash column chromatography was carried out on silica gel 60 GF₂₅₄, with the crude material applied to the column using the 'dry loading' technique (in which the sample is absorbed onto a minimum of silica prior to loading). All eluent compositions have been reported by volume ratio of their component solvents.

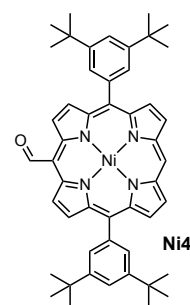
Thin layer chromatography (TLC) was carried out using aluminum-backed silica gel 60 F₂₅₄ plates. Electronic absorption spectra were recorded using a Perkin Elmer Lambda 20 spectrometer (glass cell, 1 cm path length). Infrared spectra were recorded using a Perkin Elmer 1750 FT-IR spectrometer, with the sample mounted as a KBr disc. NMR spectra were recorded at ambient probe temperature on Varian 200 MHz, Bruker 400 MHz or Bruker 500 MHz instruments. Samples were dissolved in CDCl₃, CD₂Cl₂ or d₈-THF, with the residual protonated solvent providing internal calibration for δ_H/δ_C as follows: 7.27/77.0 ppm (CDCl₃), 5.32/54.0 ppm (CD₂Cl₂) and 3.58/67.6 ppm (d₈-THF). The vast majority of the mass spectra were recorded at the EPSRC National Mass Spectrometry Service Centre, using a Voyager-DE-STR for MALDI-TOF, and a Finnigan MAT900 for ESI, EI, CI and FAB. Oxford-based mass spectrometry was carried out using a Micromass Tof Spec 2E for MALDI-TOF, and a Micromass LCT for ESI. X-ray crystal structures were determined at Daresbury Laboratory using Station 9.8 of the SRS synchrotron facility.

Electrochemical measurements were performed at room temperature, under nitrogen, using a custom-built Autolab Potentiostat. Nitrogen-saturated dichloromethane was used as the solvent, along with tetrabutylammonium tetrafluoroborate (0.1 M) as the supporting electrolyte. A 3 mm glassy carbon working electrode was used, along with a platinum wire counter-electrode and a Ag/Ag⁺ pseudo-reference electrode. Ferrocene was used as an internal standard, with its first oxidation taken as 0.00 V (the ferrocene oxidation occurred at ca. 250 mV against the pseudo-reference electrode). The scan rate was 0.1 V/s for cyclic voltammetry, and 20 mV/s for normal pulse and square wave voltammetries. Prior to the analysis of each sample, the working electrode was polished using Micropolish II powdered alumina (1.0 μ m and 0.3 μ m particle size, manufactured by Buehler).

Experimental Synthetic Procedures

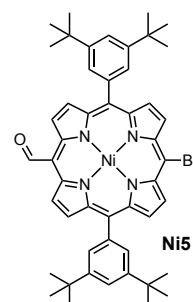
Preparation of Ni4

This known compound was prepared using a slight modification of the published procedures.¹⁻³ POCl₃ (5.0 mL, 54 mmol) was added dropwise to DMF (5.0 mL, 65 mmol) under argon, at 0 °C with stirring. The resulting pale orange formylating solution was then stirred at room temperature for 30 min. A suspension of **Ni3** (1.30 g, 1.75 mmol) in 1,2-dichloroethane (100 mL) was added dropwise to the formylating solution with stirring at 50 °C. After 2 h, the mixture was cooled to 0 °C and cautiously quenched with saturated aqueous NaOAc (100 mL). The layers were separated, the organic layer washed with saturated aqueous NaOAc (2 × 100 mL), water (100 mL) and the solvents removed by evaporation. Flash chromatography (4:1 petroleum ether (bp 40–60 °C) : CH₂Cl₂) and recrystallization from CH₂Cl₂ by layered addition of methanol afforded **Ni4** (1.10 g, 82%) in purple, crystalline form. UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 419 (5.36), 544 (4.15), 590 (4.30) nm. IR (KBr): ν_{max} 2958, 2864, 1680 cm⁻¹. ¹H NMR (200 MHz, CDCl₃): δ_{H} 12.14 (1 H, s, CHO), 9.88 (2 H, d, *J* 5.0, β H), 9.69 (1 H, s, meso H), 9.04 (2 H, d, *J* 5.0, β H), 8.98 (2 H, d, *J* 5.0, β H), 8.81 (2 H, d, *J* 5.0, β H), 7.88 (4 H, d, *J* 1.8, *o*-aryl H), 7.81 (2 H, t, *J* 1.8, *p*-aryl H), 1.55 (36 H, s, *t*-Bu H). ¹³C NMR (50.3 MHz, CDCl₃): δ_{C} 193.1, 149.3, 144.5, 144.2, 141.6, 141.3, 139.1, 135.6, 133.0, 132.6, 130.3, 128.7, 121.8, 121.6, 108.4, 106.2, 35.0, 31.7. MS (MALDI-TOF): *m/z* 771.8 (M+H⁺, C₄₉H₅₃N₄ONi requires 771.4).



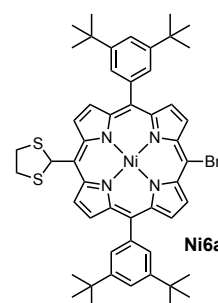
Preparation of Ni5

Ni4 (1.30 g, 1.68 mmol) was dissolved in CHCl₃ (30 mL) and pyridine (1 mL). The mixture was stirred at 0 °C while NBS (330 mg, 1.85 mmol) was added in small portions. The mixture was stirred at room temperature for 1 h before acetone (5 mL) was added and the solvents removed by evaporation. Flash chromatography (4:1 petroleum ether (bp 60–80 °C) : CH₂Cl₂) and then recrystallization from CH₂Cl₂ by layered addition of methanol afforded **Ni5** (1.26 g, 88%) in purple, crystalline form. *R*_f 0.56 (1:1 petroleum ether (bp 40–60 °C) : CH₂Cl₂). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 317 (4.28), 427 (5.35), 555 (4.04), 598 (4.29) nm. IR (KBr): ν_{max} 2962, 1687 cm⁻¹. ¹H NMR (200 MHz, CDCl₃): δ_{H} 11.96 (1 H, s, formyl H), 9.72 (2 H, d, *J* 5.0, β H), 9.37 (2 H, d, *J* 5.0, β H), 8.84 (2 H, d, *J* 5.0, β H), 8.65 (2 H, d, *J* 5.0, β H), 7.78 (6 H, m, aryl H), 1.50 (36 H, s, *t*-Bu H). ¹³C NMR (50.3 MHz, CDCl₃): δ_{C} 192.5, 149.4, 144.8, 144.7, 141.4, 141.2, 138.5, 135.9, 134.0, 133.2, 130.9, 128.6, 122.5, 121.7, 107.8, 106.1, 35.0, 31.7. MS (MALDI-TOF): *m/z* 848.6 (M⁺, C₄₉H₅₁N₄OBrNi requires 848.3).



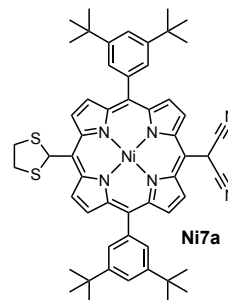
Preparation of Ni6a

Ni5 (915 mg, 1.08 mmol), 1,2-ethanedithiol (4.2 mL, 50 mmol) and Na₂CO₃ (1.0 g) were stirred in CH₂Cl₂ (40 mL) under argon at 40 °C. TiCl₄ (0.40 mL, 0.90 M in CH₂Cl₂, 0.36 mmol) was added causing the purple mixture to become red almost immediately. After 15 min, the mixture was cooled to 0 °C, quenched with aqueous NaOH (10 mL, 0.25 M) and the layers separated. The organic layer was washed with aqueous NaOH (6 × 20 mL, 0.25 M) and water (20 mL). The solvents were evaporated and the crude product purified by eluting through silica (5:1 petroleum ether (bp 40–60 °C) : CH₂Cl₂). Recrystallization from CH₂Cl₂ by layered addition of methanol afforded **Ni6a** (803 mg, 81%) in red, crystalline form. *R*_f 0.55 (3:2 petroleum ether (bp 60–80 °C) : CH₂Cl₂). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 304 (4.26), 425 (5.39), 543 (4.23), 576 (3.83) nm. IR (KBr): ν_{max} 2961, 2867 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ_{H} 9.70 (2 H, d, *J* 5.0, β H), 9.43 (2 H, d, *J* 5.0, β H), 8.76 (4 H, m, β H), 7.82 (4 H, d, *J* 2.0, *o*-aryl H), 7.77 (2 H, t, *J* 2.0, *p*-aryl H), 7.66 (1 H, s, CHS₂), 4.05 (2 H, m, C₂H₄), 3.81 (2 H, m, C₂H₄), 1.52 (36 H, s, *t*-Bu H). ¹³C NMR (100 MHz, CDCl₃): δ_{C} 149.2, 143.2, 142.3, 141.6 (two coincident signals), 139.0, 133.5, 133.4, 133.3, 131.3, 128.6, 121.4, 120.5, 109.1, 102.9, 56.2, 41.8, 35.0, 31.7. MS (FAB+): *m/z* 924.2 (M⁺, C₅₁H₅₅N₄S₂BrNi requires 924.2).



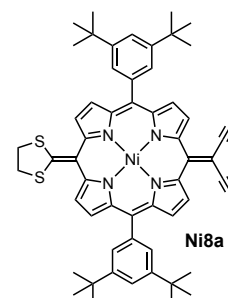
Preparation of Ni7a

THF (50 mL) was added to a mixture of **Ni6a** (190 mg, 0.205 mmol), malononitrile (76.0 mg, 1.15 mmol), Pd₂(dba)₃ (19 mg, 21 μmol), PPh₃ (27 mg, 0.10 mmol), CuI (7.9 mg, 41 μmol) and NaH (124 mg, 3.10 mmol, 60% in mineral oil) under argon, producing a red solution which turned green almost immediately. The solution was heated to reflux for 90 min then cooled, quenched with CHCl₃/0.5% HOAc (40 mL) and washed with aqueous HOAc (3 × 50 mL, 0.1 M). Flash chromatography (3:2 petroleum ether (bp 60–80 °C) : CH₂Cl₂) afforded **Ni7a** (150 mg, 79%) as a purple solid, which was unstable and therefore characterized without recrystallization. *R*_f 0.36 (1:1 petroleum ether (bp 60–80 °C) : CH₂Cl₂). UV/vis (CH₂Cl₂): λ_{max} (log ε) 309 (4.20), 425 (5.29), 546 (4.12), 587 (4.00) nm. IR (KBr): ν_{max} 2960, 2206 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ_H 9.77 (2 H, d, *J* 5.2, βH), 9.34 (2 H, d, *J* 5.2, βH), 8.94 (2 H, d, *J* 5.2, βH), 8.83 (2 H, d, *J* 5.2, βH), 7.86 (4 H, d, *J* 1.4, *o*-aryl *H*), 7.83 (2 H, t, *J* 1.4, *p*-aryl *H*), 7.64 (1 H, s, CHS₂), 6.95 (1 H, s, CH(CN)₂), 4.07 (2 H, m, C₂H₄), 3.82 (2 H, m, C₂H₄), 1.56 (36 H, s, *t*-Bu *H*). ¹³C NMR (100 MHz, CDCl₃): δ_C 149.3, 142.6, 142.4, 142.1, 139.3, 138.5, 135.0, 133.6, 132.2, 128.5, 127.5, 121.6, 121.3, 113.5, 111.5, 99.0, 55.9, 41.8, 34.9, 31.6, 26.8. MS (FAB+): *m/z* 910.3 (M⁺, C₅₄H₅₆N₆S₂Ni requires 910.3).



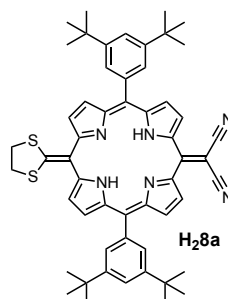
Preparation of Ni8a

DDQ (25 mg, 0.11 mmol) was added to a stirred solution of **Ni7a** (75 mg, 82 μmol) in CH₂Cl₂ (3 mL) at room temperature. The purple solution became dark green as the reaction proceeded. After 10 min, the solvent was evaporated and the crude product purified by flash chromatography (10:1 petroleum ether (bp 60–80 °C) : EtOAc). Precipitation from CH₂Cl₂/petroleum ether (bp 60–80 °C) afforded **Ni8a** as a black powder (50 mg, 67%). *R*_f 0.13 (4:1 petroleum ether (bp 60–80 °C) : EtOAc). UV/vis (CH₂Cl₂): λ_{max} (log ε) 306 (4.35), 371 (4.64), 415 (4.72), 461 (4.98), 683 (4.68) nm. IR (KBr): ν_{max} 2961, 2209 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ_H 7.56 (2 H, t, *J* 1.6, *p*-aryl *H*), 7.44 (2 H, d, *J* 4.5, βH), 7.34 (6 H, m, *o*-aryl 4H, β2H), 7.00 (2 H, d, *J* 4.5, βH), 6.77 (2 H, d, *J* 4.5, βH), 3.66 (4 H, m, C₂H₄), 1.38 (36 H, s, *t*-Bu *H*). ¹³C NMR (100 MHz, CDCl₃): δ_C 158.4, 154.1, 150.8, 150.0, 143.6, 143.3, 140.3, 137.3, 135.6, 135.0, 129.5, 125.2, 124.7, 122.7, 121.6, 116.9, 113.4, 69.5, 39.9, 34.9, 31.4. MS (MALDI-TOF): *m/z* 908.2 (M⁺, C₅₄H₅₄N₆S₂Ni requires 908.3). Anal Calcd for C₅₄H₅₄N₆S₂Ni: C 71.28, H 5.98, N 9.24. Found C 71.00, H 5.95, N 8.88. Vapor diffusion of methanol into a solution of **Ni8a** in 1,2-dichloroethane afforded crystals from which an X-ray crystal structure was obtained.



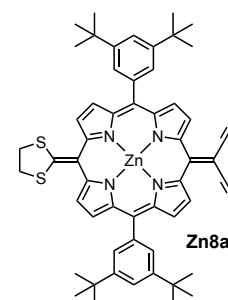
Preparation of H28a

Ni8a (21 mg, 23 μmol) and TFA/10% H₂SO₄ (3 mL) were stirred in CH₂Cl₂ (2 mL) for 2 min and then quenched with water (5 mL). The organic layer was washed with water (4 × 5 mL) and purified by flash chromatography (8:1 petroleum ether (bp 60–80 °C) : EtOAc). Precipitation from CH₂Cl₂/methanol afforded **H28a** as a black powder (16 mg, 81%). *R*_f 0.27 (4:1 petroleum ether (bp 60–80 °C) : EtOAc). UV/vis (CH₂Cl₂): λ_{max} (log ε) 295 (4.23), 361, (4.58), 411 (4.72), 434 (4.82), 475 (4.25), 613 (4.43) nm. IR (KBr): ν_{max} 3320, 2960, 2868, 2213 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ_H 12.23 (2 H, s, NH), 7.55 (2 H, br, *p*-aryl *H*), 7.42 (2 H, d, *J* 4.4, βH), 7.34 (4 H, d, *J* 1.6, *o*-aryl *H*), 7.15 (2 H, d, *J* 4.4, βH), 6.83 (2 H, d, *J* 4.4, βH), 6.73 (2 H, d, *J* 4.4, βH), 3.61 (4 H, s, C₂H₄), 1.37 (36 H, s, *t*-Bu *H*). ¹³C NMR (100 MHz, CDCl₃): δ_C 156.7, 155.2, 152.2, 149.9, 145.2, 143.6, 143.1, 141.5, 136.5, 131.6, 128.8, 125.7, 122.8, 122.3, 121.2, 116.1, 113.4, 75.5, 39.5, 34.9, 31.4. MS (FAB+): *m/z* 852.4 (M⁺, C₅₄H₅₆N₆S₂ requires 852.4). HR MS (accurate mass, ESI+): *m/z* 853.4076 (M+H⁺, C₅₄H₅₇N₆S₂ requires 853.4081).



Preparation of Zn8a

Zn(OAc)₂·2H₂O (36 mg, 0.16 mmol) was dissolved in methanol (0.6 mL) and added to a stirred solution of **H28a** (15 mg, 18 μmol) in CHCl₃ (5 mL). After 5 min the solvents were evaporated and the crude product eluted with CHCl₃/1% pyridine through a silica frit. Precipitation from CH₂Cl₂/petroleum ether (bp 60–80 °C) afforded **Zn8a** as a purple powder (15 mg, 93 %). *R*_f 0.72 (1:1 petroleum ether (bp 40–60 °C) : EtOAc). UV/vis (CH₂Cl₂): λ_{max} (log ε) 302 (4.29), 365 (4.63), 428 (4.57), 456 (5.05), 639 (4.68) nm. IR (KBr): ν_{max} 2961, 2207 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ_H 7.51 (2 H, t, *J* 2.0, *p*-aryl *H*), 7.48 (2 H, d, *J* 4.4, βH), 7.33 (4 H, br, *o*-aryl *H*), 7.23 (2 H, d, *J* 4.4, βH), 6.86 (2 H, d, *J* 4.4, βH), 6.68 (2 H, d, *J* 4.4, βH), 3.52 (4 H, s, C₂H₄), 1.36 (36 H, s, *t*-Bu *H*). ¹³C

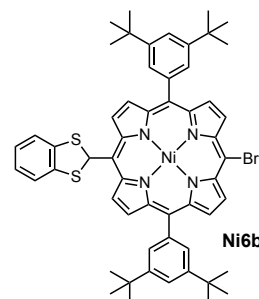


NMR (100 MHz, CDCl₃): δ_c 161.6, 153.9, 153.1, 149.4, 147.6, 147.0, 146.1, 143.8, 138.0, 133.7, 129.3, 125.5, 122.7, 122.0, 120.8, 117.9, 116.1, 71.0, 39.7, 34.8, 31.5. MS (FAB+): m/z 914.5 (M⁺, C₅₄H₅₄N₆S₂Zn requires 914.3). Vapor diffusion of methanol into a solution of **Zn8a** in CHCl₃ afforded crystals.

Preparation of Ni6b

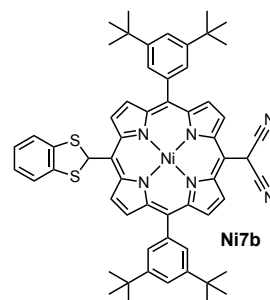
Ni5 (955 mg, 1.12 mmol), 1,2-benzenedithiol (1.09 g, 7.66 mmol) and Na₂CO₃ (1.7 g) were stirred in CH₂Cl₂ (20 mL) under argon at 40 °C. TiCl₄ (50 μ L, 2.2 M in CH₂Cl₂, 0.11 mmol) was then added causing the purple reaction mixture to become red almost immediately. After 20 min the mixture was cooled to 0 °C, quenched with aqueous NaOH (5 mL, 0.25 M) and the layers separated. The organic layer was washed with aqueous NaOH (3 $\times$ 10 mL, 0.25 M) and water (10 mL). The solvents were evaporated and the crude product purified by eluting through silica (5:1 petroleum ether (bp 40–60 °C) : CH₂Cl₂, some neat CH₂Cl₂ was required to dissolve the crude). Recrystallization from CH₂Cl₂ by layered addition of methanol afforded

Ni6b (1.01 g, 92%) as red crystals. R_f 0.60 (4:1 petroleum ether (bp 60–80 °C) : CH₂Cl₂). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 302 (4.55), 425 (5.42), 544 (4.31), 580 (4.00) nm. IR (KBr): ν_{max} 2961, 2862 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): δ_H 9.84 (2 H, d, J 5.0, βH), 9.44 (2 H, d, J 5.0, βH), 8.77 (4 H, m, βH), 8.73 (1 H, s, CHS₂), 7.83 (4 H, d, J 1.6, o -aryl H), 7.77 (2 H, t, J 1.6, p -aryl H), 7.27 (2 H, m, dithio aryl H), 7.20 (2 H, m, dithio aryl H), 1.52 (36 H, s, t -Bu H). ¹³C NMR (100 MHz, CDCl₃): δ_c 149.2, 143.4, 142.3, 141.8, 141.7, 138.9, 138.1, 133.7, 133.5, 133.5, 130.9, 128.6, 126.4, 121.5, 121.4, 121.0, 108.2, 103.3, 56.3, 35.0, 31.7. MS (MALDI-TOF): m/z 972.2 (M⁺, C₅₅H₅₅N₄S₂BrNi requires 972.2).



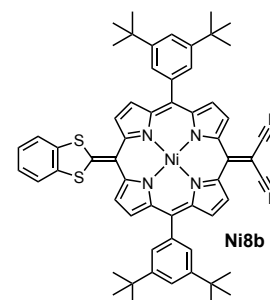
Preparation of Ni7b

THF (45 mL) was added to a mixture of **Ni6b** (200 mg, 0.210 mmol), malononitrile (95 mg, 1.4 mmol), Pd₂(dba)₃ (18 mg, 20 μ mol), PPh₃ (26 mg, 0.10 mmol), CuI (7.6 mg, 40 μ mol) and NaH (120 mg, 3.00 mmol, 60% in mineral oil) under argon, producing a red solution which turned green almost immediately. The solution was heated to reflux for 1 h then cooled, quenched with CHCl₃/0.5% HOAc (40 mL) and washed with aqueous HOAc (3 $\times$ 50 mL, 0.1 M). Flash chromatography (3:1 petroleum ether (bp 60–80 °C) : EtOAc) afforded **Ni7b** (83 mg, 42%) as a purple solid, which was unstable and therefore characterized without recrystallization. R_f 0.25 (3:1 petroleum ether (bp 60–80 °C) : EtOAc). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 307 (4.35), 424 (5.34), 547 (4.19), 588 (4.11) nm. IR (KBr): ν_{max} 2961, 2213 cm⁻¹. ¹H NMR (500 MHz, CDCl₃): δ_H 9.85 (2 H, d, J 5.3, βH), 9.31 (2 H, d, J 5.3, βH), 8.91 (2 H, d, J 5.3, βH), 8.79 (2 H, d, J 5.3, βH), 8.67 (1 H, s, CHS₂), 7.81 (4 H, t, J 1.5, o -aryl H), 7.79 (2 H, t, J 1.5, p -aryl H), 7.28 (2 H, m, dithio aryl H), 7.21 (2 H, m, dithio aryl H), 6.91 (1 H, s, CH(CN)₂), 1.51 (36 H, s, t -Bu H). ¹³C NMR (125 MHz, CDCl₃): δ_c 149.4, 142.8, 142.6, 142.2, 139.4, 138.4, 137.9, 135.2, 133.9, 131.8, 128.6, 127.8, 126.6, 121.8, 121.7, 121.4, 113.5, 110.6, 99.4, 55.9, 35.0, 31.5, 26.8. MS (FAB+): m/z 959.3 (M⁺, C₅₈H₅₆N₆S₂Ni requires 959.3).



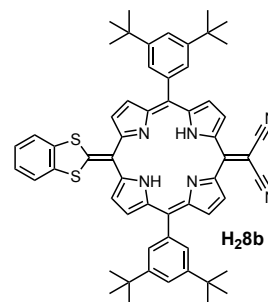
Preparation of Ni8b

DDQ (20 mg, 88 μ mol) was added to a stirred solution of **Ni7b** (69 mg, 72 μ mol) in CH₂Cl₂ (3 mL) at room temperature. The purple solution became olive green as the reaction proceeded. After 10 min the solvent was evaporated and the crude product purified by flash chromatography (25:1 petroleum ether (bp 60–80 °C) : EtOAc). Precipitation from CH₂Cl₂/petroleum ether (bp 60–80 °C) afforded **Ni8b** as a black powder (65 mg, 94%). R_f 0.43 (5:1 petroleum ether (bp 60–80 °C) : EtOAc). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 312 (4.27), 377 (4.53), 436 (4.73), 469 (4.87), 523 (4.16), 562 (4.12), 686 (4.50), 747 (4.73) nm. IR (KBr): ν_{max} 2960, 2207 cm⁻¹. ¹H NMR (500 MHz, CDCl₃): δ_H 7.57 (2 H, t, J 1.5, p -aryl H), 7.53 (2 H, d, J 4.6, βH), 7.51 (2 H, d, J 4.6, βH), 7.50 (2 H, m, dithio aryl H), 7.36 (4 H, br, o -aryl H), 7.32 (2 H, m, dithio aryl H), 7.13 (2 H, d, J 4.6, βH), 6.85 (2 H, d, J 4.6, βH), 1.39 (36 H, s, t -Bu H). ¹³C NMR (125 MHz, CDCl₃): δ_c 152.0, 152.0, 150.0, 149.9, 143.7, 142.5, 140.2, 137.0, 137.0, 135.8, 135.4, 129.9, 127.0, 125.3, 123.5, 122.7, 122.4, 122.0, 117.0, 110.2, 69.7, 34.9, 31.5. MS (FAB+): m/z 956.3 (M⁺, C₅₈H₅₄N₆S₂Ni requires 956.3). MS (accurate mass, EI+): m/z 956.3190 (M⁺, C₅₈H₅₄N₆S₂Ni requires 956.3205). Anal Calcd for C₅₈H₅₄N₆S₂Ni: C 72.72, H 5.68, N 8.77. Found C 71.84, H 5.69, N 8.42.



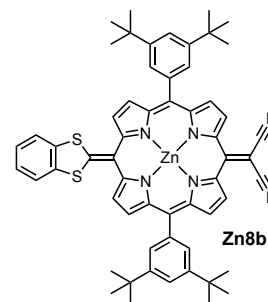
Preparation of H₂8b

Ni8b (10 mg, 10 μ mol) and TFA/10% H₂SO₄ (1.5 mL) were stirred in CH₂Cl₂ (2 mL) for 2 min and then quenched with water (5 mL). The organic layer was washed with water (4 $\times$ 5 mL) and purified by flash chromatography (25:2 petroleum ether (bp 60–80 $^{\circ}$ C) : EtOAc). Precipitation from CH₂Cl₂/petroleum ether (bp 60–80 $^{\circ}$ C) afforded **H₂8b** as a black powder (8.0 mg, 85%). *R_f* 0.43 (5:1 petroleum ether (bp 60–80 $^{\circ}$ C) : EtOAc). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 303 (4.27), 368 (4.59), 441 (4.88), 498 (4.28), 530 (4.25), 724 (4.59) nm. IR (KBr): ν_{max} 3318, 2963, 2869, 2214 cm⁻¹. ¹H NMR (500 MHz, CDCl₃): δ_{H} 11.94 (2 H, s, NH), 7.57 (2 H, t, *J* 1.8, *p*-aryl *H*), 7.49 (2 H, d, *J* 4.5, β H), 7.43 (2 H, m, dithio aryl *H*), 7.36 (4 H, d, *J* 1.8, *o*-aryl *H*), 7.31 (2 H, d, *J* 4.5, β H), 7.26 (2 H, m, dithio aryl *H*), 6.94 (2 H, d, *J* 4.5, β H), 6.79 (2 H, d, *J* 4.5, β H), 1.39 (36 H, s, *t*-Bu *H*). ¹³C NMR (125 MHz, CDCl₃): δ_{C} 155.0, 151.7, 150.0, 149.6, 145.3, 143.7, 142.9, 141.3, 136.8, 136.7, 132.2, 129.2, 126.7, 125.9, 122.9, 122.1, 121.5, 121.2, 116.2, 110.6, 75.9, 34.9, 31.5. MS (accurate mass, ESI⁺): *m/z* 901.4089 (M+H⁺, C₅₈H₅₇N₆S₂ requires 901.4086). Vapor diffusion of pentane into a solution of **H₂8b** in 1,2-dichloroethane afforded crystals from which an X-ray crystal structure was obtained.



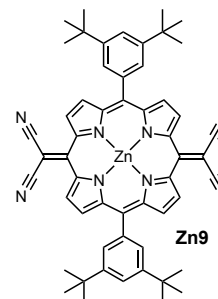
Preparation of Zn8b

This compound was prepared as reported previously.⁴ Zn(OAc)₂·2H₂O (24 mg, 0.11 mmol) was dissolved in methanol (0.4 mL) and added to a stirred solution of **H₂8b** (8.0 mg, 8.9 μ mol) in CHCl₃ (4 mL). After 10 min the solvents were removed by evaporation and the crude product purified by flash chromatography (8:1 petroleum ether (bp 60–80 $^{\circ}$ C) : EtOAc). Precipitation from CH₂Cl₂/petroleum ether (bp 60–80 $^{\circ}$ C) afforded **Zn8b** in dark green, microcrystalline form (7.0 mg, 82 %). *R_f* 0.43 (4:1 petroleum ether (bp 60–80 $^{\circ}$ C) : EtOAc). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 308 (4.21), 373 (4.55), 462 (5.06), 504 (4.33), 666 (4.55), 719 (4.58) nm. IR (KBr): ν_{max} 2963, 2863, 2209 cm⁻¹. ¹H NMR (500 MHz, CDCl₃/1% d₅-pyridine): δ_{H} 7.55 (2 H, d, *J* 4.3, β H), 7.53 (2 H, t, *J* 2.0, *p*-aryl *H*), 7.37 (8 H, m, dithio aryl 2*H*, *o*-aryl 4*H*, β 2*H*), 7.22 (2 H, m, dithio aryl *H*), 6.96 (2 H, d, *J* 4.3, β H), 6.75 (2 H, d, *J* 4.3, β H), 1.38 (36 H, s, *t*-Bu *H*). ¹³C NMR (125 MHz, CDCl₃/1% d₅-pyridine): δ_{C} 159.6, 153.4, 149.4, 147.7, 147.3, 146.8, 146.1, 143.6, 138.1, 137.1, 134.0, 129.7, 126.4, 125.6, 122.0, 121.8, 121.3, 121.1, 117.9, 113.2, 71.4, 34.8, 31.5. MS (FAB⁺): *m/z* 962.5 (M⁺, C₅₈H₅₄N₆S₂Zn requires 962.3). Vapor diffusion of methanol into a solution of **Zn8b** in CHCl₃ afforded crystals from which an X-ray crystal structure was obtained (this has already been reported).



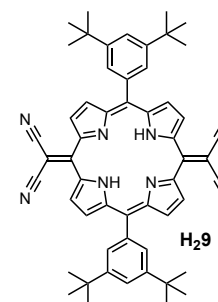
Preparation of Zn9

This compound was prepared as reported previously.⁴ **Zn12** (423 mg, 0.466 mmol), malononitrile (308 mg, 4.66 mmol), Pd₂(dba)₃ (43 mg, 0.047 mmol), PPh₃ (49 mg, 0.19 mmol) and CuI (18 mg, 0.093 mmol) were dissolved in THF (150 mL) and pyridine (1.5 mL) under an inert atmosphere. The solution was degassed and sodium hydride then added as a 60% in oil (279 mg, 6.99 mmol). The reaction was heated to reflux for 15 h. On completion, acetic acid (0.4 mL, 7.0 mmol) was added and the mixture then poured into silica and the solvents removed under reduced pressure. The silica residue was then loaded onto a silica column and the product isolated by eluting with CH₂Cl₂. Crystallization from CH₂Cl₂ by layered addition of petroleum ether (bp 30–40 $^{\circ}$ C) yielded the pure product **Zn9** as dark green crystals (300 mg, 53%). UV/vis (CH₂Cl₂): λ_{max} (log ϵ) 309 (4.28), 458 (4.83), 637 (4.79) nm. IR (KBr): ν_{max} 2216 cm⁻¹. ¹H NMR (500 MHz, CDCl₃): δ_{H} 7.55 (2H, t, *J* 1.6, *p*-aryl *H*), 7.25 (4H, d, *J* 1.6, *o*-aryl *H*), 7.06 (4H, d, *J* 4.4, β H), 6.56 (4H, d, *J* 4.4, β H), 1.36 (36 H, s, *t*-Bu *H*). ¹³C NMR (125 MHz, CDCl₃): δ_{C} 155.7, 154.1, 153.8, 150.3, 147.7, 136.9, 133.5, 125.1, 123.7, 121.9, 115.3, 76.5, 35.1, 31.6. MS (FAB⁺): *m/z* 876 (MH⁺). Anal Calcd for C₅₄H₅₀N₈Zn·H₂O: C 72.51, H 5.86, N 12.53. Found C 72.21, H 5.70, N 12.34. The crystal structure has already been reported.



Preparation of H₂9

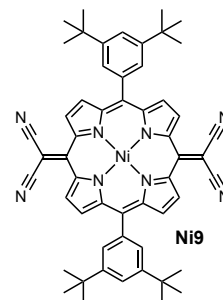
Zinc 5,15-bis(3,5-di-*tert*-butylphenyl)-10,20-bis(dicyanomethylene)porphyrin **Zn9** (140 mg, 0.160 mmol) was dissolved in CH₂Cl₂ (50 mL) and trifluoroacetic acid (1.2 mL, 0.016 mol) added. The reaction was stirred for 15 min at room temperature then was washed with water (4 $\times$ 50 mL), the organic phase reduced to 3 mL, and the product precipitated by layered addition of 1% water in methanol to give a dull green solid (118 mg, 91%). mp > 250 $^{\circ}$ C. UV/vis (CH₂Cl₂): λ_{max} (log ϵ): 412 (4.76), 568 (4.53) nm. IR (KBr): ν_{max} 2219 cm⁻¹ (CN). ¹H NMR (500 MHz, CDCl₃): δ_{H} 13.86 (2H, s, NH), 7.60 (2H, t, *J* 1.6, *p*-aryl *H*), 7.26 (4H, d, *J* 1.6 *o*-aryl *H*), 7.19 (4H, d, *J* 4.5, β H), 6.68 (4H, d, *J* 4.5, β H), 1.36 (36 H, s, *t*-Bu *H*). ¹³C NMR (125 MHz, CDCl₃): δ_{C} 153.0, 150.9, 147.5, 135.5, 131.8, 125.7, 124.5,



122.7, 114.4, 79.7, 35.2, 31.6. FAB-MS (NOBA): m/z 814.4 (M^+ , $C_{54}H_{52}N_8$ requires 814.06). Crystals were obtained from aqueous methanol, and an X-ray crystal structure obtained.

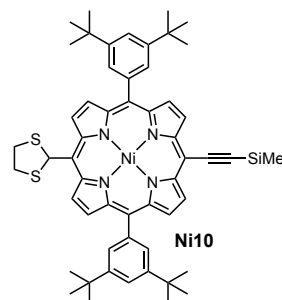
Preparation of Ni9

5,15-Bis(3,5-di-*tert*-butylphenyl)-10,20-bis(dicyanomethylene) porphyrin **H29** (10 mg, 0.0123 mmol) was dissolved in chloroform (4 mL) and nickel acetate tetrahydrate (30 mg, 0.123 mmol) added in methanol (1 mL). The reaction was heated to reflux for 20 min and the reaction mixture then passed through a short silica plug. The solvents were removed and the product crystallized from chloroform by layered addition of methanol. Yield (11 mg, 99%). mp > 250 °C. UV/vis (CH_2Cl_2): λ_{max} (log ϵ): 321 (4.31), 458 (4.77), 615 (4.34) nm. IR (KBr): ν_{max} 2217 cm^{-1} (CN). 1H NMR (500 MHz, $CDCl_3$) δ_H 7.57 (t, 2H, J 1.7 Hz), 7.21 (br, 4H), 6.87 (d, 4H, J 4.5 Hz), 6.48 (d, 4H, J 4.5 Hz), 1.36 (s, 36H). ^{13}C NMR (125 MHz, $CDCl_3$) δ_C 154.9, 152.5, 151.3, 148.8, 142.9, 134.5, 134.4, 124.7, 122.4, 114.6, 75.8, 35.4, 31.8. MS (APCI+): m/z 869.4 [M^+], $C_{54}H_{50}N_8Ni$ requires 869.71.



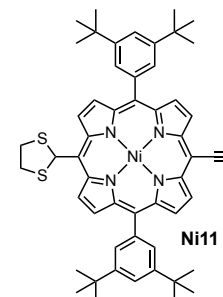
Preparation of Ni10

Toluene (40 mL) and Et_3N (35 mL) were added to **Ni6a** (500 mg, 0.540 mmol), $Pd_2(dba)_3$ (17 mg, 19 μ mol), PPh_3 (30 mg, 0.11 mmol) and CuI (8.0 mg, 42 μ mol) under argon. The solution was degassed, trimethylsilylacetylene (0.40 mL, 2.8 mmol) was added, and the mixture was heated with stirring at 40 °C for 2 h. After cooling to room temperature, the solution was washed with water (2 $\times$ 50 mL). Flash chromatography (60:1 petroleum ether (bp 60–80 °C): $EtOAc$) and recrystallization from CH_2Cl_2 by layered addition of methanol afforded **Ni10** (410 mg, 80%) as red crystals. R_f 0.35 (3:1 petroleum ether (bp 40–60 °C) : CH_2Cl_2). UV/vis (CH_2Cl_2): λ_{max} (log ϵ) 432 (5.49), 553 (4.28), 593 (4.25) nm. IR (KBr) ν_{max} 2948, 2865, 2144, 1591 cm^{-1} . 1H NMR (400 MHz, $CDCl_3$) δ_H 9.76 (2 H, d, J 5.1, βH), 9.52 (2 H, d, J 5.1, βH), 8.84 (2 H, d, J 5.1, βH), 8.82 (2 H, d, J 5.1, βH), 7.90 (4 H, d, J 1.8, *o*-aryl H), 7.82 (2 H, t, J 1.8, *p*-aryl H), 7.74 (1 H, s, CHS_2), 4.06 (2 H, m, $C_2H_4 H$), 3.81 (2 H, m, $C_2H_4 H$), 1.58 (36 H, s, *t*-Bu H), 0.62 (9 H, s, TMS). ^{13}C NMR (100 MHz, $CDCl_3$) δ_C 149.2, 144.3, 142.5, 142.1, 141.8, 139.2, 133.1, 133.1, 131.9, 131.1, 128.7, 121.4, 120.9, 110.2, 105.0, 102.6, 99.2, 56.3, 41.8, 35.1, 31.7, 0.3. MS (FAB+): m/z 942.5 (M^+ , $C_{56}H_{64}N_4S_2SiNi$ requires 942.4). Vapor diffusion of methanol into a solution of **Ni10** in 1,2-dichloroethane afforded crystals from which an X-ray crystal structure was obtained.



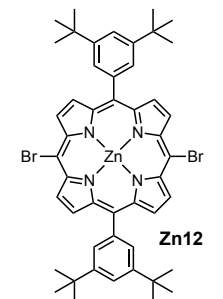
Preparation of Ni11

TBAF (1.0 M in THF, 0.64 mL, 0.64 mmol) was added to a stirred solution of **Ni10** (500 mg, 0.530 mmol) in CH_2Cl_2 (10 mL). After 2 min, water was added (10 mL) and the layers separated. The organic layer was washed with water (10 mL) and the solvent removed by evaporation. Flash chromatography (40:1 petroleum ether (bp 60–80 °C) : $EtOAc$) and precipitation from CH_2Cl_2 /petroleum ether (bp 60–80 °C) afforded **Ni11** (420 mg, 91%) as a purple powder. R_f 0.29 (3:1 petroleum ether (bp 40–60 °C) : CH_2Cl_2). UV/vis (CH_2Cl_2): λ_{max} (log ϵ) 309 (4.30), 429 (5.42), 550 (4.21), 590 (4.12) nm. IR (KBr): ν_{max} 3281, 2961, 2867, 2096, 1593 cm^{-1} . 1H NMR (500 MHz, $CDCl_3$) δ_H 9.73 (2 H, d, J 4.8, βH), 9.48 (2 H, d, J 4.8, βH), 8.81 (2 H, d, J 4.8, βH), 8.78 (2 H, d, J 4.8, βH), 7.86 (4 H, br, *o*-aryl H), 7.79 (2 H, br, *p*-aryl H), 7.71 (1 H, s, CHS_2), 4.07 (1 H, s, ethynyl H), 4.05 (2 H, m, $C_2H_4 H$), 3.81 (2 H, m, $C_2H_4 H$), 1.54 (36 H, s, *t*-Bu H). ^{13}C NMR (125 MHz, $CDCl_3$) δ_C 149.1, 144.3, 142.5, 142.0, 141.7, 139.0, 133.2, 133.0, 131.7, 131.1, 128.5, 121.3, 120.8, 110.3, 97.6, 84.5, 83.6, 56.2, 41.7, 34.9, 31.6. MS (MALDI-TOF): m/z 870.2 (M^+ , $C_{53}H_{56}N_4S_2Ni$ requires 870.3).



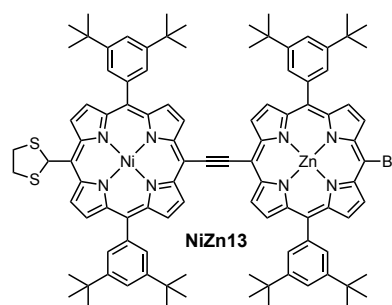
Preparation of Zn12

This known compound was prepared using a slight modification of the published procedure.^{3,6} 5,15-Bis(3,5-di-*tert*-butylphenyl)porphyrinato zinc(II) **Zn3** (400 mg, 0.533 mmol) was dissolved in $CHCl_3$ (60 mL) and pyridine (0.25 mL). The solution was cooled to 0 °C and *N*-bromosuccinimide (190 mg, 1.07 mmol) added. The reaction mixture was stirred for 15 min and then quenched with acetone (1 mL). The solvents were removed under reduced pressure and the residue washed with methanol to yield the pure product **Zn12** as a purple solid (412 mg, 85%). UV/vis (CH_2Cl_2 /1% pyridine): λ_{max} (log ϵ) 316 (4.32), 435 (5.61), 572 (4.23), 615 (4.18) nm. 1H NMR (500 MHz, $CDCl_3$ /1% d_5 -pyridine): δ_H 9.62 (4H, d, J 4.6, βH), 8.88 (4H, d, J 4.6, βH), 7.96 (4H, d, J 1.8, *o*-aryl H), 7.77 (2H, t, J 1.8, *p*-aryl H), 1.50 (36H, s, *t*-Bu H). ^{13}C NMR (125 MHz, $CDCl_3$ /1% d_5 -pyridine): δ_C 151.1, 150.0, 148.5, 141.7, 133.6, 132.7, 130.0, 123.3, 120.9, 104.6, 35.0, 31.8. MS (FAB+): m/z 908 (M^+ , $C_{48}H_{50}Br_2N_4Zn$ requires 908.14). Anal Calcd for $C_{48}H_{50}Br_2N_4Zn$: C 63.48, H 5.55, N 6.17. Found C 63.47, H 5.77, N 6.01.



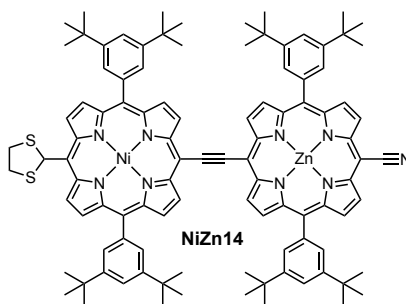
Preparation of NiZn13

Toluene (30 mL), Et₃N (30 mL) and pyridine (4 mL) were added to **Ni11** (110 mg, 0.126 mmol), **Zn12** (1.32 g, 1.45 mmol), Pd₂(dba)₃ (6.0 mg, 6.6 μmol), PPh₃ (8.0 mg, 30 μmol) and CuI (3.0 mg, 16 μmol) under argon. The solution was degassed, heated to 90 °C and stirred. After 2 h the reaction mixture was cooled, eluted with CH₂Cl₂ through a short plug of silica and the solvent evaporated to recover the crude product. Flash chromatography (initially 12:1 petroleum ether (bp 60–80 °C) : pyridine, to remove unreacted **Zn12** and then increasing the polarity to 6:1 petroleum ether (bp 60–80 °C): pyridine, to separate dimeric products) and precipitation from CHCl₃/petroleum ether (bp 60–80 °C) afforded **NiZn13** (65 mg, 30%) as a brown powder. *R*_f 0.32 (5:1 petroleum ether (bp 40–60 °C) : pyridine). UV/vis (CH₂Cl₂/1% pyridine): λ_{max} (log ε) 317 (4.55), 433 (5.12), 480 (5.40), 550 (4.32), 708 (4.86) nm. IR (KBr): ν_{max} 2962, 2172, 1593 cm⁻¹. ¹H NMR (500 MHz, CDCl₃/1% d₅-pyridine): δ_H 10.20 (2 H, d, *J* 4.8, βH), 10.13 (2 H, d, *J* 4.8, βH), 9.70 (2 H, d, *J* 4.8, βH), 9.67 (2 H, d, *J* 4.8, βH), 9.09 (2 H, d, *J* 4.8, βH), 8.94 (2 H, d, *J* 4.8, βH), 8.92 (2 H, d, *J* 4.8, βH), 8.76 (2 H, d, *J* 4.8, βH), 8.07 (4 H, d, *J* 1.8, *o*-aryl H), 7.89 (4 H, d, *J* 1.8, *o*-aryl H), 7.84 (2 H, t, *J* 1.8, *p*-aryl H), 7.77 (2 H, t, *J* 1.8, *p*-aryl H), 7.71 (1 H, s, CHS₂), 4.07 (2 H, m, C₂H₄ H), 3.83 (2 H, m, C₂H₄ H), 1.59 (36 H, s, *t*-Bu H), 1.53 (36 H, s, *t*-Bu H). ¹³C NMR (125 MHz, CDCl₃/1% d₅-pyridine): δ_C 153.0, 151.2, 150.2, 149.1, 148.4, 144.4, 142.4, 142.1, 141.9, 141.6, 139.1, 133.6, 133.3, 133.2, 133.0, 132.5, 131.8, 131.1, 130.5, 129.7, 128.5, 124.0, 123.5, 121.2, 121.1, 120.8, 109.7, 106.2, 102.7, 101.3, 100.1, 96.8, 56.2, 41.7, 34.9, 34.9, 31.7, 31.6. MS (MALDI-TOF): *m/z* 1694.5 (M⁺, C₁₀₁H₁₀₅N₈S₂NiZnBr requires 1694.6).



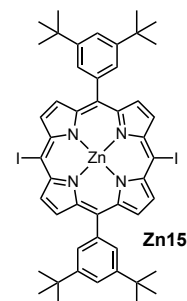
Preparation of NiZn14

THF (5 mL) was added to a mixture of **NiZn13** (20 mg, 12 μmol), malononitrile (100 mg, 1.51 mmol), Pd₂(dba)₃ (2.0 mg, 2.1 μmol), PPh₃ (3.0 mg, 11 μmol), CuI (1.0 mg, 5.2 μmol) and NaH (5.0 mg, 0.13 mmol, 60% in mineral oil) under argon. The solution was heated to reflux for 2 h, then cooled and quenched with CHCl₃/0.5% HOAc (5 mL). The mixture was washed with water (2 × 10 mL) and purified by flash chromatography (3:2 petroleum ether (bp 60–80 °C) : pyridine). Precipitation from CHCl₃/petroleum ether (bp 60–80 °C) afforded **NiZn14** (15 mg, 77%) as a brown powder. *R*_f 0.28 (5:1 petroleum ether (bp 40–60 °C) : pyridine). UV/vis (CH₂Cl₂/1% pyridine): λ_{max} (log ε) 312 (4.56), 446 (5.16), 481 (5.45), 553 (4.33), 709 (4.89) nm. IR (KBr): ν_{max} 2961, 2855, 2201, 1590 cm⁻¹. ¹H NMR (500 MHz, CDCl₃/1% d₅-pyridine): δ_H 10.20 (2 H, d, *J* 4.5, βH), 10.10 (2 H, d, *J* 4.5, βH), 9.71 (2 H, d, *J* 4.5, βH), 9.54 (2 H, d, *J* 4.5, βH), 9.04 (2 H, d, *J* 4.5, βH), 8.99 (2 H, d, *J* 4.5, βH), 8.93 (2 H, d, *J* 4.5, βH), 8.75 (2 H, d, *J* 4.5, βH), 8.02 (4 H, d, *J* 1.5, *o*-aryl H), 7.84 (4 H, d, *J* 1.5, *o*-aryl H), 7.82 (2 H, br, *p*-aryl H), 7.74 (2 H, br, *p*-aryl H), 7.67 (1 H, s, CHS₂), 4.04 (2 H, m, C₂H₄ H), 3.80 (2 H, m, C₂H₄ H), 1.54 (36 H, s, *t*-Bu H), 1.48 (36 H, s, *t*-Bu H). ¹³C NMR (125 MHz, CDCl₃/1% d₅-pyridine): δ_C 151.7, 151.6, 151.3, 150.8, 149.1, 148.6, 144.7, 142.7, 142.3, 141.0, 139.0, 135.6, 134.4, 133.8, 133.5, 133.2, 132.0, 131.9, 131.5, 131.1, 129.5, 125.4, 123.3, 121.3, 121.2, 121.1, 110.3, 104.7, 101.8, 100.3, 98.2, 85.2, 56.1, 41.7, 34.9, 34.9, 31.6, 31.5. MS (MALDI-TOF): *m/z* 1641.7 (M⁺, C₁₀₂H₁₀₅N₉S₂NiZn requires 1641.7). Vapor diffusion of methanol into a solution of **NiZn14** in CHCl₃/1% pyridine afforded crystals from which an X-ray crystal structure was obtained.



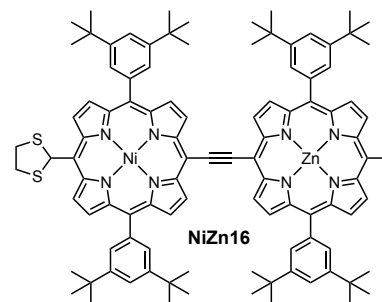
Preparation of Zn15

The bis-aryl porphyrin **Zn3** was iodinated using conditions reported by Wytke *et al.*⁷ A solution of iodine (91 mg, 0.36 mmol) in chloroform (10 mL) was added to a light-protected solution of trifluoroacetoxyiodobenzene (186 mg, 0.43 mmol) in chloroform (15 mL). Pyridine (1 mL) was then added to the solution which turned a pale yellow color over 15 min. This solution was then added slowly over several minutes to a solution of **Zn3** (180 mg, 0.24 mmol) in chloroform (75 mL) and the reaction mixture was stirred at room temperature for a further 1 h. The reaction mixture was washed with a saturated aqueous solution of sodium thiosulfate (100 mL), water (2 × 100 mL) and dried over magnesium sulfate. The solvent was removed and the residue washed with methanol to yield the pure product as a purple solid (211 mg, 88%). mp > 250 °C. UV/vis (1% C₅H₅N/CH₂Cl₂): λ_{max} (log ε) 319 (4.35), 436 (5.64), 440 (5.62), 578 (4.21), 623 (4.28) nm. ¹H NMR (500 MHz, CDCl₃/C₅D₅N): δ_H 9.68 (d, 4H, *J* 4.6 Hz), 8.86 (d, 4H, *J* 4.6 Hz), 7.97 (d, 4H, *J* 1.8 Hz), 7.80 (t, 2H, *J* 1.8 Hz), 1.54 (s, 36H). ¹³C NMR (125 MHz, CDCl₃/C₅D₅N): δ_C 152.4, 151.8, 148.5, 141.8, 137.7, 133.9, 130.1, 123.7, 121.0, 81.5, 35.2, 31.9. FAB-MS (NOBA): *m/z* 1002 (M⁺, C₄₈H₅₀I₂N₄Zn requires 1002.14). Anal Calcd for C₄₈H₅₀I₂N₄Zn: C 57.53, H 5.03, N 5.59. Found: C 56.76, H 5.05, N 5.39.



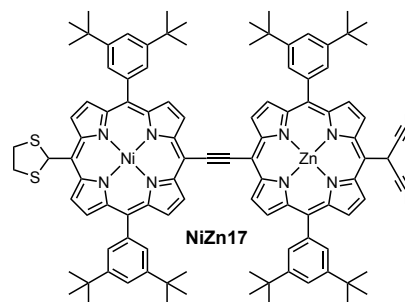
Preparation of NiZn16

THF (40 mL) and Et₃N (65 mL) were added to **Ni11** (222 mg, 0.255 mmol), **Zn15** (676 mg, 0.675 mmol), Pd₂(dba)₃ (8.0 mg, 8.7 μmol), PPh₃ (12 mg, 46 μmol) and CuI (3.0 mg, 16 μmol) under argon. The solution was degassed, heated to 50 °C and stirred. After 4 h, a mixture of Pd₂(dba)₃ (4.0 mg, 4.4 μmol), PPh₃ (6.0 mg, 23 μmol) and CuI (1.5 mg, 7.9 μmol) was dissolved in THF (0.3 mL) and added to the reaction, which was then stirred for a further 4 h before cooling to room temperature. The solvents were removed by evaporation without heating and the crude product was purified by eluting through silica (5:1, petroleum ether (bp 40–60 °C) : pyridine, 20 cm × 3 cm silica). Precipitation from CHCl₃/petroleum ether (bp 60–80 °C) afforded **NiZn16** (148 mg, 33%) as a brown powder. *R*_f 0.15 (5:1 petroleum ether (bp 40–60 °C) : pyridine). UV/vis (CHCl₃/1% pyridine): λ_{max} (log ε) 318 (4.58), 434 (5.11), 448 (5.09), 482 (5.41), 552 (4.31), 713 (4.88) nm. IR (KBr): ν_{max} 2958, 2180, 1594 cm⁻¹. ¹H NMR (500 MHz, CDCl₃/1% d₅-pyridine): δ_H 10.21 (2 H, br, βH), 10.15 (2 H, br, βH), 9.72 (2 H, d, *J* 4.5, βH), 9.71 (2 H, br, βH), 9.09 (2 H, d, *J* 4.5, βH), 8.95 (2 H, d, *J* 4.5, βH), 8.90 (2 H, d, *J* 4.5, βH), 8.78 (2 H, d, *J* 4.5, βH), 8.08 (4 H, br, *o*-aryl H), 7.91 (4 H, br, *o*-aryl H), 7.86 (2 H, br, *p*-aryl H), 7.79 (2 H, br, *p*-aryl H), 7.72 (1 H, s, CHS₂), 4.05 (2 H, br, C₂H₄ H), 3.82 (2 H, br, C₂H₄ H), 1.59 (36 H, s, *t*-Bu H), 1.54 (36 H, s, *t*-Bu H). ¹³C NMR (125 MHz, CDCl₃/1% d₅-pyridine): δ_C 152.8, 151.8, 150.3, 149.1, 148.4, 144.7, 142.7, 142.5, 142.2, 141.6, 139.1, 137.4, 134.6, 133.6, 133.5, 133.4, 132.1, 131.5, 130.6, 129.6, 128.5, 124.2, 121.3, 121.2, 120.8, 109.8, 102.6, 101.3, 100.4, 96.9, 83.0, 56.1, 41.7, 34.9, 34.9, 31.7, 31.6. MS (FAB⁺): *m/z* 1765.6 (M+Na⁺, C₁₀₁H₁₀₅N₈S₂NiZnNa requires 1765.5).



Preparation of NiZn17

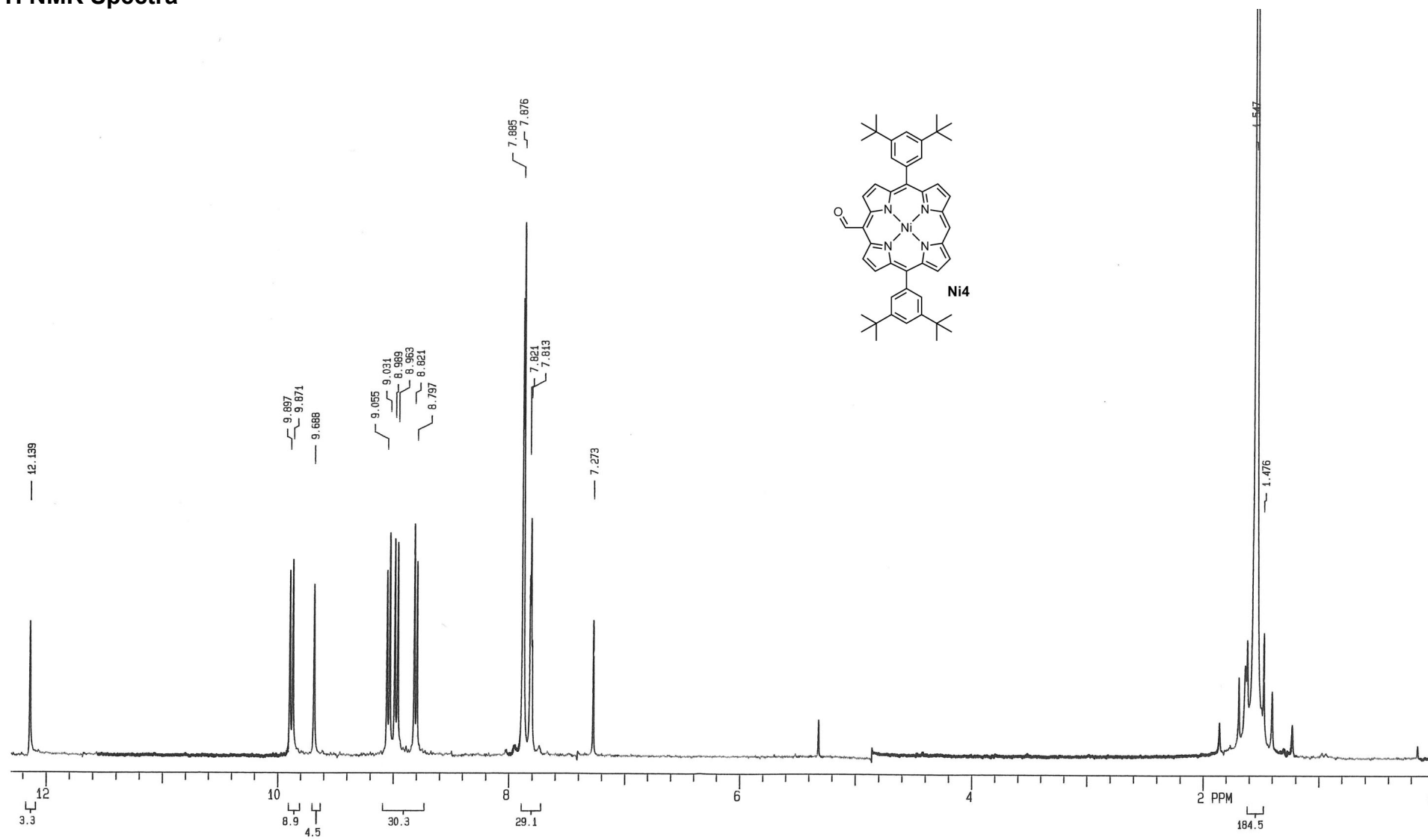
THF (5 mL) was added to a mixture of **NiZn16** (135 mg, 77 μmol), malononitrile (55 mg, 0.83 mmol), Pd₂(dba)₃ (10 mg, 11 μmol), PPh₃ (15 mg, 57 μmol), CuI (4.0 mg, 21 μmol) and NaH (60 mg, 1.5 mmol, 60% in mineral oil) under argon, producing a brown solution which became dark orange almost immediately. The solution was heated to reflux for 30 min, cooled to room temperature and quenched with aqueous HOAc (10 mL, 0.17 M). The solution was then extracted into CHCl₃ (10 mL) by washing with aqueous HOAc (aq) (3 × 10 mL, 0.17 M) and the solvents removed by evaporation. Flash chromatography (1:4 petroleum ether (bp 40–60 °C) : CHCl₃) and precipitation from CHCl₃/petroleum ether (bp 60–80 °C) afforded **NiZn17** (72 mg, 55%) as a black powder. *R*_f 0.15 (5:1 petroleum ether (bp 40–60 °C) : pyridine). UV/vis (CHCl₃)/nm: λ_{max} (log ε) 312 (4.50), 415 (5.09), 434 (5.12), 479 (5.40), 562 (4.34), 688 (4.84) nm. IR (KBr): ν_{max} 2958, 2171, 1592 cm⁻¹. ¹H NMR (400 MHz, d₈-THF) δ_H 10.29 (2 H, d, *J* 4.8, βH), 10.16 (2 H, d, *J* 4.8, βH), 9.79 (4 H, br, βH), 9.09 (2 H, d, *J* 4.8, βH), 9.06 (2 H, d, *J* 4.8, βH), 8.95 (2 H, d, *J* 4.8, βH), 8.70 (2 H, d, *J* 4.8, βH), 8.32 (1 H, s, CH(CN)₂), 8.17 (4 H, br, *o*-aryl H), 7.98 (6 H, br, *o*-aryl H, *p*-aryl H), 7.88 (2 H, br, *p*-aryl H), 7.80 (1 H, s, CHS₂), 4.08 (2 H, m, C₂H₄ H), 3.84 (2 H, m, C₂H₄ H), 1.62 (36 H, s, *t*-Bu H), 1.56 (36 H, s, *t*-Bu H). ¹³C NMR (125 MHz, d₈-THF) δ_C 153.8, 152.1, 150.4, 150.0, 149.8, 149.6, 145.5, 143.7, 143.7, 143.4, 142.9, 140.7, 134.9, 134.4, 134.0, 133.6, 132.6, 132.3, 130.6, 130.4, 129.7, 128.9, 125.4, 122.5, 122.4, 122.2, 116.6, 112.1, 104.4, 103.1, 102.8, 101.4, 98.8, 57.3, 42.6, 35.9, 32.2, 32.2, 28.8. MS (ESI⁻): *m/z* 1679.7 (M⁻H⁺, C₁₀₄H₁₀₅N₁₀S₂NiZn requires 1679.7).



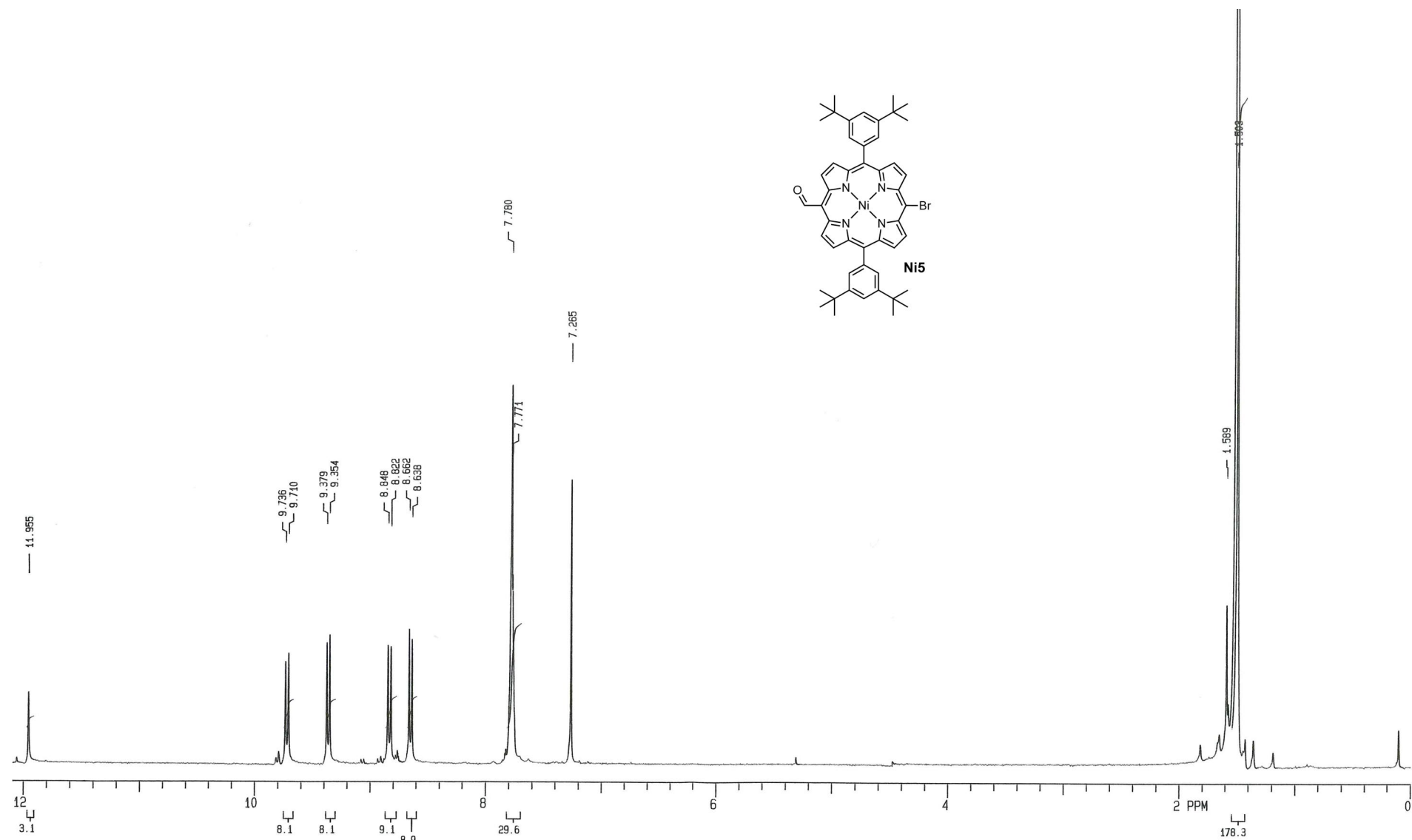
References

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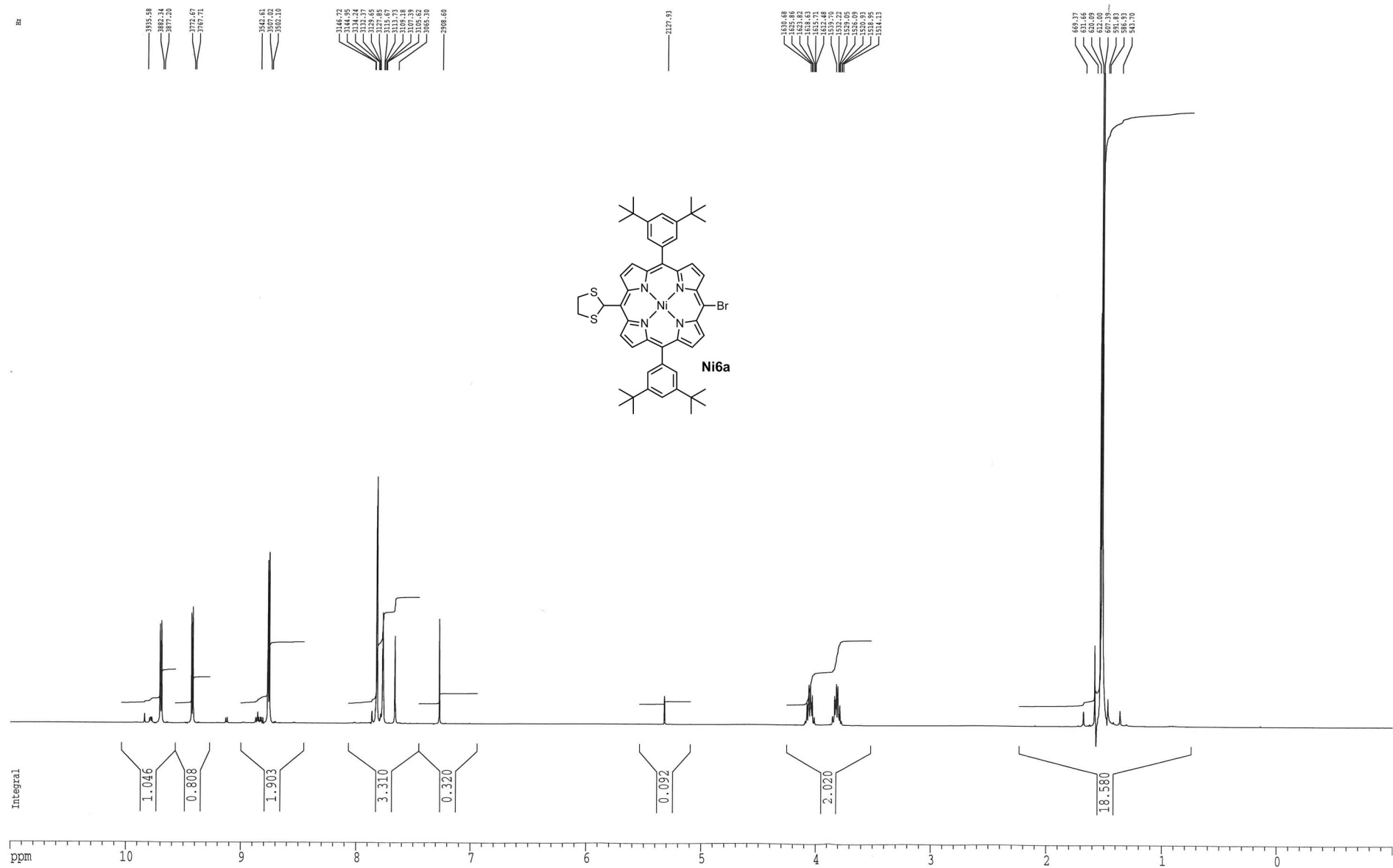
¹H NMR Spectra



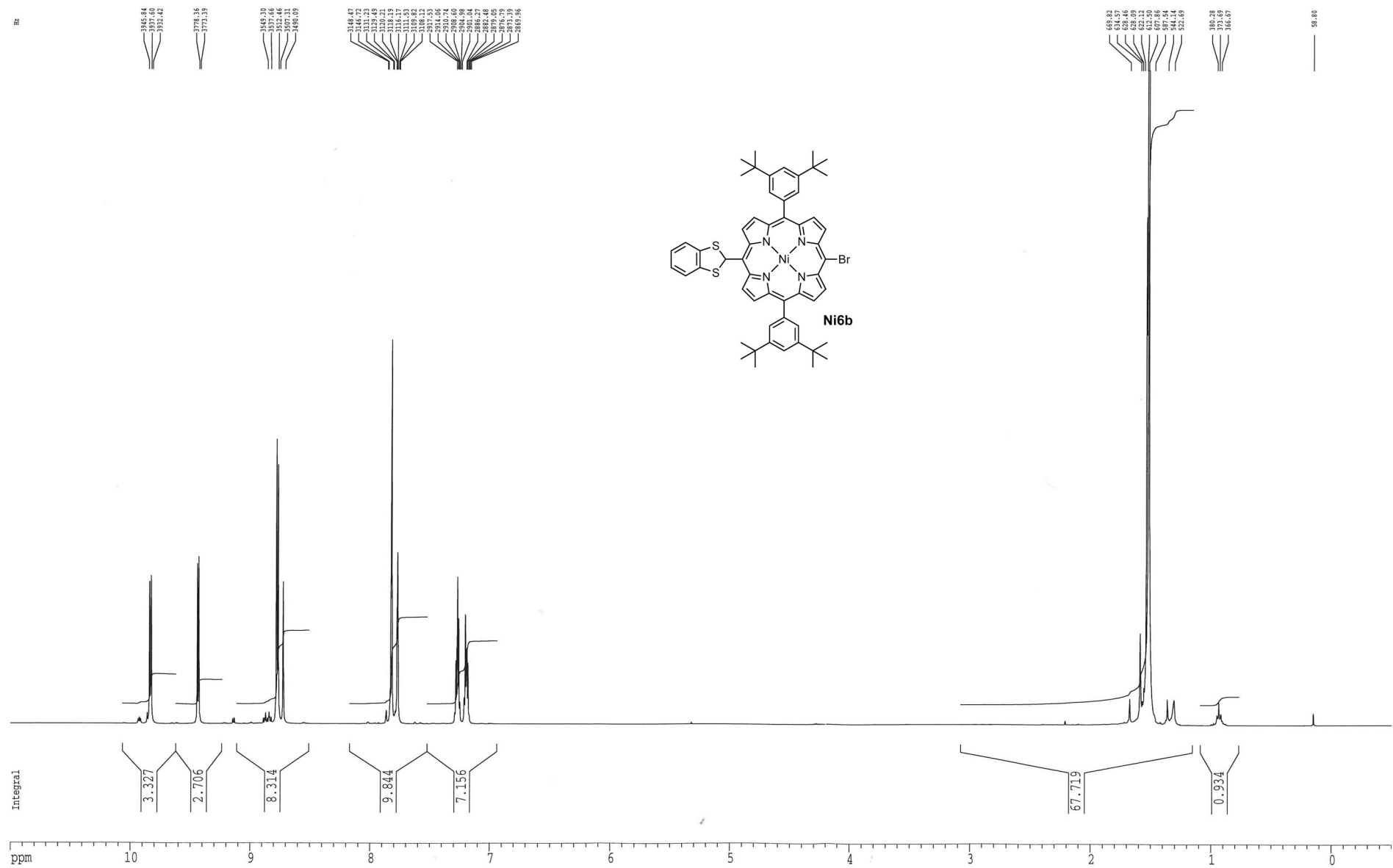
¹H NMR spectrum of **Ni4** (200 MHz, CDCl₃, 298 K)



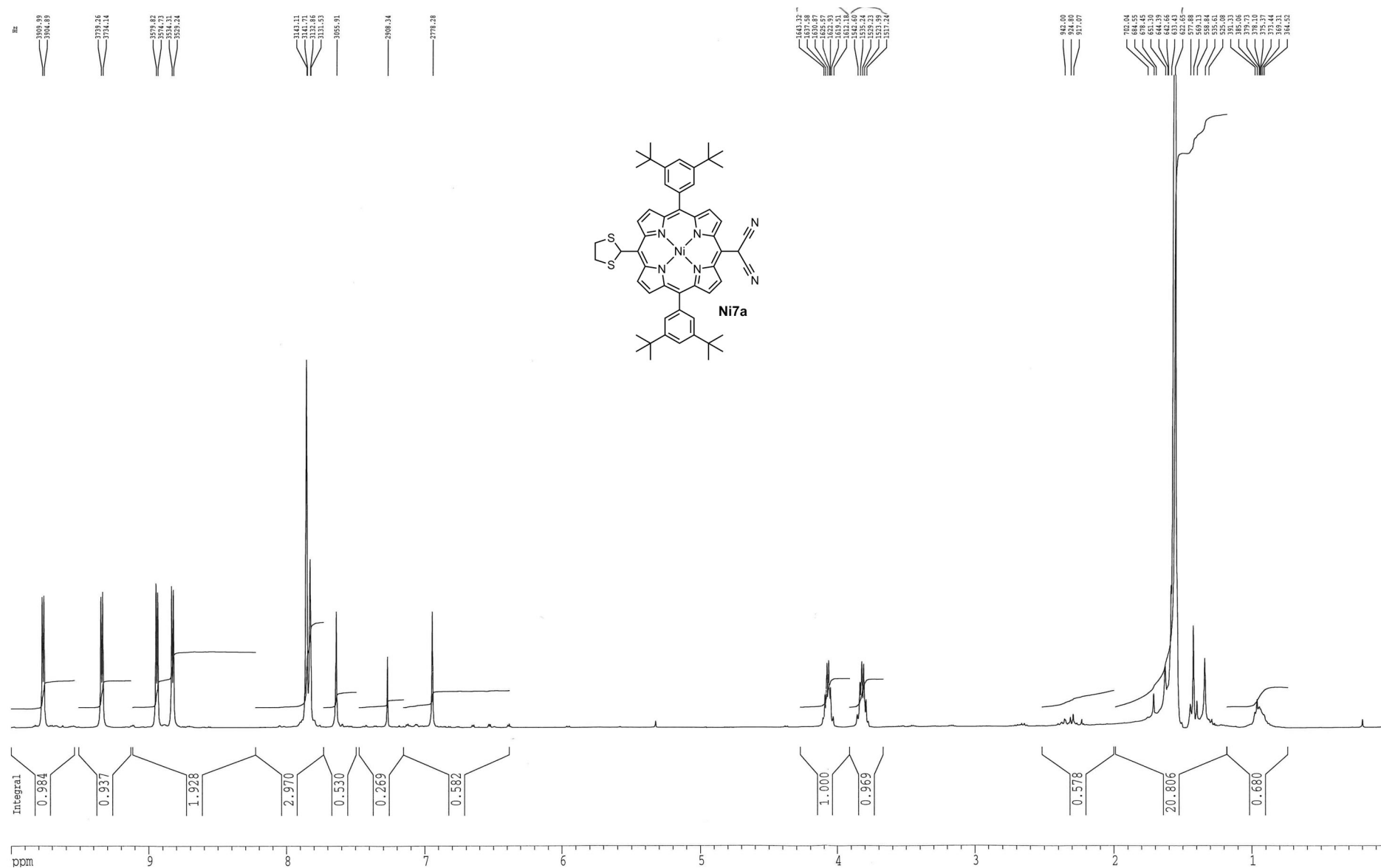
¹H NMR spectrum of **Ni5** (200 MHz, CDCl₃, 298 K)



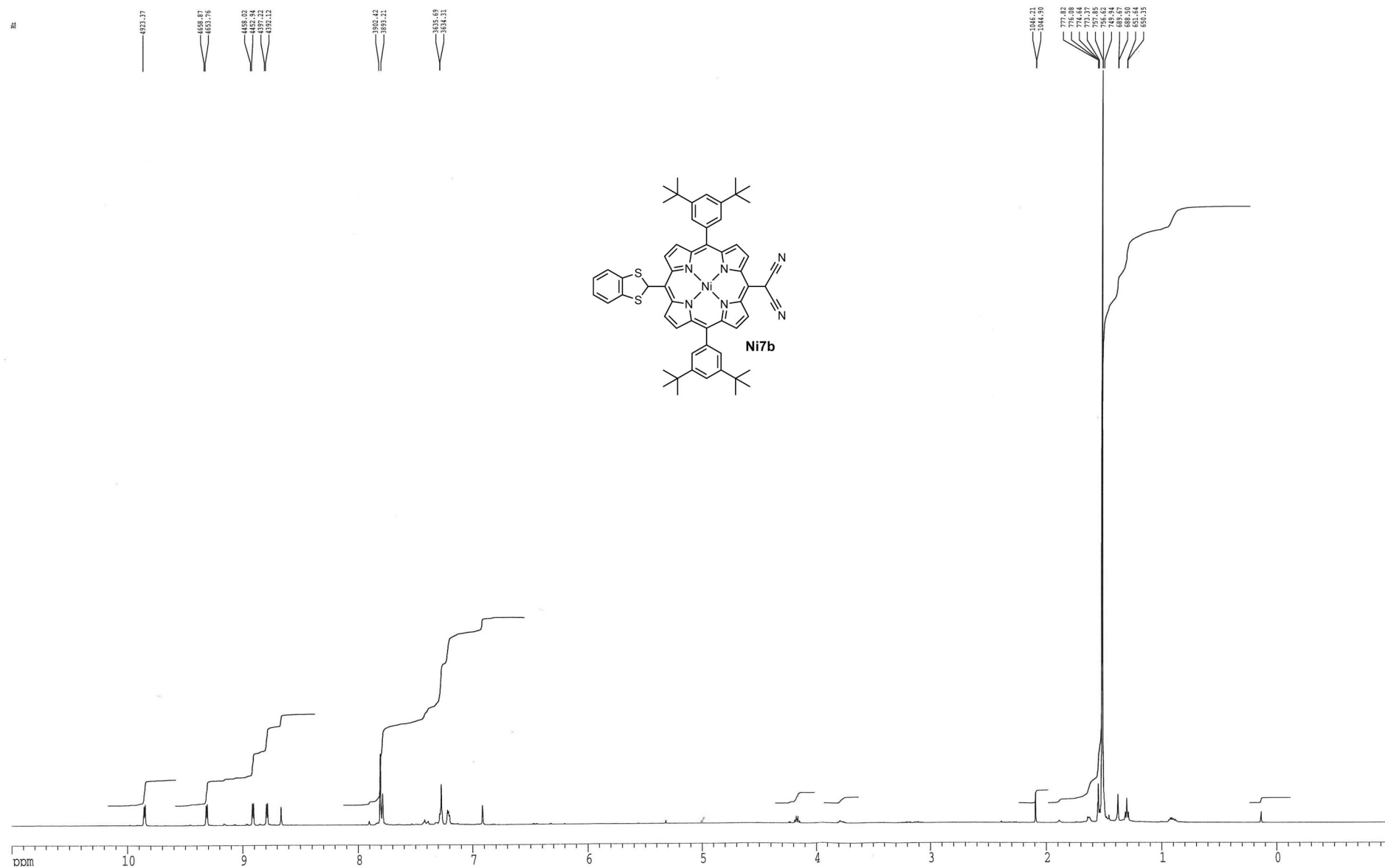
¹H NMR spectrum of **Ni6a** (400 MHz, CDCl₃, 298 K)



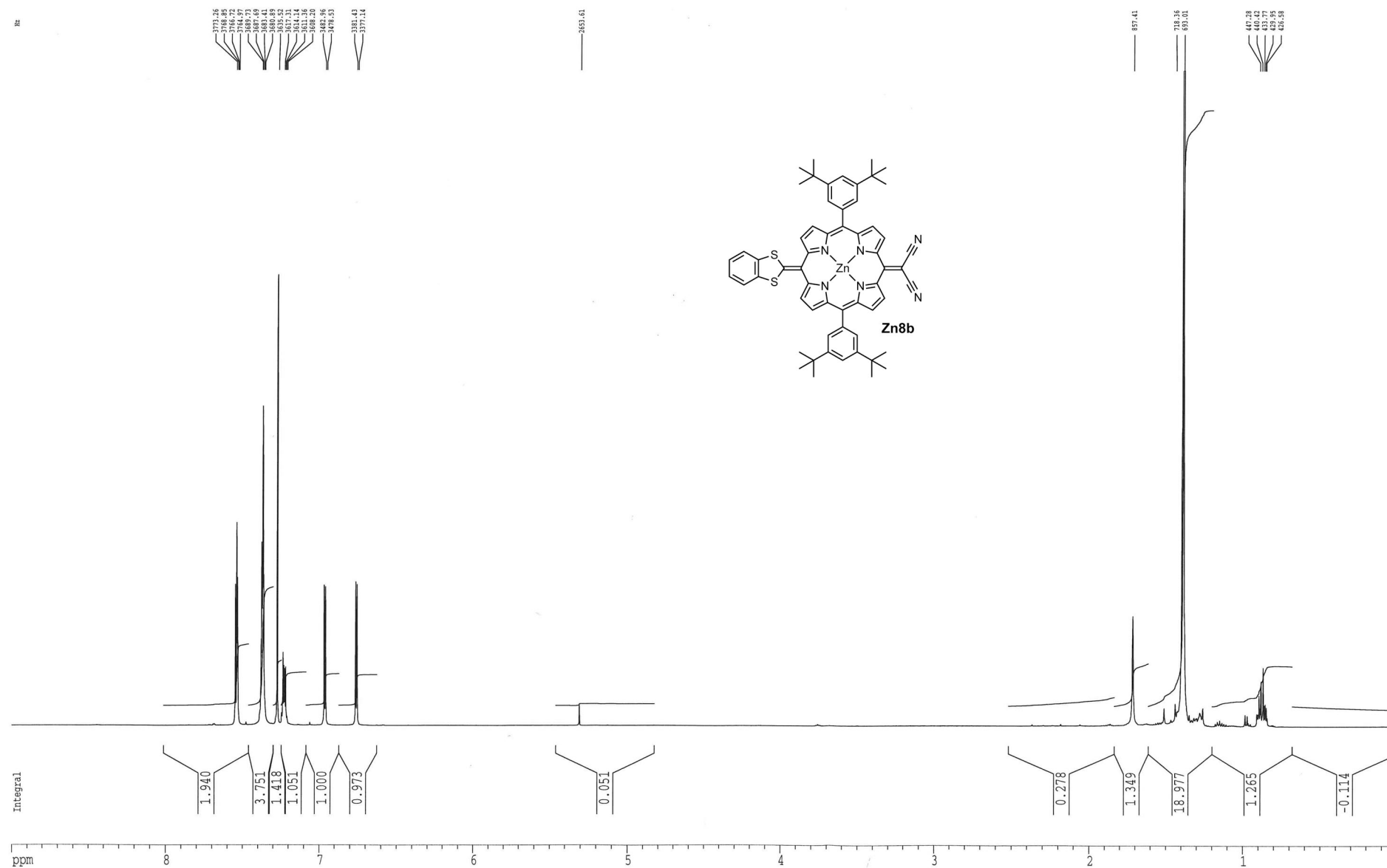
¹H NMR spectrum of **Ni6b** (400 MHz, CDCl₃, 298 K)



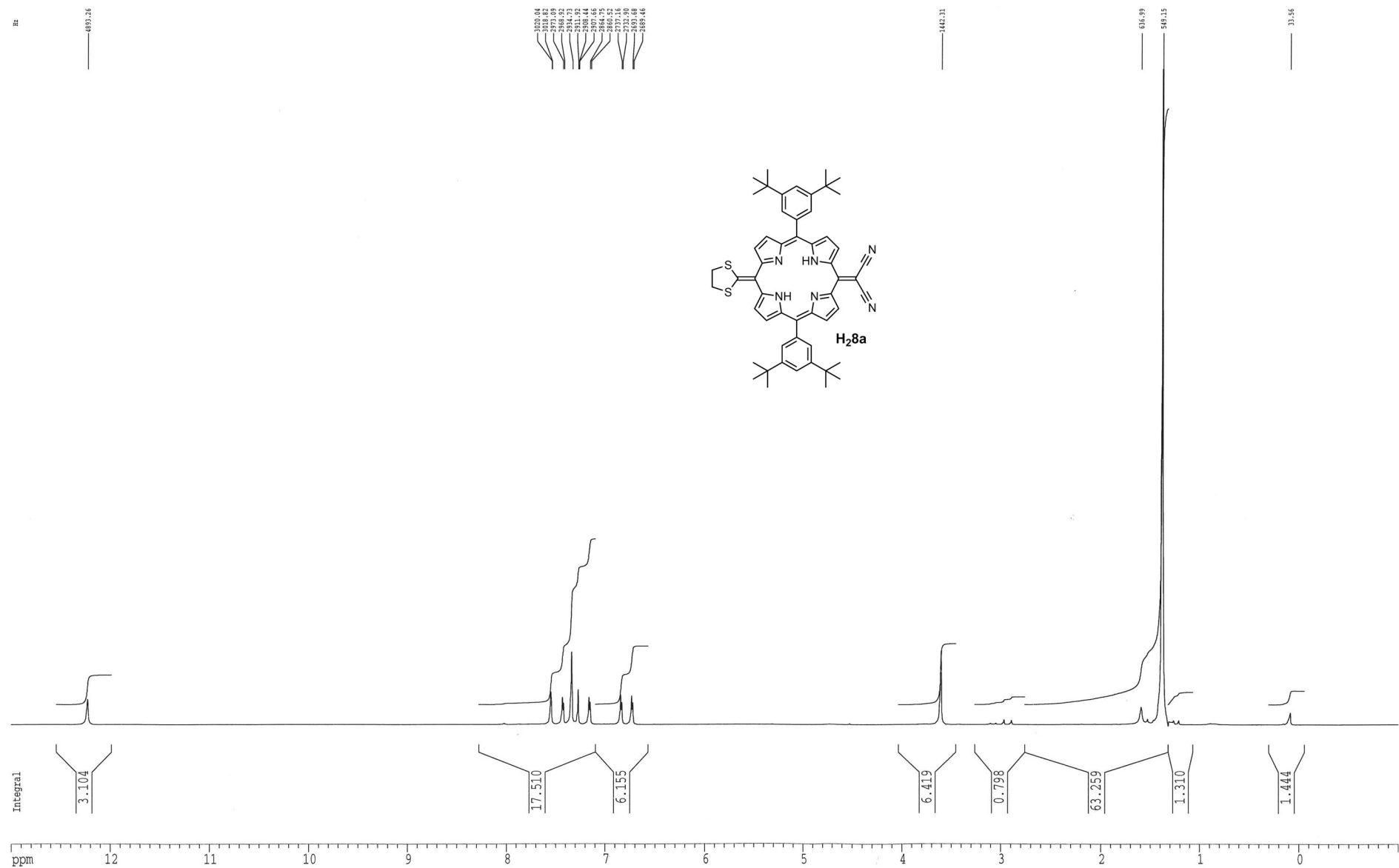
^1H NMR spectrum of **Ni7a** (400 MHz, CDCl_3 , 298 K)



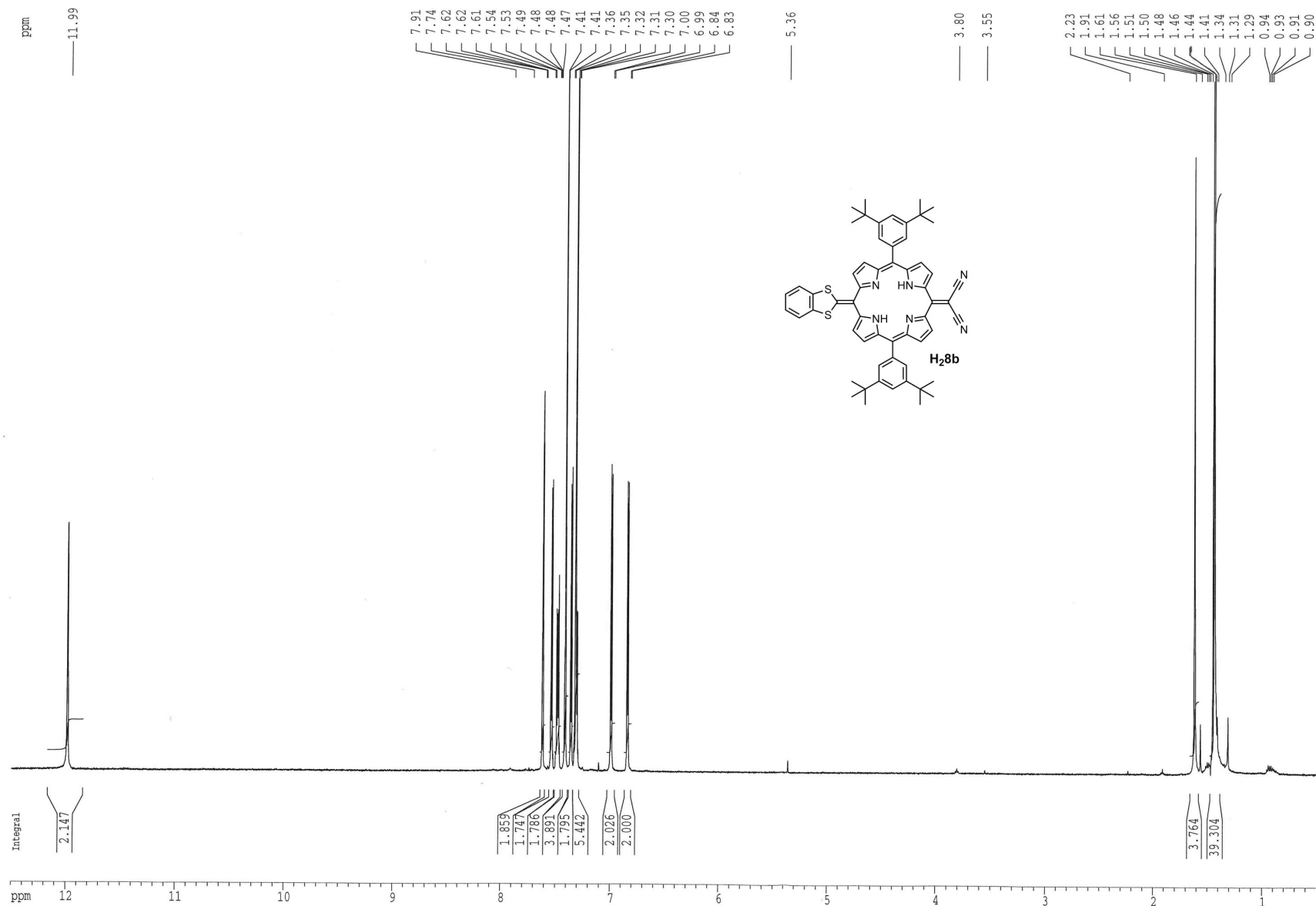
¹H NMR spectrum of Ni7b (500 MHz, CDCl₃, 298 K)



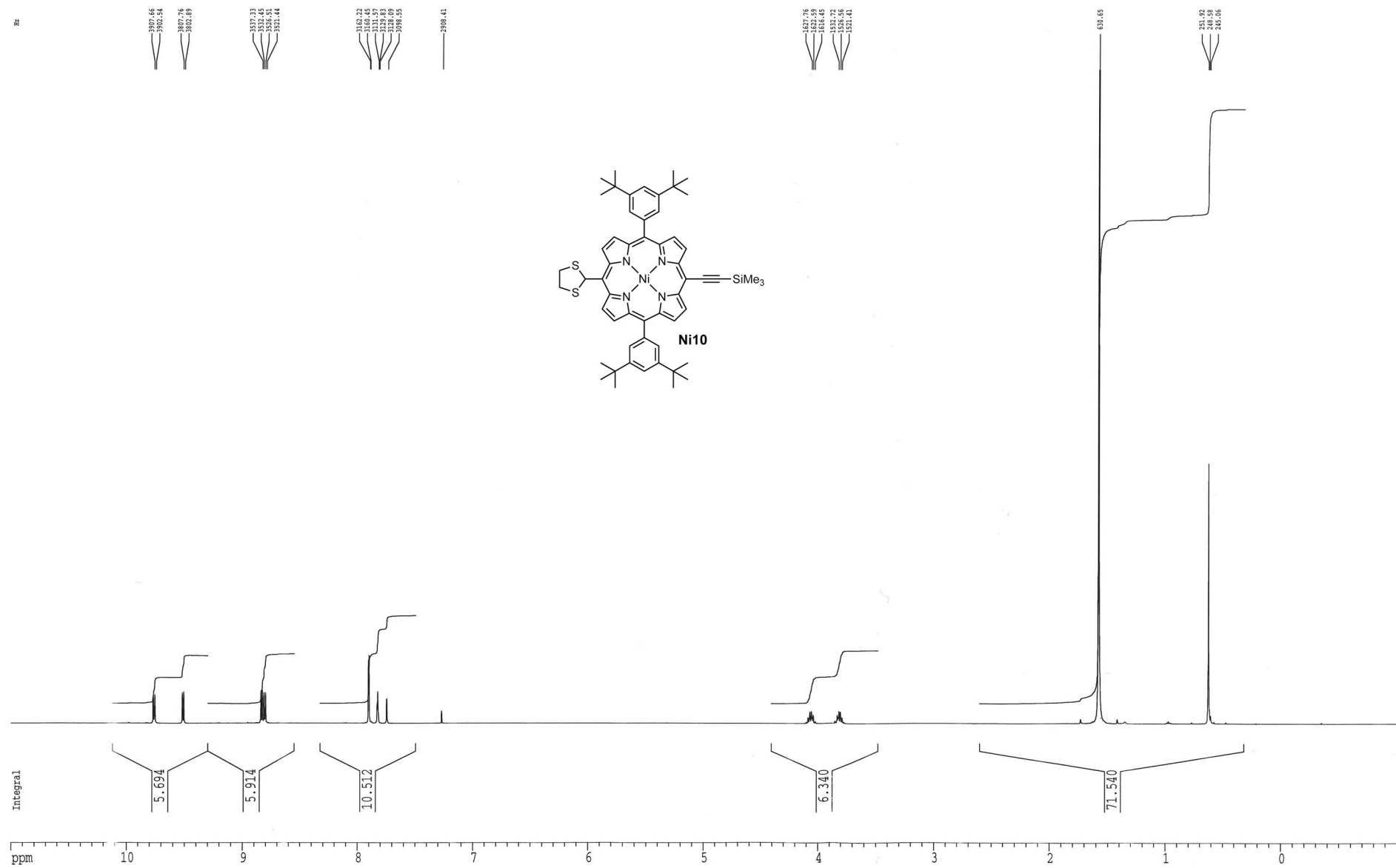
¹H NMR spectrum of **Zn8b** (500 MHz, CDCl₃ with 1% d₅-pyridine, 298 K)



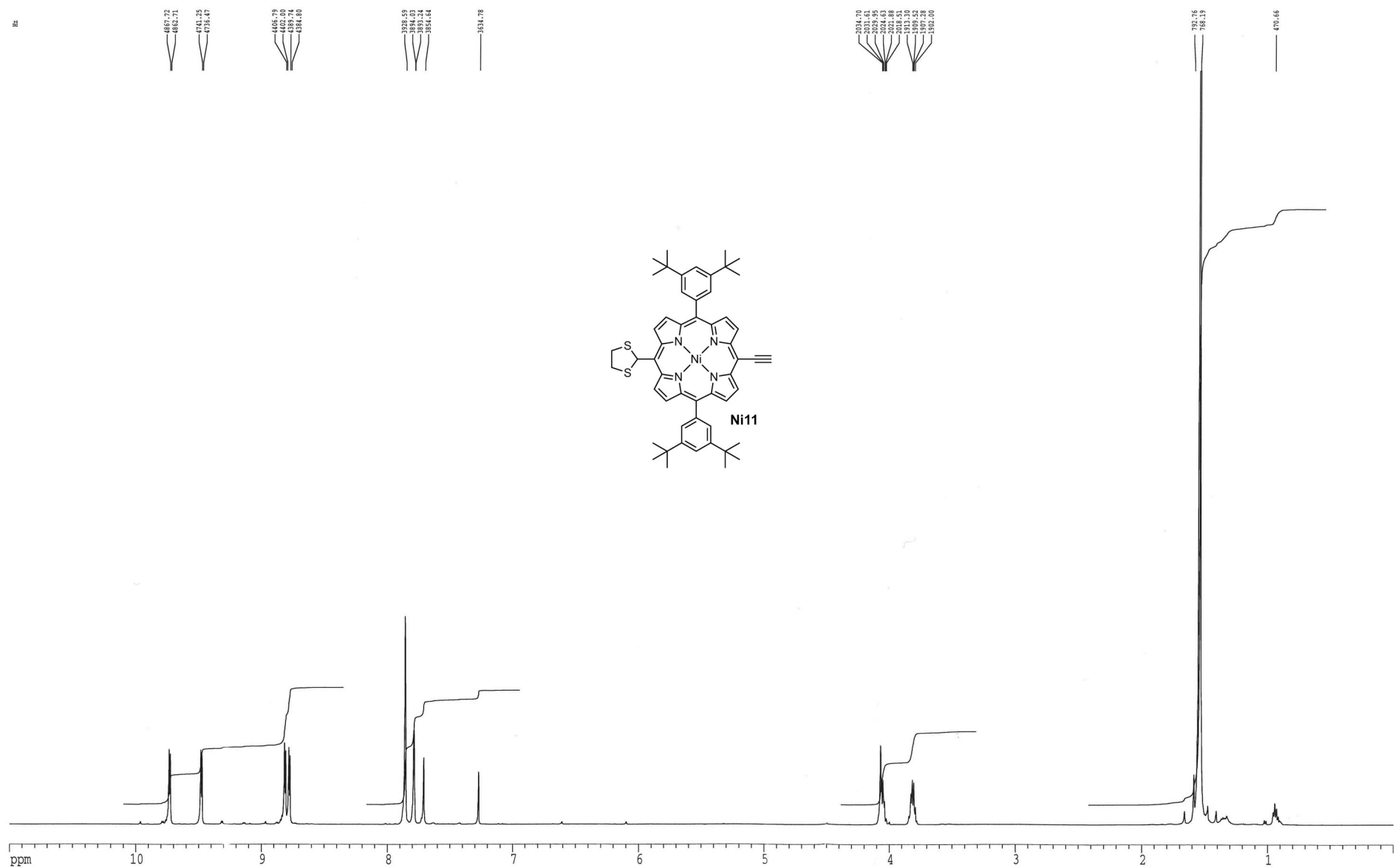
¹H NMR spectrum of **H₂8a** (400 MHz, CDCl₃, 298 K)



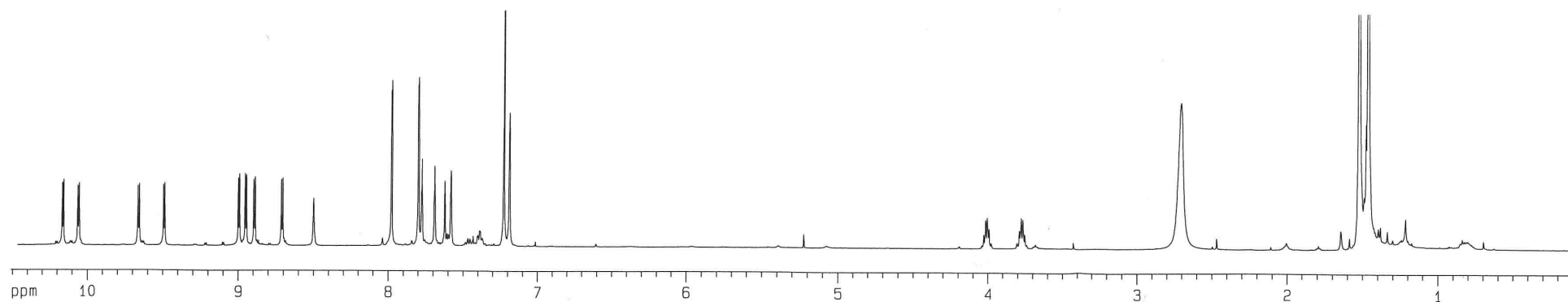
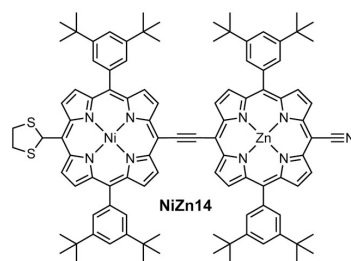
¹H NMR spectrum of **H₂8b** (500 MHz, CDCl₃, 298 K)



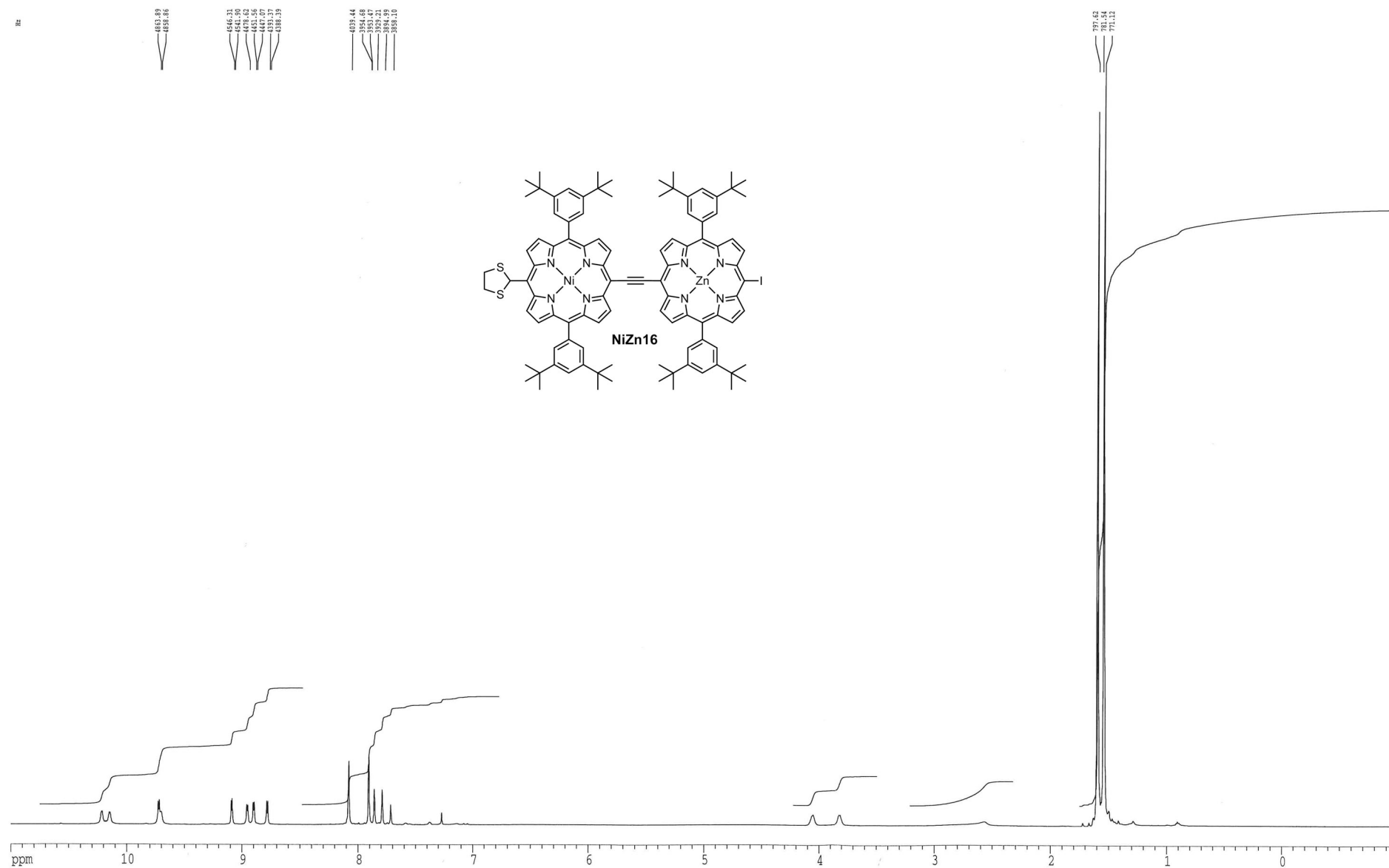
¹H NMR spectrum of **Ni10** (400 MHz, CDCl₃, 298 K)



¹H NMR spectrum of **Ni11** (500 MHz, CDCl₃, 298 K)

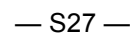


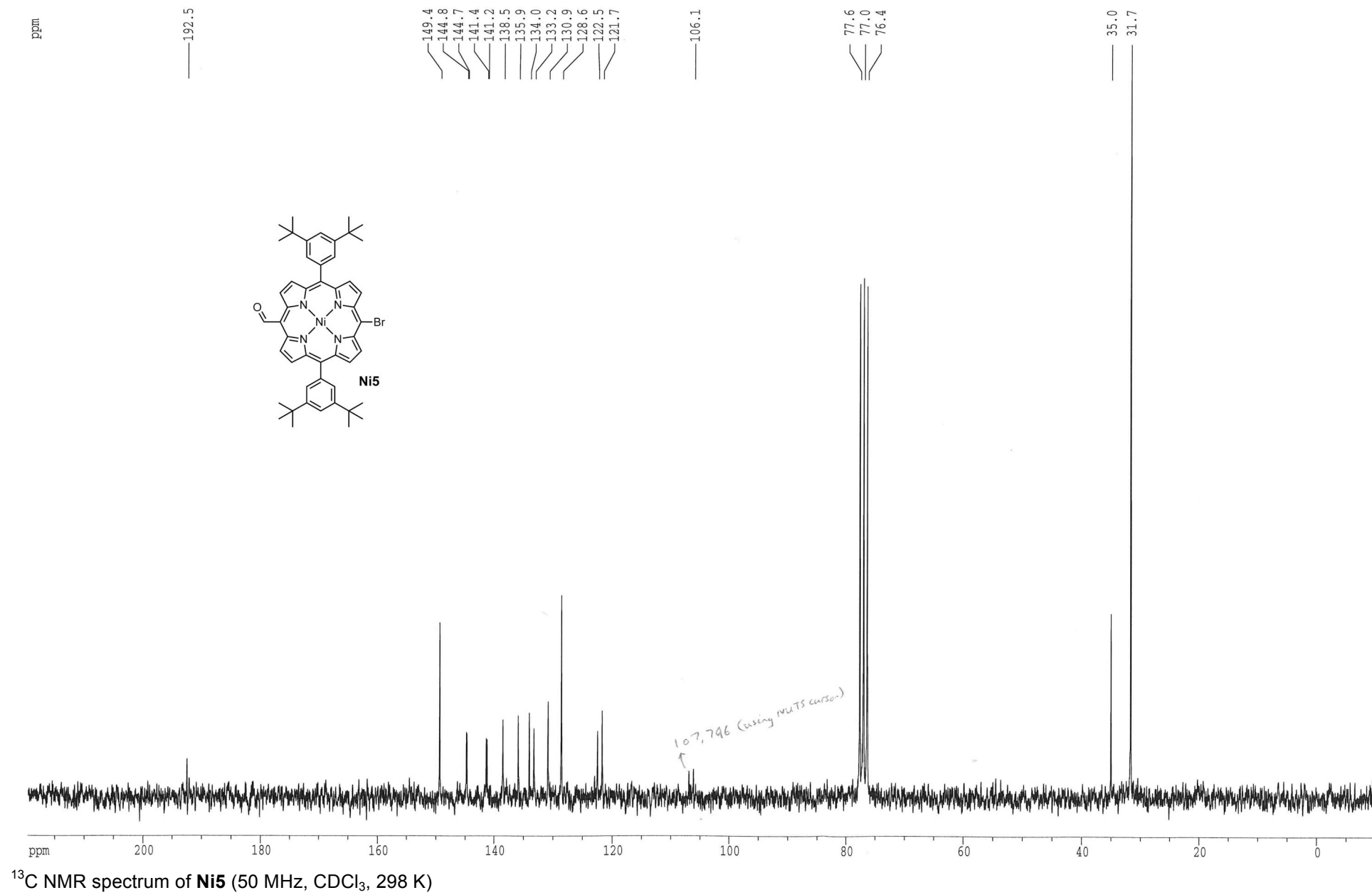
^1H NMR spectrum of **NiZn14** (500 MHz, CDCl_3 with 1% d_5 -pyridine, 298 K)



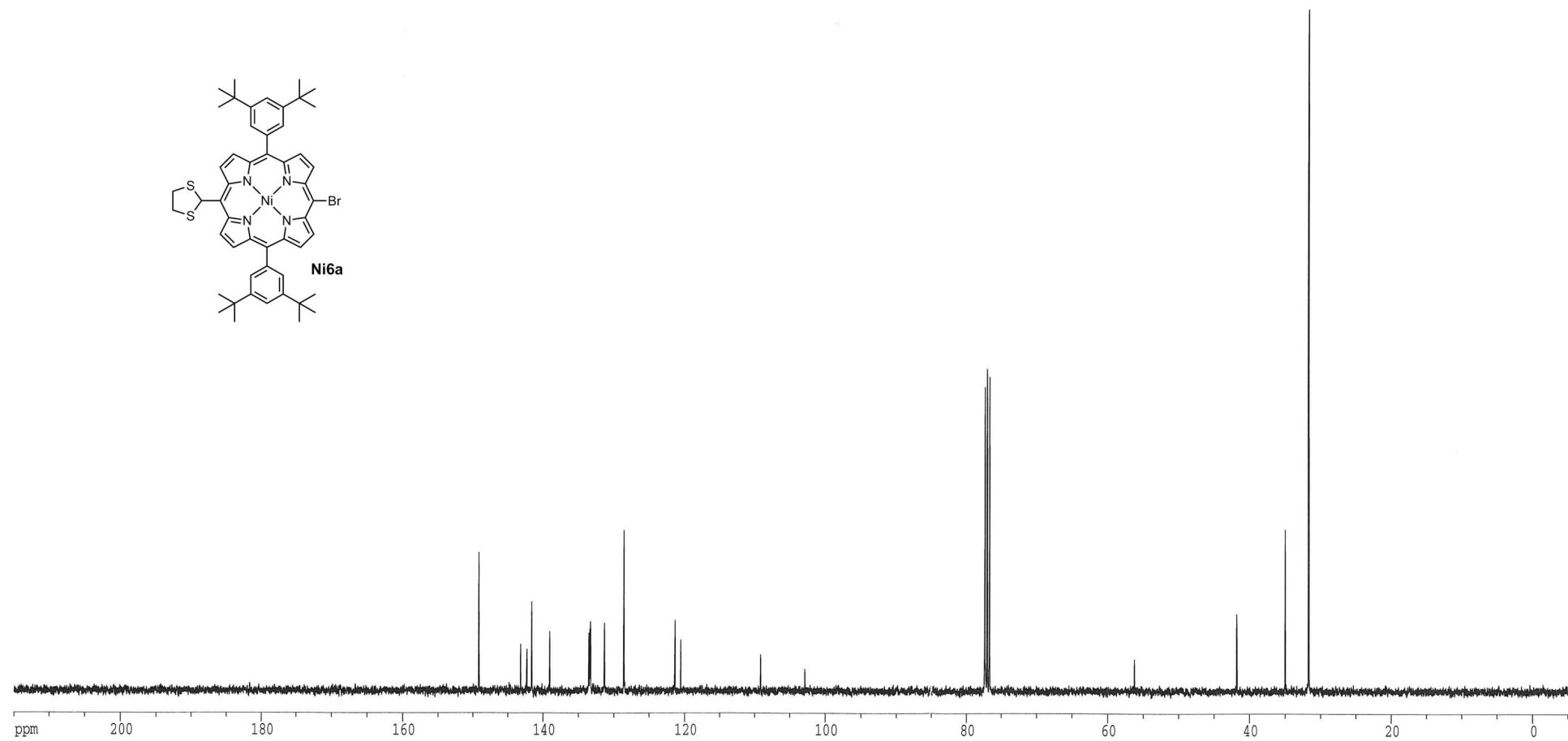
^1H NMR spectrum of **NiZn16** (500 MHz, CDCl_3 with 1% d_5 -pyridine, 298 K)

¹³C NMR spectrum of **Ni4** (50 MHz, CDCl₃, 298 K)

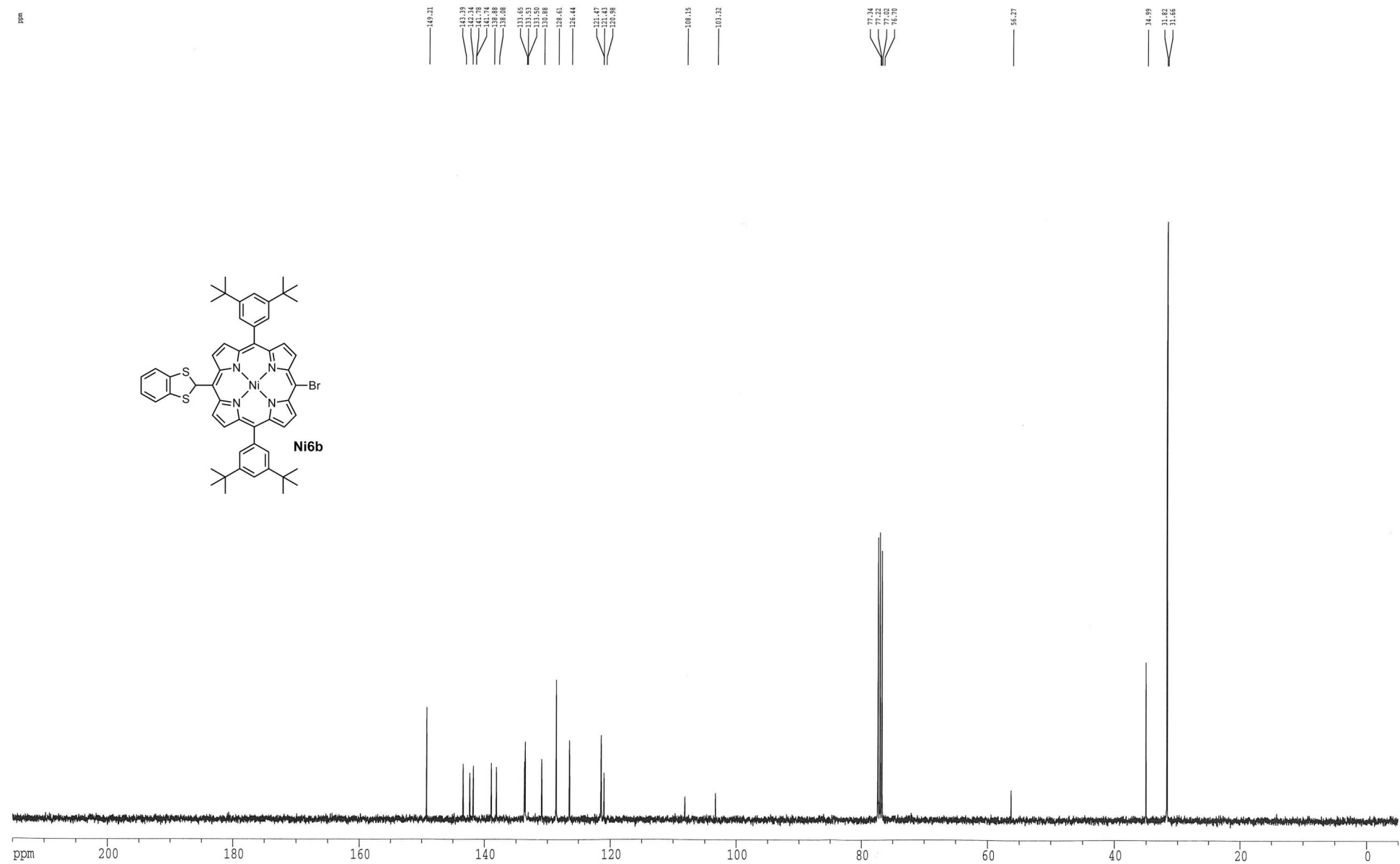




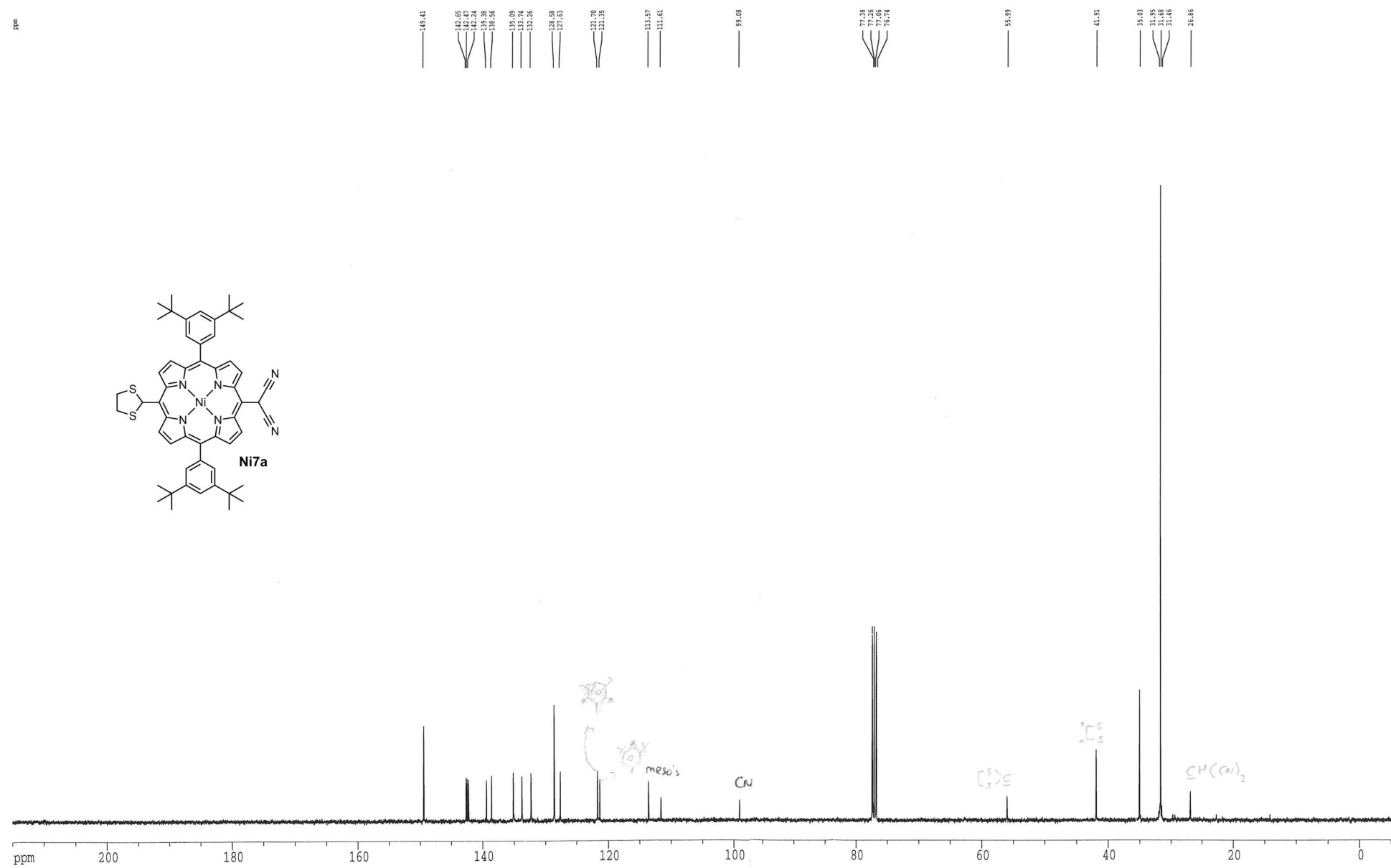
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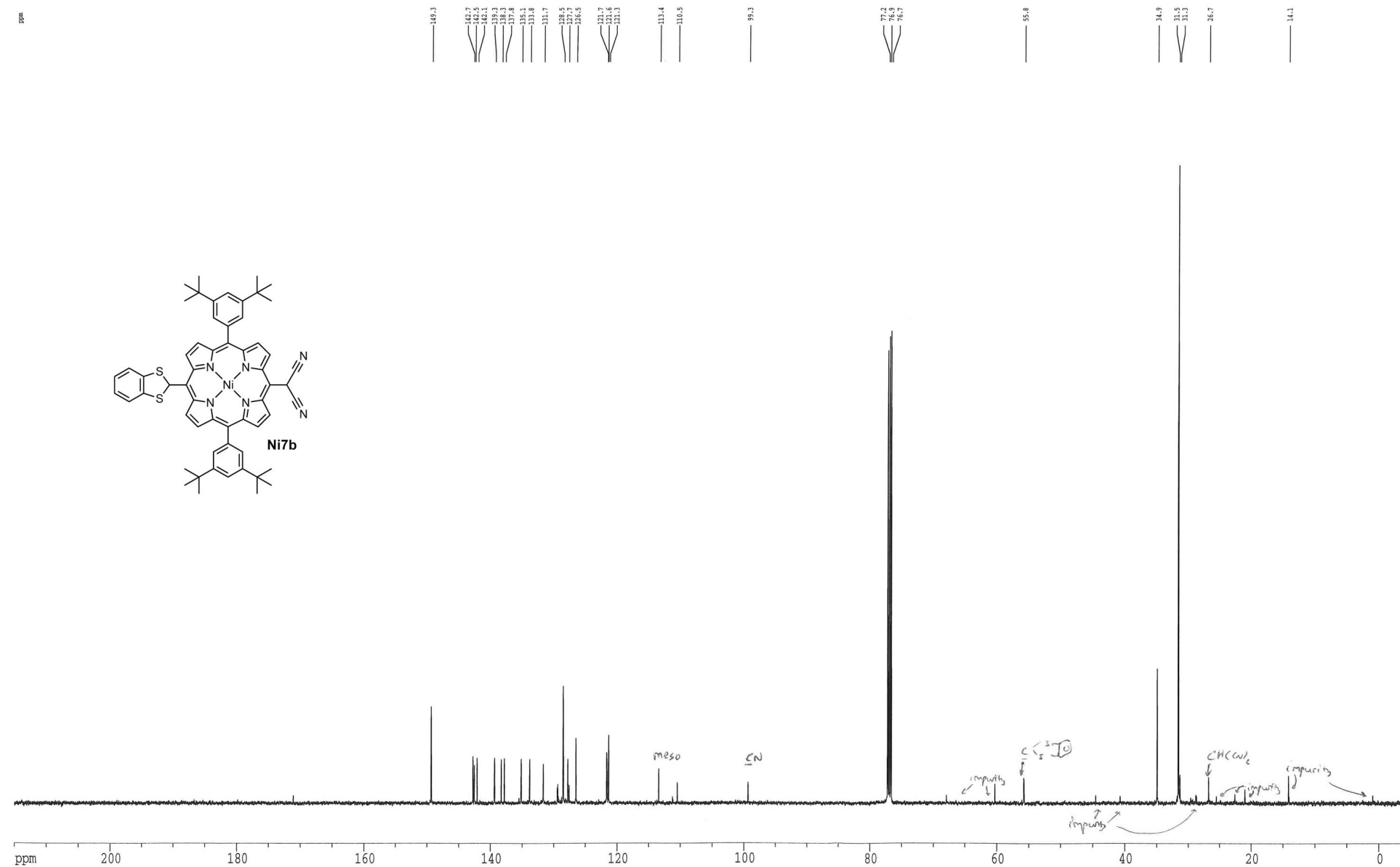
^{13}C NMR spectrum of **Ni6a** (100 MHz, CDCl_3 , 298 K)



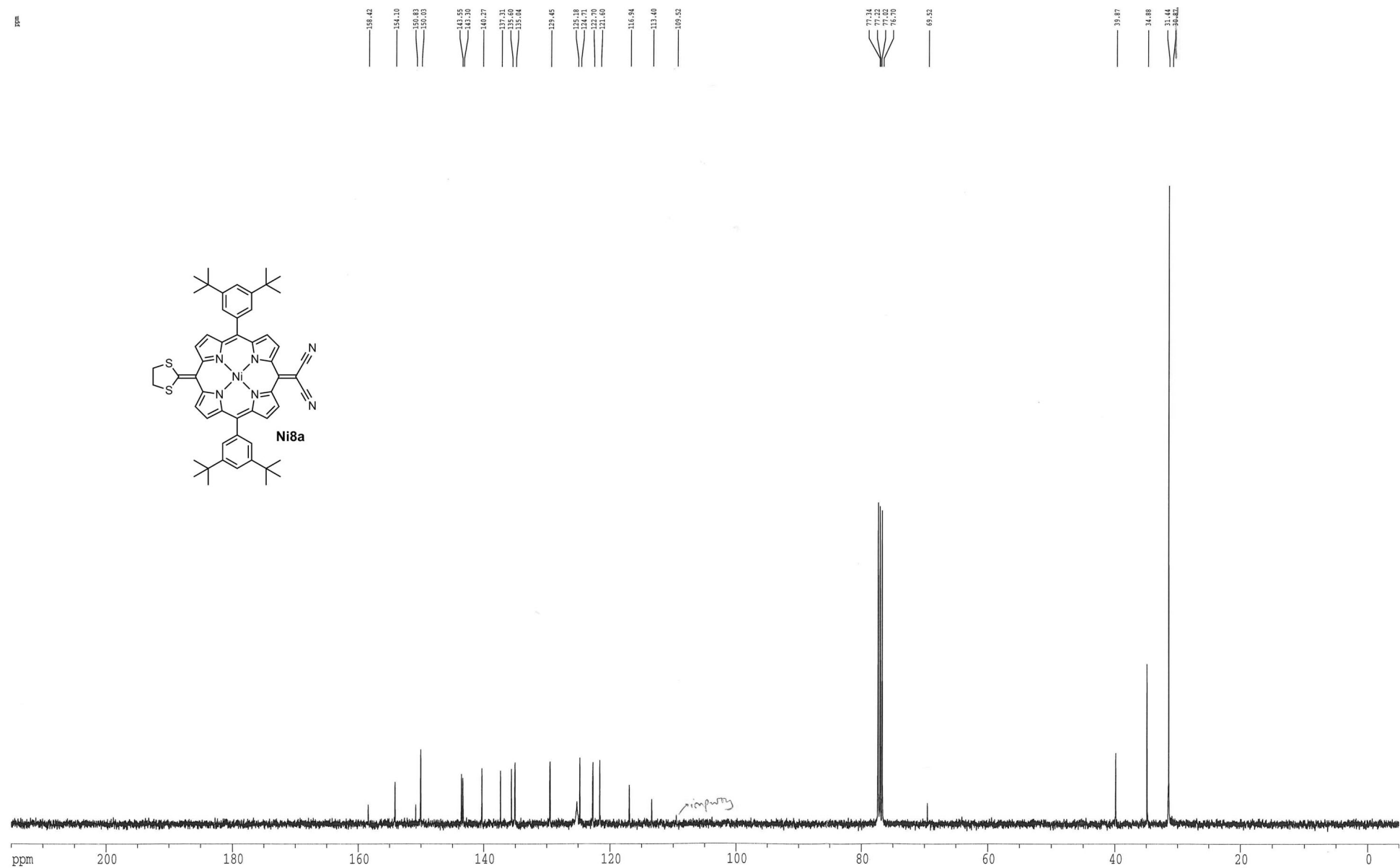
^{13}C NMR spectrum of **Ni6b** (100 MHz, CDCl_3 , 298 K)



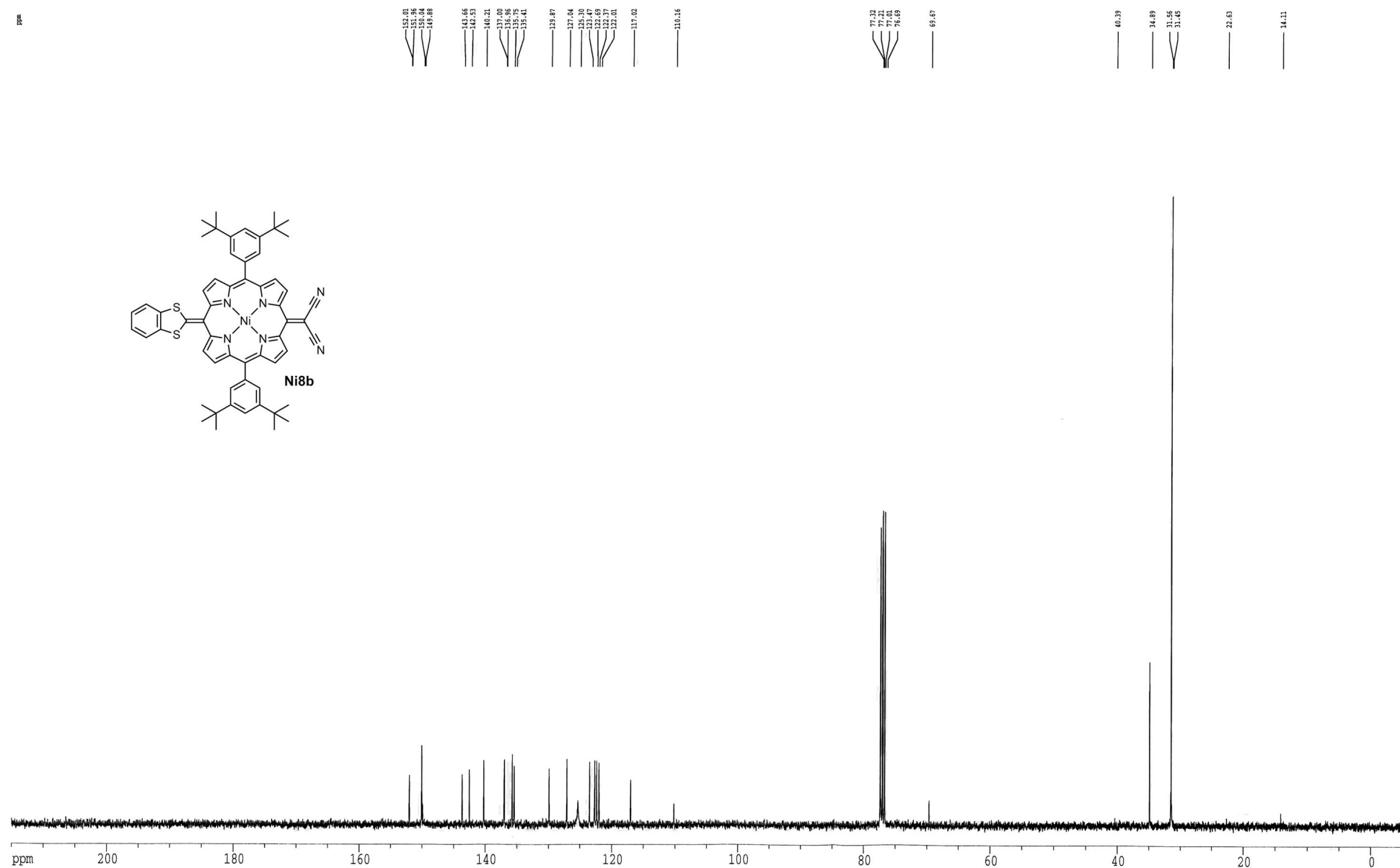
¹³C NMR spectrum of **Ni7a** (100 MHz, CDCl₃, 298 K)



¹³C NMR spectrum of **Ni7b** (125 MHz, CDCl₃, 298 K)

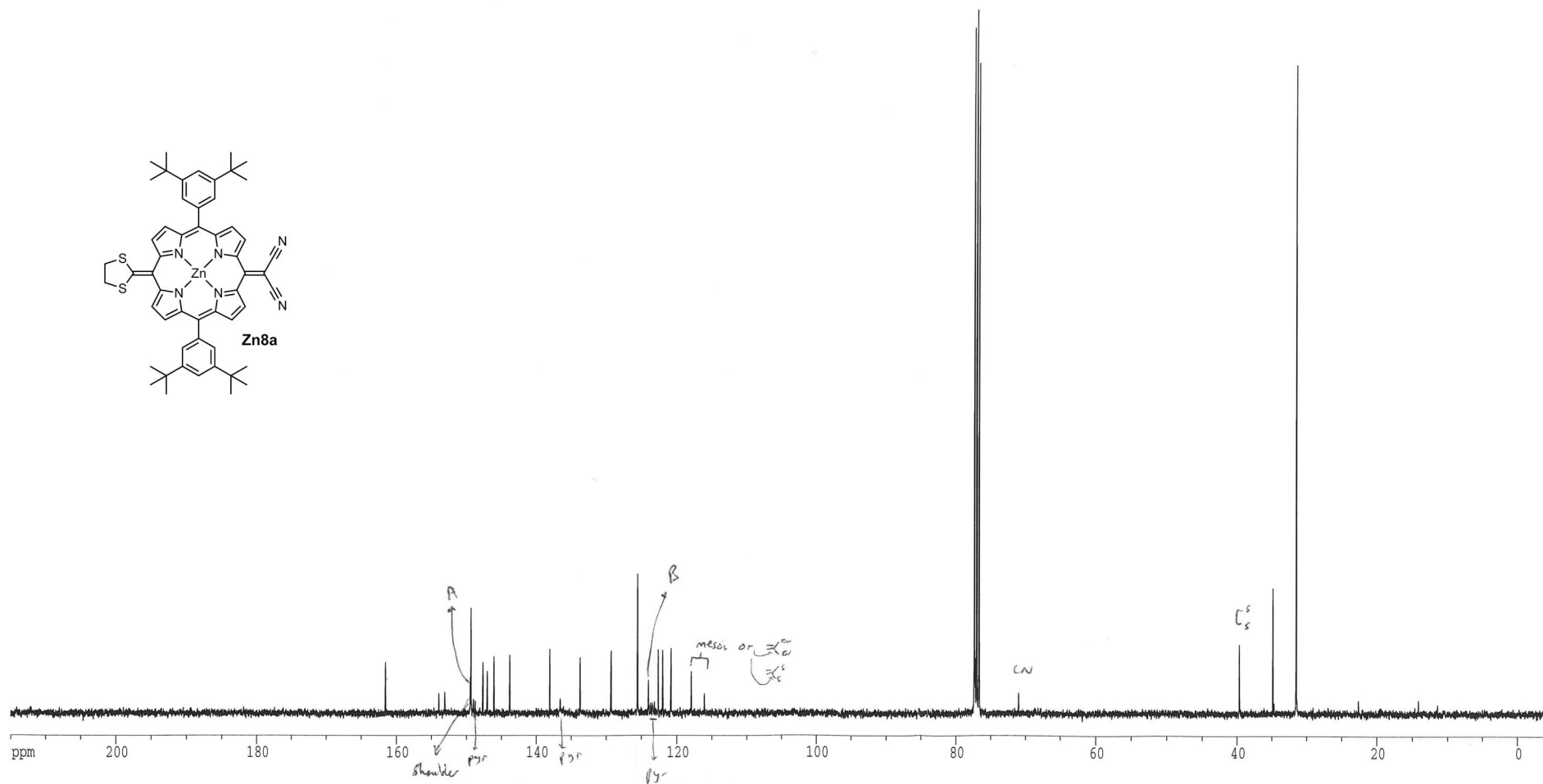


¹³C NMR spectrum of **Ni8a** (100 MHz, CDCl₃, 298 K)

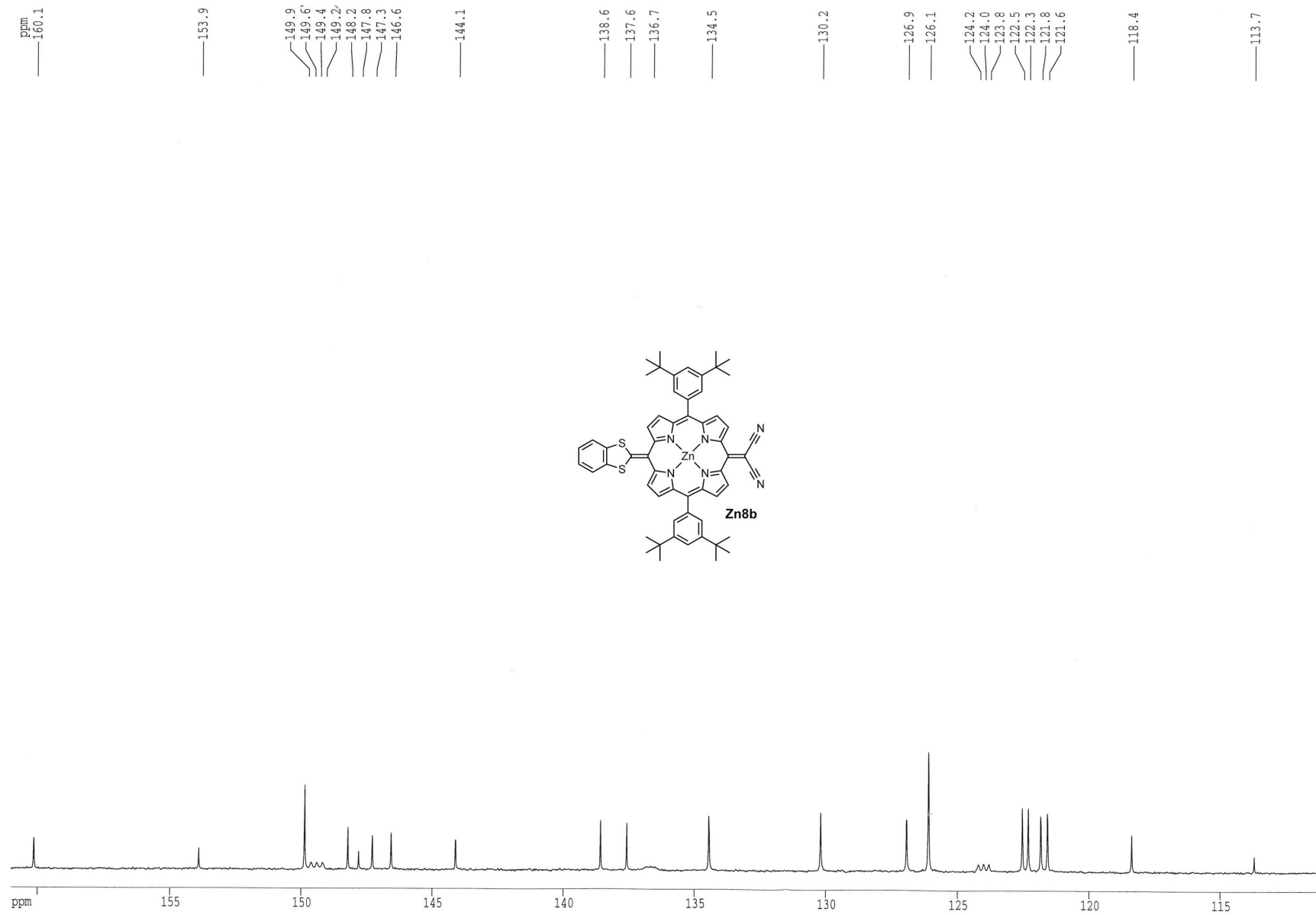


¹³C NMR spectrum of **Ni8b** (125 MHz, CDCl₃, 298 K)

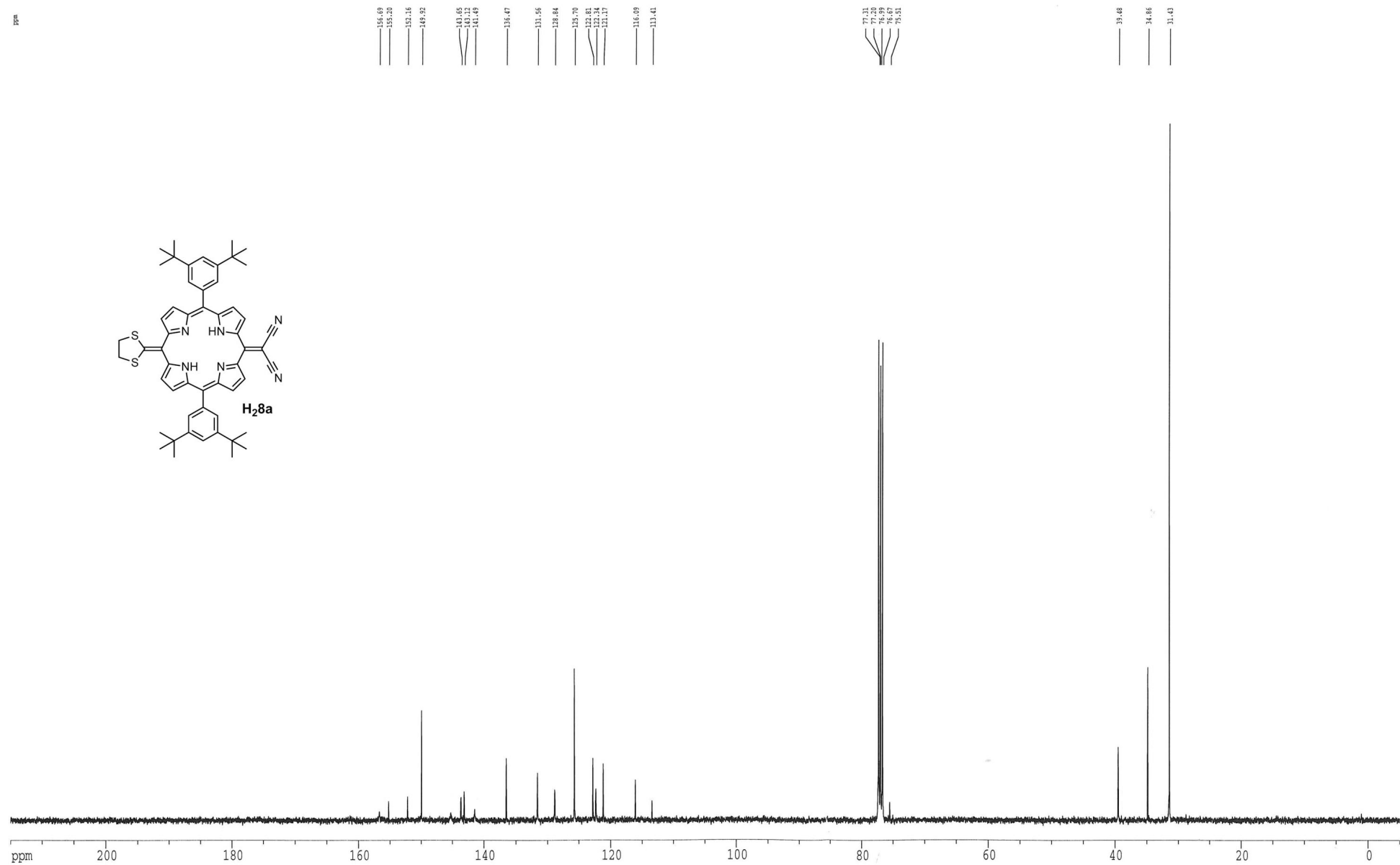
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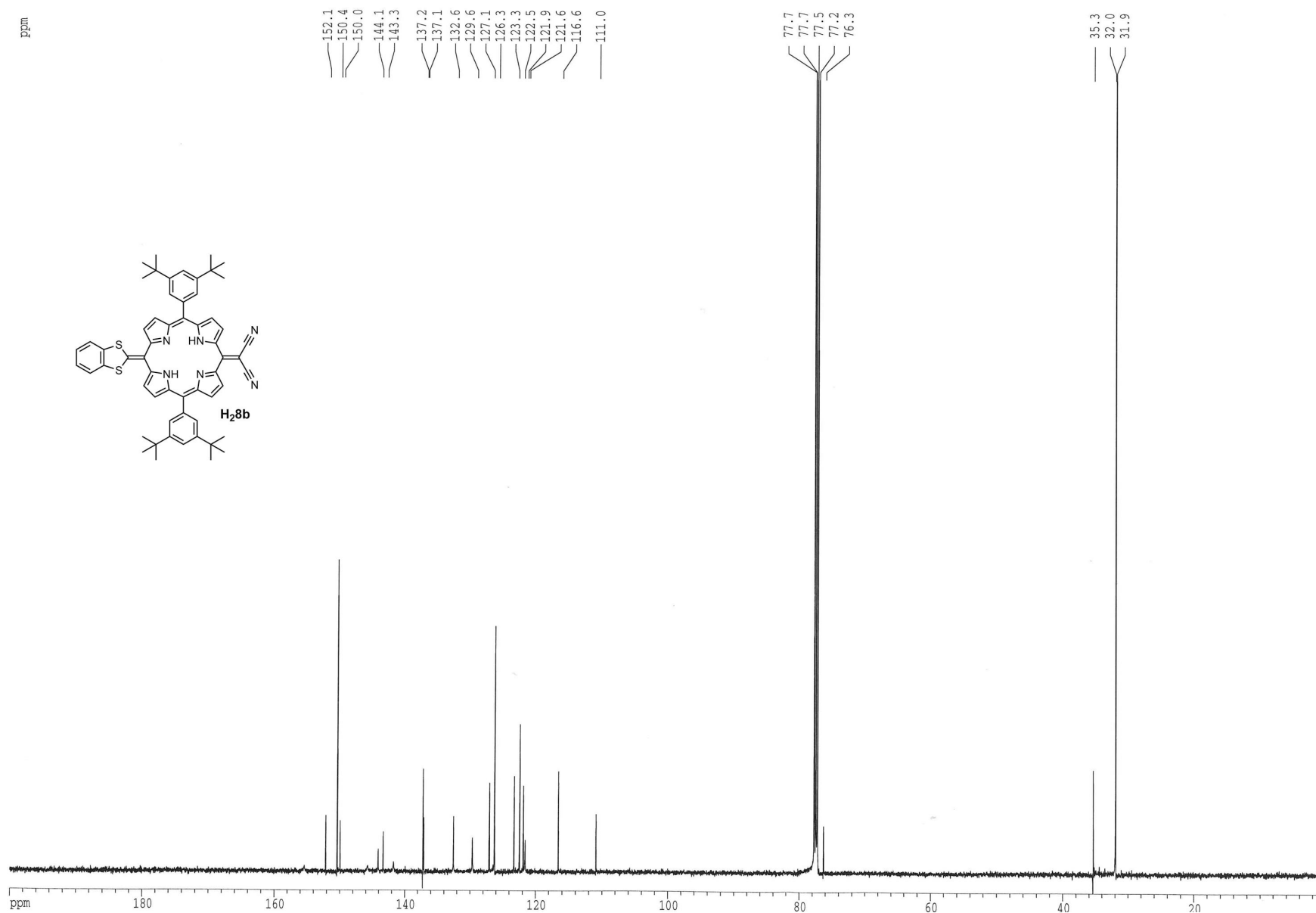
^{13}C NMR spectrum of **Zn8a** (100 MHz, CDCl_3 with 1% d_5 -pyridine, 298 K)



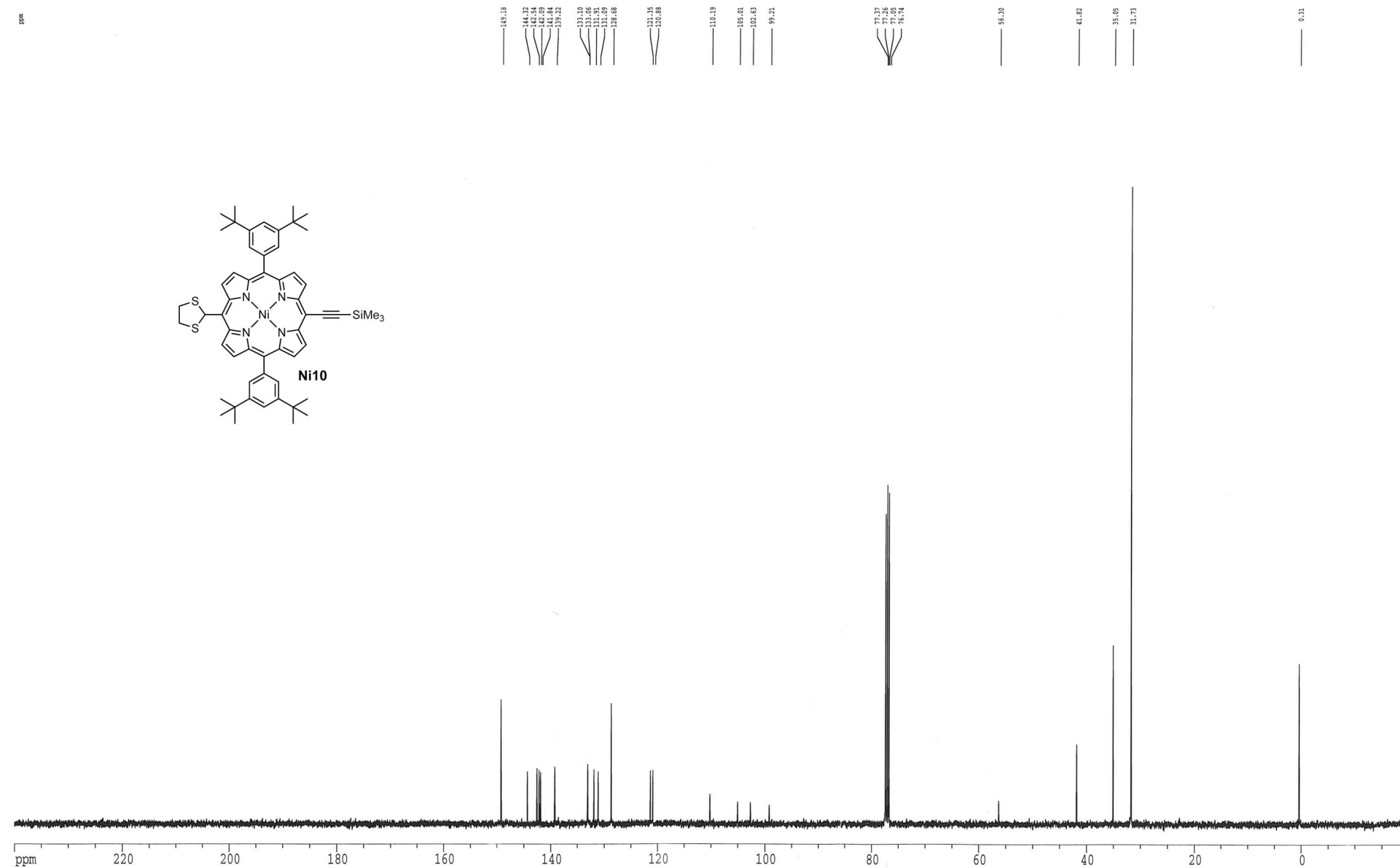
¹³C NMR spectrum of **Zn8b (125 MHz, CDCl₃ with 1% d₅-pyridine, 298 K)**



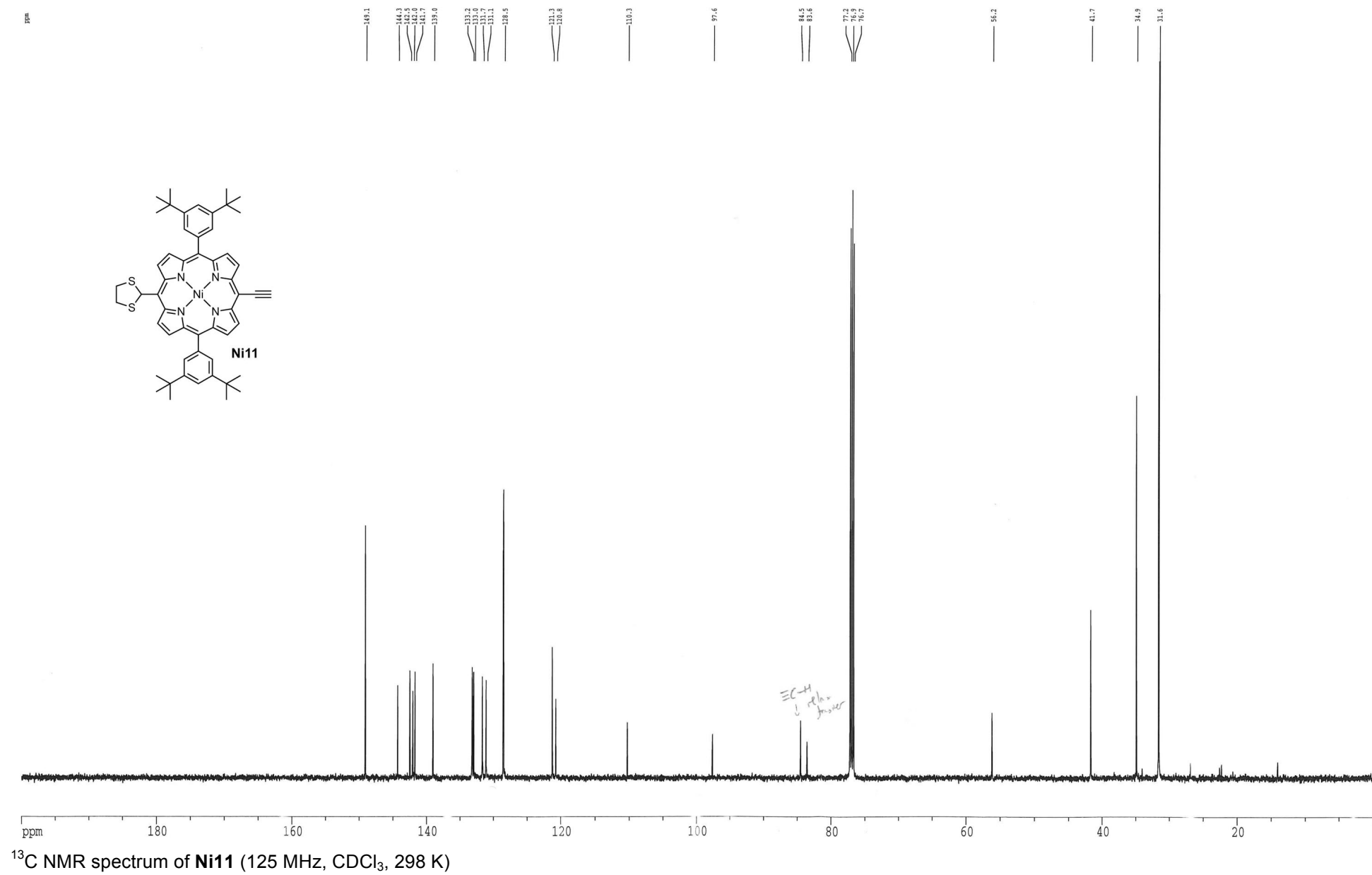
¹³C NMR spectrum of **H₂8a** (100 MHz, CDCl₃, 298 K)

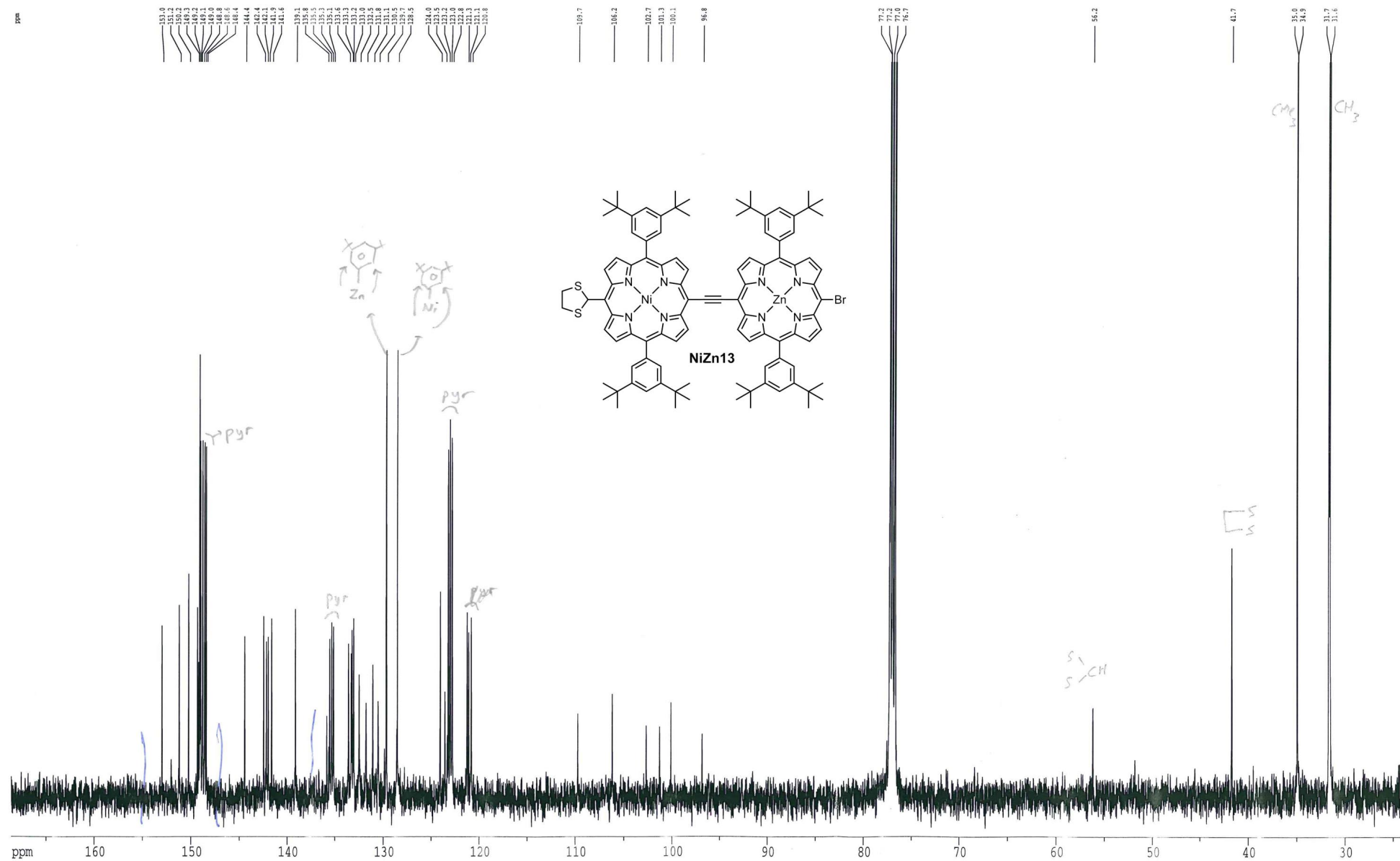


¹³C NMR spectrum of **H₂8b** (125 MHz, CDCl₃, 298 K)

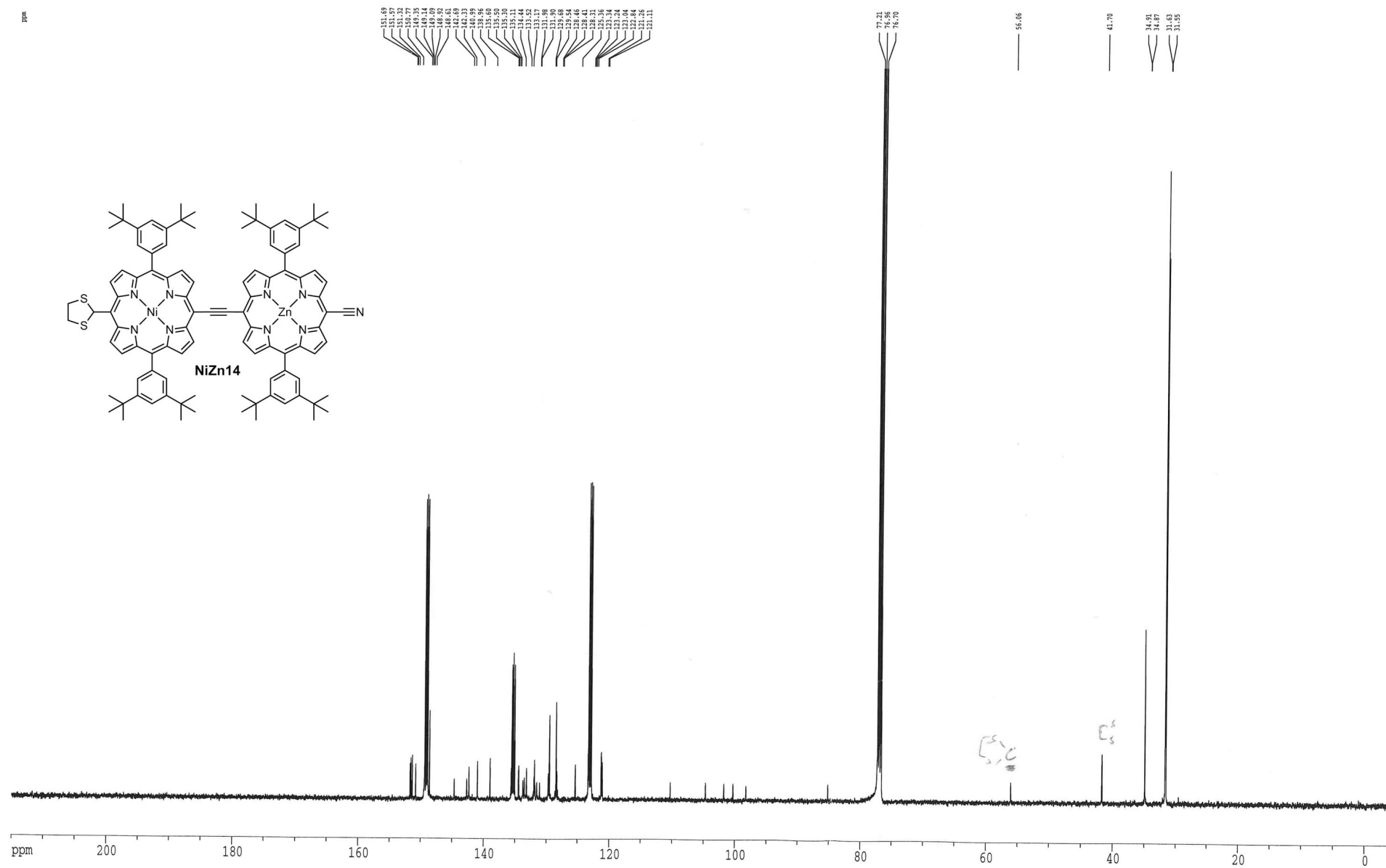


^{13}C NMR spectrum of **Ni10** (100 MHz, CDCl_3 , 298 K)

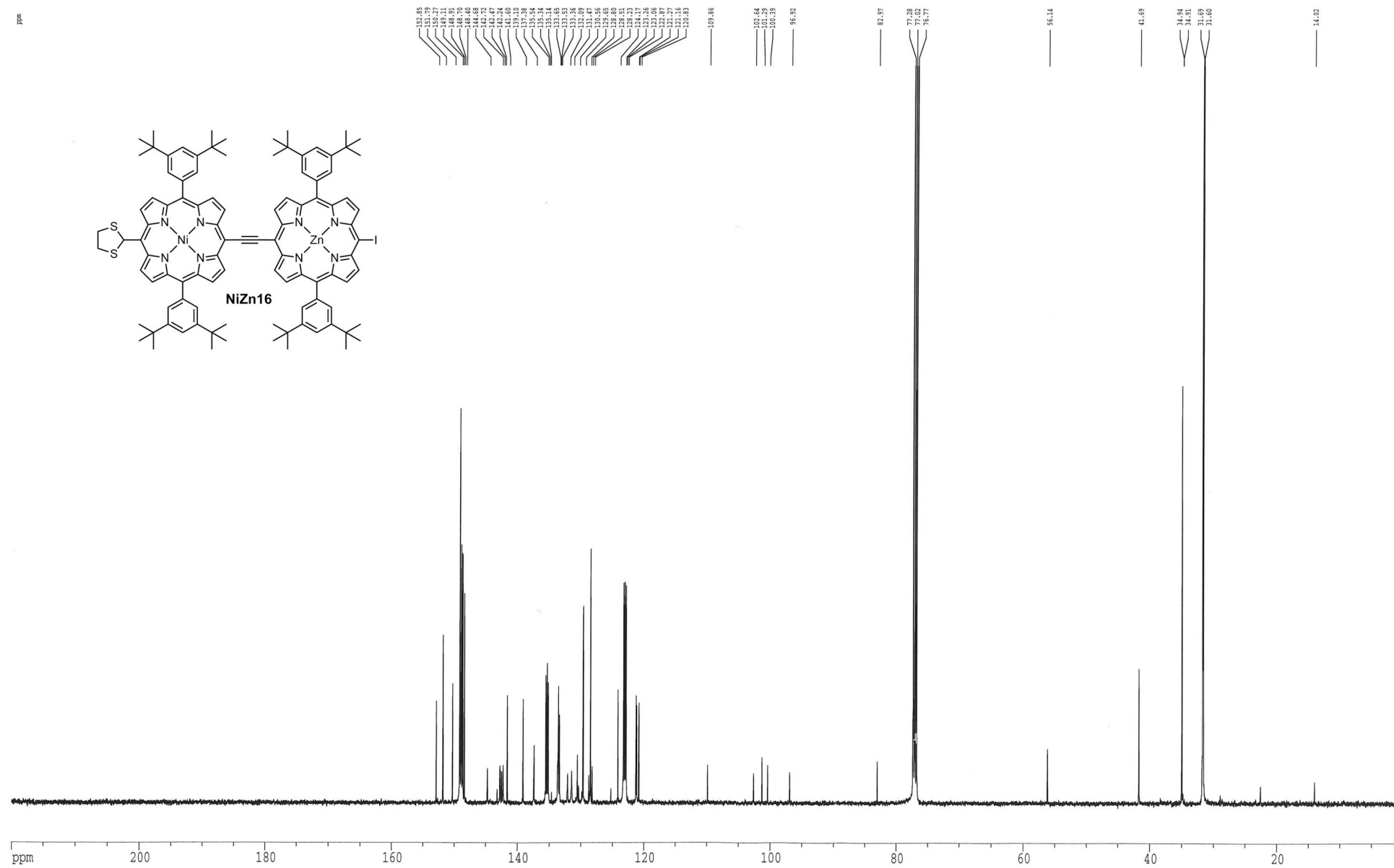




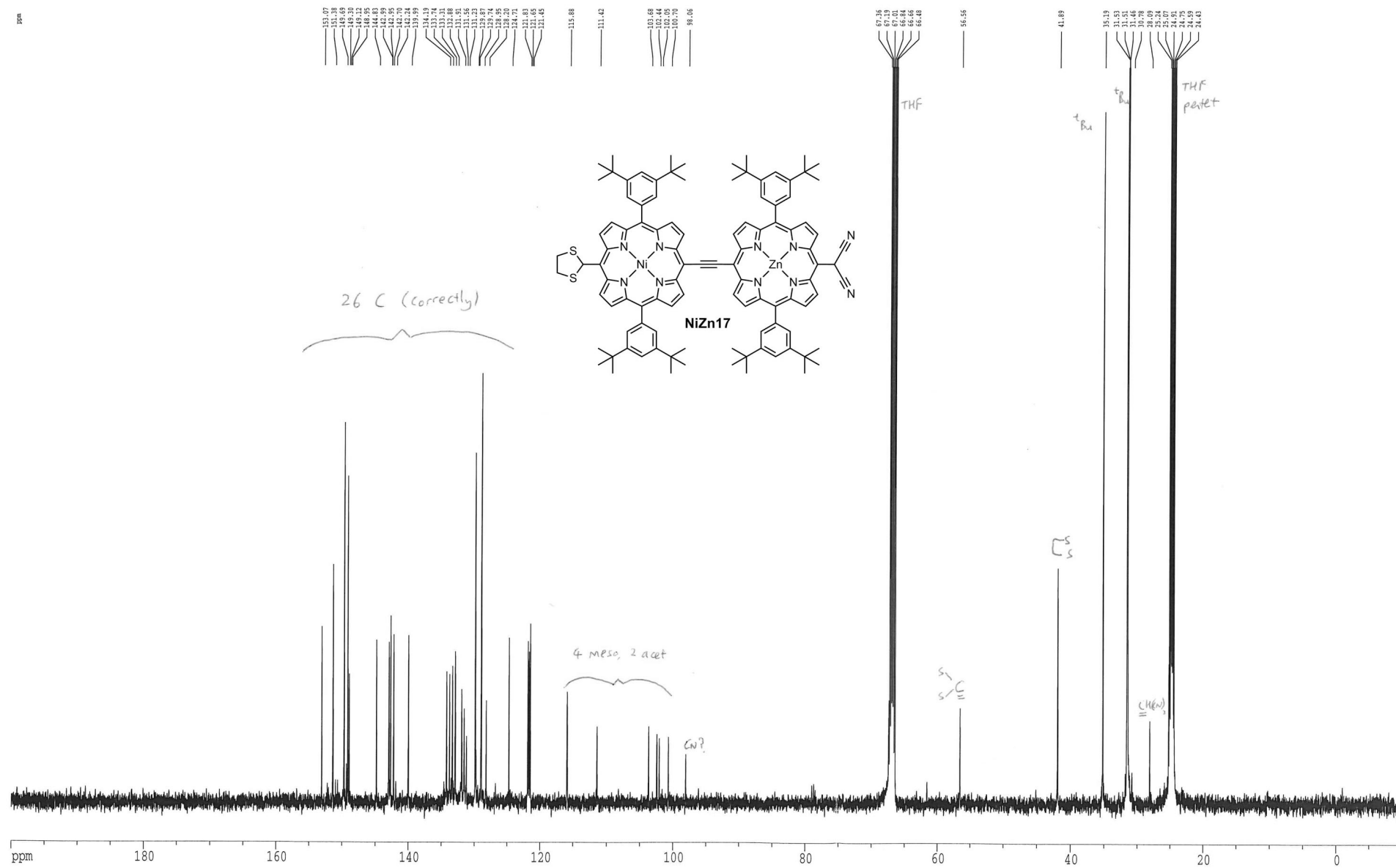
^{13}C NMR spectrum of **NiZn13** (125 MHz, CDCl_3 with 1% d_5 -pyridine, 298 K)



^{13}C NMR spectrum of **NiZn14** (125 MHz, CDCl_3 with 1% d_5 -pyridine, 298 K)



¹³C NMR spectrum of NiZn16 (125 MHz, CDCl₃ with 1% d₅-pyridine, 298 K)



¹³C NMR spectrum of **NiZn17** (100 MHz, d₈-THF, 298 K)

X-Ray Crystallography

The crystal structures of **Ni8a**, **H₂8b**, **H₂9**, **Ni10**, and **NiZn14** were determined using synchrotron single-crystal diffraction data, collected at Station 9.8 of the Daresbury Laboratory Synchrotron Radiation Source (SRS). The use of synchrotron radiation was required because of extensive structural disorder and crystal twinning, and the weak diffraction generated by very small crystals. The X-ray wavelength was close to the Zr absorption edge, and was calibrated on each occasion by measurement of unit cell parameters for a standard crystal. Corrections were made for the significant intensity decay of this second-generation synchrotron source and, where appropriate, for absorption effects, using multiple and symmetry-equivalent reflections in the measured data. The equipment included a Bruker SMART 1K CCD detector and diffractometer, and the sample temperature was maintained at 150 K by an Oxford Cryostream system.

The structures were solved by automatic direct methods, and were refined on all unique measured F^2 values, using the most recent release of SHELXL (2018/1). For non-merohedrally twinned structures, merging of symmetry-equivalent reflections before refinement is not possible, so the number of 'unique' reflections reported is misleading, and there are no statistics for merging (R_{int} etc.).

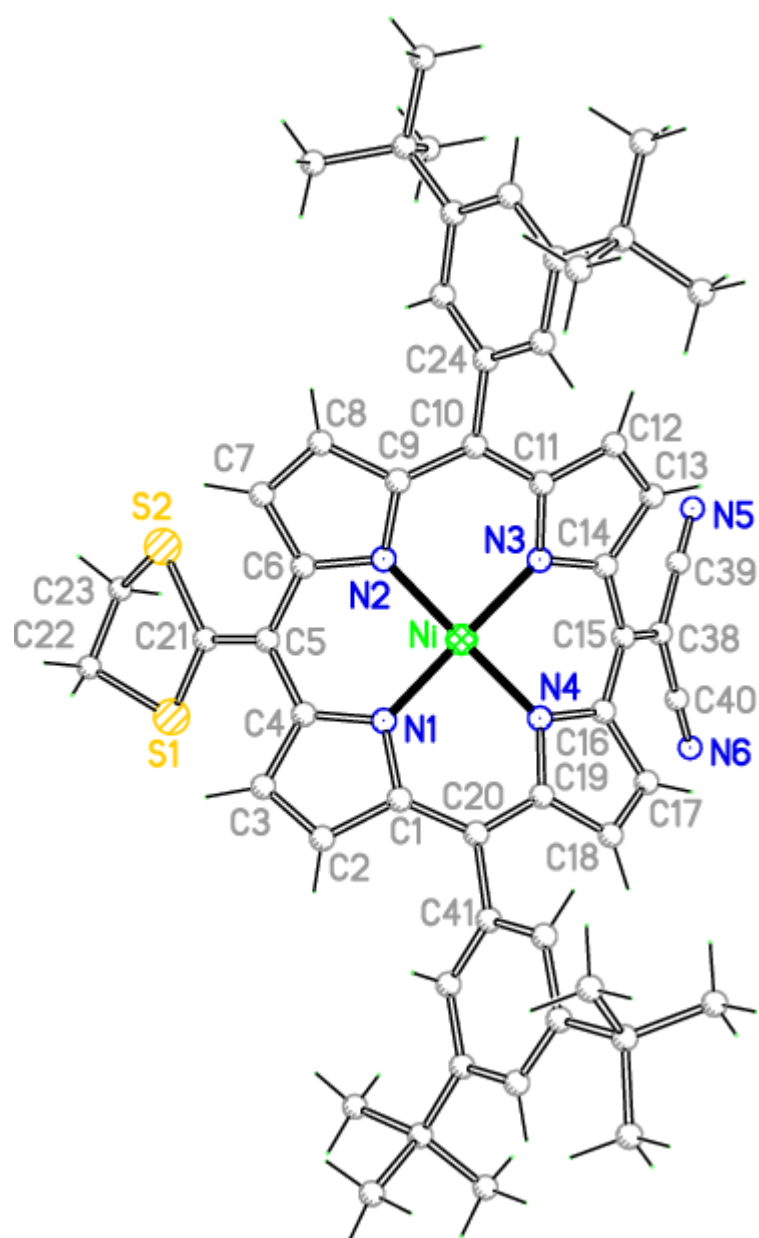
Disorder (limited to two components) was identified and refined for parts of the structures, particularly tertiary butyl substituents, with the aid of similarity restraints on geometry and on anisotropic displacement parameters. Hydrogen atoms were included in geometrically calculated positions, with a riding model for refinement, where such positions could be assigned unambiguously.

Some solvent disorder was too extensive to be modeled by discrete atom positions. These cases were treated by the SQUEEZE procedure of PLATON, in which the contributions to the scattering by disordered solvent regions of the structure are calculated by Fourier transform of the diffuse electron density regions. The solvents treated in this way are not included in the chemical formulae and derived properties (calculated density, absorption coefficient, etc.).

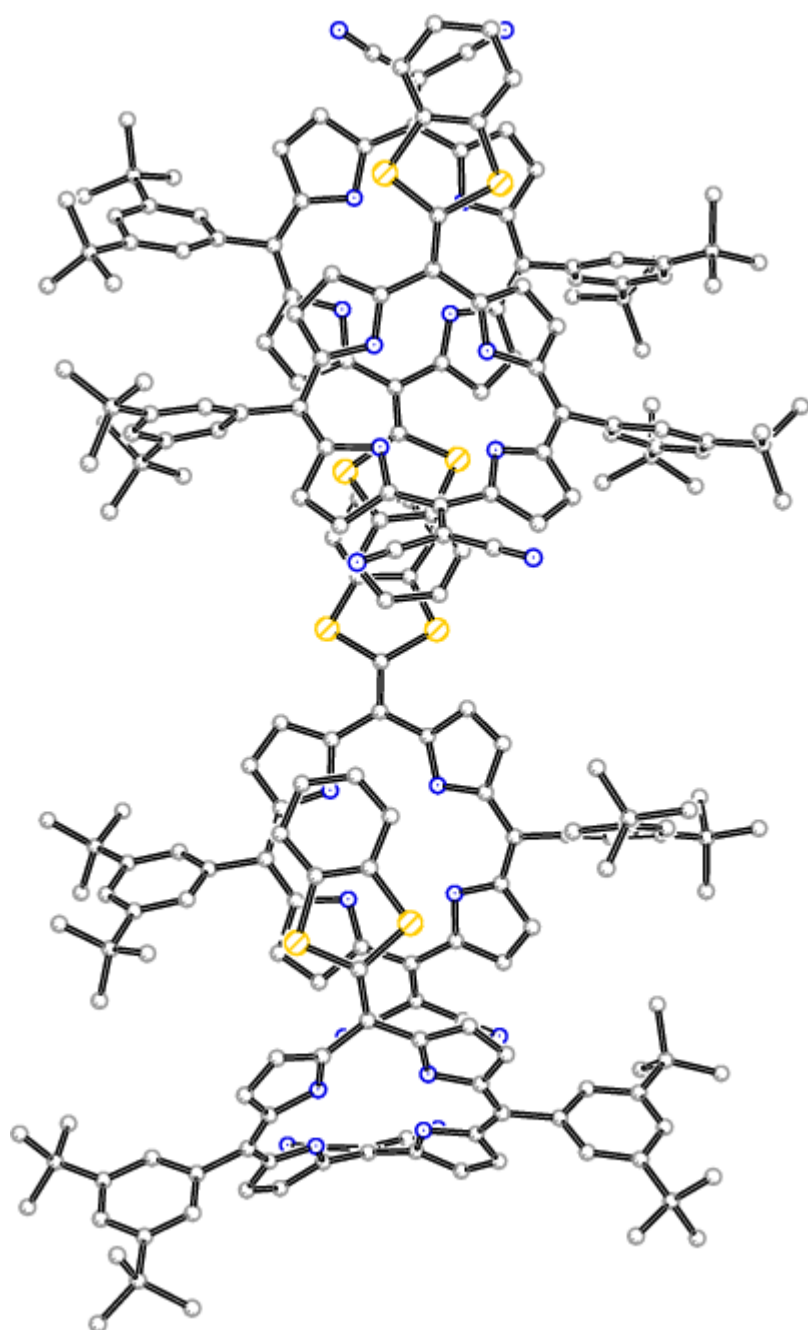
For the two uncoordinated porphyrin structures, H atoms were allocated to porphyrin N atoms on the basis of a consistent pattern of bond lengths, angles, and non-bonded distances resulting from localized alternating single and double bonds.

All the structures have been validated with PLATON/CheckCIF and programs from the CCDC (Mercury, Mogul) to check for consistency with expected results.

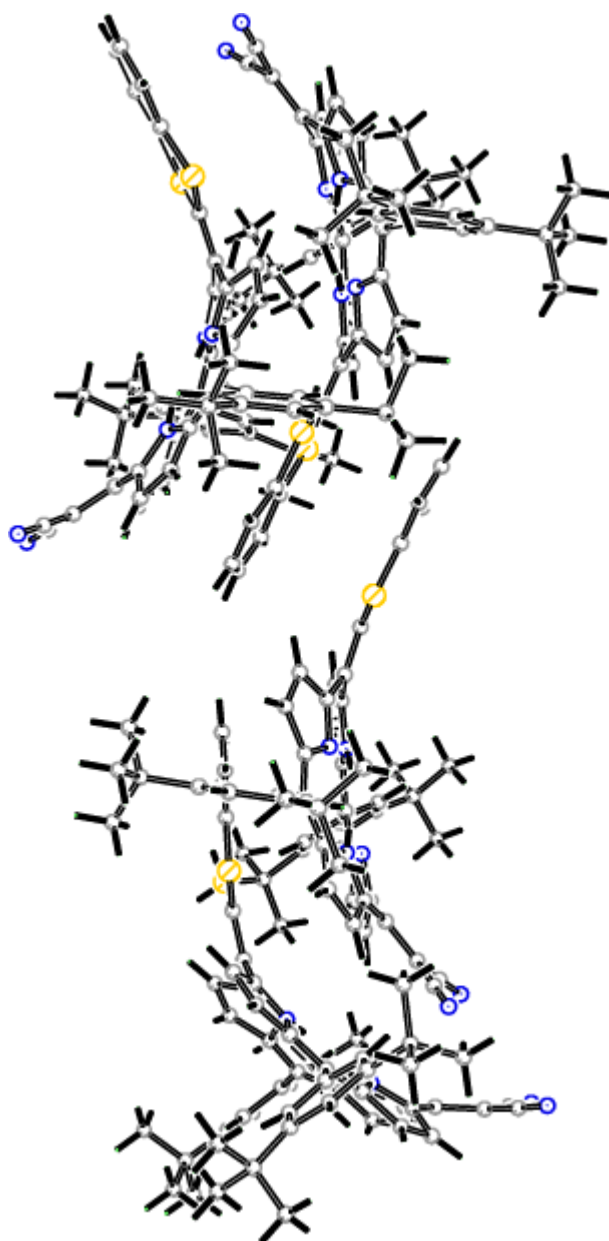
Ni8a:	$Z' = 1$. Disorder modeled for some <i>t</i> -Bu groups, dithiolane substituent, and solvent molecules.
H₂8b:	$Z' = 4$. Disorder modeled for some <i>t</i> -Bu groups. Twinned. Solvent treated by SQUEEZE.
H₂9:	$Z' = 2$. Disorder modeled for some <i>t</i> -Bu groups. Solvent treated by SQUEEZE.
Ni10:	$Z' = 4$. No disorder modeled (solvent also ordered). Twinned.
NiZn14:	$Z' = 1$. Disorder modeled for some <i>t</i> -Bu groups and part of the dithiolane-substituted porphyrin group. Solvent treated by SQUEEZE.



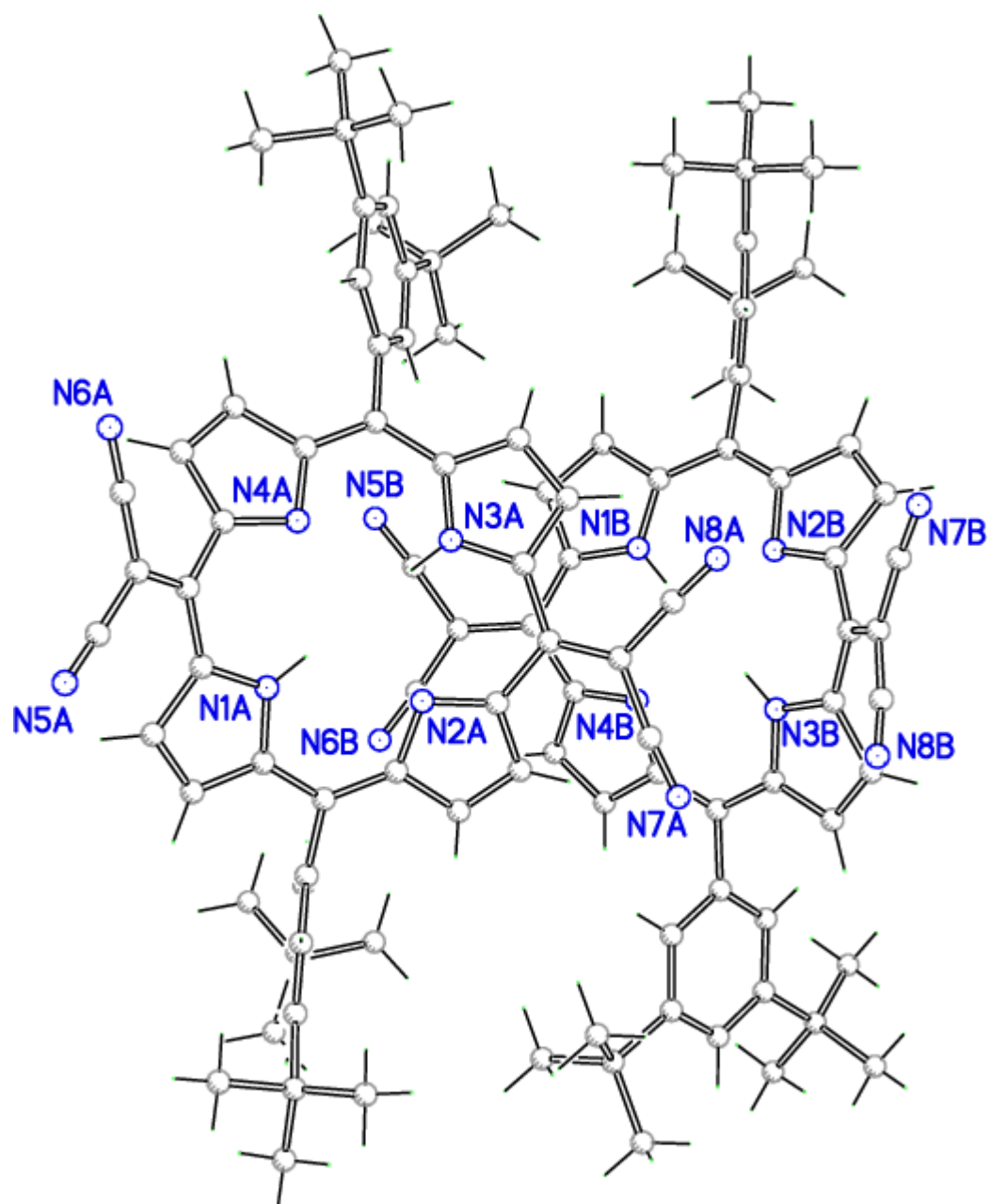
The molecular structure of **Ni8a**. In all these Figures, only one disorder component is shown, and solvent molecules are not included.



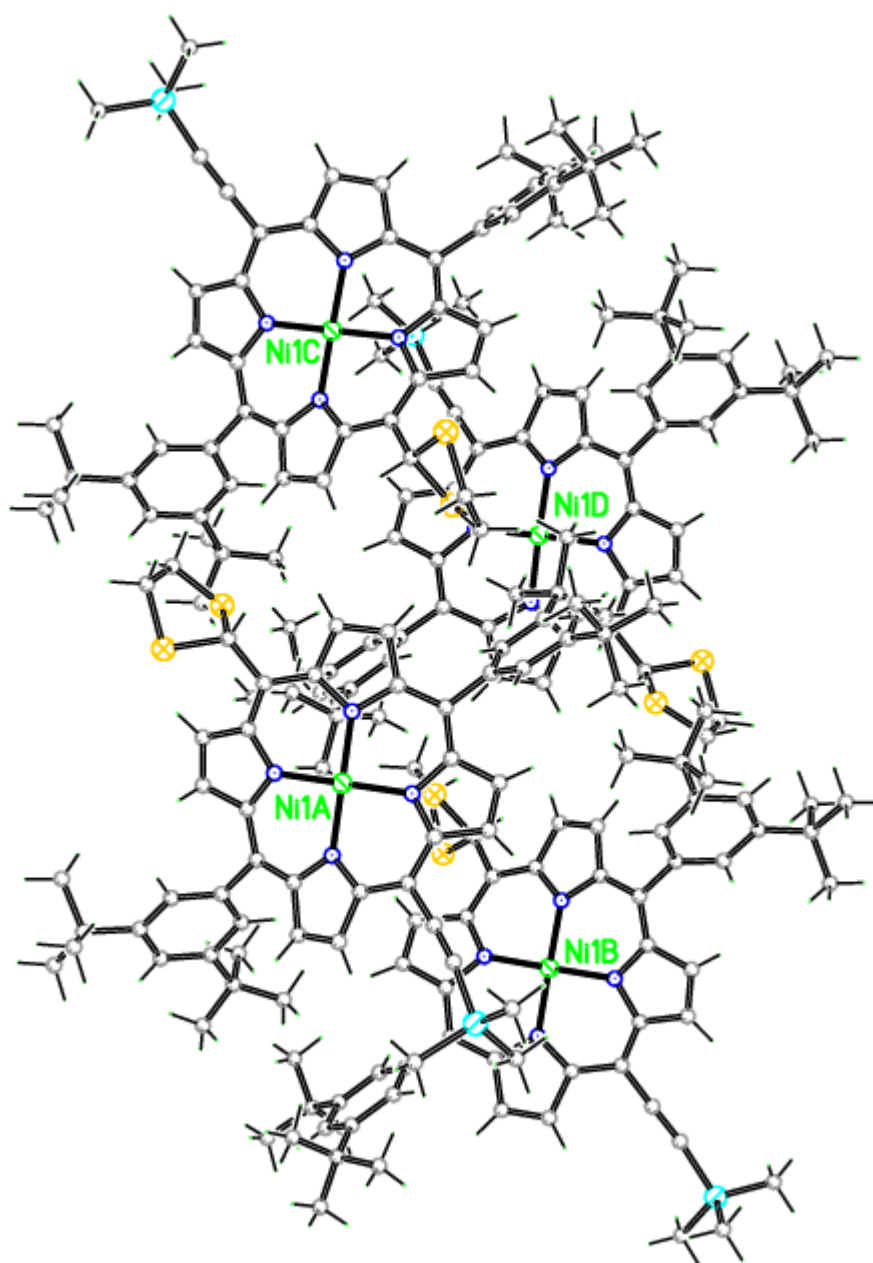
The four independent molecules of **H₂8b** in the asymmetric unit (without H atoms).



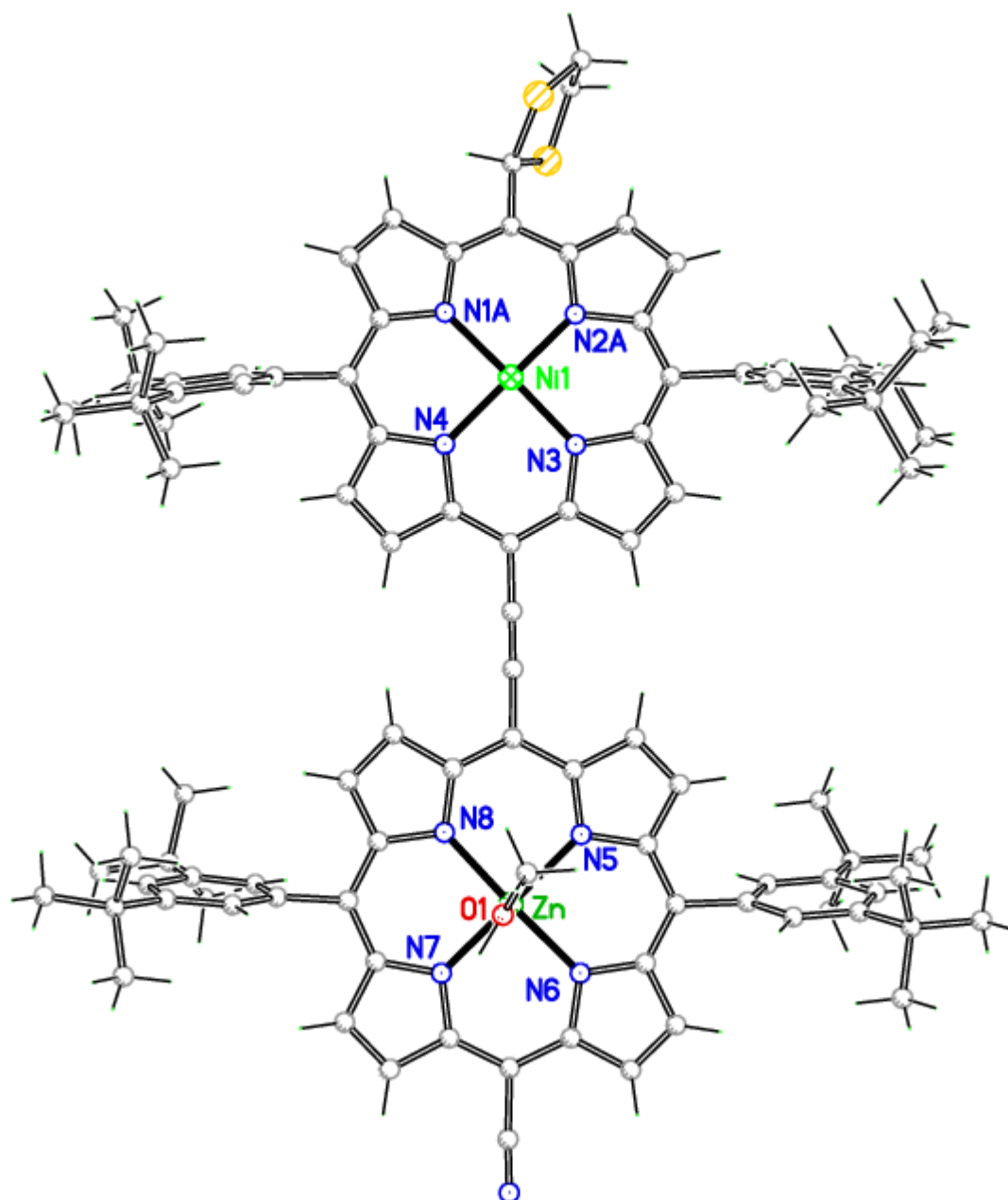
A side view of the four molecules of **H₂8b**, including H atoms.



The two molecules of **H₂9** in the asymmetric unit.



The four molecules of **Ni10** in the asymmetric unit.



The molecular structure of **NiZn14**.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) oxdp21_Ni8a, oxdp22_H29, oxdp25_NiZn14, oxdp26_H28b, oxdp28_Ni10

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: oxdp21_Ni8a

Bond precision: C-C = 0.0050 Å Wavelength=0.68930

Cell: a=39.247(4) b=12.6465(11) c=21.5421(19)

alpha=90 beta=93.847(2) gamma=90

Temperature: 150 K

Calculated Reported

Volume 10668.1(17) 10668.1(17)

Space group C 2/c C 2/c

Hall group -C 2yc -C 2yc

Moiety formula

C54 H54 N6 Ni S2, C2 H4

Cl2, O

C54 H54 N6 Ni S2, C2 H4

Cl2, H2 O

Sum formula C56 H58 Cl2 N6 Ni O S2 C56 H60 Cl2 N6 Ni O S2

Mr 1024.79 1026.83

Dx, g cm⁻³ 1.276 1.279

Z 8 8

Mu (mm⁻¹) 0.536 0.542

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F000' 4311.83

h,k,lmax 55,17,30 55,17,29

Nref 15888 14512

Tmin, Tmax 0.897, 0.984 0.852, 0.928

Tmin' 0.897

Correction method= # Reported T Limits: Tmin=0.852 Tmax=0.928

AbsCorr = MULTI-SCAN

Data completeness= 0.913 Theta(max)= 29.225

R(reflections)= 0.0701(10061) wR2(reflections)= 0.2007(14512)

S = 1.066 Npar= 763

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT430_ALERT_2_B Short Inter D...A Contact N6 ..O1 . 2.76 Ång.

Author Response: This is a hydrogen bond, but the relevant H atoms have not been located.

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 2.04 Check

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT220_ALERT_2_C Non-Solvent Resd N Ueq(max)/Ueq(min) Range 3.1 Ratio

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C30 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C34 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C47 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C51 Check
 PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C55 Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.676 Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report
 PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
 PLAT977_ALERT_2_C Check Negative Difference Density on H55B -0.42 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H55C -0.34 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H56D -0.35 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: C56 H60 Cl2 N6 Ni1 O1 S2
 Atom count from the _atom_site data: C56 H58 Cl2 N6 Ni1 O1 S2
 ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
 not performed for this radiation type.
 CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
 CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
 From the CIF: _cell_formula_units_Z 8
 From the CIF: _chemical_formula_sum C56 H60 Cl2 N6 Ni O S2
 TEST: Compare cell contents of formula and atom_site data
 atom Z*formula cif sites diff
 C 448.00 448.00 0.00
 H 480.00 464.00 16.00
 Cl 16.00 16.00 0.00
 N 48.00 48.00 0.00
 Ni 8.00 8.00 0.00
 O 8.00 8.00 0.00
 S 16.00 16.00 0.00
 PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 36 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 83 Report
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 22.63 Why ?
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
 PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 13 Report
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 4 Report
 PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
 PLAT301_ALERT_3_G Main Residue Disorder (Resd 1) 21% Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 50% Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
 PLAT304_ALERT_4_G Non-Integer Number of Atoms in 3. Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms in 4. Check
 PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O1' Check
 PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O1 Check
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 1672 Note
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1324 Note
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info
 PLAT984_ALERT_1_G The Ni-f²= 0.358 Deviates from the B&C-Value 0.343 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 25 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 16 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

Datablock: oxdp26_H28b

Bond precision: C-C = 0.0140 Å Wavelength=0.69320
 Cell: a=36.962(8) b=14.668(3) c=40.822(9)
 alpha=90 beta=91.783(2) gamma=90
 Temperature: 150 K

Calculated Reported
 Volume 22121(8) 22121(8)
 Space group P 21/n P 21/n
 Hall group -P 2yn -P 2yn
 Moiety formula C58 H56 N6 S2 [+ solvent] C58 H56 ClO N6 S2
 Sum formula C58 H56 N6 S2 [+ solvent] C58 H56 ClO N6 S2
 Mr 901.21 901.20
 Dx,g cm-3 1.082 1.082
 Z 16 16
 Mu (mm-1) 0.126 0.129
 F000 7648.0 7648.0
 F000' 7653.77
 h,k,lmax 46,18,51 46,18,49
 Nref 45822 42452
 Tmin,Tmax 0.977,0.999
 Tmin' 0.977
 Correction method= Not given
 Data completeness= 0.926 Theta(max)= 25.787
 R(reflections)= 0.2034(28286) wR2(reflections)= 0.5174(42452)
 S = 1.071 Npar= 2575

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
 Click on the hyperlinks for more details of the test.

Alert level A

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.52 Report

Author Response: Weak and relatively imprecise diffraction data from challenging samples.

PLAT413_ALERT_2_A Short Inter XH3 .. XHn H43L ..H57M . 1.85 Ang.

Author Response: Probably a consequence of unresolved disorder.

PLAT910_ALERT_3_A Missing # of FCF Reflection(s) Below Theta(Min). 284 Note

Author Response: Low-angle reflections rejected because of beam stop and high background scattering.

PLAT930_ALERT_2_A Check Twin Law (2-1 1)[2-5 1] Estimated BASF 0.95

Author Response: The most probable twin law has been used in the refinement.

PLAT930_ALERT_2_A Check Twin Law (2 1 -1)[2 5 -1] Estimated BASF 0.95

Author Response: The most probable twin law has been used in the refinement.

Alert level B

PLAT082_ALERT_2_B High R1 Value 0.20 Report

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.94 eA-3

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01396 Ang.

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75

_refine_diff_density_min given = -1.418

Test value = -1.200

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75

The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -1.42 eA-3

PLAT213_ALERT_2_C Atom C40A has ADP max/min Ratio 3.1 prolata

PLAT213_ALERT_2_C Atom C39W has ADP max/min Ratio 3.9 prolata

PLAT213_ALERT_2_C Atom C22B has ADP max/min Ratio 3.1 prolata

PLAT213_ALERT_2_C Atom C23B has ADP max/min Ratio 3.6 prolata

PLAT213_ALERT_2_C Atom C24B has ADP max/min Ratio 3.1 prolata

PLAT213_ALERT_2_C Atom C44D has ADP max/min Ratio 3.1 prolata

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 4.1 Ratio

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 3.5 Ratio

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 4.6 Ratio

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 4.1 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 5.1 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 4.1 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 4.9 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 5.0 Ratio

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C41A Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C55A Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C41B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C51B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C55B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C41D Check

PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C22D -C27D 1.37 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 14.778 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.585 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.715 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.017 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 578 Report

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 16

From the CIF: _chemical_formula_sum C58 H56 Cl0 N6 S2

TEST: Compare cell contents of formula and atom_site data

atom Z*formula cif sites diff

C 928.00 928.00 0.00

H 896.00 896.00 0.00

Cl 16.00 0.00 16.00

N 96.00 96.00 0.00

S 32.00 32.00 0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 285 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 285 Report

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 8 Report

PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 264.59 Why ?

PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 27 Report

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 8 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 9% Note

PLAT301_ALERT_3_G Main Residue Disorder(Resd 2) 9% Note

PLAT301_ALERT_3_G Main Residue Disorder(Resd 3) 9% Note

PLAT301_ALERT_3_G Main Residue Disorder(Resd 4) 5% Note

PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 8 Note

PLAT722_ALERT_1_G Angle Calc 108.00, Rep 109.50 Dev... 1.50 Degree

C37A -C40W -H40O 1.555 1.555 1.555 # 969 Check

PLAT722_ALERT_1_G Angle Calc 111.00, Rep 109.50 Dev... 1.50 Degree

H40M -C40W -H40N 1.555 1.555 1.555 # 970 Check

PLAT860_ALERT_3_G Number of Least-Squares Restraints 11126 Note

PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info

PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2422 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT931_ALERT_5_G Found Twin Law (0 0 1)[] Est. BASF 0.34 Check
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ 2 Units

5 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
30 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
30 **ALERT level G** = General information/check it is not something unexpected

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 ALERT type 2 Indicator that the structure model may be wrong or deficient
18 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: oxdp22_H29

Bond precision: C-C = 0.0139 Å Wavelength=0.68930

Cell: a=34.85(3) b=13.785(11) c=40.21(3)

alpha=90 beta=92.378(10) gamma=90

Temperature: 150 K

Calculated Reported

Volume 19301(27) 19302(26)

Space group I 2/a I 2/a

Hall group -I 2ya -I 2ya

Moiety formula C₅₄ H₅₂ N₈ [+ solvent] C₅₄ H₅₂ N₈

Sum formula C₅₄ H₅₂ N₈ [+ solvent] C₅₄ H₅₂ N₈

Mr 813.04 813.03

Dx,g cm⁻³ 1.119 1.119

Z 16 16

Mu (mm⁻¹) 0.063 0.063

F000 6912.0 6912.0

F000' 6913.76

h,k,lmax 40,16,46 40,15,45

Nref 15993 14281

Tmin,Tmax 0.986,0.998

Tmin' 0.986

Correction method= Not given

Data completeness= 0.893 Theta(max)= 23.677

R(reflections)= 0.1812(8224) wR2(reflections)= 0.4153(14281)

S = 1.142 Npar= 1202

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.893 Why?

Author Response: Incomplete coverage of diffraction pattern and some data rejected as poor during integration and scaling.

PLAT213_ALERT_2_A Atom C53Y has ADP max/min Ratio 6.0 prolate

Author Response: Consequence of imperfect disorder modelling.

Alert level B

PLAT082_ALERT_2_B High R1 Value 0.18 Report

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.42 Report
Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.23 eA-3
Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT213_ALERT_2_B Atom C53B has ADP max/min Ratio 4.1 prolata
Author Response: Consequence of imperfect disorder modelling.

PLAT213_ALERT_2_B Atom C54B has ADP max/min Ratio 4.3 prolata
Author Response: Consequence of imperfect disorder modelling.

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01391 Ang.
Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 14 Note
Author Response: Low-angle reflections rejected because of beam stop and high background scattering.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.583 1665 Report
Author Response: Incomplete coverage of diffraction pattern and some data rejected as poor during integration and scaling.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5826

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.76 Report

PLAT213_ALERT_2_C Atom C10A has ADP max/min Ratio 3.4 oblate
Author Response: Consequence of imperfect disorder modelling.

PLAT213_ALERT_2_C Atom C24A has ADP max/min Ratio 3.3 prolata
Author Response: Consequence of imperfect disorder modelling.

PLAT213_ALERT_2_C Atom C11B has ADP max/min Ratio 3.4 oblate
Author Response: Consequence of imperfect disorder modelling.

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 3.4 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 4.1 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference C37A --C39A 0.17 Ang.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C37A Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C37B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C47B Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.7 Note

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H40F ..H48I . 2.12 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 35.783 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 8.315 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.029 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.356 Check

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 133 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 133 Report

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 309.89 Why ?

PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 13 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report

PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 10% Note

PLAT301_ALERT_3_G Main Residue Disorder(Resd 2) 5% Note

PLAT432_ALERT_2_G Short Inter X...Y Contact N8B ..C22A 3.03 Ang.

PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 323 A**3

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 4 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 3291 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note

2 **ALERT level A** = Most likely a serious problem - resolve or explain
8 **ALERT level B** = A potentially serious problem, consider carefully
19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 ALERT type 2 Indicator that the structure model may be wrong or deficient
15 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: oxdp28_Ni10

Bond precision: C-C = 0.0211 Å Wavelength=0.69320

Cell: a=26.289(2) b=15.6605(14) c=28.462(2)

alpha=90 beta=109.794(2) gamma=90

Temperature: 150 K

Calculated Reported

Volume 11025.4(15) 11025.4(15)

Space group P 21 P 21

Hall group P 2yb P 2yb

Moiety formula

C56 H64 N4 Ni S2 Si, C2 H4

Cl2

C56 H64 N4 Ni S2 Si,C2 H4

Cl2

Sum formula C58 H68 Cl2 N4 Ni S2 Si C58 H68 Cl2 N4 Ni S2 Si

Mr 1042.96 1042.98

Dx,g cm-3 1.257 1.257

Z 8 8

Mu (mm-1) 0.544 0.550

F000 4416.0 4416.0

F000' 4424.46

h,k,lmax 33,19,35 32,19,35

Nref 45832[23789] 31817

Tmin,Tmax 0.926,0.978 0.920,0.980

Tmin' 0.926

Correction method= # Reported T Limits: Tmin=0.920 Tmax=0.980

AbsCorr = MULTI-SCAN

Data completeness= 1.34/0.69 Theta(max)= 25.817

R(reflections)= 0.1419(29230) wR2(reflections)= 0.4066(31817)

S = 1.646 Npar= 2412

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density 5.90 eA-3

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT910_ALERT_3_A Missing # of FCF Reflection(s) Below Theta(Min). 67 Note

Author Response: Low-angle reflections rejected because of beam stop and high background scattering.

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.41 Report

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT220_ALERT_2_B Non-Solvent Resd C Ueq(max)/Ueq(min) Range 7.2 Ratio

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.0211 Ang.

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT082_ALERT_2_C High R1 Value 0.14 Report

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.94 Report

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 8 Check

PLAT213_ALERT_2_C Atom N1B has ADP max/min Ratio 3.1 prolate

PLAT213_ALERT_2_C Atom N1B has ADP max/min Ratio 3.1 prolate

PLAT213_ALERT_2_C Atom N3B has ADP max/min Ratio 3.1 oblate

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 4.3 Ratio

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 4.5 Ratio

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 5.1 Ratio

Author Response: Weak and relatively imprecise diffraction data from challenging samples, and limitations of structure model with extensive disorder.

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 5.1 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 8.1 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 4.4 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 4.9 Ratio

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35A Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C49A Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C49B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35C Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C49C Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35D Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C49D Check

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C2S Check

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C4S Check

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C5S Check

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C7S Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C1S Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C3S Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C6S Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C8S Check

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H28G ..H54D . 2.10 Ang.

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H4S1 ..H51C . 2.04 Ang.

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 276 Report

PLAT914_ALERT_3_C No Bijvoet Pairs in FCF for Non-centro Structure Please Check

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 129 Check

PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 26.41 Check

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu

not performed for this radiation type.

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 272 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 264 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.186 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.25 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 7 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C5A - C21A . 1.42 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C5B - C21B . 1.42 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C5C - C21C . 1.42 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C5D - C21D . 1.42 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 16 Note
PLAT722_ALERT_1_G Angle Calc 112.00, Rep 110.40 Dev... 1.60 Degree
C1S -C2S -H2S1 1.555 1.555 1.555 # 1031 Check
PLAT722_ALERT_1_G Angle Calc 109.00, Rep 110.40 Dev... 1.40 Degree
H2S2 -C2S -CL2 1.555 1.555 1.555 # 1036 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
C56 H64 N4 Ni S2 Si
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 7 Note
C2 H4 Cl2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 8 Note
C2 H4 Cl2
PLAT860_ALERT_3_G Number of Least-Squares Restraints 5129 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 369 Note
PLAT984_ALERT_1_G The Ni-f²= 0.358 Deviates from the B&C-Value 0.343 Check
PLAT984_ALERT_1_G The Si-f²= 0.078 Deviates from the B&C-Value 0.079 Check

2 **ALERT level A** = Most likely a serious problem - resolve or explain

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36 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

25 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

27 ALERT type 2 Indicator that the structure model may be wrong or deficient

13 ALERT type 3 Indicator that the structure quality may be low

18 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

Datablock: oxdp25_NiZn14

Bond precision: C-C = 0.0120 Å Wavelength=0.69320

Cell: a=14.218(5) b=20.122(6) c=21.975(7)

alpha=69.445(3) beta=72.044(3) gamma=82.393(3)

Temperature: 150 K

Calculated Reported

Volume 5598(3) 5598(3)

Space group P -1 P -1

Hall group -P 1 -P 1

Moiety formula

C103 H109 N9 Ni O S2 Zn [+]

solvent]

C103 H109 N9 Ni O S2 Zn

Sum formula

C103 H109 N9 Ni O S2 Zn [+]

solvent]

C103 H109 N9 Ni O S2 Zn

Mr 1677.19 1677.19

Dx,g cm⁻³ 0.995 0.995

Z 2 2

Mu (mm⁻¹) 0.432 0.435

F000 1776.0 1776.0
 F000' 1778.17
 h,k,lmax 15,22,24 15,22,24
 Nref 16414 15633
 Tmin,Tmax 0.959,0.996 0.930,0.990
 Tmin' 0.937
 Correction method= # Reported T Limits: Tmin=0.930 Tmax=0.990
 AbsCorr = MULTI-SCAN
 Data completeness= 0.952 Theta(max)= 22.810
 R(reflections)= 0.1004(8508) wR2(reflections)= 0.3328(15633)
 S = 1.039 Npar= 1348

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
 Click on the hyperlinks for more details of the test.

Alert level A

PLAT910_ALERT_3_A Missing # of FCF Reflection(s) Below Theta(Min). 151 Note

Author Response: Low-angle reflections rejected because of beam stop and high background scattering.

Alert level B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575

Calculated sin(theta_max)/wavelength = 0.5593

Author Response: Weak diffraction, especially at higher angles; this structure shows considerable disorder of the main molecule and (unmodelled) solvent.

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full value Low . 0.952 Why?

Author Response: Incomplete coverage of diffraction pattern and some data rejected as poor during integration and scaling.

PLAT234_ALERT_4_B Large Hirshfeld Difference O1 --C103 0.28 Ang.

Author Response: Consequence of incompletely modelled disorder.

PLAT412_ALERT_2_B Short Intra XH3 .. XHn H63 ..H67B .. 1.74 Ang.

Author Response: Probably a consequence of unresolved disorder.

PLAT420_ALERT_2_B D-H Without Acceptor O1 -- H1 . Please Check

Author Response: Possibly a potential hydrogen bond to the unmodelled solvent, but more likely no hydrogen bond possible for this coordinated methanol molecule.

Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.33 Report

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.40 Report

PLAT213_ALERT_2_C Atom Ni2 has ADP max/min Ratio 3.3 prolate

PLAT213_ALERT_2_C Atom N2B has ADP max/min Ratio 3.4 prolate

PLAT213_ALERT_2_C Atom C10B has ADP max/min Ratio 3.2 oblate

PLAT220_ALERT_2_C Non-Solvent Resd C Ueq(max)/Ueq(min) Range 4.7 Ratio

PLAT220_ALERT_2_C Non-Solvent Resd N Ueq(max)/Ueq(min) Range 3.8 Ratio

PLAT222_ALERT_3_C Non-Solv. Resd H Uiso(max)/Uiso(min) Range 5.4 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference Zn --O1 0.16 Ang.

Author Response: Consequence of incompletely modelled disorder.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C56 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C70 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C84 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C102 Check

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.01203 Ang.

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C10 - C46 . 1.53 Ang.

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H23 ..H95C . 2.05 Ang.

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -7.946 Report

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.148 Report

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.559 633 Report

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.86A From O1 -0.45 eA-3

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 91 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 148 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.17 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.53 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 16 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for S1A --C43A . 7.3 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 27% Note
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C15 - C41 . 1.41 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C40 - C42 . 1.43 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact S1B ..C102 3.26 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N9 ..C5B 2.41 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N9 ..C4B 2.80 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N9 ..C6B 2.85 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N9 ..C43B 3.05 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C30 ..C44B 3.19 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C102 ..C44B 3.10 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C102 ..C5B 3.18 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT722_ALERT_1_G Angle Calc 111.00, Rep 109.50 Dev... 1.50 Degree
C94 -C95 -H95B 1.555 1.555 1.555 # 438 Check
PLAT722_ALERT_1_G Angle Calc 108.00, Rep 109.50 Dev... 1.50 Degree
H95A -C95 -H95C 1.555 1.555 1.555 # 441 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 4477 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT984_ALERT_1_G The Ni-f² = 0.358 Deviates from the B&C-Value 0.343 Check
PLAT984_ALERT_1_G The Zn-f² = 0.324 Deviates from the B&C-Value 0.304 Check
PLAT985_ALERT_1_G The Zn-f² = 1.403 Deviates from the B&C-Value 1.376 Check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta*

Crystallographica Section C or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 12/12/2017

Datablock oxdp21_Ni8a - ellipsoid plot
Datablock oxdp26_H28b - ellipsoid plot
Datablock oxdp22_H29 - ellipsoid plot
Datablock oxdp28_Ni10 - ellipsoid plot
Datablock oxdp25_NiZn14 - ellipsoid plot

Table S1. Crystal data and structure refinement for **Ni8a**.

Identification code	oxdp21	
CCDC deposition number	1822190	
Chemical formula (moiety)	$C_{54}H_{54}N_6NiS_2 \cdot C_2H_4Cl_2 \cdot H_2O$	
Chemical formula (total)	$C_{56}H_{60}Cl_2N_6NiOS_2$	
Formula weight	1026.83	
Temperature	150(2) K	
Radiation, wavelength	synchrotron, 0.6893 Å	
Crystal system, space group	monoclinic, C2/c	
Unit cell parameters	$a = 39.247(4)$ Å	$\alpha = 90^\circ$
	$b = 12.6465(11)$ Å	$\beta = 93.847(2)^\circ$
	$c = 21.5421(19)$ Å	$\gamma = 90^\circ$
Cell volume	$10668.1(17)$ Å ³	
Z	8	
Calculated density	1.279 g/cm ³	
Absorption coefficient μ	0.542 mm ⁻¹	
F(000)	4320	
Crystal color and size	black, $0.200 \times 0.200 \times 0.030$ mm ³	
Reflections for cell refinement	13074 (θ range 2.2 to 28.7°)	
Data collection method	Bruker SMART 1K CCD diffractometer	
	thick-slice ω scans	
θ range for data collection	1.9 to 29.2°	
Index ranges	$h -50$ to 55 , $k -17$ to 16 , $l -29$ to 16	
Completeness to $\theta = 24.4^\circ$	99.8 %	
Reflections collected	36156	
Independent reflections	14512 ($R_{\text{int}} = 0.0363$)	
Reflections with $F^2 > 2\sigma$	10061	
Absorption correction	multi-scan	
Min. and max. transmission	0.852 and 0.928	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0890, 22.6250	
Data / restraints / parameters	14512 / 1672 / 763	
Final R indices [$F^2 > 2\sigma$]	$R1 = 0.0701$, $wR2 = 0.1767$	
R indices (all data)	$R1 = 0.1045$, $wR2 = 0.2007$	
Goodness-of-fit on F^2	1.066	
Largest and mean shift/su	0.003 and 0.000	
Largest diff. peak and hole	0.89 and -0.55 e Å ⁻³	

Table S2. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$) for **Ni8a**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ni	0.62376(2)	0.41905(3)	0.65823(2)	0.03138(11)
N1	0.63945(6)	0.48496(18)	0.73348(11)	0.0344(5)
N2	0.59413(6)	0.33323(19)	0.70176(11)	0.0367(5)
N3	0.60688(6)	0.35827(17)	0.58273(11)	0.0339(5)
N4	0.65223(6)	0.50722(18)	0.61387(11)	0.0347(5)
N5	0.66613(12)	0.1683(3)	0.4249(2)	0.0838(12)
N6	0.74188(13)	0.3984(5)	0.4757(3)	0.1044(16)
C1	0.65035(8)	0.5905(2)	0.73989(16)	0.0389(6)
C2	0.65462(9)	0.6144(3)	0.80499(17)	0.0497(8)
C3	0.64893(9)	0.5240(3)	0.83668(16)	0.0506(8)
C4	0.63931(8)	0.4447(3)	0.79089(14)	0.0406(6)
C5	0.62704(9)	0.3382(3)	0.80182(14)	0.0435(7)
C6	0.59789(9)	0.3048(3)	0.76206(14)	0.0452(7)
C7	0.56845(11)	0.2492(3)	0.77995(17)	0.0631(11)
C8	0.54643(11)	0.2448(3)	0.72902(18)	0.0597(10)
C9	0.56243(8)	0.2934(2)	0.67872(15)	0.0430(7)
C10	0.55219(8)	0.2903(2)	0.61601(15)	0.0391(6)
C11	0.57457(8)	0.3167(2)	0.56997(14)	0.0374(6)
C12	0.57086(9)	0.2875(2)	0.50618(15)	0.0460(7)
C13	0.60132(10)	0.3060(3)	0.48120(15)	0.0498(8)
C14	0.62328(8)	0.3499(2)	0.52940(14)	0.0408(6)
C15	0.65777(9)	0.3888(3)	0.52453(14)	0.0425(7)
C16	0.66657(8)	0.4840(2)	0.55956(14)	0.0409(6)
C17	0.68668(10)	0.5692(3)	0.54137(17)	0.0507(8)
C18	0.68411(9)	0.6467(3)	0.58505(17)	0.0495(8)
C19	0.66323(8)	0.6069(2)	0.63116(15)	0.0387(6)
C20	0.66010(7)	0.6503(2)	0.69051(15)	0.0385(6)
C21	0.64269(11)	0.2727(3)	0.84576(16)	0.0574(9)
S1	0.68079(15)	0.2936(4)	0.8854(3)	0.0678(11)
S2	0.6238(2)	0.1456(4)	0.8582(3)	0.0796(15)
C22	0.6789(4)	0.1800(8)	0.9375(5)	0.083(2)
C23	0.6645(3)	0.0917(7)	0.8965(6)	0.088(2)
S1'	0.67662(19)	0.3241(5)	0.8966(3)	0.0790(14)
S2'	0.63707(15)	0.1399(4)	0.8520(3)	0.0652(11)
C22'	0.6929(3)	0.1955(9)	0.9235(6)	0.082(2)
C23'	0.6630(3)	0.1225(10)	0.9238(6)	0.086(2)
C24	0.51830(8)	0.2444(2)	0.59502(15)	0.0407(7)
C25	0.50994(8)	0.1409(2)	0.61013(14)	0.0384(6)
C26	0.47842(8)	0.0974(2)	0.58998(14)	0.0366(6)
C27	0.45558(8)	0.1606(2)	0.55394(14)	0.0376(6)
C28	0.46340(8)	0.2643(2)	0.53706(16)	0.0420(7)
C29	0.49489(8)	0.3050(2)	0.55878(17)	0.0446(7)
C30	0.47029(9)	−0.0168(2)	0.60801(14)	0.0405(7)
C31	0.47187(15)	−0.0255(3)	0.67900(18)	0.0772(14)
C32	0.43466(10)	−0.0521(3)	0.5825(2)	0.0598(10)
C33	0.49633(10)	−0.0917(3)	0.5815(2)	0.0566(9)

C34	0.43781(9)	0.3319(3)	0.49781(19)	0.0543(9)
C35	0.4232(5)	0.4142(12)	0.5434(5)	0.093(5)
C36	0.4098(4)	0.2655(9)	0.4670(10)	0.099(5)
C37	0.4566(3)	0.3931(12)	0.4505(6)	0.069(3)
C35'	0.4070(4)	0.3584(18)	0.5331(8)	0.091(5)
C36'	0.4248(6)	0.2675(10)	0.4373(7)	0.082(5)
C37'	0.4524(4)	0.4315(10)	0.4695(9)	0.067(4)
C38	0.68007(10)	0.3400(3)	0.48619(16)	0.0543(8)
C39	0.67169(12)	0.2446(3)	0.45225(18)	0.0624(10)
C40	0.71424(12)	0.3756(4)	0.4811(2)	0.0675(11)
C41	0.67225(8)	0.7610(2)	0.70122(17)	0.0447(7)
C42	0.65491(9)	0.8435(2)	0.67027(18)	0.0500(8)
C43	0.66595(9)	0.9479(3)	0.6786(2)	0.0567(10)
C44	0.69474(9)	0.9662(3)	0.7176(2)	0.0597(10)
C45	0.71307(9)	0.8855(3)	0.7488(2)	0.0528(9)
C46	0.70114(8)	0.7823(2)	0.74054(18)	0.0476(8)
C47	0.64599(10)	1.0374(3)	0.6433(2)	0.0746(13)
C48	0.6089(5)	1.033(3)	0.6650(18)	0.094(7)
C49	0.6446(9)	1.022(3)	0.5726(7)	0.085(6)
C50	0.6607(6)	1.1463(10)	0.6611(16)	0.081(6)
C48'	0.6093(4)	1.046(3)	0.6638(17)	0.101(7)
C49'	0.6463(10)	1.009(4)	0.5737(7)	0.109(8)
C50'	0.6642(8)	1.1450(12)	0.653(2)	0.108(8)
C51	0.74557(10)	0.9079(3)	0.7903(2)	0.0655(11)
C52	0.7705(2)	0.9600(11)	0.7509(5)	0.090(4)
C53	0.7353(2)	0.9954(7)	0.8405(5)	0.073(3)
C54	0.7579(3)	0.8162(8)	0.8298(7)	0.095(5)
C52'	0.7574(3)	1.0198(7)	0.7912(6)	0.104(5)
C53'	0.7443(3)	0.8603(10)	0.8534(4)	0.085(3)
C54'	0.77639(18)	0.8435(9)	0.7607(5)	0.086(3)
C55	0.5593(3)	0.4251(11)	0.2923(6)	0.256(5)
C56	0.5566(3)	0.3876(7)	0.2267(6)	0.254(5)
Cl1	0.52824(14)	0.3839(5)	0.3424(2)	0.200(2)
Cl2	0.57053(15)	0.2510(4)	0.2300(4)	0.235(3)
Cl1'	0.5300(3)	0.5073(10)	0.3239(7)	0.249(5)
Cl2'	0.5345(4)	0.2694(10)	0.2160(8)	0.288(6)
O1	0.7367(4)	0.8947(14)	0.5326(10)	0.179(5)
O1'	0.7369(3)	0.8883(12)	0.5857(8)	0.172(5)

Table S3. Bond lengths [Å] and angles [°] for **Ni8a**.

Ni–N1	1.889(2)	Ni–N2	1.886(3)
Ni–N3	1.879(2)	Ni–N4	1.884(2)
N1–C1	1.406(3)	N1–C4	1.338(4)
N2–C6	1.346(4)	N2–C9	1.402(4)
N3–C11	1.383(4)	N3–C14	1.358(4)
N4–C16	1.364(4)	N4–C19	1.375(4)
N5–C39	1.145(6)	N6–C40	1.136(6)
C1–C2	1.433(5)	C1–C20	1.380(5)
C2–H2	0.950	C2–C3	1.357(5)
C3–H3	0.950	C3–C4	1.439(4)
C4–C5	1.455(4)	C5–C6	1.446(4)
C5–C21	1.372(5)	C6–C7	1.427(5)
C7–H7	0.950	C7–C8	1.352(5)
C8–H8	0.950	C8–C9	1.427(5)
C9–C10	1.384(4)	C10–C11	1.408(5)
C10–C24	1.494(4)	C11–C12	1.421(4)
C12–H12	0.950	C12–C13	1.364(5)
C13–H13	0.950	C13–C14	1.417(4)
C14–C15	1.450(5)	C15–C16	1.451(5)
C15–C38	1.388(5)	C16–C17	1.406(5)
C17–H17	0.950	C17–C18	1.367(5)
C18–H18	0.950	C18–C19	1.421(5)
C19–C20	1.405(5)	C20–C41	1.492(4)
C21–S1	1.692(6)	C21–S2	1.797(6)
C21–S1'	1.789(7)	C21–S2'	1.701(7)
S1–C22	1.827(9)	S2–C23	1.877(11)
C22–H22A	0.990	C22–H22B	0.990
C22–C23	1.510(12)	C23–H23A	0.990
C23–H23B	0.990	S1'–C22'	1.827(10)
S2'–C23'	1.808(10)	C22'–H22C	0.990
C22'–H22D	0.990	C22'–C23'	1.493(14)
C23'–H23C	0.990	C23'–H23D	0.990
C24–C25	1.393(4)	C24–C29	1.395(4)
C25–H25	0.950	C25–C26	1.397(4)
C26–C27	1.397(4)	C26–C30	1.535(4)
C27–H27	0.950	C27–C28	1.401(4)
C28–C29	1.390(4)	C28–C34	1.530(4)
C29–H29	0.950	C30–C31	1.530(5)
C30–C32	1.534(5)	C30–C33	1.532(5)
C31–H31A	0.980	C31–H31B	0.980
C31–H31C	0.980	C32–H32A	0.980
C32–H32B	0.980	C32–H32C	0.980
C33–H33A	0.980	C33–H33B	0.980
C33–H33C	0.980	C34–C35	1.567(8)
C34–C36	1.501(8)	C34–C37	1.512(9)
C34–C35'	1.509(10)	C34–C36'	1.593(10)
C34–C37'	1.528(9)	C35–H35A	0.980
C35–H35B	0.980	C35–H35C	0.980
C36–H36A	0.980	C36–H36B	0.980

C36–H36C	0.980	C37–H37A	0.980
C37–H37B	0.980	C37–H37C	0.980
C35'–H35D	0.980	C35'–H35E	0.980
C35'–H35F	0.980	C36'–H36D	0.980
C36'–H36E	0.980	C36'–H36F	0.980
C37'–H37D	0.980	C37'–H37E	0.980
C37'–H37F	0.980	C38–C39	1.437(6)
C38–C40	1.426(6)	C41–C42	1.391(4)
C41–C46	1.395(4)	C42–H42	0.950
C42–C43	1.398(4)	C43–C44	1.383(5)
C43–C47	1.546(5)	C44–H44	0.950
C44–C45	1.395(5)	C45–C46	1.394(4)
C45–C51	1.535(5)	C46–H46	0.950
C47–C48	1.558(12)	C47–C49	1.532(12)
C47–C50	1.532(11)	C47–C48'	1.538(11)
C47–C49'	1.542(12)	C47–C50'	1.545(11)
C48–H48A	0.980	C48–H48B	0.980
C48–H48C	0.980	C49–H49A	0.980
C49–H49B	0.980	C49–H49C	0.980
C50–H50A	0.980	C50–H50B	0.980
C50–H50C	0.980	C48'–H48D	0.980
C48'–H48E	0.980	C48'–H48F	0.980
C49'–H49D	0.980	C49'–H49E	0.980
C49'–H49F	0.980	C50'–H50D	0.980
C50'–H50E	0.980	C50'–H50F	0.980
C51–C52	1.492(9)	C51–C53	1.616(9)
C51–C54	1.499(9)	C51–C52'	1.490(8)
C51–C53'	1.491(9)	C51–C54'	1.624(9)
C52–H52A	0.980	C52–H52B	0.980
C52–H52C	0.980	C53–H53A	0.980
C53–H53B	0.980	C53–H53C	0.980
C54–H54A	0.980	C54–H54B	0.980
C54–H54C	0.980	C52'–H52D	0.980
C52'–H52E	0.980	C52'–H52F	0.980
C53'–H53D	0.980	C53'–H53E	0.980
C53'–H53F	0.980	C54'–H54D	0.980
C54'–H54E	0.980	C54'–H54F	0.980
C55–H55A	0.990	C55–H55B	0.990
C55–H55C	0.990	C55–H55D	0.990
C55–C56	1.489(9)	C55–Cl1	1.761(8)
C55–Cl1'	1.723(8)	C56–H56A	0.990
C56–H56B	0.990	C56–H56C	0.990
C56–H56D	0.990	C56–Cl2	1.812(8)
C56–Cl2'	1.738(8)		
N1–Ni–N2	90.20(10)	N1–Ni–N3	177.59(10)
N1–Ni–N4	90.22(11)	N2–Ni–N3	90.09(10)
N2–Ni–N4	178.29(11)	N3–Ni–N4	89.41(11)
Ni–N1–C1	125.7(2)	Ni–N1–C4	127.2(2)
C1–N1–C4	106.9(2)	Ni–N2–C6	127.0(2)
Ni–N2–C9	126.4(2)	C6–N2–C9	106.4(3)

Ni-N3-C11	126.4(2)	Ni-N3-C14	127.2(2)
C11-N3-C14	106.4(2)	Ni-N4-C16	126.9(2)
Ni-N4-C19	126.2(2)	C16-N4-C19	106.8(3)
N1-C1-C2	108.1(3)	N1-C1-C20	122.9(3)
C2-C1-C20	128.2(3)	C1-C2-H2	126.2
C1-C2-C3	107.6(3)	H2-C2-C3	126.2
C2-C3-H3	126.7	C2-C3-C4	106.6(3)
H3-C3-C4	126.7	N1-C4-C3	110.6(3)
N1-C4-C5	121.6(3)	C3-C4-C5	127.5(3)
C4-C5-C6	115.6(3)	C4-C5-C21	122.2(3)
C6-C5-C21	122.2(3)	N2-C6-C5	121.6(3)
N2-C6-C7	110.7(3)	C5-C6-C7	127.4(3)
C6-C7-H7	126.7	C6-C7-C8	106.6(3)
H7-C7-C8	126.7	C7-C8-H8	126.0
C7-C8-C9	108.0(3)	H8-C8-C9	126.0
N2-C9-C8	108.1(3)	N2-C9-C10	123.3(3)
C8-C9-C10	128.0(3)	C9-C10-C11	121.8(3)
C9-C10-C24	120.1(3)	C11-C10-C24	117.6(3)
N3-C11-C10	123.8(3)	N3-C11-C12	108.9(3)
C10-C11-C12	126.2(3)	C11-C12-H12	126.2
C11-C12-C13	107.5(3)	H12-C12-C13	126.2
C12-C13-H13	126.7	C12-C13-C14	106.5(3)
H13-C13-C14	126.7	N3-C14-C13	110.5(3)
N3-C14-C15	122.2(3)	C13-C14-C15	127.2(3)
C14-C15-C16	115.7(3)	C14-C15-C38	121.4(3)
C16-C15-C38	122.7(3)	N4-C16-C15	121.8(3)
N4-C16-C17	110.2(3)	C15-C16-C17	127.6(3)
C16-C17-H17	126.6	C16-C17-C18	106.8(3)
H17-C17-C18	126.6	C17-C18-H18	126.3
C17-C18-C19	107.4(3)	H18-C18-C19	126.3
N4-C19-C18	108.7(3)	N4-C19-C20	124.1(3)
C18-C19-C20	126.0(3)	C1-C20-C19	122.2(3)
C1-C20-C41	119.8(3)	C19-C20-C41	117.5(3)
C5-C21-S1	126.4(3)	C5-C21-S2	118.2(3)
C5-C21-S1'	118.9(3)	C5-C21-S2'	126.6(3)
S1-C21-S2	115.1(3)	S1'-C21-S2'	113.9(3)
C21-S1-C22	96.7(5)	C21-S2-C23	92.5(4)
S1-C22-H22A	110.8	S1-C22-H22B	110.8
S1-C22-C23	104.6(7)	H22A-C22-H22B	108.9
H22A-C22-C23	110.8	H22B-C22-C23	110.8
S2-C23-C22	105.2(8)	S2-C23-H23A	110.7
S2-C23-H23B	110.7	C22-C23-H23A	110.7
C22-C23-H23B	110.7	H23A-C23-H23B	108.8
C21-S1'-C22'	95.8(4)	C21-S2'-C23'	96.8(5)
S1'-C22'-H22C	110.3	S1'-C22'-H22D	110.3
S1'-C22'-C23'	107.1(8)	H22C-C22'-H22D	108.6
H22C-C22'-C23'	110.3	H22D-C22'-C23'	110.3
S2'-C23'-C22'	108.5(8)	S2'-C23'-H23C	110.0
S2'-C23'-H23D	110.0	C22'-C23'-H23C	110.0
C22'-C23'-H23D	110.0	H23C-C23'-H23D	108.4
C10-C24-C25	120.9(3)	C10-C24-C29	119.7(3)

C25-C24-C29	119.4(3)	C24-C25-H25	119.5
C24-C25-C26	121.0(3)	H25-C25-C26	119.5
C25-C26-C27	118.0(3)	C25-C26-C30	119.1(3)
C27-C26-C30	122.9(3)	C26-C27-H27	118.8
C26-C27-C28	122.4(3)	H27-C27-C28	118.8
C27-C28-C29	117.7(3)	C27-C28-C34	121.3(3)
C29-C28-C34	121.0(3)	C24-C29-C28	121.5(3)
C24-C29-H29	119.3	C28-C29-H29	119.3
C26-C30-C31	109.0(3)	C26-C30-C32	112.5(3)
C26-C30-C33	109.4(3)	C31-C30-C32	108.2(3)
C31-C30-C33	110.2(3)	C32-C30-C33	107.5(3)
C30-C31-H31A	109.5	C30-C31-H31B	109.5
C30-C31-H31C	109.5	H31A-C31-H31B	109.5
H31A-C31-H31C	109.5	H31B-C31-H31C	109.5
C30-C32-H32A	109.5	C30-C32-H32B	109.5
C30-C32-H32C	109.5	H32A-C32-H32B	109.5
H32A-C32-H32C	109.5	H32B-C32-H32C	109.5
C30-C33-H33A	109.5	C30-C33-H33B	109.5
C30-C33-H33C	109.5	H33A-C33-H33B	109.5
H33A-C33-H33C	109.5	H33B-C33-H33C	109.5
C28-C34-C35	106.2(5)	C28-C34-C36	111.4(5)
C28-C34-C37	109.0(5)	C28-C34-C35'	111.4(6)
C28-C34-C36'	109.2(6)	C28-C34-C37'	115.6(6)
C35-C34-C36	111.1(7)	C35-C34-C37	107.4(6)
C36-C34-C37	111.4(8)	C35'-C34-C36'	107.6(8)
C35'-C34-C37'	110.7(7)	C36'-C34-C37'	101.7(8)
C34-C35-H35A	109.5	C34-C35-H35B	109.5
C34-C35-H35C	109.5	H35A-C35-H35B	109.5
H35A-C35-H35C	109.5	H35B-C35-H35C	109.5
C34-C36-H36A	109.5	C34-C36-H36B	109.5
C34-C36-H36C	109.5	H36A-C36-H36B	109.5
H36A-C36-H36C	109.5	H36B-C36-H36C	109.5
C34-C37-H37A	109.5	C34-C37-H37B	109.5
C34-C37-H37C	109.5	H37A-C37-H37B	109.5
H37A-C37-H37C	109.5	H37B-C37-H37C	109.5
C34-C35'-H35D	109.5	C34-C35'-H35E	109.5
C34-C35'-H35F	109.5	H35D-C35'-H35E	109.5
H35D-C35'-H35F	109.5	H35E-C35'-H35F	109.5
C34-C36'-H36D	109.5	C34-C36'-H36E	109.5
C34-C36'-H36F	109.5	H36D-C36'-H36E	109.5
H36D-C36'-H36F	109.5	H36E-C36'-H36F	109.5
C34-C37'-H37D	109.5	C34-C37'-H37E	109.5
C34-C37'-H37F	109.5	H37D-C37'-H37E	109.5
H37D-C37'-H37F	109.5	H37E-C37'-H37F	109.5
C15-C38-C39	122.9(4)	C15-C38-C40	122.7(4)
C39-C38-C40	114.2(4)	N5-C39-C38	177.7(5)
N6-C40-C38	176.0(6)	C20-C41-C42	119.2(3)
C20-C41-C46	120.9(3)	C42-C41-C46	119.9(3)
C41-C42-H42	119.7	C41-C42-C43	120.6(3)
H42-C42-C43	119.7	C42-C43-C44	118.0(3)
C42-C43-C47	119.1(3)	C44-C43-C47	122.9(3)

C43-C44-H44	118.5	C43-C44-C45	123.0(3)
H44-C44-C45	118.5	C44-C45-C46	117.8(3)
C44-C45-C51	121.8(3)	C46-C45-C51	120.4(3)
C41-C46-C45	120.7(3)	C41-C46-H46	119.7
C45-C46-H46	119.7	C43-C47-C48	106.1(15)
C43-C47-C49	112.4(16)	C43-C47-C50	111.4(8)
C43-C47-C48'	111.3(16)	C43-C47-C49'	105.8(18)
C43-C47-C50'	111.3(10)	C48-C47-C49	108.8(14)
C48-C47-C50	107.5(12)	C49-C47-C50	110.4(13)
C48'-C47-C49'	111.4(13)	C48'-C47-C50'	109.3(12)
C49'-C47-C50'	107.6(14)	C47-C48-H48A	109.5
C47-C48-H48B	109.5	C47-C48-H48C	109.5
H48A-C48-H48B	109.5	H48A-C48-H48C	109.5
H48B-C48-H48C	109.5	C47-C49-H49A	109.5
C47-C49-H49B	109.5	C47-C49-H49C	109.5
H49A-C49-H49B	109.5	H49A-C49-H49C	109.5
H49B-C49-H49C	109.5	C47-C50-H50A	109.5
C47-C50-H50B	109.5	C47-C50-H50C	109.5
H50A-C50-H50B	109.5	H50A-C50-H50C	109.5
H50B-C50-H50C	109.5	C47-C48'-H48D	109.5
C47-C48'-H48E	109.5	C47-C48'-H48F	109.5
H48D-C48'-H48E	109.5	H48D-C48'-H48F	109.5
H48E-C48'-H48F	109.5	C47-C49'-H49D	109.5
C47-C49'-H49E	109.5	C47-C49'-H49F	109.5
H49D-C49'-H49E	109.5	H49D-C49'-H49F	109.5
H49E-C49'-H49F	109.5	C47-C50'-H50D	109.5
C47-C50'-H50E	109.5	C47-C50'-H50F	109.5
H50D-C50'-H50E	109.5	H50D-C50'-H50F	109.5
H50E-C50'-H50F	109.5	C45-C51-C52	107.5(5)
C45-C51-C53	106.4(4)	C45-C51-C54	114.4(5)
C45-C51-C52'	115.4(5)	C45-C51-C53'	112.3(5)
C45-C51-C54'	106.9(4)	C52-C51-C53	106.3(6)
C52-C51-C54	117.7(8)	C53-C51-C54	103.6(7)
C52'-C51-C53'	113.7(7)	C52'-C51-C54'	103.9(7)
C53'-C51-C54'	103.2(7)	C51-C52-H52A	109.5
C51-C52-H52B	109.5	C51-C52-H52C	109.5
H52A-C52-H52B	109.5	H52A-C52-H52C	109.5
H52B-C52-H52C	109.5	C51-C53-H53A	109.5
C51-C53-H53B	109.5	C51-C53-H53C	109.5
H53A-C53-H53B	109.5	H53A-C53-H53C	109.5
H53B-C53-H53C	109.5	C51-C54-H54A	109.5
C51-C54-H54B	109.5	C51-C54-H54C	109.5
H54A-C54-H54B	109.5	H54A-C54-H54C	109.5
H54B-C54-H54C	109.5	C51-C52'-H52D	109.5
C51-C52'-H52E	109.5	C51-C52'-H52F	109.5
H52D-C52'-H52E	109.5	H52D-C52'-H52F	109.5
H52E-C52'-H52F	109.5	C51-C53'-H53D	109.5
C51-C53'-H53E	109.5	C51-C53'-H53F	109.5
H53D-C53'-H53E	109.5	H53D-C53'-H53F	109.5
H53E-C53'-H53F	109.5	C51-C54'-H54D	109.5
C51-C54'-H54E	109.5	C51-C54'-H54F	109.5

H54D–C54'–H54E	109.5	H54D–C54'–H54F	109.5
H54E–C54'–H54F	109.5	H55A–C55–H55B	107.1
H55A–C55–C56	107.6	H55A–C55–C11	107.6
H55B–C55–C56	107.6	H55B–C55–C11	107.6
H55C–C55–H55D	106.4	H55C–C55–C56	106.3
H55C–C55–C11'	106.3	H55D–C55–C56	106.3
H55D–C55–C11'	106.3	C56–C55–C11	118.7(9)
C56–C55–C11'	124.1(12)	C55–C56–H56A	110.7
C55–C56–H56B	110.7	C55–C56–H56C	108.8
C55–C56–H56D	108.8	C55–C56–C12	105.3(9)
C55–C56–C12'	113.7(10)	H56A–C56–H56B	108.8
H56A–C56–C12	110.7	H56B–C56–C12	110.7
H56C–C56–H56D	107.7	H56C–C56–C12'	108.8
H56D–C56–C12'	108.8		

Table S4. Torsion angles [°] for **Ni8a**.

N2–Ni–N1–C1	–148.0(2)	N2–Ni–N1–C4	25.1(3)
N4–Ni–N1–C1	30.3(2)	N4–Ni–N1–C4	–156.6(3)
N1–Ni–N2–C6	–25.5(3)	N1–Ni–N2–C9	149.1(3)
N3–Ni–N2–C6	156.9(3)	N3–Ni–N2–C9	–28.5(3)
N2–Ni–N3–C11	28.4(2)	N2–Ni–N3–C14	–154.3(2)
N4–Ni–N3–C11	–150.0(2)	N4–Ni–N3–C14	27.3(2)
N1–Ni–N4–C16	151.0(2)	N1–Ni–N4–C19	–27.2(2)
N3–Ni–N4–C16	–31.4(2)	N3–Ni–N4–C19	150.4(2)
Ni–N1–C1–C2	170.4(2)	Ni–N1–C1–C20	–19.1(4)
C4–N1–C1–C2	–3.9(3)	C4–N1–C1–C20	166.7(3)
N1–C1–C2–C3	4.3(4)	C20–C1–C2–C3	–165.6(3)
C1–C2–C3–C4	–2.9(4)	Ni–N1–C4–C3	–172.0(2)
Ni–N1–C4–C5	1.6(5)	C1–N1–C4–C3	2.1(4)
C1–N1–C4–C5	175.8(3)	C2–C3–C4–N1	0.6(4)
C2–C3–C4–C5	–172.6(3)	N1–C4–C5–C6	–37.3(5)
N1–C4–C5–C21	140.9(4)	C3–C4–C5–C6	135.2(4)
C3–C4–C5–C21	–46.6(6)	Ni–N2–C6–C5	–0.8(5)
Ni–N2–C6–C7	173.6(3)	C9–N2–C6–C5	–176.2(3)
C9–N2–C6–C7	–1.9(4)	C4–C5–C6–N2	36.9(5)
C4–C5–C6–C7	–136.5(4)	C21–C5–C6–N2	–141.4(4)
C21–C5–C6–C7	45.3(6)	N2–C6–C7–C8	–0.3(5)
C5–C6–C7–C8	173.7(4)	C6–C7–C8–C9	2.3(5)
Ni–N2–C9–C8	–172.2(2)	Ni–N2–C9–C10	16.4(4)
C6–N2–C9–C8	3.2(4)	C6–N2–C9–C10	–168.1(3)
C7–C8–C9–N2	–3.5(5)	C7–C8–C9–C10	167.4(4)
N2–C9–C10–C11	7.0(5)	N2–C9–C10–C24	178.6(3)
C8–C9–C10–C11	–162.6(4)	C8–C9–C10–C24	9.0(5)
Ni–N3–C11–C10	–16.1(4)	Ni–N3–C11–C12	174.72(19)
C14–N3–C11–C10	166.1(3)	C14–N3–C11–C12	–3.0(3)
C9–C10–C11–N3	–7.2(4)	C9–C10–C11–C12	160.0(3)
C24–C10–C11–N3	–179.0(3)	C24–C10–C11–C12	–11.8(4)
N3–C11–C12–C13	3.1(3)	C10–C11–C12–C13	–165.7(3)
C11–C12–C13–C14	–1.9(4)	Ni–N3–C14–C13	–175.8(2)
Ni–N3–C14–C15	0.4(4)	C11–N3–C14–C13	1.9(3)
C11–N3–C14–C15	178.1(3)	C12–C13–C14–N3	0.0(4)
C12–C13–C14–C15	–176.0(3)	N3–C14–C15–C16	–34.8(4)
N3–C14–C15–C38	148.2(3)	C13–C14–C15–C16	140.7(3)
C13–C14–C15–C38	–36.2(5)	Ni–N4–C16–C15	7.7(4)
Ni–N4–C16–C17	–179.0(2)	C19–N4–C16–C15	–173.7(3)
C19–N4–C16–C17	–0.5(3)	C14–C15–C16–N4	30.6(4)
C14–C15–C16–C17	–141.5(3)	C38–C15–C16–N4	–152.5(3)
C38–C15–C16–C17	35.5(5)	N4–C16–C17–C18	–0.9(4)
C15–C16–C17–C18	171.8(3)	C16–C17–C18–C19	1.9(4)
Ni–N4–C19–C18	–179.78(19)	Ni–N4–C19–C20	12.6(4)
C16–N4–C19–C18	1.7(3)	C16–N4–C19–C20	–166.0(3)
C17–C18–C19–N4	–2.3(3)	C17–C18–C19–C20	165.1(3)
N1–C1–C20–C19	–6.7(4)	N1–C1–C20–C41	–178.4(3)

C2-C1-C20-C19	161.8(3)	C2-C1-C20-C41	-9.8(5)
N4-C19-C20-C1	10.2(4)	N4-C19-C20-C41	-178.0(2)
C18-C19-C20-C1	-155.3(3)	C18-C19-C20-C41	16.5(4)
C4-C5-C21-S1	-10.2(6)	C4-C5-C21-S2	176.5(4)
C4-C5-C21-S1'	6.4(6)	C4-C5-C21-S2'	-164.8(4)
C6-C5-C21-S1	167.9(4)	C6-C5-C21-S2	-5.4(6)
C6-C5-C21-S1'	-175.5(4)	C6-C5-C21-S2'	13.3(6)
C5-C21-S1-C22	173.9(6)	S2-C21-S1-C22	-12.7(6)
C5-C21-S2-C23	160.8(5)	S1-C21-S2-C23	-13.2(6)
C21-S1-C22-C23	41.2(11)	S1-C22-C23-S2	-53.6(12)
C21-S2-C23-C22	40.9(10)	C5-C21-S1'-C22'	-164.3(6)
S2'-C21-S1'-C22'	8.0(7)	C5-C21-S2'-C23'	-174.7(6)
S1'-C21-S2'-C23'	13.7(6)	C21-S1'-C22'-C23'	-32.3(12)
S1'-C22'-C23'-S2'	45.3(15)	C21-S2'-C23'-C22'	-36.7(12)
C9-C10-C24-C25	-57.3(4)	C9-C10-C24-C29	123.9(4)
C11-C10-C24-C25	114.6(3)	C11-C10-C24-C29	-64.2(4)
C10-C24-C25-C26	-179.3(3)	C29-C24-C25-C26	-0.5(5)
C24-C25-C26-C27	0.3(5)	C24-C25-C26-C30	-179.8(3)
C25-C26-C27-C28	0.7(5)	C30-C26-C27-C28	-179.2(3)
C26-C27-C28-C29	-1.6(5)	C26-C27-C28-C34	-179.7(3)
C27-C28-C29-C24	1.4(5)	C34-C28-C29-C24	179.5(3)
C10-C24-C29-C28	178.4(3)	C25-C24-C29-C28	-0.4(5)
C25-C26-C30-C31	59.7(4)	C25-C26-C30-C32	179.7(3)
C25-C26-C30-C33	-60.8(4)	C27-C26-C30-C31	-120.4(4)
C27-C26-C30-C32	-0.4(5)	C27-C26-C30-C33	119.1(3)
C27-C28-C34-C35	105.4(9)	C27-C28-C34-C36	-15.7(11)
C27-C28-C34-C37	-139.1(8)	C27-C28-C34-C35'	67.1(12)
C27-C28-C34-C36'	-51.6(10)	C27-C28-C34-C37'	-165.5(10)
C29-C28-C34-C35	-72.6(10)	C29-C28-C34-C36	166.2(11)
C29-C28-C34-C37	42.8(8)	C29-C28-C34-C35'	-110.9(12)
C29-C28-C34-C36'	130.4(10)	C29-C28-C34-C37'	16.5(11)
C14-C15-C38-C39	-4.4(5)	C14-C15-C38-C40	-179.2(3)
C16-C15-C38-C39	178.9(3)	C16-C15-C38-C40	4.1(5)
C1-C20-C41-C42	-120.6(4)	C1-C20-C41-C46	60.9(5)
C19-C20-C41-C42	67.3(4)	C19-C20-C41-C46	-111.1(4)
C20-C41-C42-C43	-179.0(4)	C46-C41-C42-C43	-0.6(6)
C41-C42-C43-C44	0.8(7)	C41-C42-C43-C47	179.9(4)
C42-C43-C44-C45	0.1(7)	C47-C43-C44-C45	-179.0(4)
C43-C44-C45-C46	-1.2(7)	C43-C44-C45-C51	178.1(4)
C44-C45-C46-C41	1.5(6)	C51-C45-C46-C41	-177.9(4)
C20-C41-C46-C45	177.8(4)	C42-C41-C46-C45	-0.6(6)
C42-C43-C47-C48	60.0(16)	C42-C43-C47-C49	-58.7(14)
C42-C43-C47-C50	176.7(16)	C42-C43-C47-C48'	63.7(13)
C42-C43-C47-C49'	-57.5(16)	C42-C43-C47-C50'	-174(2)
C44-C43-C47-C48	-120.9(15)	C44-C43-C47-C49	120.4(14)
C44-C43-C47-C50	-4.2(17)	C44-C43-C47-C48'	-117.2(13)
C44-C43-C47-C49'	121.5(15)	C44-C43-C47-C50'	5(2)
C44-C45-C51-C52	-58.9(8)	C44-C45-C51-C53	54.6(6)
C44-C45-C51-C54	168.4(8)	C44-C45-C51-C52'	-4.4(9)

C44–C45–C51–C53'	128.1(7)	C44–C45–C51–C54'	–119.4(6)
C46–C45–C51–C52	120.4(7)	C46–C45–C51–C53	–126.0(5)
C46–C45–C51–C54	–12.3(9)	C46–C45–C51–C52'	174.9(8)
C46–C45–C51–C53'	–52.5(8)	C46–C45–C51–C54'	59.9(6)
C11–C55–C56–C12	–75.3(13)	C11'–C55–C56–C12'	–90.3(14)

Table S5. Anisotropic displacement parameters ($\text{\AA}^2$) for **Ni8a**.The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	0.03581(19)	0.02429(16)	0.03294(18)	0.00049(13)	-0.00584(13)	0.00047(13)
N1	0.0353(12)	0.0275(11)	0.0396(12)	-0.0032(9)	-0.0038(10)	-0.0023(9)
N2	0.0440(13)	0.0327(12)	0.0327(11)	-0.0043(9)	-0.0030(10)	-0.0070(10)
N3	0.0424(12)	0.0257(10)	0.0323(11)	0.0015(9)	-0.0067(9)	0.0032(9)
N4	0.0347(12)	0.0314(11)	0.0367(12)	0.0072(9)	-0.0084(9)	0.0031(9)
N5	0.112(3)	0.072(2)	0.069(2)	-0.018(2)	0.020(2)	0.011(2)
N6	0.079(3)	0.133(4)	0.103(4)	-0.017(3)	0.024(3)	-0.001(3)
C1	0.0363(14)	0.0274(12)	0.0518(16)	-0.0067(12)	-0.0065(12)	-0.0016(11)
C2	0.0525(19)	0.0440(17)	0.0523(18)	-0.0178(14)	0.0006(15)	-0.0129(14)
C3	0.059(2)	0.0502(19)	0.0419(17)	-0.0124(14)	-0.0019(15)	-0.0164(16)
C4	0.0444(16)	0.0409(15)	0.0356(14)	-0.0057(12)	-0.0025(12)	-0.0082(12)
C5	0.0582(19)	0.0418(16)	0.0303(14)	-0.0039(12)	0.0014(13)	-0.0140(14)
C6	0.0611(19)	0.0401(16)	0.0340(14)	-0.0048(12)	0.0009(13)	-0.0168(14)
C7	0.084(3)	0.067(2)	0.0380(17)	-0.0072(16)	0.0074(17)	-0.041(2)
C8	0.065(2)	0.064(2)	0.0500(19)	-0.0117(17)	0.0079(17)	-0.0321(19)
C9	0.0469(17)	0.0370(15)	0.0446(16)	-0.0078(13)	-0.0020(13)	-0.0083(13)
C10	0.0429(15)	0.0262(12)	0.0467(16)	-0.0042(11)	-0.0078(12)	-0.0016(11)
C11	0.0462(15)	0.0254(12)	0.0387(14)	-0.0006(11)	-0.0120(12)	0.0022(11)
C12	0.0600(19)	0.0354(15)	0.0401(15)	-0.0012(12)	-0.0146(14)	-0.0017(13)
C13	0.070(2)	0.0460(18)	0.0319(15)	-0.0017(13)	-0.0085(14)	-0.0017(16)
C14	0.0520(17)	0.0313(13)	0.0379(14)	0.0046(11)	-0.0072(12)	0.0032(12)
C15	0.0535(17)	0.0414(15)	0.0315(14)	0.0085(12)	-0.0040(12)	0.0068(13)
C16	0.0437(16)	0.0406(15)	0.0370(14)	0.0114(12)	-0.0068(12)	0.0032(12)
C17	0.057(2)	0.0474(18)	0.0471(18)	0.0133(14)	-0.0004(15)	-0.0030(15)
C18	0.0491(18)	0.0403(16)	0.0572(19)	0.0181(14)	-0.0094(15)	-0.0060(13)
C19	0.0370(14)	0.0286(13)	0.0481(16)	0.0086(11)	-0.0142(12)	0.0000(10)
C20	0.0313(13)	0.0272(12)	0.0547(17)	0.0021(12)	-0.0133(12)	-0.0001(10)
C21	0.086(2)	0.0523(18)	0.0331(15)	0.0018(13)	-0.0041(16)	-0.0130(17)
S1	0.090(2)	0.059(2)	0.0515(18)	0.0124(15)	-0.0168(14)	-0.0106(17)
S2	0.136(4)	0.0551(19)	0.0454(14)	0.0125(13)	-0.011(2)	-0.037(2)
C22	0.123(5)	0.066(4)	0.055(4)	0.027(3)	-0.023(4)	-0.020(4)
C23	0.137(5)	0.062(4)	0.060(4)	0.015(3)	-0.021(4)	-0.016(4)
S1'	0.111(3)	0.062(3)	0.058(2)	0.0062(17)	-0.039(2)	0.000(2)
S2'	0.085(3)	0.0490(14)	0.060(2)	0.0079(12)	-0.0089(19)	0.0012(17)
C22'	0.115(5)	0.071(4)	0.055(4)	0.013(3)	-0.027(4)	-0.007(4)
C23'	0.130(5)	0.067(4)	0.058(4)	0.020(4)	-0.011(4)	-0.003(4)
C24	0.0434(15)	0.0280(13)	0.0491(17)	-0.0052(12)	-0.0087(13)	-0.0015(11)
C25	0.0437(15)	0.0292(13)	0.0408(15)	-0.0024(11)	-0.0094(12)	0.0023(11)
C26	0.0469(15)	0.0258(12)	0.0361(14)	-0.0044(10)	-0.0055(12)	-0.0020(11)
C27	0.0411(15)	0.0300(13)	0.0404(15)	-0.0039(11)	-0.0078(12)	-0.0013(11)
C28	0.0453(16)	0.0275(13)	0.0516(18)	-0.0026(12)	-0.0098(13)	0.0039(11)
C29	0.0464(16)	0.0250(13)	0.061(2)	-0.0009(13)	-0.0093(14)	-0.0004(11)
C30	0.0569(18)	0.0266(13)	0.0366(14)	-0.0018(11)	-0.0075(13)	-0.0046(12)

C31	0.138(4)	0.050(2)	0.0420(19)	0.0023(16)	-0.004(2)	-0.028(3)
C32	0.060(2)	0.0310(15)	0.086(3)	-0.0022(17)	-0.012(2)	-0.0108(14)
C33	0.066(2)	0.0279(15)	0.074(2)	-0.0006(15)	-0.0063(19)	0.0025(14)
C34	0.0508(18)	0.0344(15)	0.075(2)	0.0077(15)	-0.0167(16)	0.0077(13)
C35	0.110(10)	0.076(7)	0.092(6)	0.013(5)	0.000(6)	0.058(7)
C36	0.084(8)	0.067(5)	0.136(12)	0.042(6)	-0.073(8)	-0.018(5)
C37	0.073(5)	0.058(6)	0.074(6)	0.026(5)	-0.020(4)	0.012(5)
C35'	0.063(7)	0.095(12)	0.114(10)	0.032(9)	0.002(6)	0.040(7)
C36'	0.103(12)	0.051(5)	0.085(8)	0.019(5)	-0.056(7)	-0.011(6)
C37'	0.058(6)	0.034(5)	0.106(11)	0.024(6)	-0.018(6)	0.008(4)
C38	0.065(2)	0.060(2)	0.0386(17)	0.0074(15)	0.0055(15)	0.0059(17)
C39	0.086(3)	0.057(2)	0.046(2)	0.0022(16)	0.0157(19)	0.013(2)
C40	0.067(2)	0.084(3)	0.053(2)	-0.003(2)	0.0116(19)	0.013(2)
C41	0.0397(15)	0.0275(13)	0.064(2)	0.0011(13)	-0.0169(14)	-0.0045(11)
C42	0.0438(16)	0.0300(14)	0.072(2)	0.0028(14)	-0.0229(16)	-0.0022(12)
C43	0.0523(19)	0.0286(14)	0.086(3)	0.0036(16)	-0.0228(18)	0.0001(13)
C44	0.055(2)	0.0291(15)	0.091(3)	0.0036(16)	-0.0239(19)	-0.0089(14)
C45	0.0415(17)	0.0371(15)	0.077(2)	0.0021(16)	-0.0203(16)	-0.0068(13)
C46	0.0411(16)	0.0292(14)	0.069(2)	0.0053(14)	-0.0194(15)	-0.0051(12)
C47	0.072(2)	0.0295(16)	0.116(3)	0.0088(19)	-0.041(2)	0.0034(16)
C48	0.070(7)	0.049(10)	0.160(17)	0.016(11)	-0.026(10)	0.032(7)
C49	0.103(14)	0.036(7)	0.109(6)	0.022(6)	-0.043(8)	0.009(7)
C50	0.075(10)	0.030(6)	0.130(14)	0.018(7)	-0.049(9)	0.009(6)
C48'	0.064(6)	0.044(9)	0.186(19)	-0.015(11)	-0.043(8)	0.007(6)
C49'	0.157(19)	0.060(14)	0.103(6)	0.030(7)	-0.053(9)	0.016(10)
C50'	0.124(14)	0.026(6)	0.168(19)	0.012(8)	-0.035(14)	-0.012(7)
C51	0.054(2)	0.055(2)	0.083(3)	0.0029(18)	-0.0303(19)	-0.0182(16)
C52	0.046(5)	0.108(9)	0.114(8)	-0.014(6)	-0.012(5)	-0.025(5)
C53	0.061(5)	0.058(5)	0.097(7)	-0.001(4)	-0.023(4)	-0.007(4)
C54	0.080(8)	0.059(6)	0.136(11)	-0.003(6)	-0.070(7)	0.005(5)
C52'	0.089(7)	0.071(5)	0.143(11)	0.018(6)	-0.063(8)	-0.041(5)
C53'	0.079(7)	0.102(9)	0.070(5)	0.010(5)	-0.026(4)	-0.036(6)
C54'	0.039(4)	0.120(8)	0.094(7)	-0.003(6)	-0.024(4)	-0.012(4)
C55	0.221(8)	0.271(9)	0.278(10)	0.001(9)	0.036(9)	-0.075(8)
C56	0.218(8)	0.255(9)	0.291(10)	0.000(9)	0.024(9)	-0.078(8)
Cl1	0.206(4)	0.254(6)	0.142(3)	0.040(3)	0.031(3)	-0.047(4)
Cl2	0.180(4)	0.166(4)	0.370(8)	0.008(4)	0.092(5)	-0.064(4)
Cl1'	0.276(10)	0.193(9)	0.281(10)	-0.023(8)	0.036(9)	-0.051(8)
Cl2'	0.256(11)	0.265(11)	0.350(12)	0.018(10)	0.063(11)	-0.061(9)
O1	0.174(8)	0.195(9)	0.164(11)	0.005(11)	-0.010(10)	-0.100(8)
O1'	0.149(7)	0.199(9)	0.168(11)	0.048(10)	0.015(9)	-0.061(7)

Table S6. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for **Ni8a**.

	x	y	z	U
H2	0.660385	0.681311	0.822747	0.060
H3	0.650909	0.514916	0.880547	0.061
H7	0.565005	0.220911	0.819887	0.076
H8	0.524214	0.214650	0.727037	0.072
H12	0.550822	0.259986	0.484831	0.055
H13	0.606754	0.292264	0.439649	0.060
H17	0.699555	0.572261	0.505614	0.061
H18	0.694393	0.714643	0.584660	0.059
H22A	0.701977	0.161717	0.955816	0.099
H22B	0.663886	0.194982	0.971549	0.099
H23A	0.659914	0.028389	0.921709	0.105
H23B	0.680662	0.072137	0.865056	0.105
H22C	0.709771	0.168419	0.895191	0.098
H22D	0.704203	0.201672	0.965816	0.098
H23C	0.649428	0.138588	0.959754	0.103
H23D	0.670996	0.048353	0.927587	0.103
H25	0.525935	0.099313	0.634521	0.046
H27	0.433947	0.132149	0.540371	0.045
H29	0.500581	0.375736	0.548730	0.054
H31A	0.455115	0.022726	0.695430	0.116
H31B	0.466684	−0.098218	0.690903	0.116
H31C	0.494814	−0.006471	0.696130	0.116
H32A	0.433118	−0.047166	0.537006	0.090
H32B	0.430745	−0.125438	0.594929	0.090
H32C	0.417360	−0.006312	0.599292	0.090
H33A	0.495079	−0.085458	0.536013	0.085
H33B	0.519350	−0.072892	0.598292	0.085
H33C	0.491220	−0.164638	0.593065	0.085
H35A	0.441907	0.456467	0.562851	0.140
H35B	0.406941	0.460896	0.520208	0.140
H35C	0.411470	0.376878	0.575700	0.140
H36A	0.398140	0.226873	0.498792	0.149
H36B	0.393466	0.311221	0.443497	0.149
H36C	0.419658	0.215056	0.438648	0.149
H37A	0.474701	0.435591	0.471981	0.104
H37B	0.466822	0.343661	0.422017	0.104
H37C	0.440630	0.439825	0.426866	0.104
H35D	0.397997	0.293608	0.550914	0.136
H35E	0.413558	0.408233	0.566618	0.136
H35F	0.389361	0.390474	0.504708	0.136
H36D	0.444325	0.249090	0.413312	0.124
H36E	0.413357	0.202641	0.449607	0.124
H36F	0.408712	0.311001	0.411612	0.124
H37D	0.472361	0.412777	0.446773	0.100
H37E	0.434994	0.463961	0.440765	0.100
H37F	0.459192	0.481721	0.502675	0.100
H42	0.635366	0.828674	0.643235	0.060

H44	0.702393	1.036991	0.723532	0.072
H46	0.712796	0.725861	0.761925	0.057
H48A	0.598842	0.963684	0.654188	0.142
H48B	0.609519	1.042742	0.710157	0.142
H48C	0.595172	1.088683	0.644284	0.142
H49A	0.635168	0.952399	0.561876	0.127
H49B	0.630010	1.077031	0.552441	0.127
H49C	0.667676	1.027962	0.558159	0.127
H50A	0.661393	1.154719	0.706427	0.122
H50B	0.683803	1.152379	0.647057	0.122
H50C	0.646138	1.201448	0.641339	0.122
H48D	0.609967	1.063867	0.708150	0.151
H48E	0.597057	1.101348	0.639610	0.151
H48F	0.597573	0.978224	0.656801	0.151
H49D	0.669991	1.004343	0.562052	0.164
H49E	0.634861	0.941221	0.565978	0.164
H49F	0.634345	1.064345	0.548786	0.164
H50D	0.687550	1.139778	0.640093	0.162
H50E	0.651711	1.199285	0.628335	0.162
H50F	0.664760	1.164301	0.697268	0.162
H52A	0.759242	1.018243	0.727595	0.135
H52B	0.789710	0.987627	0.777452	0.135
H52C	0.778931	0.908260	0.721692	0.135
H53A	0.718883	0.964840	0.867689	0.110
H53B	0.755838	1.017668	0.865537	0.110
H53C	0.725061	1.056708	0.818605	0.110
H54A	0.739183	0.789456	0.853214	0.143
H54B	0.765962	0.759940	0.803111	0.143
H54C	0.776742	0.839306	0.858871	0.143
H52D	0.757691	1.046044	0.748397	0.156
H52E	0.741891	1.063159	0.814237	0.156
H52F	0.780511	1.023812	0.811418	0.156
H53D	0.736298	0.787034	0.849534	0.127
H53E	0.767119	0.861678	0.874738	0.127
H53F	0.728499	0.901025	0.877557	0.127
H54D	0.770658	0.768078	0.758394	0.129
H54E	0.779605	0.870291	0.718822	0.129
H54F	0.797510	0.853142	0.787027	0.129
H55A	0.559178	0.503380	0.291582	0.307
H55B	0.581886	0.402936	0.311151	0.307
H55C	0.581719	0.460819	0.298636	0.307
H55D	0.560658	0.360885	0.318658	0.307
H56A	0.571497	0.430121	0.200908	0.305
H56B	0.532800	0.392864	0.208762	0.305
H56C	0.579939	0.378412	0.212519	0.305
H56D	0.545061	0.442678	0.200256	0.305

Table S7. Crystal data and structure refinement for **H₂8b**.

Identification code	oxdp26	
CCDC deposition number	1822191	
Chemical formula (moiety)	C ₅₈ H ₅₆ Cl ₀ N ₆ S ₂	
Chemical formula (total)	C ₅₈ H ₅₆ Cl ₀ N ₆ S ₂	
Formula weight	901.20	
Temperature	150(2) K	
Radiation, wavelength	synchrotron, 0.6932 Å	
Crystal system, space group	monoclinic, P2 ₁ /n	
Unit cell parameters	a = 36.962(8) Å	α = 90°
	b = 14.668(3) Å	β = 91.783(2)°
	c = 40.822(9) Å	γ = 90°
Cell volume	22121(8) Å ³	
Z	16	
Calculated density	1.082 g/cm ³	
Absorption coefficient μ	0.129 mm ⁻¹	
F(000)	7648	
Crystal color and size	dark green, 0.180 × 0.150 × 0.010 mm ³	
Reflections for cell refinement	21035 (θ range 4.6 to 25.4°)	
Data collection method	Bruker SMART 1K CCD diffractometer	
	thin-slice ω scans	
θ range for data collection	4.6 to 25.8°	
Index ranges	h -45 to 46, k -18 to 18, l -2 to 49	
Completeness to θ = 24.6°	98.1 %	
Reflections collected	42452	
Reflections with F ² > 2σ	28286	
Absorption correction	none	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F ²	
Weighting parameters a, b	0.1954, 264.5945	
Data / restraints / parameters	42452 / 11126 / 2575	
Final R indices [F ² > 2σ]	R1 = 0.2034, wR2 = 0.4944	
R indices (all data)	R1 = 0.2409, wR2 = 0.5174	
Goodness-of-fit on F ²	1.071	
Extinction coefficient	0.0293(16)	
Largest and mean shift/su	0.003 and 0.000	
Largest diff. peak and hole	1.94 and -1.42 e Å ⁻³	

Table S8. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$) for **H₂8b**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
N1A	0.6560(2)	0.0864(5)	0.26623(18)	0.0266(16)
N2A	0.5951(2)	−0.0366(5)	0.26153(18)	0.0267(16)
N3A	0.5905(2)	−0.0221(6)	0.1911(2)	0.0361(19)
N4A	0.6492(2)	0.1020(6)	0.19650(19)	0.0308(18)
N5A	0.5444(3)	−0.3378(7)	0.2730(3)	0.053(3)
N6A	0.5443(4)	−0.3292(8)	0.1705(3)	0.067(3)
C1A	0.6879(2)	0.1269(6)	0.2625(2)	0.0276(19)
C2A	0.7008(3)	0.1583(7)	0.2930(2)	0.035(2)
C3A	0.6754(3)	0.1348(7)	0.3154(2)	0.033(2)
C4A	0.6478(2)	0.0858(6)	0.2987(2)	0.0281(19)
C5A	0.6176(2)	0.0395(6)	0.3115(2)	0.0312(19)
C6A	0.5945(2)	−0.0178(6)	0.2947(2)	0.0294(19)
C7A	0.5647(2)	−0.0675(8)	0.3092(2)	0.040(2)
C8A	0.5495(3)	−0.1197(7)	0.2849(2)	0.040(2)
C9A	0.5696(2)	−0.0992(6)	0.2557(2)	0.032(2)
C10A	0.5636(3)	−0.1451(6)	0.2246(2)	0.033(2)
C11A	0.5668(3)	−0.0932(7)	0.1941(2)	0.037(2)
C12A	0.5463(3)	−0.0990(8)	0.1651(2)	0.041(2)
C13A	0.5581(3)	−0.0317(8)	0.1441(2)	0.040(2)
C14A	0.5853(3)	0.0184(7)	0.1614(2)	0.036(2)
C15A	0.6058(3)	0.0927(7)	0.1495(2)	0.035(2)
C16A	0.6355(2)	0.1307(6)	0.1653(2)	0.0309(19)
C17A	0.6587(3)	0.2004(7)	0.1524(2)	0.035(2)
C18A	0.6863(3)	0.2101(7)	0.1744(2)	0.033(2)
C19A	0.6800(2)	0.1475(6)	0.2008(2)	0.0282(19)
C20A	0.7034(2)	0.1406(6)	0.2303(2)	0.0291(19)
C21A	0.7406(2)	0.1358(7)	0.2277(2)	0.033(2)
C22A	0.8090(2)	0.1015(7)	0.2371(3)	0.039(2)
C23A	0.8046(2)	0.1090(7)	0.2041(3)	0.043(2)
C24A	0.8335(3)	0.0975(8)	0.1836(3)	0.051(3)
C25A	0.8669(3)	0.0764(9)	0.1975(4)	0.062(3)
C26A	0.8714(3)	0.0667(8)	0.2313(4)	0.057(3)
C27A	0.8430(2)	0.0799(7)	0.2511(3)	0.051(3)
C28A	0.5519(3)	−0.2317(6)	0.2229(2)	0.039(2)
C29A	0.5477(3)	−0.2888(7)	0.2512(3)	0.043(3)
C30A	0.5473(3)	−0.2840(8)	0.1934(3)	0.047(3)
C31A	0.6143(3)	0.0435(6)	0.3481(2)	0.035(2)
C32A	0.5971(3)	0.1157(7)	0.3629(2)	0.041(2)
C33A	0.5903(3)	0.1174(7)	0.3960(2)	0.049(3)
C34A	0.6020(4)	0.0413(8)	0.4143(3)	0.053(3)
C35A	0.6202(3)	−0.0304(7)	0.4014(2)	0.049(3)
C36A	0.6246(3)	−0.0312(7)	0.3678(2)	0.039(2)
C37A	0.5693(4)	0.1910(9)	0.4129(3)	0.074(4)
C38A	0.5533(5)	0.2597(11)	0.3884(4)	0.084(6)
C39A	0.5939(5)	0.2413(14)	0.4375(5)	0.110(7)

C40A	0.5384(5)	0.1493(13)	0.4323(5)	0.105(7)
C41A	0.6321(4)	-0.1139(8)	0.4215(3)	0.071(4)
C42A	0.6557(13)	-0.083(2)	0.4508(8)	0.098(10)
C43A	0.5983(7)	-0.161(3)	0.4342(11)	0.095(10)
C44A	0.6530(14)	-0.180(2)	0.4007(8)	0.097(10)
C45A	0.5938(3)	0.1331(7)	0.1168(2)	0.038(2)
C46A	0.5943(3)	0.0818(7)	0.0880(2)	0.037(2)
C47A	0.5820(3)	0.1201(7)	0.0583(2)	0.038(2)
C48A	0.5686(3)	0.2082(7)	0.0587(3)	0.043(2)
C49A	0.5674(3)	0.2612(6)	0.0870(2)	0.042(2)
C50A	0.5809(3)	0.2208(7)	0.1162(2)	0.038(2)
C51A	0.5833(3)	0.0680(7)	0.0257(2)	0.048(3)
C52A	0.5992(4)	-0.0273(8)	0.0299(3)	0.057(3)
C53A	0.5443(3)	0.0606(12)	0.0121(3)	0.066(4)
C54A	0.6053(4)	0.1208(10)	0.0009(3)	0.060(4)
C55A	0.5529(3)	0.3594(7)	0.0871(3)	0.050(3)
C56A	0.5287(5)	0.3781(11)	0.0577(4)	0.095(6)
C57A	0.5850(4)	0.4241(9)	0.0865(5)	0.082(5)
C58A	0.5324(5)	0.3811(11)	0.1180(4)	0.089(5)
S1A	0.77081(7)	0.11940(19)	0.26054(7)	0.0368(6)
S2A	0.76145(7)	0.1416(2)	0.18986(7)	0.0392(7)
N1B	0.1544(2)	-0.0961(5)	0.22754(18)	0.0288(17)
N2B	0.0931(2)	0.0233(5)	0.2299(2)	0.0316(18)
N3B	0.0862(2)	-0.0005(6)	0.2992(2)	0.0333(19)
N4B	0.1479(2)	-0.1182(5)	0.29665(18)	0.0279(17)
N5B	0.0449(3)	0.3262(7)	0.2197(3)	0.047(2)
N6B	0.0373(3)	0.3049(8)	0.3215(3)	0.052(3)
C1B	0.1863(2)	-0.1374(6)	0.2329(2)	0.031(2)
C2B	0.1996(3)	-0.1649(7)	0.2026(2)	0.035(2)
C3B	0.1745(2)	-0.1382(7)	0.1791(2)	0.031(2)
C4B	0.1461(2)	-0.0942(6)	0.1943(2)	0.0296(19)
C5B	0.1164(2)	-0.0460(6)	0.1802(2)	0.0317(19)
C6B	0.0924(2)	0.0065(6)	0.1960(2)	0.032(2)
C7B	0.0625(3)	0.0582(7)	0.1807(2)	0.035(2)
C8B	0.0473(3)	0.1070(7)	0.2047(2)	0.038(2)
C9B	0.0667(2)	0.0861(6)	0.2346(2)	0.0307(19)
C10B	0.0597(2)	0.1261(6)	0.2661(2)	0.032(2)
C11B	0.0623(3)	0.0697(7)	0.2951(2)	0.039(2)
C12B	0.0420(3)	0.0734(7)	0.3233(3)	0.041(2)
C13B	0.0531(3)	0.0014(8)	0.3438(3)	0.044(3)
C14B	0.0822(3)	-0.0418(7)	0.3286(2)	0.036(2)
C15B	0.1041(3)	-0.1139(7)	0.3409(2)	0.036(2)
C16B	0.1341(3)	-0.1478(7)	0.3270(2)	0.034(2)
C17B	0.1594(3)	-0.2117(7)	0.3411(2)	0.039(2)
C18B	0.1873(3)	-0.2199(7)	0.3212(2)	0.031(2)
C19B	0.1790(2)	-0.1605(6)	0.2939(2)	0.032(2)
C20B	0.2027(2)	-0.1483(6)	0.2657(2)	0.0282(19)
C21B	0.2395(2)	-0.1449(6)	0.2714(2)	0.033(2)
C22B	0.3082(2)	-0.1109(7)	0.2655(3)	0.052(3)
C23B	0.3041(3)	-0.1181(7)	0.2986(3)	0.053(3)

C24B	0.3331(3)	-0.1043(8)	0.3208(4)	0.064(3)
C25B	0.3657(3)	-0.0813(9)	0.3079(4)	0.074(4)
C26B	0.3700(3)	-0.0774(9)	0.2748(4)	0.074(4)
C27B	0.3421(3)	-0.0887(8)	0.2529(4)	0.061(3)
C28B	0.0484(3)	0.2141(6)	0.2684(2)	0.040(2)
C29B	0.0460(3)	0.2744(7)	0.2410(3)	0.037(2)
C30B	0.0421(3)	0.2614(7)	0.2985(3)	0.040(2)
C31B	0.1125(3)	-0.0491(7)	0.1433(2)	0.035(2)
C32B	0.0987(3)	-0.1244(7)	0.1266(2)	0.042(2)
C33B	0.0929(3)	-0.1255(7)	0.0929(2)	0.046(2)
C34B	0.1038(3)	-0.0466(7)	0.0762(3)	0.046(3)
C35B	0.1177(3)	0.0304(7)	0.0914(2)	0.049(3)
C36B	0.1220(3)	0.0268(7)	0.1249(2)	0.041(2)
C37B	0.0744(3)	-0.2032(8)	0.0749(3)	0.065(3)
C38B	0.0620(5)	-0.2779(10)	0.0980(4)	0.065(5)
C39B	0.0994(6)	-0.2464(14)	0.0506(5)	0.094(6)
C40B	0.0400(4)	-0.1674(13)	0.0567(5)	0.080(6)
C41B	0.1289(3)	0.1158(8)	0.0725(3)	0.066(3)
C42B	0.1193(8)	0.1071(16)	0.0363(3)	0.084(7)
C43B	0.1092(8)	0.1985(10)	0.0865(6)	0.092(7)
C44B	0.1694(4)	0.1307(18)	0.0786(7)	0.093(7)
C45B	0.0928(3)	-0.1554(7)	0.3725(2)	0.037(2)
C46B	0.0969(3)	-0.1054(8)	0.4020(2)	0.044(3)
C47B	0.0873(3)	-0.1444(7)	0.4316(2)	0.046(3)
C48B	0.0732(3)	-0.2308(7)	0.4308(2)	0.040(2)
C49B	0.0688(3)	-0.2829(7)	0.4021(2)	0.039(2)
C50B	0.0784(3)	-0.2421(6)	0.3732(2)	0.035(2)
C51B	0.0929(3)	-0.0918(8)	0.4638(2)	0.055(3)
C52B	0.1056(5)	0.0068(9)	0.4587(4)	0.080(5)
C53B	0.0582(4)	-0.0873(15)	0.4822(4)	0.099(6)
C54B	0.1223(4)	-0.1399(11)	0.4842(4)	0.081(5)
C55B	0.0537(3)	-0.3796(7)	0.4035(2)	0.044(3)
C56B	0.0236(4)	-0.3864(11)	0.4281(4)	0.079(5)
C57B	0.0840(4)	-0.4451(10)	0.4139(4)	0.074(4)
C58B	0.0384(4)	-0.4097(11)	0.3699(3)	0.070(4)
S1B	0.27007(7)	-0.1284(2)	0.23979(8)	0.0428(7)
S2B	0.26036(8)	-0.1500(2)	0.30991(8)	0.0427(7)
N1C	0.3337(2)	0.1395(6)	0.29232(19)	0.0318(18)
N2C	0.2552(2)	0.1166(5)	0.28012(18)	0.0289(17)
N3C	0.2617(2)	0.0907(6)	0.21172(18)	0.0275(17)
N4C	0.3394(2)	0.1112(6)	0.22339(19)	0.0326(18)
N5C	0.1343(3)	0.2278(8)	0.2834(2)	0.049(3)
N6C	0.1371(3)	0.1980(6)	0.1803(2)	0.044(2)
C1C	0.3696(3)	0.1539(6)	0.2916(2)	0.031(2)
C2C	0.3828(3)	0.1508(7)	0.3243(2)	0.038(2)
C3C	0.3542(3)	0.1313(7)	0.3437(2)	0.038(2)
C4C	0.3232(2)	0.1253(7)	0.3238(2)	0.033(2)
C5C	0.2878(2)	0.1063(6)	0.3331(2)	0.032(2)
C6C	0.2572(2)	0.1001(6)	0.3138(2)	0.0305(19)
C7C	0.2211(3)	0.0771(7)	0.3246(2)	0.034(2)

C8C	0.1981(3)	0.0829(7)	0.2985(2)	0.033(2)
C9C	0.2200(2)	0.1093(7)	0.2714(2)	0.0289(19)
C10C	0.2044(2)	0.1272(6)	0.23903(19)	0.0268(18)
C11C	0.2248(2)	0.0996(6)	0.2105(2)	0.0297(19)
C12C	0.2123(2)	0.0708(8)	0.1798(2)	0.034(2)
C13C	0.2418(2)	0.0437(7)	0.1623(2)	0.031(2)
C14C	0.2729(2)	0.0559(7)	0.1825(2)	0.034(2)
C15C	0.3091(2)	0.0421(7)	0.1745(2)	0.031(2)
C16C	0.3391(2)	0.0655(8)	0.1934(2)	0.034(2)
C17C	0.3758(2)	0.0544(8)	0.1829(2)	0.038(2)
C18C	0.3970(3)	0.0949(9)	0.2055(3)	0.044(3)
C19C	0.3737(2)	0.1297(7)	0.2304(2)	0.030(2)
C20C	0.3875(2)	0.1729(7)	0.2610(2)	0.033(2)
C21C	0.4187(2)	0.2245(7)	0.2608(2)	0.032(2)
C22C	0.4703(2)	0.3375(7)	0.2766(2)	0.038(2)
C23C	0.4700(3)	0.3364(7)	0.2433(3)	0.042(2)
C24C	0.4946(3)	0.3869(8)	0.2259(3)	0.054(3)
C25C	0.5168(3)	0.4461(8)	0.2437(3)	0.050(3)
C26C	0.5184(3)	0.4488(8)	0.2773(3)	0.050(3)
C27C	0.4940(3)	0.3965(8)	0.2936(3)	0.051(3)
C28C	0.1707(2)	0.1643(6)	0.2358(2)	0.0288(19)
C29C	0.1507(3)	0.1957(7)	0.2629(2)	0.037(2)
C30C	0.1522(3)	0.1824(7)	0.2047(2)	0.034(2)
C31C	0.2825(3)	0.0976(7)	0.3697(2)	0.038(2)
C32C	0.2861(3)	0.1719(7)	0.3903(2)	0.036(2)
C33C	0.2794(3)	0.1636(7)	0.4237(2)	0.045(2)
C34C	0.2674(4)	0.0780(7)	0.4348(3)	0.053(3)
C35C	0.2648(4)	0.0025(7)	0.4149(2)	0.057(3)
C36C	0.2714(4)	0.0128(7)	0.3817(2)	0.045(3)
C37C	0.2820(3)	0.2432(8)	0.4471(2)	0.057(3)
C38C	0.2982(4)	0.3278(8)	0.4316(3)	0.052(3)
C39C	0.3056(4)	0.2193(10)	0.4770(3)	0.065(4)
C40C	0.2438(3)	0.2675(11)	0.4578(4)	0.070(4)
C41C	0.2498(4)	−0.0883(8)	0.4275(3)	0.077(4)
C42C	0.2105(5)	−0.0788(16)	0.4349(8)	0.097(7)
C43C	0.2565(7)	−0.1634(9)	0.4023(5)	0.066(6)
C44C	0.2725(9)	−0.1164(17)	0.4580(5)	0.110(8)
C45C	0.3152(3)	0.0002(6)	0.1417(2)	0.035(2)
C46C	0.3290(3)	−0.0895(6)	0.1397(2)	0.033(2)
C47C	0.3370(3)	−0.1260(6)	0.1088(2)	0.034(2)
C48C	0.3283(3)	−0.0746(6)	0.0815(2)	0.033(2)
C49C	0.3133(3)	0.0119(6)	0.0825(2)	0.034(2)
C50C	0.3070(3)	0.0486(7)	0.1135(2)	0.034(2)
C51C	0.3541(3)	−0.2209(6)	0.1081(2)	0.041(2)
C52C	0.3284(4)	−0.2909(7)	0.1225(3)	0.051(3)
C53C	0.3625(4)	−0.2477(9)	0.0730(2)	0.057(3)
C54C	0.3896(3)	−0.2206(11)	0.1284(3)	0.061(3)
C55C	0.3026(3)	0.0689(7)	0.0522(2)	0.041(2)
C56C	0.3145(5)	0.0223(10)	0.0208(3)	0.069(4)
C57C	0.3210(4)	0.1625(8)	0.0546(3)	0.057(3)
C58C	0.2615(3)	0.0789(10)	0.0509(3)	0.057(3)

S1C	0.43862(8)	0.27207(19)	0.29605(7)	0.0387(7)
S2C	0.43745(8)	0.2630(2)	0.22507(7)	0.0440(7)
N1D	0.6634(2)	0.3538(5)	0.28807(17)	0.0283(17)
N2D	0.7411(2)	0.3769(5)	0.28105(17)	0.0291(17)
N3D	0.73501(19)	0.4001(5)	0.21205(18)	0.0270(16)
N4D	0.6574(2)	0.3773(6)	0.2187(2)	0.0322(18)
N5D	0.8620(3)	0.2630(8)	0.2903(2)	0.048(2)
N6D	0.8585(3)	0.2993(7)	0.1873(3)	0.053(3)
C1D	0.6279(2)	0.3359(6)	0.28507(19)	0.0284(19)
C2D	0.6129(3)	0.3401(7)	0.3163(2)	0.037(2)
C3D	0.6407(3)	0.3616(7)	0.3378(2)	0.038(2)
C4D	0.6726(3)	0.3668(7)	0.3207(2)	0.035(2)
C5D	0.7081(2)	0.3860(7)	0.3324(2)	0.034(2)
C6D	0.7389(3)	0.3909(7)	0.3149(2)	0.036(2)
C7D	0.7750(3)	0.4123(8)	0.3283(2)	0.039(2)
C8D	0.7978(3)	0.4067(7)	0.3032(2)	0.040(2)
C9D	0.7768(2)	0.3832(7)	0.2747(2)	0.033(2)
C10D	0.7913(2)	0.3665(6)	0.2429(2)	0.0296(19)
C11D	0.7719(2)	0.3947(7)	0.2134(2)	0.031(2)
C12D	0.7845(3)	0.4264(9)	0.1841(3)	0.045(3)
C13D	0.7547(3)	0.4521(8)	0.1645(2)	0.038(2)
C14D	0.7236(2)	0.4356(7)	0.1828(2)	0.035(2)
C15D	0.6874(2)	0.4478(7)	0.1719(2)	0.035(2)
C16D	0.6572(2)	0.4239(8)	0.1884(2)	0.037(2)
C17D	0.6205(3)	0.4333(9)	0.1766(3)	0.050(3)
C18D	0.5995(3)	0.3937(9)	0.1980(2)	0.046(3)
C19D	0.6233(2)	0.3598(8)	0.2238(2)	0.037(2)
C20D	0.6098(2)	0.3163(6)	0.25361(19)	0.0278(19)
C21D	0.5811(2)	0.2578(6)	0.2508(2)	0.032(2)
C22D	0.5292(3)	0.1430(6)	0.2620(2)	0.037(2)
C23D	0.5328(3)	0.1394(7)	0.2293(2)	0.040(2)
C24D	0.5120(3)	0.0803(9)	0.2102(3)	0.059(3)
C25D	0.4867(3)	0.0259(8)	0.2245(3)	0.057(3)
C26D	0.4827(3)	0.0308(8)	0.2577(3)	0.058(3)
C27D	0.5029(3)	0.0879(7)	0.2768(3)	0.047(3)
C28D	0.8254(2)	0.3313(7)	0.2409(2)	0.035(2)
C29D	0.8449(3)	0.2956(8)	0.2694(2)	0.037(2)
C30D	0.8433(3)	0.3150(7)	0.2106(2)	0.039(2)
C31D	0.7132(3)	0.3956(7)	0.3688(2)	0.041(2)
C32D	0.7094(4)	0.3217(8)	0.3892(2)	0.046(3)
C33D	0.7157(4)	0.3286(8)	0.4230(2)	0.057(3)
C34D	0.7296(4)	0.4127(8)	0.4344(3)	0.059(3)
C35D	0.7326(4)	0.4897(7)	0.4152(3)	0.058(3)
C36D	0.7250(4)	0.4791(8)	0.3818(2)	0.048(3)
C37D	0.7138(4)	0.2482(8)	0.4458(3)	0.069(4)
C38D	0.6971(5)	0.1658(10)	0.4287(4)	0.088(5)
C39D	0.6895(5)	0.2752(13)	0.4737(4)	0.093(5)
C40D	0.7517(4)	0.2239(12)	0.4591(3)	0.083(5)
C41D	0.7501(4)	0.5784(8)	0.4274(3)	0.074(4)
C42D	0.7909(4)	0.5636(13)	0.4309(5)	0.109(6)
C43D	0.7440(6)	0.6568(9)	0.4033(4)	0.092(6)

C44D	0.7347(7)	0.5988(15)	0.4609(4)	0.130(8)
C45D	0.6819(3)	0.4914(6)	0.1388(2)	0.033(2)
C46D	0.6682(3)	0.5808(7)	0.1352(2)	0.037(2)
C47D	0.6612(3)	0.6165(6)	0.1037(2)	0.040(2)
C48D	0.6697(3)	0.5640(7)	0.0775(2)	0.043(3)
C49D	0.6841(3)	0.4770(6)	0.0798(2)	0.041(2)
C50D	0.6899(3)	0.4407(7)	0.1112(2)	0.038(2)
C51D	0.6445(3)	0.7127(7)	0.1009(2)	0.050(3)
C52D	0.6437(16)	0.757(2)	0.1346(6)	0.067(10)
C53D	0.6667(12)	0.7704(18)	0.0781(12)	0.062(9)
C54D	0.6058(7)	0.705(2)	0.0873(13)	0.057(9)
C55D	0.6955(3)	0.4191(7)	0.0505(2)	0.058(3)
C56D	0.6841(7)	0.4669(13)	0.0185(3)	0.091(6)
C57D	0.6773(5)	0.3270(8)	0.0518(4)	0.072(5)
C58D	0.7365(3)	0.4108(12)	0.0510(4)	0.070(5)
S1D	0.55814(8)	0.21437(19)	0.28447(7)	0.0366(6)
S2D	0.56537(8)	0.2126(2)	0.21339(7)	0.0467(8)
C38W	0.5301(8)	0.193(5)	0.400(2)	0.093(11)
C39W	0.5864(19)	0.2843(13)	0.407(2)	0.079(10)
C40W	0.569(3)	0.175(5)	0.4499(5)	0.097(11)
C42W	0.6261(9)	−0.0995(17)	0.4576(3)	0.097(7)
C43W	0.6119(8)	−0.1976(10)	0.4085(7)	0.104(8)
C44W	0.6727(4)	−0.1282(19)	0.4162(7)	0.093(7)
C38X	0.0912(14)	−0.2941(11)	0.0861(13)	0.070(9)
C39X	0.0801(16)	−0.195(3)	0.0380(4)	0.078(10)
C40X	0.0341(5)	−0.205(3)	0.0810(13)	0.071(9)
C42X	0.0987(10)	0.142(3)	0.0477(10)	0.080(9)
C43X	0.1357(14)	0.1944(14)	0.0961(7)	0.082(9)
C44X	0.1631(10)	0.096(2)	0.0539(12)	0.094(9)
C42Y	0.2108(7)	−0.098(3)	0.4127(12)	0.094(10)
C43Y	0.2716(11)	−0.1677(12)	0.4156(12)	0.089(9)
C44Y	0.2459(16)	−0.085(2)	0.4641(4)	0.097(10)
C52Z	0.6707(5)	0.7793(9)	0.1175(5)	0.069(5)
C53Z	0.6384(6)	0.7385(11)	0.0654(3)	0.073(5)
C54Z	0.6091(4)	0.7134(12)	0.1186(5)	0.067(5)
C56Z	0.6652(13)	0.417(6)	0.0245(12)	0.076(11)
C57Z	0.704(3)	0.323(2)	0.0621(10)	0.068(10)
C58Z	0.7296(16)	0.460(4)	0.0363(16)	0.065(10)

Table S9. Bond lengths [Å] and angles [°] for **H₂8b**.

N1A–H1NA	0.880	N1A–C1A	1.332(10)
N1A–C4A	1.368(10)	N2A–C6A	1.381(10)
N2A–C9A	1.333(10)	N3A–H3NA	0.880
N3A–C11A	1.370(10)	N3A–C14A	1.361(10)
N4A–C16A	1.420(10)	N4A–C19A	1.327(10)
N5A–C29A	1.155(11)	N6A–C30A	1.147(12)
C1A–C2A	1.398(11)	C1A–C20A	1.465(10)
C2A–H2A	0.950	C2A–C3A	1.374(12)
C3A–H3A	0.950	C3A–C4A	1.407(11)
C4A–C5A	1.419(10)	C5A–C6A	1.368(11)
C5A–C31A	1.502(11)	C6A–C7A	1.464(11)
C7A–H7A	0.950	C7A–C8A	1.358(12)
C8A–H8A	0.950	C8A–C9A	1.455(11)
C9A–C10A	1.450(11)	C10A–C11A	1.468(11)
C10A–C28A	1.342(11)	C11A–C12A	1.386(11)
C12A–H12A	0.950	C12A–C13A	1.386(12)
C13A–H13A	0.950	C13A–C14A	1.414(12)
C14A–C15A	1.420(11)	C15A–C16A	1.374(11)
C15A–C45A	1.514(10)	C16A–C17A	1.445(11)
C17A–H17A	0.950	C17A–C18A	1.345(11)
C18A–H18A	0.950	C18A–C19A	1.441(11)
C19A–C20A	1.466(10)	C20A–C21A	1.381(11)
C21A–S1A	1.737(9)	C21A–S2A	1.749(9)
C22A–C23A	1.356(13)	C22A–C27A	1.402(11)
C22A–S1A	1.748(9)	C23A–C24A	1.388(12)
C23A–S2A	1.747(9)	C24A–H24A	0.950
C24A–C25A	1.376(14)	C25A–H25A	0.950
C25A–C26A	1.393(15)	C26A–H26A	0.950
C26A–C27A	1.358(14)	C27A–H27A	0.950
C28A–C29A	1.440(12)	C28A–C30A	1.434(12)
C31A–C32A	1.386(12)	C31A–C36A	1.405(12)
C32A–H32A	0.950	C32A–C33A	1.382(12)
C33A–C34A	1.405(13)	C33A–C37A	1.508(11)
C34A–H34A	0.950	C34A–C35A	1.365(13)
C35A–C36A	1.388(12)	C35A–C41A	1.531(12)
C36A–H36A	0.950	C37A–C38A	1.527(11)
C37A–C39A	1.521(12)	C37A–C40A	1.538(12)
C37A–C38W	1.527(14)	C37A–C39W	1.532(14)
C37A–C40W	1.525(13)	C38A–H38A	0.980
C38A–H38B	0.980	C38A–H38C	0.980
C39A–H39A	0.980	C39A–H39B	0.980
C39A–H39C	0.980	C40A–H40A	0.980
C40A–H40B	0.980	C40A–H40C	0.980
C41A–C42A	1.526(13)	C41A–C43A	1.534(13)
C41A–C44A	1.517(13)	C41A–C42W	1.510(12)
C41A–C43W	1.524(12)	C41A–C44W	1.537(12)
C42A–H42A	0.980	C42A–H42B	0.980
C42A–H42C	0.980	C43A–H43A	0.980
C43A–H43B	0.980	C43A–H43C	0.980

C44A–H44A	0.980	C44A–H44B	0.980
C44A–H44C	0.980	C45A–C46A	1.396(12)
C45A–C50A	1.372(12)	C46A–H46A	0.950
C46A–C47A	1.400(11)	C47A–C48A	1.384(12)
C47A–C51A	1.538(12)	C48A–H48A	0.950
C48A–C49A	1.395(12)	C49A–C50A	1.407(11)
C49A–C55A	1.538(12)	C50A–H50A	0.950
C51A–C52A	1.523(11)	C51A–C53A	1.533(11)
C51A–C54A	1.528(11)	C52A–H52A	0.980
C52A–H52B	0.980	C52A–H52C	0.980
C53A–H53A	0.980	C53A–H53B	0.980
C53A–H53C	0.980	C54A–H54A	0.980
C54A–H54B	0.980	C54A–H54C	0.980
C55A–C56A	1.499(11)	C55A–C57A	1.523(12)
C55A–C58A	1.523(12)	C56A–H56A	0.980
C56A–H56B	0.980	C56A–H56C	0.980
C57A–H57A	0.980	C57A–H57B	0.980
C57A–H57C	0.980	C58A–H58A	0.980
C58A–H58B	0.980	C58A–H58C	0.980
N1B–H1NB	0.880	N1B–C1B	1.337(10)
N1B–C4B	1.383(10)	N2B–C6B	1.403(11)
N2B–C9B	1.359(10)	N3B–H3NB	0.880
N3B–C11B	1.365(11)	N3B–C14B	1.360(11)
N4B–C16B	1.422(10)	N4B–C19B	1.315(10)
N5B–C29B	1.155(11)	N6B–C30B	1.154(11)
C1B–C2B	1.404(11)	C1B–C20B	1.459(11)
C2B–H2B	0.950	C2B–C3B	1.373(12)
C3B–H3B	0.950	C3B–C4B	1.395(11)
C4B–C5B	1.412(11)	C5B–C6B	1.355(11)
C5B–C31B	1.507(11)	C6B–C7B	1.465(11)
C7B–H7B	0.950	C7B–C8B	1.348(12)
C8B–H8B	0.950	C8B–C9B	1.433(11)
C9B–C10B	1.441(11)	C10B–C11B	1.447(11)
C10B–C28B	1.361(11)	C11B–C12B	1.394(11)
C12B–H12B	0.950	C12B–C13B	1.403(12)
C13B–H13B	0.950	C13B–C14B	1.407(11)
C14B–C15B	1.414(11)	C15B–C16B	1.356(11)
C15B–C45B	1.496(11)	C16B–C17B	1.430(11)
C17B–H17B	0.950	C17B–C18B	1.338(11)
C18B–H18B	0.950	C18B–C19B	1.438(11)
C19B–C20B	1.480(10)	C20B–C21B	1.376(10)
C21B–S1B	1.757(9)	C21B–S2B	1.731(9)
C22B–C23B	1.370(13)	C22B–C27B	1.410(12)
C22B–S1B	1.749(10)	C23B–C24B	1.397(13)
C23B–S2B	1.757(10)	C24B–H24B	0.950
C24B–C25B	1.374(15)	C25B–H25B	0.950
C25B–C26B	1.367(15)	C26B–H26B	0.950
C26B–C27B	1.354(14)	C27B–H27B	0.950
C28B–C29B	1.427(12)	C28B–C30B	1.437(12)
C31B–C32B	1.388(12)	C31B–C36B	1.395(12)
C32B–H32B	0.950	C32B–C33B	1.387(12)

C33B–C34B	1.408(12)	C33B–C37B	1.508(12)
C34B–H34B	0.950	C34B–C35B	1.380(13)
C35B–C36B	1.373(12)	C35B–C41B	1.534(11)
C36B–H36B	0.950	C37B–C38B	1.526(11)
C37B–C39B	1.513(12)	C37B–C40B	1.545(11)
C37B–C38X	1.536(13)	C37B–C39X	1.532(13)
C37B–C40X	1.518(13)	C38B–H38D	0.980
C38B–H38E	0.980	C38B–H38F	0.980
C39B–H39D	0.980	C39B–H39E	0.980
C39B–H39F	0.980	C40B–H40D	0.980
C40B–H40E	0.980	C40B–H40F	0.980
C41B–C42B	1.515(12)	C41B–C43B	1.535(12)
C41B–C44B	1.526(12)	C41B–C42X	1.530(13)
C41B–C43X	1.519(13)	C41B–C44X	1.523(13)
C42B–H42D	0.980	C42B–H42E	0.980
C42B–H42F	0.980	C43B–H43D	0.980
C43B–H43E	0.980	C43B–H43F	0.980
C44B–H44D	0.980	C44B–H44E	0.980
C44B–H44F	0.980	C45B–C46B	1.412(12)
C45B–C50B	1.380(12)	C46B–H46B	0.950
C46B–C47B	1.395(12)	C47B–C48B	1.369(12)
C47B–C51B	1.530(12)	C48B–H48B	0.950
C48B–C49B	1.404(12)	C49B–C50B	1.381(11)
C49B–C55B	1.524(12)	C50B–H50B	0.950
C51B–C52B	1.536(12)	C51B–C53B	1.510(12)
C51B–C54B	1.522(12)	C52B–H52D	0.980
C52B–H52E	0.980	C52B–H52F	0.980
C53B–H53D	0.980	C53B–H53E	0.980
C53B–H53F	0.980	C54B–H54D	0.980
C54B–H54E	0.980	C54B–H54F	0.980
C55B–C56B	1.527(11)	C55B–C57B	1.527(11)
C55B–C58B	1.533(11)	C56B–H56D	0.980
C56B–H56E	0.980	C56B–H56F	0.980
C57B–H57D	0.980	C57B–H57E	0.980
C57B–H57F	0.980	C58B–H58D	0.980
C58B–H58E	0.980	C58B–H58F	0.980
N1C–H1NC	0.880	N1C–C1C	1.343(11)
N1C–C4C	1.370(10)	N2C–C6C	1.397(10)
N2C–C9C	1.341(10)	N3C–H3NC	0.880
N3C–C11C	1.368(10)	N3C–C14C	1.372(10)
N4C–C16C	1.397(10)	N4C–C19C	1.317(10)
N5C–C29C	1.150(11)	N6C–C30C	1.148(11)
C1C–C2C	1.407(11)	C1C–C20C	1.459(11)
C2C–H2C	0.950	C2C–C3C	1.371(12)
C3C–H3C	0.950	C3C–C4C	1.387(11)
C4C–C5C	1.403(11)	C5C–C6C	1.360(11)
C5C–C31C	1.519(11)	C6C–C7C	1.455(11)
C7C–H7C	0.950	C7C–C8C	1.342(12)
C8C–H8C	0.950	C8C–C9C	1.444(11)
C9C–C10C	1.451(11)	C10C–C11C	1.464(10)
C10C–C28C	1.360(11)	C11C–C12C	1.387(11)

C12C–H12C	0.950	C12C–C13C	1.381(11)
C13C–H13C	0.950	C13C–C14C	1.405(11)
C14C–C15C	1.404(11)	C15C–C16C	1.375(11)
C15C–C45C	1.496(11)	C16C–C17C	1.444(11)
C17C–H17C	0.950	C17C–C18C	1.331(12)
C18C–H18C	0.950	C18C–C19C	1.444(11)
C19C–C20C	1.480(10)	C20C–C21C	1.378(11)
C21C–S1C	1.741(9)	C21C–S2C	1.731(9)
C22C–C23C	1.361(12)	C22C–C27C	1.400(12)
C22C–S1C	1.726(9)	C23C–C24C	1.384(12)
C23C–S2C	1.761(9)	C24C–H24C	0.950
C24C–C25C	1.385(14)	C25C–H25C	0.950
C25C–C26C	1.369(14)	C26C–H26C	0.950
C26C–C27C	1.370(13)	C27C–H27C	0.950
C28C–C29C	1.425(11)	C28C–C30C	1.450(11)
C31C–C32C	1.382(12)	C31C–C36C	1.403(12)
C32C–H32C	0.950	C32C–C33C	1.395(11)
C33C–C34C	1.412(13)	C33C–C37C	1.511(12)
C34C–H34C	0.950	C34C–C35C	1.376(13)
C35C–C36C	1.392(11)	C35C–C41C	1.537(11)
C36C–H36C	0.950	C37C–C38C	1.526(11)
C37C–C39C	1.518(11)	C37C–C40C	1.531(12)
C38C–H38G	0.980	C38C–H38H	0.980
C38C–H38I	0.980	C39C–H39G	0.980
C39C–H39H	0.980	C39C–H39I	0.980
C40C–H40G	0.980	C40C–H40H	0.980
C40C–H40I	0.980	C41C–C42C	1.501(12)
C41C–C43C	1.533(12)	C41C–C44C	1.536(12)
C41C–C42Y	1.554(13)	C41C–C43Y	1.505(13)
C41C–C44Y	1.509(13)	C42C–H42G	0.980
C42C–H42H	0.980	C42C–H42I	0.980
C43C–H43G	0.980	C43C–H43H	0.980
C43C–H43I	0.980	C44C–H44G	0.980
C44C–H44H	0.980	C44C–H44I	0.980
C45C–C46C	1.414(11)	C45C–C50C	1.379(11)
C46C–H46C	0.950	C46C–C47C	1.410(11)
C47C–C48C	1.373(11)	C47C–C51C	1.531(11)
C48C–H48C	0.950	C48C–C49C	1.386(11)
C49C–C50C	1.399(11)	C49C–C55C	1.537(11)
C50C–H50C	0.950	C51C–C52C	1.529(11)
C51C–C53C	1.527(10)	C51C–C54C	1.531(11)
C52C–H52G	0.980	C52C–H52H	0.980
C52C–H52I	0.980	C53C–H53G	0.980
C53C–H53H	0.980	C53C–H53I	0.980
C54C–H54G	0.980	C54C–H54H	0.980
C54C–H54I	0.980	C55C–C56C	1.530(11)
C55C–C57C	1.533(11)	C55C–C58C	1.524(11)
C56C–H56G	0.980	C56C–H56H	0.980
C56C–H56I	0.980	C57C–H57G	0.980
C57C–H57H	0.980	C57C–H57I	0.980
C58C–H58G	0.980	C58C–H58H	0.980

C58C–H58I	0.980	N1D–H1ND	0.880
N1D–C1D	1.339(10)	N1D–C4D	1.377(10)
N2D–C6D	1.404(10)	N2D–C9D	1.355(11)
N3D–H3ND	0.880	N3D–C11D	1.365(10)
N3D–C14D	1.359(10)	N4D–C16D	1.413(10)
N4D–C19D	1.309(10)	N5D–C29D	1.151(11)
N6D–C30D	1.142(11)	C1D–C2D	1.406(11)
C1D–C20D	1.459(10)	C2D–H2D	0.950
C2D–C3D	1.368(12)	C3D–H3D	0.950
C3D–C4D	1.391(12)	C4D–C5D	1.412(11)
C5D–C6D	1.361(11)	C5D–C31D	1.498(11)
C6D–C7D	1.462(11)	C7D–H7D	0.950
C7D–C8D	1.347(12)	C8D–H8D	0.950
C8D–C9D	1.422(11)	C9D–C10D	1.440(11)
C10D–C11D	1.445(11)	C10D–C28D	1.366(11)
C11D–C12D	1.378(11)	C12D–H12D	0.950
C12D–C13D	1.391(12)	C13D–H13D	0.950
C13D–C14D	1.408(11)	C14D–C15D	1.408(11)
C15D–C16D	1.369(11)	C15D–C45D	1.502(11)
C16D–C17D	1.431(12)	C17D–H17D	0.950
C17D–C18D	1.319(12)	C18D–H18D	0.950
C18D–C19D	1.439(11)	C19D–C20D	1.475(10)
C20D–C21D	1.366(11)	C21D–S1D	1.757(9)
C21D–S2D	1.748(9)	C22D–C23D	1.350(12)
C22D–C27D	1.413(12)	C22D–S1D	1.737(9)
C23D–C24D	1.383(13)	C23D–S2D	1.751(10)
C24D–H24D	0.950	C24D–C25D	1.373(14)
C25D–H25D	0.950	C25D–C26D	1.372(15)
C26D–H26D	0.950	C26D–C27D	1.352(14)
C27D–H27D	0.950	C28D–C29D	1.446(11)
C28D–C30D	1.442(12)	C31D–C32D	1.377(12)
C31D–C36D	1.400(12)	C32D–H32D	0.950
C32D–C33D	1.396(12)	C33D–C34D	1.410(13)
C33D–C37D	1.507(13)	C34D–H34D	0.950
C34D–C35D	1.380(13)	C35D–C36D	1.391(12)
C35D–C41D	1.529(13)	C36D–H36D	0.950
C37D–C38D	1.517(12)	C37D–C39D	1.522(12)
C37D–C40D	1.527(12)	C38D–H38J	0.980
C38D–H38K	0.980	C38D–H38L	0.980
C39D–H39J	0.980	C39D–H39K	0.980
C39D–H39L	0.980	C40D–H40J	0.980
C40D–H40K	0.980	C40D–H40L	0.980
C41D–C42D	1.527(13)	C41D–C43D	1.524(12)
C41D–C44D	1.526(12)	C42D–H42J	0.980
C42D–H42K	0.980	C42D–H42L	0.980
C43D–H43J	0.980	C43D–H43K	0.980
C43D–H43L	0.980	C44D–H44J	0.980
C44D–H44K	0.980	C44D–H44L	0.980
C45D–C46D	1.411(11)	C45D–C50D	1.389(11)
C46D–H46D	0.950	C46D–C47D	1.407(11)
C47D–C48D	1.363(11)	C47D–C51D	1.542(10)

C48D–H48D	0.950	C48D–C49D	1.385(11)
C49D–C50D	1.399(11)	C49D–C55D	1.537(11)
C50D–H50D	0.950	C51D–C52D	1.521(13)
C51D–C53D	1.518(13)	C51D–C54D	1.524(13)
C51D–C52Z	1.519(11)	C51D–C53Z	1.510(11)
C51D–C54Z	1.516(11)	C52D–H52J	0.980
C52D–H52K	0.980	C52D–H52L	0.980
C53D–H53J	0.980	C53D–H53K	0.980
C53D–H53L	0.980	C54D–H54J	0.980
C54D–H54K	0.980	C54D–H54L	0.980
C55D–C56D	1.531(11)	C55D–C57D	1.512(12)
C55D–C58D	1.520(12)	C55D–C56Z	1.517(13)
C55D–C57Z	1.522(13)	C55D–C58Z	1.525(14)
C56D–H56J	0.980	C56D–H56K	0.980
C56D–H56L	0.980	C57D–H57J	0.980
C57D–H57K	0.980	C57D–H57L	0.980
C58D–H58J	0.980	C58D–H58K	0.980
C58D–H58L	0.980	C38W–H38M	0.980
C38W–H38N	0.980	C38W–H38O	0.980
C39W–H39M	0.980	C39W–H39N	0.980
C39W–H39O	0.980	C40W–H40M	0.980
C40W–H40N	0.980	C40W–H40O	0.980
C42W–H42M	0.980	C42W–H42N	0.980
C42W–H42O	0.980	C43W–H43M	0.980
C43W–H43N	0.980	C43W–H43O	0.980
C44W–H44M	0.980	C44W–H44N	0.980
C44W–H44O	0.980	C38X–H38P	0.980
C38X–H38Q	0.980	C38X–H38R	0.980
C39X–H39P	0.980	C39X–H39Q	0.980
C39X–H39R	0.980	C40X–H40P	0.980
C40X–H40Q	0.980	C40X–H40R	0.980
C42X–H42P	0.980	C42X–H42Q	0.980
C42X–H42R	0.980	C43X–H43P	0.980
C43X–H43Q	0.980	C43X–H43R	0.980
C44X–H44P	0.980	C44X–H44Q	0.980
C44X–H44R	0.980	C42Y–H42S	0.980
C42Y–H42T	0.980	C42Y–H42U	0.980
C43Y–H43S	0.980	C43Y–H43T	0.980
C43Y–H43U	0.980	C44Y–H44S	0.980
C44Y–H44T	0.980	C44Y–H44U	0.980
C52Z–H52M	0.980	C52Z–H52N	0.980
C52Z–H52O	0.980	C53Z–H53M	0.980
C53Z–H53N	0.980	C53Z–H53O	0.980
C54Z–H54M	0.980	C54Z–H54N	0.980
C54Z–H54O	0.980	C56Z–H56M	0.980
C56Z–H56N	0.980	C56Z–H56O	0.980
C57Z–H57M	0.980	C57Z–H57N	0.980
C57Z–H57O	0.980	C58Z–H58M	0.980
C58Z–H58N	0.980	C58Z–H58O	0.980

H1NA–N1A–C1A

125.1

H1NA–N1A–C4A

125.1

C1A-N1A-C4A	109.7(7)	C6A-N2A-C9A	106.3(7)
H3NA-N3A-C11A	125.2	H3NA-N3A-C14A	125.2
C11A-N3A-C14A	109.7(8)	C16A-N4A-C19A	104.5(7)
N1A-C1A-C2A	108.9(7)	N1A-C1A-C20A	122.5(8)
C2A-C1A-C20A	128.4(8)	C1A-C2A-H2A	126.7
C1A-C2A-C3A	106.7(8)	H2A-C2A-C3A	126.7
C2A-C3A-H3A	126.1	C2A-C3A-C4A	107.9(8)
H3A-C3A-C4A	126.1	N1A-C4A-C3A	106.6(7)
N1A-C4A-C5A	124.2(8)	C3A-C4A-C5A	129.1(8)
C4A-C5A-C6A	126.3(8)	C4A-C5A-C31A	116.0(8)
C6A-C5A-C31A	117.0(8)	N2A-C6A-C5A	126.0(8)
N2A-C6A-C7A	109.3(7)	C5A-C6A-C7A	124.7(8)
C6A-C7A-H7A	126.7	C6A-C7A-C8A	106.6(8)
H7A-C7A-C8A	126.7	C7A-C8A-H8A	127.1
C7A-C8A-C9A	105.7(8)	H8A-C8A-C9A	127.1
N2A-C9A-C8A	111.9(8)	N2A-C9A-C10A	124.3(8)
C8A-C9A-C10A	123.7(8)	C9A-C10A-C11A	119.3(8)
C9A-C10A-C28A	121.6(8)	C11A-C10A-C28A	118.8(8)
N3A-C11A-C10A	122.6(8)	N3A-C11A-C12A	107.8(8)
C10A-C11A-C12A	129.4(8)	C11A-C12A-H12A	126.0
C11A-C12A-C13A	108.0(8)	H12A-C12A-C13A	126.0
C12A-C13A-H13A	126.4	C12A-C13A-C14A	107.1(8)
H13A-C13A-C14A	126.4	N3A-C14A-C13A	107.2(8)
N3A-C14A-C15A	125.2(8)	C13A-C14A-C15A	127.4(8)
C14A-C15A-C16A	125.3(8)	C14A-C15A-C45A	117.1(8)
C16A-C15A-C45A	117.6(8)	N4A-C16A-C15A	124.1(8)
N4A-C16A-C17A	109.6(7)	C15A-C16A-C17A	126.2(8)
C16A-C17A-H17A	126.8	C16A-C17A-C18A	106.3(8)
H17A-C17A-C18A	126.8	C17A-C18A-H18A	126.5
C17A-C18A-C19A	107.0(8)	H18A-C18A-C19A	126.5
N4A-C19A-C18A	112.4(7)	N4A-C19A-C20A	123.7(8)
C18A-C19A-C20A	123.7(8)	C1A-C20A-C19A	120.6(7)
C1A-C20A-C21A	118.9(7)	C19A-C20A-C21A	120.0(8)
C20A-C21A-S1A	124.3(7)	C20A-C21A-S2A	122.3(7)
S1A-C21A-S2A	113.4(5)	C23A-C22A-C27A	120.1(9)
C23A-C22A-S1A	117.2(7)	C27A-C22A-S1A	122.7(9)
C22A-C23A-C24A	121.2(9)	C22A-C23A-S2A	115.7(7)
C24A-C23A-S2A	123.0(9)	C23A-C24A-H24A	120.7
C23A-C24A-C25A	118.5(11)	H24A-C24A-C25A	120.7
C24A-C25A-H25A	119.7	C24A-C25A-C26A	120.6(10)
H25A-C25A-C26A	119.7	C25A-C26A-H26A	119.9
C25A-C26A-C27A	120.3(10)	H26A-C26A-C27A	119.9
C22A-C27A-C26A	119.3(11)	C22A-C27A-H27A	120.3
C26A-C27A-H27A	120.3	C10A-C28A-C29A	123.5(9)
C10A-C28A-C30A	125.4(9)	C29A-C28A-C30A	110.5(9)
N5A-C29A-C28A	177.0(13)	N6A-C30A-C28A	176.9(15)
C5A-C31A-C32A	121.1(8)	C5A-C31A-C36A	120.6(8)
C32A-C31A-C36A	117.8(9)	C31A-C32A-H32A	118.6
C31A-C32A-C33A	122.8(9)	H32A-C32A-C33A	118.6
C32A-C33A-C34A	116.4(9)	C32A-C33A-C37A	124.9(9)
C34A-C33A-C37A	118.6(8)	C33A-C34A-H34A	118.2

C33A–C34A–C35A	123.7(9)	H34A–C34A–C35A	118.2
C34A–C35A–C36A	117.6(9)	C34A–C35A–C41A	123.0(9)
C36A–C35A–C41A	119.0(8)	C31A–C36A–C35A	121.4(9)
C31A–C36A–H36A	119.3	C35A–C36A–H36A	119.3
C33A–C37A–C38A	111.5(8)	C33A–C37A–C39A	110.1(9)
C33A–C37A–C40A	110.6(9)	C33A–C37A–C38W	110.7(12)
C33A–C37A–C39W	110.1(12)	C33A–C37A–C40W	111.0(12)
C38A–C37A–C39A	108.8(13)	C38A–C37A–C40A	108.7(11)
C39A–C37A–C40A	107.0(12)	C38W–C37A–C39W	108.4(18)
C38W–C37A–C40W	108.6(18)	C39W–C37A–C40W	108.0(18)
C37A–C38A–H38A	109.5	C37A–C38A–H38B	109.5
C37A–C38A–H38C	109.5	H38A–C38A–H38B	109.5
H38A–C38A–H38C	109.5	H38B–C38A–H38C	109.5
C37A–C39A–H39A	109.5	C37A–C39A–H39B	109.5
C37A–C39A–H39C	109.5	H39A–C39A–H39B	109.5
H39A–C39A–H39C	109.5	H39B–C39A–H39C	109.5
C37A–C40A–H40A	109.5	C37A–C40A–H40B	109.5
C37A–C40A–H40C	109.5	H40A–C40A–H40B	109.5
H40A–C40A–H40C	109.5	H40B–C40A–H40C	109.5
C35A–C41A–C42A	109.5(11)	C35A–C41A–C43A	108.6(10)
C35A–C41A–C44A	110.6(10)	C35A–C41A–C42W	111.4(10)
C35A–C41A–C43W	109.2(9)	C35A–C41A–C44W	107.3(9)
C42A–C41A–C43A	108.7(16)	C42A–C41A–C44A	109.8(16)
C43A–C41A–C44A	109.5(16)	C42W–C41A–C43W	111.5(14)
C42W–C41A–C44W	109.3(13)	C43W–C41A–C44W	108.1(14)
C41A–C42A–H42A	109.5	C41A–C42A–H42B	109.5
C41A–C42A–H42C	109.5	H42A–C42A–H42B	109.5
H42A–C42A–H42C	109.5	H42B–C42A–H42C	109.5
C41A–C43A–H43A	109.5	C41A–C43A–H43B	109.5
C41A–C43A–H43C	109.5	H43A–C43A–H43B	109.5
H43A–C43A–H43C	109.5	H43B–C43A–H43C	109.5
C41A–C44A–H44A	109.5	C41A–C44A–H44B	109.5
C41A–C44A–H44C	109.5	H44A–C44A–H44B	109.5
H44A–C44A–H44C	109.5	H44B–C44A–H44C	109.5
C15A–C45A–C46A	121.3(9)	C15A–C45A–C50A	118.3(9)
C46A–C45A–C50A	120.4(8)	C45A–C46A–H46A	120.0
C45A–C46A–C47A	120.0(9)	H46A–C46A–C47A	120.0
C46A–C47A–C48A	118.1(9)	C46A–C47A–C51A	122.1(9)
C48A–C47A–C51A	119.7(8)	C47A–C48A–H48A	118.3
C47A–C48A–C49A	123.3(9)	H48A–C48A–C49A	118.3
C48A–C49A–C50A	116.7(9)	C48A–C49A–C55A	122.8(9)
C50A–C49A–C55A	120.5(9)	C45A–C50A–C49A	121.5(9)
C45A–C50A–H50A	119.3	C49A–C50A–H50A	119.3
C47A–C51A–C52A	112.5(8)	C47A–C51A–C53A	107.0(9)
C47A–C51A–C54A	110.6(9)	C52A–C51A–C53A	109.3(10)
C52A–C51A–C54A	109.1(9)	C53A–C51A–C54A	108.1(10)
C51A–C52A–H52A	109.5	C51A–C52A–H52B	109.5
C51A–C52A–H52C	109.5	H52A–C52A–H52B	109.5
H52A–C52A–H52C	109.5	H52B–C52A–H52C	109.5
C51A–C53A–H53A	109.5	C51A–C53A–H53B	109.5
C51A–C53A–H53C	109.5	H53A–C53A–H53B	109.5

H53A–C53A–H53C	109.5	H53B–C53A–H53C	109.5
C51A–C54A–H54A	109.5	C51A–C54A–H54B	109.5
C51A–C54A–H54C	109.5	H54A–C54A–H54B	109.5
H54A–C54A–H54C	109.5	H54B–C54A–H54C	109.5
C49A–C55A–C56A	111.8(9)	C49A–C55A–C57A	108.1(9)
C49A–C55A–C58A	112.2(9)	C56A–C55A–C57A	108.6(11)
C56A–C55A–C58A	109.1(12)	C57A–C55A–C58A	106.9(11)
C55A–C56A–H56A	109.5	C55A–C56A–H56B	109.5
C55A–C56A–H56C	109.5	H56A–C56A–H56B	109.5
H56A–C56A–H56C	109.5	H56B–C56A–H56C	109.5
C55A–C57A–H57A	109.5	C55A–C57A–H57B	109.5
C55A–C57A–H57C	109.5	H57A–C57A–H57B	109.5
H57A–C57A–H57C	109.5	H57B–C57A–H57C	109.5
C55A–C58A–H58A	109.5	C55A–C58A–H58B	109.5
C55A–C58A–H58C	109.5	H58A–C58A–H58B	109.5
H58A–C58A–H58C	109.5	H58B–C58A–H58C	109.5
C21A–S1A–C22A	96.3(4)	C21A–S2A–C23A	96.7(5)
H1NB–N1B–C1B	125.1	H1NB–N1B–C4B	125.1
C1B–N1B–C4B	109.9(7)	C6B–N2B–C9B	105.6(7)
H3NB–N3B–C11B	124.6	H3NB–N3B–C14B	124.6
C11B–N3B–C14B	110.8(7)	C16B–N4B–C19B	105.5(7)
N1B–C1B–C2B	108.4(7)	N1B–C1B–C20B	122.5(8)
C2B–C1B–C20B	129.0(8)	C1B–C2B–H2B	126.7
C1B–C2B–C3B	106.7(8)	H2B–C2B–C3B	126.7
C2B–C3B–H3B	125.6	C2B–C3B–C4B	108.9(8)
H3B–C3B–C4B	125.6	N1B–C4B–C3B	106.2(7)
N1B–C4B–C5B	123.9(8)	C3B–C4B–C5B	129.5(8)
C4B–C5B–C6B	127.0(8)	C4B–C5B–C31B	116.1(8)
C6B–C5B–C31B	116.7(8)	N2B–C6B–C5B	125.3(8)
N2B–C6B–C7B	108.7(7)	C5B–C6B–C7B	126.0(8)
C6B–C7B–H7B	126.6	C6B–C7B–C8B	106.9(8)
H7B–C7B–C8B	126.6	C7B–C8B–H8B	126.4
C7B–C8B–C9B	107.3(8)	H8B–C8B–C9B	126.4
N2B–C9B–C8B	111.4(8)	N2B–C9B–C10B	123.6(8)
C8B–C9B–C10B	125.0(8)	C9B–C10B–C11B	119.2(8)
C9B–C10B–C28B	120.8(8)	C11B–C10B–C28B	119.8(8)
N3B–C11B–C10B	123.8(8)	N3B–C11B–C12B	107.1(8)
C10B–C11B–C12B	129.1(9)	C11B–C12B–H12B	126.1
C11B–C12B–C13B	107.9(8)	H12B–C12B–C13B	126.1
C12B–C13B–H13B	126.5	C12B–C13B–C14B	107.0(8)
H13B–C13B–C14B	126.5	N3B–C14B–C13B	107.1(8)
N3B–C14B–C15B	124.8(8)	C13B–C14B–C15B	128.1(8)
C14B–C15B–C16B	126.3(8)	C14B–C15B–C45B	116.0(8)
C16B–C15B–C45B	117.7(8)	N4B–C16B–C15B	124.9(8)
N4B–C16B–C17B	107.8(7)	C15B–C16B–C17B	127.1(8)
C16B–C17B–H17B	125.7	C16B–C17B–C18B	108.6(8)
H17B–C17B–C18B	125.7	C17B–C18B–H18B	127.3
C17B–C18B–C19B	105.5(8)	H18B–C18B–C19B	127.3
N4B–C19B–C18B	112.7(7)	N4B–C19B–C20B	123.3(8)
C18B–C19B–C20B	124.0(8)	C1B–C20B–C19B	119.3(8)
C1B–C20B–C21B	122.0(8)	C19B–C20B–C21B	118.7(8)

C20B-C21B-S1B	122.4(7)	C20B-C21B-S2B	124.2(7)
S1B-C21B-S2B	113.3(5)	C23B-C22B-C27B	120.4(10)
C23B-C22B-S1B	118.0(7)	C27B-C22B-S1B	121.5(9)
C22B-C23B-C24B	121.5(10)	C22B-C23B-S2B	114.2(7)
C24B-C23B-S2B	124.2(10)	C23B-C24B-H24B	121.6
C23B-C24B-C25B	116.9(12)	H24B-C24B-C25B	121.6
C24B-C25B-H25B	119.3	C24B-C25B-C26B	121.4(12)
H25B-C25B-C26B	119.3	C25B-C26B-H26B	118.7
C25B-C26B-C27B	122.6(12)	H26B-C26B-C27B	118.7
C22B-C27B-C26B	117.0(12)	C22B-C27B-H27B	121.5
C26B-C27B-H27B	121.5	C10B-C28B-C29B	123.0(9)
C10B-C28B-C30B	125.2(9)	C29B-C28B-C30B	111.3(9)
N5B-C29B-C28B	176.9(13)	N6B-C30B-C28B	175.2(12)
C5B-C31B-C32B	122.5(8)	C5B-C31B-C36B	119.9(8)
C32B-C31B-C36B	117.6(9)	C31B-C32B-H32B	118.6
C31B-C32B-C33B	122.8(9)	H32B-C32B-C33B	118.6
C32B-C33B-C34B	115.6(9)	C32B-C33B-C37B	123.1(8)
C34B-C33B-C37B	121.2(8)	C33B-C34B-H34B	117.8
C33B-C34B-C35B	124.3(9)	H34B-C34B-C35B	117.8
C34B-C35B-C36B	116.5(9)	C34B-C35B-C41B	123.1(8)
C36B-C35B-C41B	120.4(8)	C31B-C36B-C35B	123.0(9)
C31B-C36B-H36B	118.5	C35B-C36B-H36B	118.5
C33B-C37B-C38B	112.4(8)	C33B-C37B-C39B	111.0(9)
C33B-C37B-C40B	109.4(9)	C33B-C37B-C38X	109.7(11)
C33B-C37B-C39X	110.2(12)	C33B-C37B-C40X	111.3(12)
C38B-C37B-C39B	107.8(12)	C38B-C37B-C40B	106.4(11)
C39B-C37B-C40B	109.8(12)	C38X-C37B-C39X	107.3(17)
C38X-C37B-C40X	109.1(17)	C39X-C37B-C40X	109.1(17)
C37B-C38B-H38D	109.5	C37B-C38B-H38E	109.5
C37B-C38B-H38F	109.5	H38D-C38B-H38E	109.5
H38D-C38B-H38F	109.5	H38E-C38B-H38F	109.5
C37B-C39B-H39D	109.5	C37B-C39B-H39E	109.5
C37B-C39B-H39F	109.5	H39D-C39B-H39E	109.5
H39D-C39B-H39F	109.5	H39E-C39B-H39F	109.5
C37B-C40B-H40D	109.5	C37B-C40B-H40E	109.5
C37B-C40B-H40F	109.5	H40D-C40B-H40E	109.5
H40D-C40B-H40F	109.5	H40E-C40B-H40F	109.5
C35B-C41B-C42B	111.3(9)	C35B-C41B-C43B	108.6(9)
C35B-C41B-C44B	108.4(9)	C35B-C41B-C42X	109.2(11)
C35B-C41B-C43X	110.1(11)	C35B-C41B-C44X	109.6(11)
C42B-C41B-C43B	109.3(13)	C42B-C41B-C44B	111.7(13)
C43B-C41B-C44B	107.4(14)	C42X-C41B-C43X	109.5(16)
C42X-C41B-C44X	108.5(16)	C43X-C41B-C44X	109.9(16)
C41B-C42B-H42D	109.5	C41B-C42B-H42E	109.5
C41B-C42B-H42F	109.5	H42D-C42B-H42E	109.5
H42D-C42B-H42F	109.5	H42E-C42B-H42F	109.5
C41B-C43B-H43D	109.5	C41B-C43B-H43E	109.5
C41B-C43B-H43F	109.5	H43D-C43B-H43E	109.5
H43D-C43B-H43F	109.5	H43E-C43B-H43F	109.5
C41B-C44B-H44D	109.5	C41B-C44B-H44E	109.5
C41B-C44B-H44F	109.5	H44D-C44B-H44E	109.5

H44D–C44B–H44F	109.5	H44E–C44B–H44F	109.5
C15B–C45B–C46B	119.8(9)	C15B–C45B–C50B	120.8(9)
C46B–C45B–C50B	119.5(8)	C45B–C46B–H46B	119.9
C45B–C46B–C47B	120.2(9)	H46B–C46B–C47B	119.9
C46B–C47B–C48B	117.7(9)	C46B–C47B–C51B	120.4(9)
C48B–C47B–C51B	121.9(9)	C47B–C48B–H48B	118.0
C47B–C48B–C49B	124.0(9)	H48B–C48B–C49B	118.0
C48B–C49B–C50B	116.8(9)	C48B–C49B–C55B	120.6(8)
C50B–C49B–C55B	122.6(9)	C45B–C50B–C49B	121.8(9)
C45B–C50B–H50B	119.1	C49B–C50B–H50B	119.1
C47B–C51B–C52B	113.2(9)	C47B–C51B–C53B	110.7(10)
C47B–C51B–C54B	108.1(10)	C52B–C51B–C53B	107.0(12)
C52B–C51B–C54B	107.1(11)	C53B–C51B–C54B	110.6(12)
C51B–C52B–H52D	109.5	C51B–C52B–H52E	109.5
C51B–C52B–H52F	109.5	H52D–C52B–H52E	109.5
H52D–C52B–H52F	109.5	H52E–C52B–H52F	109.5
C51B–C53B–H53D	109.5	C51B–C53B–H53E	109.5
C51B–C53B–H53F	109.5	H53D–C53B–H53E	109.5
H53D–C53B–H53F	109.5	H53E–C53B–H53F	109.5
C51B–C54B–H54D	109.5	C51B–C54B–H54E	109.5
C51B–C54B–H54F	109.5	H54D–C54B–H54E	109.5
H54D–C54B–H54F	109.5	H54E–C54B–H54F	109.5
C49B–C55B–C56B	111.1(9)	C49B–C55B–C57B	109.3(9)
C49B–C55B–C58B	111.1(8)	C56B–C55B–C57B	108.6(11)
C56B–C55B–C58B	108.3(10)	C57B–C55B–C58B	108.4(10)
C55B–C56B–H56D	109.5	C55B–C56B–H56E	109.5
C55B–C56B–H56F	109.5	H56D–C56B–H56E	109.5
H56D–C56B–H56F	109.5	H56E–C56B–H56F	109.5
C55B–C57B–H57D	109.5	C55B–C57B–H57E	109.5
C55B–C57B–H57F	109.5	H57D–C57B–H57E	109.5
H57D–C57B–H57F	109.5	H57E–C57B–H57F	109.5
C55B–C58B–H58D	109.5	C55B–C58B–H58E	109.5
C55B–C58B–H58F	109.5	H58D–C58B–H58E	109.5
H58D–C58B–H58F	109.5	H58E–C58B–H58F	109.5
C21B–S1B–C22B	95.9(5)	C21B–S2B–C23B	97.9(5)
H1NC–N1C–C1C	124.7	H1NC–N1C–C4C	124.7
C1C–N1C–C4C	110.6(8)	C6C–N2C–C9C	105.5(7)
H3NC–N3C–C11C	125.3	H3NC–N3C–C14C	125.3
C11C–N3C–C14C	109.4(7)	C16C–N4C–C19C	105.6(7)
N1C–C1C–C2C	106.7(8)	N1C–C1C–C20C	121.6(8)
C2C–C1C–C20C	131.6(9)	C1C–C2C–H2C	126.1
C1C–C2C–C3C	107.8(8)	H2C–C2C–C3C	126.1
C2C–C3C–H3C	126.0	C2C–C3C–C4C	108.0(8)
H3C–C3C–C4C	126.0	N1C–C4C–C3C	106.8(8)
N1C–C4C–C5C	125.3(8)	C3C–C4C–C5C	128.0(8)
C4C–C5C–C6C	128.7(8)	C4C–C5C–C31C	115.6(8)
C6C–C5C–C31C	115.5(8)	N2C–C6C–C5C	125.0(8)
N2C–C6C–C7C	108.4(7)	C5C–C6C–C7C	126.6(8)
C6C–C7C–H7C	126.0	C6C–C7C–C8C	108.1(8)
H7C–C7C–C8C	126.0	C7C–C8C–H8C	127.2
C7C–C8C–C9C	105.5(8)	H8C–C8C–C9C	127.2

N2C-C9C-C8C	112.3(8)	N2C-C9C-C10C	125.6(8)
C8C-C9C-C10C	122.0(8)	C9C-C10C-C11C	118.3(7)
C9C-C10C-C28C	119.8(7)	C11C-C10C-C28C	121.8(8)
N3C-C11C-C10C	122.4(8)	N3C-C11C-C12C	107.8(7)
C10C-C11C-C12C	129.6(8)	C11C-C12C-H12C	125.9
C11C-C12C-C13C	108.2(8)	H12C-C12C-C13C	125.9
C12C-C13C-H13C	126.2	C12C-C13C-C14C	107.5(8)
H13C-C13C-C14C	126.2	N3C-C14C-C13C	107.2(7)
N3C-C14C-C15C	124.9(8)	C13C-C14C-C15C	127.8(8)
C14C-C15C-C16C	126.4(8)	C14C-C15C-C45C	116.1(8)
C16C-C15C-C45C	117.5(8)	N4C-C16C-C15C	126.5(8)
N4C-C16C-C17C	109.4(7)	C15C-C16C-C17C	123.8(8)
C16C-C17C-H17C	126.8	C16C-C17C-C18C	106.3(8)
H17C-C17C-C18C	126.8	C17C-C18C-H18C	126.4
C17C-C18C-C19C	107.1(8)	H18C-C18C-C19C	126.4
N4C-C19C-C18C	111.5(7)	N4C-C19C-C20C	125.2(8)
C18C-C19C-C20C	123.2(8)	C1C-C20C-C19C	119.2(8)
C1C-C20C-C21C	120.7(8)	C19C-C20C-C21C	119.9(8)
C20C-C21C-S1C	123.3(7)	C20C-C21C-S2C	122.7(7)
S1C-C21C-S2C	113.3(5)	C23C-C22C-C27C	119.2(9)
C23C-C22C-S1C	118.0(7)	C27C-C22C-S1C	122.7(8)
C22C-C23C-C24C	121.4(9)	C22C-C23C-S2C	114.4(7)
C24C-C23C-S2C	124.2(9)	C23C-C24C-H24C	121.5
C23C-C24C-C25C	117.0(11)	H24C-C24C-C25C	121.5
C24C-C25C-H25C	118.3	C24C-C25C-C26C	123.3(10)
H25C-C25C-C26C	118.3	C25C-C26C-H26C	121.3
C25C-C26C-C27C	117.5(11)	H26C-C26C-C27C	121.3
C22C-C27C-C26C	121.1(11)	C22C-C27C-H27C	119.4
C26C-C27C-H27C	119.4	C10C-C28C-C29C	123.4(8)
C10C-C28C-C30C	124.2(8)	C29C-C28C-C30C	112.2(8)
N5C-C29C-C28C	174.4(12)	N6C-C30C-C28C	178.6(12)
C5C-C31C-C32C	121.4(8)	C5C-C31C-C36C	117.8(8)
C32C-C31C-C36C	120.6(8)	C31C-C32C-H32C	119.7
C31C-C32C-C33C	120.6(9)	H32C-C32C-C33C	119.7
C32C-C33C-C34C	117.4(9)	C32C-C33C-C37C	122.8(9)
C34C-C33C-C37C	119.7(9)	C33C-C34C-H34C	118.6
C33C-C34C-C35C	122.7(9)	H34C-C34C-C35C	118.6
C34C-C35C-C36C	118.5(9)	C34C-C35C-C41C	121.3(8)
C36C-C35C-C41C	119.6(8)	C31C-C36C-C35C	119.9(9)
C31C-C36C-H36C	120.1	C35C-C36C-H36C	120.1
C33C-C37C-C38C	112.4(8)	C33C-C37C-C39C	110.8(10)
C33C-C37C-C40C	108.6(10)	C38C-C37C-C39C	107.3(10)
C38C-C37C-C40C	107.9(10)	C39C-C37C-C40C	109.8(10)
C37C-C38C-H38G	109.5	C37C-C38C-H38H	109.5
C37C-C38C-H38I	109.5	H38G-C38C-H38H	109.5
H38G-C38C-H38I	109.5	H38H-C38C-H38I	109.5
C37C-C39C-H39G	109.5	C37C-C39C-H39H	109.5
C37C-C39C-H39I	109.5	H39G-C39C-H39H	109.5
H39G-C39C-H39I	109.5	H39H-C39C-H39I	109.5
C37C-C40C-H40G	109.5	C37C-C40C-H40H	109.5
C37C-C40C-H40I	109.5	H40G-C40C-H40H	109.5

H40G-C40C-H40I	109.5	H40H-C40C-H40I	109.5
C35C-C41C-C42C	110.4(10)	C35C-C41C-C43C	109.4(8)
C35C-C41C-C44C	108.1(10)	C35C-C41C-C42Y	106.8(10)
C35C-C41C-C43Y	111.1(11)	C35C-C41C-C44Y	110.5(11)
C42C-C41C-C43C	112.2(13)	C42C-C41C-C44C	111.6(13)
C43C-C41C-C44C	104.9(13)	C42Y-C41C-C43Y	107.8(16)
C42Y-C41C-C44Y	105.7(16)	C43Y-C41C-C44Y	114.5(16)
C41C-C42C-H42G	109.5	C41C-C42C-H42H	109.5
C41C-C42C-H42I	109.5	H42G-C42C-H42H	109.5
H42G-C42C-H42I	109.5	H42H-C42C-H42I	109.5
C41C-C43C-H43G	109.5	C41C-C43C-H43H	109.5
C41C-C43C-H43I	109.5	H43G-C43C-H43H	109.5
H43G-C43C-H43I	109.5	H43H-C43C-H43I	109.5
C41C-C44C-H44G	109.5	C41C-C44C-H44H	109.5
C41C-C44C-H44I	109.5	H44G-C44C-H44H	109.5
H44G-C44C-H44I	109.5	H44H-C44C-H44I	109.5
C15C-C45C-C46C	120.0(8)	C15C-C45C-C50C	120.1(8)
C46C-C45C-C50C	120.0(8)	C45C-C46C-H46C	120.3
C45C-C46C-C47C	119.4(8)	H46C-C46C-C47C	120.3
C46C-C47C-C48C	117.9(8)	C46C-C47C-C51C	117.4(8)
C48C-C47C-C51C	124.8(8)	C47C-C48C-H48C	117.9
C47C-C48C-C49C	124.1(8)	H48C-C48C-C49C	117.9
C48C-C49C-C50C	117.2(8)	C48C-C49C-C55C	124.5(8)
C50C-C49C-C55C	118.3(8)	C45C-C50C-C49C	121.2(9)
C45C-C50C-H50C	119.4	C49C-C50C-H50C	119.4
C47C-C51C-C52C	110.0(8)	C47C-C51C-C53C	110.3(8)
C47C-C51C-C54C	109.6(9)	C52C-C51C-C53C	109.6(9)
C52C-C51C-C54C	109.1(9)	C53C-C51C-C54C	108.2(9)
C51C-C52C-H52G	109.5	C51C-C52C-H52H	109.5
C51C-C52C-H52I	109.5	H52G-C52C-H52H	109.5
H52G-C52C-H52I	109.5	H52H-C52C-H52I	109.5
C51C-C53C-H53G	109.5	C51C-C53C-H53H	109.5
C51C-C53C-H53I	109.5	H53G-C53C-H53H	109.5
H53G-C53C-H53I	109.5	H53H-C53C-H53I	109.5
C51C-C54C-H54G	109.5	C51C-C54C-H54H	109.5
C51C-C54C-H54I	109.5	H54G-C54C-H54H	109.5
H54G-C54C-H54I	109.5	H54H-C54C-H54I	109.5
C49C-C55C-C56C	111.0(8)	C49C-C55C-C57C	109.5(8)
C49C-C55C-C58C	108.1(8)	C56C-C55C-C57C	108.4(9)
C56C-C55C-C58C	109.0(10)	C57C-C55C-C58C	110.8(9)
C55C-C56C-H56G	109.5	C55C-C56C-H56H	109.5
C55C-C56C-H56I	109.5	H56G-C56C-H56H	109.5
H56G-C56C-H56I	109.5	H56H-C56C-H56I	109.5
C55C-C57C-H57G	109.5	C55C-C57C-H57H	109.5
C55C-C57C-H57I	109.5	H57G-C57C-H57H	109.5
H57G-C57C-H57I	109.5	H57H-C57C-H57I	109.5
C55C-C58C-H58G	109.5	C55C-C58C-H58H	109.5
C55C-C58C-H58I	109.5	H58G-C58C-H58H	109.5
H58G-C58C-H58I	109.5	H58H-C58C-H58I	109.5
C21C-S1C-C22C	96.8(4)	C21C-S2C-C23C	97.5(4)
H1ND-N1D-C1D	125.4	H1ND-N1D-C4D	125.4

C1D-N1D-C4D	109.1(7)	C6D-N2D-C9D	105.6(7)
H3ND-N3D-C11D	125.1	H3ND-N3D-C14D	125.1
C11D-N3D-C14D	109.7(7)	C16D-N4D-C19D	104.8(7)
N1D-C1D-C2D	108.7(8)	N1D-C1D-C20D	122.7(7)
C2D-C1D-C20D	128.5(8)	C1D-C2D-H2D	126.8
C1D-C2D-C3D	106.4(8)	H2D-C2D-C3D	126.8
C2D-C3D-H3D	125.7	C2D-C3D-C4D	108.7(8)
H3D-C3D-C4D	125.7	N1D-C4D-C3D	106.9(8)
N1D-C4D-C5D	123.7(8)	C3D-C4D-C5D	129.4(8)
C4D-C5D-C6D	128.0(8)	C4D-C5D-C31D	116.2(8)
C6D-C5D-C31D	115.6(8)	N2D-C6D-C5D	125.8(8)
N2D-C6D-C7D	108.4(8)	C5D-C6D-C7D	125.7(8)
C6D-C7D-H7D	126.6	C6D-C7D-C8D	106.8(8)
H7D-C7D-C8D	126.6	C7D-C8D-H8D	126.3
C7D-C8D-C9D	107.5(9)	H8D-C8D-C9D	126.3
N2D-C9D-C8D	111.6(8)	N2D-C9D-C10D	123.7(8)
C8D-C9D-C10D	124.7(8)	C9D-C10D-C11D	120.8(8)
C9D-C10D-C28D	119.3(8)	C11D-C10D-C28D	119.7(8)
N3D-C11D-C10D	121.3(7)	N3D-C11D-C12D	108.1(8)
C10D-C11D-C12D	130.4(8)	C11D-C12D-H12D	126.1
C11D-C12D-C13D	107.8(8)	H12D-C12D-C13D	126.1
C12D-C13D-H13D	126.4	C12D-C13D-C14D	107.1(8)
H13D-C13D-C14D	126.4	N3D-C14D-C13D	107.2(8)
N3D-C14D-C15D	126.2(8)	C13D-C14D-C15D	126.4(8)
C14D-C15D-C16D	126.4(8)	C14D-C15D-C45D	116.1(8)
C16D-C15D-C45D	117.5(8)	N4D-C16D-C15D	125.0(8)
N4D-C16D-C17D	108.6(7)	C15D-C16D-C17D	126.1(8)
C16D-C17D-H17D	126.1	C16D-C17D-C18D	107.8(8)
H17D-C17D-C18D	126.1	C17D-C18D-H18D	126.9
C17D-C18D-C19D	106.1(9)	H18D-C18D-C19D	126.9
N4D-C19D-C18D	112.6(8)	N4D-C19D-C20D	124.5(8)
C18D-C19D-C20D	122.8(8)	C1D-C20D-C19D	119.0(7)
C1D-C20D-C21D	122.1(7)	C19D-C20D-C21D	118.9(8)
C20D-C21D-S1D	123.7(7)	C20D-C21D-S2D	123.2(6)
S1D-C21D-S2D	112.9(5)	C23D-C22D-C27D	119.4(9)
C23D-C22D-S1D	117.8(7)	C27D-C22D-S1D	122.8(8)
C22D-C23D-C24D	120.7(10)	C22D-C23D-S2D	115.7(7)
C24D-C23D-S2D	123.6(9)	C23D-C24D-H24D	119.9
C23D-C24D-C25D	120.1(12)	H24D-C24D-C25D	119.9
C24D-C25D-H25D	120.5	C24D-C25D-C26D	119.0(11)
H25D-C25D-C26D	120.5	C25D-C26D-H26D	119.1
C25D-C26D-C27D	121.8(11)	H26D-C26D-C27D	119.1
C22D-C27D-C26D	119.0(11)	C22D-C27D-H27D	120.5
C26D-C27D-H27D	120.5	C10D-C28D-C29D	121.8(9)
C10D-C28D-C30D	124.2(9)	C29D-C28D-C30D	113.5(9)
N5D-C29D-C28D	174.5(12)	N6D-C30D-C28D	176.9(13)
C5D-C31D-C32D	121.0(8)	C5D-C31D-C36D	119.1(8)
C32D-C31D-C36D	119.7(8)	C31D-C32D-H32D	119.2
C31D-C32D-C33D	121.6(9)	H32D-C32D-C33D	119.2
C32D-C33D-C34D	115.9(9)	C32D-C33D-C37D	123.0(10)
C34D-C33D-C37D	120.4(9)	C33D-C34D-H34D	117.9

C33D-C34D-C35D	124.3(9)	H34D-C34D-C35D	117.9
C34D-C35D-C36D	116.6(9)	C34D-C35D-C41D	123.6(9)
C36D-C35D-C41D	118.9(10)	C31D-C36D-C35D	121.3(10)
C31D-C36D-H36D	119.3	C35D-C36D-H36D	119.3
C33D-C37D-C38D	111.5(10)	C33D-C37D-C39D	107.3(11)
C33D-C37D-C40D	110.0(10)	C38D-C37D-C39D	108.1(12)
C38D-C37D-C40D	109.4(12)	C39D-C37D-C40D	110.5(11)
C37D-C38D-H38J	109.5	C37D-C38D-H38K	109.5
C37D-C38D-H38L	109.5	H38J-C38D-H38K	109.5
H38J-C38D-H38L	109.5	H38K-C38D-H38L	109.5
C37D-C39D-H39J	109.5	C37D-C39D-H39K	109.5
C37D-C39D-H39L	109.5	H39J-C39D-H39K	109.5
H39J-C39D-H39L	109.5	H39K-C39D-H39L	109.5
C37D-C40D-H40J	109.5	C37D-C40D-H40K	109.5
C37D-C40D-H40L	109.5	H40J-C40D-H40K	109.5
H40J-C40D-H40L	109.5	H40K-C40D-H40L	109.5
C35D-C41D-C42D	108.3(11)	C35D-C41D-C43D	112.4(10)
C35D-C41D-C44D	107.1(11)	C42D-C41D-C43D	107.0(12)
C42D-C41D-C44D	109.7(13)	C43D-C41D-C44D	112.3(13)
C41D-C42D-H42J	109.5	C41D-C42D-H42K	109.5
C41D-C42D-H42L	109.5	H42J-C42D-H42K	109.5
H42J-C42D-H42L	109.5	H42K-C42D-H42L	109.5
C41D-C43D-H43J	109.5	C41D-C43D-H43K	109.5
C41D-C43D-H43L	109.5	H43J-C43D-H43K	109.5
H43J-C43D-H43L	109.5	H43K-C43D-H43L	109.5
C41D-C44D-H44J	109.5	C41D-C44D-H44K	109.5
C41D-C44D-H44L	109.5	H44J-C44D-H44K	109.5
H44J-C44D-H44L	109.5	H44K-C44D-H44L	109.5
C15D-C45D-C46D	121.8(8)	C15D-C45D-C50D	118.3(8)
C46D-C45D-C50D	119.9(8)	C45D-C46D-H46D	120.1
C45D-C46D-C47D	119.7(8)	H46D-C46D-C47D	120.1
C46D-C47D-C48D	117.9(8)	C46D-C47D-C51D	118.0(8)
C48D-C47D-C51D	124.1(8)	C47D-C48D-H48D	117.8
C47D-C48D-C49D	124.3(9)	H48D-C48D-C49D	117.8
C48D-C49D-C50D	117.5(8)	C48D-C49D-C55D	124.8(8)
C50D-C49D-C55D	117.7(8)	C45D-C50D-C49D	120.6(8)
C45D-C50D-H50D	119.7	C49D-C50D-H50D	119.7
C47D-C51D-C52D	110.0(11)	C47D-C51D-C53D	109.5(10)
C47D-C51D-C54D	109.2(10)	C47D-C51D-C52Z	108.0(8)
C47D-C51D-C53Z	110.4(8)	C47D-C51D-C54Z	108.7(8)
C52D-C51D-C53D	110.2(17)	C52D-C51D-C54D	108.3(16)
C53D-C51D-C54D	109.6(17)	C52Z-C51D-C53Z	110.0(11)
C52Z-C51D-C54Z	109.3(11)	C53Z-C51D-C54Z	110.4(11)
C51D-C52D-H52J	109.5	C51D-C52D-H52K	109.5
C51D-C52D-H52L	109.5	H52J-C52D-H52K	109.5
H52J-C52D-H52L	109.5	H52K-C52D-H52L	109.5
C51D-C53D-H53J	109.5	C51D-C53D-H53K	109.5
C51D-C53D-H53L	109.5	H53J-C53D-H53K	109.5
H53J-C53D-H53L	109.5	H53K-C53D-H53L	109.5
C51D-C54D-H54J	109.5	C51D-C54D-H54K	109.5
C51D-C54D-H54L	109.5	H54J-C54D-H54K	109.5

H54J-C54D-H54L	109.5	H54K-C54D-H54L	109.5
C49D-C55D-C56D	109.7(8)	C49D-C55D-C57D	109.5(8)
C49D-C55D-C58D	109.3(8)	C49D-C55D-C56Z	109.8(12)
C49D-C55D-C57Z	109.4(12)	C49D-C55D-C58Z	109.2(12)
C56D-C55D-C57D	109.2(11)	C56D-C55D-C58D	107.3(11)
C57D-C55D-C58D	111.9(11)	C56Z-C55D-C57Z	110.2(18)
C56Z-C55D-C58Z	109.9(18)	C57Z-C55D-C58Z	108.3(17)
C55D-C56D-H56J	109.5	C55D-C56D-H56K	109.5
C55D-C56D-H56L	109.5	H56J-C56D-H56K	109.5
H56J-C56D-H56L	109.5	H56K-C56D-H56L	109.5
C55D-C57D-H57J	109.5	C55D-C57D-H57K	109.5
C55D-C57D-H57L	109.5	H57J-C57D-H57K	109.5
H57J-C57D-H57L	109.5	H57K-C57D-H57L	109.5
C55D-C58D-H58J	109.5	C55D-C58D-H58K	109.5
C55D-C58D-H58L	109.5	H58J-C58D-H58K	109.5
H58J-C58D-H58L	109.5	H58K-C58D-H58L	109.5
C21D-S1D-C22D	96.4(4)	C21D-S2D-C23D	97.1(4)
C37A-C38W-H38M	109.5	C37A-C38W-H38N	109.5
C37A-C38W-H38O	109.5	H38M-C38W-H38N	109.5
H38M-C38W-H38O	109.5	H38N-C38W-H38O	109.5
C37A-C39W-H39M	109.5	C37A-C39W-H39N	109.5
C37A-C39W-H39O	109.5	H39M-C39W-H39N	109.5
H39M-C39W-H39O	109.5	H39N-C39W-H39O	109.5
C37A-C40W-H40M	109.5	C37A-C40W-H40N	109.5
C37A-C40W-H40O	109.5	H40M-C40W-H40N	109.5
H40M-C40W-H40O	109.5	H40N-C40W-H40O	109.5
C41A-C42W-H42M	109.5	C41A-C42W-H42N	109.5
C41A-C42W-H42O	109.5	H42M-C42W-H42N	109.5
H42M-C42W-H42O	109.5	H42N-C42W-H42O	109.5
C41A-C43W-H43M	109.5	C41A-C43W-H43N	109.5
C41A-C43W-H43O	109.5	H43M-C43W-H43N	109.5
H43M-C43W-H43O	109.5	H43N-C43W-H43O	109.5
C41A-C44W-H44M	109.5	C41A-C44W-H44N	109.5
C41A-C44W-H44O	109.5	H44M-C44W-H44N	109.5
H44M-C44W-H44O	109.5	H44N-C44W-H44O	109.5
C37B-C38X-H38P	109.5	C37B-C38X-H38Q	109.5
C37B-C38X-H38R	109.5	H38P-C38X-H38Q	109.5
H38P-C38X-H38R	109.5	H38Q-C38X-H38R	109.5
C37B-C39X-H39P	109.5	C37B-C39X-H39Q	109.5
C37B-C39X-H39R	109.5	H39P-C39X-H39Q	109.5
H39P-C39X-H39R	109.5	H39Q-C39X-H39R	109.5
C37B-C40X-H40P	109.5	C37B-C40X-H40Q	109.5
C37B-C40X-H40R	109.5	H40P-C40X-H40Q	109.5
H40P-C40X-H40R	109.5	H40Q-C40X-H40R	109.5
C41B-C42X-H42P	109.5	C41B-C42X-H42Q	109.5
C41B-C42X-H42R	109.5	H42P-C42X-H42Q	109.5
H42P-C42X-H42R	109.5	H42Q-C42X-H42R	109.5
C41B-C43X-H43P	109.5	C41B-C43X-H43Q	109.5
C41B-C43X-H43R	109.5	H43P-C43X-H43Q	109.5
H43P-C43X-H43R	109.5	H43Q-C43X-H43R	109.5
C41B-C44X-H44P	109.5	C41B-C44X-H44Q	109.5

C41B–C44X–H44R	109.5	H44P–C44X–H44Q	109.5
H44P–C44X–H44R	109.5	H44Q–C44X–H44R	109.5
C41C–C42Y–H42S	109.5	C41C–C42Y–H42T	109.5
C41C–C42Y–H42U	109.5	H42S–C42Y–H42T	109.5
H42S–C42Y–H42U	109.5	H42T–C42Y–H42U	109.5
C41C–C43Y–H43S	109.5	C41C–C43Y–H43T	109.5
C41C–C43Y–H43U	109.5	H43S–C43Y–H43T	109.5
H43S–C43Y–H43U	109.5	H43T–C43Y–H43U	109.5
C41C–C44Y–H44S	109.5	C41C–C44Y–H44T	109.5
C41C–C44Y–H44U	109.5	H44S–C44Y–H44T	109.5
H44S–C44Y–H44U	109.5	H44T–C44Y–H44U	109.5
C51D–C52Z–H52M	109.5	C51D–C52Z–H52N	109.5
C51D–C52Z–H52O	109.5	H52M–C52Z–H52N	109.5
H52M–C52Z–H52O	109.5	H52N–C52Z–H52O	109.5
C51D–C53Z–H53M	109.5	C51D–C53Z–H53N	109.5
C51D–C53Z–H53O	109.5	H53M–C53Z–H53N	109.5
H53M–C53Z–H53O	109.5	H53N–C53Z–H53O	109.5
C51D–C54Z–H54M	109.5	C51D–C54Z–H54N	109.5
C51D–C54Z–H54O	109.5	H54M–C54Z–H54N	109.5
H54M–C54Z–H54O	109.5	H54N–C54Z–H54O	109.5
C55D–C56Z–H56M	109.5	C55D–C56Z–H56N	109.5
C55D–C56Z–H56O	109.5	H56M–C56Z–H56N	109.5
H56M–C56Z–H56O	109.5	H56N–C56Z–H56O	109.5
C55D–C57Z–H57M	109.5	C55D–C57Z–H57N	109.5
C55D–C57Z–H57O	109.5	H57M–C57Z–H57N	109.5
H57M–C57Z–H57O	109.5	H57N–C57Z–H57O	109.5
C55D–C58Z–H58M	109.5	C55D–C58Z–H58N	109.5
C55D–C58Z–H58O	109.5	H58M–C58Z–H58N	109.5
H58M–C58Z–H58O	109.5	H58N–C58Z–H58O	109.5

Table S10. Torsion angles [°] for **H₂8b**.

C4A–N1A–C1A–C2A	–2.8(11)	C4A–N1A–C1A–C20A	–177.9(8)
N1A–C1A–C2A–C3A	0.2(11)	C20A–C1A–C2A–C3A	174.9(9)
C1A–C2A–C3A–C4A	2.4(12)	C1A–N1A–C4A–C3A	4.2(11)
C1A–N1A–C4A–C5A	–173.0(9)	C2A–C3A–C4A–N1A	–4.0(11)
C2A–C3A–C4A–C5A	173.0(10)	N1A–C4A–C5A–C6A	6.6(16)
N1A–C4A–C5A–C31A	177.2(9)	C3A–C4A–C5A–C6A	–170.0(10)
C3A–C4A–C5A–C31A	0.5(15)	C4A–C5A–C6A–N2A	–4.1(16)
C4A–C5A–C6A–C7A	177.2(10)	C31A–C5A–C6A–N2A	–174.6(9)
C31A–C5A–C6A–C7A	6.7(14)	C9A–N2A–C6A–C5A	176.5(10)
C9A–N2A–C6A–C7A	–4.7(11)	N2A–C6A–C7A–C8A	4.0(12)
C5A–C6A–C7A–C8A	–177.1(10)	C6A–C7A–C8A–C9A	–1.7(12)
C6A–N2A–C9A–C8A	3.7(11)	C6A–N2A–C9A–C10A	–173.3(9)
C7A–C8A–C9A–N2A	–1.2(12)	C7A–C8A–C9A–C10A	175.8(10)
N2A–C9A–C10A–C11A	–39.2(14)	N2A–C9A–C10A–C28A	147.0(10)
C8A–C9A–C10A–C11A	144.1(10)	C8A–C9A–C10A–C28A	–29.6(15)
C14A–N3A–C11A–C10A	–174.3(10)	C14A–N3A–C11A–C12A	1.0(13)
C9A–C10A–C11A–N3A	32.4(15)	C9A–C10A–C11A–C12A	–141.9(12)
C28A–C10A–C11A–N3A	–153.7(11)	C28A–C10A–C11A–C12A	32.0(18)
N3A–C11A–C12A–C13A	1.0(14)	C10A–C11A–C12A–C13A	176.0(12)
C11A–C12A–C13A–C14A	–2.6(14)	C11A–N3A–C14A–C13A	–2.6(13)
C11A–N3A–C14A–C15A	–178.0(11)	C12A–C13A–C14A–N3A	3.2(13)
C12A–C13A–C14A–C15A	178.4(11)	N3A–C14A–C15A–C16A	4.6(19)
N3A–C14A–C15A–C45A	–175.2(10)	C13A–C14A–C15A–C16A	–169.8(12)
C13A–C14A–C15A–C45A	10.4(17)	C14A–C15A–C16A–N4A	–1.8(18)
C14A–C15A–C16A–C17A	174.0(11)	C45A–C15A–C16A–N4A	178.0(9)
C45A–C15A–C16A–C17A	–6.2(17)	C19A–N4A–C16A–C15A	172.4(10)
C19A–N4A–C16A–C17A	–3.9(11)	N4A–C16A–C17A–C18A	2.9(12)
C15A–C16A–C17A–C18A	–173.4(11)	C16A–C17A–C18A–C19A	–0.7(12)
C16A–N4A–C19A–C18A	3.6(11)	C16A–N4A–C19A–C20A	178.6(9)
C17A–C18A–C19A–N4A	–1.9(12)	C17A–C18A–C19A–C20A	–177.0(9)
N1A–C1A–C20A–C19A	26.3(14)	N1A–C1A–C20A–C21A	–145.8(9)
C2A–C1A–C20A–C19A	–147.8(10)	C2A–C1A–C20A–C21A	40.1(15)
N4A–C19A–C20A–C1A	–33.9(14)	N4A–C19A–C20A–C21A	138.2(10)
C18A–C19A–C20A–C1A	140.6(10)	C18A–C19A–C20A–C21A	–47.3(14)
C1A–C20A–C21A–S1A	–3.0(14)	C1A–C20A–C21A–S2A	174.4(7)
C19A–C20A–C21A–S1A	–175.2(7)	C19A–C20A–C21A–S2A	2.3(13)
C27A–C22A–C23A–C24A	–1.3(16)	C27A–C22A–C23A–S2A	–177.0(8)
S1A–C22A–C23A–C24A	178.9(9)	S1A–C22A–C23A–S2A	3.2(11)
C22A–C23A–C24A–C25A	1.2(17)	S2A–C23A–C24A–C25A	176.6(9)
C23A–C24A–C25A–C26A	0.2(18)	C24A–C25A–C26A–C27A	–1.5(19)
C25A–C26A–C27A–C22A	1.3(17)	C23A–C22A–C27A–C26A	0.0(16)
S1A–C22A–C27A–C26A	179.8(9)	C9A–C10A–C28A–C29A	–6.2(16)
C9A–C10A–C28A–C30A	–176.1(10)	C11A–C10A–C28A–C29A	–179.9(10)
C11A–C10A–C28A–C30A	10.1(17)	C4A–C5A–C31A–C32A	86.0(12)
C4A–C5A–C31A–C36A	–101.9(12)	C6A–C5A–C31A–C32A	–102.6(12)
C6A–C5A–C31A–C36A	69.5(13)	C5A–C31A–C32A–C33A	173.3(10)
C36A–C31A–C32A–C33A	0.9(17)	C31A–C32A–C33A–C34A	0.3(18)

C31A-C32A-C33A-C37A	-175.4(11)	C32A-C33A-C34A-C35A	2(2)
C37A-C33A-C34A-C35A	178.2(12)	C33A-C34A-C35A-C36A	-6(2)
C33A-C34A-C35A-C41A	-178.7(12)	C34A-C35A-C36A-C31A	6.9(18)
C41A-C35A-C36A-C31A	-179.9(10)	C5A-C31A-C36A-C35A	-177.0(10)
C32A-C31A-C36A-C35A	-4.6(17)	C32A-C33A-C37A-C38A	5.4(18)
C32A-C33A-C37A-C39A	-115.5(15)	C32A-C33A-C37A-C40A	126.5(15)
C32A-C33A-C37A-C38W	64(4)	C32A-C33A-C37A-C39W	-56(4)
C32A-C33A-C37A-C40W	-176(5)	C34A-C33A-C37A-C38A	-170.2(14)
C34A-C33A-C37A-C39A	68.9(16)	C34A-C33A-C37A-C40A	-49.1(16)
C34A-C33A-C37A-C38W	-112(4)	C34A-C33A-C37A-C39W	128(4)
C34A-C33A-C37A-C40W	9(5)	C34A-C35A-C41A-C42A	-57(3)
C34A-C35A-C41A-C43A	62(3)	C34A-C35A-C41A-C44A	-178(3)
C34A-C35A-C41A-C42W	-8.6(19)	C34A-C35A-C41A-C43W	114.9(18)
C34A-C35A-C41A-C44W	-128.2(17)	C36A-C35A-C41A-C42A	130(2)
C36A-C35A-C41A-C43A	-111(2)	C36A-C35A-C41A-C44A	9(3)
C36A-C35A-C41A-C42W	178.5(16)	C36A-C35A-C41A-C43W	-57.9(17)
C36A-C35A-C41A-C44W	58.9(17)	C14A-C15A-C45A-C46A	-63.4(15)
C14A-C15A-C45A-C50A	114.1(12)	C16A-C15A-C45A-C46A	116.8(12)
C16A-C15A-C45A-C50A	-65.8(14)	C15A-C45A-C46A-C47A	178.0(10)
C50A-C45A-C46A-C47A	0.6(17)	C45A-C46A-C47A-C48A	-1.8(16)
C45A-C46A-C47A-C51A	177.6(10)	C46A-C47A-C48A-C49A	1.5(17)
C51A-C47A-C48A-C49A	-178.0(10)	C47A-C48A-C49A-C50A	0.0(17)
C47A-C48A-C49A-C55A	179.2(10)	C15A-C45A-C50A-C49A	-176.5(10)
C46A-C45A-C50A-C49A	0.9(17)	C48A-C49A-C50A-C45A	-1.3(16)
C55A-C49A-C50A-C45A	179.6(10)	C46A-C47A-C51A-C52A	0.0(15)
C46A-C47A-C51A-C53A	120.1(12)	C46A-C47A-C51A-C54A	-122.4(12)
C48A-C47A-C51A-C52A	179.4(11)	C48A-C47A-C51A-C53A	-60.5(14)
C48A-C47A-C51A-C54A	57.0(13)	C48A-C49A-C55A-C56A	20.7(16)
C48A-C49A-C55A-C57A	-98.8(13)	C48A-C49A-C55A-C58A	143.6(13)
C50A-C49A-C55A-C56A	-160.2(12)	C50A-C49A-C55A-C57A	80.4(14)
C50A-C49A-C55A-C58A	-37.3(15)	C20A-C21A-S1A-C22A	170.2(9)
S2A-C21A-S1A-C22A	-7.5(7)	C23A-C22A-S1A-C21A	2.7(9)
C27A-C22A-S1A-C21A	-177.1(9)	C22A-C23A-S2A-C21A	-7.3(9)
C24A-C23A-S2A-C21A	177.1(10)	C20A-C21A-S2A-C23A	-168.9(9)
S1A-C21A-S2A-C23A	8.9(7)	C4B-N1B-C1B-C2B	-0.7(11)
C4B-N1B-C1B-C20B	178.9(9)	N1B-C1B-C2B-C3B	0.2(12)
C20B-C1B-C2B-C3B	-179.4(10)	C1B-C2B-C3B-C4B	0.4(12)
C1B-N1B-C4B-C3B	0.9(11)	C1B-N1B-C4B-C5B	-172.2(9)
C2B-C3B-C4B-N1B	-0.8(11)	C2B-C3B-C4B-C5B	171.8(10)
N1B-C4B-C5B-C6B	1.7(17)	N1B-C4B-C5B-C31B	177.7(9)
C3B-C4B-C5B-C6B	-169.7(11)	C3B-C4B-C5B-C31B	6.3(16)
C4B-C5B-C6B-N2B	0.7(17)	C4B-C5B-C6B-C7B	177.9(10)
C31B-C5B-C6B-N2B	-175.3(9)	C31B-C5B-C6B-C7B	1.9(15)
C9B-N2B-C6B-C5B	173.9(10)	C9B-N2B-C6B-C7B	-3.8(11)
N2B-C6B-C7B-C8B	2.8(12)	C5B-C6B-C7B-C8B	-174.8(10)
C6B-C7B-C8B-C9B	-0.7(12)	C6B-N2B-C9B-C8B	3.4(11)
C6B-N2B-C9B-C10B	-176.4(9)	C7B-C8B-C9B-N2B	-1.8(12)
C7B-C8B-C9B-C10B	178.1(9)	N2B-C9B-C10B-C11B	-38.5(14)
N2B-C9B-C10B-C28B	146.0(10)	C8B-C9B-C10B-C11B	141.7(10)

C8B-C9B-C10B-C28B	-33.8(15)	C14B-N3B-C11B-C10B	-179.3(10)
C14B-N3B-C11B-C12B	-0.2(13)	C9B-C10B-C11B-N3B	33.5(15)
C9B-C10B-C11B-C12B	-145.5(12)	C28B-C10B-C11B-N3B	-151.0(11)
C28B-C10B-C11B-C12B	30.0(18)	N3B-C11B-C12B-C13B	-2.4(14)
C10B-C11B-C12B-C13B	176.7(12)	C11B-C12B-C13B-C14B	4.0(15)
C11B-N3B-C14B-C13B	2.7(13)	C11B-N3B-C14B-C15B	-176.7(11)
C12B-C13B-C14B-N3B	-4.1(14)	C12B-C13B-C14B-C15B	175.2(12)
N3B-C14B-C15B-C16B	6.1(19)	N3B-C14B-C15B-C45B	-174.4(10)
C13B-C14B-C15B-C16B	-173.1(12)	C13B-C14B-C15B-C45B	6.5(18)
C14B-C15B-C16B-N4B	-2.6(19)	C14B-C15B-C16B-C17B	170.8(12)
C45B-C15B-C16B-N4B	177.9(10)	C45B-C15B-C16B-C17B	-8.8(18)
C19B-N4B-C16B-C15B	173.2(11)	C19B-N4B-C16B-C17B	-1.2(11)
N4B-C16B-C17B-C18B	1.2(13)	C15B-C16B-C17B-C18B	-173.1(11)
C16B-C17B-C18B-C19B	-0.7(12)	C16B-N4B-C19B-C18B	0.8(11)
C16B-N4B-C19B-C20B	-179.3(9)	C17B-C18B-C19B-N4B	-0.1(12)
C17B-C18B-C19B-C20B	-179.9(10)	N1B-C1B-C20B-C19B	32.5(14)
N1B-C1B-C20B-C21B	-145.6(10)	C2B-C1B-C20B-C19B	-148.0(10)
C2B-C1B-C20B-C21B	33.9(16)	N4B-C19B-C20B-C1B	-37.2(14)
N4B-C19B-C20B-C21B	141.0(10)	C18B-C19B-C20B-C1B	142.6(10)
C18B-C19B-C20B-C21B	-39.2(14)	C1B-C20B-C21B-S1B	-0.6(14)
C1B-C20B-C21B-S2B	175.6(7)	C19B-C20B-C21B-S1B	-178.7(7)
C19B-C20B-C21B-S2B	-2.5(13)	C27B-C22B-C23B-C24B	-0.4(17)
C27B-C22B-C23B-S2B	-177.9(8)	S1B-C22B-C23B-C24B	-179.5(9)
S1B-C22B-C23B-S2B	3.0(12)	C22B-C23B-C24B-C25B	1.4(17)
S2B-C23B-C24B-C25B	178.7(9)	C23B-C24B-C25B-C26B	-3.7(19)
C24B-C25B-C26B-C27B	5(2)	C25B-C26B-C27B-C22B	-4.0(19)
C23B-C22B-C27B-C26B	1.6(17)	S1B-C22B-C27B-C26B	-179.4(9)
C9B-C10B-C28B-C29B	-6.1(16)	C9B-C10B-C28B-C30B	-177.3(10)
C11B-C10B-C28B-C29B	178.5(10)	C11B-C10B-C28B-C30B	7.3(17)
C4B-C5B-C31B-C32B	77.3(13)	C4B-C5B-C31B-C36B	-104.5(12)
C6B-C5B-C31B-C32B	-106.3(12)	C6B-C5B-C31B-C36B	72.0(13)
C5B-C31B-C32B-C33B	175.7(10)	C36B-C31B-C32B-C33B	-2.6(17)
C31B-C32B-C33B-C34B	3.5(17)	C31B-C32B-C33B-C37B	-173.4(10)
C32B-C33B-C34B-C35B	-3.4(18)	C37B-C33B-C34B-C35B	173.6(11)
C33B-C34B-C35B-C36B	2.3(19)	C33B-C34B-C35B-C41B	-179.3(11)
C34B-C35B-C36B-C31B	-1.2(18)	C41B-C35B-C36B-C31B	-179.6(10)
C5B-C31B-C36B-C35B	-177.0(10)	C32B-C31B-C36B-C35B	1.4(17)
C32B-C33B-C37B-C38B	1.9(16)	C32B-C33B-C37B-C39B	-119.0(15)
C32B-C33B-C37B-C40B	119.8(14)	C32B-C33B-C37B-C38X	-49(3)
C32B-C33B-C37B-C39X	-167(3)	C32B-C33B-C37B-C40X	72(3)
C34B-C33B-C37B-C38B	-174.9(13)	C34B-C33B-C37B-C39B	64.3(16)
C34B-C33B-C37B-C40B	-57.0(15)	C34B-C33B-C37B-C38X	135(3)
C34B-C33B-C37B-C39X	17(3)	C34B-C33B-C37B-C40X	-105(3)
C34B-C35B-C41B-C42B	5.6(19)	C34B-C35B-C41B-C43B	126.0(17)
C34B-C35B-C41B-C44B	-117.6(17)	C34B-C35B-C41B-C42X	48(2)
C34B-C35B-C41B-C43X	168(2)	C34B-C35B-C41B-C44X	-71(3)
C36B-C35B-C41B-C42B	-176.1(16)	C36B-C35B-C41B-C43B	-55.7(17)
C36B-C35B-C41B-C44B	60.7(17)	C36B-C35B-C41B-C42X	-134(2)

C36B–C35B–C41B–C43X	–13(2)	C36B–C35B–C41B–C44X	108(2)
C14B–C15B–C45B–C46B	–70.6(14)	C14B–C15B–C45B–C50B	109.2(12)
C16B–C15B–C45B–C46B	109.0(13)	C16B–C15B–C45B–C50B	–71.2(15)
C15B–C45B–C46B–C47B	–178.5(11)	C50B–C45B–C46B–C47B	1.7(18)
C45B–C46B–C47B–C48B	–1.4(18)	C45B–C46B–C47B–C51B	177.7(11)
C46B–C47B–C48B–C49B	1.5(19)	C51B–C47B–C48B–C49B	–177.6(11)
C47B–C48B–C49B–C50B	–1.9(17)	C47B–C48B–C49B–C55B	178.6(11)
C15B–C45B–C50B–C49B	178.0(10)	C46B–C45B–C50B–C49B	–2.2(17)
C48B–C49B–C50B–C45B	2.2(16)	C55B–C49B–C50B–C45B	–178.3(10)
C46B–C47B–C51B–C52B	6.3(17)	C46B–C47B–C51B–C53B	126.5(14)
C46B–C47B–C51B–C54B	–112.2(13)	C48B–C47B–C51B–C52B	–174.6(13)
C48B–C47B–C51B–C53B	–54.5(17)	C48B–C47B–C51B–C54B	66.8(15)
C48B–C49B–C55B–C56B	38.5(15)	C48B–C49B–C55B–C57B	–81.3(13)
C48B–C49B–C55B–C58B	159.2(11)	C50B–C49B–C55B–C56B	–140.9(12)
C50B–C49B–C55B–C57B	99.3(13)	C50B–C49B–C55B–C58B	–20.2(15)
C23B–C22B–S1B–C21B	2.4(10)	C27B–C22B–S1B–C21B	–176.6(9)
C20B–C21B–S1B–C22B	169.6(9)	S2B–C21B–S1B–C22B	–7.0(7)
C20B–C21B–S2B–C23B	–168.2(9)	S1B–C21B–S2B–C23B	8.4(6)
C22B–C23B–S2B–C21B	–6.9(9)	C24B–C23B–S2B–C21B	175.6(10)
C4C–N1C–C1C–C2C	–1.3(11)	C4C–N1C–C1C–C20C	–178.6(9)
N1C–C1C–C2C–C3C	2.0(12)	C20C–C1C–C2C–C3C	179.0(10)
C1C–C2C–C3C–C4C	–2.0(12)	C1C–N1C–C4C–C3C	0.0(11)
C1C–N1C–C4C–C5C	–178.5(9)	C2C–C3C–C4C–N1C	1.3(12)
C2C–C3C–C4C–C5C	179.7(10)	N1C–C4C–C5C–C6C	–1.7(17)
N1C–C4C–C5C–C31C	–177.2(9)	C3C–C4C–C5C–C6C	–179.9(11)
C3C–C4C–C5C–C31C	4.6(15)	C4C–C5C–C6C–N2C	–3.3(17)
C4C–C5C–C6C–C7C	177.8(10)	C31C–C5C–C6C–N2C	172.2(9)
C31C–C5C–C6C–C7C	–6.7(14)	C9C–N2C–C6C–C5C	–175.7(9)
C9C–N2C–C6C–C7C	3.3(10)	N2C–C6C–C7C–C8C	–2.3(11)
C5C–C6C–C7C–C8C	176.8(10)	C6C–C7C–C8C–C9C	0.3(11)
C6C–N2C–C9C–C8C	–3.3(11)	C6C–N2C–C9C–C10C	175.4(9)
C7C–C8C–C9C–N2C	1.9(12)	C7C–C8C–C9C–C10C	–176.8(9)
N2C–C9C–C10C–C11C	38.1(14)	N2C–C9C–C10C–C28C	–145.3(10)
C8C–C9C–C10C–C11C	–143.3(9)	C8C–C9C–C10C–C28C	33.3(14)
C14C–N3C–C11C–C10C	174.3(9)	C14C–N3C–C11C–C12C	–0.7(12)
C9C–C10C–C11C–N3C	–25.3(13)	C9C–C10C–C11C–C12C	148.5(11)
C28C–C10C–C11C–N3C	158.1(9)	C28C–C10C–C11C–C12C	–28.1(16)
N3C–C11C–C12C–C13C	0.3(12)	C10C–C11C–C12C–C13C	–174.2(10)
C11C–C12C–C13C–C14C	0.1(13)	C11C–N3C–C14C–C13C	0.7(12)
C11C–N3C–C14C–C15C	176.6(10)	C12C–C13C–C14C–N3C	–0.5(12)
C12C–C13C–C14C–C15C	–176.3(11)	N3C–C14C–C15C–C16C	–4.0(19)
N3C–C14C–C15C–C45C	177.9(10)	C13C–C14C–C15C–C16C	171.0(11)
C13C–C14C–C15C–C45C	–7.0(17)	C14C–C15C–C16C–N4C	–3.1(19)
C14C–C15C–C16C–C17C	–176.2(11)	C45C–C15C–C16C–N4C	174.9(10)
C45C–C15C–C16C–C17C	1.8(17)	C19C–N4C–C16C–C15C	–171.9(11)
C19C–N4C–C16C–C17C	2.0(13)	N4C–C16C–C17C–C18C	–2.0(14)
C15C–C16C–C17C–C18C	172.2(12)	C16C–C17C–C18C–C19C	1.1(14)
C16C–N4C–C19C–C18C	–1.3(13)	C16C–N4C–C19C–C20C	–176.0(10)
C17C–C18C–C19C–N4C	0.1(15)	C17C–C18C–C19C–C20C	174.9(10)

N1C-C1C-C20C-C19C	-33.5(14)	N1C-C1C-C20C-C21C	151.6(10)
C2C-C1C-C20C-C19C	149.9(11)	C2C-C1C-C20C-C21C	-25.0(17)
N4C-C19C-C20C-C1C	33.6(15)	N4C-C19C-C20C-C21C	-151.5(11)
C18C-C19C-C20C-C1C	-140.5(11)	C18C-C19C-C20C-C21C	34.5(16)
C1C-C20C-C21C-S1C	-1.0(15)	C1C-C20C-C21C-S2C	-170.4(8)
C19C-C20C-C21C-S1C	-175.9(8)	C19C-C20C-C21C-S2C	14.7(14)
C27C-C22C-C23C-C24C	5.2(17)	C27C-C22C-C23C-S2C	-177.3(9)
S1C-C22C-C23C-C24C	-179.9(9)	S1C-C22C-C23C-S2C	-2.4(12)
C22C-C23C-C24C-C25C	-6.9(18)	S2C-C23C-C24C-C25C	175.9(9)
C23C-C24C-C25C-C26C	7.7(18)	C24C-C25C-C26C-C27C	-6.5(18)
C25C-C26C-C27C-C22C	4.5(18)	C23C-C22C-C27C-C26C	-4.0(17)
S1C-C22C-C27C-C26C	-178.6(9)	C9C-C10C-C28C-C29C	6.4(14)
C9C-C10C-C28C-C30C	-178.1(9)	C11C-C10C-C28C-C29C	-177.1(9)
C11C-C10C-C28C-C30C	-1.7(15)	C4C-C5C-C31C-C32C	67.8(14)
C4C-C5C-C31C-C36C	-116.4(12)	C6C-C5C-C31C-C32C	-108.3(12)
C6C-C5C-C31C-C36C	67.5(14)	C5C-C31C-C32C-C33C	176.9(10)
C36C-C31C-C32C-C33C	1.2(18)	C31C-C32C-C33C-C34C	-2.7(18)
C31C-C32C-C33C-C37C	-178.4(11)	C32C-C33C-C34C-C35C	5(2)
C37C-C33C-C34C-C35C	-179.2(13)	C33C-C34C-C35C-C36C	-5(2)
C33C-C34C-C35C-C41C	-176.8(12)	C34C-C35C-C36C-C31C	4(2)
C41C-C35C-C36C-C31C	175.2(12)	C5C-C31C-C36C-C35C	-177.4(11)
C32C-C31C-C36C-C35C	-2(2)	C32C-C33C-C37C-C38C	-9.0(17)
C32C-C33C-C37C-C39C	-129.1(13)	C32C-C33C-C37C-C40C	110.3(13)
C34C-C33C-C37C-C38C	175.3(12)	C34C-C33C-C37C-C39C	55.3(16)
C34C-C33C-C37C-C40C	-65.4(15)	C34C-C35C-C41C-C42C	66.1(19)
C34C-C35C-C41C-C43C	-169.9(17)	C34C-C35C-C41C-C44C	-56.2(19)
C34C-C35C-C41C-C42Y	104(2)	C34C-C35C-C41C-C43Y	-139(3)
C34C-C35C-C41C-C44Y	-10(3)	C36C-C35C-C41C-C42C	-105.3(18)
C36C-C35C-C41C-C43C	18.7(19)	C36C-C35C-C41C-C44C	132.4(18)
C36C-C35C-C41C-C42Y	-67(2)	C36C-C35C-C41C-C43Y	50(3)
C36C-C35C-C41C-C44Y	178(3)	C14C-C15C-C45C-C46C	-110.7(12)
C14C-C15C-C45C-C50C	68.4(13)	C16C-C15C-C45C-C46C	71.0(14)
C16C-C15C-C45C-C50C	-109.9(12)	C15C-C45C-C46C-C47C	-175.8(9)
C50C-C45C-C46C-C47C	5.1(16)	C45C-C46C-C47C-C48C	-4.9(16)
C45C-C46C-C47C-C51C	176.1(9)	C46C-C47C-C48C-C49C	1.9(17)
C51C-C47C-C48C-C49C	-179.1(10)	C47C-C48C-C49C-C50C	0.8(16)
C47C-C48C-C49C-C55C	-178.4(10)	C15C-C45C-C50C-C49C	178.5(9)
C46C-C45C-C50C-C49C	-2.3(16)	C48C-C49C-C50C-C45C	-0.6(15)
C55C-C49C-C50C-C45C	178.6(9)	C46C-C47C-C51C-C52C	61.7(12)
C46C-C47C-C51C-C53C	-177.3(10)	C46C-C47C-C51C-C54C	-58.2(12)
C48C-C47C-C51C-C52C	-117.3(12)	C48C-C47C-C51C-C53C	3.7(15)
C48C-C47C-C51C-C54C	122.8(12)	C48C-C49C-C55C-C56C	-6.1(15)
C48C-C49C-C55C-C57C	-125.8(11)	C48C-C49C-C55C-C58C	113.4(12)
C50C-C49C-C55C-C56C	174.7(11)	C50C-C49C-C55C-C57C	55.0(12)
C50C-C49C-C55C-C58C	-65.7(12)	C23C-C22C-S1C-C21C	2.2(10)
C27C-C22C-S1C-C21C	176.9(10)	C20C-C21C-S1C-C22C	-171.5(9)
S2C-C21C-S1C-C22C	-1.2(7)	C20C-C21C-S2C-C23C	170.6(9)
S1C-C21C-S2C-C23C	0.2(7)	C22C-C23C-S2C-C21C	1.3(9)
C24C-C23C-S2C-C21C	178.7(11)	C4D-N1D-C1D-C2D	2.0(11)

C4D–N1D–C1D–C20D	–178.3(9)	N1D–C1D–C2D–C3D	0.3(12)
C20D–C1D–C2D–C3D	–179.4(10)	C1D–C2D–C3D–C4D	–2.4(12)
C1D–N1D–C4D–C3D	–3.5(11)	C1D–N1D–C4D–C5D	179.2(9)
C2D–C3D–C4D–N1D	3.6(12)	C2D–C3D–C4D–C5D	–179.3(11)
N1D–C4D–C5D–C6D	–3.2(17)	N1D–C4D–C5D–C31D	–178.4(9)
C3D–C4D–C5D–C6D	–179.9(11)	C3D–C4D–C5D–C31D	5.0(16)
C4D–C5D–C6D–N2D	–0.3(18)	C4D–C5D–C6D–C7D	179.1(10)
C31D–C5D–C6D–N2D	174.8(9)	C31D–C5D–C6D–C7D	–5.7(15)
C9D–N2D–C6D–C5D	–176.6(10)	C9D–N2D–C6D–C7D	3.9(11)
N2D–C6D–C7D–C8D	–2.7(12)	C5D–C6D–C7D–C8D	177.8(10)
C6D–C7D–C8D–C9D	0.5(12)	C6D–N2D–C9D–C8D	–3.7(11)
C6D–N2D–C9D–C10D	175.3(9)	C7D–C8D–C9D–N2D	2.0(13)
C7D–C8D–C9D–C10D	–176.9(9)	N2D–C9D–C10D–C11D	37.6(14)
N2D–C9D–C10D–C28D	–148.5(10)	C8D–C9D–C10D–C11D	–143.5(10)
C8D–C9D–C10D–C28D	30.4(14)	C14D–N3D–C11D–C10D	174.7(9)
C14D–N3D–C11D–C12D	–0.8(12)	C9D–C10D–C11D–N3D	–29.0(14)
C9D–C10D–C11D–C12D	145.3(12)	C28D–C10D–C11D–N3D	157.1(10)
C28D–C10D–C11D–C12D	–28.5(17)	N3D–C11D–C12D–C13D	0.3(13)
C10D–C11D–C12D–C13D	–174.6(11)	C11D–C12D–C13D–C14D	0.3(14)
C11D–N3D–C14D–C13D	1.0(12)	C11D–N3D–C14D–C15D	177.0(10)
C12D–C13D–C14D–N3D	–0.8(13)	C12D–C13D–C14D–C15D	–176.8(11)
N3D–C14D–C15D–C16D	–1.7(19)	N3D–C14D–C15D–C45D	178.1(9)
C13D–C14D–C15D–C16D	173.5(11)	C13D–C14D–C15D–C45D	–6.6(16)
C14D–C15D–C16D–N4D	–4.3(19)	C14D–C15D–C16D–C17D	–177.4(12)
C45D–C15D–C16D–N4D	175.9(10)	C45D–C15D–C16D–C17D	2.7(18)
C19D–N4D–C16D–C15D	–173.3(11)	C19D–N4D–C16D–C17D	0.9(13)
N4D–C16D–C17D–C18D	–1.0(15)	C15D–C16D–C17D–C18D	173.1(12)
C16D–C17D–C18D–C19D	0.7(15)	C16D–N4D–C19D–C18D	–0.5(13)
C16D–N4D–C19D–C20D	–176.3(10)	C17D–C18D–C19D–N4D	–0.1(16)
C17D–C18D–C19D–C20D	175.8(11)	N1D–C1D–C20D–C19D	–31.8(14)
N1D–C1D–C20D–C21D	147.2(10)	C2D–C1D–C20D–C19D	147.8(11)
C2D–C1D–C20D–C21D	–33.2(16)	N4D–C19D–C20D–C1D	34.9(16)
N4D–C19D–C20D–C21D	–144.1(11)	C18D–C19D–C20D–C1D	–140.5(11)
C18D–C19D–C20D–C21D	40.5(16)	C1D–C20D–C21D–S1D	10.8(14)
C1D–C20D–C21D–S2D	–164.9(8)	C19D–C20D–C21D–S1D	–170.2(8)
C19D–C20D–C21D–S2D	14.0(14)	C27D–C22D–C23D–C24D	–2.3(16)
C27D–C22D–C23D–S2D	178.3(8)	S1D–C22D–C23D–C24D	176.5(9)
S1D–C22D–C23D–S2D	–2.9(12)	C22D–C23D–C24D–C25D	1.5(18)
S2D–C23D–C24D–C25D	–179.1(9)	C23D–C24D–C25D–C26D	–0.4(18)
C24D–C25D–C26D–C27D	0.2(18)	C25D–C26D–C27D–C22D	–1.0(18)
C23D–C22D–C27D–C26D	2.0(16)	S1D–C22D–C27D–C26D	–176.7(9)
C9D–C10D–C28D–C29D	10.9(15)	C9D–C10D–C28D–C30D	–177.5(10)
C11D–C10D–C28D–C29D	–175.1(9)	C11D–C10D–C28D–C30D	–3.6(15)
C4D–C5D–C31D–C32D	67.8(15)	C4D–C5D–C31D–C36D	–117.6(12)
C6D–C5D–C31D–C32D	–108.0(13)	C6D–C5D–C31D–C36D	66.7(15)
C5D–C31D–C32D–C33D	177.1(12)	C36D–C31D–C32D–C33D	3(2)
C31D–C32D–C33D–C34D	–6(2)	C31D–C32D–C33D–C37D	–176.5(13)
C32D–C33D–C34D–C35D	9(2)	C37D–C33D–C34D–C35D	179.5(14)
C33D–C34D–C35D–C36D	–8(2)	C33D–C34D–C35D–C41D	–176.0(14)

C34D–C35D–C36D–C31D	3(2)	C41D–C35D–C36D–C31D	172.1(13)
C5D–C31D–C36D–C35D	–175.4(12)	C32D–C31D–C36D–C35D	–1(2)
C32D–C33D–C37D–C38D	–12(2)	C32D–C33D–C37D–C39D	–129.9(15)
C32D–C33D–C37D–C40D	109.9(15)	C34D–C33D–C37D–C38D	178.7(15)
C34D–C33D–C37D–C39D	60.4(18)	C34D–C33D–C37D–C40D	–59.8(17)
C34D–C35D–C41D–C42D	71.8(18)	C34D–C35D–C41D–C43D	–170.2(15)
C34D–C35D–C41D–C44D	–46(2)	C36D–C35D–C41D–C42D	–96.5(16)
C36D–C35D–C41D–C43D	21.6(19)	C36D–C35D–C41D–C44D	145.3(15)
C14D–C15D–C45D–C46D	–109.4(12)	C14D–C15D–C45D–C50D	72.1(13)
C16D–C15D–C45D–C46D	70.5(14)	C16D–C15D–C45D–C50D	–108.1(12)
C15D–C45D–C46D–C47D	–175.7(10)	C50D–C45D–C46D–C47D	2.8(16)
C45D–C46D–C47D–C48D	–3.0(17)	C45D–C46D–C47D–C51D	177.2(10)
C46D–C47D–C48D–C49D	1.3(19)	C51D–C47D–C48D–C49D	–178.9(11)
C47D–C48D–C49D–C50D	0.8(19)	C47D–C48D–C49D–C55D	–176.8(11)
C15D–C45D–C50D–C49D	177.9(10)	C46D–C45D–C50D–C49D	–0.7(17)
C48D–C49D–C50D–C45D	–1.1(17)	C55D–C49D–C50D–C45D	176.7(10)
C46D–C47D–C51D–C52D	8(3)	C46D–C47D–C51D–C53D	129(3)
C46D–C47D–C51D–C54D	–111(2)	C46D–C47D–C51D–C52Z	60.8(13)
C46D–C47D–C51D–C53Z	–179.0(13)	C46D–C47D–C51D–C54Z	–57.7(14)
C48D–C47D–C51D–C52D	–172(3)	C48D–C47D–C51D–C53D	–51(3)
C48D–C47D–C51D–C54D	69(3)	C48D–C47D–C51D–C52Z	–119.0(14)
C48D–C47D–C51D–C53Z	1.2(16)	C48D–C47D–C51D–C54Z	122.5(14)
C48D–C49D–C55D–C56D	–7.1(17)	C48D–C49D–C55D–C57D	–126.9(13)
C48D–C49D–C55D–C58D	110.2(14)	C48D–C49D–C55D–C56Z	–50(4)
C48D–C49D–C55D–C57Z	–171(4)	C48D–C49D–C55D–C58Z	71(4)
C50D–C49D–C55D–C56D	175.3(14)	C50D–C49D–C55D–C57D	55.5(14)
C50D–C49D–C55D–C58D	–67.4(14)	C50D–C49D–C55D–C56Z	133(4)
C50D–C49D–C55D–C57Z	12(4)	C50D–C49D–C55D–C58Z	–107(4)
C23D–C22D–S1D–C21D	1.7(9)	C27D–C22D–S1D–C21D	–179.6(9)
C20D–C21D–S1D–C22D	–176.0(9)	S2D–C21D–S1D–C22D	0.1(6)
C20D–C21D–S2D–C23D	174.8(9)	S1D–C21D–S2D–C23D	–1.3(7)
C22D–C23D–S2D–C21D	2.5(9)	C24D–C23D–S2D–C21D	–176.8(10)

Table S11. Anisotropic displacement parameters ($\text{\AA}^2$) for **H₂8b**.The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N1A	0.026(4)	0.018(4)	0.036(4)	0.004(3)	0.000(3)	0.004(3)
N2A	0.021(4)	0.020(4)	0.039(4)	0.008(3)	0.003(3)	0.001(3)
N3A	0.032(4)	0.037(5)	0.039(4)	0.010(4)	-0.006(3)	-0.007(4)
N4A	0.028(4)	0.028(4)	0.036(4)	0.008(3)	-0.003(3)	0.004(3)
N5A	0.043(6)	0.032(5)	0.083(8)	0.012(5)	0.004(5)	-0.002(5)
N6A	0.068(8)	0.046(7)	0.086(8)	-0.012(6)	-0.003(7)	-0.016(6)
C1A	0.026(4)	0.021(4)	0.035(4)	0.007(4)	0.001(3)	0.005(4)
C2A	0.035(5)	0.025(5)	0.044(5)	0.003(4)	-0.001(4)	-0.003(4)
C3A	0.036(5)	0.022(5)	0.041(5)	-0.005(4)	0.002(4)	0.002(4)
C4A	0.030(4)	0.016(4)	0.038(5)	0.000(4)	0.001(4)	-0.001(3)
C5A	0.024(4)	0.024(4)	0.046(5)	0.006(4)	0.003(4)	0.001(4)
C6A	0.015(4)	0.030(5)	0.044(5)	0.018(4)	0.000(4)	0.002(3)
C7A	0.021(4)	0.055(6)	0.044(5)	0.024(5)	0.010(4)	0.002(4)
C8A	0.030(5)	0.033(5)	0.056(6)	0.011(5)	-0.002(4)	-0.004(4)
C9A	0.022(4)	0.023(4)	0.052(5)	0.014(4)	0.003(4)	-0.001(4)
C10A	0.018(4)	0.031(5)	0.051(5)	0.008(4)	-0.004(4)	-0.003(4)
C11A	0.026(5)	0.042(5)	0.044(5)	0.006(4)	-0.002(4)	-0.013(4)
C12A	0.041(6)	0.043(6)	0.038(5)	0.005(5)	-0.007(4)	-0.012(5)
C13A	0.036(5)	0.046(6)	0.038(5)	0.003(5)	-0.003(4)	-0.012(5)
C14A	0.033(5)	0.037(5)	0.039(5)	0.011(4)	0.005(4)	0.002(4)
C15A	0.033(5)	0.036(5)	0.036(5)	0.012(4)	-0.009(4)	-0.002(4)
C16A	0.036(5)	0.022(4)	0.035(5)	0.006(4)	0.007(4)	0.002(4)
C17A	0.039(5)	0.030(5)	0.035(5)	0.002(4)	0.001(4)	0.000(4)
C18A	0.034(5)	0.026(5)	0.040(5)	-0.002(4)	0.000(4)	0.002(4)
C19A	0.028(4)	0.022(4)	0.034(4)	-0.001(4)	0.000(3)	0.007(4)
C20A	0.035(5)	0.015(4)	0.037(4)	-0.005(4)	-0.004(4)	0.000(4)
C21A	0.029(4)	0.024(5)	0.046(5)	-0.003(4)	0.007(4)	-0.011(4)
C22A	0.021(4)	0.015(4)	0.082(6)	0.009(5)	-0.006(4)	-0.003(4)
C23A	0.026(4)	0.024(5)	0.079(7)	-0.003(5)	0.010(4)	-0.016(4)
C24A	0.024(5)	0.034(6)	0.096(7)	0.000(6)	0.012(5)	-0.004(5)
C25A	0.025(5)	0.033(6)	0.131(9)	-0.006(7)	0.027(6)	-0.002(5)
C26A	0.020(5)	0.026(5)	0.125(9)	0.004(7)	-0.004(6)	0.004(4)
C27A	0.022(5)	0.021(5)	0.108(8)	0.008(6)	-0.010(5)	-0.006(4)
C28A	0.027(5)	0.028(5)	0.062(6)	0.007(4)	0.004(4)	0.001(4)
C29A	0.037(6)	0.024(5)	0.068(6)	0.010(5)	0.009(5)	-0.002(5)
C30A	0.038(6)	0.031(6)	0.070(7)	-0.006(5)	0.001(5)	-0.014(5)
C31A	0.029(5)	0.030(5)	0.046(5)	0.002(4)	0.002(4)	-0.005(4)
C32A	0.039(6)	0.038(5)	0.047(5)	0.005(4)	0.007(5)	0.004(5)
C33A	0.051(6)	0.053(6)	0.045(6)	0.002(5)	0.015(5)	0.004(5)
C34A	0.062(7)	0.060(7)	0.039(5)	0.005(5)	0.011(5)	-0.005(6)
C35A	0.052(6)	0.044(5)	0.051(6)	0.015(5)	0.005(5)	-0.003(5)
C36A	0.039(5)	0.038(5)	0.040(5)	0.002(4)	-0.002(4)	0.005(5)
C37A	0.096(9)	0.074(8)	0.054(7)	0.013(6)	0.035(7)	0.034(7)
C38A	0.094(12)	0.074(11)	0.084(11)	0.012(9)	0.045(9)	0.048(10)

C39A	0.139(15)	0.104(14)	0.087(12)	-0.039(11)	0.020(10)	0.054(11)
C40A	0.102(12)	0.120(14)	0.096(13)	0.043(11)	0.071(10)	0.068(10)
C41A	0.090(9)	0.062(7)	0.061(7)	0.024(6)	0.002(7)	-0.002(7)
C42A	0.11(2)	0.10(2)	0.083(16)	0.050(15)	-0.012(16)	0.015(18)
C43A	0.125(19)	0.09(2)	0.07(2)	0.059(16)	0.004(15)	-0.005(16)
C44A	0.12(2)	0.078(17)	0.094(18)	0.047(15)	-0.004(17)	0.045(16)
C45A	0.042(5)	0.036(5)	0.037(5)	0.013(4)	-0.008(4)	-0.008(4)
C46A	0.031(5)	0.040(5)	0.040(5)	0.001(4)	-0.005(4)	0.000(4)
C47A	0.039(5)	0.038(5)	0.038(5)	0.010(4)	-0.002(4)	-0.005(4)
C48A	0.037(5)	0.050(6)	0.043(5)	0.013(4)	-0.002(4)	-0.004(5)
C49A	0.046(6)	0.032(5)	0.049(6)	0.017(4)	-0.007(5)	-0.012(4)
C50A	0.035(5)	0.041(5)	0.039(5)	0.005(4)	-0.006(4)	-0.010(4)
C51A	0.051(6)	0.060(7)	0.033(5)	0.003(5)	0.005(5)	0.000(6)
C52A	0.068(8)	0.052(7)	0.050(7)	-0.001(6)	0.011(6)	0.002(6)
C53A	0.057(7)	0.089(11)	0.052(7)	-0.029(7)	-0.001(6)	-0.005(7)
C54A	0.062(8)	0.068(9)	0.052(7)	0.011(7)	0.025(6)	0.011(7)
C55A	0.047(6)	0.040(6)	0.062(7)	0.015(5)	0.000(5)	0.008(5)
C56A	0.113(13)	0.043(8)	0.127(12)	0.003(9)	-0.054(11)	0.032(9)
C57A	0.083(10)	0.032(6)	0.131(14)	-0.017(8)	0.008(9)	0.000(7)
C58A	0.094(12)	0.058(9)	0.118(11)	0.028(9)	0.028(10)	0.023(9)
S1A	0.0305(13)	0.0269(13)	0.0528(16)	0.0035(12)	-0.0006(11)	-0.0026(11)
S2A	0.0300(13)	0.0367(15)	0.0514(16)	-0.0061(13)	0.0093(12)	-0.0058(12)
N1B	0.028(4)	0.023(4)	0.036(4)	-0.001(3)	0.004(3)	0.002(3)
N2B	0.018(4)	0.025(4)	0.052(5)	0.001(4)	0.007(3)	-0.002(3)
N3B	0.028(4)	0.031(4)	0.042(4)	0.006(4)	0.013(3)	0.006(3)
N4B	0.028(4)	0.024(4)	0.031(4)	0.004(3)	0.003(3)	-0.004(3)
N5B	0.040(5)	0.039(6)	0.064(6)	0.012(5)	0.007(5)	0.003(5)
N6B	0.052(6)	0.048(6)	0.057(6)	0.005(5)	0.011(5)	0.000(5)
C1B	0.034(5)	0.018(4)	0.042(4)	-0.003(4)	0.001(4)	0.000(4)
C2B	0.030(5)	0.024(5)	0.051(5)	0.006(4)	0.006(4)	0.004(4)
C3B	0.033(5)	0.024(5)	0.037(4)	-0.001(4)	0.006(4)	0.000(4)
C4B	0.033(4)	0.022(4)	0.034(4)	0.003(4)	0.003(4)	0.000(4)
C5B	0.027(4)	0.021(4)	0.047(5)	-0.001(4)	-0.001(4)	-0.003(4)
C6B	0.024(4)	0.023(4)	0.048(5)	0.005(4)	0.002(4)	0.003(4)
C7B	0.027(5)	0.032(5)	0.047(5)	-0.002(4)	0.007(4)	-0.002(4)
C8B	0.025(5)	0.033(5)	0.055(6)	0.007(5)	-0.003(4)	0.008(4)
C9B	0.023(4)	0.021(4)	0.049(5)	0.006(4)	0.006(4)	-0.004(4)
C10B	0.018(4)	0.027(4)	0.053(5)	0.001(4)	0.004(4)	-0.006(4)
C11B	0.037(5)	0.033(5)	0.047(5)	0.005(4)	0.013(4)	-0.002(4)
C12B	0.042(6)	0.031(5)	0.050(6)	0.007(5)	0.015(5)	0.014(4)
C13B	0.043(6)	0.040(6)	0.049(6)	0.012(5)	0.017(5)	0.012(5)
C14B	0.030(5)	0.033(5)	0.045(5)	0.006(4)	0.004(4)	0.004(4)
C15B	0.036(5)	0.030(5)	0.042(5)	0.010(4)	0.009(4)	0.004(4)
C16B	0.044(5)	0.027(5)	0.030(5)	0.002(4)	0.002(4)	0.007(4)
C17B	0.041(5)	0.035(5)	0.040(5)	0.005(4)	0.004(4)	0.006(4)
C18B	0.031(5)	0.032(5)	0.031(5)	-0.006(4)	0.000(4)	0.009(4)
C19B	0.038(5)	0.020(4)	0.039(5)	-0.003(4)	0.006(4)	-0.001(4)
C20B	0.028(4)	0.017(4)	0.040(4)	0.003(4)	0.009(4)	0.003(4)
C21B	0.029(4)	0.016(4)	0.053(6)	-0.008(4)	0.000(4)	-0.002(4)

C22B	0.032(5)	0.018(5)	0.107(7)	-0.005(6)	0.000(5)	0.012(4)
C23B	0.039(5)	0.013(4)	0.105(8)	-0.016(5)	-0.012(5)	0.009(4)
C24B	0.043(6)	0.024(5)	0.124(9)	-0.019(6)	-0.020(6)	0.016(5)
C25B	0.040(6)	0.026(6)	0.152(10)	-0.021(8)	-0.035(8)	0.010(5)
C26B	0.032(6)	0.031(6)	0.160(11)	-0.010(8)	-0.009(7)	0.008(5)
C27B	0.028(5)	0.019(5)	0.135(9)	0.007(6)	0.003(6)	0.004(4)
C28B	0.032(5)	0.035(5)	0.053(5)	0.004(4)	-0.001(4)	0.007(4)
C29B	0.016(4)	0.030(5)	0.064(6)	0.006(5)	0.008(4)	0.009(4)
C30B	0.039(6)	0.030(5)	0.051(6)	0.002(5)	-0.001(5)	0.008(5)
C31B	0.021(4)	0.034(5)	0.049(5)	0.003(4)	-0.002(4)	-0.002(4)
C32B	0.041(6)	0.035(5)	0.049(5)	-0.003(4)	-0.004(5)	0.003(5)
C33B	0.049(6)	0.046(5)	0.043(5)	0.011(5)	-0.004(5)	0.002(5)
C34B	0.056(7)	0.049(6)	0.033(5)	-0.004(4)	-0.002(5)	0.013(5)
C35B	0.051(6)	0.049(6)	0.048(6)	0.009(5)	0.004(5)	0.000(5)
C36B	0.043(6)	0.036(5)	0.045(5)	-0.002(4)	0.005(5)	-0.006(5)
C37B	0.084(8)	0.068(7)	0.042(6)	0.004(6)	-0.020(6)	-0.001(7)
C38B	0.088(12)	0.054(9)	0.051(9)	0.005(7)	-0.018(8)	-0.027(9)
C39B	0.098(13)	0.095(14)	0.090(13)	-0.029(11)	0.028(11)	-0.016(11)
C40B	0.067(10)	0.096(13)	0.074(11)	0.037(10)	-0.032(8)	-0.026(9)
C41B	0.082(8)	0.062(7)	0.055(7)	0.023(6)	0.001(6)	-0.011(7)
C42B	0.114(17)	0.065(14)	0.073(11)	0.030(10)	0.001(11)	-0.022(13)
C43B	0.131(17)	0.055(10)	0.089(14)	0.029(10)	-0.003(14)	0.017(13)
C44B	0.077(12)	0.108(17)	0.095(15)	0.045(14)	0.004(11)	-0.035(11)
C45B	0.043(5)	0.034(5)	0.036(5)	0.003(4)	0.010(4)	0.008(4)
C46B	0.053(6)	0.041(6)	0.038(5)	0.003(4)	0.010(5)	0.001(5)
C47B	0.060(6)	0.043(6)	0.035(5)	0.002(4)	0.004(5)	0.005(5)
C48B	0.043(6)	0.046(6)	0.032(5)	0.014(4)	0.005(4)	0.001(5)
C49B	0.031(5)	0.045(5)	0.043(5)	0.008(4)	0.008(4)	0.008(4)
C50B	0.039(5)	0.029(5)	0.037(5)	0.003(4)	0.011(4)	0.012(4)
C51B	0.064(7)	0.059(7)	0.041(6)	-0.001(5)	0.005(5)	-0.001(6)
C52B	0.116(13)	0.060(8)	0.065(9)	-0.007(7)	-0.007(9)	-0.016(9)
C53B	0.096(11)	0.144(17)	0.058(9)	-0.048(10)	0.029(8)	-0.025(10)
C54B	0.096(11)	0.080(10)	0.064(9)	0.003(8)	-0.025(8)	-0.025(9)
C55B	0.047(6)	0.045(6)	0.040(6)	0.010(5)	0.015(5)	-0.003(5)
C56B	0.086(10)	0.062(9)	0.093(10)	-0.004(8)	0.043(9)	-0.019(8)
C57B	0.087(10)	0.052(8)	0.081(10)	0.003(8)	-0.014(8)	0.013(8)
C58B	0.079(10)	0.070(10)	0.062(8)	0.016(7)	-0.003(7)	-0.040(8)
S1B	0.0274(13)	0.0306(14)	0.071(2)	0.0054(14)	0.0104(13)	0.0031(11)
S2B	0.0384(15)	0.0344(15)	0.0547(17)	-0.0122(13)	-0.0056(13)	0.0025(12)
N1C	0.042(4)	0.020(4)	0.034(4)	-0.006(3)	0.002(3)	-0.002(4)
N2C	0.037(4)	0.018(4)	0.032(4)	-0.005(3)	0.003(3)	0.003(3)
N3C	0.027(4)	0.029(4)	0.026(4)	-0.002(3)	0.005(3)	-0.008(3)
N4C	0.031(4)	0.036(5)	0.031(4)	-0.007(4)	0.006(3)	-0.001(4)
N5C	0.045(6)	0.055(6)	0.049(6)	0.005(5)	0.013(5)	0.009(5)
N6C	0.049(6)	0.028(5)	0.054(6)	-0.005(4)	0.000(5)	0.004(4)
C1C	0.047(5)	0.015(4)	0.030(4)	-0.002(4)	-0.003(4)	-0.004(4)
C2C	0.048(5)	0.028(5)	0.037(5)	0.001(4)	-0.001(4)	0.001(5)
C3C	0.061(6)	0.026(5)	0.026(4)	0.000(4)	-0.005(4)	-0.014(5)
C4C	0.054(5)	0.015(4)	0.031(5)	0.003(4)	0.002(4)	0.002(4)

C5C	0.049(5)	0.013(4)	0.035(4)	0.005(4)	0.006(4)	0.000(4)
C6C	0.043(5)	0.015(4)	0.034(4)	0.003(4)	0.004(4)	0.001(4)
C7C	0.040(5)	0.022(5)	0.042(5)	0.004(4)	0.003(4)	0.000(4)
C8C	0.038(5)	0.026(5)	0.035(5)	0.002(4)	0.008(4)	-0.003(4)
C9C	0.028(4)	0.022(4)	0.037(4)	-0.008(4)	0.007(3)	0.001(4)
C10C	0.032(4)	0.019(4)	0.030(4)	0.000(3)	0.007(3)	-0.012(4)
C11C	0.037(5)	0.021(4)	0.032(4)	0.002(4)	0.009(4)	-0.005(4)
C12C	0.024(4)	0.041(6)	0.038(5)	-0.005(4)	0.002(4)	-0.008(4)
C13C	0.032(5)	0.037(5)	0.025(4)	-0.003(4)	0.005(4)	-0.003(4)
C14C	0.024(4)	0.034(5)	0.044(5)	-0.010(4)	-0.002(4)	-0.003(4)
C15C	0.032(4)	0.036(5)	0.025(4)	-0.004(4)	0.005(3)	-0.002(4)
C16C	0.024(4)	0.039(5)	0.038(5)	-0.011(4)	0.005(4)	0.001(4)
C17C	0.033(5)	0.055(6)	0.027(5)	-0.011(4)	0.008(4)	0.007(5)
C18C	0.026(4)	0.058(7)	0.048(6)	-0.011(5)	0.004(4)	0.000(5)
C19C	0.031(5)	0.028(5)	0.033(4)	-0.008(4)	0.002(4)	0.002(4)
C20C	0.036(5)	0.025(5)	0.037(4)	-0.003(4)	-0.002(4)	0.003(4)
C21C	0.031(4)	0.027(5)	0.040(5)	-0.004(4)	0.007(4)	-0.001(4)
C22C	0.019(4)	0.034(5)	0.060(6)	-0.010(5)	0.008(4)	0.005(4)
C23C	0.023(4)	0.032(5)	0.070(6)	0.006(5)	0.006(5)	0.000(4)
C24C	0.028(5)	0.049(7)	0.087(7)	0.015(6)	0.021(5)	-0.004(5)
C25C	0.018(5)	0.035(6)	0.098(8)	-0.004(6)	0.016(5)	0.001(4)
C26C	0.023(5)	0.031(5)	0.098(8)	-0.006(6)	0.014(5)	0.001(4)
C27C	0.033(5)	0.032(6)	0.088(7)	-0.014(5)	0.002(5)	-0.007(5)
C28C	0.030(4)	0.019(4)	0.038(5)	0.002(4)	0.009(4)	-0.003(4)
C29C	0.034(5)	0.031(5)	0.046(5)	0.005(5)	0.002(4)	-0.001(4)
C30C	0.028(5)	0.026(5)	0.048(5)	0.005(4)	0.006(4)	-0.003(4)
C31C	0.052(6)	0.034(5)	0.028(4)	0.002(4)	0.004(4)	-0.003(5)
C32C	0.047(6)	0.029(5)	0.033(5)	0.008(4)	0.005(4)	0.001(5)
C33C	0.058(6)	0.044(5)	0.034(5)	0.001(4)	0.005(5)	0.005(5)
C34C	0.076(8)	0.056(6)	0.026(5)	0.015(5)	0.004(5)	-0.006(6)
C35C	0.092(8)	0.048(5)	0.030(5)	0.009(5)	0.011(5)	-0.013(6)
C36C	0.067(7)	0.033(5)	0.036(5)	0.009(4)	0.007(5)	-0.008(5)
C37C	0.073(8)	0.066(7)	0.033(5)	-0.006(5)	0.005(6)	-0.008(7)
C38C	0.070(8)	0.047(7)	0.039(6)	-0.024(5)	0.003(6)	-0.011(6)
C39C	0.089(10)	0.064(9)	0.042(6)	-0.015(6)	0.003(6)	-0.003(8)
C40C	0.071(8)	0.074(10)	0.065(9)	-0.024(8)	0.024(7)	-0.003(7)
C41C	0.140(11)	0.059(7)	0.034(6)	0.015(6)	0.014(7)	-0.029(8)
C42C	0.143(15)	0.070(14)	0.083(16)	-0.002(13)	0.053(12)	-0.039(12)
C43C	0.098(16)	0.040(9)	0.059(12)	0.021(8)	0.003(11)	-0.026(10)
C44C	0.20(2)	0.081(16)	0.052(11)	0.029(10)	0.007(14)	-0.024(17)
C45C	0.034(5)	0.032(5)	0.038(5)	-0.002(4)	0.008(4)	-0.003(4)
C46C	0.036(5)	0.024(4)	0.038(5)	0.001(4)	0.003(4)	0.003(4)
C47C	0.034(5)	0.030(5)	0.039(5)	-0.001(4)	0.007(4)	0.001(4)
C48C	0.033(5)	0.035(5)	0.031(4)	-0.001(4)	0.008(4)	0.008(4)
C49C	0.031(5)	0.033(5)	0.039(5)	-0.007(4)	0.003(4)	-0.003(4)
C50C	0.034(5)	0.033(5)	0.034(4)	-0.003(4)	0.009(4)	0.001(4)
C51C	0.058(7)	0.034(5)	0.030(5)	0.001(4)	0.008(5)	0.012(5)
C52C	0.076(8)	0.027(5)	0.050(7)	-0.002(5)	0.016(6)	0.007(6)
C53C	0.085(10)	0.042(7)	0.043(6)	-0.004(5)	0.007(6)	0.020(7)

C54C	0.060(7)	0.075(10)	0.047(7)	0.008(7)	-0.001(6)	0.028(7)
C55C	0.047(6)	0.039(6)	0.038(5)	0.004(5)	0.012(5)	0.010(5)
C56C	0.100(11)	0.065(9)	0.042(6)	0.012(6)	0.010(7)	0.019(8)
C57C	0.058(7)	0.053(7)	0.060(8)	0.019(6)	0.010(6)	0.015(6)
C58C	0.063(7)	0.048(7)	0.058(8)	0.006(6)	-0.008(6)	0.009(6)
S1C	0.0381(14)	0.0315(14)	0.0466(15)	-0.0081(12)	0.0007(12)	-0.0037(12)
S2C	0.0310(14)	0.0550(19)	0.0464(16)	-0.0050(14)	0.0097(12)	-0.0081(13)
N1D	0.040(4)	0.020(4)	0.025(4)	0.000(3)	0.008(3)	-0.001(3)
N2D	0.049(5)	0.010(3)	0.027(4)	-0.003(3)	-0.005(3)	-0.004(3)
N3D	0.027(4)	0.022(4)	0.032(4)	0.003(3)	0.003(3)	-0.004(3)
N4D	0.029(4)	0.030(4)	0.038(4)	0.006(4)	0.006(3)	0.001(4)
N5D	0.037(5)	0.052(6)	0.057(6)	-0.002(5)	0.004(4)	0.007(5)
N6D	0.053(6)	0.039(6)	0.069(7)	-0.004(5)	0.015(5)	-0.005(5)
C1D	0.044(5)	0.016(4)	0.025(4)	0.004(3)	0.011(3)	0.002(4)
C2D	0.051(5)	0.031(5)	0.029(5)	-0.001(4)	0.012(4)	0.001(5)
C3D	0.064(6)	0.022(5)	0.028(4)	-0.005(4)	0.005(4)	0.002(5)
C4D	0.056(5)	0.021(4)	0.029(4)	0.005(4)	-0.004(4)	0.002(4)
C5D	0.050(5)	0.020(4)	0.032(4)	0.001(4)	-0.007(4)	-0.001(4)
C6D	0.052(5)	0.024(5)	0.031(4)	0.006(4)	-0.011(4)	0.004(4)
C7D	0.043(5)	0.030(5)	0.043(5)	-0.005(4)	-0.016(4)	0.002(5)
C8D	0.049(5)	0.026(5)	0.045(5)	0.004(4)	-0.009(5)	-0.006(5)
C9D	0.039(5)	0.022(4)	0.036(4)	0.009(4)	-0.008(4)	0.001(4)
C10D	0.038(4)	0.008(4)	0.042(4)	0.004(4)	-0.003(4)	-0.009(4)
C11D	0.028(4)	0.027(5)	0.039(4)	0.008(4)	0.007(4)	-0.011(4)
C12D	0.037(5)	0.048(6)	0.050(6)	0.008(5)	0.004(4)	-0.018(5)
C13D	0.042(5)	0.033(5)	0.039(5)	0.010(4)	0.004(4)	-0.013(5)
C14D	0.040(4)	0.029(5)	0.036(5)	-0.002(4)	0.002(4)	-0.007(4)
C15D	0.038(4)	0.028(5)	0.039(5)	0.003(4)	0.003(4)	0.000(4)
C16D	0.042(5)	0.036(5)	0.033(5)	0.006(4)	0.001(4)	0.000(4)
C17D	0.048(6)	0.064(7)	0.037(5)	0.020(5)	0.005(5)	0.015(6)
C18D	0.040(5)	0.074(8)	0.025(5)	0.011(5)	-0.001(4)	0.013(5)
C19D	0.036(5)	0.050(6)	0.024(4)	0.005(4)	0.001(4)	-0.007(5)
C20D	0.033(4)	0.030(5)	0.021(4)	0.001(4)	0.012(3)	0.005(4)
C21D	0.028(4)	0.028(5)	0.041(5)	-0.001(4)	0.007(4)	0.006(4)
C22D	0.032(5)	0.016(4)	0.062(6)	0.002(4)	-0.001(4)	0.012(4)
C23D	0.028(5)	0.039(5)	0.051(6)	0.002(5)	-0.004(4)	0.010(4)
C24D	0.033(6)	0.055(7)	0.089(8)	-0.015(6)	-0.013(5)	0.017(5)
C25D	0.033(6)	0.040(6)	0.097(8)	-0.007(6)	-0.024(6)	0.009(5)
C26D	0.035(6)	0.030(6)	0.108(9)	0.001(6)	-0.010(6)	0.009(5)
C27D	0.034(5)	0.031(5)	0.076(7)	0.018(5)	-0.001(5)	0.005(5)
C28D	0.027(4)	0.031(5)	0.048(5)	0.007(4)	0.001(4)	-0.012(4)
C29D	0.033(5)	0.035(6)	0.041(5)	-0.001(5)	-0.004(4)	0.003(5)
C30D	0.046(6)	0.025(5)	0.046(5)	-0.001(5)	0.003(5)	0.000(5)
C31D	0.059(6)	0.037(5)	0.025(4)	-0.009(4)	-0.009(4)	-0.001(5)
C32D	0.059(7)	0.048(6)	0.030(5)	-0.001(4)	-0.007(5)	-0.017(6)
C33D	0.077(8)	0.059(6)	0.033(5)	-0.001(5)	-0.006(5)	-0.008(6)
C34D	0.090(9)	0.064(7)	0.023(5)	-0.012(5)	0.004(5)	-0.001(7)
C35D	0.087(8)	0.045(6)	0.041(6)	-0.018(5)	-0.006(6)	-0.001(6)
C36D	0.070(7)	0.042(6)	0.030(5)	-0.004(4)	-0.002(5)	-0.005(6)

C37D	0.099(10)	0.075(8)	0.034(6)	0.017(6)	-0.001(6)	-0.016(8)
C38D	0.131(14)	0.060(9)	0.073(10)	0.022(7)	0.017(9)	-0.011(10)
C39D	0.125(14)	0.095(13)	0.061(9)	0.020(8)	0.009(9)	0.004(12)
C40D	0.135(12)	0.078(11)	0.035(7)	0.025(7)	0.005(7)	0.009(9)
C41D	0.124(11)	0.058(7)	0.040(6)	-0.023(6)	-0.006(7)	-0.001(8)
C42D	0.120(12)	0.075(12)	0.129(16)	0.001(11)	-0.038(11)	-0.040(10)
C43D	0.147(16)	0.052(8)	0.077(10)	-0.020(7)	-0.025(10)	-0.004(10)
C44D	0.22(2)	0.105(15)	0.064(9)	-0.055(9)	0.017(13)	-0.039(16)
C45D	0.036(5)	0.027(5)	0.038(5)	0.002(4)	0.001(4)	-0.010(4)
C46D	0.048(6)	0.031(5)	0.032(5)	-0.002(4)	0.005(4)	0.004(5)
C47D	0.047(6)	0.036(5)	0.037(5)	0.005(4)	-0.002(4)	0.008(4)
C48D	0.056(6)	0.038(5)	0.034(5)	0.008(4)	0.003(5)	0.012(5)
C49D	0.053(6)	0.036(5)	0.034(5)	0.000(4)	0.000(4)	0.011(5)
C50D	0.044(6)	0.029(5)	0.041(5)	0.004(4)	0.005(4)	0.004(4)
C51D	0.072(7)	0.039(6)	0.040(6)	0.004(5)	0.001(5)	0.023(6)
C52D	0.09(2)	0.042(18)	0.067(16)	-0.007(15)	-0.003(16)	0.012(19)
C53D	0.087(19)	0.025(15)	0.073(19)	0.011(16)	0.002(18)	0.030(16)
C54D	0.074(14)	0.038(19)	0.060(19)	-0.009(17)	0.002(15)	0.039(13)
C55D	0.087(8)	0.046(6)	0.041(6)	-0.004(5)	-0.005(6)	0.030(6)
C56D	0.156(16)	0.073(11)	0.045(7)	-0.021(7)	-0.015(9)	0.056(11)
C57D	0.099(12)	0.064(9)	0.051(8)	-0.033(7)	-0.010(8)	0.023(8)
C58D	0.098(10)	0.057(10)	0.057(9)	-0.007(8)	0.026(8)	0.032(8)
S1D	0.0371(14)	0.0303(14)	0.0427(15)	0.0038(12)	0.0045(11)	-0.0029(11)
S2D	0.0405(16)	0.0566(19)	0.0428(16)	-0.0071(14)	-0.0011(12)	-0.0044(14)
C38W	0.096(15)	0.09(2)	0.09(2)	0.02(2)	0.043(18)	0.050(15)
C39W	0.10(2)	0.062(13)	0.07(2)	-0.004(18)	0.04(2)	0.055(18)
C40W	0.12(2)	0.10(2)	0.067(15)	0.004(17)	0.046(16)	0.05(2)
C42W	0.131(19)	0.091(15)	0.070(11)	0.050(10)	0.011(12)	0.009(15)
C43W	0.138(17)	0.059(11)	0.115(16)	0.046(11)	-0.015(16)	-0.011(13)
C44W	0.083(12)	0.101(17)	0.093(15)	0.042(14)	-0.009(11)	0.033(11)
C38X	0.10(2)	0.056(12)	0.057(19)	-0.022(16)	-0.01(2)	-0.007(17)
C39X	0.08(2)	0.09(2)	0.061(14)	-0.004(14)	-0.018(15)	-0.01(2)
C40X	0.078(14)	0.07(2)	0.06(2)	0.00(2)	-0.023(16)	-0.018(13)
C42X	0.104(18)	0.052(18)	0.083(18)	0.030(14)	-0.019(16)	-0.027(16)
C43X	0.10(2)	0.063(13)	0.079(18)	0.023(15)	-0.022(16)	-0.021(16)
C44X	0.091(17)	0.09(2)	0.10(2)	0.027(17)	0.023(15)	-0.035(17)
C42Y	0.118(17)	0.08(2)	0.08(2)	0.00(2)	0.033(17)	-0.043(14)
C43Y	0.15(2)	0.053(12)	0.069(19)	0.027(16)	0.012(19)	-0.017(17)
C44Y	0.16(2)	0.074(19)	0.060(14)	0.026(13)	0.034(15)	-0.038(19)
C52Z	0.091(11)	0.034(7)	0.081(11)	0.010(8)	-0.014(9)	0.002(8)
C53Z	0.124(15)	0.044(9)	0.051(8)	0.006(7)	-0.007(8)	0.046(10)
C54Z	0.061(9)	0.054(10)	0.088(11)	-0.007(9)	0.006(8)	0.021(7)
C56Z	0.11(2)	0.07(2)	0.047(17)	-0.023(17)	-0.012(18)	0.032(19)
C57Z	0.10(2)	0.053(14)	0.05(2)	-0.016(16)	0.003(19)	0.027(17)
C58Z	0.106(18)	0.06(2)	0.03(2)	-0.015(19)	0.014(14)	0.035(18)

Table S12. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for **H₂8b**.

	x	y	z	U
H1NA	0.642329	0.063538	0.250238	0.032
H3NA	0.606703	−0.005114	0.206196	0.043
H2A	0.722870	0.189829	0.297433	0.042
H3A	0.676286	0.149110	0.338073	0.039
H7A	0.557327	−0.063927	0.331224	0.048
H8A	0.529881	−0.161070	0.286705	0.048
H12A	0.527522	−0.141649	0.160514	0.050
H13A	0.549563	−0.021309	0.122280	0.048
H17A	0.655076	0.232982	0.132480	0.042
H18A	0.706259	0.250601	0.172718	0.040
H24A	0.830334	0.103967	0.160584	0.061
H25A	0.887001	0.068389	0.183885	0.075
H26A	0.894439	0.050709	0.240579	0.069
H27A	0.846195	0.074536	0.274224	0.061
H32A	0.589616	0.166246	0.349798	0.049
H34A	0.596857	0.039570	0.436999	0.064
H36A	0.634868	−0.083400	0.357832	0.047
H38A	0.539858	0.306453	0.400164	0.125
H38B	0.572819	0.288508	0.376486	0.125
H38C	0.536824	0.228235	0.372886	0.125
H39A	0.579992	0.288868	0.448301	0.164
H39B	0.603452	0.198178	0.453882	0.164
H39C	0.613943	0.269168	0.425963	0.164
H40A	0.525079	0.198058	0.443157	0.157
H40B	0.521877	0.116109	0.417349	0.157
H40C	0.548426	0.107258	0.448910	0.157
H42A	0.642109	−0.040709	0.464227	0.148
H42B	0.662696	−0.136683	0.464083	0.148
H42C	0.677493	−0.053280	0.443065	0.148
H43A	0.584801	−0.118378	0.447692	0.143
H43B	0.582855	−0.181086	0.415605	0.143
H43C	0.605507	−0.214185	0.447470	0.143
H44A	0.637669	−0.199331	0.381905	0.145
H44B	0.674734	−0.150016	0.392831	0.145
H44C	0.659937	−0.233419	0.413849	0.145
H46A	0.603049	0.020918	0.088597	0.045
H48A	0.559655	0.233844	0.038681	0.052
H50A	0.581033	0.255073	0.135996	0.046
H52A	0.585242	−0.061474	0.045746	0.068
H52B	0.598256	−0.058967	0.008732	0.068
H52C	0.624473	−0.022644	0.037818	0.068
H53A	0.534022	0.121789	0.009441	0.079
H53B	0.544135	0.029604	−0.009141	0.079
H53C	0.529822	0.025599	0.027429	0.079
H54A	0.595194	0.182187	−0.001823	0.073
H54B	0.630541	0.125257	0.008924	0.073

H54C	0.604324	0.088933	-0.020162	0.073
H56A	0.541694	0.364263	0.037687	0.114
H56B	0.507029	0.339800	0.058514	0.114
H56C	0.521600	0.442473	0.057528	0.114
H57A	0.601094	0.412654	0.105573	0.098
H57B	0.598360	0.414142	0.066375	0.098
H57C	0.576408	0.487262	0.087014	0.098
H58A	0.548100	0.368973	0.137291	0.107
H58B	0.525332	0.445447	0.117749	0.107
H58C	0.510762	0.342774	0.118735	0.107
H1NB	0.140817	-0.073590	0.242872	0.035
H3NB	0.102128	-0.016868	0.284655	0.040
H2B	0.221722	-0.195995	0.199130	0.042
H3B	0.176179	-0.148106	0.156194	0.038
H7B	0.055160	0.057525	0.158181	0.042
H8B	0.027361	0.147643	0.202143	0.045
H12B	0.023734	0.116927	0.327737	0.049
H13B	0.043027	-0.015066	0.364066	0.052
H17B	0.156763	-0.243036	0.361267	0.046
H18B	0.208122	-0.257001	0.324388	0.038
H24B	0.330371	-0.110599	0.343794	0.077
H25B	0.385712	-0.067904	0.322271	0.088
H26B	0.393488	-0.066227	0.266843	0.089
H27B	0.345289	-0.081978	0.229974	0.073
H32B	0.093088	-0.177508	0.138743	0.050
H34B	0.101395	-0.046382	0.052944	0.055
H36B	0.131972	0.078374	0.135989	0.050
H38D	0.050161	-0.326687	0.085196	0.097
H38E	0.082959	-0.302665	0.110231	0.097
H38F	0.044813	-0.252276	0.113304	0.097
H39D	0.086813	-0.296587	0.039251	0.140
H39E	0.106600	-0.200620	0.034598	0.140
H39F	0.120989	-0.269970	0.062322	0.140
H40D	0.027931	-0.217826	0.044960	0.119
H40E	0.023518	-0.141486	0.072557	0.119
H40F	0.046679	-0.120277	0.040970	0.119
H42D	0.093160	0.097636	0.033301	0.126
H42E	0.126280	0.163045	0.024956	0.126
H42F	0.132245	0.055130	0.027161	0.126
H43D	0.115427	0.204200	0.109979	0.138
H43E	0.116713	0.253825	0.075122	0.138
H43F	0.083043	0.190295	0.083513	0.138
H44D	0.174614	0.135939	0.102212	0.140
H44E	0.182797	0.078891	0.069857	0.140
H44F	0.176832	0.186806	0.067652	0.140
H46B	0.106225	-0.045080	0.401576	0.053
H48B	0.066084	-0.257003	0.450891	0.048
H50B	0.074918	-0.274607	0.353214	0.041
H52D	0.128178	0.006733	0.446820	0.096
H52E	0.086987	0.040477	0.446093	0.096

H52F	0.109630	0.036120	0.480115	0.096
H53D	0.039566	-0.056151	0.468675	0.118
H53E	0.050007	-0.149240	0.487101	0.118
H53F	0.062323	-0.053589	0.502660	0.118
H54D	0.144618	-0.142216	0.471841	0.097
H54E	0.126759	-0.106452	0.504662	0.097
H54F	0.114443	-0.202103	0.489103	0.097
H56D	0.014394	-0.449088	0.428537	0.095
H56E	0.033132	-0.369818	0.449994	0.095
H56F	0.003879	-0.344832	0.421686	0.095
H57D	0.074446	-0.507333	0.414846	0.088
H57E	0.103341	-0.442514	0.398037	0.088
H57F	0.093812	-0.427645	0.435635	0.088
H58D	0.028939	-0.471840	0.371421	0.084
H58E	0.018890	-0.368274	0.362810	0.084
H58F	0.057684	-0.408083	0.353921	0.084
H1NC	0.319019	0.139257	0.274952	0.038
H3NC	0.275951	0.105016	0.228579	0.033
H2C	0.407138	0.160466	0.331558	0.045
H3C	0.355436	0.123202	0.366834	0.046
H7C	0.214953	0.060759	0.346208	0.041
H8C	0.172803	0.072028	0.298072	0.040
H12C	0.187799	0.069934	0.172209	0.041
H13C	0.241202	0.020985	0.140474	0.038
H17C	0.383385	0.024124	0.163717	0.046
H18C	0.422585	0.100016	0.205346	0.052
H24C	0.496113	0.381302	0.202824	0.065
H25C	0.531722	0.486728	0.232094	0.060
H26C	0.535626	0.485665	0.288811	0.061
H27C	0.493281	0.400242	0.316770	0.061
H32C	0.293162	0.229182	0.381761	0.044
H34C	0.260893	0.072265	0.457083	0.063
H36C	0.268424	-0.037518	0.367235	0.054
H38G	0.299381	0.377336	0.447658	0.063
H38H	0.322701	0.313825	0.424427	0.063
H38I	0.283091	0.346437	0.412612	0.063
H39G	0.306938	0.271683	0.491887	0.078
H39H	0.295163	0.167074	0.488320	0.078
H39I	0.329997	0.203703	0.470070	0.078
H40G	0.245090	0.319011	0.473027	0.083
H40H	0.228822	0.284126	0.438466	0.083
H40I	0.233102	0.214786	0.468606	0.083
H42G	0.207501	-0.030174	0.451066	0.146
H42H	0.196692	-0.063550	0.414743	0.146
H42I	0.201551	-0.136388	0.443733	0.146
H43G	0.282397	-0.167250	0.398171	0.099
H43H	0.248035	-0.221955	0.410744	0.099
H43I	0.243176	-0.149117	0.381754	0.099
H44G	0.297932	-0.121978	0.452331	0.165
H44H	0.270123	-0.069991	0.475095	0.165

H44I	0.263779	-0.175097	0.466107	0.165
H46C	0.332831	-0.124888	0.158956	0.040
H48C	0.332981	-0.099876	0.060636	0.040
H50C	0.296955	0.107947	0.115093	0.040
H52G	0.323012	-0.273548	0.145011	0.061
H52H	0.305841	-0.292713	0.109201	0.061
H52I	0.339778	-0.351180	0.122493	0.061
H53G	0.378972	-0.202829	0.063774	0.068
H53H	0.373910	-0.308034	0.072952	0.068
H53I	0.339973	-0.249567	0.059660	0.068
H54G	0.384756	-0.203504	0.151043	0.073
H54H	0.400429	-0.281555	0.128050	0.073
H54I	0.406344	-0.176509	0.119077	0.073
H56G	0.340920	0.015635	0.021460	0.083
H56H	0.303244	-0.038063	0.019005	0.083
H56I	0.307048	0.059329	0.001780	0.083
H57G	0.347313	0.154578	0.055402	0.068
H57H	0.313876	0.199223	0.035387	0.068
H57I	0.313478	0.193557	0.074523	0.068
H58G	0.253715	0.108779	0.070904	0.068
H58H	0.254167	0.115860	0.031799	0.068
H58I	0.250363	0.018468	0.049023	0.068
H1ND	0.678451	0.356815	0.271806	0.034
H3ND	0.720743	0.383049	0.227792	0.032
H2D	0.588360	0.330002	0.321374	0.044
H3D	0.638602	0.371239	0.360682	0.046
H7D	0.781284	0.427278	0.350388	0.047
H8D	0.823176	0.416635	0.304394	0.048
H12D	0.809140	0.430088	0.178242	0.054
H13D	0.755219	0.476173	0.142950	0.046
H17D	0.612678	0.462789	0.156941	0.060
H18D	0.573905	0.388653	0.196562	0.056
H24D	0.515188	0.077343	0.187235	0.071
H25D	0.472150	-0.014543	0.211483	0.069
H26D	0.465224	-0.006946	0.267622	0.069
H27D	0.499411	0.090991	0.299714	0.057
H32D	0.702385	0.264591	0.380074	0.055
H34D	0.737524	0.416676	0.456709	0.071
H36D	0.727893	0.529661	0.367579	0.057
H38J	0.696221	0.114716	0.444179	0.106
H38K	0.672454	0.180663	0.420867	0.106
H38L	0.711742	0.148697	0.410113	0.106
H39J	0.687720	0.224180	0.489076	0.112
H39K	0.699946	0.328188	0.485201	0.112
H39L	0.665388	0.290634	0.464820	0.112
H40J	0.750202	0.171570	0.473873	0.099
H40K	0.767084	0.208513	0.440774	0.099
H40L	0.761990	0.276185	0.471034	0.099
H42J	0.795889	0.513460	0.446226	0.131
H42K	0.800500	0.548315	0.409443	0.131

H42L	0.802482	0.619400	0.439184	0.131
H43J	0.754249	0.640790	0.382185	0.111
H43K	0.718005	0.668164	0.400249	0.111
H43L	0.755926	0.711811	0.411954	0.111
H44J	0.739206	0.546799	0.475482	0.156
H44K	0.746538	0.653216	0.470145	0.156
H44L	0.708617	0.609570	0.458439	0.156
H46D	0.663695	0.616609	0.154065	0.044
H48D	0.665399	0.588706	0.056204	0.051
H50D	0.699367	0.380849	0.113717	0.045
H52J	0.629322	0.718978	0.149164	0.101
H52K	0.668413	0.762349	0.143752	0.101
H52L	0.632724	0.817477	0.132684	0.101
H53J	0.667031	0.741308	0.056485	0.092
H53K	0.655782	0.831087	0.075982	0.092
H53L	0.691471	0.775959	0.087051	0.092
H54J	0.591528	0.667811	0.102126	0.085
H54K	0.595089	0.766099	0.085517	0.085
H54L	0.605789	0.676518	0.065643	0.085
H56J	0.695827	0.526739	0.017525	0.137
H56K	0.691375	0.429835	-0.000157	0.137
H56L	0.657748	0.474825	0.017588	0.137
H57J	0.650992	0.335084	0.051426	0.107
H57K	0.684143	0.290564	0.032844	0.107
H57L	0.685023	0.295468	0.072024	0.107
H58J	0.747321	0.471740	0.050157	0.106
H58K	0.744782	0.380106	0.071239	0.106
H58L	0.743902	0.375202	0.032059	0.106
H38M	0.516932	0.241416	0.411268	0.140
H38N	0.529574	0.205643	0.376400	0.140
H38O	0.518610	0.134291	0.404039	0.140
H39M	0.572641	0.331569	0.417874	0.119
H39N	0.611487	0.284338	0.415379	0.119
H39O	0.586128	0.296562	0.383187	0.119
H40M	0.555672	0.223706	0.460302	0.145
H40N	0.558264	0.116066	0.454419	0.145
H40O	0.594415	0.175519	0.458622	0.145
H42M	0.639440	-0.045329	0.465181	0.146
H42N	0.600240	-0.091015	0.461115	0.146
H42O	0.634831	-0.152963	0.469923	0.146
H43M	0.616328	-0.204955	0.385145	0.157
H43N	0.620492	-0.251802	0.420466	0.157
H43O	0.585900	-0.189854	0.411658	0.157
H44M	0.676625	-0.137478	0.392761	0.139
H44N	0.686177	-0.074305	0.423801	0.139
H44O	0.681147	-0.181840	0.428470	0.139
H38P	0.079148	-0.344440	0.074374	0.105
H38Q	0.117072	-0.294418	0.081432	0.105
H38R	0.088200	-0.301550	0.109732	0.105
H39P	0.067941	-0.245684	0.026520	0.118

H39Q	0.069849	-0.137094	0.029958	0.118
H39R	0.106022	-0.196611	0.033776	0.118
H40P	0.022851	-0.255843	0.069004	0.106
H40Q	0.030340	-0.212126	0.104487	0.106
H40R	0.023148	-0.147427	0.073397	0.106
H42P	0.094336	0.090769	0.032526	0.120
H42Q	0.076499	0.154686	0.059389	0.120
H42R	0.105904	0.195656	0.035479	0.120
H43P	0.113607	0.206939	0.108019	0.123
H43Q	0.155310	0.178294	0.111740	0.123
H43R	0.142507	0.248840	0.083810	0.123
H44P	0.158510	0.044967	0.038693	0.142
H44Q	0.169938	0.149980	0.041488	0.142
H44R	0.182742	0.079434	0.069418	0.142
H42S	0.195934	-0.046851	0.420086	0.140
H42T	0.211466	-0.097228	0.388718	0.140
H42U	0.200213	-0.155419	0.419960	0.140
H43S	0.272890	-0.164918	0.391640	0.134
H43T	0.296119	-0.164924	0.425384	0.134
H43U	0.260010	-0.224802	0.421903	0.134
H44S	0.231416	-0.031554	0.469857	0.145
H44T	0.233765	-0.140417	0.471428	0.145
H44U	0.269873	-0.080539	0.474909	0.145
H52M	0.674536	0.762024	0.140566	0.104
H52N	0.693842	0.777775	0.106476	0.104
H52O	0.660564	0.840949	0.116241	0.104
H53M	0.661516	0.737702	0.054300	0.110
H53N	0.621728	0.694800	0.054796	0.110
H53O	0.627906	0.799821	0.064004	0.110
H54M	0.613495	0.696545	0.141623	0.101
H54N	0.598484	0.774651	0.117437	0.101
H54O	0.592306	0.669629	0.108229	0.101
H56M	0.659863	0.479755	0.017298	0.114
H56N	0.672745	0.380939	0.005818	0.114
H56O	0.643547	0.390325	0.033758	0.114
H57M	0.723811	0.324668	0.078802	0.101
H57N	0.682662	0.295367	0.071381	0.101
H57O	0.711859	0.285981	0.043442	0.101
H58M	0.749003	0.460976	0.053159	0.098
H58N	0.737062	0.423056	0.017688	0.098
H58O	0.724501	0.522427	0.028855	0.098

Table S13. Crystal data and structure refinement for **H₂9**.

Identification code	oxdp22	
CCDC deposition number	1822192	
Chemical formula (moiety)	C ₅₄ H ₅₂ N ₈	
Chemical formula (total)	C ₅₄ H ₅₂ N ₈	
Formula weight	813.03	
Temperature	150(2) K	
Radiation, wavelength	synchrotron, 0.6893 Å	
Crystal system, space group	monoclinic, I2/a	
Unit cell parameters	a = 34.85(3) Å	α = 90°
	b = 13.785(11) Å	β = 92.378(10)°
	c = 40.21(3) Å	γ = 90°
Cell volume	19302(26) Å ³	
Z	16	
Calculated density	1.119 g/cm ³	
Absorption coefficient μ	0.063 mm ⁻¹	
F(000)	6912	
Crystal color and size	black, 0.220 × 0.220 × 0.030 mm ³	
Reflections for cell refinement	5490 (θ range 2.3 to 22.1°)	
Data collection method	Bruker SMART 1K CCD diffractometer	
	thin-slice ω scans	
θ range for data collection	2.3 to 23.7°	
Index ranges	h -38 to 40, k -15 to 13, l -45 to 40	
Completeness to θ = 23.7°	89.3 %	
Reflections collected	33400	
Independent reflections	14281 (R _{int} = 0.1012)	
Reflections with F ² > 2σ	8224	
Absorption correction	none	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F ²	
Weighting parameters a, b	0.1111, 309.8881	
Data / restraints / parameters	14281 / 3291 / 1202	
Final R indices [F ² > 2σ]	R1 = 0.1812, wR2 = 0.3842	
R indices (all data)	R1 = 0.2429, wR2 = 0.4153	
Goodness-of-fit on F ²	1.142	
Extinction coefficient	0.00044(9)	
Largest and mean shift/su	0.002 and 0.000	
Largest diff. peak and hole	1.23 and -0.44 e Å ⁻³	

Table S14. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$) for **H₂9**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
N1A	0.6690(2)	0.2113(5)	0.79707(18)	0.0351(18)
N2A	0.6170(2)	0.3692(5)	0.79202(19)	0.0391(19)
N3A	0.6301(2)	0.4060(5)	0.72319(19)	0.0368(18)
N4A	0.6818(2)	0.2488(5)	0.72663(18)	0.0327(17)
N5A	0.6874(3)	−0.1419(6)	0.7886(3)	0.062(3)
N6A	0.7152(3)	−0.0600(6)	0.6907(2)	0.058(3)
N7A	0.4851(3)	0.4718(7)	0.7965(3)	0.068(3)
N8A	0.4953(2)	0.4719(6)	0.6924(3)	0.055(3)
C1A	0.6864(3)	0.1252(6)	0.7902(2)	0.035(2)
C2A	0.6950(3)	0.0831(7)	0.8219(2)	0.044(2)
C3A	0.6819(3)	0.1449(6)	0.8459(2)	0.038(2)
C4A	0.6651(3)	0.2240(6)	0.8304(2)	0.036(2)
C5A	0.6458(3)	0.3056(6)	0.8444(2)	0.038(2)
C6A	0.6235(3)	0.3723(6)	0.8269(2)	0.037(2)
C7A	0.6000(3)	0.4477(6)	0.8408(3)	0.042(2)
C8A	0.5786(3)	0.4845(7)	0.8159(2)	0.042(2)
C9A	0.5893(3)	0.4346(6)	0.7863(2)	0.039(2)
C10A	0.5716(3)	0.4502(6)	0.7526(2)	0.037(2)
C11A	0.5965(2)	0.4528(6)	0.7249(2)	0.034(2)
C12A	0.5918(3)	0.5050(7)	0.6947(2)	0.042(2)
C13A	0.6236(3)	0.4878(6)	0.6765(2)	0.041(2)
C14A	0.6478(3)	0.4243(6)	0.6942(2)	0.034(2)
C15A	0.6819(3)	0.3778(6)	0.6838(2)	0.036(2)
C16A	0.6988(3)	0.2967(6)	0.6996(2)	0.035(2)
C17A	0.7327(3)	0.2475(6)	0.6901(2)	0.035(2)
C18A	0.7364(3)	0.1691(6)	0.7103(2)	0.040(2)
C19A	0.7044(3)	0.1720(6)	0.7322(2)	0.035(2)
C20A	0.6971(3)	0.0988(6)	0.7576(2)	0.037(2)
C21A	0.7005(3)	0.0017(6)	0.7489(2)	0.042(2)
C22A	0.6933(3)	−0.0773(6)	0.7717(3)	0.043(2)
C23A	0.7089(3)	−0.0310(7)	0.7168(3)	0.046(3)
C24A	0.5332(2)	0.4637(6)	0.7487(3)	0.042(2)
C25A	0.5072(3)	0.4669(7)	0.7766(3)	0.043(2)
C26A	0.5129(3)	0.4687(7)	0.7168(3)	0.040(2)
C27A	0.6483(3)	0.3147(7)	0.8815(2)	0.041(2)
C28A	0.6275(3)	0.2519(7)	0.9023(2)	0.046(2)
C29A	0.6256(4)	0.2677(8)	0.9358(3)	0.061(3)
C30A	0.6465(3)	0.3472(8)	0.9498(3)	0.061(3)
C31A	0.6673(3)	0.4096(8)	0.9301(3)	0.057(3)
C32A	0.6683(3)	0.3933(7)	0.8966(2)	0.046(2)
C33A	0.6012(4)	0.2036(9)	0.9576(3)	0.080(4)
C34A	0.5600(5)	0.201(2)	0.9444(8)	0.095(8)
C35A	0.6198(9)	0.1018(14)	0.9543(8)	0.103(8)
C36A	0.6047(11)	0.232(3)	0.9946(4)	0.116(9)
C37A	0.6881(3)	0.4994(8)	0.9458(2)	0.065(3)
C38A	0.7286(3)	0.5082(11)	0.9326(4)	0.092(5)

C39A	0.6913(5)	0.4936(11)	0.9838(3)	0.104(5)
C40A	0.6648(4)	0.5887(9)	0.9346(4)	0.098(5)
C41A	0.7000(3)	0.4196(6)	0.6542(2)	0.035(2)
C42A	0.7062(3)	0.3654(7)	0.6259(2)	0.046(2)
C43A	0.7227(3)	0.4062(7)	0.5977(3)	0.055(3)
C44A	0.7343(3)	0.5026(7)	0.6001(3)	0.052(3)
C45A	0.7289(3)	0.5598(6)	0.6281(2)	0.043(2)
C46A	0.7113(3)	0.5185(6)	0.6550(2)	0.040(2)
C47A	0.7286(3)	0.3491(8)	0.5656(3)	0.071(3)
C48A	0.7512(10)	0.2555(18)	0.5768(8)	0.079(8)
C49A	0.7537(10)	0.399(2)	0.5405(7)	0.086(9)
C50A	0.6901(7)	0.315(3)	0.5499(9)	0.091(9)
C51A	0.7419(3)	0.6673(6)	0.6273(2)	0.056(3)
C52A	0.7850(3)	0.6706(8)	0.6199(3)	0.066(3)
C53A	0.7189(4)	0.7197(9)	0.5990(3)	0.088(4)
C54A	0.7356(3)	0.7196(7)	0.6603(3)	0.062(3)
N1B	0.5933(2)	0.7317(5)	0.72324(19)	0.0392(19)
N2B	0.5129(2)	0.7173(5)	0.6994(2)	0.0404(19)
N3B	0.4881(2)	0.7069(5)	0.7664(2)	0.0394(19)
N4B	0.5695(2)	0.7144(6)	0.7887(2)	0.044(2)
N5B	0.7125(3)	0.5500(8)	0.7408(2)	0.064(3)
N6B	0.6862(3)	0.5765(7)	0.8409(3)	0.067(3)
N7B	0.4099(3)	0.5388(7)	0.6447(3)	0.074(3)
N8B	0.3887(3)	0.4815(7)	0.7464(3)	0.069(3)
C1B	0.6278(3)	0.7127(6)	0.7381(2)	0.036(2)
C2B	0.6555(3)	0.7350(7)	0.7144(2)	0.043(2)
C3B	0.6356(3)	0.7645(7)	0.6860(3)	0.048(2)
C4B	0.5972(3)	0.7625(7)	0.6916(2)	0.040(2)
C5B	0.5656(3)	0.7819(6)	0.6683(2)	0.043(2)
C6B	0.5277(3)	0.7597(6)	0.6711(2)	0.036(2)
C7B	0.4964(3)	0.7744(7)	0.6471(2)	0.042(2)
C8B	0.4643(3)	0.7398(7)	0.6594(2)	0.046(2)
C9B	0.4760(2)	0.7042(6)	0.6917(2)	0.035(2)
C10B	0.4505(3)	0.6599(7)	0.7160(2)	0.042(2)
C11B	0.4544(2)	0.6851(6)	0.7507(2)	0.036(2)
C12B	0.4260(3)	0.6943(7)	0.7747(2)	0.043(2)
C13B	0.4443(3)	0.7178(7)	0.8046(3)	0.048(2)
C14B	0.4831(3)	0.7256(7)	0.7997(2)	0.039(2)
C15B	0.5133(3)	0.7401(6)	0.8242(2)	0.042(2)
C16B	0.5523(3)	0.7393(7)	0.8192(2)	0.041(2)
C17B	0.5820(3)	0.7529(7)	0.8445(3)	0.047(2)
C18B	0.6158(3)	0.7392(7)	0.8305(3)	0.051(3)
C19B	0.6065(3)	0.7113(7)	0.7962(2)	0.044(2)
C20B	0.6340(3)	0.6818(6)	0.7716(2)	0.040(2)
C21B	0.6653(3)	0.6261(7)	0.7818(2)	0.043(2)
C22B	0.6913(3)	0.5861(8)	0.7582(3)	0.044(2)
C23B	0.6757(3)	0.5995(8)	0.8147(3)	0.050(3)
C24B	0.4238(3)	0.5919(7)	0.7054(3)	0.050(2)
C25B	0.4174(3)	0.5637(8)	0.6707(3)	0.054(3)
C26B	0.4029(3)	0.5334(8)	0.7279(3)	0.051(3)
C27B	0.5787(3)	0.8304(7)	0.6376(2)	0.046(2)

C28B	0.5767(3)	0.7881(8)	0.6055(2)	0.053(3)
C29B	0.5934(3)	0.8293(7)	0.5785(3)	0.056(3)
C30B	0.6122(3)	0.9201(7)	0.5833(3)	0.058(3)
C31B	0.6133(3)	0.9650(7)	0.6147(3)	0.054(3)
C32B	0.5969(3)	0.9213(7)	0.6413(3)	0.047(2)
C33B	0.5924(3)	0.7772(8)	0.5449(3)	0.072(3)
C34B	0.6137(4)	0.6800(8)	0.5491(3)	0.079(4)
C35B	0.5507(3)	0.7557(9)	0.5338(3)	0.081(4)
C36B	0.6113(5)	0.8343(10)	0.5179(3)	0.096(5)
C37B	0.6362(3)	1.0622(7)	0.6193(3)	0.058(3)
C38B	0.6362(4)	1.0975(8)	0.6555(3)	0.073(4)
C39B	0.6172(4)	1.1396(8)	0.5970(4)	0.090(5)
C40B	0.6774(3)	1.0428(9)	0.6100(4)	0.080(4)
C41B	0.5013(3)	0.7445(6)	0.8594(2)	0.045(2)
C42B	0.5068(3)	0.6617(7)	0.8789(2)	0.052(3)
C43B	0.4964(3)	0.6614(6)	0.9119(2)	0.050(3)
C44B	0.4823(3)	0.7468(6)	0.9251(2)	0.049(3)
C45B	0.4778(4)	0.8310(7)	0.9064(3)	0.061(3)
C46B	0.4869(3)	0.8294(7)	0.8733(3)	0.057(3)
C47B	0.5050(3)	0.5715(6)	0.9341(2)	0.055(3)
C48B	0.4993(4)	0.4797(7)	0.9130(3)	0.067(3)
C49B	0.4765(4)	0.5658(8)	0.9621(3)	0.079(4)
C50B	0.5462(3)	0.5746(10)	0.9482(4)	0.097(5)
C51B	0.4600(4)	0.9227(7)	0.9214(3)	0.078(4)
C52B	0.4173(4)	0.9042(14)	0.9262(8)	0.088(6)
C53B	0.4804(9)	0.9423(14)	0.9555(5)	0.089(6)
C54B	0.4648(9)	1.0123(10)	0.8992(5)	0.080(6)
C34X	0.5721(8)	0.143(2)	0.9370(6)	0.084(7)
C35X	0.6253(7)	0.140(2)	0.9814(7)	0.099(8)
C36X	0.5766(9)	0.2718(18)	0.9789(8)	0.099(8)
C48X	0.7070(7)	0.2530(13)	0.5648(6)	0.106(7)
C49X	0.7714(4)	0.3389(15)	0.5605(5)	0.075(5)
C50X	0.7103(6)	0.4112(14)	0.5365(4)	0.083(6)
C52Y	0.4178(12)	0.924(7)	0.909(3)	0.086(12)
C53Y	0.463(4)	0.925(7)	0.9596(5)	0.080(12)
C54Y	0.481(3)	1.012(5)	0.908(3)	0.087(12)

Table S15. Bond lengths [Å] and angles [°] for **H₂9**.

N1A–H1NA	0.880	N1A–C1A	1.367(10)
N1A–C4A	1.365(10)	N2A–C6A	1.410(11)
N2A–C9A	1.334(10)	N3A–H3NA	0.880
N3A–C11A	1.343(10)	N3A–C14A	1.366(10)
N4A–C16A	1.422(10)	N4A–C19A	1.333(10)
N5A–C22A	1.144(11)	N6A–C23A	1.152(11)
N7A–C25A	1.137(12)	N8A–C26A	1.138(11)
C1A–C2A	1.421(12)	C1A–C20A	1.424(11)
C2A–H2A	0.950	C2A–C3A	1.381(12)
C3A–H3A	0.950	C3A–C4A	1.375(11)
C4A–C5A	1.438(11)	C5A–C6A	1.378(11)
C5A–C27A	1.497(12)	C6A–C7A	1.452(12)
C7A–H7A	0.950	C7A–C8A	1.325(12)
C8A–H8A	0.950	C8A–C9A	1.437(12)
C9A–C10A	1.481(12)	C10A–C11A	1.439(11)
C10A–C24A	1.354(11)	C11A–C12A	1.416(12)
C12A–H12A	0.950	C12A–C13A	1.375(12)
C13A–H13A	0.950	C13A–C14A	1.389(11)
C14A–C15A	1.427(11)	C15A–C16A	1.403(11)
C15A–C41A	1.486(11)	C16A–C17A	1.430(11)
C17A–H17A	0.950	C17A–C18A	1.356(12)
C18A–H18A	0.950	C18A–C19A	1.447(12)
C19A–C20A	1.465(11)	C20A–C21A	1.391(11)
C21A–C22A	1.452(12)	C21A–C23A	1.407(13)
C24A–C25A	1.472(13)	C24A–C26A	1.438(13)
C27A–C28A	1.421(12)	C27A–C32A	1.411(12)
C28A–H28A	0.950	C28A–C29A	1.369(13)
C29A–C30A	1.420(13)	C29A–C33A	1.527(14)
C30A–H30A	0.950	C30A–C31A	1.396(13)
C31A–C32A	1.366(12)	C31A–C37A	1.556(13)
C32A–H32A	0.950	C33A–C34A	1.513(13)
C33A–C35A	1.553(13)	C33A–C36A	1.535(13)
C33A–C34X	1.534(13)	C33A–C35X	1.520(13)
C33A–C36X	1.555(13)	C34A–H34A	0.980
C34A–H34B	0.980	C34A–H34C	0.980
C35A–H35A	0.980	C35A–H35B	0.980
C35A–H35C	0.980	C36A–H36A	0.980
C36A–H36B	0.980	C36A–H36C	0.980
C37A–C38A	1.533(11)	C37A–C39A	1.527(11)
C37A–C40A	1.533(11)	C38A–H38A	0.980
C38A–H38B	0.980	C38A–H38C	0.980
C39A–H39A	0.980	C39A–H39B	0.980
C39A–H39C	0.980	C40A–H40A	0.980
C40A–H40B	0.980	C40A–H40C	0.980
C41A–C42A	1.387(12)	C41A–C46A	1.418(12)
C42A–H42A	0.950	C42A–C43A	1.409(12)
C43A–C44A	1.391(12)	C43A–C47A	1.534(12)
C44A–H44A	0.950	C44A–C45A	1.391(12)
C45A–C46A	1.390(12)	C45A–C51A	1.549(12)

C46A–H46A	0.950	C47A–C48A	1.569(13)
C47A–C49A	1.523(13)	C47A–C50A	1.533(13)
C47A–C48X	1.524(12)	C47A–C49X	1.519(12)
C47A–C50X	1.565(12)	C48A–H48A	0.980
C48A–H48B	0.980	C48A–H48C	0.980
C49A–H49A	0.980	C49A–H49B	0.980
C49A–H49C	0.980	C50A–H50A	0.980
C50A–H50B	0.980	C50A–H50C	0.980
C51A–C52A	1.543(11)	C51A–C53A	1.544(11)
C51A–C54A	1.534(10)	C52A–H52A	0.980
C52A–H52B	0.980	C52A–H52C	0.980
C53A–H53A	0.980	C53A–H53B	0.980
C53A–H53C	0.980	C54A–H54A	0.980
C54A–H54B	0.980	C54A–H54C	0.980
N1B–H1NB	0.880	N1B–C1B	1.348(10)
N1B–C4B	1.353(11)	N2B–C6B	1.396(11)
N2B–C9B	1.321(10)	N3B–H3NB	0.880
N3B–C11B	1.346(10)	N3B–C14B	1.382(11)
N4B–C16B	1.430(11)	N4B–C19B	1.311(11)
N5B–C22B	1.152(11)	N6B–C23B	1.145(11)
N7B–C25B	1.118(12)	N8B–C26B	1.158(12)
C1B–C2B	1.418(12)	C1B–C20B	1.419(12)
C2B–H2B	0.950	C2B–C3B	1.375(12)
C3B–H3B	0.950	C3B–C4B	1.367(12)
C4B–C5B	1.442(12)	C5B–C6B	1.365(12)
C5B–C27B	1.492(12)	C6B–C7B	1.442(12)
C7B–H7B	0.950	C7B–C8B	1.330(12)
C8B–H8B	0.950	C8B–C9B	1.435(12)
C9B–C10B	1.480(12)	C10B–C11B	1.438(12)
C10B–C24B	1.376(12)	C11B–C12B	1.414(12)
C12B–H12B	0.950	C12B–C13B	1.376(12)
C13B–H13B	0.950	C13B–C14B	1.378(12)
C14B–C15B	1.429(12)	C15B–C16B	1.382(12)
C15B–C41B	1.493(11)	C16B–C17B	1.432(12)
C17B–H17B	0.950	C17B–C18B	1.338(12)
C18B–H18B	0.950	C18B–C19B	1.453(12)
C19B–C20B	1.467(12)	C20B–C21B	1.381(12)
C21B–C22B	1.445(13)	C21B–C23B	1.409(13)
C24B–C25B	1.459(14)	C24B–C26B	1.432(13)
C27B–C28B	1.413(13)	C27B–C32B	1.410(12)
C28B–H28B	0.950	C28B–C29B	1.377(13)
C29B–C30B	1.421(13)	C29B–C33B	1.530(13)
C30B–H30B	0.950	C30B–C31B	1.406(13)
C31B–C32B	1.373(13)	C31B–C37B	1.567(12)
C32B–H32B	0.950	C33B–C34B	1.538(11)
C33B–C35B	1.532(11)	C33B–C36B	1.514(11)
C34B–H34D	0.980	C34B–H34E	0.980
C34B–H34F	0.980	C35B–H35D	0.980
C35B–H35E	0.980	C35B–H35F	0.980
C36B–H36D	0.980	C36B–H36E	0.980
C36B–H36F	0.980	C37B–C38B	1.533(11)

C37B–C39B	1.527(11)	C37B–C40B	1.522(11)
C38B–H38D	0.980	C38B–H38E	0.980
C38B–H38F	0.980	C39B–H39D	0.980
C39B–H39E	0.980	C39B–H39F	0.980
C40B–H40D	0.980	C40B–H40E	0.980
C40B–H40F	0.980	C41B–C42B	1.394(12)
C41B–C46B	1.398(12)	C42B–H42B	0.950
C42B–C43B	1.390(12)	C43B–C44B	1.388(12)
C43B–C47B	1.548(12)	C44B–H44B	0.950
C44B–C45B	1.388(12)	C45B–C46B	1.382(12)
C45B–C51B	1.542(12)	C46B–H46B	0.950
C47B–C48B	1.532(10)	C47B–C49B	1.534(11)
C47B–C50B	1.521(11)	C48B–H48D	0.980
C48B–H48E	0.980	C48B–H48F	0.980
C49B–H49D	0.980	C49B–H49E	0.980
C49B–H49F	0.980	C50B–H50D	0.980
C50B–H50E	0.980	C50B–H50F	0.980
C51B–C52B	1.533(12)	C51B–C53B	1.541(12)
C51B–C54B	1.537(11)	C51B–C52Y	1.531(15)
C51B–C53Y	1.535(15)	C51B–C54Y	1.536(15)
C52B–H52D	0.980	C52B–H52E	0.980
C52B–H52F	0.980	C53B–H53D	0.980
C53B–H53E	0.980	C53B–H53F	0.980
C54B–H54D	0.980	C54B–H54E	0.980
C54B–H54F	0.980	C34X–H34G	0.980
C34X–H34H	0.980	C34X–H34I	0.980
C35X–H35G	0.980	C35X–H35H	0.980
C35X–H35I	0.980	C36X–H36G	0.980
C36X–H36H	0.980	C36X–H36I	0.980
C48X–H48G	0.980	C48X–H48H	0.980
C48X–H48I	0.980	C49X–H49G	0.980
C49X–H49H	0.980	C49X–H49I	0.980
C50X–H50G	0.980	C50X–H50H	0.980
C50X–H50I	0.980	C52Y–H52G	0.980
C52Y–H52H	0.980	C52Y–H52I	0.980
C53Y–H53G	0.980	C53Y–H53H	0.980
C53Y–H53I	0.980	C54Y–H54G	0.980
C54Y–H54H	0.980	C54Y–H54I	0.980
H1NA–N1A–C1A	124.0	H1NA–N1A–C4A	124.0
C1A–N1A–C4A	112.0(7)	C6A–N2A–C9A	103.6(7)
H3NA–N3A–C11A	123.8	H3NA–N3A–C14A	123.8
C11A–N3A–C14A	112.4(8)	C16A–N4A–C19A	103.7(7)
N1A–C1A–C2A	104.5(8)	N1A–C1A–C20A	122.9(8)
C2A–C1A–C20A	131.9(8)	C1A–C2A–H2A	125.9
C1A–C2A–C3A	108.3(8)	H2A–C2A–C3A	125.9
C2A–C3A–H3A	125.7	C2A–C3A–C4A	108.5(8)
H3A–C3A–C4A	125.7	N1A–C4A–C3A	106.6(8)
N1A–C4A–C5A	123.5(8)	C3A–C4A–C5A	129.8(8)
C4A–C5A–C6A	125.8(8)	C4A–C5A–C27A	116.5(8)
C6A–C5A–C27A	117.7(8)	N2A–C6A–C5A	123.5(8)

N2A-C6A-C7A	109.6(7)	C5A-C6A-C7A	126.5(8)
C6A-C7A-H7A	126.5	C6A-C7A-C8A	107.0(8)
H7A-C7A-C8A	126.5	C7A-C8A-H8A	126.7
C7A-C8A-C9A	106.5(8)	H8A-C8A-C9A	126.7
N2A-C9A-C8A	113.1(8)	N2A-C9A-C10A	121.7(8)
C8A-C9A-C10A	125.2(8)	C9A-C10A-C11A	118.1(8)
C9A-C10A-C24A	119.9(9)	C11A-C10A-C24A	122.0(9)
N3A-C11A-C10A	125.7(8)	N3A-C11A-C12A	105.6(8)
C10A-C11A-C12A	128.7(8)	C11A-C12A-H12A	126.2
C11A-C12A-C13A	107.7(8)	H12A-C12A-C13A	126.2
C12A-C13A-H13A	125.6	C12A-C13A-C14A	108.7(8)
H13A-C13A-C14A	125.6	N3A-C14A-C13A	105.6(8)
N3A-C14A-C15A	125.2(8)	C13A-C14A-C15A	128.9(8)
C14A-C15A-C16A	124.4(8)	C14A-C15A-C41A	116.5(8)
C16A-C15A-C41A	119.1(8)	N4A-C16A-C15A	122.4(8)
N4A-C16A-C17A	111.0(7)	C15A-C16A-C17A	126.5(8)
C16A-C17A-H17A	127.0	C16A-C17A-C18A	106.0(8)
H17A-C17A-C18A	127.0	C17A-C18A-H18A	126.7
C17A-C18A-C19A	106.7(8)	H18A-C18A-C19A	126.7
N4A-C19A-C18A	112.6(8)	N4A-C19A-C20A	123.0(8)
C18A-C19A-C20A	124.4(8)	C1A-C20A-C19A	121.7(8)
C1A-C20A-C21A	120.4(8)	C19A-C20A-C21A	117.9(8)
C20A-C21A-C22A	122.9(9)	C20A-C21A-C23A	124.2(9)
C22A-C21A-C23A	112.8(8)	N5A-C22A-C21A	177.1(11)
N6A-C23A-C21A	178.1(12)	C10A-C24A-C25A	123.6(9)
C10A-C24A-C26A	123.9(9)	C25A-C24A-C26A	112.4(8)
N7A-C25A-C24A	175.1(11)	N8A-C26A-C24A	176.8(11)
C5A-C27A-C28A	121.6(8)	C5A-C27A-C32A	120.0(8)
C28A-C27A-C32A	118.0(9)	C27A-C28A-H28A	119.0
C27A-C28A-C29A	121.9(9)	H28A-C28A-C29A	119.0
C28A-C29A-C30A	117.9(10)	C28A-C29A-C33A	121.7(10)
C30A-C29A-C33A	120.4(10)	C29A-C30A-H30A	119.3
C29A-C30A-C31A	121.4(10)	H30A-C30A-C31A	119.3
C30A-C31A-C32A	119.6(10)	C30A-C31A-C37A	120.2(9)
C32A-C31A-C37A	120.1(9)	C27A-C32A-C31A	121.2(9)
C27A-C32A-H32A	119.4	C31A-C32A-H32A	119.4
C29A-C33A-C34A	110.9(13)	C29A-C33A-C35A	103.3(13)
C29A-C33A-C36A	112.7(14)	C29A-C33A-C34X	112.1(13)
C29A-C33A-C35X	112.9(14)	C29A-C33A-C36X	107.4(14)
C34A-C33A-C35A	109.8(15)	C34A-C33A-C36A	112.5(15)
C35A-C33A-C36A	107.2(14)	C34X-C33A-C35X	111.2(15)
C34X-C33A-C36X	105.1(14)	C35X-C33A-C36X	107.7(14)
C33A-C34A-H34A	109.5	C33A-C34A-H34B	109.5
C33A-C34A-H34C	109.5	H34A-C34A-H34B	109.5
H34A-C34A-H34C	109.5	H34B-C34A-H34C	109.5
C33A-C35A-H35A	109.5	C33A-C35A-H35B	109.5
C33A-C35A-H35C	109.5	H35A-C35A-H35B	109.5
H35A-C35A-H35C	109.5	H35B-C35A-H35C	109.5
C33A-C36A-H36A	109.5	C33A-C36A-H36B	109.5
C33A-C36A-H36C	109.5	H36A-C36A-H36B	109.5
H36A-C36A-H36C	109.5	H36B-C36A-H36C	109.5

C31A-C37A-C38A	109.9(9)	C31A-C37A-C39A	112.3(9)
C31A-C37A-C40A	106.7(9)	C38A-C37A-C39A	108.6(10)
C38A-C37A-C40A	108.6(10)	C39A-C37A-C40A	110.7(10)
C37A-C38A-H38A	109.5	C37A-C38A-H38B	109.5
C37A-C38A-H38C	109.5	H38A-C38A-H38B	109.5
H38A-C38A-H38C	109.5	H38B-C38A-H38C	109.5
C37A-C39A-H39A	109.5	C37A-C39A-H39B	109.5
C37A-C39A-H39C	109.5	H39A-C39A-H39B	109.5
H39A-C39A-H39C	109.5	H39B-C39A-H39C	109.5
C37A-C40A-H40A	109.5	C37A-C40A-H40B	109.5
C37A-C40A-H40C	109.5	H40A-C40A-H40B	109.5
H40A-C40A-H40C	109.5	H40B-C40A-H40C	109.5
C15A-C41A-C42A	122.3(8)	C15A-C41A-C46A	118.8(8)
C42A-C41A-C46A	118.9(8)	C41A-C42A-H42A	119.1
C41A-C42A-C43A	121.9(9)	H42A-C42A-C43A	119.1
C42A-C43A-C44A	116.9(9)	C42A-C43A-C47A	123.1(9)
C44A-C43A-C47A	120.0(9)	C43A-C44A-H44A	118.4
C43A-C44A-C45A	123.3(9)	H44A-C44A-C45A	118.4
C44A-C45A-C46A	118.4(8)	C44A-C45A-C51A	118.4(8)
C46A-C45A-C51A	123.1(8)	C41A-C46A-C45A	120.5(9)
C41A-C46A-H46A	119.7	C45A-C46A-H46A	119.7
C43A-C47A-C48A	105.3(13)	C43A-C47A-C49A	115.4(15)
C43A-C47A-C50A	111.1(15)	C43A-C47A-C48X	112.4(11)
C43A-C47A-C49X	109.2(11)	C43A-C47A-C50X	106.6(10)
C48A-C47A-C49A	105.2(15)	C48A-C47A-C50A	106.6(16)
C49A-C47A-C50A	112.5(16)	C48X-C47A-C49X	113.8(12)
C48X-C47A-C50X	105.9(12)	C49X-C47A-C50X	108.7(11)
C47A-C48A-H48A	109.5	C47A-C48A-H48B	109.5
C47A-C48A-H48C	109.5	H48A-C48A-H48B	109.5
H48A-C48A-H48C	109.5	H48B-C48A-H48C	109.5
C47A-C49A-H49A	109.5	C47A-C49A-H49B	109.5
C47A-C49A-H49C	109.5	H49A-C49A-H49B	109.5
H49A-C49A-H49C	109.5	H49B-C49A-H49C	109.5
C47A-C50A-H50A	109.5	C47A-C50A-H50B	109.5
C47A-C50A-H50C	109.5	H50A-C50A-H50B	109.5
H50A-C50A-H50C	109.5	H50B-C50A-H50C	109.5
C45A-C51A-C52A	108.7(8)	C45A-C51A-C53A	108.6(8)
C45A-C51A-C54A	112.3(8)	C52A-C51A-C53A	108.9(9)
C52A-C51A-C54A	109.2(8)	C53A-C51A-C54A	109.2(9)
C51A-C52A-H52A	109.5	C51A-C52A-H52B	109.5
C51A-C52A-H52C	109.5	H52A-C52A-H52B	109.5
H52A-C52A-H52C	109.5	H52B-C52A-H52C	109.5
C51A-C53A-H53A	109.5	C51A-C53A-H53B	109.5
C51A-C53A-H53C	109.5	H53A-C53A-H53B	109.5
H53A-C53A-H53C	109.5	H53B-C53A-H53C	109.5
C51A-C54A-H54A	109.5	C51A-C54A-H54B	109.5
C51A-C54A-H54C	109.5	H54A-C54A-H54B	109.5
H54A-C54A-H54C	109.5	H54B-C54A-H54C	109.5
H1NB-N1B-C1B	124.6	H1NB-N1B-C4B	124.6
C1B-N1B-C4B	110.9(8)	C6B-N2B-C9B	104.9(7)
H3NB-N3B-C11B	124.7	H3NB-N3B-C14B	124.7

C11B-N3B-C14B	110.6(8)	C16B-N4B-C19B	104.6(8)
N1B-C1B-C2B	106.2(8)	N1B-C1B-C20B	125.3(8)
C2B-C1B-C20B	128.4(8)	C1B-C2B-H2B	126.6
C1B-C2B-C3B	106.8(8)	H2B-C2B-C3B	126.6
C2B-C3B-H3B	125.7	C2B-C3B-C4B	108.7(9)
H3B-C3B-C4B	125.7	N1B-C4B-C3B	107.4(8)
N1B-C4B-C5B	124.5(8)	C3B-C4B-C5B	128.0(9)
C4B-C5B-C6B	128.3(8)	C4B-C5B-C27B	111.7(8)
C6B-C5B-C27B	120.1(8)	N2B-C6B-C5B	123.7(8)
N2B-C6B-C7B	108.0(8)	C5B-C6B-C7B	128.3(8)
C6B-C7B-H7B	125.5	C6B-C7B-C8B	109.0(8)
H7B-C7B-C8B	125.5	C7B-C8B-H8B	127.8
C7B-C8B-C9B	104.3(8)	H8B-C8B-C9B	127.8
N2B-C9B-C8B	113.7(8)	N2B-C9B-C10B	120.5(8)
C8B-C9B-C10B	125.8(8)	C9B-C10B-C11B	120.4(8)
C9B-C10B-C24B	119.6(9)	C11B-C10B-C24B	120.0(9)
N3B-C11B-C10B	123.5(8)	N3B-C11B-C12B	106.4(8)
C10B-C11B-C12B	130.0(8)	C11B-C12B-H12B	126.1
C11B-C12B-C13B	107.8(9)	H12B-C12B-C13B	126.1
C12B-C13B-H13B	125.8	C12B-C13B-C14B	108.4(9)
H13B-C13B-C14B	125.8	N3B-C14B-C13B	106.8(8)
N3B-C14B-C15B	125.1(8)	C13B-C14B-C15B	127.8(9)
C14B-C15B-C16B	126.9(8)	C14B-C15B-C41B	115.6(8)
C16B-C15B-C41B	117.0(9)	N4B-C16B-C15B	125.2(9)
N4B-C16B-C17B	108.9(8)	C15B-C16B-C17B	125.6(9)
C16B-C17B-H17B	126.1	C16B-C17B-C18B	107.8(9)
H17B-C17B-C18B	126.1	C17B-C18B-H18B	127.2
C17B-C18B-C19B	105.7(9)	H18B-C18B-C19B	127.2
N4B-C19B-C18B	112.9(9)	N4B-C19B-C20B	121.2(9)
C18B-C19B-C20B	125.9(9)	C1B-C20B-C19B	118.6(8)
C1B-C20B-C21B	122.3(9)	C19B-C20B-C21B	119.0(8)
C20B-C21B-C22B	121.7(9)	C20B-C21B-C23B	126.3(9)
C22B-C21B-C23B	112.0(9)	N5B-C22B-C21B	176.1(12)
N6B-C23B-C21B	176.0(13)	C10B-C24B-C25B	123.6(9)
C10B-C24B-C26B	122.9(10)	C25B-C24B-C26B	113.1(9)
N7B-C25B-C24B	174.6(13)	N8B-C26B-C24B	174.4(12)
C5B-C27B-C28B	124.3(8)	C5B-C27B-C32B	117.5(9)
C28B-C27B-C32B	118.1(9)	C27B-C28B-H28B	118.6
C27B-C28B-C29B	122.8(10)	H28B-C28B-C29B	118.6
C28B-C29B-C30B	117.7(10)	C28B-C29B-C33B	120.5(9)
C30B-C29B-C33B	121.8(9)	C29B-C30B-H30B	119.9
C29B-C30B-C31B	120.2(10)	H30B-C30B-C31B	119.9
C30B-C31B-C32B	120.8(9)	C30B-C31B-C37B	118.4(9)
C32B-C31B-C37B	120.6(9)	C27B-C32B-C31B	120.4(10)
C27B-C32B-H32B	119.8	C31B-C32B-H32B	119.8
C29B-C33B-C34B	108.6(9)	C29B-C33B-C35B	109.6(10)
C29B-C33B-C36B	113.2(9)	C34B-C33B-C35B	108.2(9)
C34B-C33B-C36B	108.0(10)	C35B-C33B-C36B	109.1(10)
C33B-C34B-H34D	109.5	C33B-C34B-H34E	109.5
C33B-C34B-H34F	109.5	H34D-C34B-H34E	109.5
H34D-C34B-H34F	109.5	H34E-C34B-H34F	109.5

C33B-C35B-H35D	109.5	C33B-C35B-H35E	109.5
C33B-C35B-H35F	109.5	H35D-C35B-H35E	109.5
H35D-C35B-H35F	109.5	H35E-C35B-H35F	109.5
C33B-C36B-H36D	109.5	C33B-C36B-H36E	109.5
C33B-C36B-H36F	109.5	H36D-C36B-H36E	109.5
H36D-C36B-H36F	109.5	H36E-C36B-H36F	109.5
C31B-C37B-C38B	111.3(8)	C31B-C37B-C39B	108.7(8)
C31B-C37B-C40B	107.6(8)	C38B-C37B-C39B	108.6(9)
C38B-C37B-C40B	109.1(9)	C39B-C37B-C40B	111.6(10)
C37B-C38B-H38D	109.5	C37B-C38B-H38E	109.5
C37B-C38B-H38F	109.5	H38D-C38B-H38E	109.5
H38D-C38B-H38F	109.5	H38E-C38B-H38F	109.5
C37B-C39B-H39D	109.5	C37B-C39B-H39E	109.5
C37B-C39B-H39F	109.5	H39D-C39B-H39E	109.5
H39D-C39B-H39F	109.5	H39E-C39B-H39F	109.5
C37B-C40B-H40D	109.5	C37B-C40B-H40E	109.5
C37B-C40B-H40F	109.5	H40D-C40B-H40E	109.5
H40D-C40B-H40F	109.5	H40E-C40B-H40F	109.5
C15B-C41B-C42B	117.5(8)	C15B-C41B-C46B	122.1(8)
C42B-C41B-C46B	120.3(9)	C41B-C42B-H42B	119.9
C41B-C42B-C43B	120.3(9)	H42B-C42B-C43B	119.9
C42B-C43B-C44B	118.2(9)	C42B-C43B-C47B	120.0(8)
C44B-C43B-C47B	121.5(8)	C43B-C44B-H44B	118.8
C43B-C44B-C45B	122.4(9)	H44B-C44B-C45B	118.8
C44B-C45B-C46B	118.9(9)	C44B-C45B-C51B	120.8(8)
C46B-C45B-C51B	120.1(8)	C41B-C46B-C45B	119.8(9)
C41B-C46B-H46B	120.1	C45B-C46B-H46B	120.1
C43B-C47B-C48B	109.0(8)	C43B-C47B-C49B	110.4(8)
C43B-C47B-C50B	110.4(9)	C48B-C47B-C49B	106.8(9)
C48B-C47B-C50B	109.2(9)	C49B-C47B-C50B	110.9(10)
C47B-C48B-H48D	109.5	C47B-C48B-H48E	109.5
C47B-C48B-H48F	109.5	H48D-C48B-H48E	109.5
H48D-C48B-H48F	109.5	H48E-C48B-H48F	109.5
C47B-C49B-H49D	109.5	C47B-C49B-H49E	109.5
C47B-C49B-H49F	109.5	H49D-C49B-H49E	109.5
H49D-C49B-H49F	109.5	H49E-C49B-H49F	109.5
C47B-C50B-H50D	109.5	C47B-C50B-H50E	109.5
C47B-C50B-H50F	109.5	H50D-C50B-H50E	109.5
H50D-C50B-H50F	109.5	H50E-C50B-H50F	109.5
C45B-C51B-C52B	108.8(10)	C45B-C51B-C53B	108.3(12)
C45B-C51B-C54B	112.2(10)	C45B-C51B-C52Y	106(3)
C45B-C51B-C53Y	113(4)	C45B-C51B-C54Y	108(4)
C52B-C51B-C53B	109.3(11)	C52B-C51B-C54B	109.6(11)
C53B-C51B-C54B	108.7(11)	C52Y-C51B-C53Y	110(2)
C52Y-C51B-C54Y	110(2)	C53Y-C51B-C54Y	108(2)
C51B-C52B-H52D	109.5	C51B-C52B-H52E	109.5
C51B-C52B-H52F	109.5	H52D-C52B-H52E	109.5
H52D-C52B-H52F	109.5	H52E-C52B-H52F	109.5
C51B-C53B-H53D	109.5	C51B-C53B-H53E	109.5
C51B-C53B-H53F	109.5	H53D-C53B-H53E	109.5
H53D-C53B-H53F	109.5	H53E-C53B-H53F	109.5

C51B–C54B–H54D	109.5	C51B–C54B–H54E	109.5
C51B–C54B–H54F	109.5	H54D–C54B–H54E	109.5
H54D–C54B–H54F	109.5	H54E–C54B–H54F	109.5
C33A–C34X–H34G	109.5	C33A–C34X–H34H	109.5
C33A–C34X–H34I	109.5	H34G–C34X–H34H	109.5
H34G–C34X–H34I	109.5	H34H–C34X–H34I	109.5
C33A–C35X–H35G	109.5	C33A–C35X–H35H	109.5
C33A–C35X–H35I	109.5	H35G–C35X–H35H	109.5
H35G–C35X–H35I	109.5	H35H–C35X–H35I	109.5
C33A–C36X–H36G	109.5	C33A–C36X–H36H	109.5
C33A–C36X–H36I	109.5	H36G–C36X–H36H	109.5
H36G–C36X–H36I	109.5	H36H–C36X–H36I	109.5
C47A–C48X–H48G	109.5	C47A–C48X–H48H	109.5
C47A–C48X–H48I	109.5	H48G–C48X–H48H	109.5
H48G–C48X–H48I	109.5	H48H–C48X–H48I	109.5
C47A–C49X–H49G	109.5	C47A–C49X–H49H	109.5
C47A–C49X–H49I	109.5	H49G–C49X–H49H	109.5
H49G–C49X–H49I	109.5	H49H–C49X–H49I	109.5
C47A–C50X–H50G	109.5	C47A–C50X–H50H	109.5
C47A–C50X–H50I	109.5	H50G–C50X–H50H	109.5
H50G–C50X–H50I	109.5	H50H–C50X–H50I	109.5
C51B–C52Y–H52G	109.5	C51B–C52Y–H52H	109.5
C51B–C52Y–H52I	109.5	H52G–C52Y–H52H	109.5
H52G–C52Y–H52I	109.5	H52H–C52Y–H52I	109.5
C51B–C53Y–H53G	109.5	C51B–C53Y–H53H	109.5
C51B–C53Y–H53I	109.5	H53G–C53Y–H53H	109.5
H53G–C53Y–H53I	109.5	H53H–C53Y–H53I	109.5
C51B–C54Y–H54G	109.5	C51B–C54Y–H54H	109.5
C51B–C54Y–H54I	109.5	H54G–C54Y–H54H	109.5
H54G–C54Y–H54I	109.5	H54H–C54Y–H54I	109.5

Table S16. Torsion angles [°] for **H₂9**.

C4A–N1A–C1A–C2A	–2.0(10)	C4A–N1A–C1A–C20A	–173.9(9)
N1A–C1A–C2A–C3A	0.9(11)	C20A–C1A–C2A–C3A	171.8(10)
C1A–C2A–C3A–C4A	0.5(12)	C1A–N1A–C4A–C3A	2.3(11)
C1A–N1A–C4A–C5A	–176.2(9)	C2A–C3A–C4A–N1A	–1.6(11)
C2A–C3A–C4A–C5A	176.7(10)	N1A–C4A–C5A–C6A	11.2(15)
N1A–C4A–C5A–C27A	–172.7(8)	C3A–C4A–C5A–C6A	–166.9(10)
C3A–C4A–C5A–C27A	9.2(15)	C4A–C5A–C6A–N2A	–0.5(16)
C4A–C5A–C6A–C7A	171.8(9)	C27A–C5A–C6A–N2A	–176.6(8)
C27A–C5A–C6A–C7A	–4.3(15)	C9A–N2A–C6A–C5A	169.6(9)
C9A–N2A–C6A–C7A	–3.9(10)	N2A–C6A–C7A–C8A	3.5(11)
C5A–C6A–C7A–C8A	–169.7(10)	C6A–C7A–C8A–C9A	–1.7(11)
C6A–N2A–C9A–C8A	2.9(11)	C6A–N2A–C9A–C10A	–175.7(8)
C7A–C8A–C9A–N2A	–0.8(12)	C7A–C8A–C9A–C10A	177.7(9)
N2A–C9A–C10A–C11A	–42.7(13)	N2A–C9A–C10A–C24A	138.9(9)
C8A–C9A–C10A–C11A	138.8(10)	C8A–C9A–C10A–C24A	–39.6(14)
C14A–N3A–C11A–C10A	–178.4(8)	C14A–N3A–C11A–C12A	0.4(10)
C9A–C10A–C11A–N3A	29.0(13)	C9A–C10A–C11A–C12A	–149.5(9)
C24A–C10A–C11A–N3A	–152.6(9)	C24A–C10A–C11A–C12A	28.8(14)
N3A–C11A–C12A–C13A	–1.0(10)	C10A–C11A–C12A–C13A	177.7(9)
C11A–C12A–C13A–C14A	1.3(11)	C11A–N3A–C14A–C13A	0.4(10)
C11A–N3A–C14A–C15A	–173.5(8)	C12A–C13A–C14A–N3A	–1.0(11)
C12A–C13A–C14A–C15A	172.6(9)	N3A–C14A–C15A–C16A	10.0(15)
N3A–C14A–C15A–C41A	–170.1(8)	C13A–C14A–C15A–C16A	–162.5(10)
C13A–C14A–C15A–C41A	17.4(14)	C14A–C15A–C16A–N4A	4.1(14)
C14A–C15A–C16A–C17A	179.8(9)	C41A–C15A–C16A–N4A	–175.8(8)
C41A–C15A–C16A–C17A	–0.1(14)	C19A–N4A–C16A–C15A	174.4(9)
C19A–N4A–C16A–C17A	–1.9(10)	N4A–C16A–C17A–C18A	1.4(10)
C15A–C16A–C17A–C18A	–174.7(9)	C16A–C17A–C18A–C19A	–0.3(10)
C16A–N4A–C19A–C18A	1.7(10)	C16A–N4A–C19A–C20A	–177.9(9)
C17A–C18A–C19A–N4A	–0.9(11)	C17A–C18A–C19A–C20A	178.7(9)
N1A–C1A–C20A–C19A	24.4(14)	N1A–C1A–C20A–C21A	–154.9(9)
C2A–C1A–C20A–C19A	–145.1(10)	C2A–C1A–C20A–C21A	35.7(16)
N4A–C19A–C20A–C1A	–44.4(14)	N4A–C19A–C20A–C21A	134.9(10)
C18A–C19A–C20A–C1A	136.1(10)	C18A–C19A–C20A–C21A	–44.6(14)
C1A–C20A–C21A–C22A	0.4(16)	C1A–C20A–C21A–C23A	176.6(10)
C19A–C20A–C21A–C22A	–178.9(9)	C19A–C20A–C21A–C23A	–2.7(15)
C9A–C10A–C24A–C25A	1.9(13)	C9A–C10A–C24A–C26A	–173.0(8)
C11A–C10A–C24A–C25A	–176.5(8)	C11A–C10A–C24A–C26A	8.7(14)
C4A–C5A–C27A–C28A	–73.1(12)	C4A–C5A–C27A–C32A	114.0(10)
C6A–C5A–C27A–C28A	103.3(11)	C6A–C5A–C27A–C32A	–69.5(13)
C5A–C27A–C28A–C29A	–171.0(10)	C32A–C27A–C28A–C29A	2.0(16)
C27A–C28A–C29A–C30A	–2.6(17)	C27A–C28A–C29A–C33A	176.2(10)
C28A–C29A–C30A–C31A	2.1(18)	C33A–C29A–C30A–C31A	–176.7(11)
C29A–C30A–C31A–C32A	–1.0(18)	C29A–C30A–C31A–C37A	176.6(11)
C30A–C31A–C32A–C27A	0.2(17)	C37A–C31A–C32A–C27A	–177.3(10)
C5A–C27A–C32A–C31A	172.4(10)	C28A–C27A–C32A–C31A	–0.7(16)
C28A–C29A–C33A–C34A	–55(2)	C28A–C29A–C33A–C35A	62.2(19)

C28A-C29A-C33A-C36A	177.5(19)	C28A-C29A-C33A-C34X	-16(2)
C28A-C29A-C33A-C35X	110.5(19)	C28A-C29A-C33A-C36X	-131.0(18)
C30A-C29A-C33A-C34A	123.5(18)	C30A-C29A-C33A-C35A	-119.0(17)
C30A-C29A-C33A-C36A	-4(2)	C30A-C29A-C33A-C34X	162.8(17)
C30A-C29A-C33A-C35X	-70.7(19)	C30A-C29A-C33A-C36X	47.9(19)
C30A-C31A-C37A-C38A	135.9(12)	C30A-C31A-C37A-C39A	14.9(16)
C30A-C31A-C37A-C40A	-106.5(13)	C32A-C31A-C37A-C38A	-46.6(15)
C32A-C31A-C37A-C39A	-167.6(12)	C32A-C31A-C37A-C40A	71.0(14)
C14A-C15A-C41A-C42A	-122.2(10)	C14A-C15A-C41A-C46A	57.6(12)
C16A-C15A-C41A-C42A	57.7(13)	C16A-C15A-C41A-C46A	-122.5(10)
C15A-C41A-C42A-C43A	178.7(10)	C46A-C41A-C42A-C43A	-1.1(16)
C41A-C42A-C43A-C44A	3.1(17)	C41A-C42A-C43A-C47A	-177.8(10)
C42A-C43A-C44A-C45A	-2.8(18)	C47A-C43A-C44A-C45A	178.0(11)
C43A-C44A-C45A-C46A	0.6(17)	C43A-C44A-C45A-C51A	-178.0(11)
C44A-C45A-C46A-C41A	1.5(15)	C51A-C45A-C46A-C41A	-180.0(9)
C15A-C41A-C46A-C45A	179.0(9)	C42A-C41A-C46A-C45A	-1.2(14)
C42A-C43A-C47A-C48A	-53.0(19)	C42A-C43A-C47A-C49A	-168(2)
C42A-C43A-C47A-C50A	62(2)	C42A-C43A-C47A-C48X	12.7(18)
C42A-C43A-C47A-C49X	-114.5(14)	C42A-C43A-C47A-C50X	128.3(14)
C44A-C43A-C47A-C48A	126.1(18)	C44A-C43A-C47A-C49A	11(2)
C44A-C43A-C47A-C50A	-119(2)	C44A-C43A-C47A-C48X	-168.2(15)
C44A-C43A-C47A-C49X	64.6(16)	C44A-C43A-C47A-C50X	-52.6(16)
C44A-C45A-C51A-C52A	-56.8(12)	C44A-C45A-C51A-C53A	61.5(13)
C44A-C45A-C51A-C54A	-177.6(10)	C46A-C45A-C51A-C52A	124.7(10)
C46A-C45A-C51A-C53A	-117.0(11)	C46A-C45A-C51A-C54A	3.8(14)
C4B-N1B-C1B-C2B	1.2(10)	C4B-N1B-C1B-C20B	178.1(9)
N1B-C1B-C2B-C3B	-1.3(11)	C20B-C1B-C2B-C3B	-178.1(9)
C1B-C2B-C3B-C4B	0.9(12)	C1B-N1B-C4B-C3B	-0.7(11)
C1B-N1B-C4B-C5B	175.3(9)	C2B-C3B-C4B-N1B	-0.2(12)
C2B-C3B-C4B-C5B	-176.0(9)	N1B-C4B-C5B-C6B	-11.2(16)
N1B-C4B-C5B-C27B	170.4(9)	C3B-C4B-C5B-C6B	163.9(11)
C3B-C4B-C5B-C27B	-14.5(14)	C4B-C5B-C6B-N2B	3.9(16)
C4B-C5B-C6B-C7B	-176.3(10)	C27B-C5B-C6B-N2B	-177.8(8)
C27B-C5B-C6B-C7B	2.0(15)	C9B-N2B-C6B-C5B	-177.5(9)
C9B-N2B-C6B-C7B	2.6(10)	N2B-C6B-C7B-C8B	-2.1(11)
C5B-C6B-C7B-C8B	178.1(10)	C6B-C7B-C8B-C9B	0.7(11)
C6B-N2B-C9B-C8B	-2.3(11)	C6B-N2B-C9B-C10B	179.9(8)
C7B-C8B-C9B-N2B	1.1(12)	C7B-C8B-C9B-C10B	178.7(9)
N2B-C9B-C10B-C11B	40.3(13)	N2B-C9B-C10B-C24B	-137.6(10)
C8B-C9B-C10B-C11B	-137.1(10)	C8B-C9B-C10B-C24B	44.9(14)
C14B-N3B-C11B-C10B	-178.5(8)	C14B-N3B-C11B-C12B	2.6(10)
C9B-C10B-C11B-N3B	-33.4(13)	C9B-C10B-C11B-C12B	145.3(9)
C24B-C10B-C11B-N3B	144.6(9)	C24B-C10B-C11B-C12B	-36.8(15)
N3B-C11B-C12B-C13B	-2.5(10)	C10B-C11B-C12B-C13B	178.7(9)
C11B-C12B-C13B-C14B	1.4(11)	C12B-C13B-C14B-N3B	0.1(11)
C12B-C13B-C14B-C15B	-173.8(9)	C11B-N3B-C14B-C13B	-1.8(10)
C11B-N3B-C14B-C15B	172.4(8)	N3B-C14B-C15B-C16B	0.9(15)
N3B-C14B-C15B-C41B	-171.2(8)	C13B-C14B-C15B-C16B	173.8(10)
C13B-C14B-C15B-C41B	1.7(14)	C14B-C15B-C16B-N4B	-6.3(15)

C14B-C15B-C16B-C17B	-179.2(9)	C41B-C15B-C16B-N4B	165.7(8)
C41B-C15B-C16B-C17B	-7.2(14)	C19B-N4B-C16B-C15B	-172.2(9)
C19B-N4B-C16B-C17B	1.7(10)	N4B-C16B-C17B-C18B	1.1(11)
C15B-C16B-C17B-C18B	175.0(10)	C16B-C17B-C18B-C19B	-3.1(11)
C16B-N4B-C19B-C18B	-3.8(11)	C16B-N4B-C19B-C20B	176.1(8)
C17B-C18B-C19B-N4B	4.6(12)	C17B-C18B-C19B-C20B	-175.3(9)
N1B-C1B-C20B-C19B	-28.7(14)	N1B-C1B-C20B-C21B	152.2(9)
C2B-C1B-C20B-C19B	147.5(10)	C2B-C1B-C20B-C21B	-31.6(15)
N4B-C19B-C20B-C1B	38.6(13)	N4B-C19B-C20B-C21B	-142.2(10)
C18B-C19B-C20B-C1B	-141.5(10)	C18B-C19B-C20B-C21B	37.6(14)
C1B-C20B-C21B-C22B	-7.6(15)	C1B-C20B-C21B-C23B	173.9(10)
C19B-C20B-C21B-C22B	173.3(9)	C19B-C20B-C21B-C23B	-5.2(15)
C9B-C10B-C24B-C25B	-3.5(15)	C9B-C10B-C24B-C26B	168.6(9)
C11B-C10B-C24B-C25B	178.5(9)	C11B-C10B-C24B-C26B	-9.4(15)
C4B-C5B-C27B-C28B	114.3(11)	C4B-C5B-C27B-C32B	-60.7(12)
C6B-C5B-C27B-C28B	-64.2(14)	C6B-C5B-C27B-C32B	120.7(11)
C5B-C27B-C28B-C29B	-171.4(10)	C32B-C27B-C28B-C29B	3.6(17)
C27B-C28B-C29B-C30B	-2.4(18)	C27B-C28B-C29B-C33B	176.2(10)
C28B-C29B-C30B-C31B	-0.1(17)	C33B-C29B-C30B-C31B	-178.8(11)
C29B-C30B-C31B-C32B	1.4(18)	C29B-C30B-C31B-C37B	176.7(10)
C30B-C31B-C32B-C27B	-0.2(17)	C37B-C31B-C32B-C27B	-175.4(9)
C5B-C27B-C32B-C31B	173.2(10)	C28B-C27B-C32B-C31B	-2.2(15)
C28B-C29B-C33B-C34B	-61.6(14)	C28B-C29B-C33B-C35B	56.4(14)
C28B-C29B-C33B-C36B	178.5(12)	C30B-C29B-C33B-C34B	117.1(12)
C30B-C29B-C33B-C35B	-125.0(12)	C30B-C29B-C33B-C36B	-2.9(16)
C30B-C31B-C37B-C38B	-176.7(10)	C30B-C31B-C37B-C39B	63.7(13)
C30B-C31B-C37B-C40B	-57.2(13)	C32B-C31B-C37B-C38B	-1.3(14)
C32B-C31B-C37B-C39B	-120.9(12)	C32B-C31B-C37B-C40B	118.1(11)
C14B-C15B-C41B-C42B	101.2(12)	C14B-C15B-C41B-C46B	-82.1(13)
C16B-C15B-C41B-C42B	-71.7(13)	C16B-C15B-C41B-C46B	105.0(12)
C15B-C41B-C42B-C43B	179.7(10)	C46B-C41B-C42B-C43B	2.9(18)
C41B-C42B-C43B-C44B	-3.1(18)	C41B-C42B-C43B-C47B	-176.1(10)
C42B-C43B-C44B-C45B	1.0(19)	C47B-C43B-C44B-C45B	173.8(11)
C43B-C44B-C45B-C46B	1(2)	C43B-C44B-C45B-C51B	176.7(11)
C44B-C45B-C46B-C41B	-1.6(19)	C51B-C45B-C46B-C41B	-176.9(11)
C15B-C41B-C46B-C45B	-177.1(11)	C42B-C41B-C46B-C45B	-0.5(19)
C42B-C43B-C47B-C48B	-36.9(14)	C42B-C43B-C47B-C49B	-153.9(11)
C42B-C43B-C47B-C50B	83.1(13)	C44B-C43B-C47B-C48B	150.4(11)
C44B-C43B-C47B-C49B	33.3(15)	C44B-C43B-C47B-C50B	-89.6(14)
C44B-C45B-C51B-C52B	-69.6(19)	C44B-C45B-C51B-C53B	49.1(19)
C44B-C45B-C51B-C54B	169.0(16)	C44B-C45B-C51B-C52Y	-99(5)
C44B-C45B-C51B-C53Y	22(6)	C44B-C45B-C51B-C54Y	143(5)
C46B-C45B-C51B-C52B	105.7(18)	C46B-C45B-C51B-C53B	-135.7(17)
C46B-C45B-C51B-C54B	-16(2)	C46B-C45B-C51B-C52Y	77(5)
C46B-C45B-C51B-C53Y	-162(5)	C46B-C45B-C51B-C54Y	-42(5)

Table S17. Anisotropic displacement parameters ($\text{\AA}^2$) for **H₂9**.The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N1A	0.053(5)	0.017(4)	0.036(4)	0.009(3)	0.007(4)	-0.005(3)
N2A	0.054(5)	0.020(4)	0.043(4)	0.004(3)	-0.002(4)	-0.003(3)
N3A	0.037(4)	0.026(4)	0.047(5)	0.001(3)	-0.001(4)	-0.006(3)
N4A	0.038(4)	0.017(4)	0.042(4)	-0.001(3)	-0.010(3)	-0.002(3)
N5A	0.089(7)	0.016(5)	0.079(7)	0.000(5)	-0.008(6)	-0.006(5)
N6A	0.089(7)	0.015(5)	0.069(6)	-0.002(4)	0.011(6)	0.008(4)
N7A	0.050(6)	0.041(6)	0.114(9)	0.027(6)	0.019(6)	0.012(5)
N8A	0.044(5)	0.036(5)	0.084(7)	-0.015(5)	-0.026(5)	0.018(4)
C1A	0.038(5)	0.018(4)	0.049(5)	0.000(4)	0.001(4)	-0.004(4)
C2A	0.055(6)	0.028(5)	0.048(5)	0.006(4)	-0.012(5)	0.001(4)
C3A	0.059(6)	0.021(5)	0.035(5)	0.007(4)	0.001(5)	-0.003(4)
C4A	0.047(5)	0.026(4)	0.036(5)	0.011(4)	0.014(4)	-0.004(4)
C5A	0.052(5)	0.024(5)	0.038(5)	0.005(4)	0.005(4)	-0.003(4)
C6A	0.048(5)	0.021(5)	0.042(5)	0.003(4)	0.000(4)	-0.002(4)
C7A	0.051(6)	0.022(5)	0.052(5)	-0.009(4)	-0.005(5)	0.005(4)
C8A	0.050(6)	0.023(5)	0.051(6)	-0.008(4)	-0.003(5)	0.001(4)
C9A	0.041(5)	0.020(5)	0.056(5)	-0.009(4)	-0.006(4)	0.007(4)
C10A	0.049(5)	0.006(4)	0.055(5)	-0.006(4)	-0.004(4)	-0.003(4)
C11A	0.028(4)	0.024(5)	0.050(5)	-0.001(4)	-0.013(4)	-0.003(4)
C12A	0.049(5)	0.022(5)	0.054(6)	-0.003(4)	-0.003(5)	0.003(4)
C13A	0.059(6)	0.022(5)	0.041(5)	0.007(4)	-0.014(5)	-0.001(4)
C14A	0.046(5)	0.024(5)	0.032(5)	-0.006(4)	-0.004(4)	-0.004(4)
C15A	0.051(5)	0.017(4)	0.040(5)	-0.009(4)	0.006(4)	-0.007(4)
C16A	0.042(5)	0.023(4)	0.040(5)	-0.001(4)	0.007(4)	-0.003(4)
C17A	0.049(5)	0.024(5)	0.032(5)	-0.012(4)	0.000(4)	-0.004(4)
C18A	0.054(6)	0.017(5)	0.050(6)	-0.010(4)	0.004(5)	-0.004(4)
C19A	0.041(5)	0.014(4)	0.050(5)	0.003(4)	-0.011(4)	-0.006(4)
C20A	0.045(5)	0.018(4)	0.049(5)	0.002(4)	0.001(4)	0.001(4)
C21A	0.048(5)	0.020(4)	0.058(6)	-0.002(4)	0.004(5)	-0.002(4)
C22A	0.057(6)	0.012(5)	0.059(6)	-0.005(4)	0.000(5)	-0.003(4)
C23A	0.057(6)	0.020(5)	0.061(6)	-0.004(5)	0.017(6)	0.001(5)
C24A	0.035(5)	0.010(4)	0.079(6)	-0.005(4)	-0.012(4)	-0.006(4)
C25A	0.033(5)	0.018(5)	0.078(7)	0.010(5)	-0.010(5)	0.004(4)
C26A	0.023(5)	0.019(5)	0.078(7)	-0.007(5)	-0.014(5)	0.005(4)
C27A	0.056(6)	0.030(5)	0.037(5)	0.005(4)	-0.004(4)	0.005(4)
C28A	0.072(7)	0.025(5)	0.041(5)	0.005(4)	-0.003(5)	-0.003(5)
C29A	0.088(7)	0.047(6)	0.047(6)	0.007(5)	0.001(5)	-0.005(5)
C30A	0.081(7)	0.051(6)	0.051(6)	-0.002(5)	0.000(6)	0.004(5)
C31A	0.073(7)	0.046(6)	0.051(6)	-0.008(5)	0.002(5)	-0.004(5)
C32A	0.061(6)	0.027(5)	0.049(5)	-0.010(4)	-0.001(5)	-0.006(4)
C33A	0.115(9)	0.064(7)	0.063(7)	0.011(6)	0.017(7)	-0.015(7)
C34A	0.112(13)	0.081(18)	0.094(17)	0.024(16)	0.034(14)	-0.020(13)
C35A	0.140(18)	0.080(13)	0.090(17)	0.042(13)	0.017(17)	-0.006(14)
C36A	0.15(2)	0.133(19)	0.065(12)	0.019(14)	0.035(13)	-0.030(18)

C37A	0.092(8)	0.055(7)	0.046(6)	-0.012(5)	-0.006(6)	-0.013(6)
C38A	0.087(9)	0.076(10)	0.115(11)	-0.029(9)	0.005(8)	-0.030(7)
C39A	0.156(14)	0.083(11)	0.072(9)	-0.027(7)	-0.003(8)	-0.042(10)
C40A	0.140(12)	0.045(7)	0.108(11)	-0.029(7)	0.004(10)	0.001(8)
C41A	0.038(5)	0.024(5)	0.043(5)	0.002(4)	-0.008(4)	0.006(4)
C42A	0.067(6)	0.022(5)	0.050(6)	-0.009(4)	0.006(5)	-0.002(5)
C43A	0.084(7)	0.034(5)	0.048(5)	-0.010(4)	0.015(5)	-0.009(5)
C44A	0.070(7)	0.034(5)	0.053(6)	0.001(5)	0.001(5)	-0.007(5)
C45A	0.051(5)	0.022(4)	0.055(6)	0.004(4)	0.002(5)	-0.002(4)
C46A	0.051(6)	0.024(5)	0.045(5)	0.006(4)	-0.005(5)	0.003(4)
C47A	0.107(8)	0.051(7)	0.056(6)	-0.014(5)	0.014(6)	-0.008(6)
C48A	0.115(19)	0.063(14)	0.058(17)	-0.030(12)	0.002(15)	0.002(14)
C49A	0.116(18)	0.090(18)	0.055(15)	-0.015(14)	0.027(15)	0.004(16)
C50A	0.112(17)	0.09(2)	0.071(18)	-0.030(16)	-0.008(14)	-0.007(15)
C51A	0.083(7)	0.019(5)	0.066(7)	0.007(5)	0.007(6)	-0.007(5)
C52A	0.093(8)	0.043(7)	0.064(8)	-0.011(6)	0.028(6)	-0.028(6)
C53A	0.144(11)	0.032(7)	0.085(9)	0.026(7)	-0.014(9)	-0.003(8)
C54A	0.081(8)	0.025(6)	0.081(8)	-0.009(5)	0.017(7)	-0.006(6)
N1B	0.042(4)	0.023(4)	0.052(5)	0.000(4)	-0.009(4)	-0.008(3)
N2B	0.051(5)	0.019(4)	0.050(5)	0.000(4)	-0.002(4)	0.003(4)
N3B	0.044(4)	0.019(4)	0.055(5)	0.010(4)	0.000(4)	0.006(3)
N4B	0.061(5)	0.019(4)	0.051(5)	0.005(4)	0.004(4)	0.005(4)
N5B	0.054(6)	0.072(7)	0.065(7)	-0.003(6)	0.000(5)	0.014(5)
N6B	0.076(7)	0.049(6)	0.072(7)	0.011(5)	-0.031(6)	0.002(5)
N7B	0.082(7)	0.048(6)	0.087(8)	0.007(6)	-0.040(7)	-0.003(5)
N8B	0.072(7)	0.049(6)	0.086(8)	0.019(6)	0.001(6)	-0.006(5)
C1B	0.045(5)	0.020(5)	0.043(5)	-0.013(4)	-0.004(4)	-0.009(4)
C2B	0.042(5)	0.034(5)	0.050(6)	-0.003(5)	-0.013(4)	0.003(4)
C3B	0.054(5)	0.033(5)	0.055(6)	0.003(5)	-0.008(5)	0.002(5)
C4B	0.047(5)	0.020(5)	0.053(5)	0.006(4)	-0.005(4)	-0.001(4)
C5B	0.061(5)	0.015(4)	0.052(5)	0.000(4)	0.006(4)	0.008(4)
C6B	0.053(5)	0.020(5)	0.035(5)	0.001(4)	0.000(4)	-0.001(4)
C7B	0.063(6)	0.028(5)	0.034(5)	0.004(4)	0.005(4)	0.006(5)
C8B	0.056(5)	0.030(5)	0.053(6)	0.008(5)	-0.003(5)	0.002(5)
C9B	0.041(5)	0.013(4)	0.051(5)	0.004(4)	-0.009(4)	0.004(4)
C10B	0.043(5)	0.026(5)	0.057(5)	0.003(4)	0.001(4)	0.005(4)
C11B	0.039(5)	0.019(5)	0.048(5)	0.019(4)	-0.004(4)	0.012(4)
C12B	0.041(5)	0.036(6)	0.053(6)	0.016(5)	0.002(4)	0.015(4)
C13B	0.056(6)	0.032(5)	0.055(6)	0.016(5)	-0.001(5)	0.006(5)
C14B	0.051(5)	0.021(5)	0.045(5)	0.002(4)	0.015(4)	0.002(4)
C15B	0.065(5)	0.012(4)	0.049(5)	0.007(4)	0.017(4)	-0.004(4)
C16B	0.060(5)	0.017(5)	0.045(5)	0.003(4)	0.007(4)	-0.005(4)
C17B	0.074(6)	0.021(5)	0.045(5)	-0.009(4)	0.005(5)	0.000(5)
C18B	0.073(6)	0.025(5)	0.056(6)	-0.006(5)	-0.001(5)	-0.001(5)
C19B	0.062(6)	0.022(5)	0.049(5)	0.003(4)	0.006(5)	0.002(4)
C20B	0.045(5)	0.023(5)	0.050(5)	0.003(4)	-0.006(4)	-0.007(4)
C21B	0.045(5)	0.033(5)	0.049(5)	0.003(4)	-0.010(4)	-0.008(4)
C22B	0.034(5)	0.042(6)	0.056(6)	0.006(5)	0.001(5)	-0.002(4)
C23B	0.058(7)	0.037(6)	0.053(6)	0.001(5)	-0.026(5)	-0.004(5)

C24B	0.045(5)	0.036(5)	0.070(6)	0.007(5)	−0.006(5)	0.001(4)
C25B	0.054(7)	0.036(6)	0.070(7)	0.017(6)	−0.030(6)	−0.004(5)
C26B	0.044(6)	0.044(6)	0.065(7)	0.012(6)	−0.009(5)	0.004(5)
C27B	0.052(6)	0.024(5)	0.061(5)	0.003(4)	−0.003(5)	−0.002(4)
C28B	0.072(7)	0.032(5)	0.056(6)	0.006(5)	0.004(6)	−0.008(5)
C29B	0.078(7)	0.032(5)	0.057(5)	0.006(5)	0.003(5)	−0.003(5)
C30B	0.076(7)	0.026(5)	0.072(7)	0.003(5)	0.015(6)	−0.005(5)
C31B	0.060(6)	0.027(5)	0.074(7)	−0.002(5)	0.004(6)	−0.005(4)
C32B	0.053(6)	0.023(5)	0.065(6)	0.005(4)	0.002(5)	0.004(4)
C33B	0.110(9)	0.049(7)	0.056(7)	−0.004(6)	0.004(7)	−0.016(7)
C34B	0.120(10)	0.045(7)	0.072(9)	−0.021(6)	0.022(8)	−0.007(7)
C35B	0.126(10)	0.050(8)	0.066(9)	−0.001(7)	0.001(8)	−0.012(7)
C36B	0.152(13)	0.078(10)	0.059(8)	0.002(7)	0.019(9)	−0.024(9)
C37B	0.059(6)	0.032(6)	0.083(8)	0.003(5)	0.001(6)	−0.014(5)
C38B	0.095(10)	0.031(7)	0.093(9)	−0.019(6)	0.008(7)	−0.010(6)
C39B	0.106(10)	0.036(7)	0.126(11)	0.020(8)	−0.034(9)	−0.020(7)
C40B	0.078(8)	0.054(8)	0.109(11)	−0.013(7)	0.026(8)	−0.022(6)
C41B	0.070(6)	0.022(5)	0.044(5)	0.001(4)	0.020(5)	0.005(5)
C42B	0.079(7)	0.026(5)	0.051(6)	−0.001(4)	0.018(6)	0.012(5)
C43B	0.086(7)	0.020(4)	0.046(5)	−0.008(4)	0.009(5)	0.006(5)
C44B	0.089(7)	0.018(5)	0.038(5)	−0.002(4)	0.005(5)	0.007(5)
C45B	0.114(8)	0.017(4)	0.053(6)	0.007(4)	0.038(6)	0.007(5)
C46B	0.088(8)	0.024(5)	0.062(6)	0.013(5)	0.030(6)	0.009(5)
C47B	0.093(8)	0.016(5)	0.054(6)	0.008(4)	−0.008(6)	0.004(5)
C48B	0.110(10)	0.021(5)	0.070(8)	0.012(5)	0.008(7)	0.000(6)
C49B	0.145(11)	0.033(7)	0.060(8)	0.014(6)	0.012(8)	0.021(7)
C50B	0.114(10)	0.048(8)	0.125(13)	0.019(8)	−0.036(9)	−0.003(8)
C51B	0.146(10)	0.019(5)	0.072(7)	0.002(5)	0.029(8)	0.010(6)
C52B	0.134(11)	0.041(10)	0.092(16)	0.007(10)	0.050(9)	0.024(8)
C53B	0.178(17)	0.011(8)	0.079(9)	−0.005(7)	0.007(11)	−0.005(11)
C54B	0.160(17)	0.010(6)	0.073(10)	−0.002(7)	0.017(10)	0.013(8)
C34X	0.120(16)	0.082(17)	0.054(13)	0.007(12)	0.029(12)	−0.038(13)
C35X	0.123(17)	0.095(17)	0.081(16)	0.047(13)	0.011(13)	−0.006(14)
C36X	0.141(19)	0.072(15)	0.088(17)	−0.009(12)	0.045(14)	−0.011(13)
C48X	0.152(16)	0.075(12)	0.093(15)	−0.038(10)	0.037(14)	−0.030(12)
C49X	0.094(11)	0.084(13)	0.047(11)	−0.019(10)	0.011(9)	0.021(9)
C50X	0.106(13)	0.094(13)	0.046(9)	−0.016(9)	−0.010(10)	0.016(11)
C52Y	0.139(17)	0.04(2)	0.08(3)	0.02(3)	0.04(2)	0.032(15)
C53Y	0.16(3)	0.01(2)	0.073(16)	−0.008(15)	0.037(19)	0.02(3)
C54Y	0.16(3)	0.020(13)	0.08(3)	0.00(2)	0.04(2)	0.01(2)

Table S18. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for **H₂9**.

	x	y	z	U
H1NA	0.661249	0.253559	0.781819	0.042
H3NA	0.639706	0.367808	0.738980	0.044
H2A	0.707603	0.022862	0.825835	0.053
H3A	0.684144	0.134527	0.869300	0.046
H7A	0.599985	0.467023	0.863503	0.050
H8A	0.559789	0.534133	0.817354	0.050
H12A	0.570545	0.544729	0.688203	0.050
H13A	0.628290	0.514743	0.655286	0.049
H17A	0.749367	0.265931	0.673079	0.042
H18A	0.756058	0.121430	0.710193	0.048
H28A	0.614643	0.197440	0.892633	0.055
H30A	0.646227	0.358135	0.973141	0.073
H32A	0.682575	0.435791	0.883229	0.055
H34A	0.544904	0.159155	0.958778	0.142
H34B	0.549289	0.266370	0.944152	0.142
H34C	0.558960	0.174301	0.921750	0.142
H35A	0.646490	0.104071	0.962923	0.154
H35B	0.605458	0.054488	0.967146	0.154
H35C	0.619081	0.082492	0.930859	0.154
H36A	0.631850	0.232819	1.001949	0.174
H36B	0.593553	0.296388	0.997543	0.174
H36C	0.590923	0.184446	1.007746	0.174
H38A	0.726956	0.511996	0.908278	0.139
H38B	0.740961	0.566922	0.941679	0.139
H38C	0.743780	0.451238	0.939507	0.139
H39A	0.665606	0.487994	0.992535	0.156
H39B	0.706634	0.436717	0.990457	0.156
H39C	0.703815	0.552400	0.992630	0.156
H40A	0.663015	0.591243	0.910215	0.147
H40B	0.638906	0.584543	0.943152	0.147
H40C	0.677483	0.647525	0.943210	0.147
H42A	0.699104	0.298891	0.625494	0.056
H44A	0.746591	0.530795	0.581806	0.063
H46A	0.706730	0.556771	0.674102	0.048
H48A	0.736516	0.219903	0.593117	0.118
H48B	0.755057	0.214086	0.557422	0.118
H48C	0.776234	0.273932	0.586936	0.118
H49A	0.777907	0.419081	0.551705	0.130
H49B	0.759177	0.352901	0.522639	0.130
H49C	0.740297	0.455301	0.531142	0.130
H50A	0.675020	0.283632	0.566889	0.137
H50B	0.675953	0.370634	0.540585	0.137
H50C	0.694833	0.268234	0.532082	0.137
H52A	0.789197	0.637235	0.598864	0.099
H52B	0.793290	0.738280	0.618283	0.099
H52C	0.799848	0.638344	0.637960	0.099
H53A	0.722893	0.686501	0.577838	0.132

H53B	0.691544	0.718831	0.603620	0.132
H53C	0.727746	0.786988	0.597494	0.132
H54A	0.708222	0.717681	0.665038	0.093
H54B	0.750475	0.687284	0.678242	0.093
H54C	0.743917	0.787220	0.658565	0.093
H1NB	0.571208	0.724914	0.732793	0.047
H3NB	0.510321	0.708999	0.756781	0.047
H2B	0.682638	0.730386	0.717605	0.051
H3B	0.646698	0.783274	0.665773	0.057
H7B	0.498393	0.803975	0.625872	0.050
H8B	0.439301	0.738810	0.649024	0.056
H12B	0.399126	0.685849	0.770798	0.052
H13B	0.432227	0.726937	0.825096	0.057
H17B	0.578396	0.768805	0.867126	0.056
H18B	0.640632	0.746358	0.840780	0.061
H28B	0.563153	0.728691	0.602514	0.064
H30B	0.624117	0.950515	0.565185	0.069
H32B	0.597907	0.952437	0.662430	0.057
H34D	0.601939	0.641673	0.566533	0.094
H34E	0.612058	0.644130	0.528085	0.094
H34F	0.640738	0.692217	0.555485	0.094
H35D	0.538309	0.718700	0.551222	0.097
H35E	0.536887	0.816873	0.529964	0.097
H35F	0.550183	0.717774	0.513203	0.097
H36D	0.609753	0.797474	0.497090	0.115
H36E	0.598088	0.896605	0.514754	0.115
H36F	0.638308	0.845924	0.524510	0.115
H38D	0.609742	1.110206	0.661619	0.088
H38E	0.647548	1.047614	0.670167	0.088
H38F	0.651277	1.157341	0.657711	0.088
H39D	0.590814	1.150299	0.603609	0.108
H39E	0.631729	1.200274	0.599159	0.108
H39F	0.616912	1.117752	0.573748	0.108
H40D	0.688667	0.992940	0.624768	0.096
H40E	0.677574	1.020136	0.586890	0.096
H40F	0.692391	1.102658	0.612302	0.096
H42B	0.517742	0.605233	0.869626	0.062
H44B	0.475520	0.747588	0.947716	0.058
H46B	0.483390	0.885912	0.859939	0.069
H48D	0.472792	0.477412	0.903833	0.080
H48E	0.517040	0.480458	0.894717	0.080
H48F	0.504338	0.422394	0.926921	0.080
H49D	0.450259	0.563905	0.952408	0.095
H49E	0.481517	0.506974	0.975219	0.095
H49F	0.479624	0.622906	0.976447	0.095
H50D	0.549978	0.633304	0.961690	0.116
H50E	0.551195	0.517257	0.962091	0.116
H50F	0.563897	0.575320	0.929887	0.116
H52D	0.414307	0.847099	0.940390	0.105
H52E	0.405958	0.960867	0.936846	0.105
H52F	0.404137	0.892962	0.904539	0.105

H53D	0.507746	0.954125	0.952479	0.107
H53E	0.468931	0.999327	0.965713	0.107
H53F	0.477402	0.885804	0.969958	0.107
H54D	0.492156	1.023985	0.896108	0.097
H54E	0.451707	1.001129	0.877461	0.097
H54F	0.453528	1.069034	0.909768	0.097
H34G	0.556998	0.185400	0.921923	0.101
H34H	0.585706	0.094789	0.923935	0.101
H34I	0.554859	0.109474	0.951895	0.101
H35G	0.608271	0.100794	0.994722	0.119
H35H	0.641658	0.097608	0.968595	0.119
H35I	0.641332	0.181434	0.996115	0.119
H36G	0.560745	0.313631	0.964212	0.119
H36H	0.559948	0.232775	0.992733	0.119
H36I	0.593530	0.312008	0.993277	0.119
H48G	0.679733	0.264780	0.568247	0.127
H48H	0.709857	0.221671	0.543157	0.127
H48I	0.717557	0.210577	0.582485	0.127
H49G	0.783402	0.403182	0.561268	0.090
H49H	0.782973	0.297988	0.578083	0.090
H49I	0.775273	0.309082	0.538755	0.090
H50G	0.682679	0.418301	0.539488	0.099
H50H	0.722351	0.475433	0.536431	0.099
H50I	0.714393	0.378762	0.515212	0.099
H52G	0.416172	0.922773	0.884872	0.103
H52H	0.404612	0.867592	0.918010	0.103
H52I	0.405606	0.983626	0.917126	0.103
H53G	0.490129	0.924096	0.967089	0.096
H53H	0.450925	0.984439	0.967539	0.096
H53I	0.449931	0.868405	0.968423	0.096
H54G	0.508036	1.009964	0.915988	0.104
H54H	0.479592	1.010887	0.883706	0.104
H54I	0.468968	1.070944	0.916117	0.104

Table S19. Crystal data and structure refinement for **Ni10**.

Identification code	oxdp28	
CCDC deposition number	1822193	
Chemical formula (moiety)	$C_{56}H_{64}N_4NiS_2Si \cdot C_2H_4Cl_2$	
Chemical formula (total)	$C_{58}H_{68}Cl_2N_4NiS_2Si$	
Formula weight	1042.98	
Temperature	150(2) K	
Radiation, wavelength	synchrotron, 0.6932 Å	
Crystal system, space group	monoclinic, $P2_1$	
Unit cell parameters	$a = 26.289(2)$ Å	$\alpha = 90^\circ$
	$b = 15.6605(14)$ Å	$\beta = 109.794(2)^\circ$
	$c = 28.462(2)$ Å	$\gamma = 90^\circ$
Cell volume	$11025.4(15)$ Å ³	
Z	8	
Calculated density	1.257 g/cm ³	
Absorption coefficient μ	0.550 mm ⁻¹	
F(000)	4416	
Crystal color and size	red, $0.140 \times 0.140 \times 0.040$ mm ³	
Reflections for cell refinement	15432 (θ range 3.4 to 25.8°)	
Data collection method	Bruker SMART 1K CCD diffractometer	
	thin-slice ω scans	
θ range for data collection	3.3 to 25.8°	
Index ranges	$h -32$ to 30, $k 0$ to 19, $l 0$ to 35	
Completeness to $\theta = 24.6^\circ$	99.6 %	
Reflections collected	31817	
Independent reflections	31817 ($R_{int} = 0.0000$)	
Reflections with $F^2 > 2\sigma$	29230	
Absorption correction	multi-scan	
Min. and max. transmission	0.92 and 0.98	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.2500,	
Data / restraints / parameters	31817 / 5129 / 2412	
Final R indices [$F^2 > 2\sigma$]	$R1 = 0.1419$, $wR2 = 0.3897$	
R indices (all data)	$R1 = 0.1506$, $wR2 = 0.4066$	
Goodness-of-fit on F^2	1.646	
Absolute structure parameter	0.186(8)	
Largest and mean shift/su	0.005 and 0.000	
Largest diff. peak and hole	5.90 and -2.01 e Å ⁻³	

Table S20. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$) for **Ni10**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ni1A	0.31871(7)	0.20042(10)	0.89369(6)	0.0159(4)
N1A	0.3319(4)	0.3209(5)	0.8869(4)	0.016(2)
N2A	0.3891(4)	0.1753(6)	0.8911(5)	0.021(2)
N3A	0.3043(4)	0.0809(6)	0.8973(4)	0.019(2)
N4A	0.2499(4)	0.2273(6)	0.8989(5)	0.025(2)
C1A	0.2932(4)	0.3852(7)	0.8731(5)	0.021(3)
C2A	0.3191(5)	0.4644(7)	0.8679(5)	0.024(3)
C3A	0.3721(5)	0.4498(7)	0.8821(5)	0.022(3)
C4A	0.3795(4)	0.3603(7)	0.8928(5)	0.022(3)
C5A	0.4296(4)	0.3184(7)	0.9064(5)	0.021(2)
C6A	0.4324(5)	0.2297(7)	0.9016(5)	0.023(3)
C7A	0.4798(5)	0.1861(9)	0.9001(7)	0.033(3)
C8A	0.4645(5)	0.1052(8)	0.8877(6)	0.028(3)
C9A	0.4092(5)	0.0981(7)	0.8831(5)	0.021(3)
C10A	0.3782(5)	0.0235(7)	0.8712(5)	0.022(3)
C11A	0.3296(5)	0.0159(7)	0.8802(5)	0.025(3)
C12A	0.3023(5)	−0.0638(7)	0.8808(5)	0.020(3)
C13A	0.2629(6)	−0.0463(7)	0.9000(5)	0.026(3)
C14A	0.2625(5)	0.0435(7)	0.9085(5)	0.019(2)
C15A	0.2264(5)	0.0880(7)	0.9246(5)	0.021(3)
C16A	0.2188(5)	0.1748(7)	0.9171(5)	0.024(3)
C17A	0.1715(5)	0.2187(9)	0.9171(6)	0.032(3)
C18A	0.1726(6)	0.2979(9)	0.8974(6)	0.034(3)
C19A	0.2211(5)	0.3037(7)	0.8859(6)	0.025(3)
C20A	0.2406(4)	0.3783(7)	0.8720(5)	0.021(2)
C21A	0.4778(5)	0.3677(8)	0.9174(5)	0.023(3)
C22A	0.5205(5)	0.4063(9)	0.9300(5)	0.027(3)
C23A	0.6352(6)	0.3615(10)	0.9792(6)	0.038(4)
C24A	0.6016(6)	0.4830(12)	0.8897(6)	0.039(4)
C25A	0.5947(7)	0.5380(10)	0.9904(6)	0.044(4)
C26A	0.1886(5)	0.0409(8)	0.9460(5)	0.026(3)
C27A	0.1497(6)	−0.0700(14)	0.9919(6)	0.047(4)
C28A	0.1073(7)	−0.0587(14)	0.9429(6)	0.055(5)
C29A	0.4038(5)	−0.0535(7)	0.8572(4)	0.019(2)
C30A	0.4143(5)	−0.0512(8)	0.8129(4)	0.022(3)
C31A	0.4394(6)	−0.1214(8)	0.7985(4)	0.025(3)
C32A	0.4532(6)	−0.1928(8)	0.8305(5)	0.028(3)
C33A	0.4411(6)	−0.1962(7)	0.8743(4)	0.022(3)
C34A	0.4179(6)	−0.1252(7)	0.8878(5)	0.020(3)
C35A	0.4503(6)	−0.1170(9)	0.7493(5)	0.030(3)
C36A	0.4658(10)	−0.0294(12)	0.7398(8)	0.061(5)
C37A	0.4899(10)	−0.1808(15)	0.7462(9)	0.073(6)
C38A	0.3997(8)	−0.1353(18)	0.7070(7)	0.073(6)
C39A	0.4544(6)	−0.2760(8)	0.9079(5)	0.033(3)
C40A	0.4922(8)	−0.2530(11)	0.9594(6)	0.048(4)

C41A	0.4771(7)	−0.3509(9)	0.8865(7)	0.039(4)
C42A	0.4006(7)	−0.3106(13)	0.9116(8)	0.055(5)
C43A	0.2037(5)	0.4542(7)	0.8591(5)	0.024(3)
C44A	0.1578(5)	0.4514(8)	0.8164(5)	0.029(3)
C45A	0.1243(5)	0.5215(8)	0.8018(4)	0.026(3)
C46A	0.1384(5)	0.5966(8)	0.8311(4)	0.022(3)
C47A	0.1843(5)	0.6010(7)	0.8732(4)	0.022(3)
C48A	0.2168(5)	0.5280(7)	0.8879(5)	0.022(3)
C49A	0.0741(6)	0.5215(10)	0.7542(5)	0.034(3)
C50A	0.0592(10)	0.4350(13)	0.7331(9)	0.082(7)
C51A	0.0232(7)	0.5509(15)	0.7655(8)	0.058(5)
C52A	0.0830(9)	0.5865(16)	0.7175(7)	0.067(6)
C53A	0.2000(5)	0.6814(7)	0.9064(4)	0.020(3)
C54A	0.1941(7)	0.6643(9)	0.9564(5)	0.033(3)
C55A	0.1648(6)	0.7571(9)	0.8817(6)	0.034(3)
C56A	0.2589(5)	0.7073(11)	0.9144(7)	0.036(3)
Si1A	0.58865(16)	0.4500(3)	0.94710(17)	0.0292(9)
S1A	0.21615(17)	−0.0445(3)	0.99071(16)	0.0346(9)
S2A	0.12833(16)	−0.0024(3)	0.89807(17)	0.0330(9)
Ni1B	0.39540(7)	0.39091(10)	0.60923(7)	0.0173(4)
N1B	0.4112(4)	0.5111(6)	0.6087(5)	0.023(2)
N2B	0.4677(4)	0.3649(6)	0.6121(5)	0.023(2)
N3B	0.3799(4)	0.2720(6)	0.6123(5)	0.021(2)
N4B	0.3236(4)	0.4182(6)	0.6056(5)	0.023(2)
C1B	0.3832(5)	0.5807(7)	0.6203(5)	0.019(3)
C2B	0.4119(5)	0.6581(8)	0.6201(6)	0.028(3)
C3B	0.4544(6)	0.6398(8)	0.6070(6)	0.029(3)
C4B	0.4551(5)	0.5490(7)	0.6015(5)	0.021(3)
C5B	0.4945(5)	0.5045(7)	0.5893(5)	0.020(3)
C6B	0.5008(5)	0.4158(7)	0.5972(5)	0.018(2)
C7B	0.5487(5)	0.3703(9)	0.5979(6)	0.031(3)
C8B	0.5445(5)	0.2929(8)	0.6160(6)	0.029(3)
C9B	0.4937(5)	0.2888(7)	0.6242(5)	0.023(3)
C10B	0.4721(4)	0.2143(7)	0.6354(5)	0.022(3)
C11B	0.4178(4)	0.2069(8)	0.6304(5)	0.024(3)
C12B	0.3902(5)	0.1290(8)	0.6322(5)	0.027(3)
C13B	0.3364(5)	0.1445(7)	0.6120(5)	0.024(3)
C14B	0.3305(4)	0.2342(7)	0.5994(5)	0.022(3)
C15B	0.2817(4)	0.2775(7)	0.5829(5)	0.021(3)
C16B	0.2796(5)	0.3645(7)	0.5911(5)	0.021(3)
C17B	0.2319(5)	0.4116(9)	0.5867(6)	0.032(3)
C18B	0.2476(5)	0.4914(8)	0.6048(6)	0.029(3)
C19B	0.3039(5)	0.4976(7)	0.6139(6)	0.029(3)
C20B	0.3331(5)	0.5725(7)	0.6242(5)	0.022(3)
C21B	0.5329(5)	0.5496(9)	0.5736(5)	0.025(3)
C22B	0.5663(5)	0.5909(9)	0.5614(5)	0.025(3)
C23B	0.6469(6)	0.5581(11)	0.5111(7)	0.042(4)
C24B	0.6734(6)	0.6787(12)	0.6003(5)	0.041(4)
C25B	0.5911(8)	0.7297(11)	0.5009(6)	0.049(4)
C26B	0.2278(5)	0.2332(8)	0.5614(5)	0.027(3)
C27B	0.1551(6)	0.1227(12)	0.5153(6)	0.039(4)

C28B	0.1496(6)	0.1272(12)	0.5657(6)	0.041(4)
C29B	0.5087(5)	0.1381(7)	0.6528(5)	0.024(3)
C30B	0.5534(6)	0.1409(10)	0.6964(5)	0.039(4)
C31B	0.5888(6)	0.0692(10)	0.7111(6)	0.043(4)
C32B	0.5779(6)	−0.0013(9)	0.6792(5)	0.035(3)
C33B	0.5342(6)	−0.0035(8)	0.6348(5)	0.028(3)
C34B	0.4997(5)	0.0672(7)	0.6210(5)	0.020(3)
C35B	0.6383(8)	0.0717(13)	0.7583(7)	0.071(6)
C36B	0.6561(11)	0.1587(16)	0.7749(12)	0.096(8)
C37B	0.6865(9)	0.0319(19)	0.7523(11)	0.091(7)
C38B	0.6318(14)	0.018(2)	0.7986(11)	0.130(10)
C39B	0.5240(6)	−0.0810(8)	0.5991(5)	0.034(3)
C40B	0.5282(8)	−0.0558(13)	0.5489(6)	0.050(4)
C41B	0.5628(7)	−0.1559(10)	0.6206(7)	0.047(4)
C42B	0.4671(6)	−0.1171(11)	0.5909(7)	0.043(4)
C43B	0.3056(5)	0.6488(7)	0.6367(5)	0.023(3)
C44B	0.2933(6)	0.6490(9)	0.6803(5)	0.028(3)
C45B	0.2674(6)	0.7192(8)	0.6927(5)	0.026(3)
C46B	0.2590(6)	0.7918(8)	0.6628(5)	0.027(3)
C47B	0.2709(6)	0.7926(7)	0.6186(5)	0.026(3)
C48B	0.2949(6)	0.7205(7)	0.6057(5)	0.022(3)
C49B	0.2526(6)	0.7216(9)	0.7408(5)	0.033(3)
C50B	0.2512(10)	0.6350(13)	0.7619(8)	0.066(6)
C51B	0.1965(8)	0.7610(17)	0.7281(9)	0.074(6)
C52B	0.2918(10)	0.7803(18)	0.7784(9)	0.086(7)
C53B	0.2614(6)	0.8724(8)	0.5848(5)	0.031(3)
C54B	0.2120(8)	0.8558(14)	0.5390(7)	0.060(5)
C55B	0.2465(8)	0.9487(10)	0.6112(7)	0.043(4)
C56B	0.3117(7)	0.8959(14)	0.5728(8)	0.053(5)
Si1B	0.61955(16)	0.6417(3)	0.54312(15)	0.0246(8)
S1B	0.22393(17)	0.1457(3)	0.51824(16)	0.0346(9)
S2B	0.20126(17)	0.1900(3)	0.60872(16)	0.0365(10)
Ni1C	−0.14477(7)	0.21795(11)	0.89473(7)	0.0197(4)
N1C	−0.1610(4)	0.0992(6)	0.8952(5)	0.024(2)
N2C	−0.2170(4)	0.2462(6)	0.8925(4)	0.023(2)
N3C	−0.1296(4)	0.3383(6)	0.8926(4)	0.022(2)
N4C	−0.0727(4)	0.1930(7)	0.8978(5)	0.025(2)
C1C	−0.1325(5)	0.0321(7)	0.8825(6)	0.024(3)
C2C	−0.1619(6)	−0.0453(9)	0.8803(7)	0.036(3)
C3C	−0.2032(6)	−0.0281(8)	0.8967(6)	0.033(3)
C4C	−0.2033(5)	0.0618(7)	0.9045(5)	0.021(3)
C5C	−0.2446(5)	0.1064(7)	0.9143(5)	0.025(3)
C6C	−0.2507(5)	0.1945(7)	0.9069(5)	0.023(3)
C7C	−0.2995(6)	0.2386(9)	0.9045(6)	0.036(3)
C8C	−0.2959(6)	0.3166(9)	0.8860(7)	0.036(4)
C9C	−0.2437(5)	0.3221(7)	0.8798(5)	0.025(3)
C10C	−0.2223(5)	0.3960(7)	0.8675(5)	0.024(3)
C11C	−0.1673(4)	0.4025(7)	0.8741(5)	0.024(3)
C12C	−0.1398(5)	0.4814(9)	0.8732(6)	0.032(3)
C13C	−0.0867(5)	0.4662(8)	0.8918(6)	0.034(3)

C14C	-0.0795(4)	0.3758(8)	0.9016(6)	0.027(3)
C15C	-0.0300(5)	0.3334(8)	0.9190(6)	0.031(3)
C16C	-0.0279(5)	0.2460(7)	0.9137(5)	0.027(3)
C17C	0.0195(6)	0.2027(9)	0.9128(7)	0.038(4)
C18C	0.0039(5)	0.1209(9)	0.8985(7)	0.036(3)
C19C	-0.0525(5)	0.1142(7)	0.8893(6)	0.024(3)
C20C	-0.0828(5)	0.0398(7)	0.8768(5)	0.026(3)
C21C	-0.2838(5)	0.0588(9)	0.9273(5)	0.026(3)
C22C	-0.3178(6)	0.0179(10)	0.9380(6)	0.035(3)
C23C	-0.3990(8)	0.0426(13)	0.9875(8)	0.056(5)
C24C	-0.4238(6)	-0.0672(12)	0.8932(5)	0.039(4)
C25C	-0.3448(8)	-0.1281(11)	0.9914(7)	0.048(4)
C26C	0.0227(5)	0.3799(8)	0.9403(5)	0.031(3)
C27C	0.0924(6)	0.4973(13)	0.9833(6)	0.049(5)
C28C	0.0976(7)	0.4911(13)	0.9319(6)	0.050(5)
C29C	-0.2581(5)	0.4729(8)	0.8509(5)	0.030(3)
C30C	-0.2998(6)	0.4714(9)	0.8057(5)	0.035(3)
C31C	-0.3363(7)	0.5412(10)	0.7889(6)	0.045(4)
C32C	-0.3256(6)	0.6131(9)	0.8205(5)	0.032(3)
C33C	-0.2837(6)	0.6166(8)	0.8659(5)	0.030(3)
C34C	-0.2495(6)	0.5457(8)	0.8805(5)	0.026(3)
C35C	-0.3806(7)	0.5363(12)	0.7381(6)	0.059(5)
C36C	-0.4138(11)	0.4594(16)	0.7327(10)	0.086(7)
C37C	-0.4093(11)	0.6146(16)	0.7182(11)	0.094(8)
C38C	-0.3553(10)	0.5246(18)	0.6980(8)	0.077(6)
C39C	-0.2747(6)	0.6955(8)	0.8999(5)	0.032(3)
C40C	-0.2866(9)	0.6704(12)	0.9467(6)	0.053(5)
C41C	-0.3085(8)	0.7724(10)	0.8747(8)	0.049(4)
C42C	-0.2154(7)	0.7239(13)	0.9147(9)	0.058(5)
C43C	-0.0567(5)	-0.0365(7)	0.8630(5)	0.022(3)
C44C	-0.0414(6)	-0.0336(9)	0.8205(5)	0.029(3)
C45C	-0.0193(6)	-0.1032(8)	0.8054(5)	0.029(3)
C46C	-0.0107(6)	-0.1782(8)	0.8348(5)	0.029(3)
C47C	-0.0246(6)	-0.1836(8)	0.8775(5)	0.029(3)
C48C	-0.0461(6)	-0.1106(7)	0.8922(5)	0.027(3)
C49C	-0.0041(6)	-0.0999(10)	0.7584(5)	0.040(4)
C50C	-0.0033(10)	-0.0120(12)	0.7391(9)	0.064(5)
C51C	0.0526(7)	-0.1359(15)	0.7680(8)	0.061(5)
C52C	-0.0441(9)	-0.1552(17)	0.7180(7)	0.076(6)
C53C	-0.0154(6)	-0.2641(9)	0.9101(6)	0.040(4)
C54C	0.0314(7)	-0.2497(10)	0.9591(6)	0.045(4)
C55C	-0.0005(7)	-0.3406(8)	0.8839(6)	0.035(3)
C56C	-0.0651(7)	-0.2872(12)	0.9235(8)	0.046(4)
Si1C	-0.37258(18)	-0.0359(3)	0.95266(16)	0.0308(9)
Si1C	0.0255(2)	0.4682(3)	0.98169(17)	0.0416(10)
Si2C	0.04741(17)	0.4196(3)	0.89128(17)	0.0352(9)
Ni1D	-0.07193(7)	0.40941(11)	0.60303(7)	0.0202(4)
N1D	-0.0851(4)	0.2903(6)	0.6067(5)	0.026(2)
N2D	-0.1428(4)	0.4362(7)	0.6053(5)	0.028(3)

N3D	−0.0565(4)	0.5312(6)	0.6010(4)	0.023(2)
N4D	−0.0022(4)	0.3863(6)	0.5994(4)	0.023(2)
C1D	−0.0465(5)	0.2252(7)	0.6233(5)	0.025(3)
C2D	−0.0738(5)	0.1481(9)	0.6276(6)	0.033(3)
C3D	−0.1266(5)	0.1632(8)	0.6118(6)	0.033(3)
C4D	−0.1337(5)	0.2522(8)	0.6017(6)	0.028(3)
C5D	−0.1826(5)	0.2943(8)	0.5904(6)	0.030(3)
C6D	−0.1858(5)	0.3841(8)	0.5954(6)	0.032(3)
C7D	−0.2325(6)	0.4290(9)	0.5968(7)	0.037(4)
C8D	−0.2162(5)	0.5092(8)	0.6111(6)	0.030(3)
C9D	−0.1610(5)	0.5139(7)	0.6157(6)	0.027(3)
C10D	−0.1322(5)	0.5903(7)	0.6240(5)	0.019(2)
C11D	−0.0829(5)	0.5973(7)	0.6163(5)	0.021(3)
C12D	−0.0549(6)	0.6750(8)	0.6158(6)	0.029(3)
C13D	−0.0158(6)	0.6582(8)	0.5968(5)	0.026(3)
C14D	−0.0168(5)	0.5679(7)	0.5878(5)	0.020(3)
C15D	0.0225(5)	0.5246(7)	0.5737(5)	0.026(3)
C16D	0.0308(5)	0.4388(7)	0.5847(5)	0.027(3)
C17D	0.0788(6)	0.3941(10)	0.5847(7)	0.042(4)
C18D	0.0764(6)	0.3152(9)	0.6038(6)	0.031(3)
C19D	0.0259(5)	0.3085(7)	0.6111(5)	0.024(3)
C20D	0.0066(5)	0.2336(7)	0.6253(5)	0.029(3)
C21D	−0.2315(5)	0.2470(9)	0.5796(6)	0.029(3)
C22D	−0.2736(5)	0.2047(10)	0.5682(6)	0.033(3)
C23D	−0.3910(7)	0.2384(11)	0.5199(7)	0.051(5)
C24D	−0.3487(7)	0.1207(13)	0.6117(6)	0.047(4)
C25D	−0.3480(7)	0.0651(10)	0.5117(7)	0.043(4)
C26D	0.0607(5)	0.5711(8)	0.5543(5)	0.025(3)
C27D	0.1013(6)	0.6832(13)	0.5110(6)	0.045(4)
C28D	0.1413(7)	0.6847(12)	0.5632(6)	0.049(5)
C29D	−0.1560(6)	0.6672(8)	0.6401(5)	0.030(3)
C30D	−0.1680(6)	0.6631(9)	0.6841(5)	0.030(3)
C31D	−0.1905(6)	0.7331(8)	0.7005(5)	0.032(3)
C32D	−0.2019(6)	0.8068(8)	0.6697(5)	0.027(3)
C33D	−0.1903(6)	0.8109(8)	0.6254(5)	0.031(3)
C34D	−0.1690(6)	0.7395(8)	0.6097(5)	0.028(3)
C35D	−0.2050(7)	0.7323(11)	0.7484(6)	0.046(4)
C36D	−0.2016(11)	0.6471(13)	0.7702(9)	0.073(6)
C37D	−0.2585(8)	0.7687(18)	0.7407(10)	0.076(6)
C38D	−0.1688(10)	0.7947(17)	0.7840(9)	0.081(7)
C39D	−0.2049(6)	0.8895(9)	0.5913(5)	0.035(3)
C40D	−0.2520(8)	0.8679(12)	0.5437(7)	0.055(5)
C41D	−0.2205(7)	0.9668(9)	0.6161(7)	0.038(4)
C42D	−0.1560(7)	0.9168(13)	0.5779(8)	0.058(5)
C43D	0.0430(5)	0.1587(8)	0.6414(5)	0.027(3)
C44D	0.0893(5)	0.1644(9)	0.6843(5)	0.031(3)
C45D	0.1236(6)	0.0947(9)	0.6984(5)	0.032(3)
C46D	0.1107(6)	0.0179(9)	0.6700(5)	0.032(3)
C47D	0.0656(5)	0.0108(7)	0.6280(4)	0.024(3)

C48D	0.0323(5)	0.0831(7)	0.6138(5)	0.024(3)
C49D	0.1747(6)	0.0973(10)	0.7449(6)	0.044(4)
C50D	0.1886(10)	0.1869(13)	0.7627(9)	0.076(7)
C51D	0.2236(8)	0.0592(16)	0.7350(9)	0.071(6)
C52D	0.1671(11)	0.0431(18)	0.7858(9)	0.091(8)
C53D	0.0511(5)	−0.0712(8)	0.5967(5)	0.028(3)
C54D	0.0610(8)	−0.0556(11)	0.5477(6)	0.042(4)
C55D	0.0851(6)	−0.1469(8)	0.6238(6)	0.033(3)
C56D	−0.0087(6)	−0.0936(11)	0.5866(7)	0.041(4)
Si1D	−0.34084(17)	0.1568(3)	0.55329(18)	0.0321(10)
S1D	0.0338(2)	0.6583(4)	0.51097(17)	0.0490(12)
S2D	0.12051(17)	0.6122(3)	0.60301(16)	0.0349(9)
Cl1	0.3674(5)	0.2039(11)	0.7559(5)	0.163(5)
C1S	0.3161(15)	0.276(2)	0.7171(13)	0.140(16)
C2S	0.310(2)	0.334(4)	0.755(2)	0.33(5)
Cl2	0.2481(6)	0.3935(6)	0.7261(6)	0.164(5)
Cl3	0.0029(10)	0.2283(16)	0.7738(9)	0.277(11)
C3S	−0.0562(16)	0.293(3)	0.7411(16)	0.156(19)
C4S	−0.057(3)	0.362(5)	0.776(2)	0.38(6)
Cl4	−0.1174(6)	0.4215(12)	0.7414(5)	0.173(6)
Cl5	−0.1573(6)	0.1263(15)	0.7540(6)	0.213(7)
C5S	−0.203(2)	0.205(3)	0.7155(16)	0.24(3)
C6S	−0.2187(14)	0.262(2)	0.7493(13)	0.116(13)
Cl6	−0.2736(9)	0.3255(17)	0.7075(8)	0.276(11)
Cl7	−0.4719(7)	0.2888(9)	0.7926(6)	0.178(6)
C7S	−0.5362(15)	0.334(3)	0.7528(16)	0.16(2)
C8S	−0.5411(12)	0.4078(19)	0.7834(12)	0.104(11)
Cl8	−0.5932(5)	0.4757(10)	0.7462(5)	0.153(5)

Table S21. Bond lengths [Å] and angles [°] for **Ni10**.

Ni1A–N1A	1.939(8)	Ni1A–N2A	1.918(9)
Ni1A–N3A	1.919(9)	Ni1A–N4A	1.910(9)
N1A–C1A	1.391(12)	N1A–C4A	1.353(12)
N2A–C6A	1.371(13)	N2A–C9A	1.369(12)
N3A–C11A	1.391(13)	N3A–C14A	1.374(12)
N4A–C16A	1.380(13)	N4A–C19A	1.397(12)
C1A–C2A	1.447(13)	C1A–C20A	1.375(13)
C2A–H2A	0.950	C2A–C3A	1.333(14)
C3A–H3A	0.950	C3A–C4A	1.435(13)
C4A–C5A	1.402(13)	C5A–C6A	1.400(13)
C5A–C21A	1.426(13)	C6A–C7A	1.434(14)
C7A–H7A	0.950	C7A–C8A	1.340(15)
C8A–H8A	0.950	C8A–C9A	1.419(13)
C9A–C10A	1.398(13)	C10A–C11A	1.390(13)
C10A–C29A	1.499(12)	C11A–C12A	1.442(13)
C12A–H12A	0.950	C12A–C13A	1.353(14)
C13A–H13A	0.950	C13A–C14A	1.428(13)
C14A–C15A	1.376(13)	C15A–C16A	1.380(13)
C15A–C26A	1.520(13)	C16A–C17A	1.420(14)
C17A–H17A	0.950	C17A–C18A	1.365(15)
C18A–H18A	0.950	C18A–C19A	1.423(14)
C19A–C20A	1.387(13)	C20A–C43A	1.500(12)
C21A–C22A	1.216(13)	C22A–Si1A	1.823(11)
C23A–H23A	0.980	C23A–H23B	0.980
C23A–H23C	0.980	C23A–Si1A	1.869(12)
C24A–H24A	0.980	C24A–H24B	0.980
C24A–H24C	0.980	C24A–Si1A	1.853(13)
C25A–H25A	0.980	C25A–H25B	0.980
C25A–H25C	0.980	C25A–Si1A	1.820(13)
C26A–H26A	1.000	C26A–S1A	1.819(12)
C26A–S2A	1.834(12)	C27A–H27A	0.990
C27A–H27B	0.990	C27A–C28A	1.474(17)
C27A–S1A	1.804(13)	C28A–H28A	0.990
C28A–H28B	0.990	C28A–S2A	1.785(14)
C29A–C30A	1.380(13)	C29A–C34A	1.393(13)
C30A–H30A	0.950	C30A–C31A	1.411(14)
C31A–C32A	1.411(14)	C31A–C35A	1.524(14)
C32A–H32A	0.950	C32A–C33A	1.387(14)
C33A–C34A	1.384(13)	C33A–C39A	1.540(13)
C34A–H34A	0.950	C35A–C36A	1.481(18)
C35A–C37A	1.465(18)	C35A–C38A	1.488(19)
C36A–H36A	0.980	C36A–H36B	0.980
C36A–H36C	0.980	C37A–H37A	0.980
C37A–H37B	0.980	C37A–H37C	0.980
C38A–H38A	0.980	C38A–H38B	0.980
C38A–H38C	0.980	C39A–C40A	1.509(16)
C39A–C41A	1.533(14)	C39A–C42A	1.552(16)
C40A–H40A	0.980	C40A–H40B	0.980
C40A–H40C	0.980	C41A–H41A	0.980

C41A–H41B	0.980	C41A–H41C	0.980
C42A–H42A	0.980	C42A–H42B	0.980
C42A–H42C	0.980	C43A–C44A	1.394(14)
C43A–C48A	1.391(13)	C44A–H44A	0.950
C44A–C45A	1.380(14)	C45A–C46A	1.417(13)
C45A–C49A	1.539(14)	C46A–H46A	0.950
C46A–C47A	1.385(13)	C47A–C48A	1.404(13)
C47A–C53A	1.542(12)	C48A–H48A	0.950
C49A–C50A	1.479(18)	C49A–C51A	1.548(17)
C49A–C52A	1.534(18)	C50A–H50A	0.980
C50A–H50B	0.980	C50A–H50C	0.980
C51A–H51A	0.980	C51A–H51B	0.980
C51A–H51C	0.980	C52A–H52A	0.980
C52A–H52B	0.980	C52A–H52C	0.980
C53A–C54A	1.508(15)	C53A–C55A	1.522(14)
C53A–C56A	1.542(15)	C54A–H54A	0.980
C54A–H54B	0.980	C54A–H54C	0.980
C55A–H55A	0.980	C55A–H55B	0.980
C55A–H55C	0.980	C56A–H56A	0.980
C56A–H56B	0.980	C56A–H56C	0.980
Ni1B–N1B	1.930(9)	Ni1B–N2B	1.919(9)
Ni1B–N3B	1.914(9)	Ni1B–N4B	1.905(9)
N1B–C1B	1.414(12)	N1B–C4B	1.373(12)
N2B–C6B	1.348(12)	N2B–C9B	1.359(13)
N3B–C11B	1.397(13)	N3B–C14B	1.360(13)
N4B–C16B	1.376(13)	N4B–C19B	1.397(13)
C1B–C2B	1.428(14)	C1B–C20B	1.365(13)
C2B–H2B	0.950	C2B–C3B	1.324(15)
C3B–H3B	0.950	C3B–C4B	1.432(14)
C4B–C5B	1.385(13)	C5B–C6B	1.409(13)
C5B–C21B	1.423(13)	C6B–C7B	1.442(14)
C7B–H7B	0.950	C7B–C8B	1.335(15)
C8B–H8B	0.950	C8B–C9B	1.432(13)
C9B–C10B	1.383(13)	C10B–C11B	1.391(13)
C10B–C29B	1.508(13)	C11B–C12B	1.428(14)
C12B–H12B	0.950	C12B–C13B	1.357(14)
C13B–H13B	0.950	C13B–C14B	1.446(13)
C14B–C15B	1.386(13)	C15B–C16B	1.386(13)
C15B–C26B	1.510(13)	C16B–C17B	1.423(14)
C17B–H17B	0.950	C17B–C18B	1.362(15)
C18B–H18B	0.950	C18B–C19B	1.417(14)
C19B–C20B	1.377(13)	C20B–C43B	1.500(12)
C21B–C22B	1.231(13)	C22B–Si1B	1.832(10)
C23B–H23D	0.980	C23B–H23E	0.980
C23B–H23F	0.980	C23B–Si1B	1.871(13)
C24B–H24D	0.980	C24B–H24E	0.980
C24B–H24F	0.980	C24B–Si1B	1.851(13)
C25B–H25D	0.980	C25B–H25E	0.980
C25B–H25F	0.980	C25B–Si1B	1.817(14)
C26B–H26B	1.000	C26B–S1B	1.819(12)
C26B–S2B	1.842(12)	C27B–H27C	0.990

C27B–H27D	0.990	C27B–C28B	1.492(17)
C27B–S1B	1.818(13)	C28B–H28C	0.990
C28B–H28D	0.990	C28B–S2B	1.785(13)
C29B–C30B	1.390(14)	C29B–C34B	1.403(13)
C30B–H30B	0.950	C30B–C31B	1.428(15)
C31B–C32B	1.397(15)	C31B–C35B	1.523(17)
C32B–H32B	0.950	C32B–C33B	1.391(14)
C33B–C34B	1.400(13)	C33B–C39B	1.547(14)
C34B–H34B	0.950	C35B–C36B	1.47(2)
C35B–C37B	1.47(2)	C35B–C38B	1.48(2)
C36B–H36D	0.980	C36B–H36E	0.980
C36B–H36F	0.980	C37B–H37D	0.980
C37B–H37E	0.980	C37B–H37F	0.980
C38B–H38D	0.980	C38B–H38E	0.980
C38B–H38F	0.980	C39B–C40B	1.521(16)
C39B–C41B	1.539(15)	C39B–C42B	1.539(16)
C40B–H40D	0.980	C40B–H40E	0.980
C40B–H40F	0.980	C41B–H41D	0.980
C41B–H41E	0.980	C41B–H41F	0.980
C42B–H42D	0.980	C42B–H42E	0.980
C42B–H42F	0.980	C43B–C44B	1.385(14)
C43B–C48B	1.395(13)	C44B–H44B	0.950
C44B–C45B	1.400(14)	C45B–C46B	1.392(14)
C45B–C49B	1.545(14)	C46B–H46B	0.950
C46B–C47B	1.395(14)	C47B–C48B	1.401(13)
C47B–C53B	1.545(14)	C48B–H48B	0.950
C49B–C50B	1.489(18)	C49B–C51B	1.526(17)
C49B–C52B	1.518(19)	C50B–H50D	0.980
C50B–H50E	0.980	C50B–H50F	0.980
C51B–H51D	0.980	C51B–H51E	0.980
C51B–H51F	0.980	C52B–H52D	0.980
C52B–H52E	0.980	C52B–H52F	0.980
C53B–C54B	1.520(16)	C53B–C55B	1.531(15)
C53B–C56B	1.519(15)	C54B–H54D	0.980
C54B–H54E	0.980	C54B–H54F	0.980
C55B–H55D	0.980	C55B–H55E	0.980
C55B–H55F	0.980	C56B–H56D	0.980
C56B–H56E	0.980	C56B–H56F	0.980
Ni1C–N1C	1.909(9)	Ni1C–N2C	1.930(9)
Ni1C–N3C	1.932(9)	Ni1C–N4C	1.908(9)
N1C–C1C	1.406(12)	N1C–C4C	1.359(12)
N2C–C6C	1.362(13)	N2C–C9C	1.366(13)
N3C–C11C	1.385(13)	N3C–C14C	1.382(13)
N4C–C16C	1.386(13)	N4C–C19C	1.396(13)
C1C–C2C	1.428(14)	C1C–C20C	1.377(13)
C2C–H2C	0.950	C2C–C3C	1.345(15)
C3C–H3C	0.950	C3C–C4C	1.425(14)
C4C–C5C	1.397(13)	C5C–C6C	1.396(13)
C5C–C21C	1.419(13)	C6C–C7C	1.439(14)
C7C–H7C	0.950	C7C–C8C	1.347(16)
C8C–H8C	0.950	C8C–C9C	1.444(14)

C9C–C10C	1.382(13)	C10C–C11C	1.396(13)
C10C–C29C	1.503(13)	C11C–C12C	1.437(14)
C12C–H12C	0.950	C12C–C13C	1.335(15)
C13C–H13C	0.950	C13C–C14C	1.443(14)
C14C–C15C	1.395(14)	C15C–C16C	1.381(14)
C15C–C26C	1.499(14)	C16C–C17C	1.425(14)
C17C–H17C	0.950	C17C–C18C	1.364(16)
C18C–H18C	0.950	C18C–C19C	1.417(14)
C19C–C20C	1.389(13)	C20C–C43C	1.496(13)
C21C–C22C	1.218(14)	C22C–Si1C	1.835(11)
C23C–H23G	0.980	C23C–H23H	0.980
C23C–H23I	0.980	C23C–Si1C	1.855(14)
C24C–H24G	0.980	C24C–H24H	0.980
C24C–H24I	0.980	C24C–Si1C	1.836(13)
C25C–H25G	0.980	C25C–H25H	0.980
C25C–H25I	0.980	C25C–Si1C	1.814(14)
C26C–H26C	1.000	C26C–S1C	1.803(12)
C26C–S2C	1.834(12)	C27C–H27E	0.990
C27C–H27F	0.990	C27C–C28C	1.518(18)
C27C–S1C	1.802(14)	C28C–H28E	0.990
C28C–H28F	0.990	C28C–S2C	1.817(14)
C29C–C30C	1.380(14)	C29C–C34C	1.391(14)
C30C–H30C	0.950	C30C–C31C	1.425(15)
C31C–C32C	1.409(15)	C31C–C35C	1.520(16)
C32C–H32C	0.950	C32C–C33C	1.387(14)
C33C–C34C	1.401(14)	C33C–C39C	1.538(14)
C34C–H34C	0.950	C35C–C36C	1.46(2)
C35C–C37C	1.45(2)	C35C–C38C	1.52(2)
C36C–H36G	0.980	C36C–H36H	0.980
C36C–H36I	0.980	C37C–H37G	0.980
C37C–H37H	0.980	C37C–H37I	0.980
C38C–H38G	0.980	C38C–H38H	0.980
C38C–H38I	0.980	C39C–C40C	1.518(16)
C39C–C41C	1.524(15)	C39C–C42C	1.538(16)
C40C–H40G	0.980	C40C–H40H	0.980
C40C–H40I	0.980	C41C–H41G	0.980
C41C–H41H	0.980	C41C–H41I	0.980
C42C–H42G	0.980	C42C–H42H	0.980
C42C–H42I	0.980	C43C–C44C	1.395(14)
C43C–C48C	1.400(13)	C44C–H44C	0.950
C44C–C45C	1.371(14)	C45C–C46C	1.414(14)
C45C–C49C	1.523(14)	C46C–H46C	0.950
C46C–C47C	1.383(14)	C47C–C48C	1.402(14)
C47C–C53C	1.536(14)	C48C–H48C	0.950
C49C–C50C	1.485(17)	C49C–C51C	1.529(17)
C49C–C52C	1.536(18)	C50C–H50G	0.980
C50C–H50H	0.980	C50C–H50I	0.980
C51C–H51G	0.980	C51C–H51H	0.980
C51C–H51I	0.980	C52C–H52G	0.980
C52C–H52H	0.980	C52C–H52I	0.980
C53C–C54C	1.530(16)	C53C–C55C	1.530(15)

C53C–C56C	1.525(15)	C54C–H54G	0.980
C54C–H54H	0.980	C54C–H54I	0.980
C55C–H55G	0.980	C55C–H55H	0.980
C55C–H55I	0.980	C56C–H56G	0.980
C56C–H56H	0.980	C56C–H56I	0.980
Ni1D–N1D	1.907(9)	Ni1D–N2D	1.931(10)
Ni1D–N3D	1.954(9)	Ni1D–N4D	1.905(9)
N1D–C1D	1.403(13)	N1D–C4D	1.373(13)
N2D–C6D	1.345(13)	N2D–C9D	1.375(13)
N3D–C11D	1.397(12)	N3D–C14D	1.353(13)
N4D–C16D	1.360(13)	N4D–C19D	1.406(13)
C1D–C2D	1.431(14)	C1D–C20D	1.384(13)
C2D–H2D	0.950	C2D–C3D	1.327(15)
C3D–H3D	0.950	C3D–C4D	1.423(14)
C4D–C5D	1.382(14)	C5D–C6D	1.418(14)
C5D–C21D	1.422(14)	C6D–C7D	1.429(15)
C7D–H7D	0.950	C7D–C8D	1.345(15)
C8D–H8D	0.950	C8D–C9D	1.414(14)
C9D–C10D	1.393(13)	C10D–C11D	1.387(13)
C10D–C29D	1.500(13)	C11D–C12D	1.426(14)
C12D–H12D	0.950	C12D–C13D	1.339(15)
C13D–H13D	0.950	C13D–C14D	1.436(13)
C14D–C15D	1.404(13)	C15D–C16D	1.381(13)
C15D–C26D	1.489(13)	C16D–C17D	1.444(15)
C17D–H17D	0.950	C17D–C18D	1.361(16)
C18D–H18D	0.950	C18D–C19D	1.416(14)
C19D–C20D	1.391(13)	C20D–C43D	1.485(13)
C21D–C22D	1.235(14)	C22D–Si1D	1.834(11)
C23D–H23J	0.980	C23D–H23K	0.980
C23D–H23L	0.980	C23D–Si1D	1.851(14)
C24D–H24J	0.980	C24D–H24K	0.980
C24D–H24L	0.980	C24D–Si1D	1.834(14)
C25D–H25J	0.980	C25D–H25K	0.980
C25D–H25L	0.980	C25D–Si1D	1.829(13)
C26D–H26D	1.000	C26D–S1D	1.815(12)
C26D–S2D	1.826(12)	C27D–H27G	0.990
C27D–H27H	0.990	C27D–C28D	1.500(17)
C27D–S1D	1.815(14)	C28D–H28G	0.990
C28D–H28H	0.990	C28D–S2D	1.814(14)
C29D–C30D	1.394(14)	C29D–C34D	1.394(14)
C30D–H30D	0.950	C30D–C31D	1.398(14)
C31D–C32D	1.417(14)	C31D–C35D	1.536(15)
C32D–H32D	0.950	C32D–C33D	1.398(14)
C33D–C34D	1.390(14)	C33D–C39D	1.534(14)
C34D–H34D	0.950	C35D–C36D	1.461(19)
C35D–C37D	1.462(19)	C35D–C38D	1.49(2)
C36D–H36J	0.980	C36D–H36K	0.980
C36D–H36L	0.980	C37D–H37J	0.980
C37D–H37K	0.980	C37D–H37L	0.980
C38D–H38J	0.980	C38D–H38K	0.980
C38D–H38L	0.980	C39D–C40D	1.532(17)

C39D–C41D	1.527(15)	C39D–C42D	1.520(16)
C40D–H40J	0.980	C40D–H40K	0.980
C40D–H40L	0.980	C41D–H41J	0.980
C41D–H41K	0.980	C41D–H41L	0.980
C42D–H42J	0.980	C42D–H42K	0.980
C42D–H42L	0.980	C43D–C44D	1.405(14)
C43D–C48D	1.396(13)	C44D–H44D	0.950
C44D–C45D	1.385(14)	C45D–C46D	1.426(14)
C45D–C49D	1.533(15)	C46D–H46D	0.950
C46D–C47D	1.373(14)	C47D–C48D	1.405(13)
C47D–C53D	1.536(13)	C48D–H48D	0.950
C49D–C50D	1.494(18)	C49D–C51D	1.526(18)
C49D–C52D	1.508(19)	C50D–H50J	0.980
C50D–H50K	0.980	C50D–H50L	0.980
C51D–H51J	0.980	C51D–H51K	0.980
C51D–H51L	0.980	C52D–H52J	0.980
C52D–H52K	0.980	C52D–H52L	0.980
C53D–C54D	1.522(15)	C53D–C55D	1.526(14)
C53D–C56D	1.541(15)	C54D–H54J	0.980
C54D–H54K	0.980	C54D–H54L	0.980
C55D–H55J	0.980	C55D–H55K	0.980
C55D–H55L	0.980	C56D–H56J	0.980
C56D–H56K	0.980	C56D–H56L	0.980
Cl1–C1S	1.82(2)	C1S–H1S1	0.990
C1S–H1S2	0.990	C1S–C2S	1.47(4)
C2S–H2S1	0.990	C2S–H2S2	0.990
C2S–Cl2	1.81(2)	Cl3–C3S	1.83(2)
C3S–H3S1	0.990	C3S–H3S2	0.990
C3S–C4S	1.47(4)	C4S–H4S1	0.990
C4S–H4S2	0.990	C4S–Cl4	1.82(3)
Cl5–C5S	1.81(2)	C5S–H5S1	0.990
C5S–H5S2	0.990	C5S–C6S	1.47(4)
C6S–H6S1	0.990	C6S–H6S2	0.990
C6S–Cl6	1.82(2)	Cl7–C7S	1.83(2)
C7S–H7S1	0.990	C7S–H7S2	0.990
C7S–C8S	1.48(4)	C8S–H8S1	0.990
C8S–H8S2	0.990	C8S–Cl8	1.77(2)
N1A–Ni1A–N2A	89.3(4)	N1A–Ni1A–N3A	177.6(5)
N1A–Ni1A–N4A	89.9(4)	N2A–Ni1A–N3A	90.7(4)
N2A–Ni1A–N4A	177.7(5)	N3A–Ni1A–N4A	90.1(4)
Ni1A–N1A–C1A	126.4(7)	Ni1A–N1A–C4A	128.3(7)
C1A–N1A–C4A	105.2(8)	Ni1A–N2A–C6A	127.2(8)
Ni1A–N2A–C9A	128.2(7)	C6A–N2A–C9A	104.3(9)
Ni1A–N3A–C11A	124.6(8)	Ni1A–N3A–C14A	128.0(7)
C11A–N3A–C14A	106.5(8)	Ni1A–N4A–C16A	126.5(8)
Ni1A–N4A–C19A	127.7(8)	C16A–N4A–C19A	105.8(9)
N1A–C1A–C2A	109.0(9)	N1A–C1A–C20A	125.7(10)
C2A–C1A–C20A	124.7(10)	C1A–C2A–H2A	126.2
C1A–C2A–C3A	107.5(10)	H2A–C2A–C3A	126.2
C2A–C3A–H3A	126.7	C2A–C3A–C4A	106.6(10)

H3A-C3A-C4A	126.7	N1A-C4A-C3A	111.4(9)
N1A-C4A-C5A	124.3(10)	C3A-C4A-C5A	124.3(11)
C4A-C5A-C6A	120.8(10)	C4A-C5A-C21A	119.3(10)
C6A-C5A-C21A	119.1(10)	N2A-C6A-C5A	124.8(10)
N2A-C6A-C7A	111.3(10)	C5A-C6A-C7A	123.4(11)
C6A-C7A-H7A	127.2	C6A-C7A-C8A	105.7(11)
H7A-C7A-C8A	127.2	C7A-C8A-H8A	126.1
C7A-C8A-C9A	107.9(11)	H8A-C8A-C9A	126.1
N2A-C9A-C8A	110.8(9)	N2A-C9A-C10A	123.6(10)
C8A-C9A-C10A	125.7(10)	C9A-C10A-C11A	121.6(10)
C9A-C10A-C29A	117.3(10)	C11A-C10A-C29A	120.2(10)
N3A-C11A-C10A	125.5(10)	N3A-C11A-C12A	109.3(9)
C10A-C11A-C12A	124.6(10)	C11A-C12A-H12A	126.8
C11A-C12A-C13A	106.3(10)	H12A-C12A-C13A	126.8
C12A-C13A-H13A	125.7	C12A-C13A-C14A	108.6(10)
H13A-C13A-C14A	125.7	N3A-C14A-C13A	109.1(9)
N3A-C14A-C15A	123.9(10)	C13A-C14A-C15A	126.9(10)
C14A-C15A-C16A	121.7(10)	C14A-C15A-C26A	120.5(10)
C16A-C15A-C26A	117.5(10)	N4A-C16A-C15A	125.0(10)
N4A-C16A-C17A	110.0(9)	C15A-C16A-C17A	123.8(11)
C16A-C17A-H17A	126.2	C16A-C17A-C18A	107.5(11)
H17A-C17A-C18A	126.2	C17A-C18A-H18A	126.4
C17A-C18A-C19A	107.2(11)	H18A-C18A-C19A	126.4
N4A-C19A-C18A	109.5(10)	N4A-C19A-C20A	125.2(10)
C18A-C19A-C20A	124.5(11)	C1A-C20A-C19A	121.7(10)
C1A-C20A-C43A	120.3(10)	C19A-C20A-C43A	117.8(10)
C5A-C21A-C22A	175.2(15)	C21A-C22A-Si1A	171.9(13)
H23A-C23A-H23B	109.5	H23A-C23A-H23C	109.5
H23A-C23A-Si1A	109.5	H23B-C23A-H23C	109.5
H23B-C23A-Si1A	109.5	H23C-C23A-Si1A	109.5
H24A-C24A-H24B	109.5	H24A-C24A-H24C	109.5
H24A-C24A-Si1A	109.5	H24B-C24A-H24C	109.5
H24B-C24A-Si1A	109.5	H24C-C24A-Si1A	109.5
H25A-C25A-H25B	109.5	H25A-C25A-H25C	109.5
H25A-C25A-Si1A	109.5	H25B-C25A-H25C	109.5
H25B-C25A-Si1A	109.5	H25C-C25A-Si1A	109.5
C15A-C26A-H26A	105.7	C15A-C26A-S1A	118.5(9)
C15A-C26A-S2A	113.5(9)	H26A-C26A-S1A	105.7
H26A-C26A-S2A	105.7	S1A-C26A-S2A	106.7(6)
H27A-C27A-H27B	107.8	H27A-C27A-C28A	109.1
H27A-C27A-S1A	109.1	H27B-C27A-C28A	109.1
H27B-C27A-S1A	109.1	C28A-C27A-S1A	112.4(10)
C27A-C28A-H28A	108.6	C27A-C28A-H28B	108.6
C27A-C28A-S2A	114.7(11)	H28A-C28A-H28B	107.6
H28A-C28A-S2A	108.6	H28B-C28A-S2A	108.6
C10A-C29A-C30A	118.0(10)	C10A-C29A-C34A	122.0(10)
C30A-C29A-C34A	120.0(10)	C29A-C30A-H30A	119.9
C29A-C30A-C31A	120.2(10)	H30A-C30A-C31A	119.9
C30A-C31A-C32A	118.2(10)	C30A-C31A-C35A	118.9(10)
C32A-C31A-C35A	122.9(11)	C31A-C32A-H32A	119.2
C31A-C32A-C33A	121.6(11)	H32A-C32A-C33A	119.2

C32A-C33A-C34A	118.4(10)	C32A-C33A-C39A	121.1(10)
C34A-C33A-C39A	120.5(10)	C29A-C34A-C33A	121.5(10)
C29A-C34A-H34A	119.2	C33A-C34A-H34A	119.2
C31A-C35A-C36A	111.1(12)	C31A-C35A-C37A	112.5(13)
C31A-C35A-C38A	109.8(13)	C36A-C35A-C37A	112.1(15)
C36A-C35A-C38A	104.8(15)	C37A-C35A-C38A	106.1(16)
C35A-C36A-H36A	109.5	C35A-C36A-H36B	109.5
C35A-C36A-H36C	109.5	H36A-C36A-H36B	109.5
H36A-C36A-H36C	109.5	H36B-C36A-H36C	109.5
C35A-C37A-H37A	109.5	C35A-C37A-H37B	109.5
C35A-C37A-H37C	109.5	H37A-C37A-H37B	109.5
H37A-C37A-H37C	109.5	H37B-C37A-H37C	109.5
C35A-C38A-H38A	109.5	C35A-C38A-H38B	109.5
C35A-C38A-H38C	109.5	H38A-C38A-H38B	109.5
H38A-C38A-H38C	109.5	H38B-C38A-H38C	109.5
C33A-C39A-C40A	110.3(11)	C33A-C39A-C41A	114.3(11)
C33A-C39A-C42A	107.7(12)	C40A-C39A-C41A	110.6(12)
C40A-C39A-C42A	109.5(14)	C41A-C39A-C42A	104.2(13)
C39A-C40A-H40A	109.5	C39A-C40A-H40B	109.5
C39A-C40A-H40C	109.5	H40A-C40A-H40B	109.5
H40A-C40A-H40C	109.5	H40B-C40A-H40C	109.5
C39A-C41A-H41A	109.5	C39A-C41A-H41B	109.5
C39A-C41A-H41C	109.5	H41A-C41A-H41B	109.5
H41A-C41A-H41C	109.5	H41B-C41A-H41C	109.5
C39A-C42A-H42A	109.5	C39A-C42A-H42B	109.5
C39A-C42A-H42C	109.5	H42A-C42A-H42B	109.5
H42A-C42A-H42C	109.5	H42B-C42A-H42C	109.5
C20A-C43A-C44A	119.1(10)	C20A-C43A-C48A	120.3(10)
C44A-C43A-C48A	120.5(10)	C43A-C44A-H44A	119.6
C43A-C44A-C45A	120.8(11)	H44A-C44A-C45A	119.6
C44A-C45A-C46A	118.1(10)	C44A-C45A-C49A	122.3(11)
C46A-C45A-C49A	119.5(10)	C45A-C46A-H46A	119.1
C45A-C46A-C47A	121.9(10)	H46A-C46A-C47A	119.1
C46A-C47A-C48A	118.7(10)	C46A-C47A-C53A	123.0(10)
C48A-C47A-C53A	118.2(10)	C43A-C48A-C47A	119.9(10)
C43A-C48A-H48A	120.1	C47A-C48A-H48A	120.1
C45A-C49A-C50A	112.8(13)	C45A-C49A-C51A	111.2(12)
C45A-C49A-C52A	108.5(12)	C50A-C49A-C51A	103.2(15)
C50A-C49A-C52A	114.2(16)	C51A-C49A-C52A	106.7(14)
C49A-C50A-H50A	109.5	C49A-C50A-H50B	109.5
C49A-C50A-H50C	109.5	H50A-C50A-H50B	109.5
H50A-C50A-H50C	109.5	H50B-C50A-H50C	109.5
C49A-C51A-H51A	109.5	C49A-C51A-H51B	109.5
C49A-C51A-H51C	109.5	H51A-C51A-H51B	109.5
H51A-C51A-H51C	109.5	H51B-C51A-H51C	109.5
C49A-C52A-H52A	109.5	C49A-C52A-H52B	109.5
C49A-C52A-H52C	109.5	H52A-C52A-H52B	109.5
H52A-C52A-H52C	109.5	H52B-C52A-H52C	109.5
C47A-C53A-C54A	109.9(10)	C47A-C53A-C55A	111.0(10)
C47A-C53A-C56A	110.8(11)	C54A-C53A-C55A	109.4(11)
C54A-C53A-C56A	109.0(11)	C55A-C53A-C56A	106.7(11)

C53A–C54A–H54A	109.5	C53A–C54A–H54B	109.5
C53A–C54A–H54C	109.5	H54A–C54A–H54B	109.5
H54A–C54A–H54C	109.5	H54B–C54A–H54C	109.5
C53A–C55A–H55A	109.5	C53A–C55A–H55B	109.5
C53A–C55A–H55C	109.5	H55A–C55A–H55B	109.5
H55A–C55A–H55C	109.5	H55B–C55A–H55C	109.5
C53A–C56A–H56A	109.5	C53A–C56A–H56B	109.5
C53A–C56A–H56C	109.5	H56A–C56A–H56B	109.5
H56A–C56A–H56C	109.5	H56B–C56A–H56C	109.5
C22A–Si1A–C23A	105.9(7)	C22A–Si1A–C24A	109.0(7)
C22A–Si1A–C25A	108.5(7)	C23A–Si1A–C24A	110.7(8)
C23A–Si1A–C25A	109.7(8)	C24A–Si1A–C25A	112.7(9)
C26A–S1A–C27A	91.0(7)	C26A–S2A–C28A	92.8(7)
N1B–Ni1B–N2B	89.7(4)	N1B–Ni1B–N3B	177.9(5)
N1B–Ni1B–N4B	89.6(4)	N2B–Ni1B–N3B	90.8(4)
N2B–Ni1B–N4B	179.0(5)	N3B–Ni1B–N4B	89.9(4)
Ni1B–N1B–C1B	128.2(7)	Ni1B–N1B–C4B	128.1(8)
C1B–N1B–C4B	103.5(8)	Ni1B–N2B–C6B	126.6(8)
Ni1B–N2B–C9B	127.1(7)	C6B–N2B–C9B	105.9(9)
Ni1B–N3B–C11B	126.3(8)	Ni1B–N3B–C14B	127.6(8)
C11B–N3B–C14B	106.1(9)	Ni1B–N4B–C16B	126.6(8)
Ni1B–N4B–C19B	127.4(8)	C16B–N4B–C19B	105.9(9)
N1B–C1B–C2B	109.6(9)	N1B–C1B–C20B	122.7(10)
C2B–C1B–C20B	127.2(10)	C1B–C2B–H2B	125.8
C1B–C2B–C3B	108.4(11)	H2B–C2B–C3B	125.8
C2B–C3B–H3B	126.6	C2B–C3B–C4B	106.8(11)
H3B–C3B–C4B	126.6	N1B–C4B–C3B	111.7(10)
N1B–C4B–C5B	123.9(10)	C3B–C4B–C5B	124.4(11)
C4B–C5B–C6B	120.8(10)	C4B–C5B–C21B	120.0(11)
C6B–C5B–C21B	118.8(10)	N2B–C6B–C5B	125.4(10)
N2B–C6B–C7B	111.0(10)	C5B–C6B–C7B	123.0(10)
C6B–C7B–H7B	127.2	C6B–C7B–C8B	105.5(11)
H7B–C7B–C8B	127.2	C7B–C8B–H8B	126.1
C7B–C8B–C9B	107.8(11)	H8B–C8B–C9B	126.1
N2B–C9B–C8B	109.7(9)	N2B–C9B–C10B	126.0(10)
C8B–C9B–C10B	123.7(10)	C9B–C10B–C11B	122.4(10)
C9B–C10B–C29B	118.5(10)	C11B–C10B–C29B	119.1(10)
N3B–C11B–C10B	123.7(10)	N3B–C11B–C12B	109.3(9)
C10B–C11B–C12B	125.7(11)	C11B–C12B–H12B	126.2
C11B–C12B–C13B	107.5(11)	H12B–C12B–C13B	126.2
C12B–C13B–H13B	126.7	C12B–C13B–C14B	106.7(10)
H13B–C13B–C14B	126.7	N3B–C14B–C13B	110.2(9)
N3B–C14B–C15B	124.7(10)	C13B–C14B–C15B	124.6(10)
C14B–C15B–C16B	120.6(10)	C14B–C15B–C26B	123.2(10)
C16B–C15B–C26B	115.8(10)	N4B–C16B–C15B	125.0(10)
N4B–C16B–C17B	109.6(9)	C15B–C16B–C17B	125.4(11)
C16B–C17B–H17B	126.4	C16B–C17B–C18B	107.3(11)
H17B–C17B–C18B	126.4	C17B–C18B–H18B	126.4
C17B–C18B–C19B	107.2(11)	H18B–C18B–C19B	126.4
N4B–C19B–C18B	109.4(10)	N4B–C19B–C20B	125.6(10)
C18B–C19B–C20B	124.7(11)	C1B–C20B–C19B	123.1(10)

C1B-C20B-C43B	120.0(10)	C19B-C20B-C43B	116.8(10)
C5B-C21B-C22B	177.6(16)	C21B-C22B-Si1B	174.0(14)
H23D-C23B-H23E	109.5	H23D-C23B-H23F	109.5
H23D-C23B-Si1B	109.5	H23E-C23B-H23F	109.5
H23E-C23B-Si1B	109.5	H23F-C23B-Si1B	109.5
H24D-C24B-H24E	109.5	H24D-C24B-H24F	109.5
H24D-C24B-Si1B	109.5	H24E-C24B-H24F	109.5
H24E-C24B-Si1B	109.5	H24F-C24B-Si1B	109.5
H25D-C25B-H25E	109.5	H25D-C25B-H25F	109.5
H25D-C25B-Si1B	109.5	H25E-C25B-H25F	109.5
H25E-C25B-Si1B	109.5	H25F-C25B-Si1B	109.5
C15B-C26B-H26B	106.6	C15B-C26B-S1B	116.8(9)
C15B-C26B-S2B	114.0(9)	H26B-C26B-S1B	106.6
H26B-C26B-S2B	106.6	S1B-C26B-S2B	105.6(6)
H27C-C27B-H27D	108.0	H27C-C27B-C28B	109.3
H27C-C27B-S1B	109.3	H27D-C27B-C28B	109.3
H27D-C27B-S1B	109.3	C28B-C27B-S1B	111.5(10)
C27B-C28B-H28C	109.1	C27B-C28B-H28D	109.1
C27B-C28B-S2B	112.6(10)	H28C-C28B-H28D	107.8
H28C-C28B-S2B	109.1	H28D-C28B-S2B	109.1
C10B-C29B-C30B	121.4(11)	C10B-C29B-C34B	117.7(10)
C30B-C29B-C34B	120.6(11)	C29B-C30B-H30B	119.8
C29B-C30B-C31B	120.4(12)	H30B-C30B-C31B	119.8
C30B-C31B-C32B	117.4(12)	C30B-C31B-C35B	121.0(13)
C32B-C31B-C35B	121.4(13)	C31B-C32B-H32B	118.8
C31B-C32B-C33B	122.4(12)	H32B-C32B-C33B	118.8
C32B-C33B-C34B	119.5(11)	C32B-C33B-C39B	121.5(11)
C34B-C33B-C39B	119.0(10)	C29B-C34B-C33B	119.5(11)
C29B-C34B-H34B	120.2	C33B-C34B-H34B	120.2
C31B-C35B-C36B	113.2(16)	C31B-C35B-C37B	113.4(17)
C31B-C35B-C38B	112.3(18)	C36B-C35B-C37B	103.8(19)
C36B-C35B-C38B	113(2)	C37B-C35B-C38B	100.4(19)
C35B-C36B-H36D	109.5	C35B-C36B-H36E	109.5
C35B-C36B-H36F	109.5	H36D-C36B-H36E	109.5
H36D-C36B-H36F	109.5	H36E-C36B-H36F	109.5
C35B-C37B-H37D	109.5	C35B-C37B-H37E	109.5
C35B-C37B-H37F	109.5	H37D-C37B-H37E	109.5
H37D-C37B-H37F	109.5	H37E-C37B-H37F	109.5
C35B-C38B-H38D	109.5	C35B-C38B-H38E	109.5
C35B-C38B-H38F	109.5	H38D-C38B-H38E	109.5
H38D-C38B-H38F	109.5	H38E-C38B-H38F	109.5
C33B-C39B-C40B	111.1(12)	C33B-C39B-C41B	113.1(11)
C33B-C39B-C42B	109.4(12)	C40B-C39B-C41B	108.8(13)
C40B-C39B-C42B	109.2(13)	C41B-C39B-C42B	105.0(12)
C39B-C40B-H40D	109.5	C39B-C40B-H40E	109.5
C39B-C40B-H40F	109.5	H40D-C40B-H40E	109.5
H40D-C40B-H40F	109.5	H40E-C40B-H40F	109.5
C39B-C41B-H41D	109.5	C39B-C41B-H41E	109.5
C39B-C41B-H41F	109.5	H41D-C41B-H41E	109.5
H41D-C41B-H41F	109.5	H41E-C41B-H41F	109.5
C39B-C42B-H42D	109.5	C39B-C42B-H42E	109.5

C39B–C42B–H42F	109.5	H42D–C42B–H42E	109.5
H42D–C42B–H42F	109.5	H42E–C42B–H42F	109.5
C20B–C43B–C44B	119.4(10)	C20B–C43B–C48B	120.2(10)
C44B–C43B–C48B	120.3(10)	C43B–C44B–H44B	119.7
C43B–C44B–C45B	120.6(11)	H44B–C44B–C45B	119.7
C44B–C45B–C46B	118.5(11)	C44B–C45B–C49B	122.2(10)
C46B–C45B–C49B	119.1(10)	C45B–C46B–H46B	119.3
C45B–C46B–C47B	121.4(11)	H46B–C46B–C47B	119.3
C46B–C47B–C48B	119.1(10)	C46B–C47B–C53B	122.0(10)
C48B–C47B–C53B	118.8(10)	C43B–C48B–C47B	119.8(10)
C43B–C48B–H48B	120.1	C47B–C48B–H48B	120.1
C45B–C49B–C50B	112.5(12)	C45B–C49B–C51B	108.2(13)
C45B–C49B–C52B	109.0(13)	C50B–C49B–C51B	108.0(15)
C50B–C49B–C52B	111.7(16)	C51B–C49B–C52B	107.1(16)
C49B–C50B–H50D	109.5	C49B–C50B–H50E	109.5
C49B–C50B–H50F	109.5	H50D–C50B–H50E	109.5
H50D–C50B–H50F	109.5	H50E–C50B–H50F	109.5
C49B–C51B–H51D	109.5	C49B–C51B–H51E	109.5
C49B–C51B–H51F	109.5	H51D–C51B–H51E	109.5
H51D–C51B–H51F	109.5	H51E–C51B–H51F	109.5
C49B–C52B–H52D	109.5	C49B–C52B–H52E	109.5
C49B–C52B–H52F	109.5	H52D–C52B–H52E	109.5
H52D–C52B–H52F	109.5	H52E–C52B–H52F	109.5
C47B–C53B–C54B	107.9(12)	C47B–C53B–C55B	109.9(11)
C47B–C53B–C56B	111.5(12)	C54B–C53B–C55B	105.6(13)
C54B–C53B–C56B	113.8(14)	C55B–C53B–C56B	108.0(13)
C53B–C54B–H54D	109.5	C53B–C54B–H54E	109.5
C53B–C54B–H54F	109.5	H54D–C54B–H54E	109.5
H54D–C54B–H54F	109.5	H54E–C54B–H54F	109.5
C53B–C55B–H55D	109.5	C53B–C55B–H55E	109.5
C53B–C55B–H55F	109.5	H55D–C55B–H55E	109.5
H55D–C55B–H55F	109.5	H55E–C55B–H55F	109.5
C53B–C56B–H56D	109.5	C53B–C56B–H56E	109.5
C53B–C56B–H56F	109.5	H56D–C56B–H56E	109.5
H56D–C56B–H56F	109.5	H56E–C56B–H56F	109.5
C22B–Si1B–C23B	106.9(7)	C22B–Si1B–C24B	108.5(7)
C22B–Si1B–C25B	109.5(8)	C23B–Si1B–C24B	110.0(8)
C23B–Si1B–C25B	110.4(8)	C24B–Si1B–C25B	111.4(9)
C26B–S1B–C27B	90.4(6)	C26B–S2B–C28B	95.1(6)
N1C–Ni1C–N2C	90.2(4)	N1C–Ni1C–N3C	178.6(6)
N1C–Ni1C–N4C	91.2(4)	N2C–Ni1C–N3C	89.3(4)
N2C–Ni1C–N4C	178.4(5)	N3C–Ni1C–N4C	89.4(4)
Ni1C–N1C–C1C	125.9(8)	Ni1C–N1C–C4C	128.4(8)
C1C–N1C–C4C	105.6(9)	Ni1C–N2C–C6C	126.0(8)
Ni1C–N2C–C9C	128.3(8)	C6C–N2C–C9C	105.6(9)
Ni1C–N3C–C11C	126.2(8)	Ni1C–N3C–C14C	127.0(8)
C11C–N3C–C14C	106.1(9)	Ni1C–N4C–C16C	127.8(8)
Ni1C–N4C–C19C	127.2(8)	C16C–N4C–C19C	104.7(9)
N1C–C1C–C2C	108.6(10)	N1C–C1C–C20C	125.1(10)
C2C–C1C–C20C	126.2(11)	C1C–C2C–H2C	126.2
C1C–C2C–C3C	107.6(11)	H2C–C2C–C3C	126.2

C2C–C3C–H3C	126.4	C2C–C3C–C4C	107.2(11)
H3C–C3C–C4C	126.4	N1C–C4C–C3C	110.6(10)
N1C–C4C–C5C	124.4(10)	C3C–C4C–C5C	124.6(11)
C4C–C5C–C6C	121.5(10)	C4C–C5C–C21C	118.2(11)
C6C–C5C–C21C	120.1(11)	N2C–C6C–C5C	125.4(10)
N2C–C6C–C7C	111.1(10)	C5C–C6C–C7C	122.5(11)
C6C–C7C–H7C	127.0	C6C–C7C–C8C	105.9(12)
H7C–C7C–C8C	127.0	C7C–C8C–H8C	126.3
C7C–C8C–C9C	107.4(11)	H8C–C8C–C9C	126.3
N2C–C9C–C8C	109.9(10)	N2C–C9C–C10C	125.4(10)
C8C–C9C–C10C	124.5(11)	C9C–C10C–C11C	121.3(10)
C9C–C10C–C29C	119.0(10)	C11C–C10C–C29C	119.5(10)
N3C–C11C–C10C	125.0(10)	N3C–C11C–C12C	109.2(10)
C10C–C11C–C12C	124.5(11)	C11C–C12C–H12C	126.1
C11C–C12C–C13C	107.8(11)	H12C–C12C–C13C	126.1
C12C–C13C–H13C	126.2	C12C–C13C–C14C	107.6(11)
H13C–C13C–C14C	126.2	N3C–C14C–C13C	109.0(10)
N3C–C14C–C15C	125.4(10)	C13C–C14C–C15C	125.5(11)
C14C–C15C–C16C	120.0(11)	C14C–C15C–C26C	122.5(11)
C16C–C15C–C26C	117.4(11)	N4C–C16C–C15C	124.6(11)
N4C–C16C–C17C	111.1(10)	C15C–C16C–C17C	122.8(11)
C16C–C17C–H17C	127.0	C16C–C17C–C18C	106.0(11)
H17C–C17C–C18C	127.0	C17C–C18C–H18C	125.9
C17C–C18C–C19C	108.3(11)	H18C–C18C–C19C	125.8
N4C–C19C–C18C	109.8(10)	N4C–C19C–C20C	124.5(10)
C18C–C19C–C20C	125.6(11)	C1C–C20C–C19C	121.9(10)
C1C–C20C–C43C	120.1(10)	C19C–C20C–C43C	117.5(10)
C5C–C21C–C22C	179.4(18)	C21C–C22C–Si1C	175.2(16)
H23G–C23C–H23H	109.5	H23G–C23C–H23I	109.5
H23G–C23C–Si1C	109.5	H23H–C23C–H23I	109.5
H23H–C23C–Si1C	109.5	H23I–C23C–Si1C	109.5
H24G–C24C–H24H	109.5	H24G–C24C–H24I	109.5
H24G–C24C–Si1C	109.5	H24H–C24C–H24I	109.5
H24H–C24C–Si1C	109.5	H24I–C24C–Si1C	109.5
H25G–C25C–H25H	109.5	H25G–C25C–H25I	109.5
H25G–C25C–Si1C	109.5	H25H–C25C–H25I	109.5
H25H–C25C–Si1C	109.5	H25I–C25C–Si1C	109.5
C15C–C26C–H26C	106.6	C15C–C26C–S1C	117.6(9)
C15C–C26C–S2C	112.0(9)	H26C–C26C–S1C	106.6
H26C–C26C–S2C	106.6	S1C–C26C–S2C	106.9(7)
H27E–C27C–H27F	108.0	H27E–C27C–C28C	109.4
H27E–C27C–S1C	109.4	H27F–C27C–C28C	109.4
H27F–C27C–S1C	109.4	C28C–C27C–S1C	111.4(11)
C27C–C28C–H28E	109.3	C27C–C28C–H28F	109.3
C27C–C28C–S2C	111.7(11)	H28E–C28C–H28F	107.9
H28E–C28C–S2C	109.3	H28F–C28C–S2C	109.3
C10C–C29C–C30C	119.8(11)	C10C–C29C–C34C	120.6(11)
C30C–C29C–C34C	119.6(11)	C29C–C30C–H30C	118.9
C29C–C30C–C31C	122.2(12)	H30C–C30C–C31C	118.9
C30C–C31C–C32C	115.7(12)	C30C–C31C–C35C	119.4(12)
C32C–C31C–C35C	124.8(13)	C31C–C32C–H32C	118.3

C31C-C32C-C33C	123.3(12)	H32C-C32C-C33C	118.3
C32C-C33C-C34C	118.2(11)	C32C-C33C-C39C	121.5(11)
C34C-C33C-C39C	120.3(11)	C29C-C34C-C33C	120.9(11)
C29C-C34C-H34C	119.5	C33C-C34C-H34C	119.5
C31C-C35C-C36C	112.3(16)	C31C-C35C-C37C	117.3(16)
C31C-C35C-C38C	109.4(15)	C36C-C35C-C37C	116.2(18)
C36C-C35C-C38C	102.7(17)	C37C-C35C-C38C	96.3(17)
C35C-C36C-H36G	109.5	C35C-C36C-H36H	109.5
C35C-C36C-H36I	109.5	H36G-C36C-H36H	109.5
H36G-C36C-H36I	109.5	H36H-C36C-H36I	109.5
C35C-C37C-H37G	109.5	C35C-C37C-H37H	109.5
C35C-C37C-H37I	109.5	H37G-C37C-H37H	109.5
H37G-C37C-H37I	109.5	H37H-C37C-H37I	109.5
C35C-C38C-H38G	109.5	C35C-C38C-H38H	109.5
C35C-C38C-H38I	109.5	H38G-C38C-H38H	109.5
H38G-C38C-H38I	109.5	H38H-C38C-H38I	109.5
C33C-C39C-C40C	108.1(12)	C33C-C39C-C41C	113.4(12)
C33C-C39C-C42C	109.2(12)	C40C-C39C-C41C	111.0(13)
C40C-C39C-C42C	109.0(14)	C41C-C39C-C42C	106.0(13)
C39C-C40C-H40G	109.5	C39C-C40C-H40H	109.5
C39C-C40C-H40I	109.5	H40G-C40C-H40H	109.5
H40G-C40C-H40I	109.5	H40H-C40C-H40I	109.5
C39C-C41C-H41G	109.5	C39C-C41C-H41H	109.5
C39C-C41C-H41I	109.5	H41G-C41C-H41H	109.5
H41G-C41C-H41I	109.5	H41H-C41C-H41I	109.5
C39C-C42C-H42G	109.5	C39C-C42C-H42H	109.5
C39C-C42C-H42I	109.5	H42G-C42C-H42H	109.5
H42G-C42C-H42I	109.5	H42H-C42C-H42I	109.5
C20C-C43C-C44C	119.7(10)	C20C-C43C-C48C	121.4(10)
C44C-C43C-C48C	118.9(10)	C43C-C44C-H44C	119.3
C43C-C44C-C45C	121.5(11)	H44C-C44C-C45C	119.3
C44C-C45C-C46C	118.3(11)	C44C-C45C-C49C	120.9(11)
C46C-C45C-C49C	120.8(11)	C45C-C46C-H46C	118.9
C45C-C46C-C47C	122.2(11)	H46C-C46C-C47C	118.9
C46C-C47C-C48C	117.7(11)	C46C-C47C-C53C	123.2(11)
C48C-C47C-C53C	119.0(11)	C43C-C48C-C47C	121.2(11)
C43C-C48C-H48C	119.4	C47C-C48C-H48C	119.4
C45C-C49C-C50C	113.5(13)	C45C-C49C-C51C	111.1(13)
C45C-C49C-C52C	108.7(13)	C50C-C49C-C51C	105.9(15)
C50C-C49C-C52C	109.7(16)	C51C-C49C-C52C	107.8(15)
C49C-C50C-H50G	109.5	C49C-C50C-H50H	109.5
C49C-C50C-H50I	109.5	H50G-C50C-H50H	109.5
H50G-C50C-H50I	109.5	H50H-C50C-H50I	109.5
C49C-C51C-H51G	109.5	C49C-C51C-H51H	109.5
C49C-C51C-H51I	109.5	H51G-C51C-H51H	109.5
H51G-C51C-H51I	109.5	H51H-C51C-H51I	109.5
C49C-C52C-H52G	109.5	C49C-C52C-H52H	109.5
C49C-C52C-H52I	109.5	H52G-C52C-H52H	109.5
H52G-C52C-H52I	109.5	H52H-C52C-H52I	109.5
C47C-C53C-C54C	110.1(12)	C47C-C53C-C55C	111.1(11)
C47C-C53C-C56C	111.9(12)	C54C-C53C-C55C	107.5(12)

C54C–C53C–C56C	107.4(13)	C55C–C53C–C56C	108.6(12)
C53C–C54C–H54G	109.5	C53C–C54C–H54H	109.5
C53C–C54C–H54I	109.5	H54G–C54C–H54H	109.5
H54G–C54C–H54I	109.5	H54H–C54C–H54I	109.5
C53C–C55C–H55G	109.5	C53C–C55C–H55H	109.5
C53C–C55C–H55I	109.5	H55G–C55C–H55H	109.5
H55G–C55C–H55I	109.5	H55H–C55C–H55I	109.5
C53C–C56C–H56G	109.5	C53C–C56C–H56H	109.5
C53C–C56C–H56I	109.5	H56G–C56C–H56H	109.5
H56G–C56C–H56I	109.5	H56H–C56C–H56I	109.5
C22C–Si1C–C23C	106.4(9)	C22C–Si1C–C24C	107.5(7)
C22C–Si1C–C25C	108.6(8)	C23C–Si1C–C24C	112.3(9)
C23C–Si1C–C25C	110.4(9)	C24C–Si1C–C25C	111.4(9)
C26C–S1C–C27C	91.9(7)	C26C–S2C–C28C	95.3(7)
N1D–Ni1D–N2D	90.9(4)	N1D–Ni1D–N3D	178.4(5)
N1D–Ni1D–N4D	90.8(4)	N2D–Ni1D–N3D	90.0(4)
N2D–Ni1D–N4D	178.1(5)	N3D–Ni1D–N4D	88.3(4)
Ni1D–N1D–C1D	127.2(8)	Ni1D–N1D–C4D	126.8(8)
C1D–N1D–C4D	105.1(9)	Ni1D–N2D–C6D	127.8(8)
Ni1D–N2D–C9D	127.5(8)	C6D–N2D–C9D	104.7(9)
Ni1D–N3D–C11D	125.8(8)	Ni1D–N3D–C14D	127.6(8)
C11D–N3D–C14D	106.5(9)	Ni1D–N4D–C16D	128.9(8)
Ni1D–N4D–C19D	126.1(8)	C16D–N4D–C19D	104.9(9)
N1D–C1D–C2D	108.4(10)	N1D–C1D–C20D	123.4(10)
C2D–C1D–C20D	127.2(11)	C1D–C2D–H2D	125.8
C1D–C2D–C3D	108.5(11)	H2D–C2D–C3D	125.8
C2D–C3D–H3D	126.4	C2D–C3D–C4D	107.2(11)
H3D–C3D–C4D	126.4	N1D–C4D–C3D	110.4(10)
N1D–C4D–C5D	125.2(11)	C3D–C4D–C5D	124.3(11)
C4D–C5D–C6D	122.0(11)	C4D–C5D–C21D	120.1(11)
C6D–C5D–C21D	117.3(11)	N2D–C6D–C5D	123.3(11)
N2D–C6D–C7D	111.4(10)	C5D–C6D–C7D	124.8(11)
C6D–C7D–H7D	126.9	C6D–C7D–C8D	106.1(12)
H7D–C7D–C8D	126.9	C7D–C8D–H8D	126.6
C7D–C8D–C9D	106.8(11)	H8D–C8D–C9D	126.6
N2D–C9D–C8D	110.8(10)	N2D–C9D–C10D	126.0(11)
C8D–C9D–C10D	122.8(11)	C9D–C10D–C11D	121.6(10)
C9D–C10D–C29D	118.8(10)	C11D–C10D–C29D	119.6(10)
N3D–C11D–C10D	125.4(10)	N3D–C11D–C12D	108.4(9)
C10D–C11D–C12D	125.6(10)	C11D–C12D–H12D	126.0
C11D–C12D–C13D	107.9(11)	H12D–C12D–C13D	126.0
C12D–C13D–H13D	126.4	C12D–C13D–C14D	107.1(11)
H13D–C13D–C14D	126.4	N3D–C14D–C13D	109.8(10)
N3D–C14D–C15D	125.9(10)	C13D–C14D–C15D	123.8(11)
C14D–C15D–C16D	118.7(10)	C14D–C15D–C26D	121.5(10)
C16D–C15D–C26D	119.1(10)	N4D–C16D–C15D	126.1(11)
N4D–C16D–C17D	110.9(10)	C15D–C16D–C17D	122.9(11)
C16D–C17D–H17D	126.9	C16D–C17D–C18D	106.3(11)
H17D–C17D–C18D	126.9	C17D–C18D–H18D	126.3
C17D–C18D–C19D	107.5(11)	H18D–C18D–C19D	126.3
N4D–C19D–C18D	110.1(10)	N4D–C19D–C20D	125.9(10)

C18D–C19D–C20D	123.9(11)	C1D–C20D–C19D	122.0(11)
C1D–C20D–C43D	118.3(11)	C19D–C20D–C43D	119.7(11)
C5D–C21D–C22D	177.0(17)	C21D–C22D–Si1D	171.2(15)
H23J–C23D–H23K	109.5	H23J–C23D–H23L	109.5
H23J–C23D–Si1D	109.5	H23K–C23D–H23L	109.5
H23K–C23D–Si1D	109.5	H23L–C23D–Si1D	109.5
H24J–C24D–H24K	109.5	H24J–C24D–H24L	109.5
H24J–C24D–Si1D	109.5	H24K–C24D–H24L	109.5
H24K–C24D–Si1D	109.5	H24L–C24D–Si1D	109.5
H25J–C25D–H25K	109.5	H25J–C25D–H25L	109.5
H25J–C25D–Si1D	109.5	H25K–C25D–H25L	109.5
H25K–C25D–Si1D	109.5	H25L–C25D–Si1D	109.5
C15D–C26D–H26D	105.9	C15D–C26D–S1D	117.6(9)
C15D–C26D–S2D	114.0(9)	H26D–C26D–S1D	105.9
H26D–C26D–S2D	105.9	S1D–C26D–S2D	106.7(6)
H27G–C27D–H27H	108.0	H27G–C27D–C28D	109.4
H27G–C27D–S1D	109.4	H27H–C27D–C28D	109.4
H27H–C27D–S1D	109.4	C28D–C27D–S1D	111.2(10)
C27D–C28D–H28G	109.6	C27D–C28D–H28H	109.6
C27D–C28D–S2D	110.5(10)	H28G–C28D–H28H	108.1
H28G–C28D–S2D	109.6	H28H–C28D–S2D	109.6
C10D–C29D–C30D	119.0(11)	C10D–C29D–C34D	120.1(11)
C30D–C29D–C34D	120.9(11)	C29D–C30D–H30D	119.6
C29D–C30D–C31D	120.9(12)	H30D–C30D–C31D	119.6
C30D–C31D–C32D	117.2(11)	C30D–C31D–C35D	123.3(12)
C32D–C31D–C35D	119.4(11)	C31D–C32D–H32D	119.0
C31D–C32D–C33D	122.0(11)	H32D–C32D–C33D	119.0
C32D–C33D–C34D	119.2(11)	C32D–C33D–C39D	121.6(11)
C34D–C33D–C39D	119.0(11)	C29D–C34D–C33D	119.7(11)
C29D–C34D–H34D	120.2	C33D–C34D–H34D	120.2
C31D–C35D–C36D	112.8(14)	C31D–C35D–C37D	112.2(15)
C31D–C35D–C38D	107.6(14)	C36D–C35D–C37D	109.7(17)
C36D–C35D–C38D	112.1(17)	C37D–C35D–C38D	101.9(17)
C35D–C36D–H36J	109.5	C35D–C36D–H36K	109.5
C35D–C36D–H36L	109.5	H36J–C36D–H36K	109.5
H36J–C36D–H36L	109.5	H36K–C36D–H36L	109.5
C35D–C37D–H37J	109.5	C35D–C37D–H37K	109.5
C35D–C37D–H37L	109.5	H37J–C37D–H37K	109.5
H37J–C37D–H37L	109.5	H37K–C37D–H37L	109.5
C35D–C38D–H38J	109.5	C35D–C38D–H38K	109.5
C35D–C38D–H38L	109.5	H38J–C38D–H38K	109.5
H38J–C38D–H38L	109.5	H38K–C38D–H38L	109.5
C33D–C39D–C40D	109.7(12)	C33D–C39D–C41D	113.1(11)
C33D–C39D–C42D	109.4(12)	C40D–C39D–C41D	108.7(13)
C40D–C39D–C42D	109.8(14)	C41D–C39D–C42D	106.0(13)
C39D–C40D–H40J	109.5	C39D–C40D–H40K	109.5
C39D–C40D–H40L	109.5	H40J–C40D–H40K	109.5
H40J–C40D–H40L	109.5	H40K–C40D–H40L	109.5
C39D–C41D–H41J	109.5	C39D–C41D–H41K	109.5
C39D–C41D–H41L	109.5	H41J–C41D–H41K	109.5
H41J–C41D–H41L	109.5	H41K–C41D–H41L	109.5

C39D-C42D-H42J	109.5	C39D-C42D-H42K	109.5
C39D-C42D-H42L	109.5	H42J-C42D-H42K	109.5
H42J-C42D-H42L	109.5	H42K-C42D-H42L	109.5
C20D-C43D-C44D	119.8(11)	C20D-C43D-C48D	120.6(11)
C44D-C43D-C48D	119.6(10)	C43D-C44D-H44D	120.4
C43D-C44D-C45D	119.3(11)	H44D-C44D-C45D	120.4
C44D-C45D-C46D	119.6(11)	C44D-C45D-C49D	121.6(11)
C46D-C45D-C49D	118.8(11)	C45D-C46D-H46D	118.9
C45D-C46D-C47D	122.1(11)	H46D-C46D-C47D	118.9
C46D-C47D-C48D	117.1(11)	C46D-C47D-C53D	122.9(10)
C48D-C47D-C53D	120.0(10)	C43D-C48D-C47D	122.3(11)
C43D-C48D-H48D	118.9	C47D-C48D-H48D	118.9
C45D-C49D-C50D	111.1(13)	C45D-C49D-C51D	112.1(14)
C45D-C49D-C52D	110.1(15)	C50D-C49D-C51D	107.7(16)
C50D-C49D-C52D	110.4(17)	C51D-C49D-C52D	105.3(16)
C49D-C50D-H50J	109.5	C49D-C50D-H50K	109.5
C49D-C50D-H50L	109.5	H50J-C50D-H50K	109.5
H50J-C50D-H50L	109.5	H50K-C50D-H50L	109.5
C49D-C51D-H51J	109.5	C49D-C51D-H51K	109.5
C49D-C51D-H51L	109.5	H51J-C51D-H51K	109.5
H51J-C51D-H51L	109.5	H51K-C51D-H51L	109.5
C49D-C52D-H52J	109.5	C49D-C52D-H52K	109.5
C49D-C52D-H52L	109.5	H52J-C52D-H52K	109.5
H52J-C52D-H52L	109.5	H52K-C52D-H52L	109.5
C47D-C53D-C54D	108.1(11)	C47D-C53D-C55D	111.6(10)
C47D-C53D-C56D	109.6(11)	C54D-C53D-C55D	109.7(12)
C54D-C53D-C56D	110.2(12)	C55D-C53D-C56D	107.6(12)
C53D-C54D-H54J	109.5	C53D-C54D-H54K	109.5
C53D-C54D-H54L	109.5	H54J-C54D-H54K	109.5
H54J-C54D-H54L	109.5	H54K-C54D-H54L	109.5
C53D-C55D-H55J	109.5	C53D-C55D-H55K	109.5
C53D-C55D-H55L	109.5	H55J-C55D-H55K	109.5
H55J-C55D-H55L	109.5	H55K-C55D-H55L	109.5
C53D-C56D-H56J	109.5	C53D-C56D-H56K	109.5
C53D-C56D-H56L	109.5	H56J-C56D-H56K	109.5
H56J-C56D-H56L	109.5	H56K-C56D-H56L	109.5
C22D-Si1D-C23D	107.5(8)	C22D-Si1D-C24D	108.2(7)
C22D-Si1D-C25D	110.5(8)	C23D-Si1D-C24D	113.5(9)
C23D-Si1D-C25D	108.1(9)	C24D-Si1D-C25D	109.0(9)
C26D-S1D-C27D	90.3(7)	C26D-S2D-C28D	96.3(6)
Cl1-C1S-H1S1	111.7	Cl1-C1S-H1S2	111.7
Cl1-C1S-C2S	100(2)	H1S1-C1S-H1S2	109.5
H1S1-C1S-C2S	111.7	H1S2-C1S-C2S	111.7
C1S-C2S-H2S1	110.4	C1S-C2S-H2S2	110.4
C1S-C2S-Cl2	107(3)	H2S1-C2S-H2S2	108.6
H2S1-C2S-Cl2	110.4	H2S2-C2S-Cl2	110.4
Cl3-C3S-H3S1	110.6	Cl3-C3S-H3S2	110.7
Cl3-C3S-C4S	105(2)	H3S1-C3S-H3S2	108.8
H3S1-C3S-C4S	110.6	H3S2-C3S-C4S	110.7
C3S-C4S-H4S1	111.3	C3S-C4S-H4S2	111.2
C3S-C4S-Cl4	103(3)	H4S1-C4S-H4S2	109.2

H4S1-C4S-C14	111.3	H4S2-C4S-C14	111.3
Cl5-C5S-H5S1	110.3	Cl5-C5S-H5S2	110.3
Cl5-C5S-C6S	107(3)	H5S1-C5S-H5S2	108.6
H5S1-C5S-C6S	110.3	H5S2-C5S-C6S	110.3
C5S-C6S-H6S1	111.0	C5S-C6S-H6S2	111.0
C5S-C6S-Cl6	104(2)	H6S1-C6S-H6S2	109.0
H6S1-C6S-Cl6	111.0	H6S2-C6S-Cl6	111.0
Cl7-C7S-H7S1	111.7	Cl7-C7S-H7S2	111.7
Cl7-C7S-C8S	101(2)	H7S1-C7S-H7S2	109.4
H7S1-C7S-C8S	111.7	H7S2-C7S-C8S	111.7
C7S-C8S-H8S1	110.0	C7S-C8S-H8S2	110.0
C7S-C8S-Cl8	109(2)	H8S1-C8S-H8S2	108.3
H8S1-C8S-Cl8	110.0	H8S2-C8S-Cl8	110.0

Table S22. Torsion angles [°] for **Ni10**.

Ni1A–N1A–C1A–C2A	–174.5(9)	Ni1A–N1A–C1A–C20A	14.6(19)
C4A–N1A–C1A–C2A	3.6(15)	C4A–N1A–C1A–C20A	–167.3(13)
N1A–C1A–C2A–C3A	–5.0(17)	C20A–C1A–C2A–C3A	166.0(13)
C1A–C2A–C3A–C4A	4.2(16)	Ni1A–N1A–C4A–C3A	177.0(9)
Ni1A–N1A–C4A–C5A	–1(2)	C1A–N1A–C4A–C3A	–1.0(15)
C1A–N1A–C4A–C5A	–179.4(13)	C2A–C3A–C4A–N1A	–2.1(17)
C2A–C3A–C4A–C5A	176.3(13)	N1A–C4A–C5A–C6A	18(2)
N1A–C4A–C5A–C21A	–172.4(13)	C3A–C4A–C5A–C6A	–160.4(14)
C3A–C4A–C5A–C21A	9(2)	Ni1A–N2A–C6A–C5A	–14(2)
Ni1A–N2A–C6A–C7A	174.6(11)	C9A–N2A–C6A–C5A	171.7(14)
C9A–N2A–C6A–C7A	0.0(17)	C4A–C5A–C6A–N2A	–10(2)
C4A–C5A–C6A–C7A	160.6(14)	C21A–C5A–C6A–N2A	180.0(13)
C21A–C5A–C6A–C7A	–9(2)	N2A–C6A–C7A–C8A	1.1(19)
C5A–C6A–C7A–C8A	–170.8(15)	C6A–C7A–C8A–C9A	–1.7(19)
Ni1A–N2A–C9A–C8A	–175.6(10)	Ni1A–N2A–C9A–C10A	5(2)
C6A–N2A–C9A–C8A	–1.0(17)	C6A–N2A–C9A–C10A	179.8(13)
C7A–C8A–C9A–N2A	1.7(19)	C7A–C8A–C9A–C10A	–179.1(15)
N2A–C9A–C10A–C11A	–18(2)	N2A–C9A–C10A–C29A	172.5(12)
C8A–C9A–C10A–C11A	162.7(15)	C8A–C9A–C10A–C29A	–7(2)
C9A–C10A–C11A–N3A	6(2)	C9A–C10A–C11A–C12A	–164.0(14)
C29A–C10A–C11A–N3A	174.5(13)	C29A–C10A–C11A–C12A	5(2)
Ni1A–N3A–C11A–C10A	19(2)	Ni1A–N3A–C11A–C12A	–169.9(9)
C14A–N3A–C11A–C10A	–170.7(14)	C14A–N3A–C11A–C12A	0.1(15)
N3A–C11A–C12A–C13A	–2.4(16)	C10A–C11A–C12A–C13A	168.5(14)
C11A–C12A–C13A–C14A	3.7(17)	Ni1A–N3A–C14A–C13A	171.7(10)
Ni1A–N3A–C14A–C15A	–8(2)	C11A–N3A–C14A–C13A	2.1(16)
C11A–N3A–C14A–C15A	–177.1(13)	C12A–C13A–C14A–N3A	–3.8(17)
C12A–C13A–C14A–C15A	175.4(14)	N3A–C14A–C15A–C16A	20(2)
N3A–C14A–C15A–C26A	–167.7(12)	C13A–C14A–C15A–C16A	–159.5(15)
C13A–C14A–C15A–C26A	13(2)	Ni1A–N4A–C16A–C15A	–15(2)
Ni1A–N4A–C16A–C17A	177.3(10)	C19A–N4A–C16A–C15A	166.1(15)
C19A–N4A–C16A–C17A	–1.9(17)	C14A–C15A–C16A–N4A	–8(2)
C14A–C15A–C16A–C17A	158.0(14)	C26A–C15A–C16A–N4A	178.8(12)
C26A–C15A–C16A–C17A	–15(2)	N4A–C16A–C17A–C18A	1.8(19)
C15A–C16A–C17A–C18A	–166.3(16)	C16A–C17A–C18A–C19A	–0.9(19)
Ni1A–N4A–C19A–C18A	–177.9(11)	Ni1A–N4A–C19A–C20A	–8(2)
C16A–N4A–C19A–C18A	1.3(17)	C16A–N4A–C19A–C20A	171.3(14)
C17A–C18A–C19A–N4A	–0.2(19)	C17A–C18A–C19A–C20A	–170.3(15)
N1A–C1A–C20A–C19A	1(2)	N1A–C1A–C20A–C43A	176.6(12)
C2A–C1A–C20A–C19A	–168.5(14)	C2A–C1A–C20A–C43A	7(2)
N4A–C19A–C20A–C1A	–5(2)	N4A–C19A–C20A–C43A	179.8(13)
C18A–C19A–C20A–C1A	163.8(15)	C18A–C19A–C20A–C43A	–12(2)
C14A–C15A–C26A–S1A	44.9(16)	C14A–C15A–C26A–S2A	–81.4(14)
C16A–C15A–C26A–S1A	–142.1(12)	C16A–C15A–C26A–S2A	91.5(14)
S1A–C27A–C28A–S2A	–12(2)	C9A–C10A–C29A–C30A	–67.7(18)
C9A–C10A–C29A–C34A	111.0(15)	C11A–C10A–C29A–C30A	122.9(14)
C11A–C10A–C29A–C34A	–58.4(19)	C10A–C29A–C30A–C31A	178.7(12)

C34A-C29A-C30A-C31A	0(2)	C29A-C30A-C31A-C32A	0(2)
C29A-C30A-C31A-C35A	179.9(12)	C30A-C31A-C32A-C33A	2(2)
C35A-C31A-C32A-C33A	-177.8(13)	C31A-C32A-C33A-C34A	-4(2)
C31A-C32A-C33A-C39A	177.7(13)	C32A-C33A-C34A-C29A	4(2)
C39A-C33A-C34A-C29A	-177.8(13)	C10A-C29A-C34A-C33A	179.4(13)
C30A-C29A-C34A-C33A	-2(2)	C30A-C31A-C35A-C36A	36.4(19)
C30A-C31A-C35A-C37A	163.0(17)	C30A-C31A-C35A-C38A	-79.1(18)
C32A-C31A-C35A-C36A	-143.6(16)	C32A-C31A-C35A-C37A	-17(2)
C32A-C31A-C35A-C38A	100.9(19)	C32A-C33A-C39A-C40A	120.6(16)
C32A-C33A-C39A-C41A	-5(2)	C32A-C33A-C39A-C42A	-120.0(16)
C34A-C33A-C39A-C40A	-57.7(18)	C34A-C33A-C39A-C41A	177.0(14)
C34A-C33A-C39A-C42A	61.7(18)	C1A-C20A-C43A-C44A	117.3(15)
C1A-C20A-C43A-C48A	-59.4(19)	C19A-C20A-C43A-C44A	-67.1(19)
C19A-C20A-C43A-C48A	116.2(15)	C20A-C43A-C44A-C45A	-176.6(14)
C48A-C43A-C44A-C45A	0(2)	C43A-C44A-C45A-C46A	1(2)
C43A-C44A-C45A-C49A	178.4(14)	C44A-C45A-C46A-C47A	0(2)
C49A-C45A-C46A-C47A	-177.5(13)	C45A-C46A-C47A-C48A	-2(2)
C45A-C46A-C47A-C53A	-178.9(13)	C20A-C43A-C48A-C47A	174.9(13)
C44A-C43A-C48A-C47A	-2(2)	C46A-C47A-C48A-C43A	3(2)
C53A-C47A-C48A-C43A	179.8(12)	C44A-C45A-C49A-C50A	13(2)
C44A-C45A-C49A-C51A	128.3(17)	C44A-C45A-C49A-C52A	-114.7(18)
C46A-C45A-C49A-C50A	-169.5(17)	C46A-C45A-C49A-C51A	-54.1(19)
C46A-C45A-C49A-C52A	63.0(19)	C46A-C47A-C53A-C54A	111.2(15)
C46A-C47A-C53A-C55A	-10.0(19)	C46A-C47A-C53A-C56A	-128.3(15)
C48A-C47A-C53A-C54A	-65.8(16)	C48A-C47A-C53A-C55A	173.0(13)
C48A-C47A-C53A-C56A	54.7(17)	C28A-C27A-S1A-C26A	35.4(17)
C15A-C26A-S1A-C27A	-175.1(12)	S2A-C26A-S1A-C27A	-45.6(9)
C27A-C28A-S2A-C26A	-17.2(18)	C15A-C26A-S2A-C28A	172.5(11)
S1A-C26A-S2A-C28A	40.2(10)	Ni1B-N1B-C1B-C2B	174.2(11)
Ni1B-N1B-C1B-C20B	-14(2)	C4B-N1B-C1B-C2B	-0.6(16)
C4B-N1B-C1B-C20B	171.5(13)	N1B-C1B-C2B-C3B	2.5(18)
C20B-C1B-C2B-C3B	-169.2(15)	C1B-C2B-C3B-C4B	-3.2(18)
Ni1B-N1B-C4B-C3B	-176.2(11)	Ni1B-N1B-C4B-C5B	5(2)
C1B-N1B-C4B-C3B	-1.4(16)	C1B-N1B-C4B-C5B	179.8(13)
C2B-C3B-C4B-N1B	3.0(19)	C2B-C3B-C4B-C5B	-178.2(14)
N1B-C4B-C5B-C6B	-18(2)	N1B-C4B-C5B-C21B	168.5(14)
C3B-C4B-C5B-C6B	163.1(14)	C3B-C4B-C5B-C21B	-10(2)
Ni1B-N2B-C6B-C5B	18(2)	Ni1B-N2B-C6B-C7B	-171.2(10)
C9B-N2B-C6B-C5B	-168.7(14)	C9B-N2B-C6B-C7B	2.3(16)
C4B-C5B-C6B-N2B	7(2)	C4B-C5B-C6B-C7B	-163.2(13)
C21B-C5B-C6B-N2B	180.0(13)	C21B-C5B-C6B-C7B	10(2)
N2B-C6B-C7B-C8B	-3.2(18)	C5B-C6B-C7B-C8B	168.0(14)
C6B-C7B-C8B-C9B	2.7(18)	Ni1B-N2B-C9B-C8B	172.9(10)
Ni1B-N2B-C9B-C10B	2(2)	C6B-N2B-C9B-C8B	-0.5(16)
C6B-N2B-C9B-C10B	-171.5(14)	C7B-C8B-C9B-N2B	-1.5(18)
C7B-C8B-C9B-C10B	169.7(15)	N2B-C9B-C10B-C11B	7(2)
N2B-C9B-C10B-C29B	-174.1(13)	C8B-C9B-C10B-C11B	-162.7(14)
C8B-C9B-C10B-C29B	16(2)	C9B-C10B-C11B-N3B	2(2)
C9B-C10B-C11B-C12B	167.7(14)	C29B-C10B-C11B-N3B	-176.8(12)

C29B–C10B–C11B–C12B	–11(2)	Ni1B–N3B–C11B–C10B	–19(2)
Ni1B–N3B–C11B–C12B	172.8(10)	C14B–N3B–C11B–C10B	162.9(13)
C14B–N3B–C11B–C12B	–4.8(16)	N3B–C11B–C12B–C13B	4.5(17)
C10B–C11B–C12B–C13B	–162.9(14)	C11B–C12B–C13B–C14B	–2.3(17)
Ni1B–N3B–C14B–C13B	–174.2(10)	Ni1B–N3B–C14B–C15B	–2(2)
C11B–N3B–C14B–C13B	3.3(15)	C11B–N3B–C14B–C15B	175.4(13)
C12B–C13B–C14B–N3B	–0.6(17)	C12B–C13B–C14B–C15B	–172.7(14)
N3B–C14B–C15B–C16B	–18(2)	N3B–C14B–C15B–C26B	170.1(13)
C13B–C14B–C15B–C16B	153.0(14)	C13B–C14B–C15B–C26B	–19(2)
Ni1B–N4B–C16B–C15B	9(2)	Ni1B–N4B–C16B–C17B	–172.0(10)
C19B–N4B–C16B–C15B	–174.6(14)	C19B–N4B–C16B–C17B	4.3(17)
C14B–C15B–C16B–N4B	14(2)	C14B–C15B–C16B–C17B	–164.4(14)
C26B–C15B–C16B–N4B	–173.1(12)	C26B–C15B–C16B–C17B	8(2)
N4B–C16B–C17B–C18B	–7.8(18)	C15B–C16B–C17B–C18B	171.1(15)
C16B–C17B–C18B–C19B	7.9(19)	Ni1B–N4B–C19B–C18B	176.9(11)
Ni1B–N4B–C19B–C20B	3(2)	C16B–N4B–C19B–C18B	0.6(17)
C16B–N4B–C19B–C20B	–173.1(15)	C17B–C18B–C19B–N4B	–5.5(19)
C17B–C18B–C19B–C20B	168.3(16)	N1B–C1B–C20B–C19B	–5(2)
N1B–C1B–C20B–C43B	179.9(12)	C2B–C1B–C20B–C19B	166.2(15)
C2B–C1B–C20B–C43B	–9(2)	N4B–C19B–C20B–C1B	10(3)
N4B–C19B–C20B–C43B	–174.4(14)	C18B–C19B–C20B–C1B	–162.8(15)
C18B–C19B–C20B–C43B	13(2)	C14B–C15B–C26B–S1B	–42.3(17)
C14B–C15B–C26B–S2B	81.4(15)	C16B–C15B–C26B–S1B	145.3(11)
C16B–C15B–C26B–S2B	–90.9(13)	S1B–C27B–C28B–S2B	21.9(18)
C9B–C10B–C29B–C30B	61.4(19)	C9B–C10B–C29B–C34B	–111.9(15)
C11B–C10B–C29B–C30B	–119.7(16)	C11B–C10B–C29B–C34B	67.0(18)
C10B–C29B–C30B–C31B	–177.5(15)	C34B–C29B–C30B–C31B	–4(2)
C29B–C30B–C31B–C32B	3(3)	C29B–C30B–C31B–C35B	179.2(16)
C30B–C31B–C32B–C33B	–1(3)	C35B–C31B–C32B–C33B	–177.1(17)
C31B–C32B–C33B–C34B	0(3)	C31B–C32B–C33B–C39B	178.0(16)
C32B–C33B–C34B–C29B	–2(2)	C39B–C33B–C34B–C29B	–179.6(12)
C10B–C29B–C34B–C33B	177.3(12)	C30B–C29B–C34B–C33B	4(2)
C30B–C31B–C35B–C36B	–21(3)	C30B–C31B–C35B–C37B	–139(2)
C30B–C31B–C35B–C38B	108(2)	C32B–C31B–C35B–C36B	155(2)
C32B–C31B–C35B–C37B	37(3)	C32B–C31B–C35B–C38B	–76(3)
C32B–C33B–C39B–C40B	–116.8(17)	C32B–C33B–C39B–C41B	6(2)
C32B–C33B–C39B–C42B	122.6(16)	C34B–C33B–C39B–C40B	61.0(18)
C34B–C33B–C39B–C41B	–176.3(14)	C34B–C33B–C39B–C42B	–59.6(17)
C1B–C20B–C43B–C44B	–117.7(15)	C1B–C20B–C43B–C48B	59.3(19)
C19B–C20B–C43B–C44B	66.4(19)	C19B–C20B–C43B–C48B	–116.6(16)
C20B–C43B–C44B–C45B	–179.6(13)	C48B–C43B–C44B–C45B	3(2)
C43B–C44B–C45B–C46B	–6(2)	C43B–C44B–C45B–C49B	179.5(13)
C44B–C45B–C46B–C47B	6(2)	C49B–C45B–C46B–C47B	–179.0(13)
C45B–C46B–C47B–C48B	–4(2)	C45B–C46B–C47B–C53B	179.5(13)
C20B–C43B–C48B–C47B	–177.8(13)	C44B–C43B–C48B–C47B	–1(2)
C46B–C47B–C48B–C43B	1(2)	C53B–C47B–C48B–C43B	177.7(13)
C44B–C45B–C49B–C50B	–20(2)	C44B–C45B–C49B–C51B	–138.8(17)
C44B–C45B–C49B–C52B	105.0(19)	C46B–C45B–C49B–C50B	166.1(16)
C46B–C45B–C49B–C51B	46.8(19)	C46B–C45B–C49B–C52B	–69.3(19)

C46B–C47B–C53B–C54B	–106.0(17)	C46B–C47B–C53B–C55B	9(2)
C46B–C47B–C53B–C56B	128.3(16)	C48B–C47B–C53B–C54B	77.4(18)
C48B–C47B–C53B–C55B	–168.0(14)	C48B–C47B–C53B–C56B	–48.3(19)
C15B–C26B–S1B–C27B	174.8(11)	S2B–C26B–S1B–C27B	46.9(8)
C28B–C27B–S1B–C26B	–42.5(14)	C27B–C28B–S2B–C26B	10.1(15)
C15B–C26B–S2B–C28B	–167.4(10)	S1B–C26B–S2B–C28B	–37.9(9)
Ni1C–N1C–C1C–C2C	–171.4(11)	Ni1C–N1C–C1C–C20C	13(2)
C4C–N1C–C1C–C2C	5.0(17)	C4C–N1C–C1C–C20C	–170.8(14)
N1C–C1C–C2C–C3C	–6.9(19)	C20C–C1C–C2C–C3C	168.8(15)
C1C–C2C–C3C–C4C	5.8(19)	Ni1C–N1C–C4C–C3C	174.8(11)
Ni1C–N1C–C4C–C5C	2(2)	C1C–N1C–C4C–C3C	–1.5(17)
C1C–N1C–C4C–C5C	–174.4(14)	C2C–C3C–C4C–N1C	–2.8(19)
C2C–C3C–C4C–C5C	170.1(15)	N1C–C4C–C5C–C6C	11(2)
N1C–C4C–C5C–C21C	–175.0(14)	C3C–C4C–C5C–C6C	–160.6(15)
C3C–C4C–C5C–C21C	13(2)	Ni1C–N2C–C6C–C5C	–16(2)
Ni1C–N2C–C6C–C7C	174.7(10)	C9C–N2C–C6C–C5C	167.5(15)
C9C–N2C–C6C–C7C	–1.4(17)	C4C–C5C–C6C–N2C	–4(2)
C4C–C5C–C6C–C7C	164.0(14)	C21C–C5C–C6C–N2C	–177.3(14)
C21C–C5C–C6C–C7C	–10(2)	N2C–C6C–C7C–C8C	3.0(19)
C5C–C6C–C7C–C8C	–166.2(15)	C6C–C7C–C8C–C9C	–3.3(19)
Ni1C–N2C–C9C–C8C	–176.7(11)	Ni1C–N2C–C9C–C10C	–3(2)
C6C–N2C–C9C–C8C	–0.7(17)	C6C–N2C–C9C–C10C	173.3(14)
C7C–C8C–C9C–N2C	2.6(19)	C7C–C8C–C9C–C10C	–171.5(15)
N2C–C9C–C10C–C11C	–9(2)	N2C–C9C–C10C–C29C	175.8(13)
C8C–C9C–C10C–C11C	163.9(15)	C8C–C9C–C10C–C29C	–11(2)
Ni1C–N3C–C11C–C10C	20(2)	Ni1C–N3C–C11C–C12C	–172.7(10)
C14C–N3C–C11C–C10C	–169.2(14)	C14C–N3C–C11C–C12C	–1.8(16)
C9C–C10C–C11C–N3C	0(2)	C9C–C10C–C11C–C12C	–165.2(14)
C29C–C10C–C11C–N3C	175.2(12)	C29C–C10C–C11C–C12C	10(2)
N3C–C11C–C12C–C13C	–1.5(19)	C10C–C11C–C12C–C13C	166.0(15)
C11C–C12C–C13C–C14C	4(2)	Ni1C–N3C–C14C–C13C	175.0(11)
Ni1C–N3C–C14C–C15C	–7(2)	C11C–N3C–C14C–C13C	4.3(17)
C11C–N3C–C14C–C15C	–177.8(15)	C12C–C13C–C14C–N3C	–5(2)
C12C–C13C–C14C–C15C	176.7(16)	N3C–C14C–C15C–C16C	21(2)
N3C–C14C–C15C–C26C	–164.0(14)	C13C–C14C–C15C–C16C	–161.6(16)
C13C–C14C–C15C–C26C	14(3)	C14C–C15C–C16C–N4C	–9(3)
C14C–C15C–C16C–C17C	156.1(15)	C26C–C15C–C16C–N4C	175.6(13)
C26C–C15C–C16C–C17C	–19(2)	Ni1C–N4C–C16C–C15C	–16(2)
Ni1C–N4C–C16C–C17C	177.0(11)	C19C–N4C–C16C–C15C	169.5(15)
C19C–N4C–C16C–C17C	2.9(17)	N4C–C16C–C17C–C18C	–3(2)
C15C–C16C–C17C–C18C	–169.8(16)	C16C–C17C–C18C–C19C	2(2)
Ni1C–N4C–C19C–C18C	–176.0(11)	Ni1C–N4C–C19C–C20C	0(2)
C16C–N4C–C19C–C18C	–1.9(18)	C16C–N4C–C19C–C20C	174.3(14)
C17C–C18C–C19C–N4C	0(2)	C17C–C18C–C19C–C20C	–175.9(16)
N1C–C1C–C20C–C19C	8(2)	N1C–C1C–C20C–C43C	–179.6(13)
C2C–C1C–C20C–C19C	–166.9(16)	C2C–C1C–C20C–C43C	5(2)
N4C–C19C–C20C–C1C	–15(2)	N4C–C19C–C20C–C43C	172.8(13)
C18C–C19C–C20C–C1C	160.7(16)	C18C–C19C–C20C–C43C	–12(2)
C14C–C15C–C26C–S1C	42.1(19)	C14C–C15C–C26C–S2C	–82.4(16)

C16C–C15C–C26C–S1C	–142.6(13)	C16C–C15C–C26C–S2C	92.9(15)
S1C–C27C–C28C–S2C	–23(2)	C9C–C10C–C29C–C30C	–68(2)
C9C–C10C–C29C–C34C	112.1(16)	C11C–C10C–C29C–C30C	116.9(17)
C11C–C10C–C29C–C34C	–63(2)	C10C–C29C–C30C–C31C	177.5(15)
C34C–C29C–C30C–C31C	–3(3)	C29C–C30C–C31C–C32C	3(3)
C29C–C30C–C31C–C35C	178.5(16)	C30C–C31C–C32C–C33C	–2(3)
C35C–C31C–C32C–C33C	–177.8(17)	C31C–C32C–C33C–C34C	2(3)
C31C–C32C–C33C–C39C	–177.9(16)	C10C–C29C–C34C–C33C	–178.1(14)
C30C–C29C–C34C–C33C	2(2)	C32C–C33C–C34C–C29C	–2(2)
C39C–C33C–C34C–C29C	177.9(14)	C30C–C31C–C35C–C36C	54(3)
C30C–C31C–C35C–C37C	–167(2)	C30C–C31C–C35C–C38C	–59(2)
C32C–C31C–C35C–C36C	–130(2)	C32C–C31C–C35C–C37C	8(3)
C32C–C31C–C35C–C38C	116(2)	C32C–C33C–C39C–C40C	112.5(17)
C32C–C33C–C39C–C41C	–11(2)	C32C–C33C–C39C–C42C	–129.0(17)
C34C–C33C–C39C–C40C	–67.0(18)	C34C–C33C–C39C–C41C	169.4(15)
C34C–C33C–C39C–C42C	51.5(19)	C1C–C20C–C43C–C44C	123.9(15)
C1C–C20C–C43C–C48C	–57(2)	C19C–C20C–C43C–C44C	–63.6(19)
C19C–C20C–C43C–C48C	115.2(16)	C20C–C43C–C44C–C45C	–177.4(14)
C48C–C43C–C44C–C45C	4(2)	C43C–C44C–C45C–C46C	–2(2)
C43C–C44C–C45C–C49C	178.6(14)	C44C–C45C–C46C–C47C	1(2)
C49C–C45C–C46C–C47C	–179.4(14)	C45C–C46C–C47C–C48C	–2(2)
C45C–C46C–C47C–C53C	–179.6(14)	C20C–C43C–C48C–C47C	176.1(13)
C44C–C43C–C48C–C47C	–5(2)	C46C–C47C–C48C–C43C	4(2)
C53C–C47C–C48C–C43C	–178.1(13)	C44C–C45C–C49C–C50C	14(2)
C44C–C45C–C49C–C51C	132.8(17)	C44C–C45C–C49C–C52C	–108.8(19)
C46C–C45C–C49C–C50C	–166.2(16)	C46C–C45C–C49C–C51C	–47(2)
C46C–C45C–C49C–C52C	72(2)	C46C–C47C–C53C–C54C	107.3(17)
C46C–C47C–C53C–C55C	–12(2)	C46C–C47C–C53C–C56C	–133.3(17)
C48C–C47C–C53C–C54C	–70.1(18)	C48C–C47C–C53C–C55C	170.9(14)
C48C–C47C–C53C–C56C	49.2(19)	C28C–C27C–S1C–C26C	41.8(16)
C15C–C26C–S1C–C27C	–172.5(12)	S2C–C26C–S1C–C27C	–45.6(9)
C27C–C28C–S2C–C26C	–8.0(16)	C15C–C26C–S2C–C28C	165.6(11)
S1C–C26C–S2C–C28C	35.4(10)	Ni1D–N1D–C1D–C2D	170.4(11)
Ni1D–N1D–C1D–C20D	–20(2)	C4D–N1D–C1D–C2D	0.3(17)
C4D–N1D–C1D–C20D	169.4(14)	N1D–C1D–C2D–C3D	3.6(19)
C20D–C1D–C2D–C3D	–165.0(16)	C1D–C2D–C3D–C4D	–6(2)
Ni1D–N1D–C4D–C3D	–174.1(11)	Ni1D–N1D–C4D–C5D	4(2)
C1D–N1D–C4D–C3D	–3.9(17)	C1D–N1D–C4D–C5D	174.0(15)
C2D–C3D–C4D–N1D	6(2)	C2D–C3D–C4D–C5D	–171.7(16)
N1D–C4D–C5D–C6D	–17(3)	N1D–C4D–C5D–C21D	171.5(14)
C3D–C4D–C5D–C6D	160.6(17)	C3D–C4D–C5D–C21D	–11(3)
Ni1D–N2D–C6D–C5D	12(2)	Ni1D–N2D–C6D–C7D	–174.9(12)
C9D–N2D–C6D–C5D	–169.8(16)	C9D–N2D–C6D–C7D	2.9(19)
C4D–C5D–C6D–N2D	9(3)	C4D–C5D–C6D–C7D	–163.2(16)
C21D–C5D–C6D–N2D	–179.8(15)	C21D–C5D–C6D–C7D	9(3)
N2D–C6D–C7D–C8D	–4(2)	C5D–C6D–C7D–C8D	168.7(17)
C6D–C7D–C8D–C9D	3.0(19)	Ni1D–N2D–C9D–C8D	176.8(11)
Ni1D–N2D–C9D–C10D	4(2)	C6D–N2D–C9D–C8D	–1.0(18)
C6D–N2D–C9D–C10D	–174.0(15)	C7D–C8D–C9D–N2D	–1(2)

C7D–C8D–C9D–C10D	171.9(15)	N2D–C9D–C10D–C11D	8(2)
N2D–C9D–C10D–C29D	–173.6(14)	C8D–C9D–C10D–C11D	–164.1(14)
C8D–C9D–C10D–C29D	14(2)	C9D–C10D–C11D–N3D	–1(2)
C9D–C10D–C11D–C12D	169.1(15)	C29D–C10D–C11D–N3D	–179.5(12)
C29D–C10D–C11D–C12D	–9(2)	Ni1D–N3D–C11D–C10D	–17(2)
Ni1D–N3D–C11D–C12D	171.6(10)	C14D–N3D–C11D–C10D	167.1(13)
C14D–N3D–C11D–C12D	–4.7(16)	N3D–C11D–C12D–C13D	5.0(17)
C10D–C11D–C12D–C13D	–166.7(14)	C11D–C12D–C13D–C14D	–3.3(18)
Ni1D–N3D–C14D–C13D	–173.5(10)	Ni1D–N3D–C14D–C15D	–1(2)
C11D–N3D–C14D–C13D	2.7(16)	C11D–N3D–C14D–C15D	174.8(14)
C12D–C13D–C14D–N3D	0.4(18)	C12D–C13D–C14D–C15D	–171.9(14)
N3D–C14D–C15D–C16D	–16(2)	N3D–C14D–C15D–C26D	173.0(13)
C13D–C14D–C15D–C16D	154.7(14)	C13D–C14D–C15D–C26D	–16(2)
Ni1D–N4D–C16D–C15D	7(2)	Ni1D–N4D–C16D–C17D	–176.4(11)
C19D–N4D–C16D–C15D	–174.1(15)	C19D–N4D–C16D–C17D	2.7(17)
C14D–C15D–C16D–N4D	14(2)	C14D–C15D–C16D–C17D	–162.5(15)
C26D–C15D–C16D–N4D	–175.3(13)	C26D–C15D–C16D–C17D	8(2)
N4D–C16D–C17D–C18D	–5(2)	C15D–C16D–C17D–C18D	171.7(16)
C16D–C17D–C18D–C19D	5(2)	Ni1D–N4D–C19D–C18D	179.8(10)
Ni1D–N4D–C19D–C20D	3(2)	C16D–N4D–C19D–C18D	0.7(17)
C16D–N4D–C19D–C20D	–176.2(15)	C17D–C18D–C19D–N4D	–3.9(19)
C17D–C18D–C19D–C20D	173.1(16)	N1D–C1D–C20D–C19D	0(2)
N1D–C1D–C20D–C43D	–177.3(13)	C2D–C1D–C20D–C19D	167.3(15)
C2D–C1D–C20D–C43D	–10(2)	N4D–C19D–C20D–C1D	9(2)
N4D–C19D–C20D–C43D	–173.9(13)	C18D–C19D–C20D–C1D	–167.9(15)
C18D–C19D–C20D–C43D	10(2)	C14D–C15D–C26D–S1D	–41.4(17)
C14D–C15D–C26D–S2D	84.7(15)	C16D–C15D–C26D–S1D	148.0(12)
C16D–C15D–C26D–S2D	–85.9(15)	S1D–C27D–C28D–S2D	29.5(19)
C9D–C10D–C29D–C30D	59(2)	C9D–C10D–C29D–C34D	–117.1(16)
C11D–C10D–C29D–C30D	–122.9(15)	C11D–C10D–C29D–C34D	61(2)
C10D–C29D–C30D–C31D	–179.8(14)	C34D–C29D–C30D–C31D	–4(2)
C29D–C30D–C31D–C32D	2(2)	C29D–C30D–C31D–C35D	179.5(15)
C30D–C31D–C32D–C33D	–1(2)	C35D–C31D–C32D–C33D	–179.1(14)
C31D–C32D–C33D–C34D	3(2)	C31D–C32D–C33D–C39D	177.5(14)
C32D–C33D–C34D–C29D	–5(2)	C39D–C33D–C34D–C29D	–179.4(14)
C10D–C29D–C34D–C33D	–179.0(14)	C30D–C29D–C34D–C33D	5(2)
C30D–C31D–C35D–C36D	–10(2)	C30D–C31D–C35D–C37D	–134.3(19)
C30D–C31D–C35D–C38D	114(2)	C32D–C31D–C35D–C36D	167.8(17)
C32D–C31D–C35D–C37D	43(2)	C32D–C31D–C35D–C38D	–68(2)
C32D–C33D–C39D–C40D	–108.5(17)	C32D–C33D–C39D–C41D	13(2)
C32D–C33D–C39D–C42D	131.0(16)	C34D–C33D–C39D–C40D	66.2(19)
C34D–C33D–C39D–C41D	–172.2(14)	C34D–C33D–C39D–C42D	–54.2(19)
C1D–C20D–C43D–C44D	–119.1(16)	C1D–C20D–C43D–C48D	62(2)
C19D–C20D–C43D–C44D	63(2)	C19D–C20D–C43D–C48D	–115.6(16)
C20D–C43D–C44D–C45D	–178.7(15)	C48D–C43D–C44D–C45D	0(2)
C43D–C44D–C45D–C46D	–2(3)	C43D–C44D–C45D–C49D	180.0(15)
C44D–C45D–C46D–C47D	1(3)	C49D–C45D–C46D–C47D	180.0(15)
C45D–C46D–C47D–C48D	0(2)	C45D–C46D–C47D–C53D	179.8(14)
C20D–C43D–C48D–C47D	–179.6(13)	C44D–C43D–C48D–C47D	2(2)

C46D–C47D–C48D–C43D	–2(2)	C53D–C47D–C48D–C43D	178.7(13)
C44D–C45D–C49D–C50D	–15(2)	C44D–C45D–C49D–C51D	–135.5(19)
C44D–C45D–C49D–C52D	108(2)	C46D–C45D–C49D–C50D	166.6(18)
C46D–C45D–C49D–C51D	46(2)	C46D–C45D–C49D–C52D	–71(2)
C46D–C47D–C53D–C54D	–108.4(16)	C46D–C47D–C53D–C55D	12(2)
C46D–C47D–C53D–C56D	131.5(16)	C48D–C47D–C53D–C54D	71.3(17)
C48D–C47D–C53D–C55D	–168.0(13)	C48D–C47D–C53D–C56D	–48.9(18)
C15D–C26D–S1D–C27D	175.3(12)	S2D–C26D–S1D–C27D	45.8(9)
C28D–C27D–S1D–C26D	–46.4(15)	C27D–C28D–S2D–C26D	2.7(16)
C15D–C26D–S2D–C28D	–164.8(11)	S1D–C26D–S2D–C28D	–33.1(10)
Cl1–C1S–C2S–Cl2	–166(4)	Cl3–C3S–C4S–Cl4	–179(3)
Cl5–C5S–C6S–Cl6	–169(3)	Cl7–C7S–C8S–Cl8	167(2)

Table S23. Anisotropic displacement parameters ($\text{\AA}^2$) for **Ni10**.The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni1A	0.0162(9)	0.0086(7)	0.0266(8)	0.0003(6)	0.0121(7)	0.0018(6)
N1A	0.021(5)	0.009(4)	0.021(4)	-0.005(4)	0.011(4)	0.004(4)
N2A	0.021(5)	0.012(4)	0.032(5)	0.003(4)	0.012(5)	0.001(4)
N3A	0.020(5)	0.018(4)	0.023(5)	-0.005(4)	0.011(4)	0.000(4)
N4A	0.030(5)	0.013(4)	0.032(5)	-0.011(4)	0.010(5)	0.004(4)
C1A	0.024(4)	0.014(4)	0.025(4)	0.000(4)	0.010(4)	0.007(4)
C2A	0.022(5)	0.015(4)	0.032(5)	0.001(4)	0.007(4)	-0.003(4)
C3A	0.026(5)	0.019(4)	0.027(5)	-0.004(4)	0.015(4)	0.000(4)
C4A	0.023(4)	0.021(5)	0.022(4)	-0.003(4)	0.008(4)	0.006(4)
C5A	0.021(4)	0.024(4)	0.020(4)	-0.001(4)	0.011(4)	0.000(4)
C6A	0.016(5)	0.023(4)	0.030(5)	0.003(4)	0.009(4)	0.004(4)
C7A	0.026(5)	0.031(5)	0.046(6)	0.001(5)	0.017(4)	0.001(4)
C8A	0.024(5)	0.019(5)	0.040(5)	0.001(4)	0.011(4)	0.003(4)
C9A	0.016(4)	0.020(4)	0.031(5)	0.004(4)	0.012(4)	0.004(4)
C10A	0.022(5)	0.016(4)	0.027(5)	0.002(4)	0.009(4)	0.001(4)
C11A	0.025(5)	0.023(5)	0.028(5)	-0.001(4)	0.009(4)	-0.002(4)
C12A	0.019(5)	0.017(4)	0.026(4)	-0.002(4)	0.009(4)	-0.004(4)
C13A	0.029(5)	0.019(5)	0.033(5)	0.000(4)	0.011(4)	-0.001(4)
C14A	0.021(5)	0.015(4)	0.022(4)	0.001(4)	0.009(4)	-0.004(4)
C15A	0.021(5)	0.019(4)	0.026(5)	-0.004(4)	0.012(4)	0.001(4)
C16A	0.023(5)	0.020(4)	0.033(5)	-0.001(4)	0.014(4)	-0.001(4)
C17A	0.028(5)	0.026(5)	0.048(6)	0.000(4)	0.019(4)	0.003(4)
C18A	0.033(5)	0.031(5)	0.044(6)	0.000(4)	0.021(5)	0.003(4)
C19A	0.025(5)	0.019(4)	0.032(5)	0.001(4)	0.014(4)	0.005(4)
C20A	0.020(4)	0.015(4)	0.026(4)	-0.002(4)	0.005(4)	0.003(4)
C21A	0.019(5)	0.023(5)	0.028(5)	0.002(4)	0.010(4)	0.003(4)
C22A	0.026(5)	0.027(5)	0.029(5)	-0.004(4)	0.013(4)	0.003(4)
C23A	0.037(7)	0.040(7)	0.037(7)	0.009(6)	0.012(6)	0.014(6)
C24A	0.022(6)	0.049(8)	0.055(8)	0.009(6)	0.023(6)	0.001(6)
C25A	0.039(8)	0.040(7)	0.048(7)	-0.003(6)	0.006(7)	0.000(6)
C26A	0.028(5)	0.020(5)	0.031(5)	-0.003(4)	0.013(4)	0.002(4)
C27A	0.044(6)	0.056(7)	0.051(6)	0.006(5)	0.028(5)	-0.010(5)
C28A	0.052(7)	0.061(7)	0.061(7)	0.007(5)	0.030(5)	-0.001(5)
C29A	0.017(5)	0.014(4)	0.028(4)	0.002(4)	0.012(4)	0.005(4)
C30A	0.024(5)	0.016(4)	0.028(4)	0.004(4)	0.011(4)	0.000(4)
C31A	0.026(5)	0.023(5)	0.031(4)	-0.001(4)	0.016(4)	0.001(4)
C32A	0.029(5)	0.025(5)	0.034(5)	-0.006(4)	0.015(4)	-0.002(4)
C33A	0.027(5)	0.016(4)	0.029(4)	0.002(4)	0.017(4)	0.006(4)
C34A	0.024(5)	0.013(4)	0.025(4)	0.001(4)	0.012(4)	0.000(4)
C35A	0.030(5)	0.032(5)	0.032(5)	-0.005(4)	0.017(4)	0.001(4)
C36A	0.082(10)	0.059(8)	0.064(9)	0.007(7)	0.053(8)	-0.003(8)
C37A	0.085(10)	0.077(10)	0.078(10)	0.015(9)	0.055(8)	0.020(9)
C38A	0.074(9)	0.097(11)	0.055(8)	-0.004(9)	0.032(8)	-0.008(8)
C39A	0.040(6)	0.023(5)	0.038(5)	0.002(4)	0.017(4)	0.006(4)
C40A	0.062(9)	0.033(7)	0.045(7)	0.002(6)	0.011(7)	0.014(7)

C41A	0.047(8)	0.018(6)	0.052(8)	−0.008(6)	0.015(7)	0.014(6)
C42A	0.059(8)	0.047(9)	0.071(9)	0.013(7)	0.039(7)	−0.001(7)
C43A	0.023(5)	0.021(4)	0.030(5)	−0.002(4)	0.011(4)	0.007(4)
C44A	0.030(5)	0.024(5)	0.032(5)	−0.008(4)	0.011(4)	0.002(4)
C45A	0.025(5)	0.026(5)	0.026(4)	−0.002(4)	0.008(4)	0.002(4)
C46A	0.020(5)	0.017(4)	0.028(4)	0.003(4)	0.008(4)	0.004(4)
C47A	0.025(5)	0.014(4)	0.026(4)	0.000(4)	0.010(4)	0.001(4)
C48A	0.020(5)	0.018(4)	0.026(5)	0.001(4)	0.005(4)	0.004(4)
C49A	0.034(5)	0.036(5)	0.030(5)	−0.005(4)	0.008(4)	0.001(5)
C50A	0.085(11)	0.072(9)	0.071(10)	−0.021(8)	0.004(8)	−0.005(8)
C51A	0.035(7)	0.072(10)	0.058(9)	0.000(8)	0.005(7)	0.000(7)
C52A	0.062(10)	0.088(10)	0.043(8)	0.014(8)	0.007(7)	−0.003(9)
C53A	0.020(5)	0.010(4)	0.027(4)	−0.005(4)	0.003(4)	−0.005(4)
C54A	0.042(8)	0.018(6)	0.040(6)	−0.007(5)	0.015(6)	−0.008(6)
C55A	0.034(7)	0.021(6)	0.046(7)	−0.006(5)	0.012(6)	0.007(6)
C56A	0.029(6)	0.028(7)	0.052(8)	−0.011(6)	0.014(6)	0.000(6)
Si1A	0.0191(19)	0.029(2)	0.040(2)	0.0029(18)	0.0102(18)	−0.0048(17)
S1A	0.034(2)	0.0290(19)	0.048(2)	0.0067(17)	0.0233(19)	−0.0023(17)
S2A	0.0273(19)	0.030(2)	0.048(2)	0.0021(17)	0.0206(18)	−0.0059(16)
Ni1B	0.0207(9)	0.0126(8)	0.0289(8)	−0.0044(6)	0.0218(7)	−0.0031(7)
N1B	0.018(5)	0.022(5)	0.039(6)	−0.001(5)	0.023(5)	−0.003(4)
N2B	0.026(5)	0.015(4)	0.035(5)	−0.002(4)	0.020(5)	−0.004(4)
N3B	0.019(5)	0.020(5)	0.032(5)	−0.004(4)	0.021(5)	0.002(4)
N4B	0.025(5)	0.022(5)	0.031(5)	−0.003(4)	0.020(5)	−0.003(4)
C1B	0.024(5)	0.013(4)	0.022(4)	−0.005(4)	0.008(4)	−0.001(4)
C2B	0.026(5)	0.024(5)	0.038(5)	0.000(4)	0.015(4)	0.001(4)
C3B	0.025(5)	0.026(5)	0.038(5)	−0.003(4)	0.013(4)	−0.002(4)
C4B	0.021(5)	0.019(4)	0.025(5)	−0.002(4)	0.009(4)	−0.001(4)
C5B	0.018(5)	0.025(5)	0.021(4)	−0.001(4)	0.012(4)	−0.003(4)
C6B	0.015(4)	0.024(4)	0.021(4)	−0.005(4)	0.013(4)	0.001(4)
C7B	0.024(5)	0.032(5)	0.042(5)	0.000(4)	0.019(4)	−0.001(4)
C8B	0.029(5)	0.025(5)	0.038(5)	−0.004(4)	0.018(4)	−0.001(4)
C9B	0.019(5)	0.024(5)	0.032(5)	−0.002(4)	0.019(4)	−0.004(4)
C10B	0.025(5)	0.018(4)	0.028(5)	−0.005(4)	0.014(4)	−0.001(4)
C11B	0.027(4)	0.025(5)	0.026(5)	0.001(4)	0.016(4)	−0.004(4)
C12B	0.028(5)	0.024(5)	0.032(5)	−0.001(4)	0.016(4)	0.001(4)
C13B	0.025(5)	0.020(5)	0.031(5)	0.001(4)	0.016(4)	−0.001(4)
C14B	0.026(4)	0.019(4)	0.027(5)	−0.004(4)	0.014(4)	0.001(4)
C15B	0.017(4)	0.020(4)	0.030(5)	0.001(4)	0.012(4)	−0.004(4)
C16B	0.023(5)	0.022(4)	0.021(4)	−0.002(4)	0.013(4)	0.000(4)
C17B	0.029(5)	0.028(5)	0.043(5)	−0.006(4)	0.016(4)	−0.002(4)
C18B	0.025(5)	0.027(5)	0.040(5)	0.000(4)	0.018(4)	0.006(4)
C19B	0.030(5)	0.025(5)	0.037(5)	−0.002(4)	0.016(4)	−0.001(4)
C20B	0.024(5)	0.019(4)	0.028(5)	0.003(4)	0.016(4)	0.005(4)
C21B	0.023(5)	0.025(5)	0.031(5)	−0.004(4)	0.015(4)	−0.001(4)
C22B	0.022(5)	0.034(5)	0.030(5)	0.001(4)	0.022(4)	−0.003(4)
C23B	0.026(7)	0.058(8)	0.052(8)	−0.007(7)	0.025(6)	0.002(6)
C24B	0.037(7)	0.050(8)	0.044(7)	−0.004(6)	0.024(6)	−0.004(6)
C25B	0.066(9)	0.043(8)	0.045(7)	0.004(6)	0.028(7)	0.001(7)

C26B	0.024(5)	0.025(5)	0.035(5)	0.000(4)	0.015(4)	0.001(4)
C27B	0.036(6)	0.037(6)	0.045(6)	0.003(5)	0.012(5)	−0.008(5)
C28B	0.033(6)	0.042(6)	0.050(6)	−0.011(5)	0.015(5)	−0.006(5)
C29B	0.024(5)	0.024(5)	0.030(5)	−0.003(4)	0.016(4)	−0.002(4)
C30B	0.043(6)	0.036(5)	0.037(5)	0.002(4)	0.013(4)	−0.005(5)
C31B	0.044(6)	0.041(6)	0.043(5)	−0.002(5)	0.014(4)	0.000(5)
C32B	0.034(5)	0.036(5)	0.036(5)	0.007(4)	0.012(4)	0.005(4)
C33B	0.028(5)	0.023(5)	0.031(5)	0.005(4)	0.009(4)	0.003(4)
C34B	0.020(5)	0.022(4)	0.025(4)	0.001(4)	0.017(4)	0.004(4)
C35B	0.069(7)	0.070(8)	0.066(7)	0.005(5)	0.015(5)	0.001(5)
C36B	0.083(12)	0.098(11)	0.097(12)	−0.018(9)	0.015(9)	−0.002(9)
C37B	0.075(10)	0.090(12)	0.091(12)	−0.016(10)	0.006(8)	0.009(9)
C38B	0.133(15)	0.143(15)	0.112(12)	0.023(11)	0.038(10)	−0.006(11)
C39B	0.039(6)	0.025(5)	0.036(5)	0.002(4)	0.012(4)	0.004(5)
C40B	0.062(9)	0.047(8)	0.047(7)	0.004(6)	0.028(7)	0.004(7)
C41B	0.055(8)	0.028(7)	0.058(8)	0.004(6)	0.019(7)	0.023(7)
C42B	0.041(7)	0.029(7)	0.059(8)	−0.010(6)	0.016(7)	−0.003(6)
C43B	0.023(5)	0.020(4)	0.032(5)	−0.003(4)	0.018(4)	0.003(4)
C44B	0.029(5)	0.027(5)	0.029(5)	0.001(4)	0.013(4)	0.005(4)
C45B	0.029(5)	0.019(5)	0.034(5)	0.002(4)	0.016(4)	0.001(4)
C46B	0.031(5)	0.023(5)	0.032(5)	−0.005(4)	0.018(4)	0.002(4)
C47B	0.027(5)	0.023(5)	0.032(5)	0.002(4)	0.015(4)	0.000(4)
C48B	0.023(5)	0.019(4)	0.030(5)	−0.001(4)	0.018(4)	0.004(4)
C49B	0.037(6)	0.032(5)	0.038(5)	0.000(4)	0.023(4)	0.000(4)
C50B	0.082(11)	0.079(10)	0.057(9)	0.013(8)	0.048(8)	0.002(8)
C51B	0.076(9)	0.086(11)	0.075(10)	−0.005(9)	0.047(8)	0.017(8)
C52B	0.099(11)	0.097(11)	0.065(9)	−0.011(9)	0.031(9)	−0.010(10)
C53B	0.034(5)	0.025(5)	0.035(5)	0.000(4)	0.015(4)	−0.001(4)
C54B	0.066(9)	0.054(9)	0.053(8)	0.004(7)	0.011(7)	0.001(8)
C55B	0.052(9)	0.032(7)	0.053(8)	0.003(6)	0.030(7)	0.002(7)
C56B	0.055(8)	0.054(9)	0.070(9)	0.014(7)	0.046(7)	0.002(7)
Si1B	0.0212(19)	0.029(2)	0.0338(19)	−0.0006(16)	0.0225(17)	−0.0052(17)
S1B	0.038(2)	0.029(2)	0.041(2)	−0.0053(16)	0.0198(18)	−0.0061(17)
S2B	0.028(2)	0.046(2)	0.042(2)	−0.0006(19)	0.0209(18)	−0.0109(18)
Ni1C	0.0210(9)	0.0143(8)	0.0304(9)	−0.0024(7)	0.0172(8)	0.0000(7)
N1C	0.025(5)	0.017(4)	0.039(6)	−0.007(4)	0.022(5)	−0.002(4)
N2C	0.026(5)	0.018(5)	0.028(5)	0.000(4)	0.014(5)	0.007(4)
N3C	0.024(5)	0.026(5)	0.023(5)	−0.007(4)	0.016(4)	0.001(4)
N4C	0.022(5)	0.024(5)	0.034(5)	0.000(5)	0.015(5)	0.001(4)
C1C	0.025(5)	0.024(5)	0.029(5)	−0.001(4)	0.015(4)	0.003(4)
C2C	0.035(6)	0.030(5)	0.046(6)	0.001(4)	0.020(5)	0.004(4)
C3C	0.033(5)	0.031(5)	0.038(5)	0.006(4)	0.015(4)	−0.002(4)
C4C	0.022(5)	0.019(5)	0.026(5)	−0.003(4)	0.012(4)	0.001(4)
C5C	0.022(5)	0.028(5)	0.029(5)	0.003(4)	0.013(4)	0.000(4)
C6C	0.023(5)	0.027(4)	0.026(5)	−0.001(4)	0.016(4)	0.000(4)
C7C	0.034(5)	0.035(5)	0.043(6)	−0.004(4)	0.020(5)	0.002(4)
C8C	0.029(5)	0.036(5)	0.045(6)	0.001(5)	0.016(5)	0.002(4)
C9C	0.027(5)	0.024(5)	0.027(5)	−0.005(4)	0.013(4)	−0.001(4)
C10C	0.027(5)	0.020(4)	0.028(5)	0.000(4)	0.013(4)	0.003(4)
C11C	0.029(4)	0.017(5)	0.027(5)	0.003(4)	0.009(4)	0.000(4)

C12C	0.030(5)	0.032(5)	0.037(5)	0.006(4)	0.016(4)	0.000(4)
C13C	0.033(5)	0.028(5)	0.041(5)	0.002(4)	0.014(4)	-0.002(4)
C14C	0.025(4)	0.024(5)	0.032(5)	-0.001(4)	0.010(4)	-0.003(4)
C15C	0.028(5)	0.032(5)	0.034(5)	0.000(4)	0.011(4)	-0.003(4)
C16C	0.029(5)	0.029(5)	0.029(5)	0.001(4)	0.017(4)	0.000(4)
C17C	0.031(5)	0.038(5)	0.048(6)	-0.004(5)	0.018(5)	0.001(4)
C18C	0.032(5)	0.034(5)	0.045(6)	-0.002(5)	0.018(5)	0.007(4)
C19C	0.022(5)	0.022(4)	0.034(5)	-0.002(4)	0.016(4)	0.005(4)
C20C	0.028(5)	0.027(5)	0.028(5)	0.000(4)	0.016(4)	0.004(4)
C21C	0.024(5)	0.026(5)	0.030(5)	-0.003(4)	0.014(4)	-0.002(4)
C22C	0.035(5)	0.035(6)	0.037(5)	0.003(4)	0.014(4)	-0.003(4)
C23C	0.058(9)	0.061(9)	0.060(9)	-0.011(8)	0.033(8)	0.009(8)
C24C	0.037(7)	0.052(8)	0.035(6)	-0.007(6)	0.019(6)	-0.005(6)
C25C	0.057(9)	0.047(8)	0.055(8)	0.010(7)	0.039(7)	0.005(7)
C26C	0.028(5)	0.034(5)	0.034(5)	-0.003(4)	0.014(4)	-0.002(4)
C27C	0.045(6)	0.048(6)	0.054(6)	0.001(5)	0.013(5)	-0.012(5)
C28C	0.044(6)	0.049(7)	0.057(7)	0.001(5)	0.016(5)	-0.008(5)
C29C	0.030(5)	0.027(5)	0.035(5)	0.001(4)	0.014(4)	-0.002(4)
C30C	0.037(5)	0.028(5)	0.035(5)	-0.002(4)	0.007(4)	0.001(4)
C31C	0.044(6)	0.044(6)	0.047(5)	0.003(5)	0.014(4)	0.000(5)
C32C	0.026(5)	0.033(5)	0.038(5)	0.006(4)	0.013(4)	0.006(4)
C33C	0.030(5)	0.031(5)	0.034(5)	0.006(4)	0.016(4)	0.002(4)
C34C	0.024(5)	0.024(5)	0.030(5)	-0.003(4)	0.009(4)	0.004(4)
C35C	0.056(7)	0.057(7)	0.059(6)	0.004(5)	0.012(5)	0.002(5)
C36C	0.080(11)	0.090(11)	0.084(11)	-0.004(9)	0.023(8)	-0.017(9)
C37C	0.087(12)	0.090(11)	0.084(11)	0.005(9)	0.001(9)	0.016(9)
C38C	0.082(11)	0.085(11)	0.057(8)	0.005(8)	0.015(8)	-0.014(9)
C39C	0.036(6)	0.026(5)	0.035(5)	-0.006(4)	0.014(4)	0.009(4)
C40C	0.079(10)	0.033(7)	0.054(8)	-0.004(6)	0.030(8)	0.005(8)
C41C	0.054(8)	0.032(7)	0.064(9)	0.007(7)	0.026(7)	0.007(7)
C42C	0.055(8)	0.046(9)	0.074(10)	-0.015(8)	0.022(7)	0.002(7)
C43C	0.025(5)	0.018(4)	0.030(5)	0.001(4)	0.016(4)	0.007(4)
C44C	0.029(5)	0.029(5)	0.032(5)	0.003(4)	0.017(4)	0.002(4)
C45C	0.030(5)	0.028(5)	0.033(5)	-0.002(4)	0.014(4)	0.004(4)
C46C	0.030(5)	0.025(5)	0.034(5)	-0.006(4)	0.013(4)	0.003(4)
C47C	0.028(5)	0.025(5)	0.036(5)	0.000(4)	0.014(4)	0.003(4)
C48C	0.031(5)	0.023(5)	0.031(5)	-0.001(4)	0.015(4)	-0.002(4)
C49C	0.046(6)	0.039(6)	0.038(5)	-0.002(4)	0.020(5)	0.003(5)
C50C	0.080(10)	0.055(8)	0.067(10)	0.011(7)	0.039(8)	0.005(8)
C51C	0.067(9)	0.070(10)	0.063(9)	0.005(8)	0.044(7)	0.010(8)
C52C	0.088(10)	0.099(11)	0.054(8)	-0.016(8)	0.041(8)	-0.038(9)
C53C	0.040(6)	0.034(5)	0.049(6)	0.002(5)	0.021(5)	-0.001(5)
C54C	0.061(8)	0.023(6)	0.048(7)	0.016(5)	0.016(7)	-0.005(7)
C55C	0.051(8)	0.014(5)	0.051(7)	0.002(5)	0.032(7)	-0.005(6)
C56C	0.046(7)	0.038(8)	0.070(9)	0.011(7)	0.040(7)	0.004(6)
Si1C	0.033(2)	0.033(2)	0.036(2)	-0.0013(18)	0.0239(19)	-0.0023(19)
S1C	0.056(3)	0.034(2)	0.040(2)	-0.0031(17)	0.023(2)	-0.012(2)
S2C	0.0278(19)	0.033(2)	0.051(2)	-0.0065(18)	0.0212(18)	-0.0058(17)
Ni1D	0.0215(9)	0.0151(9)	0.0277(8)	-0.0018(6)	0.0132(8)	0.0003(7)

N1D	0.024(5)	0.024(5)	0.034(6)	-0.003(5)	0.013(5)	-0.001(4)
N2D	0.027(5)	0.025(5)	0.033(5)	-0.009(5)	0.010(5)	0.006(4)
N3D	0.018(5)	0.022(5)	0.031(5)	0.005(4)	0.010(5)	0.004(4)
N4D	0.021(5)	0.021(5)	0.028(5)	-0.005(4)	0.009(5)	0.002(4)
C1D	0.025(4)	0.023(5)	0.028(5)	-0.003(4)	0.011(4)	0.000(4)
C2D	0.033(5)	0.026(5)	0.039(5)	0.003(4)	0.010(4)	-0.002(4)
C3D	0.031(5)	0.026(5)	0.041(5)	-0.001(4)	0.012(4)	0.001(4)
C4D	0.030(5)	0.028(5)	0.029(5)	0.006(4)	0.013(4)	0.000(4)
C5D	0.031(5)	0.033(5)	0.029(5)	-0.002(4)	0.014(4)	0.004(4)
C6D	0.026(5)	0.031(5)	0.040(5)	0.000(4)	0.014(4)	0.002(4)
C7D	0.032(5)	0.034(5)	0.047(6)	0.003(5)	0.015(5)	-0.003(4)
C8D	0.032(5)	0.025(5)	0.038(5)	-0.001(4)	0.015(4)	0.004(4)
C9D	0.028(5)	0.023(4)	0.031(5)	0.000(4)	0.011(4)	0.002(4)
C10D	0.021(5)	0.015(4)	0.024(4)	0.006(4)	0.014(4)	0.005(4)
C11D	0.027(5)	0.016(4)	0.024(4)	-0.004(4)	0.014(4)	0.002(4)
C12D	0.027(5)	0.024(5)	0.035(5)	-0.003(4)	0.009(4)	-0.005(4)
C13D	0.027(5)	0.021(5)	0.031(5)	0.001(4)	0.009(4)	0.001(4)
C14D	0.018(5)	0.019(4)	0.022(4)	0.003(4)	0.006(4)	0.002(4)
C15D	0.025(5)	0.027(5)	0.030(5)	0.001(4)	0.013(4)	0.002(4)
C16D	0.025(5)	0.028(5)	0.030(5)	-0.001(4)	0.011(4)	0.002(4)
C17D	0.038(6)	0.043(6)	0.053(6)	0.000(5)	0.026(5)	0.003(4)
C18D	0.029(5)	0.026(5)	0.041(5)	0.003(4)	0.017(4)	0.004(4)
C19D	0.022(5)	0.023(5)	0.030(5)	-0.003(4)	0.014(4)	0.001(4)
C20D	0.030(5)	0.025(5)	0.033(5)	-0.001(4)	0.010(4)	-0.001(4)
C21D	0.028(5)	0.029(5)	0.030(5)	0.000(4)	0.012(4)	0.002(4)
C22D	0.033(5)	0.038(6)	0.033(5)	-0.006(4)	0.018(4)	-0.001(4)
C23D	0.045(8)	0.052(8)	0.061(9)	-0.003(7)	0.024(7)	0.006(7)
C24D	0.038(8)	0.049(8)	0.057(8)	-0.002(7)	0.019(7)	-0.010(7)
C25D	0.038(8)	0.046(8)	0.051(8)	-0.014(7)	0.020(7)	-0.005(6)
C26D	0.023(5)	0.027(5)	0.031(5)	0.001(4)	0.016(4)	-0.004(4)
C27D	0.048(6)	0.050(6)	0.046(6)	0.004(5)	0.025(5)	-0.008(5)
C28D	0.046(6)	0.048(6)	0.056(6)	0.002(5)	0.023(5)	-0.008(5)
C29D	0.033(5)	0.026(5)	0.032(5)	-0.002(4)	0.011(4)	0.003(4)
C30D	0.030(5)	0.025(5)	0.035(5)	0.000(4)	0.014(4)	0.001(4)
C31D	0.030(5)	0.030(5)	0.033(5)	-0.002(4)	0.009(4)	-0.001(4)
C32D	0.024(5)	0.026(5)	0.032(5)	-0.006(4)	0.013(4)	0.001(4)
C33D	0.030(5)	0.028(5)	0.037(5)	-0.005(4)	0.013(4)	0.002(4)
C34D	0.031(5)	0.029(5)	0.030(5)	0.000(4)	0.017(4)	0.004(4)
C35D	0.049(6)	0.052(6)	0.045(6)	-0.002(5)	0.025(5)	-0.001(5)
C36D	0.090(11)	0.071(9)	0.072(10)	0.006(8)	0.045(9)	0.005(8)
C37D	0.069(9)	0.089(11)	0.089(11)	0.001(9)	0.052(8)	0.009(8)
C38D	0.097(11)	0.081(10)	0.065(9)	-0.023(9)	0.026(9)	-0.008(9)
C39D	0.037(6)	0.031(5)	0.040(5)	-0.002(4)	0.017(5)	0.005(5)
C40D	0.065(9)	0.040(8)	0.056(8)	0.001(7)	0.013(7)	0.013(7)
C41D	0.041(8)	0.026(6)	0.051(7)	0.003(6)	0.020(6)	0.002(6)
C42D	0.061(8)	0.049(9)	0.076(10)	0.009(7)	0.039(8)	0.006(7)
C43D	0.027(5)	0.025(5)	0.030(5)	-0.002(4)	0.012(4)	0.005(4)
C44D	0.029(5)	0.030(5)	0.035(5)	-0.009(4)	0.011(4)	0.001(4)
C45D	0.033(5)	0.031(5)	0.032(5)	-0.003(4)	0.011(4)	0.004(4)

C46D	0.030(5)	0.030(5)	0.036(5)	0.003(4)	0.011(4)	0.006(4)
C47D	0.032(5)	0.017(4)	0.026(4)	0.008(4)	0.015(4)	0.002(4)
C48D	0.023(5)	0.022(5)	0.027(5)	0.003(4)	0.009(4)	0.003(4)
C49D	0.041(6)	0.044(6)	0.043(6)	0.003(5)	0.010(4)	−0.001(5)
C50D	0.075(11)	0.063(9)	0.076(11)	−0.018(8)	0.007(8)	−0.012(8)
C51D	0.057(9)	0.072(10)	0.073(10)	−0.007(9)	0.010(8)	0.007(8)
C52D	0.095(12)	0.092(12)	0.074(10)	0.022(9)	0.014(8)	−0.011(10)
C53D	0.028(5)	0.023(5)	0.033(5)	0.001(4)	0.010(4)	0.005(4)
C54D	0.058(9)	0.034(7)	0.039(6)	0.001(6)	0.023(7)	0.003(7)
C55D	0.038(7)	0.018(6)	0.041(7)	0.004(5)	0.011(6)	0.004(6)
C56D	0.037(7)	0.031(7)	0.056(8)	−0.006(6)	0.017(6)	−0.004(6)
Si1D	0.023(2)	0.033(2)	0.042(2)	−0.0017(19)	0.0127(19)	−0.0010(18)
S1D	0.060(3)	0.053(3)	0.035(2)	0.007(2)	0.017(2)	−0.015(3)
S2D	0.031(2)	0.038(2)	0.045(2)	0.0038(18)	0.0243(19)	−0.0051(18)
Cl1	0.147(9)	0.223(14)	0.120(8)	0.015(9)	0.047(7)	−0.061(10)
Cl2	0.235(13)	0.070(5)	0.172(11)	0.027(6)	0.051(10)	−0.016(7)
Cl3	0.315(19)	0.272(19)	0.212(16)	0.021(16)	0.049(15)	−0.021(17)
Cl4	0.170(11)	0.227(14)	0.127(9)	0.023(10)	0.057(8)	0.012(11)
Cl5	0.150(11)	0.319(18)	0.145(10)	0.076(13)	0.020(9)	0.053(13)
Cl6	0.323(18)	0.34(2)	0.251(17)	−0.006(16)	0.207(16)	0.026(17)
Cl7	0.246(14)	0.129(9)	0.192(13)	−0.038(9)	0.119(12)	0.004(10)
Cl8	0.113(8)	0.190(12)	0.133(8)	0.061(9)	0.010(7)	−0.014(8)

Table S24. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for **Ni10**.

	x	y	z	U
H2A	0.301450	0.517196	0.856329	0.029
H3A	0.399548	0.490756	0.884684	0.027
H7A	0.514821	0.209719	0.906584	0.040
H8A	0.486674	0.060589	0.882940	0.033
H12A	0.310401	−0.117808	0.869830	0.024
H13A	0.239448	−0.086967	0.906656	0.032
H17A	0.144183	0.196895	0.928632	0.039
H18A	0.145873	0.341155	0.892334	0.041
H23A	0.631813	0.314272	0.955795	0.058
H23B	0.672511	0.382423	0.990984	0.058
H23C	0.625569	0.341493	1.007765	0.058
H24A	0.597863	0.433542	0.867680	0.059
H24B	0.575443	0.527025	0.872332	0.059
H24C	0.638312	0.506077	0.898577	0.059
H25A	0.631140	0.562149	0.999973	0.067
H25B	0.568059	0.582123	0.974311	0.067
H25C	0.588028	0.516987	1.020254	0.067
H26A	0.174962	0.084946	0.964280	0.031
H27A	0.149392	−0.130011	1.002837	0.057
H27B	0.141590	−0.032992	1.016698	0.057
H28A	0.076645	−0.027522	0.947676	0.066
H28B	0.093900	−0.115681	0.929163	0.066
H30A	0.404667	−0.002287	0.792013	0.026
H32A	0.471177	−0.239737	0.821939	0.034
H34A	0.411487	−0.125383	0.918727	0.024
H36A	0.438402	0.011162	0.742177	0.091
H36B	0.500888	−0.014818	0.764559	0.091
H36C	0.468326	−0.026599	0.706222	0.091
H37A	0.478167	−0.237602	0.752730	0.109
H37B	0.492651	−0.179544	0.712735	0.109
H37C	0.525213	−0.167763	0.771072	0.109
H38A	0.371785	−0.094136	0.707398	0.109
H38B	0.406725	−0.130481	0.675438	0.109
H38C	0.387409	−0.193245	0.710470	0.109
H40A	0.477001	−0.205045	0.972479	0.073
H40B	0.496566	−0.302293	0.981628	0.073
H40C	0.527404	−0.236594	0.957563	0.073
H41A	0.452097	−0.364929	0.853145	0.059
H41B	0.512290	−0.334967	0.884349	0.059
H41C	0.481451	−0.400667	0.908413	0.059
H42A	0.376044	−0.325581	0.878153	0.082
H42B	0.407872	−0.361492	0.932896	0.082
H42C	0.383761	−0.266672	0.926019	0.082
H44A	0.149357	0.400515	0.797112	0.034
H46A	0.115669	0.645355	0.821624	0.026
H48A	0.247590	0.528927	0.917436	0.026

H50A	0.054195	0.397331	0.758719	0.122
H50B	0.025475	0.438012	0.704597	0.122
H50C	0.088072	0.412452	0.722140	0.122
H51A	0.029081	0.608463	0.779876	0.087
H51B	-0.008004	0.551458	0.734529	0.087
H51C	0.016173	0.511389	0.789355	0.087
H52A	0.092644	0.641909	0.734053	0.101
H52B	0.112305	0.566705	0.706183	0.101
H52C	0.049708	0.592265	0.688640	0.101
H54A	0.216807	0.615531	0.972315	0.050
H54B	0.205514	0.714836	0.977707	0.050
H54C	0.156256	0.651408	0.951770	0.050
H55A	0.168558	0.768256	0.849182	0.051
H55B	0.126894	0.744215	0.877082	0.051
H55C	0.176152	0.807643	0.903019	0.051
H56A	0.263075	0.718541	0.882039	0.054
H56B	0.267912	0.759020	0.935008	0.054
H56C	0.283270	0.660948	0.931359	0.054
H2B	0.402032	0.713269	0.627900	0.034
H3B	0.479677	0.679314	0.602271	0.035
H7B	0.577268	0.391021	0.587645	0.037
H8B	0.570587	0.248484	0.622262	0.035
H12B	0.406607	0.076016	0.645140	0.032
H13B	0.308027	0.104184	0.607098	0.028
H17B	0.195758	0.391166	0.573566	0.039
H18B	0.225036	0.534871	0.610335	0.035
H23D	0.662090	0.511096	0.534322	0.064
H23E	0.617657	0.536447	0.482009	0.064
H23F	0.675210	0.583127	0.500207	0.064
H24D	0.687886	0.629823	0.622259	0.062
H24E	0.702398	0.705459	0.591155	0.062
H24F	0.658301	0.720302	0.617686	0.062
H25D	0.619575	0.756860	0.491110	0.073
H25E	0.562762	0.708150	0.471042	0.073
H25F	0.575477	0.771704	0.517640	0.073
H26B	0.201354	0.277349	0.542314	0.032
H27C	0.130160	0.164282	0.492865	0.047
H27D	0.144842	0.064918	0.501218	0.047
H28C	0.150874	0.068599	0.579206	0.050
H28D	0.113847	0.151853	0.562471	0.050
H30B	0.560491	0.190947	0.716466	0.046
H32B	0.601110	-0.049495	0.688085	0.042
H34B	0.470365	0.067050	0.590241	0.024
H36D	0.626234	0.190374	0.779975	0.144
H36E	0.686634	0.156403	0.806396	0.144
H36F	0.667394	0.187516	0.749497	0.144
H37D	0.678176	-0.027256	0.741098	0.136
H37E	0.696999	0.063801	0.727399	0.136
H37F	0.716239	0.032689	0.784297	0.136
H38D	0.619868	-0.039133	0.785629	0.195
H38E	0.666381	0.014113	0.826044	0.195

H38F	0.604672	0.043858	0.810908	0.195
H40D	0.503634	-0.008140	0.534884	0.074
H40E	0.565400	-0.038528	0.553543	0.074
H40F	0.518295	-0.104655	0.526092	0.074
H41D	0.560331	-0.172667	0.652999	0.070
H41E	0.552758	-0.204482	0.597605	0.070
H41F	0.599862	-0.138355	0.625056	0.070
H42D	0.464216	-0.133385	0.623090	0.065
H42E	0.439989	-0.073443	0.575135	0.065
H42F	0.461058	-0.167314	0.569136	0.065
H44B	0.302613	0.601111	0.702049	0.033
H46B	0.244873	0.841837	0.672681	0.032
H48B	0.303731	0.720345	0.576041	0.026
H50D	0.225572	0.598957	0.736638	0.100
H50E	0.287315	0.609382	0.771738	0.100
H50F	0.239758	0.639537	0.791184	0.100
H51D	0.196445	0.818157	0.714072	0.110
H51E	0.170004	0.724985	0.703511	0.110
H51F	0.186900	0.765036	0.758397	0.110
H52D	0.291669	0.836505	0.763301	0.130
H52E	0.280718	0.786146	0.807866	0.130
H52F	0.328275	0.755991	0.788420	0.130
H54D	0.181186	0.841059	0.549390	0.090
H54E	0.203447	0.907223	0.518120	0.090
H54F	0.219503	0.808420	0.519782	0.090
H55D	0.214036	0.935035	0.619348	0.064
H55E	0.276449	0.961357	0.641962	0.064
H55F	0.239324	0.998609	0.589115	0.064
H56D	0.341818	0.905700	0.603907	0.080
H56E	0.320849	0.849202	0.554185	0.080
H56F	0.304793	0.948006	0.552523	0.080
H2C	-0.153799	-0.099232	0.869293	0.043
H3C	-0.227690	-0.068352	0.902113	0.040
H7C	-0.328382	0.217156	0.914084	0.043
H8C	-0.322689	0.360011	0.878427	0.043
H12C	-0.156320	0.534790	0.861504	0.038
H13C	-0.058761	0.507419	0.897613	0.041
H17C	0.054723	0.226018	0.920610	0.045
H18C	0.026806	0.076095	0.895240	0.043
H23G	-0.413824	0.091998	0.966111	0.084
H23H	-0.427507	0.015917	0.997435	0.084
H23I	-0.369582	0.061317	1.017340	0.084
H24G	-0.437960	-0.016161	0.873207	0.059
H24H	-0.407338	-0.105050	0.874963	0.059
H24I	-0.453353	-0.097278	0.899864	0.059
H25G	-0.373695	-0.157477	0.999566	0.072
H25H	-0.328933	-0.167211	0.973324	0.072
H25I	-0.316861	-0.109487	1.022296	0.072
H26C	0.049788	0.337030	0.959917	0.037
H27E	0.100444	0.556427	0.995914	0.059

H27F	0.119249	0.458946	1.006589	0.059
H28E	0.134196	0.470301	0.935208	0.060
H28F	0.093153	0.548678	0.916613	0.060
H30C	-0.304437	0.422322	0.785054	0.042
H32C	-0.348253	0.661782	0.810125	0.038
H34C	-0.219976	0.547330	0.911078	0.032
H36G	-0.390510	0.410556	0.747352	0.128
H36H	-0.439971	0.467639	0.749971	0.128
H36I	-0.433080	0.448542	0.697215	0.128
H37G	-0.383424	0.661731	0.723793	0.141
H37H	-0.428490	0.607900	0.682307	0.141
H37I	-0.435380	0.626997	0.735062	0.141
H38G	-0.333173	0.472740	0.704810	0.115
H38H	-0.383858	0.519585	0.665361	0.115
H38I	-0.332510	0.574095	0.697870	0.115
H40G	-0.264487	0.620927	0.962239	0.080
H40H	-0.278086	0.718323	0.970230	0.080
H40I	-0.324977	0.655757	0.937797	0.080
H41G	-0.300072	0.787313	0.844656	0.073
H41H	-0.346944	0.758361	0.865327	0.073
H41I	-0.300053	0.820926	0.897760	0.073
H42G	-0.207406	0.740218	0.884716	0.088
H42H	-0.209194	0.772897	0.937408	0.088
H42I	-0.191702	0.676708	0.931509	0.088
H44C	-0.046540	0.017653	0.801693	0.035
H46C	0.005031	-0.226454	0.824866	0.035
H48C	-0.053566	-0.111361	0.922588	0.033
H50G	0.006727	-0.014155	0.708923	0.096
H50H	-0.039292	0.013637	0.730971	0.096
H50I	0.023094	0.022654	0.764529	0.096
H51G	0.054434	-0.194295	0.780949	0.092
H51H	0.060459	-0.136524	0.736751	0.092
H51I	0.079204	-0.100155	0.792571	0.092
H52G	-0.044520	-0.213091	0.730928	0.114
H52H	-0.080407	-0.130341	0.708949	0.114
H52I	-0.033017	-0.157310	0.688487	0.114
H54G	0.064093	-0.234732	0.951808	0.067
H54H	0.022111	-0.203115	0.977761	0.067
H54I	0.037767	-0.302061	0.979149	0.067
H55G	0.031504	-0.326593	0.875090	0.052
H55H	0.007388	-0.390051	0.906316	0.052
H55I	-0.030768	-0.354047	0.853523	0.052
H56G	-0.075108	-0.238685	0.940391	0.069
H56H	-0.095221	-0.300816	0.893024	0.069
H56I	-0.057066	-0.336819	0.945817	0.069
H2D	-0.056954	0.095051	0.639866	0.039
H3D	-0.154378	0.122264	0.607806	0.039
H7D	-0.268032	0.406705	0.589226	0.045

H8D	-0.237545	0.554057	0.617059	0.036
H12D	-0.062552	0.729107	0.626934	0.035
H13D	0.008146	0.698539	0.590495	0.031
H17D	0.106595	0.415464	0.573516	0.050
H18D	0.103575	0.272388	0.610931	0.037
H23J	-0.387875	0.288209	0.541575	0.076
H23K	-0.384262	0.255705	0.489491	0.076
H23L	-0.427507	0.214437	0.511084	0.076
H24J	-0.344896	0.169527	0.634208	0.071
H24K	-0.384539	0.095086	0.604581	0.071
H24L	-0.320838	0.078175	0.627669	0.071
H25J	-0.343871	0.083952	0.480407	0.065
H25K	-0.320166	0.022692	0.527833	0.065
H25L	-0.383867	0.039603	0.504745	0.065
H26D	0.074237	0.527919	0.535518	0.030
H27G	0.112478	0.639863	0.491166	0.055
H27H	0.100903	0.739547	0.495179	0.055
H28G	0.143988	0.743432	0.576750	0.059
H28H	0.177356	0.667861	0.562656	0.059
H30D	-0.160894	0.612056	0.703289	0.036
H32D	-0.217964	0.854830	0.679574	0.032
H34D	-0.163308	0.739841	0.578501	0.034
H36J	-0.165702	0.622988	0.775343	0.110
H36K	-0.207462	0.650998	0.802366	0.110
H36L	-0.229252	0.610249	0.747590	0.110
H37J	-0.260612	0.825782	0.726062	0.114
H37K	-0.286215	0.731935	0.718020	0.114
H37L	-0.264425	0.772684	0.772795	0.114
H38J	-0.172309	0.850848	0.767926	0.122
H38K	-0.179062	0.799019	0.813916	0.122
H38L	-0.131229	0.775278	0.793342	0.122
H40J	-0.283368	0.850416	0.552518	0.083
H40K	-0.261303	0.918357	0.522052	0.083
H40L	-0.241367	0.821228	0.526017	0.083
H41J	-0.252074	0.952666	0.625548	0.057
H41K	-0.190208	0.982500	0.645990	0.057
H41L	-0.229339	1.014892	0.592674	0.057
H42J	-0.144193	0.869158	0.561731	0.087
H42K	-0.165715	0.965527	0.555009	0.087
H42L	-0.126584	0.933135	0.608325	0.087
H44D	0.097010	0.215440	0.703482	0.038
H46D	0.134036	-0.029961	0.680412	0.038
H48D	0.001366	0.080490	0.584411	0.028
H50J	0.193454	0.221330	0.735729	0.115
H50K	0.159339	0.211053	0.772498	0.115
H50L	0.222222	0.187061	0.791427	0.115
H51J	0.215549	0.000307	0.723227	0.106
H51K	0.231692	0.093158	0.709446	0.106
H51L	0.254862	0.059825	0.765883	0.106

H52J	0.158021	-0.015360	0.773645	0.136
H52K	0.200628	0.042804	0.814651	0.136
H52L	0.137745	0.066795	0.795722	0.136
H54J	0.039144	-0.007041	0.530344	0.063
H54K	0.099348	-0.043184	0.554505	0.063
H54L	0.050795	-0.106667	0.526632	0.063
H55J	0.078622	-0.156733	0.655355	0.050
H55K	0.074886	-0.197963	0.602842	0.050
H55L	0.123438	-0.134481	0.630714	0.050
H56J	-0.014567	-0.103492	0.618390	0.062
H56K	-0.031584	-0.046235	0.568906	0.062
H56L	-0.018066	-0.145345	0.566091	0.062
H1S1	0.328751	0.306502	0.692685	0.168
H1S2	0.282032	0.245303	0.699127	0.168
H2S1	0.340943	0.373039	0.767375	0.391
H2S2	0.307061	0.300900	0.784146	0.391
H3S1	-0.053211	0.317037	0.709955	0.187
H3S2	-0.089666	0.258774	0.732712	0.187
H4S1	-0.024097	0.398211	0.783695	0.450
H4S2	-0.059281	0.338860	0.807511	0.450
H5S1	-0.184247	0.238620	0.696371	0.287
H5S2	-0.234872	0.177517	0.691667	0.287
H6S1	-0.188215	0.298806	0.768733	0.139
H6S2	-0.231312	0.228494	0.772788	0.139
H7S1	-0.534624	0.352202	0.720065	0.198
H7S2	-0.566414	0.293135	0.747610	0.198
H8S1	-0.506444	0.439391	0.795472	0.125
H8S2	-0.549813	0.387853	0.812836	0.125

Table S25. Crystal data and structure refinement for **NiZn14**.

Identification code	oxdp25	
CCDC deposition number	1822194	
Chemical formula (moiety)	C ₁₀₃ H ₁₀₉ N ₉ NiOS ₂ Zn	
Chemical formula (total)	C ₁₀₃ H ₁₀₉ N ₉ NiOS ₂ Zn	
Formula weight	1677.19	
Temperature	150(2) K	
Radiation, wavelength	synchrotron, 0.6932 Å	
Crystal system, space group	triclinic, P $\bar{1}$	
Unit cell parameters	a = 14.218(5) Å	$\alpha = 69.445(3)^\circ$
	b = 20.122(6) Å	$\beta = 72.044(3)^\circ$
	c = 21.975(7) Å	$\gamma = 82.393(3)^\circ$
Cell volume	5598(3) Å ³	
Z	2	
Calculated density	0.995 g/cm ³	
Absorption coefficient μ	0.435 mm ⁻¹	
F(000)	1776	
Crystal color and size	yellow-green, 0.150 × 0.080 × 0.010 mm ³	
Reflections for cell refinement	8721 (θ range 4.7 to 22.5°)	
Data collection method	Bruker SMART 1K CCD diffractometer	
	thin-slice ω scans	
θ range for data collection	4.7 to 22.8°	
Index ranges	h -15 to 15, k -22 to 22, l -24 to 24	
Completeness to $\theta = 22.8^\circ$	95.2 %	
Reflections collected	27929	
Independent reflections	15633 ($R_{\text{int}} = 0.0392$)	
Reflections with $F^2 > 2\sigma$	8508	
Absorption correction	multi-scan	
Min. and max. transmission	0.93 and 0.99	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.1697, 5.5315	
Data / restraints / parameters	15633 / 4477 / 1348	
Final R indices [$F^2 > 2\sigma$]	R1 = 0.1004, wR2 = 0.2780	
R indices (all data)	R1 = 0.1556, wR2 = 0.3328	
Goodness-of-fit on F^2	1.039	
Largest and mean shift/su	0.003 and 0.000	
Largest diff. peak and hole	1.26 and -0.53 e Å ⁻³	

Table S26. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$) for **NiZn14**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ni1	1.0323(4)	0.57847(12)	0.22507(16)	0.1466(18)
N1A	1.0776(13)	0.6575(5)	0.1419(5)	0.134(4)
N2A	1.1274(14)	0.5171(6)	0.1862(5)	0.148(5)
N3	0.9782(5)	0.4990(3)	0.3057(3)	0.0891(17)
N4	0.9274(5)	0.6395(3)	0.2625(3)	0.0860(17)
C1A	1.0524(14)	0.7277(5)	0.1324(6)	0.125(4)
C2A	1.1116(14)	0.7701(7)	0.0659(6)	0.136(4)
C3A	1.1601(16)	0.7258(7)	0.0346(7)	0.145(4)
C4A	1.1395(16)	0.6537(7)	0.0797(7)	0.146(4)
C5A	1.1831(17)	0.5917(7)	0.0653(7)	0.155(3)
C6A	1.1876(16)	0.5293(7)	0.1207(7)	0.153(4)
C7A	1.2389(15)	0.4695(7)	0.1095(8)	0.151(4)
C8A	1.2329(14)	0.4179(7)	0.1770(7)	0.145(4)
C9A	1.1520(17)	0.4466(7)	0.2192(6)	0.129(4)
C10	1.1049(8)	0.4101(4)	0.2826(5)	0.107(2)
C11	1.0266(7)	0.4329(4)	0.3235(4)	0.0903(19)
C12	0.9711(6)	0.3899(4)	0.3877(4)	0.0880(19)
C13	0.8903(6)	0.4280(3)	0.4098(4)	0.0819(18)
C14	0.8960(6)	0.4963(3)	0.3589(4)	0.0761(17)
C15	0.8310(6)	0.5524(3)	0.3662(3)	0.0734(16)
C16	0.8499(6)	0.6208(3)	0.3216(3)	0.0740(16)
C17	0.7950(6)	0.6823(3)	0.3331(4)	0.0799(18)
C18	0.8391(6)	0.7383(3)	0.2808(4)	0.0831(18)
C19	0.9194(7)	0.7134(3)	0.2379(4)	0.0849(19)
C20	0.9770(8)	0.7549(4)	0.1758(4)	0.102(2)
Zn	0.39565(6)	0.49421(4)	0.67419(4)	0.0729(3)
N5	0.5029(4)	0.4289(2)	0.6361(3)	0.0609(12)
N6	0.3301(5)	0.4063(3)	0.7510(3)	0.0781(15)
N7	0.2688(5)	0.5531(3)	0.7015(3)	0.0808(15)
N8	0.4413(4)	0.5728(2)	0.5832(3)	0.0624(13)
C21	0.5829(5)	0.4493(3)	0.5815(3)	0.0607(14)
C22	0.6539(5)	0.3913(3)	0.5796(3)	0.0687(15)
C23	0.6130(5)	0.3354(3)	0.6321(3)	0.0665(15)
C24	0.5186(5)	0.3572(3)	0.6676(3)	0.0614(14)
C25	0.4497(5)	0.3139(3)	0.7240(3)	0.0657(14)
C26	0.3632(6)	0.3365(4)	0.7625(4)	0.0764(16)
C27	0.2952(6)	0.2921(4)	0.8229(4)	0.093(2)
C28	0.2252(8)	0.3342(4)	0.8469(5)	0.107(2)
C29	0.2450(7)	0.4050(4)	0.8017(4)	0.096(2)
C30	0.1863(8)	0.4662(5)	0.8069(5)	0.111(2)
C31	0.1959(7)	0.5348(4)	0.7602(5)	0.096(2)
C32	0.1280(8)	0.5915(4)	0.7636(5)	0.108(2)
C33	0.1603(7)	0.6462(4)	0.7056(5)	0.100(2)
C34	0.2499(6)	0.6235(4)	0.6661(4)	0.0828(18)
C35	0.3076(6)	0.6621(3)	0.6024(4)	0.0742(15)
C36	0.3938(5)	0.6398(3)	0.5631(4)	0.0682(15)

C37	0.4511(5)	0.6808(3)	0.4985(4)	0.0716(16)
C38	0.5319(5)	0.6414(3)	0.4775(4)	0.0700(16)
C39	0.5232(5)	0.5745(3)	0.5319(3)	0.0623(14)
C40	0.5931(5)	0.5179(3)	0.5314(3)	0.0622(14)
C41	0.7486(6)	0.5396(3)	0.4244(4)	0.0639(15)
C42	0.6788(6)	0.5292(3)	0.4740(4)	0.0628(15)
C43A	1.2455(10)	0.5952(10)	−0.0044(9)	0.167(4)
C44A	1.3235(16)	0.5281(15)	−0.0931(12)	0.235(6)
C45A	1.4009(14)	0.5365(15)	−0.0727(13)	0.235(7)
S1A	1.2170(10)	0.5414(6)	−0.0388(6)	0.233(4)
S2A	1.3686(6)	0.5880(4)	−0.0239(3)	0.203(3)
C46	1.1492(7)	0.3369(4)	0.3133(5)	0.104(2)
C47	1.1345(6)	0.2801(4)	0.2957(5)	0.103(2)
C48	1.1647(7)	0.2125(4)	0.3299(5)	0.105(2)
C49	1.2107(7)	0.2017(5)	0.3806(6)	0.115(2)
C50	1.2262(7)	0.2583(6)	0.3990(6)	0.122(2)
C51	1.1950(7)	0.3248(5)	0.3646(5)	0.115(2)
C52	1.1436(7)	0.1485(5)	0.3128(6)	0.123(3)
C53	1.0758(16)	0.0968(10)	0.3759(9)	0.141(5)
C54	1.0938(19)	0.1690(10)	0.2559(11)	0.142(5)
C55	1.2401(12)	0.1054(11)	0.2934(14)	0.151(6)
C56	1.2696(8)	0.2473(6)	0.4573(6)	0.143(3)
C57	1.3716(9)	0.2149(8)	0.4385(7)	0.191(5)
C58	1.2054(9)	0.1975(7)	0.5249(7)	0.179(5)
C59	1.2736(10)	0.3164(6)	0.4704(7)	0.183(5)
C60	0.9521(7)	0.8336(4)	0.1574(4)	0.0909(19)
C61	0.8990(7)	0.8641(4)	0.1108(4)	0.100(2)
C62	0.8656(7)	0.9345(4)	0.0984(4)	0.103(2)
C63	0.8891(6)	0.9728(4)	0.1321(4)	0.089(2)
C64	0.9445(5)	0.9450(3)	0.1786(4)	0.0760(16)
C65	0.9760(6)	0.8739(3)	0.1893(3)	0.0772(17)
C66	0.8056(6)	0.9660(5)	0.0472(4)	0.122(3)
C67	0.758(2)	1.0339(13)	0.0647(16)	0.131(6)
C68	0.868(2)	0.990(2)	−0.0248(10)	0.125(7)
C69	0.719(2)	0.9224(18)	0.0565(19)	0.136(7)
C70	0.9691(5)	0.9863(4)	0.2167(4)	0.0903(19)
C71	1.0815(6)	0.9877(5)	0.2023(6)	0.134(3)
C72	0.9242(8)	0.9496(5)	0.2925(5)	0.125(3)
C73	0.9265(8)	1.0627(4)	0.1986(6)	0.131(3)
C74	0.4744(5)	0.2352(3)	0.7428(3)	0.0674(15)
C75	0.4519(5)	0.1968(3)	0.7088(3)	0.0685(16)
C76	0.4756(5)	0.1240(3)	0.7220(3)	0.0713(15)
C77	0.5235(5)	0.0924(3)	0.7718(4)	0.0777(18)
C78	0.5462(6)	0.1294(4)	0.8074(4)	0.0832(18)
C79	0.5204(5)	0.2016(3)	0.7929(3)	0.0762(17)
C80	0.4492(5)	0.0813(3)	0.6850(4)	0.0827(18)
C81	0.4922(19)	0.1184(11)	0.6096(7)	0.094(5)
C82	0.4892(19)	0.0064(8)	0.7086(13)	0.098(5)
C83	0.3367(10)	0.0816(12)	0.7026(12)	0.097(5)
C84	0.6022(6)	0.0953(4)	0.8622(4)	0.106(2)
C85	0.6222(8)	0.0159(4)	0.8736(5)	0.145(4)

C86	0.5402(7)	0.1044(5)	0.9291(4)	0.129(3)
C87	0.7010(6)	0.1333(5)	0.8380(5)	0.133(4)
C88	0.2725(5)	0.7368(3)	0.5696(4)	0.0774(16)
C89	0.2950(6)	0.7919(4)	0.5863(4)	0.0848(18)
C90	0.2665(6)	0.8620(4)	0.5548(5)	0.0888(18)
C91	0.2183(6)	0.8744(4)	0.5065(4)	0.0901(19)
C92	0.1939(6)	0.8200(3)	0.4878(4)	0.0822(17)
C93	0.2228(5)	0.7512(3)	0.5223(4)	0.0786(17)
C94	0.1402(6)	0.8373(3)	0.4341(4)	0.0899(19)
C95	0.220(5)	0.830(5)	0.372(3)	0.102(7)
C96	0.094(6)	0.912(2)	0.415(5)	0.105(8)
C97	0.061(5)	0.783(4)	0.454(5)	0.100(7)
C98	0.2942(7)	0.9226(4)	0.5733(5)	0.110(2)
C99	0.4066(7)	0.9209(5)	0.5617(7)	0.117(3)
C100	0.2483(10)	0.9069(6)	0.6491(6)	0.127(4)
C101	0.2630(12)	0.9957(5)	0.5325(8)	0.143(4)
N9	0.0484(12)	0.4500(7)	0.9175(7)	0.231(7)
C102	0.1063(11)	0.4582(6)	0.8694(7)	0.154(4)
O1	0.4761(6)	0.5277(4)	0.7275(4)	0.148(3)
C103	0.5708(15)	0.5199(14)	0.7192(10)	0.285(10)
Ni2	1.0108(3)	0.5779(2)	0.2194(2)	0.0869(16)
N1B	1.0398(18)	0.6560(5)	0.1344(5)	0.116(4)
N2B	1.0991(17)	0.5139(7)	0.1798(6)	0.118(4)
C1B	1.020(2)	0.7266(6)	0.1244(7)	0.123(4)
C2B	1.059(2)	0.7696(8)	0.0537(7)	0.132(4)
C3B	1.095(3)	0.7240(8)	0.0216(8)	0.138(4)
C4B	1.078(3)	0.6526(8)	0.0693(7)	0.146(4)
C5B	1.117(3)	0.5879(8)	0.0586(8)	0.154(4)
C6B	1.138(2)	0.5275(9)	0.1106(7)	0.148(4)
C7B	1.187(2)	0.4677(10)	0.0984(9)	0.150(4)
C8B	1.195(2)	0.4166(10)	0.1639(8)	0.136(4)
C9B	1.131(3)	0.4452(11)	0.2144(7)	0.125(4)
C43B	1.1548(17)	0.5961(9)	−0.0152(9)	0.171(4)
C44B	1.258(3)	0.5357(17)	−0.1053(16)	0.230(7)
C45B	1.315(3)	0.5897(18)	−0.1151(19)	0.234(6)
S1B	1.1706(14)	0.5205(9)	−0.0312(9)	0.209(5)
S2B	1.2570(11)	0.6380(6)	−0.0657(6)	0.210(5)
C53B	1.0318(10)	0.1476(11)	0.3232(14)	0.133(5)
C54B	1.1948(18)	0.1603(10)	0.2384(8)	0.141(5)
C55B	1.178(2)	0.0779(8)	0.3573(12)	0.151(6)
C67B	0.7001(8)	0.9731(9)	0.0837(6)	0.142(5)
C68B	0.8532(9)	1.0299(6)	−0.0071(6)	0.105(4)
C69B	0.8056(12)	0.9127(7)	0.0085(7)	0.144(4)
C81B	0.3987(10)	0.1246(6)	0.6306(6)	0.097(3)
C82B	0.5409(8)	0.0447(7)	0.6507(7)	0.105(3)
C83B	0.3775(10)	0.0228(6)	0.7368(6)	0.109(4)
C95B	0.1145(8)	0.7707(4)	0.4237(6)	0.101(3)
C96B	0.2060(7)	0.8820(5)	0.3678(5)	0.108(3)
C97B	0.0418(7)	0.8771(5)	0.4553(6)	0.111(3)
C99B	0.367(3)	0.970(2)	0.5097(15)	0.124(7)
C10A	0.339(4)	0.906(2)	0.6321(19)	0.126(6)

C10B	0.202(2)	0.972(2)	0.585(3)	0.115(6)
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Table S27. Bond lengths [Å] and angles [°] for **NiZn14**.

Ni1–N1A	1.946(8)	Ni1–N2A	1.915(9)
Ni1–N3	1.945(6)	Ni1–N4	1.968(7)
N1A–C1A	1.370(12)	N1A–C4A	1.400(13)
N2A–C6A	1.383(14)	N2A–C9A	1.402(14)
N3–C11	1.399(9)	N3–C14	1.366(9)
N3–Ni2	1.968(7)	N4–C16	1.388(9)
N4–C19	1.396(8)	N4–Ni2	1.893(7)
C1A–C2A	1.459(14)	C1A–C20	1.392(13)
C2A–H2A	0.950	C2A–C3A	1.312(15)
C3A–H3A	0.950	C3A–C4A	1.448(15)
C4A–C5A	1.414(17)	C5A–C6A	1.420(19)
C5A–C43A	1.497(18)	C6A–C7A	1.381(16)
C7A–H7A	0.950	C7A–C8A	1.466(19)
C8A–H8A	0.950	C8A–C9A	1.435(15)
C9A–C10	1.329(13)	C10–C11	1.340(11)
C10–C46	1.529(12)	C10–C9B	1.367(14)
C11–C12	1.415(10)	C12–H12	0.950
C12–C13	1.352(11)	C13–H13	0.950
C13–C14	1.428(9)	C14–C15	1.384(10)
C15–C16	1.383(8)	C15–C41	1.413(10)
C16–C17	1.430(9)	C17–H17	0.950
C17–C18	1.349(9)	C18–H18	0.950
C18–C19	1.399(10)	C19–C20	1.386(10)
C20–C60	1.511(10)	C20–C1B	1.382(14)
Zn–N5	2.050(5)	Zn–N6	2.054(6)
Zn–N7	2.069(6)	Zn–N8	2.042(5)
Zn–O1	2.172(7)	N5–C21	1.357(8)
N5–C24	1.386(7)	N6–C26	1.381(8)
N6–C29	1.364(10)	N7–C31	1.348(10)
N7–C34	1.392(9)	N8–C36	1.412(8)
N8–C39	1.343(8)	C21–C22	1.442(9)
C21–C40	1.421(8)	C22–H22	0.950
C22–C23	1.335(8)	C23–H23	0.950
C23–C24	1.429(9)	C24–C25	1.404(9)
C25–C26	1.384(10)	C25–C74	1.510(8)
C26–C27	1.450(10)	C27–H27	0.950
C27–C28	1.324(11)	C28–H28	0.950
C28–C29	1.427(11)	C29–C30	1.413(12)
C30–C31	1.395(11)	C30–C102	1.462(15)
C31–C32	1.400(11)	C32–H32	0.950
C32–C33	1.355(11)	C33–H33	0.950
C33–C34	1.424(11)	C34–C35	1.391(10)
C35–C36	1.386(10)	C35–C88	1.513(9)
C36–C37	1.415(9)	C37–H37	0.950
C37–C38	1.360(9)	C38–H38	0.950
C38–C39	1.442(8)	C39–C40	1.410(9)
C40–C42	1.433(10)	C41–C42	1.202(9)
C43A–H43A	1.000	C43A–S1A	1.668(12)
C43A–S2A	1.667(12)	C44A–H44A	0.990

C44A–H44B	0.990	C44A–C45A	1.36(3)
C44A–S1A	1.671(14)	C45A–H45A	0.990
C45A–H45B	0.990	C45A–S2A	1.669(14)
C46–C47	1.385(10)	C46–C51	1.407(12)
C47–H47	0.950	C47–C48	1.389(11)
C48–C49	1.400(12)	C48–C52	1.549(10)
C49–H49	0.950	C49–C50	1.399(11)
C50–C51	1.378(13)	C50–C56	1.522(14)
C51–H51	0.950	C52–C53	1.538(12)
C52–C54	1.530(12)	C52–C55	1.549(12)
C52–C53B	1.536(12)	C52–C54B	1.516(12)
C52–C55B	1.530(12)	C53–H53A	0.980
C53–H53B	0.980	C53–H53C	0.980
C54–H54A	0.980	C54–H54B	0.980
C54–H54C	0.980	C55–H55A	0.980
C55–H55B	0.980	C55–H55C	0.980
C56–C57	1.506(11)	C56–C58	1.551(11)
C56–C59	1.526(10)	C57–H57A	0.980
C57–H57B	0.980	C57–H57C	0.980
C58–H58A	0.980	C58–H58B	0.980
C58–H58C	0.980	C59–H59A	0.980
C59–H59B	0.980	C59–H59C	0.980
C60–C61	1.382(10)	C60–C65	1.372(10)
C61–H61	0.950	C61–C62	1.391(12)
C62–C63	1.368(11)	C62–C66	1.531(10)
C63–H63	0.950	C63–C64	1.399(9)
C64–C65	1.400(9)	C64–C70	1.504(10)
C65–H65	0.950	C66–C67	1.560(14)
C66–C68	1.497(13)	C66–C69	1.526(13)
C66–C67B	1.482(11)	C66–C68B	1.481(10)
C66–C69B	1.586(11)	C67–H67A	0.980
C67–H67B	0.980	C67–H67C	0.980
C68–H68A	0.980	C68–H68B	0.980
C68–H68C	0.980	C69–H69A	0.980
C69–H69B	0.980	C69–H69C	0.980
C70–C71	1.532(9)	C70–C72	1.528(9)
C70–C73	1.536(9)	C71–H71A	0.980
C71–H71B	0.980	C71–H71C	0.980
C72–H72A	0.980	C72–H72B	0.980
C72–H72C	0.980	C73–H73A	0.980
C73–H73B	0.980	C73–H73C	0.980
C74–C75	1.371(9)	C74–C79	1.380(8)
C75–H75	0.950	C75–C76	1.405(8)
C76–C77	1.386(9)	C76–C80	1.517(9)
C77–H77	0.950	C77–C78	1.378(10)
C78–C79	1.396(9)	C78–C84	1.555(10)
C79–H79	0.950	C80–C81	1.519(12)
C80–C82	1.506(12)	C80–C83	1.526(12)
C80–C81B	1.529(10)	C80–C82B	1.530(10)
C80–C83B	1.544(10)	C81–H81A	0.980
C81–H81B	0.980	C81–H81C	0.980

C82-H82A	0.980	C82-H82B	0.980
C82-H82C	0.980	C83-H83A	0.980
C83-H83B	0.980	C83-H83C	0.980
C84-C85	1.528(9)	C84-C86	1.523(10)
C84-C87	1.544(9)	C85-H85A	0.980
C85-H85B	0.980	C85-H85C	0.980
C86-H86A	0.980	C86-H86B	0.980
C86-H86C	0.980	C87-H87A	0.980
C87-H87B	0.980	C87-H87C	0.980
C88-C89	1.385(9)	C88-C93	1.360(9)
C89-H89	0.950	C89-C90	1.404(9)
C90-C91	1.371(10)	C90-C98	1.542(10)
C91-H91	0.950	C91-C92	1.410(9)
C92-C93	1.402(9)	C92-C94	1.516(10)
C93-H93	0.950	C94-C95	1.529(15)
C94-C96	1.530(15)	C94-C97	1.529(15)
C94-C95B	1.540(9)	C94-C96B	1.506(9)
C94-C97B	1.543(9)	C95-H95A	0.980
C95-H95B	0.980	C95-H95C	0.980
C96-H96A	0.980	C96-H96B	0.980
C96-H96C	0.980	C97-H97A	0.980
C97-H97B	0.980	C97-H97C	0.980
C98-C99	1.537(10)	C98-C100	1.522(10)
C98-C101	1.519(10)	C98-C99B	1.534(14)
C98-C10A	1.527(14)	C98-C10B	1.548(14)
C99-H99A	0.980	C99-H99B	0.980
C99-H99C	0.980	C100-H10A	0.980
C100-H10B	0.980	C100-H10C	0.980
C101-H10D	0.980	C101-H10E	0.980
C101-H10F	0.980	N9-C102	1.095(13)
O1-H1	0.950	O1-C103	1.298(19)
C103-H10G	0.980	C103-H10H	0.980
C103-H10I	0.980	Ni2-N1B	1.939(9)
Ni2-N2B	1.917(10)	N1B-C1B	1.365(13)
N1B-C4B	1.388(14)	N2B-C6B	1.387(14)
N2B-C9B	1.416(14)	C1B-C2B	1.456(14)
C2B-H2B	0.950	C2B-C3B	1.309(16)
C3B-H3B	0.950	C3B-C4B	1.448(16)
C4B-C5B	1.412(18)	C5B-C6B	1.42(2)
C5B-C43B	1.499(19)	C6B-C7B	1.377(17)
C7B-H7B	0.950	C7B-C8B	1.471(19)
C8B-H8B	0.950	C8B-C9B	1.438(16)
C43B-H43B	1.000	C43B-S1B	1.650(13)
C43B-S2B	1.652(13)	C44B-H44C	0.990
C44B-H44D	0.990	C44B-C45B	1.36(3)
C44B-S1B	1.669(15)	C45B-H45C	0.990
C45B-H45D	0.990	C45B-S2B	1.666(15)
C53B-H53D	0.980	C53B-H53E	0.980
C53B-H53F	0.980	C54B-H54D	0.980
C54B-H54E	0.980	C54B-H54F	0.980
C55B-H55D	0.980	C55B-H55E	0.980

C55B–H55F	0.980	C67B–H67D	0.980
C67B–H67E	0.980	C67B–H67F	0.980
C68B–H68D	0.980	C68B–H68E	0.980
C68B–H68F	0.980	C69B–H69D	0.980
C69B–H69E	0.980	C69B–H69F	0.980
C81B–H81D	0.980	C81B–H81E	0.980
C81B–H81F	0.980	C82B–H82D	0.980
C82B–H82E	0.980	C82B–H82F	0.980
C83B–H83D	0.980	C83B–H83E	0.980
C83B–H83F	0.980	C95B–H95D	0.980
C95B–H95E	0.980	C95B–H95F	0.980
C96B–H96D	0.980	C96B–H96E	0.980
C96B–H96F	0.980	C97B–H97D	0.980
C97B–H97E	0.980	C97B–H97F	0.980
C99B–H99D	0.980	C99B–H99E	0.980
C99B–H99F	0.980	C10A–H10J	0.980
C10A–H10K	0.980	C10A–H10L	0.980
C10B–H10M	0.980	C10B–H10N	0.980
C10B–H10O	0.980		
N1A–Ni1–N2A	89.5(4)	N1A–Ni1–N3	175.5(7)
N1A–Ni1–N4	90.7(4)	N2A–Ni1–N3	91.4(4)
N2A–Ni1–N4	175.8(7)	N3–Ni1–N4	88.1(3)
Ni1–N1A–C1A	126.3(7)	Ni1–N1A–C4A	127.1(8)
C1A–N1A–C4A	106.6(9)	Ni1–N2A–C6A	130.3(9)
Ni1–N2A–C9A	127.0(7)	C6A–N2A–C9A	102.7(10)
Ni1–N3–C11	123.9(6)	Ni1–N3–C14	130.0(5)
C11–N3–C14	105.8(6)	C11–N3–Ni2	128.5(6)
C14–N3–Ni2	125.4(5)	Ni1–N4–C16	129.0(4)
Ni1–N4–C19	127.1(5)	C16–N4–C19	103.7(6)
C16–N4–Ni2	127.4(4)	C19–N4–Ni2	128.3(5)
N1A–C1A–C2A	108.9(10)	N1A–C1A–C20	126.3(9)
C2A–C1A–C20	124.6(10)	C1A–C2A–H2A	126.4
C1A–C2A–C3A	107.2(10)	H2A–C2A–C3A	126.4
C2A–C3A–H3A	125.4	C2A–C3A–C4A	109.2(11)
H3A–C3A–C4A	125.4	N1A–C4A–C3A	107.5(10)
N1A–C4A–C5A	126.7(11)	C3A–C4A–C5A	125.5(12)
C4A–C5A–C6A	117.8(12)	C4A–C5A–C43A	121.1(13)
C6A–C5A–C43A	119.2(14)	N2A–C6A–C5A	124.6(13)
N2A–C6A–C7A	113.8(12)	C5A–C6A–C7A	120.2(12)
C6A–C7A–H7A	127.3	C6A–C7A–C8A	105.4(12)
H7A–C7A–C8A	127.3	C7A–C8A–H8A	129.0
C7A–C8A–C9A	102.0(12)	H8A–C8A–C9A	129.0
N2A–C9A–C8A	112.8(11)	N2A–C9A–C10	123.6(10)
C8A–C9A–C10	123.6(11)	C9A–C10–C11	126.4(10)
C9A–C10–C46	116.5(9)	C11–C10–C46	117.0(8)
C11–C10–C9B	120.2(11)	C46–C10–C9B	121.8(9)
N3–C11–C10	125.6(8)	N3–C11–C12	109.1(7)
C10–C11–C12	124.8(8)	C11–C12–H12	126.0
C11–C12–C13	108.0(7)	H12–C12–C13	126.0
C12–C13–H13	126.6	C12–C13–C14	106.9(7)

H13-C13-C14	126.6	N3-C14-C13	110.2(7)
N3-C14-C15	125.8(6)	C13-C14-C15	123.8(7)
C14-C15-C16	121.5(7)	C14-C15-C41	118.1(6)
C16-C15-C41	120.1(6)	N4-C16-C15	125.1(7)
N4-C16-C17	111.0(5)	C15-C16-C17	123.7(7)
C16-C17-H17	127.0	C16-C17-C18	105.9(7)
H17-C17-C18	127.0	C17-C18-H18	125.7
C17-C18-C19	108.7(7)	H18-C18-C19	125.7
N4-C19-C18	110.6(6)	N4-C19-C20	123.8(7)
C18-C19-C20	125.2(7)	C1A-C20-C19	123.7(8)
C1A-C20-C60	121.3(7)	C19-C20-C60	115.0(8)
C19-C20-C1B	120.4(9)	C60-C20-C1B	118.8(8)
N5-Zn-N6	89.0(2)	N5-Zn-N7	166.9(2)
N5-Zn-N8	88.1(2)	N5-Zn-O1	98.6(3)
N6-Zn-N7	88.8(2)	N6-Zn-N8	164.1(2)
N6-Zn-O1	99.0(3)	N7-Zn-N8	90.5(2)
N7-Zn-O1	94.5(3)	N8-Zn-O1	96.8(2)
Zn-N5-C21	126.6(4)	Zn-N5-C24	126.8(5)
C21-N5-C24	105.6(5)	Zn-N6-C26	127.2(5)
Zn-N6-C29	126.9(5)	C26-N6-C29	105.8(6)
Zn-N7-C31	127.1(5)	Zn-N7-C34	125.5(6)
C31-N7-C34	106.8(6)	Zn-N8-C36	125.8(5)
Zn-N8-C39	128.8(4)	C36-N8-C39	105.3(5)
N5-C21-C22	110.8(5)	N5-C21-C40	124.3(6)
C22-C21-C40	124.8(7)	C21-C22-H22	127.0
C21-C22-C23	106.0(6)	H22-C22-C23	127.0
C22-C23-H23	125.7	C22-C23-C24	108.5(6)
H23-C23-C24	125.7	N5-C24-C23	109.0(6)
N5-C24-C25	124.2(6)	C23-C24-C25	126.8(5)
C24-C25-C26	126.4(6)	C24-C25-C74	115.3(6)
C26-C25-C74	118.3(6)	N6-C26-C25	125.1(6)
N6-C26-C27	108.7(7)	C25-C26-C27	126.2(7)
C26-C27-H27	126.2	C26-C27-C28	107.6(7)
H27-C27-C28	126.2	C27-C28-H28	126.3
C27-C28-C29	107.4(8)	H28-C28-C29	126.3
N6-C29-C28	110.4(8)	N6-C29-C30	123.4(7)
C28-C29-C30	126.1(9)	C29-C30-C31	128.2(9)
C29-C30-C102	116.9(8)	C31-C30-C102	114.8(9)
N7-C31-C30	123.2(8)	N7-C31-C32	110.7(7)
C30-C31-C32	125.8(9)	C31-C32-H32	126.5
C31-C32-C33	107.0(9)	H32-C32-C33	126.5
C32-C33-H33	126.1	C32-C33-C34	107.8(8)
H33-C33-C34	126.1	N7-C34-C33	107.6(7)
N7-C34-C35	124.8(7)	C33-C34-C35	127.5(7)
C34-C35-C36	127.8(6)	C34-C35-C88	117.7(7)
C36-C35-C88	114.5(7)	N8-C36-C35	124.8(6)
N8-C36-C37	108.9(6)	C35-C36-C37	126.2(6)
C36-C37-H37	125.6	C36-C37-C38	108.8(6)
H37-C37-C38	125.6	C37-C38-H38	127.5
C37-C38-C39	105.0(7)	H38-C38-C39	127.5
N8-C39-C38	112.0(6)	N8-C39-C40	124.1(5)

C38–C39–C40	123.9(7)	C21–C40–C39	125.3(7)
C21–C40–C42	117.4(6)	C39–C40–C42	117.2(5)
C15–C41–C42	179.3(7)	C40–C42–C41	177.7(7)
C5A–C43A–H43A	104.3	C5A–C43A–S1A	117.1(11)
C5A–C43A–S2A	122.0(13)	H43A–C43A–S1A	104.3
H43A–C43A–S2A	104.3	S1A–C43A–S2A	103.0(10)
H44A–C44A–H44B	108.2	H44A–C44A–C45A	109.7
H44A–C44A–S1A	109.7	H44B–C44A–C45A	109.7
H44B–C44A–S1A	109.7	C45A–C44A–S1A	109.8(11)
C44A–C45A–H45A	109.4	C44A–C45A–H45B	109.4
C44A–C45A–S2A	111.2(10)	H45A–C45A–H45B	108.0
H45A–C45A–S2A	109.4	H45B–C45A–S2A	109.4
C43A–S1A–C44A	104.5(9)	C43A–S2A–C45A	105.3(9)
C10–C46–C47	119.6(8)	C10–C46–C51	120.6(7)
C47–C46–C51	119.4(9)	C46–C47–H47	120.5
C46–C47–C48	119.0(8)	H47–C47–C48	120.5
C47–C48–C49	120.7(7)	C47–C48–C52	119.0(8)
C49–C48–C52	120.3(8)	C48–C49–H49	119.4
C48–C49–C50	121.2(9)	H49–C49–C50	119.4
C49–C50–C51	116.9(9)	C49–C50–C56	122.2(10)
C51–C50–C56	120.8(8)	C46–C51–C50	122.8(8)
C46–C51–H51	118.6	C50–C51–H51	118.6
C48–C52–C53	109.8(10)	C48–C52–C54	114.0(9)
C48–C52–C55	110.8(10)	C48–C52–C53B	108.3(9)
C48–C52–C54B	108.2(10)	C48–C52–C55B	112.0(10)
C53–C52–C54	107.5(11)	C53–C52–C55	105.7(11)
C54–C52–C55	108.7(12)	C53B–C52–C54B	107.7(12)
C53B–C52–C55B	109.5(12)	C54B–C52–C55B	111.0(12)
C52–C53–H53A	109.5	C52–C53–H53B	109.5
C52–C53–H53C	109.5	H53A–C53–H53B	109.5
H53A–C53–H53C	109.5	H53B–C53–H53C	109.5
C52–C54–H54A	109.5	C52–C54–H54B	109.5
C52–C54–H54C	109.5	H54A–C54–H54B	109.5
H54A–C54–H54C	109.5	H54B–C54–H54C	109.5
C52–C55–H55A	109.5	C52–C55–H55B	109.5
C52–C55–H55C	109.5	H55A–C55–H55B	109.5
H55A–C55–H55C	109.5	H55B–C55–H55C	109.5
C50–C56–C57	106.4(10)	C50–C56–C58	111.4(9)
C50–C56–C59	112.4(9)	C57–C56–C58	110.3(10)
C57–C56–C59	111.0(9)	C58–C56–C59	105.3(10)
C56–C57–H57A	109.5	C56–C57–H57B	109.5
C56–C57–H57C	109.5	H57A–C57–H57B	109.5
H57A–C57–H57C	109.5	H57B–C57–H57C	109.5
C56–C58–H58A	109.5	C56–C58–H58B	109.5
C56–C58–H58C	109.5	H58A–C58–H58B	109.5
H58A–C58–H58C	109.5	H58B–C58–H58C	109.5
C56–C59–H59A	109.5	C56–C59–H59B	109.5
C56–C59–H59C	109.5	H59A–C59–H59B	109.5
H59A–C59–H59C	109.5	H59B–C59–H59C	109.5
C20–C60–C61	119.1(7)	C20–C60–C65	121.0(7)
C61–C60–C65	119.7(7)	C60–C61–H61	119.8

C60-C61-C62	120.4(7)	H61-C61-C62	119.8
C61-C62-C63	118.3(7)	C61-C62-C66	118.7(8)
C63-C62-C66	122.9(8)	C62-C63-H63	118.2
C62-C63-C64	123.6(7)	H63-C63-C64	118.2
C63-C64-C65	115.7(7)	C63-C64-C70	124.0(6)
C65-C64-C70	120.3(6)	C60-C65-C64	122.2(6)
C60-C65-H65	118.9	C64-C65-H65	118.9
C62-C66-C67	101.5(13)	C62-C66-C68	113.5(15)
C62-C66-C69	116.0(14)	C62-C66-C67B	109.5(8)
C62-C66-C68B	110.6(7)	C62-C66-C69B	110.7(9)
C67-C66-C68	106.9(15)	C67-C66-C69	105.7(16)
C68-C66-C69	111.8(16)	C67B-C66-C68B	117.4(9)
C67B-C66-C69B	104.1(9)	C68B-C66-C69B	104.2(9)
C66-C67-H67A	109.5	C66-C67-H67B	109.5
C66-C67-H67C	109.5	H67A-C67-H67B	109.5
H67A-C67-H67C	109.5	H67B-C67-H67C	109.5
C66-C68-H68A	109.5	C66-C68-H68B	109.5
C66-C68-H68C	109.5	H68A-C68-H68B	109.5
H68A-C68-H68C	109.5	H68B-C68-H68C	109.5
C66-C69-H69A	109.5	C66-C69-H69B	109.5
C66-C69-H69C	109.5	H69A-C69-H69B	109.5
H69A-C69-H69C	109.5	H69B-C69-H69C	109.5
C64-C70-C71	110.1(7)	C64-C70-C72	108.7(6)
C64-C70-C73	112.2(6)	C71-C70-C72	108.5(7)
C71-C70-C73	109.6(7)	C72-C70-C73	107.7(7)
C70-C71-H71A	109.5	C70-C71-H71B	109.5
C70-C71-H71C	109.5	H71A-C71-H71B	109.5
H71A-C71-H71C	109.5	H71B-C71-H71C	109.5
C70-C72-H72A	109.5	C70-C72-H72B	109.5
C70-C72-H72C	109.5	H72A-C72-H72B	109.5
H72A-C72-H72C	109.5	H72B-C72-H72C	109.5
C70-C73-H73A	109.5	C70-C73-H73B	109.5
C70-C73-H73C	109.5	H73A-C73-H73B	109.5
H73A-C73-H73C	109.5	H73B-C73-H73C	109.5
C25-C74-C75	119.4(5)	C25-C74-C79	121.3(6)
C75-C74-C79	119.4(6)	C74-C75-H75	118.8
C74-C75-C76	122.5(6)	H75-C75-C76	118.8
C75-C76-C77	116.4(6)	C75-C76-C80	122.3(6)
C77-C76-C80	121.3(6)	C76-C77-H77	118.7
C76-C77-C78	122.5(6)	H77-C77-C78	118.7
C77-C78-C79	119.0(6)	C77-C78-C84	123.2(7)
C79-C78-C84	117.8(7)	C74-C79-C78	120.2(7)
C74-C79-H79	119.9	C78-C79-H79	119.9
C76-C80-C81	107.7(9)	C76-C80-C82	109.0(11)
C76-C80-C83	107.7(10)	C76-C80-C81B	114.5(6)
C76-C80-C82B	111.3(7)	C76-C80-C83B	109.0(7)
C81-C80-C82	112.6(13)	C81-C80-C83	109.7(12)
C82-C80-C83	110.0(12)	C81B-C80-C82B	107.2(8)
C81B-C80-C83B	107.0(8)	C82B-C80-C83B	107.5(8)
C80-C81-H81A	109.5	C80-C81-H81B	109.5
C80-C81-H81C	109.5	H81A-C81-H81B	109.5

H81A–C81–H81C	109.5	H81B–C81–H81C	109.5
C80–C82–H82A	109.5	C80–C82–H82B	109.5
C80–C82–H82C	109.5	H82A–C82–H82B	109.5
H82A–C82–H82C	109.5	H82B–C82–H82C	109.5
C80–C83–H83A	109.5	C80–C83–H83B	109.5
C80–C83–H83C	109.5	H83A–C83–H83B	109.5
H83A–C83–H83C	109.5	H83B–C83–H83C	109.5
C78–C84–C85	111.3(7)	C78–C84–C86	109.7(7)
C78–C84–C87	108.2(6)	C85–C84–C86	108.3(7)
C85–C84–C87	109.7(8)	C86–C84–C87	109.6(8)
C84–C85–H85A	109.5	C84–C85–H85B	109.5
C84–C85–H85C	109.5	H85A–C85–H85B	109.5
H85A–C85–H85C	109.5	H85B–C85–H85C	109.5
C84–C86–H86A	109.5	C84–C86–H86B	109.5
C84–C86–H86C	109.5	H86A–C86–H86B	109.5
H86A–C86–H86C	109.5	H86B–C86–H86C	109.5
C84–C87–H87A	109.5	C84–C87–H87B	109.5
C84–C87–H87C	109.5	H87A–C87–H87B	109.5
H87A–C87–H87C	109.5	H87B–C87–H87C	109.5
C35–C88–C89	119.1(6)	C35–C88–C93	121.4(6)
C89–C88–C93	119.5(6)	C88–C89–H89	119.8
C88–C89–C90	120.3(7)	H89–C89–C90	119.8
C89–C90–C91	118.3(6)	C89–C90–C98	119.3(7)
C91–C90–C98	122.3(7)	C90–C91–H91	118.4
C90–C91–C92	123.3(6)	H91–C91–C92	118.4
C91–C92–C93	115.2(6)	C91–C92–C94	120.6(6)
C93–C92–C94	124.1(6)	C88–C93–C92	123.3(6)
C88–C93–H93	118.3	C92–C93–H93	118.3
C92–C94–C95	105(4)	C92–C94–C96	115(4)
C92–C94–C97	111(4)	C92–C94–C95B	113.1(6)
C92–C94–C96B	108.4(6)	C92–C94–C97B	109.3(7)
C95–C94–C96	108(2)	C95–C94–C97	108(2)
C96–C94–C97	109(2)	C95B–C94–C96B	107.9(7)
C95B–C94–C97B	107.1(7)	C96B–C94–C97B	111.0(7)
C94–C95–H95A	109.5	C94–C95–H95B	109.5
C94–C95–H95C	109.5	H95A–C95–H95B	109.5
H95A–C95–H95C	109.5	H95B–C95–H95C	109.5
C94–C96–H96A	109.5	C94–C96–H96B	109.5
C94–C96–H96C	109.5	H96A–C96–H96B	109.5
H96A–C96–H96C	109.5	H96B–C96–H96C	109.5
C94–C97–H97A	109.5	C94–C97–H97B	109.5
C94–C97–H97C	109.5	H97A–C97–H97B	109.5
H97A–C97–H97C	109.5	H97B–C97–H97C	109.5
C90–C98–C99	109.6(7)	C90–C98–C100	107.4(7)
C90–C98–C101	113.2(8)	C90–C98–C99B	107.4(17)
C90–C98–C10A	120.3(18)	C90–C98–C10B	108.1(14)
C99–C98–C100	105.8(8)	C99–C98–C101	108.6(8)
C100–C98–C101	111.9(9)	C99B–C98–C10A	107.6(17)
C99B–C98–C10B	103.6(16)	C10A–C98–C10B	108.6(17)
C98–C99–H99A	109.5	C98–C99–H99B	109.5
C98–C99–H99C	109.5	H99A–C99–H99B	109.5

H99A–C99–H99C	109.5	H99B–C99–H99C	109.5
C98–C100–H10A	109.5	C98–C100–H10B	109.5
C98–C100–H10C	109.5	H10A–C100–H10B	109.5
H10A–C100–H10C	109.5	H10B–C100–H10C	109.5
C98–C101–H10D	109.5	C98–C101–H10E	109.5
C98–C101–H10F	109.5	H10D–C101–H10E	109.5
H10D–C101–H10F	109.5	H10E–C101–H10F	109.5
C30–C102–N9	177.2(16)	Zn–O1–H1	117.3
Zn–O1–C103	125.4(10)	H1–O1–C103	117.3
O1–C103–H10G	109.5	O1–C103–H10H	109.5
O1–C103–H10I	109.5	H10G–C103–H10H	109.5
H10G–C103–H10I	109.5	H10H–C103–H10I	109.5
N3–Ni2–N4	89.6(3)	N3–Ni2–N1B	178.7(8)
N3–Ni2–N2B	88.3(4)	N4–Ni2–N1B	89.7(4)
N4–Ni2–N2B	176.6(7)	N1B–Ni2–N2B	92.5(5)
Ni2–N1B–C1B	128.0(8)	Ni2–N1B–C4B	128.1(9)
C1B–N1B–C4B	103.8(10)	Ni2–N2B–C6B	124.0(10)
Ni2–N2B–C9B	127.1(8)	C6B–N2B–C9B	108.9(11)
C20–C1B–N1B	124.2(10)	C20–C1B–C2B	123.5(11)
N1B–C1B–C2B	112.0(11)	C1B–C2B–H2B	127.4
C1B–C2B–C3B	105.1(12)	H2B–C2B–C3B	127.4
C2B–C3B–H3B	125.4	C2B–C3B–C4B	109.2(12)
H3B–C3B–C4B	125.4	N1B–C4B–C3B	109.1(12)
N1B–C4B–C5B	120.7(13)	C3B–C4B–C5B	128.1(14)
C4B–C5B–C6B	122.9(15)	C4B–C5B–C43B	112.1(13)
C6B–C5B–C43B	123.3(15)	N2B–C6B–C5B	126.2(15)
N2B–C6B–C7B	109.8(13)	C5B–C6B–C7B	122.8(14)
C6B–C7B–H7B	126.4	C6B–C7B–C8B	107.2(13)
H7B–C7B–C8B	126.4	C7B–C8B–H8B	127.2
C7B–C8B–C9B	105.5(13)	H8B–C8B–C9B	127.2
C10–C9B–N2B	127.5(11)	C10–C9B–C8B	125.2(12)
N2B–C9B–C8B	107.3(11)	C5B–C43B–H43B	105.1
C5B–C43B–S1B	114.2(12)	C5B–C43B–S2B	123.4(16)
H43B–C43B–S1B	105.1	H43B–C43B–S2B	105.1
S1B–C43B–S2B	102.3(11)	H44C–C44B–H44D	108.2
H44C–C44B–C45B	109.7	H44C–C44B–S1B	109.7
H44D–C44B–C45B	109.7	H44D–C44B–S1B	109.7
C45B–C44B–S1B	109.6(12)	C44B–C45B–H45C	109.4
C44B–C45B–H45D	109.4	C44B–C45B–S2B	111.0(11)
H45C–C45B–H45D	108.0	H45C–C45B–S2B	109.4
H45D–C45B–S2B	109.4	C43B–S1B–C44B	105.4(10)
C43B–S2B–C45B	106.2(10)	C52–C53B–H53D	109.5
C52–C53B–H53E	109.5	C52–C53B–H53F	109.5
H53D–C53B–H53E	109.5	H53D–C53B–H53F	109.5
H53E–C53B–H53F	109.5	C52–C54B–H54D	109.5
C52–C54B–H54E	109.5	C52–C54B–H54F	109.5
H54D–C54B–H54E	109.5	H54D–C54B–H54F	109.5
H54E–C54B–H54F	109.5	C52–C55B–H55D	109.5
C52–C55B–H55E	109.5	C52–C55B–H55F	109.5
H55D–C55B–H55E	109.5	H55D–C55B–H55F	109.5
H55E–C55B–H55F	109.5	C66–C67B–H67D	109.5

C66–C67B–H67E	109.5	C66–C67B–H67F	109.5
H67D–C67B–H67E	109.5	H67D–C67B–H67F	109.5
H67E–C67B–H67F	109.5	C66–C68B–H68D	109.5
C66–C68B–H68E	109.5	C66–C68B–H68F	109.5
H68D–C68B–H68E	109.5	H68D–C68B–H68F	109.5
H68E–C68B–H68F	109.5	C66–C69B–H69D	109.5
C66–C69B–H69E	109.5	C66–C69B–H69F	109.5
H69D–C69B–H69E	109.5	H69D–C69B–H69F	109.5
H69E–C69B–H69F	109.5	C80–C81B–H81D	109.5
C80–C81B–H81E	109.5	C80–C81B–H81F	109.5
H81D–C81B–H81E	109.5	H81D–C81B–H81F	109.5
H81E–C81B–H81F	109.5	C80–C82B–H82D	109.5
C80–C82B–H82E	109.5	C80–C82B–H82F	109.5
H82D–C82B–H82E	109.5	H82D–C82B–H82F	109.5
H82E–C82B–H82F	109.5	C80–C83B–H83D	109.5
C80–C83B–H83E	109.5	C80–C83B–H83F	109.5
H83D–C83B–H83E	109.5	H83D–C83B–H83F	109.5
H83E–C83B–H83F	109.5	C94–C95B–H95D	109.5
C94–C95B–H95E	109.5	C94–C95B–H95F	109.5
H95D–C95B–H95E	109.5	H95D–C95B–H95F	109.5
H95E–C95B–H95F	109.5	C94–C96B–H96D	109.5
C94–C96B–H96E	109.5	C94–C96B–H96F	109.5
H96D–C96B–H96E	109.5	H96D–C96B–H96F	109.5
H96E–C96B–H96F	109.5	C94–C97B–H97D	109.5
C94–C97B–H97E	109.5	C94–C97B–H97F	109.5
H97D–C97B–H97E	109.5	H97D–C97B–H97F	109.5
H97E–C97B–H97F	109.5	C98–C99B–H99D	109.5
C98–C99B–H99E	109.5	C98–C99B–H99F	109.5
H99D–C99B–H99E	109.5	H99D–C99B–H99F	109.5
H99E–C99B–H99F	109.5	C98–C10A–H10J	109.5
C98–C10A–H10K	109.5	C98–C10A–H10L	109.5
H10J–C10A–H10K	109.5	H10J–C10A–H10L	109.5
H10K–C10A–H10L	109.5	C98–C10B–H10M	109.5
C98–C10B–H10N	109.5	C98–C10B–H10O	109.5
H10M–C10B–H10N	109.5	H10M–C10B–H10O	109.5
H10N–C10B–H10O	109.5		

Table S28. Torsion angles [°] for **NiZn14**.

Ni1–N1A–C1A–C2A	173.0(14)	Ni1–N1A–C1A–C20	–12(3)
C4A–N1A–C1A–C2A	–9(2)	C4A–N1A–C1A–C20	166(2)
N1A–C1A–C2A–C3A	8(2)	C20–C1A–C2A–C3A	–167(2)
C1A–C2A–C3A–C4A	–3(3)	Ni1–N1A–C4A–C3A	–175.0(15)
Ni1–N1A–C4A–C5A	–1(3)	C1A–N1A–C4A–C3A	7(2)
C1A–N1A–C4A–C5A	–180(2)	C2A–C3A–C4A–N1A	–2(3)
C2A–C3A–C4A–C5A	–176(2)	N1A–C4A–C5A–C6A	–18(4)
N1A–C4A–C5A–C43A	178(2)	C3A–C4A–C5A–C6A	155(2)
C3A–C4A–C5A–C43A	–9(4)	Ni1–N2A–C6A–C5A	–6(4)
Ni1–N2A–C6A–C7A	–172.9(18)	C9A–N2A–C6A–C5A	173(2)
C9A–N2A–C6A–C7A	7(3)	C4A–C5A–C6A–N2A	21(3)
C4A–C5A–C6A–C7A	–173(2)	C43A–C5A–C6A–N2A	–173.9(19)
C43A–C5A–C6A–C7A	–8(3)	N2A–C6A–C7A–C8A	–16(3)
C5A–C6A–C7A–C8A	177(2)	C6A–C7A–C8A–C9A	18(2)
Ni1–N2A–C9A–C8A	–174.5(17)	Ni1–N2A–C9A–C10	6(4)
C6A–N2A–C9A–C8A	6(3)	C6A–N2A–C9A–C10	–174(2)
C7A–C8A–C9A–N2A	–15(3)	C7A–C8A–C9A–C10	164(2)
N2A–C9A–C10–C11	2(3)	N2A–C9A–C10–C46	–173.1(19)
C8A–C9A–C10–C11	–177.1(17)	C8A–C9A–C10–C46	8(3)
C9A–C10–C11–N3	2(2)	C9A–C10–C11–C12	172.1(17)
C46–C10–C11–N3	177.5(7)	C46–C10–C11–C12	–12.5(12)
C9B–C10–C11–N3	–14(3)	C9B–C10–C11–C12	156(2)
Ni1–N3–C11–C10	–14.0(11)	Ni1–N3–C11–C12	174.7(5)
C14–N3–C11–C10	172.3(8)	C14–N3–C11–C12	1.0(8)
Ni2–N3–C11–C10	–2.0(12)	Ni2–N3–C11–C12	–173.3(5)
N3–C11–C12–C13	–0.1(8)	C10–C11–C12–C13	–171.5(8)
C11–C12–C13–C14	–0.8(8)	Ni1–N3–C14–C13	–174.7(5)
Ni1–N3–C14–C15	0.4(11)	C11–N3–C14–C13	–1.5(8)
C11–N3–C14–C15	173.5(7)	Ni2–N3–C14–C13	173.0(5)
Ni2–N3–C14–C15	–11.9(10)	C12–C13–C14–N3	1.5(8)
C12–C13–C14–C15	–173.7(7)	N3–C14–C15–C16	–6.8(11)
N3–C14–C15–C41	179.0(6)	C13–C14–C15–C16	167.6(6)
C13–C14–C15–C41	–6.5(10)	C14–C15–C16–N4	7.0(10)
C14–C15–C16–C17	–168.7(7)	C41–C15–C16–N4	–178.9(6)
C41–C15–C16–C17	5.4(10)	Ni1–N4–C16–C15	–1.0(10)
Ni1–N4–C16–C17	175.1(5)	C19–N4–C16–C15	–176.1(7)
C19–N4–C16–C17	0.1(8)	Ni2–N4–C16–C15	12.4(10)
Ni2–N4–C16–C17	–171.5(5)	N4–C16–C17–C18	0.2(8)
C15–C16–C17–C18	176.4(7)	C16–C17–C18–C19	–0.4(8)
Ni1–N4–C19–C18	–175.5(5)	Ni1–N4–C19–C20	10.9(12)
C16–N4–C19–C18	–0.3(8)	C16–N4–C19–C20	–173.9(8)
Ni2–N4–C19–C18	171.1(5)	Ni2–N4–C19–C20	–2.5(12)
C17–C18–C19–N4	0.5(9)	C17–C18–C19–C20	173.9(8)
N4–C19–C20–C1A	–3.0(17)	N4–C19–C20–C60	176.7(7)
N4–C19–C20–C1B	24(2)	C18–C19–C20–C1A	–175.7(13)
C18–C19–C20–C60	4.0(12)	C18–C19–C20–C1B	–148.9(19)
N1A–C1A–C20–C19	4(3)	N1A–C1A–C20–C60	–176.0(16)

C2A-C1A-C20-C19	177.8(15)	C2A-C1A-C20-C60	-2(3)
Zn-N5-C21-C22	165.8(4)	Zn-N5-C21-C40	-16.6(8)
C24-N5-C21-C22	-3.4(6)	C24-N5-C21-C40	174.2(5)
N5-C21-C22-C23	2.8(7)	C40-C21-C22-C23	-174.8(5)
C21-C22-C23-C24	-0.9(7)	Zn-N5-C24-C23	-166.5(4)
Zn-N5-C24-C25	15.4(8)	C21-N5-C24-C23	2.8(6)
C21-N5-C24-C25	-175.4(5)	C22-C23-C24-N5	-1.1(7)
C22-C23-C24-C25	177.0(6)	N5-C24-C25-C26	-9.6(10)
N5-C24-C25-C74	170.0(5)	C23-C24-C25-C26	172.6(6)
C23-C24-C25-C74	-7.8(9)	Zn-N6-C26-C25	1.8(10)
Zn-N6-C26-C27	179.0(5)	C29-N6-C26-C25	-177.8(7)
C29-N6-C26-C27	-0.6(8)	C24-C25-C26-N6	0.5(11)
C24-C25-C26-C27	-176.2(6)	C74-C25-C26-N6	-179.1(6)
C74-C25-C26-C27	4.1(10)	N6-C26-C27-C28	-0.9(9)
C25-C26-C27-C28	176.3(7)	C26-C27-C28-C29	1.9(10)
Zn-N6-C29-C28	-177.8(5)	Zn-N6-C29-C30	2.3(12)
C26-N6-C29-C28	1.8(9)	C26-N6-C29-C30	-178.1(8)
C27-C28-C29-N6	-2.4(11)	C27-C28-C29-C30	177.5(9)
N6-C29-C30-C31	8.1(16)	N6-C29-C30-C102	-170.5(10)
C28-C29-C30-C31	-171.7(10)	C28-C29-C30-C102	9.7(16)
Zn-N7-C31-C30	-12.7(12)	Zn-N7-C31-C32	173.0(5)
C34-N7-C31-C30	175.4(8)	C34-N7-C31-C32	1.2(9)
C29-C30-C31-N7	-2.5(16)	C29-C30-C31-C32	170.8(10)
C102-C30-C31-N7	176.1(10)	C102-C30-C31-C32	-10.6(15)
N7-C31-C32-C33	-0.2(10)	C30-C31-C32-C33	-174.3(9)
C31-C32-C33-C34	-0.8(10)	Zn-N7-C34-C33	-173.6(5)
Zn-N7-C34-C35	8.9(10)	C31-N7-C34-C33	-1.6(8)
C31-N7-C34-C35	-179.0(7)	C32-C33-C34-N7	1.5(9)
C32-C33-C34-C35	178.8(8)	N7-C34-C35-C36	-1.7(11)
N7-C34-C35-C88	176.4(6)	C33-C34-C35-C36	-178.6(7)
C33-C34-C35-C88	-0.6(11)	C34-C35-C36-N8	-2.8(11)
C34-C35-C36-C37	-179.6(6)	C88-C35-C36-N8	179.1(5)
C88-C35-C36-C37	2.3(9)	Zn-N8-C36-C35	-0.7(8)
Zn-N8-C36-C37	176.5(4)	C39-N8-C36-C35	-177.5(6)
C39-N8-C36-C37	-0.3(6)	N8-C36-C37-C38	0.6(7)
C35-C36-C37-C38	177.8(6)	C36-C37-C38-C39	-0.6(6)
Zn-N8-C39-C38	-176.8(4)	Zn-N8-C39-C40	2.8(8)
C36-N8-C39-C38	-0.1(6)	C36-N8-C39-C40	179.4(5)
C37-C38-C39-N8	0.5(7)	C37-C38-C39-C40	-179.1(5)
N8-C39-C40-C21	6.1(9)	N8-C39-C40-C42	-177.4(5)
C38-C39-C40-C21	-174.4(5)	C38-C39-C40-C42	2.1(8)
N5-C21-C40-C39	1.3(9)	N5-C21-C40-C42	-175.2(5)
C22-C21-C40-C39	178.5(6)	C22-C21-C40-C42	2.1(8)
C4A-C5A-C43A-S1A	-128(2)	C4A-C5A-C43A-S2A	104(2)
C6A-C5A-C43A-S1A	68(2)	C6A-C5A-C43A-S2A	-60(2)
S1A-C44A-C45A-S2A	-24(3)	C5A-C43A-S1A-C44A	-153.2(17)
S2A-C43A-S1A-C44A	-16.4(16)	C45A-C44A-S1A-C43A	26(3)
C5A-C43A-S2A-C45A	138.5(16)	S1A-C43A-S2A-C45A	4.5(16)
C44A-C45A-S2A-C43A	12(3)	C9A-C10-C46-C47	-77.4(17)

C9A-C10-C46-C51	109.7(17)	C11-C10-C46-C47	106.7(10)
C11-C10-C46-C51	-66.1(12)	C9B-C10-C46-C47	-61(3)
C9B-C10-C46-C51	126(3)	C10-C46-C47-C48	-172.3(9)
C51-C46-C47-C48	0.6(14)	C46-C47-C48-C49	-0.9(15)
C46-C47-C48-C52	177.0(9)	C47-C48-C49-C50	0.9(16)
C52-C48-C49-C50	-177.0(9)	C48-C49-C50-C51	-0.5(16)
C48-C49-C50-C56	175.7(10)	C49-C50-C51-C46	0.1(16)
C56-C50-C51-C46	-176.1(9)	C10-C46-C51-C50	172.7(9)
C47-C46-C51-C50	-0.2(16)	C47-C48-C52-C53	-118.2(13)
C47-C48-C52-C54	2.5(16)	C47-C48-C52-C55	125.4(13)
C47-C48-C52-C53B	-56.5(15)	C47-C48-C52-C54B	59.9(14)
C47-C48-C52-C55B	-177.4(14)	C49-C48-C52-C53	59.7(14)
C49-C48-C52-C54	-179.6(13)	C49-C48-C52-C55	-56.7(15)
C49-C48-C52-C53B	121.4(13)	C49-C48-C52-C54B	-122.2(13)
C49-C48-C52-C55B	0.5(16)	C49-C50-C56-C57	61.7(14)
C49-C50-C56-C58	-58.6(14)	C49-C50-C56-C59	-176.5(10)
C51-C50-C56-C57	-122.2(12)	C51-C50-C56-C58	117.5(12)
C51-C50-C56-C59	-0.4(15)	C1A-C20-C60-C61	76.6(15)
C1A-C20-C60-C65	-107.5(14)	C19-C20-C60-C61	-103.2(9)
C19-C20-C60-C65	72.7(11)	C1B-C20-C60-C61	50(2)
C1B-C20-C60-C65	-134(2)	C20-C60-C61-C62	172.9(8)
C65-C60-C61-C62	-3.1(13)	C60-C61-C62-C63	1.8(13)
C60-C61-C62-C66	-179.0(8)	C61-C62-C63-C64	-0.3(13)
C66-C62-C63-C64	-179.5(7)	C62-C63-C64-C65	0.1(12)
C62-C63-C64-C70	-178.9(8)	C20-C60-C65-C64	-172.9(8)
C61-C60-C65-C64	2.9(12)	C63-C64-C65-C60	-1.4(11)
C70-C64-C65-C60	177.6(7)	C61-C62-C66-C67	163.9(15)
C61-C62-C66-C68	-81.7(19)	C61-C62-C66-C69	50(2)
C61-C62-C66-C67B	105.9(12)	C61-C62-C66-C68B	-123.2(10)
C61-C62-C66-C69B	-8.2(12)	C63-C62-C66-C67	-17.0(16)
C63-C62-C66-C68	97.4(19)	C63-C62-C66-C69	-131(2)
C63-C62-C66-C67B	-74.9(12)	C63-C62-C66-C68B	56.0(13)
C63-C62-C66-C69B	170.9(9)	C63-C64-C70-C71	-122.3(9)
C63-C64-C70-C72	119.0(8)	C63-C64-C70-C73	0.0(11)
C65-C64-C70-C71	58.6(10)	C65-C64-C70-C72	-60.1(9)
C65-C64-C70-C73	-179.1(8)	C24-C25-C74-C75	-82.0(8)
C24-C25-C74-C79	97.0(8)	C26-C25-C74-C75	97.7(8)
C26-C25-C74-C79	-83.4(8)	C25-C74-C75-C76	177.8(6)
C79-C74-C75-C76	-1.2(11)	C74-C75-C76-C77	0.0(10)
C74-C75-C76-C80	179.0(6)	C75-C76-C77-C78	0.6(11)
C80-C76-C77-C78	-178.4(7)	C76-C77-C78-C79	-0.1(12)
C76-C77-C78-C84	-178.4(7)	C25-C74-C79-C78	-177.3(7)
C75-C74-C79-C78	1.7(11)	C77-C78-C79-C74	-1.1(11)
C84-C78-C79-C74	177.3(7)	C75-C76-C80-C81	54.9(13)
C75-C76-C80-C82	177.3(12)	C75-C76-C80-C83	-63.3(12)
C75-C76-C80-C81B	2.3(11)	C75-C76-C80-C82B	124.0(9)
C75-C76-C80-C83B	-117.6(8)	C77-C76-C80-C81	-126.2(12)
C77-C76-C80-C82	-3.7(14)	C77-C76-C80-C83	115.6(11)
C77-C76-C80-C81B	-178.8(8)	C77-C76-C80-C82B	-57.0(10)

C77-C76-C80-C83B	61.4(10)	C77-C78-C84-C85	-3.3(11)
C77-C78-C84-C86	-123.2(9)	C77-C78-C84-C87	117.3(9)
C79-C78-C84-C85	178.3(8)	C79-C78-C84-C86	58.5(9)
C79-C78-C84-C87	-61.0(10)	C34-C35-C88-C89	83.7(9)
C34-C35-C88-C93	-98.8(9)	C36-C35-C88-C89	-98.0(8)
C36-C35-C88-C93	79.5(9)	C35-C88-C89-C90	177.7(8)
C93-C88-C89-C90	0.1(12)	C88-C89-C90-C91	-1.4(13)
C88-C89-C90-C98	-178.8(8)	C89-C90-C91-C92	1.4(13)
C98-C90-C91-C92	178.7(8)	C90-C91-C92-C93	-0.2(12)
C90-C91-C92-C94	179.8(8)	C35-C88-C93-C92	-176.2(7)
C89-C88-C93-C92	1.3(13)	C91-C92-C93-C88	-1.3(12)
C94-C92-C93-C88	178.7(8)	C91-C92-C94-C95	105(4)
C91-C92-C94-C96	-14(4)	C91-C92-C94-C97	-139(4)
C91-C92-C94-C95B	-176.5(8)	C91-C92-C94-C96B	63.8(10)
C91-C92-C94-C97B	-57.3(10)	C93-C92-C94-C95	-75(4)
C93-C92-C94-C96	166(4)	C93-C92-C94-C97	41(4)
C93-C92-C94-C95B	3.5(12)	C93-C92-C94-C96B	-116.2(9)
C93-C92-C94-C97B	122.7(9)	C89-C90-C98-C99	55.6(11)
C89-C90-C98-C100	-58.9(11)	C89-C90-C98-C101	177.0(10)
C89-C90-C98-C99B	115(2)	C89-C90-C98-C10A	-9(3)
C89-C90-C98-C10B	-134(2)	C91-C90-C98-C99	-121.7(10)
C91-C90-C98-C100	123.8(10)	C91-C90-C98-C101	-0.2(14)
C91-C90-C98-C99B	-63(2)	C91-C90-C98-C10A	174(2)
C91-C90-C98-C10B	49(2)	C16-N4-Ni2-N3	-22.2(7)
C16-N4-Ni2-N1B	156.7(10)	C19-N4-Ni2-N3	168.3(7)
C19-N4-Ni2-N1B	-12.8(10)	Ni2-N1B-C1B-C20	2(5)
Ni2-N1B-C1B-C2B	176(2)	C4B-N1B-C1B-C20	178(3)
C4B-N1B-C1B-C2B	-8(4)	C19-C20-C1B-N1B	-24(4)
C19-C20-C1B-C2B	163(3)	C60-C20-C1B-N1B	-176(2)
C60-C20-C1B-C2B	11(4)	C20-C1B-C2B-C3B	178(3)
N1B-C1B-C2B-C3B	5(4)	C1B-C2B-C3B-C4B	1(4)
Ni2-N1B-C4B-C3B	-176(2)	Ni2-N1B-C4B-C5B	-11(5)
C1B-N1B-C4B-C3B	9(4)	C1B-N1B-C4B-C5B	174(3)
C2B-C3B-C4B-N1B	-7(4)	C2B-C3B-C4B-C5B	-170(4)
N1B-C4B-C5B-C6B	-14(5)	N1B-C4B-C5B-C43B	-180(3)
C3B-C4B-C5B-C6B	148(4)	C3B-C4B-C5B-C43B	-18(5)
Ni2-N2B-C6B-C5B	-3(5)	Ni2-N2B-C6B-C7B	-172(2)
C9B-N2B-C6B-C5B	174(3)	C9B-N2B-C6B-C7B	6(4)
C4B-C5B-C6B-N2B	22(5)	C4B-C5B-C6B-C7B	-172(3)
C43B-C5B-C6B-N2B	-174(3)	C43B-C5B-C6B-C7B	-7(5)
N2B-C6B-C7B-C8B	-10(4)	C5B-C6B-C7B-C8B	-179(3)
C6B-C7B-C8B-C9B	11(4)	C11-C10-C9B-N2B	15(5)
C11-C10-C9B-C8B	-162(3)	C46-C10-C9B-N2B	-177(3)
C46-C10-C9B-C8B	5(5)	Ni2-N2B-C9B-C10	1(6)
Ni2-N2B-C9B-C8B	179(2)	C6B-N2B-C9B-C10	-176(4)
C6B-N2B-C9B-C8B	2(4)	C7B-C8B-C9B-C10	170(4)
C7B-C8B-C9B-N2B	-8(4)	C4B-C5B-C43B-S1B	-163(2)
C4B-C5B-C43B-S2B	72(3)	C6B-C5B-C43B-S1B	31(4)
C6B-C5B-C43B-S2B	-94(3)	S1B-C44B-C45B-S2B	-19(5)

C5B–C43B–S1B–C44B	–154(3)	S2B–C43B–S1B–C44B	–19(2)
C45B–C44B–S1B–C43B	25(4)	C5B–C43B–S2B–C45B	139(3)
S1B–C43B–S2B–C45B	9(3)	C44B–C45B–S2B–C43B	7(5)

Table S29. Anisotropic displacement parameters ($\text{\AA}^2$) for **NiZn14**.The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni1	0.264(4)	0.0373(14)	0.085(2)	-0.0103(12)	0.013(2)	-0.0016(18)
N1A	0.229(8)	0.069(5)	0.076(5)	-0.024(4)	0.004(6)	-0.026(6)
N2A	0.231(9)	0.077(6)	0.096(6)	-0.033(5)	0.027(7)	-0.028(6)
N3	0.139(5)	0.048(3)	0.079(4)	-0.021(3)	-0.022(3)	-0.018(3)
N4	0.150(5)	0.045(3)	0.059(3)	-0.012(2)	-0.022(3)	-0.021(3)
C1A	0.211(7)	0.065(4)	0.073(5)	-0.015(4)	-0.003(5)	-0.028(5)
C2A	0.221(7)	0.076(4)	0.081(5)	-0.020(4)	0.004(5)	-0.028(5)
C3A	0.230(7)	0.085(5)	0.088(5)	-0.025(4)	0.007(6)	-0.033(6)
C4A	0.234(7)	0.084(4)	0.095(5)	-0.038(4)	0.012(5)	-0.031(5)
C5A	0.240(6)	0.096(4)	0.107(4)	-0.046(4)	0.010(5)	-0.034(5)
C6A	0.232(7)	0.089(5)	0.113(5)	-0.049(4)	0.014(5)	-0.026(5)
C7A	0.221(7)	0.091(5)	0.121(5)	-0.054(4)	0.013(6)	-0.029(6)
C8A	0.210(7)	0.083(5)	0.121(5)	-0.055(4)	0.015(6)	-0.024(5)
C9A	0.194(7)	0.070(4)	0.115(5)	-0.056(4)	0.007(5)	-0.029(5)
C10	0.151(5)	0.064(3)	0.113(4)	-0.050(3)	-0.013(4)	-0.028(3)
C11	0.133(5)	0.052(4)	0.093(4)	-0.037(3)	-0.022(4)	-0.016(3)
C12	0.129(5)	0.041(3)	0.093(4)	-0.017(3)	-0.032(4)	-0.011(3)
C13	0.124(5)	0.036(3)	0.086(4)	-0.015(3)	-0.034(4)	-0.006(3)
C14	0.123(5)	0.039(3)	0.068(4)	-0.016(3)	-0.025(3)	-0.018(3)
C15	0.119(4)	0.034(3)	0.073(3)	-0.013(3)	-0.036(3)	-0.013(3)
C16	0.124(5)	0.039(3)	0.063(3)	-0.012(2)	-0.035(3)	-0.008(3)
C17	0.115(5)	0.042(3)	0.075(4)	-0.006(3)	-0.030(3)	-0.002(3)
C18	0.127(5)	0.042(3)	0.075(4)	-0.007(3)	-0.032(4)	-0.009(3)
C19	0.144(5)	0.038(3)	0.065(4)	-0.010(3)	-0.023(3)	-0.010(3)
C20	0.178(5)	0.049(3)	0.069(3)	-0.012(3)	-0.021(4)	-0.024(3)
Zn	0.1014(6)	0.0439(4)	0.0837(6)	-0.0176(4)	-0.0426(5)	-0.0060(4)
N5	0.089(3)	0.030(2)	0.070(3)	-0.009(2)	-0.040(3)	-0.002(2)
N6	0.106(4)	0.053(3)	0.078(4)	-0.019(3)	-0.035(3)	0.003(3)
N7	0.109(4)	0.050(3)	0.091(4)	-0.028(3)	-0.038(3)	0.007(3)
N8	0.088(4)	0.038(3)	0.074(3)	-0.020(2)	-0.039(3)	0.000(2)
C21	0.085(4)	0.028(3)	0.078(4)	-0.011(2)	-0.042(3)	0.001(2)
C22	0.086(4)	0.039(3)	0.084(4)	-0.009(3)	-0.039(3)	-0.002(3)
C23	0.085(4)	0.035(3)	0.080(4)	-0.006(3)	-0.041(3)	0.003(3)
C24	0.083(4)	0.035(3)	0.073(3)	-0.009(2)	-0.043(3)	0.002(3)
C25	0.089(4)	0.043(3)	0.071(3)	-0.009(2)	-0.040(3)	-0.008(3)
C26	0.097(4)	0.057(3)	0.074(4)	-0.012(3)	-0.033(3)	-0.008(3)
C27	0.116(5)	0.063(4)	0.090(4)	-0.011(3)	-0.028(4)	-0.010(4)
C28	0.135(6)	0.072(4)	0.097(5)	-0.020(4)	-0.016(4)	-0.010(4)
C29	0.126(5)	0.066(4)	0.086(4)	-0.021(3)	-0.018(4)	-0.007(4)
C30	0.143(5)	0.076(4)	0.100(5)	-0.034(4)	-0.008(4)	-0.006(4)
C31	0.127(5)	0.063(4)	0.093(4)	-0.032(3)	-0.018(4)	-0.002(4)
C32	0.136(6)	0.073(4)	0.112(5)	-0.042(4)	-0.014(4)	-0.005(4)
C33	0.126(5)	0.067(4)	0.112(5)	-0.040(4)	-0.032(4)	0.004(4)

C34	0.110(5)	0.051(3)	0.100(4)	-0.039(3)	-0.035(4)	0.006(3)
C35	0.096(4)	0.046(3)	0.099(4)	-0.030(3)	-0.050(3)	0.006(3)
C36	0.089(4)	0.043(3)	0.085(4)	-0.018(3)	-0.044(3)	-0.004(3)
C37	0.093(4)	0.037(3)	0.095(4)	-0.013(3)	-0.048(3)	-0.001(3)
C38	0.091(4)	0.036(3)	0.089(4)	-0.010(3)	-0.045(3)	-0.005(3)
C39	0.089(4)	0.031(3)	0.077(4)	-0.012(2)	-0.043(3)	-0.003(3)
C40	0.089(4)	0.033(3)	0.074(3)	-0.010(2)	-0.043(3)	-0.006(3)
C41	0.096(4)	0.028(3)	0.073(4)	-0.009(3)	-0.041(3)	-0.003(3)
C42	0.094(4)	0.026(3)	0.075(4)	-0.009(3)	-0.042(3)	0.000(3)
C43A	0.253(7)	0.114(6)	0.115(5)	-0.055(5)	0.004(6)	-0.031(6)
C44A	0.315(11)	0.193(9)	0.174(9)	-0.084(8)	-0.004(9)	-0.018(10)
C45A	0.308(12)	0.191(10)	0.175(9)	-0.080(8)	-0.001(9)	-0.016(10)
S1A	0.327(9)	0.177(6)	0.175(5)	-0.075(5)	-0.016(6)	-0.029(6)
S2A	0.266(8)	0.156(5)	0.142(5)	-0.062(4)	0.022(5)	-0.010(5)
C46	0.126(5)	0.070(4)	0.137(5)	-0.059(3)	-0.033(4)	-0.013(3)
C47	0.119(5)	0.074(4)	0.146(5)	-0.059(4)	-0.051(4)	-0.003(4)
C48	0.118(5)	0.067(4)	0.168(5)	-0.068(4)	-0.063(4)	0.009(3)
C49	0.118(5)	0.088(4)	0.177(6)	-0.067(4)	-0.074(5)	0.011(4)
C50	0.122(5)	0.105(5)	0.180(6)	-0.071(4)	-0.073(4)	-0.001(4)
C51	0.123(5)	0.092(5)	0.161(6)	-0.066(4)	-0.050(5)	-0.020(4)
C52	0.147(6)	0.079(4)	0.182(7)	-0.079(5)	-0.063(5)	0.004(4)
C53	0.156(11)	0.089(9)	0.209(11)	-0.078(8)	-0.055(10)	-0.021(8)
C54	0.179(12)	0.103(9)	0.194(11)	-0.091(9)	-0.071(10)	-0.008(9)
C55	0.169(11)	0.091(9)	0.208(13)	-0.084(9)	-0.036(10)	0.006(8)
C56	0.134(6)	0.153(7)	0.193(7)	-0.083(6)	-0.087(6)	-0.005(5)
C57	0.161(9)	0.249(13)	0.205(11)	-0.106(10)	-0.092(8)	0.041(9)
C58	0.169(9)	0.206(11)	0.198(10)	-0.066(9)	-0.096(8)	-0.021(9)
C59	0.206(11)	0.196(10)	0.216(11)	-0.112(9)	-0.093(9)	-0.030(8)
C60	0.145(5)	0.051(3)	0.073(4)	0.000(3)	-0.038(4)	-0.025(3)
C61	0.146(5)	0.073(4)	0.077(4)	0.012(3)	-0.046(4)	-0.053(4)
C62	0.117(4)	0.085(4)	0.095(4)	0.021(3)	-0.057(4)	-0.041(4)
C63	0.095(4)	0.059(4)	0.101(4)	0.012(3)	-0.047(4)	-0.013(3)
C64	0.091(4)	0.045(3)	0.093(4)	-0.007(3)	-0.045(3)	-0.002(3)
C65	0.111(4)	0.047(3)	0.077(4)	-0.006(3)	-0.048(3)	-0.003(3)
C66	0.118(5)	0.123(6)	0.110(5)	0.020(4)	-0.065(4)	-0.041(5)
C67	0.116(11)	0.149(11)	0.108(11)	0.016(10)	-0.062(9)	-0.023(9)
C68	0.126(11)	0.135(13)	0.105(9)	0.013(10)	-0.069(9)	-0.033(11)
C69	0.121(11)	0.149(12)	0.124(12)	0.018(11)	-0.076(9)	-0.034(10)
C70	0.098(4)	0.061(4)	0.128(5)	-0.037(4)	-0.052(4)	0.009(3)
C71	0.122(6)	0.126(7)	0.202(9)	-0.094(7)	-0.071(6)	0.011(5)
C72	0.164(8)	0.102(6)	0.134(7)	-0.056(5)	-0.067(6)	0.015(6)
C73	0.150(8)	0.067(5)	0.184(9)	-0.043(5)	-0.061(7)	0.007(5)
C74	0.083(4)	0.047(3)	0.068(3)	0.002(2)	-0.038(3)	-0.009(3)
C75	0.089(4)	0.040(3)	0.076(4)	-0.002(3)	-0.041(3)	-0.002(3)
C76	0.085(4)	0.041(3)	0.080(3)	0.000(3)	-0.032(3)	-0.007(3)
C77	0.086(4)	0.049(3)	0.084(4)	0.007(3)	-0.036(3)	-0.003(3)
C78	0.093(4)	0.065(4)	0.080(4)	0.006(3)	-0.044(3)	0.002(3)
C79	0.092(4)	0.057(3)	0.078(4)	-0.003(3)	-0.041(3)	-0.006(3)

C80	0.103(4)	0.044(3)	0.104(4)	-0.016(3)	-0.042(4)	-0.006(3)
C81	0.131(10)	0.065(9)	0.103(8)	-0.032(7)	-0.045(9)	-0.016(9)
C82	0.120(10)	0.055(8)	0.126(11)	-0.030(8)	-0.048(10)	0.007(8)
C83	0.110(9)	0.077(10)	0.118(10)	-0.025(9)	-0.051(8)	-0.018(8)
C84	0.113(5)	0.095(5)	0.096(5)	0.011(4)	-0.061(4)	0.004(4)
C85	0.180(9)	0.100(6)	0.143(8)	0.011(5)	-0.102(7)	0.032(6)
C86	0.143(7)	0.145(8)	0.086(5)	0.010(5)	-0.068(5)	-0.002(6)
C87	0.117(6)	0.135(7)	0.137(7)	0.007(6)	-0.082(6)	0.000(6)
C88	0.098(4)	0.046(3)	0.104(4)	-0.028(3)	-0.049(3)	0.004(3)
C89	0.098(4)	0.053(3)	0.125(5)	-0.040(3)	-0.053(4)	0.008(3)
C90	0.098(4)	0.051(3)	0.143(5)	-0.048(3)	-0.056(4)	0.010(3)
C91	0.101(4)	0.044(3)	0.140(5)	-0.033(3)	-0.056(4)	0.010(3)
C92	0.096(4)	0.044(3)	0.121(4)	-0.028(3)	-0.053(3)	0.006(3)
C93	0.104(4)	0.042(3)	0.109(4)	-0.030(3)	-0.051(4)	0.002(3)
C94	0.102(4)	0.056(4)	0.123(5)	-0.024(3)	-0.055(4)	0.001(3)
C95	0.124(12)	0.067(12)	0.121(10)	-0.021(11)	-0.056(10)	0.003(11)
C96	0.114(12)	0.072(10)	0.131(12)	-0.018(11)	-0.059(11)	0.006(10)
C97	0.111(11)	0.073(11)	0.130(13)	-0.026(11)	-0.063(10)	0.000(10)
C98	0.130(5)	0.063(4)	0.171(6)	-0.065(4)	-0.063(5)	0.008(4)
C99	0.133(7)	0.074(6)	0.173(9)	-0.058(6)	-0.055(7)	-0.024(5)
C100	0.144(8)	0.093(7)	0.183(8)	-0.089(6)	-0.052(7)	0.001(6)
C101	0.188(10)	0.069(6)	0.208(10)	-0.061(6)	-0.090(8)	0.004(6)
N9	0.265(15)	0.168(10)	0.147(9)	-0.026(8)	0.065(10)	0.002(10)
C102	0.183(9)	0.093(6)	0.129(7)	-0.028(6)	0.026(6)	-0.003(6)
O1	0.139(6)	0.196(7)	0.141(6)	-0.079(5)	-0.040(5)	-0.043(5)
C103	0.216(16)	0.45(3)	0.254(18)	-0.139(18)	-0.071(14)	-0.139(17)
Ni2	0.139(3)	0.074(3)	0.065(2)	-0.043(2)	-0.005(2)	-0.059(2)
N1B	0.210(9)	0.070(6)	0.074(6)	-0.040(5)	-0.007(7)	-0.055(7)
N2B	0.202(8)	0.070(6)	0.093(6)	-0.058(5)	-0.002(6)	-0.051(6)
C1B	0.209(7)	0.068(5)	0.072(5)	-0.018(4)	-0.006(6)	-0.034(5)
C2B	0.219(7)	0.076(5)	0.078(5)	-0.022(4)	-0.001(6)	-0.038(6)
C3B	0.229(7)	0.082(5)	0.085(5)	-0.034(5)	0.003(6)	-0.038(6)
C4B	0.234(7)	0.088(5)	0.094(5)	-0.038(4)	0.008(6)	-0.037(6)
C5B	0.242(6)	0.097(5)	0.107(5)	-0.052(4)	0.009(5)	-0.033(5)
C6B	0.230(7)	0.087(5)	0.111(5)	-0.056(4)	0.011(6)	-0.035(5)
C7B	0.221(7)	0.089(5)	0.122(5)	-0.059(5)	0.015(6)	-0.031(6)
C8B	0.204(7)	0.081(5)	0.118(6)	-0.063(5)	0.008(6)	-0.034(6)
C9B	0.189(7)	0.073(5)	0.114(5)	-0.058(5)	0.002(6)	-0.034(5)
C43B	0.259(8)	0.116(6)	0.120(6)	-0.059(5)	0.004(6)	-0.032(7)
C44B	0.315(12)	0.191(9)	0.167(9)	-0.085(8)	-0.008(9)	-0.021(10)
C45B	0.313(11)	0.192(9)	0.171(8)	-0.081(8)	-0.003(9)	-0.020(9)
S1B	0.303(12)	0.182(9)	0.155(8)	-0.080(7)	-0.037(8)	-0.050(8)
S2B	0.285(10)	0.165(7)	0.153(7)	-0.075(6)	0.007(7)	-0.016(7)
C53B	0.147(10)	0.095(9)	0.202(12)	-0.076(9)	-0.069(9)	-0.028(8)
C54B	0.173(11)	0.095(9)	0.196(10)	-0.098(8)	-0.050(10)	-0.005(9)
C55B	0.175(12)	0.085(8)	0.214(12)	-0.074(9)	-0.059(11)	0.010(9)
C67B	0.109(7)	0.165(10)	0.116(8)	0.026(7)	-0.061(6)	-0.013(7)
C68B	0.103(7)	0.103(7)	0.089(7)	0.017(6)	-0.054(6)	-0.003(6)

C69B	0.164(10)	0.141(9)	0.133(9)	−0.005(7)	−0.086(7)	−0.031(8)
C81B	0.130(8)	0.075(6)	0.103(7)	−0.024(5)	−0.056(7)	−0.013(6)
C82B	0.114(7)	0.083(7)	0.137(9)	−0.049(6)	−0.045(6)	−0.003(6)
C83B	0.124(8)	0.071(6)	0.132(8)	−0.015(6)	−0.044(7)	−0.030(6)
C95B	0.129(7)	0.070(5)	0.123(7)	−0.024(4)	−0.069(6)	−0.006(5)
C96B	0.129(7)	0.071(6)	0.125(6)	−0.015(5)	−0.056(5)	−0.005(5)
C97B	0.108(6)	0.093(6)	0.140(7)	−0.029(5)	−0.063(5)	0.010(5)
C99B	0.147(12)	0.071(11)	0.185(11)	−0.066(10)	−0.059(11)	−0.011(10)
C10A	0.143(12)	0.087(11)	0.179(11)	−0.069(10)	−0.060(10)	−0.005(11)
C10B	0.144(11)	0.068(10)	0.184(13)	−0.086(10)	−0.065(10)	−0.005(9)

Table S30. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for **NiZn14**.

	x	y	z	U
H2A	1.114599	0.820457	0.048603	0.164
H3A	1.201958	0.738945	−0.010582	0.174
H7A	1.271213	0.463134	0.067018	0.182
H8A	1.272394	0.376247	0.189539	0.174
H12	0.987736	0.342464	0.411309	0.106
H13	0.839427	0.412369	0.451159	0.098
H17	0.738968	0.683401	0.369953	0.096
H18	0.819030	0.786679	0.274116	0.100
H22	0.716895	0.392610	0.547597	0.082
H23	0.641865	0.288948	0.643815	0.080
H27	0.300021	0.241861	0.841862	0.112
H28	0.171677	0.319840	0.886881	0.128
H32	0.070311	0.591524	0.799725	0.130
H33	0.128702	0.691616	0.693412	0.120
H37	0.435614	0.728009	0.473828	0.086
H38	0.582889	0.654971	0.435961	0.084
H43A	1.231904	0.643969	−0.033761	0.200
H44A	1.326151	0.479509	−0.095285	0.282
H44B	1.327593	0.562311	−0.138986	0.282
H45A	1.456114	0.558187	−0.112981	0.282
H45B	1.424258	0.489469	−0.047168	0.282
H47	1.104199	0.287385	0.260796	0.123
H49	1.231667	0.155100	0.402931	0.138
H51	1.204824	0.364193	0.376131	0.138
H53A	1.105826	0.082569	0.413317	0.211
H53B	1.011315	0.120099	0.388706	0.211
H53C	1.067036	0.054613	0.365793	0.211
H54A	1.135340	0.202108	0.214861	0.213
H54B	1.084854	0.126321	0.246792	0.213
H54C	1.029133	0.191806	0.269705	0.213
H55A	1.272777	0.091950	0.329473	0.227
H55B	1.224243	0.062554	0.287489	0.227
H55C	1.284358	0.134535	0.250978	0.227
H57A	1.402717	0.206765	0.474675	0.287
H57B	1.366789	0.169600	0.432463	0.287
H57C	1.411707	0.247263	0.396168	0.287
H58A	1.139344	0.219227	0.536462	0.268
H58B	1.199958	0.151752	0.519954	0.268
H58C	1.236449	0.190157	0.560948	0.268
H59A	1.206495	0.336357	0.482439	0.275
H59B	1.302910	0.306782	0.507651	0.275
H59C	1.314050	0.350304	0.429387	0.275
H61	0.885239	0.836911	0.087075	0.120
H63	0.866492	1.020883	0.123415	0.107
H65	1.015164	0.852925	0.219668	0.093
H67A	0.716609	1.020209	0.111673	0.197
H67B	0.810755	1.064491	0.059035	0.197

H67C	0.717927	1.059714	0.034257	0.197
H68A	0.922803	1.017987	-0.028811	0.187
H68B	0.894917	0.948870	-0.039003	0.187
H68C	0.827798	1.019848	-0.053895	0.187
H69A	0.680010	0.907488	0.104191	0.203
H69B	0.677334	0.951339	0.028252	0.203
H69C	0.744453	0.880361	0.043143	0.203
H71A	1.096794	1.014763	0.227343	0.201
H71B	1.107987	0.939044	0.216811	0.201
H71C	1.111482	1.010270	0.153686	0.201
H72A	0.939796	0.976035	0.317949	0.187
H72B	0.852318	0.948021	0.302481	0.187
H72C	0.951835	0.901080	0.305817	0.187
H73A	0.944236	1.087609	0.224452	0.197
H73B	0.953686	1.087473	0.150018	0.197
H73C	0.854308	1.061678	0.209752	0.197
H75	0.419084	0.220203	0.674918	0.082
H77	0.541266	0.043353	0.781847	0.093
H79	0.534628	0.227526	0.817565	0.091
H81A	0.464035	0.166718	0.596808	0.142
H81B	0.564198	0.120279	0.598868	0.142
H81C	0.476093	0.091960	0.584292	0.142
H82A	0.472380	-0.021495	0.684870	0.147
H82B	0.561197	0.006921	0.698630	0.147
H82C	0.459852	-0.014920	0.757467	0.147
H83A	0.311374	0.130493	0.687074	0.146
H83B	0.317425	0.053386	0.680119	0.146
H83C	0.308938	0.061022	0.751712	0.146
H85A	0.662106	0.008955	0.831017	0.218
H85B	0.658155	-0.003990	0.907890	0.218
H85C	0.559312	-0.008102	0.889200	0.218
H86A	0.526528	0.155079	0.922752	0.194
H86B	0.477642	0.079997	0.944428	0.194
H86C	0.576485	0.084110	0.963117	0.194
H87A	0.740781	0.127366	0.795010	0.200
H87B	0.687822	0.184013	0.831722	0.200
H87C	0.737287	0.112782	0.872097	0.200
H89	0.329797	0.782130	0.619195	0.102
H91	0.200373	0.922005	0.484414	0.108
H93	0.206764	0.712631	0.512158	0.094
H95A	0.190507	0.839927	0.334112	0.154
H95B	0.272617	0.862782	0.358467	0.154
H95C	0.247229	0.780829	0.381961	0.154
H96A	0.061461	0.918524	0.380205	0.157
H96B	0.045901	0.919169	0.455293	0.157
H96C	0.146442	0.947110	0.397623	0.157
H97A	0.027157	0.795452	0.418663	0.150
H97B	0.091591	0.735648	0.459848	0.150
H97C	0.012424	0.783613	0.496915	0.150
H99A	0.427775	0.874007	0.587762	0.175
H99B	0.440330	0.930442	0.513427	0.175

H99C	0.423498	0.957215	0.576603	0.175
H10A	0.270113	0.859504	0.673557	0.190
H10B	0.269199	0.942354	0.663212	0.190
H10C	0.176057	0.908878	0.659326	0.190
H10D	0.293984	1.003757	0.484103	0.214
H10E	0.190915	0.998474	0.541616	0.214
H10F	0.284056	1.031951	0.545502	0.214
H1	0.438887	0.549956	0.759434	0.178
H10G	0.588692	0.539382	0.749149	0.428
H10H	0.589456	0.469299	0.730368	0.428
H10I	0.605786	0.545099	0.672026	0.428
H2B	1.058049	0.819963	0.034977	0.158
H3B	1.127014	0.735786	-0.025544	0.166
H7B	1.211646	0.460617	0.055655	0.180
H8B	1.233390	0.373823	0.171340	0.163
H43B	1.100954	0.622424	-0.035293	0.205
H44C	1.299171	0.492223	-0.105740	0.276
H44D	1.225974	0.548252	-0.142442	0.276
H45C	1.330110	0.620409	-0.163196	0.281
H45D	1.377710	0.569987	-0.104931	0.281
H53D	0.996734	0.140030	0.371038	0.160
H53E	1.009950	0.193040	0.295220	0.160
H53F	1.017515	0.109031	0.310137	0.160
H54D	1.171883	0.205704	0.210973	0.170
H54E	1.266499	0.160959	0.230182	0.170
H54F	1.179142	0.121704	0.225850	0.170
H55D	1.143491	0.071556	0.405042	0.182
H55E	1.161775	0.038839	0.345527	0.182
H55F	1.249131	0.078094	0.349859	0.182
H67D	0.677450	0.927396	0.118108	0.171
H67E	0.692460	1.009061	0.105607	0.171
H67F	0.660536	0.987439	0.051443	0.171
H68D	0.922456	1.018393	-0.027097	0.126
H68E	0.818411	1.046056	-0.042113	0.126
H68F	0.850335	1.067679	0.012051	0.126
H69D	0.774926	0.868362	0.041163	0.173
H69E	0.767939	0.934132	-0.024614	0.173
H69F	0.873760	0.902584	-0.014958	0.173
H81D	0.384185	0.093348	0.609240	0.117
H81E	0.336949	0.146192	0.651440	0.117
H81F	0.442643	0.161979	0.596291	0.117
H82D	0.521594	0.017580	0.627291	0.126
H82E	0.588407	0.080502	0.617855	0.126
H82F	0.571392	0.012399	0.684992	0.126
H83D	0.360101	-0.005035	0.713231	0.131
H83E	0.409447	-0.008478	0.770655	0.131
H83F	0.317431	0.044649	0.759245	0.131
H95D	0.071592	0.740691	0.466286	0.121
H95E	0.080091	0.785045	0.388531	0.121
H95F	0.175433	0.744073	0.409845	0.121
H96D	0.172319	0.893616	0.332410	0.130

H96E	0.220709	0.925881	0.372439	0.130
H96F	0.267813	0.855513	0.355373	0.130
H97D	0.000378	0.847004	0.498493	0.133
H97E	0.055421	0.921036	0.460515	0.133
H97F	0.007144	0.888686	0.420490	0.133
H99D	0.339769	0.981538	0.470919	0.148
H99E	0.375704	1.013643	0.516861	0.148
H99F	0.430324	0.944460	0.500588	0.148
H10J	0.294146	0.875606	0.673581	0.151
H10K	0.402858	0.880919	0.622098	0.151
H10L	0.348238	0.950102	0.638372	0.151
H10M	0.172176	0.982836	0.547479	0.138
H10N	0.153319	0.947397	0.627645	0.138
H10O	0.220802	1.015599	0.587023	0.138