Supplementary Information (SI) for Dalton Transactions.

Supporting Information

N-Bridged bis-amidine *N*-oxides – a versatile platform in metallosupramolecular chemistry

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1. Introduction

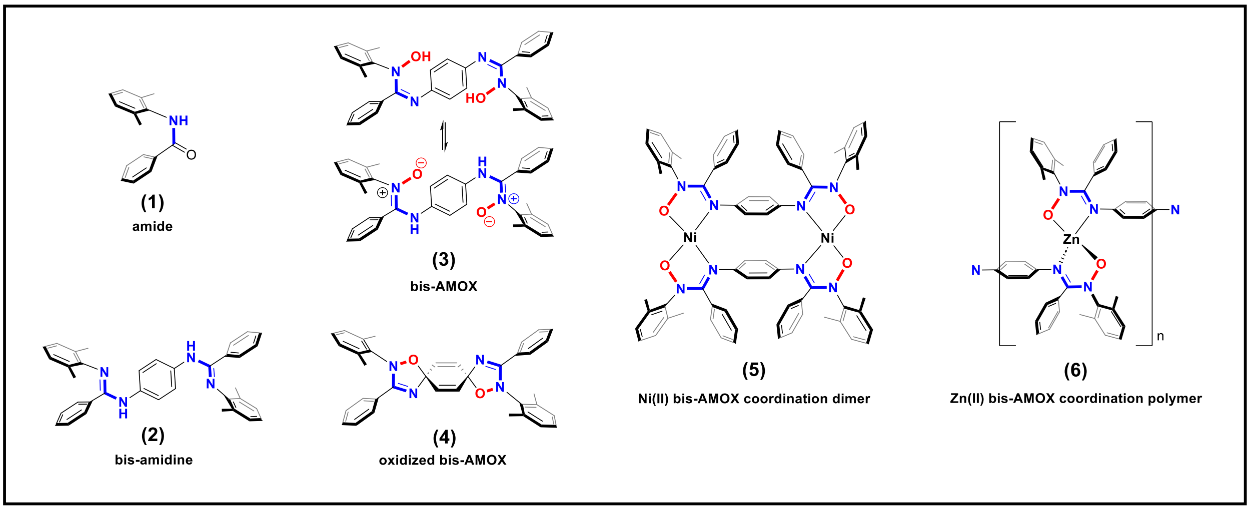


Chart S1. ChemDraw structures of compounds **1-6** presented in this work.

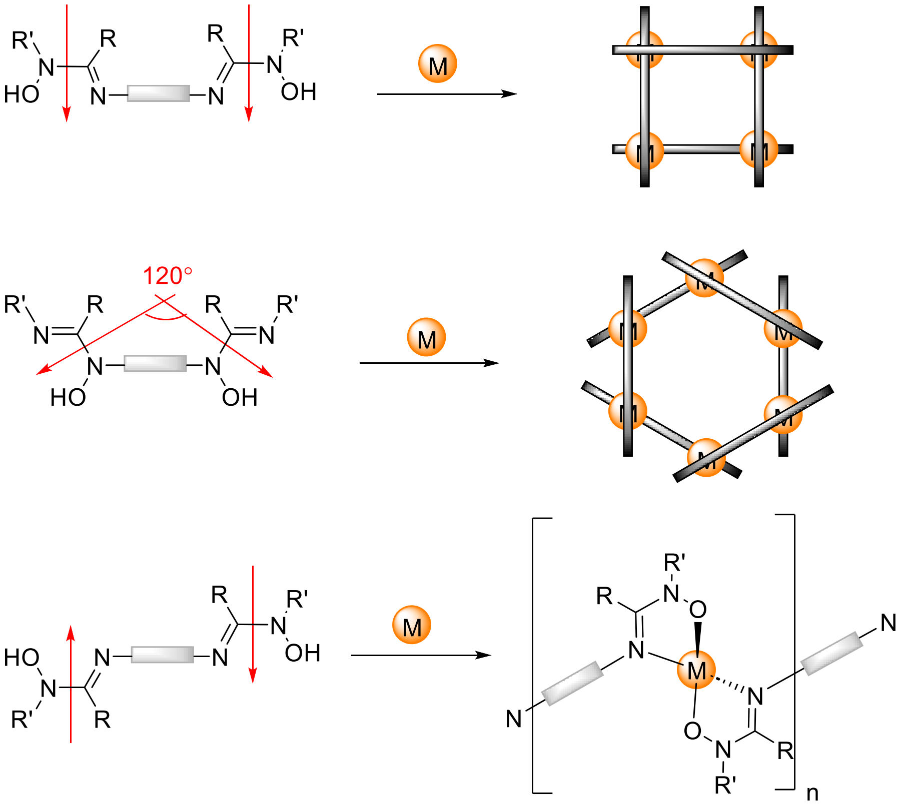


Fig. S1. *N*-bridged bis-AMOX supramolecular multimetallic systems, governed by the coordination vectors of the ligand and the preferred geometry of the metal ion (e.g., tetrahedral or square-planar), open pathways toward both discrete assemblies and polymeric structures.

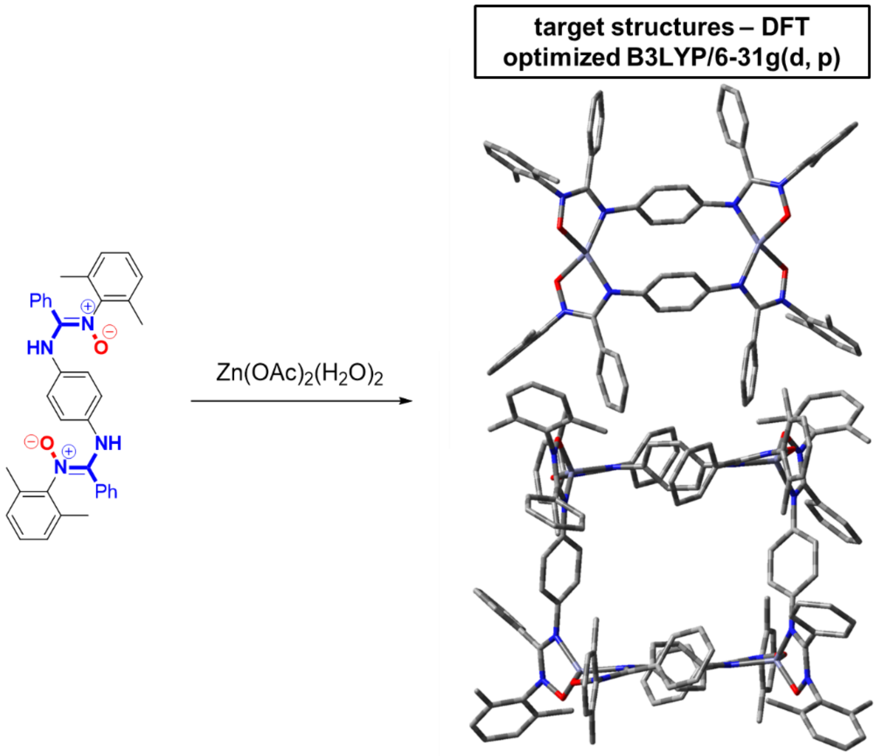


Fig. S2. Coordination of *N*-bridged bis-AMOX ligand **(3)** with Zn(II) metal-ions: expected discrete assemblies (**dimer** and **grid**) (models*).

*Gaussian09, Revision D.01[1] was used for all theoretical calculations discussed herein, with B3LYP[2] DFT method, 6,31-g(d,p)[3] basis set, in gas phase or using PCM[4] (DCM) solvation model. No symmetry constraints were used for the geometry optimization. GaussView 3.0.9[5] software was used for visualisation and plots. Initial atom coordinates for geometry optimization were obtained using Chem3D in ChemDraw (PerkinElmer). The atomic coordinates for the optimized structures are given in Tables S2 and S3.

2. Material and Instrumentation

Nuclear magnetic resonance (NMR) spectra were recorded in $CDCl_3$ and/ or DMSO-d_6 at room temperature (r.t.) (unless otherwise stated) on the following spectrometers: Bruker AV-400, AV-300, DRX-400, and ARX-300 MHz. Chemical shifts (δ) are reported in parts per million (ppm) relative to TMS, using the residual solvent protons (7.26 ppm or 2.50 ppm) as reference. Infrared (IR) spectra were recorded using a Thermo Scientific Nicolet iS10 FT-IR spectrometer. Absorption spectra were measured in toluene (concentration range 10^{-4} – 10^{-6} M) at r.t. on a Cary 500i and a Cary 6000i UV-Vis-NIR Spectrophotometer. Luminescence spectra were obtained using a Perkin Elmer LS55 Luminescence Spectrometer equipped with an accessory for measuring solid state samples. Thermogravimetric analyses (TGA) were carried out on a TA Q-500 and a TGA2950 thermogravimetric analyzer (TA Instruments) under N_2 atmosphere, in the 25 – 600 °C temperature range, at a heating rate of 10 °C/min. The mass spectrometry analyses were performed on a Bruker microTOF II instrument by electrospray ionization (ESI) method, in positive mode. The microanalyses were done by the Mass Spectrometry Service and the Elemental Analysis Service at Université de Montréal. Solvents, purchased from VWR and Fisher, were removed under reduced pressure using a rotary evaporator, unless otherwise stated. The *m*-CPBA from Acros Organics and carboxylic acids, hexamethyldisiloxane, P_2O_5, and metal salts from Aldrich, were used without further purification. The anilines from Aldrich were purified by sublimation (1,4-phenylenediamine) and distillation (2,6-dimethylaniline) before being used.

3. Experimental Procedure

3.1. Synthesis of PPSE (polyphosphoric acid trimethylsilyl ester)

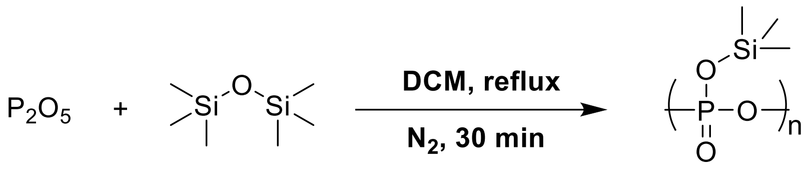
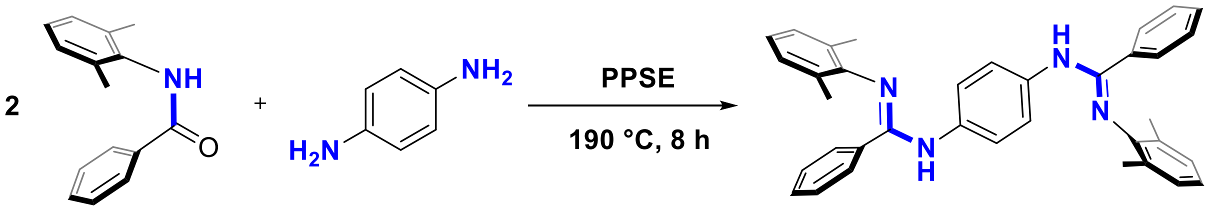


Fig. S3. Synthesis of the polymer **PPSE**

Polyphosphoric acid trimethylsilyl ester. The PPSE (a condensing and dehydrating agent) was obtained as a colorless viscous liquid by refluxing P_2O_5 with hexamethyldisiloxane (HMDS) (stoichiometry 1 to 1.5) in dry DCM for 30 min under N_2. The solvent was then evaporated. A detailed synthetic procedure, including reagent and solvent quantities for PPSE preparation, is provided in Section 3.2, which describes the preparation of **bis-amidine (2)**.

3.2. Synthesis of *N*-bridged bis-AMOX-based Compounds



(1) **(2)**

Fig. S4. Synthesis of *N*-bridged **bis-amidine (2)**.

Bis-amidine (2) – *N,N"*-(1,4-phenylene)bis(*N'*-(2,6-dimethylphenyl)benzimidamide). The synthesis of *N*-bridged **bis-amidine (2)** was carried out based on modified literature procedures for amidine synthesis, via condensation between 1,4-phenylenediamine (0.05 g, 0.47 mmol, 1 equiv.) and **amide (1)** (previously reported)[6] (0.21 g, 0.93 mmol, 2 equiv.) in polyphosphoric acid trimethylsilyl ester (PPSE).[7] PPSE was prepared by refluxing P_2O_5 (2.18 g, 15.1 mmol, 33 equiv. (vs. 1,4-phenylenediamine)) with hexamethyldisiloxane (HMDS) (5 mL, 23.5 mmol, 50 equiv. (vs. 1,4-phenylenediamine)) in dry DCM (5 mL) under N_2 for 30 min. The solvent was then evaporated. The two starting materials (1,4-phenylenediamine and **amide (1)**) were combined with the freshly prepared PPSE, and the reaction mixture was heated at 190 °C for 8 h. After cooling to room temperature, the reaction mixture was quenched with 1 M aqueous NaOH (40 mL). A beige solid was isolated, recrystallized from aqueous ethanol, and dried under vacuum to afford the pure compound as a colorless powder. Yield 0.19 g, 77%. ^{1}H NMR (400 MHz, DMSO-d_6, 110 °C) δ, ppm: 8.30 (br. s, 2H, -N***H***), 7.49 (br. s, 4H, ***H***-Ph$^{\text{bridge}}$) 7.35 – 7.25 (m, 10H, ***H***-Ph), 6.85 (br. s, 4H, $\boldsymbol{H}^{\boldsymbol{meta}}$-2,6-diMePh), 6.67 (br. s, 2H, $\boldsymbol{H}^{\boldsymbol{para}}$-2,6-diMePh), 2.07 (br. s, 12H, -C$\boldsymbol{H}_3$). ^{13}C NMR (101 MHz, DMSO-d_6, 110 °C) δ, ppm: 135.4 (2C), 128.4 (4C), 127.2 (8C), 126.8 (6C), 120.4 (6C), 17.6 (4C). (Fig. S14-S17). MS (ESI - DCM) (m/z): 523.3 $[M+H]^+$ (100%); 262.2 $[M+2H]^{2+}$ (17%). Elemental Analysis: *calc.* (%) for $C_{36}H_{34}N_4$: C 82.72, H 6.56, N 10.72; *found*: C 82.53, H 6.60, N 10.78. IR (ATR, solid sample, cm^{-1}): 3395, 3060, 3034, 3009, 2957, 2915, 1644, 1589, 1578, 1540, 1511, 1490, 1463, 1443, 1399, 1376, 1346, 1321, 1248, 1234, 1212, 1129, 1116, 1102, 1083, 1030, 922, 913, 837, 780, 758, 697, 678, 564. (Fig. S9).

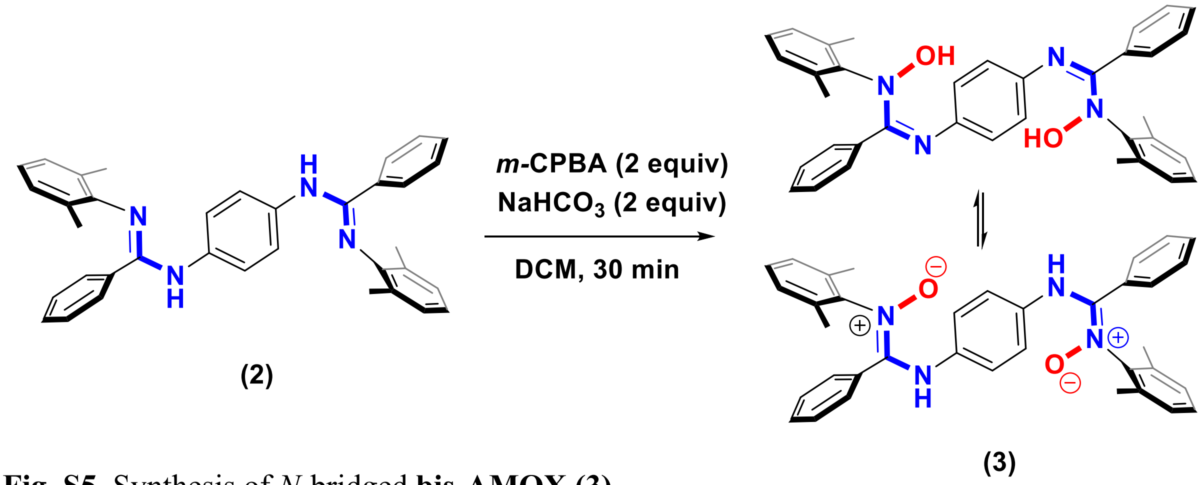
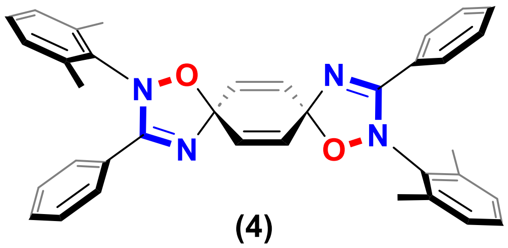


Fig. S5. Synthesis of *N*-bridged **bis-AMOX (3)**

Bis-AMOX (3) – *N,N"*-(1,4-phenylene)bis(*N'*-(2,6-dimethylphenyl)benzimidamide oxide). To a solution of the *N*-bridged **bis-amidine (2)** (0. 64 g, 1.2 mmol, 1 equiv.) in DCM (100 mL) was added $NaHCO_3$ (0.21 g, 2.4 mmol, 2 equiv.) as a solid, followed by slow addition (at 0 °C) of a solution of *m*-CPBA (0.43 g, 2.4 mmol, 2 equiv.) in DCM (100 mL). The reaction mixture was stirred and allowed to warm to room temperature over 30 min, then filtered and washed successively with 1 M aqueous NaOH (2 × 50 mL) and water (2 × 50 mL). The combined organic layers were dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure to yield a yellow-brown solid, which was further purified by flash column chromatography on silica (gradient of eluents: hexane/ EtOAc (5:5), EtOAc 100%, EtOAc/ EtOH (5:5), EtOH 100%). The purified solid was dissolved in DCM and filtered to remove any traces of silica potentially solubilized by the use of EtOH. After solvent removal under reduced pressure, the pure product was obtained as a yellow powder and dried under vacuum overnight. Yield: 0.33 g, 49%. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.23 (t, J = 7.4 Hz, 2H, $\boldsymbol{H}^{para}$-Ph) 7.12 (t, J = 7.7 Hz, 4H. $\boldsymbol{H}^{meta}$-Ph), 7.06 – 7.00 (m, 6H, $\boldsymbol{H}^{para}$-2,6-diMePh and $\boldsymbol{H}^{ortho}$-Ph,), 6.93 (d, J = 7.6 Hz, 4H, $\boldsymbol{H}^{meta}$-2,6-diMePh), 6.48 (s, 4H, $\boldsymbol{H}$-Ph^{bridge}), 2.25 (s, 12H, C$\boldsymbol{H}_3$). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 148.4 (2C), 141.2 (2C), 134.6 (2C), 134.2 (4C), 130.3(2C), 128.9 (4C), 128.8 (2C), 128.5 (8C), 127.1 (2C), 122.5 (4C), 17.6 (4C). (Fig. S14 and Fig. S18-S20)). MS (ESI - DCM) (m/z): 555.2 $[M+H]^+$ (100%). Elemental Analysis: *calc.* (%) for $C_{36}H_{34}N_4O_2$ (H_2O): C 75.50, H 6.34, N 9.78; *found*: C 75.82, H 6.22, N 9.88. IR (ATR, solid sample, cm^{-1}): 3058, 2954, 2921, 1735, 1597, 1570, 1515, 1468, 1446, 1400, 1376, 1243, 1206, 1155, 1098, 1076, 1057, 1026, 937, 915, 840. 771, 743, 695, 650, 617, 605, 579. (Fig. S10). X-ray quality yellow crystals (plates) were obtained at r. t. by slow diffusion of hexane into a DCM solution of the compound. The solid-state structure of **3** is presented in Fig. S27.

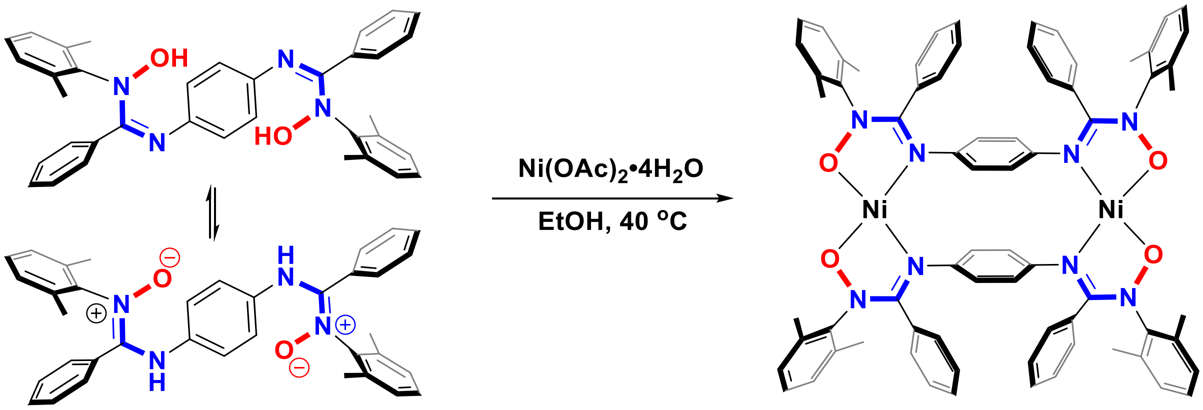


(4)

Fig. S6. Structure of **oxidized bis-AMOX (4)**.

Oxidized bis-AMOX (4) – 2,10-bis(2,6-dimethylphenyl)-3,11-diphenyl-1,9-dioxa-2,4,10,12-tetraazadispiro[4.2.4^{8}.2^{5}] tetradeca-3,6,11,13-tetraene. Compound **4** was obtained as a secondary product during the synthesis of **bis-AMOX (3)**. It was isolated as pale yellow/colorless powder following flash chromatography used for the purification of **3**. During optimization tests for the synthesis of **3**, monitored by thin layer chromatography (TLC), the formation of compound **4** was found to increase significantly with higher reactant concentrations and reached near-quantitative conversion when an excess of *m*-CPBA was used with **bis-amidine (2)**. Isolation of compound **4** and yield determination for were not performed in these test reactions. A full investigation into the direct synthesis and coordination chemistry of compound **4** is currently underway, and the findings will be reported in future publications. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.54 – 7.51 (m, 4H, $\boldsymbol{H}^{ortho}$-Ph) 7.37 – 7.33 (m, 2H, $\boldsymbol{H}^{para}$ Ph), 7.24 – 7.21 (m, 4H, $\boldsymbol{H}^{meta}$-Ph), 7.16 (t, J = 7.5 Hz, 2H, $\boldsymbol{H}^{para}$-2,6-diMePh), 7.02 (d, J = 7.3 Hz, 4H, $\boldsymbol{H}^{meta}$-2,6-

diMePh), 6.34 (s, 4H, ***H***-Ph^{bridge}), 2.37 (s, 12H, -C***H***$_3$). ^{13}C NMR (CDCl$_3$, 101 MHz) δ, ppm: 160.8 (2C), 139.3 (4C), 137.5 (2C), 131.1 (2C), 130.1 (2C), 129.7 (2C), 129.5 (2C), 129.2 (4C), 128.4 (4C), 127.9 (4C), 127.6 (2C), 96.5 (2C) 18.3 (4C). (Fig. S21-S23). MS (ESI - DCM) (m/z): 553.2 [M+H]$^+$ (100%). Elemental Analysis: *calc.* (%) for $C_{36}H_{32}N_4O_2$ $(H_2O)_2$: C 73.45, H 6.16, N 9.52; *found*: C 73.87, H 5.91, N 9.61. IR (ATR, solid sample, cm^{-1}): 3372, 3058, 3003, 2963, 2916, 2360, 1608,1597, 1566, 1494, 1473, 1447, 1408, 1350, 1313, 1294, 1131, 1067, 1027, 986, 881, 818, 791, 771, 691, 681. (Fig. S11). X- ray quality pale yellow/colourless single crystals (blocks) were formed at r. t., by diffusion of hexane into a DCM solution of the compound. Its solid-state structure is presented in Fig. S28.

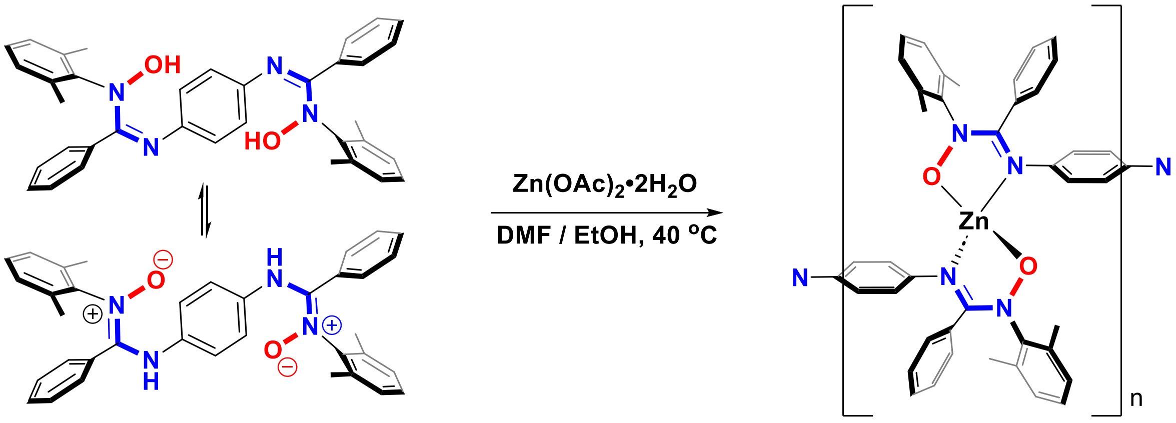


(3) **(5)**

Fig. S7. Coordination of *N*-bridged bis-AMOX ligand **(3)** with Ni(II) ions, yielding **Ni(II) bis-AMOX coordination dimer (5)**.

Ni(II) bis-AMOX coordination dimer (5). A solution of the **bis-AMOX (3)** ligand (5.5 mg, 0.01 mmol, 1 equiv.) in EtOH (5 mL) was heated for 10 min at 40 °C and added to a solution of $Ni(AcO)_2 \cdot 4H_2O$ (2.5 mg, 0.01 mmol, 1 equiv.) in EtOH (2 mL), which had also been preheated at 40 °C for 10 min. The reaction mixture was stirred at 40 °C for 1 h and then stored at 4 °C overnight. The resulting precipitate was collected by filtration and isolated as a yellow/brown solid. The product was obtained quantitatively. ^{1}H NMR (CDCl$_3$, 400 MHz) δ, ppm: 6.83 – 6.76 (m, 4H, ***H***^{para}-Ph and ***H***^{para}-2,6-diMePh), 6.71 (d, *J* = 7.8 Hz, 4H, ***H***^{meta}-2,6-diMePh) 6.66 (t, *J* = 7.7 Hz, 4H) ***H***^{meta}-Ph), 6.55 (d, *J* = 7.2 Hz, 4H, ***H***^{ortho}-Ph), 5.92 (s, 4H, ***H***-Ph^{bridge}), 2.38 (s, 12H, -C***H***$_3$). ^{13}C NMR (CDCl$_3$, 101 MHz) δ, ppm: 157.1 (2C), 140.2 (4C), 138.9 (2C), 136.9 (4C), 130.2 (2C), 128.4 (4C), 128.1 (6C), 127.6 (4C), 127.3 (4C), 18.4 (4C). (Fig. S24-S26). MS (ESI – DCM/EtOH) (m/z): 1243.3 [M+Na]$^+$ (100%). Elemental Analysis: *calc.* (%) for $C_{72}H_{64}N_8Ni_2O_4$ $(CH_3CH_2OH)(H_2O)_3$: C 67.19, H 5.79, N 8.47; *found*: C 67.05, H 5.41, N 8.24.

IR (ATR, solid sample, cm^{-1}): 3061, 3027, 2955, 2922, 2854, 1582, 1542, 1505, 1471, 1441, 1405, 1377, 1304, 1258, 1205, 1166, 1145, 1097, 1075, 1017, 979, 966, 919, 856, 819, 794, 774, 756, 725, 716, 697, 664, 650, 622, 559. (Fig. S12). X-ray quality yellow/brown crystals were obtained from aqueous EtOH at 4 ºC. The solid-state structure of **5** is presented in Figure 2 (article) and Fig. S29.



(3) **(6)**

Fig. S8. Coordination of *N*-bridged bis-AMOX ligand **(3)** with Zn(II) ions, yielding **Zn(II) bis-AMOX coordination polymer (6)**.

Zn(II) bis-AMOX coordination polymer (6). The synthesis of this compound was adapted from a previously reported protocol for the preparation of metallomacrocyclic complexes.[8] A solution of the **bis-AMOX (3)** ligand (55 mg, 0.1 mmol, 1 equiv.) in DMF (5 mL) and EtOH (2 mL) was added over 30 min (syringe pump) at 40 °C to a solution of $Zn(AcO)_2·2H_2O$ (22 mg, 0.1 mmol, 1 equiv.) in DMF (2 mL), which was had been preheated at 40 °C for 10 min. The reaction mixture was maintained at 40 °C for an additional 30 min and left at r.t. overnight. The resulting precipitate was collected by filtration and isolated as a yellow solid (42 mg obtained after drying under vacuum). The compound is very poorly soluble in common solvents, and NMR characterization was hindered by its low solubility. IR (ATR, solid sample, cm^{-1}): 3383, 3029, 2921, 1603, 1583, 1511, 1442, 1376, 1256, 1209, 1166, 1149, 1099, 1015, 961, 917, 838, 770, 745, 698, 596. (Fig. S13). Very poor quality single crystals (very fine yellow needles) were obtained by slow evaporation of a hot toluene solution of the compound. The solid-state structure of **6** is presented in Figure 3 (article) and Fig. S30. T_d (TGA, 5% weight loss): 320 °C (Fig. S32).

4. IR Spectra

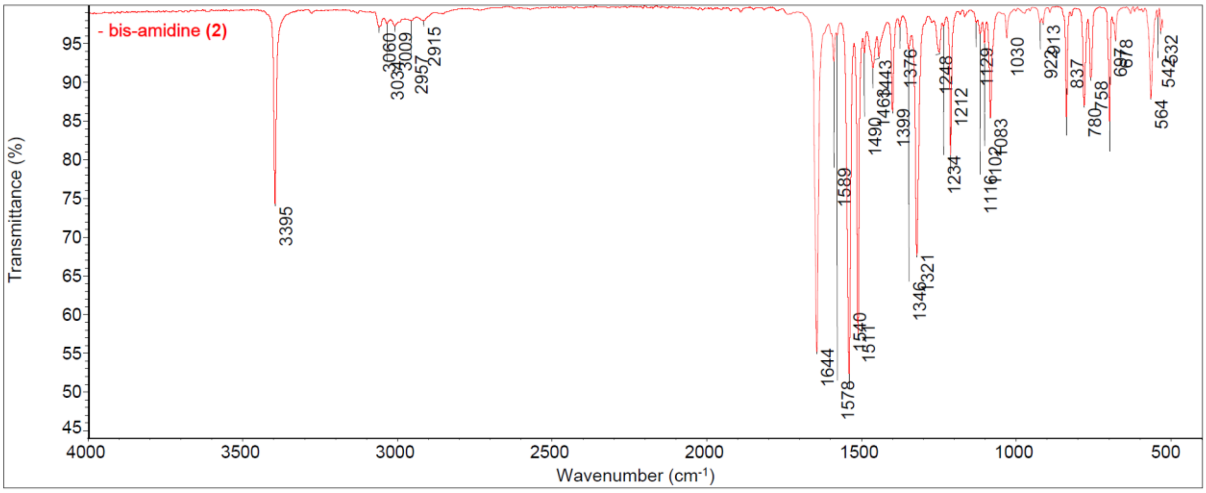


Fig. S9. IR spectrum of **bis-amidine (2)**.

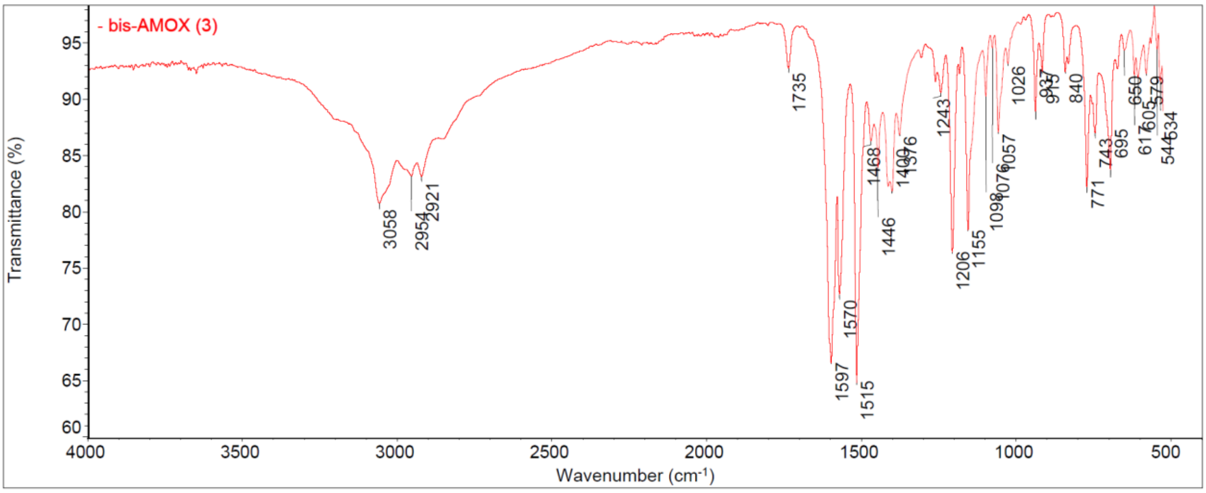


Fig. S10. IR spectrum of **bis-AMOX (3)**.

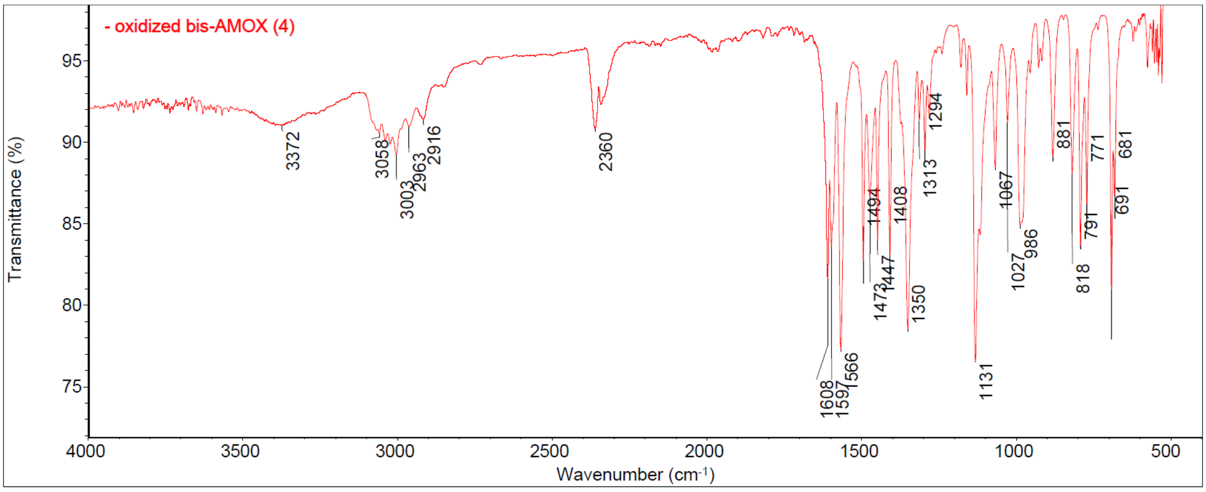


Fig. S11. IR spectrum of **oxidized bis-AMOX (4)**.

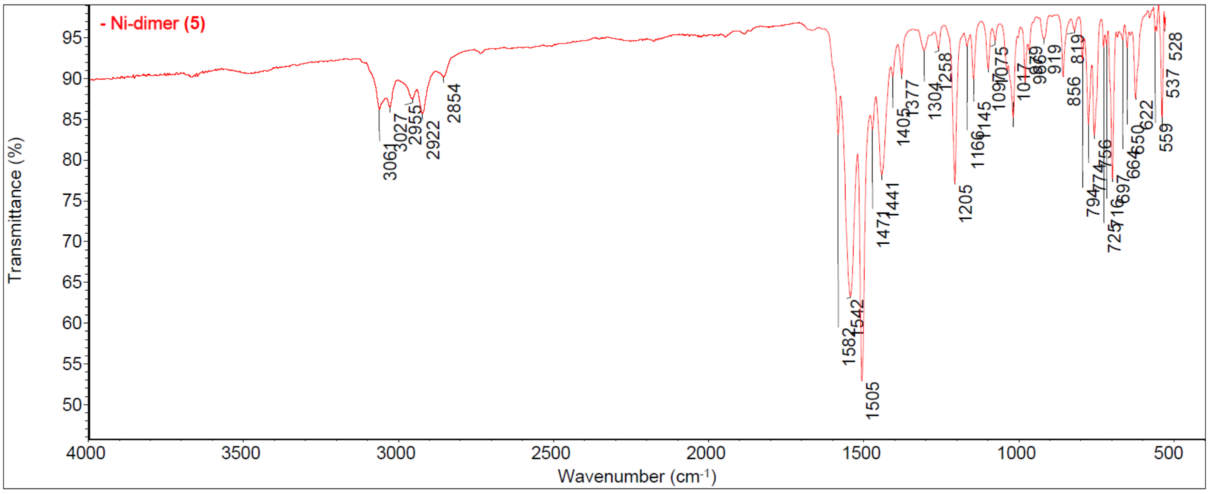


Fig. S12. IR spectrum of **Ni(II) bis-AMOX coordination dimer (5)**.

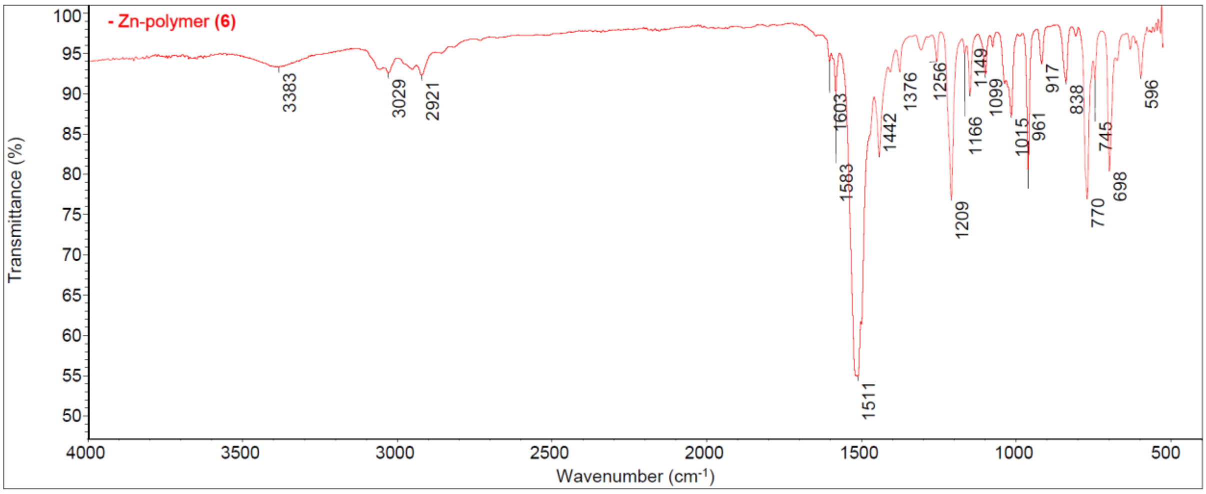


Fig. S13. IR spectrum of **Zn(II) bis-AMOX coordination polymer (6)**.

5. NMR Spectra

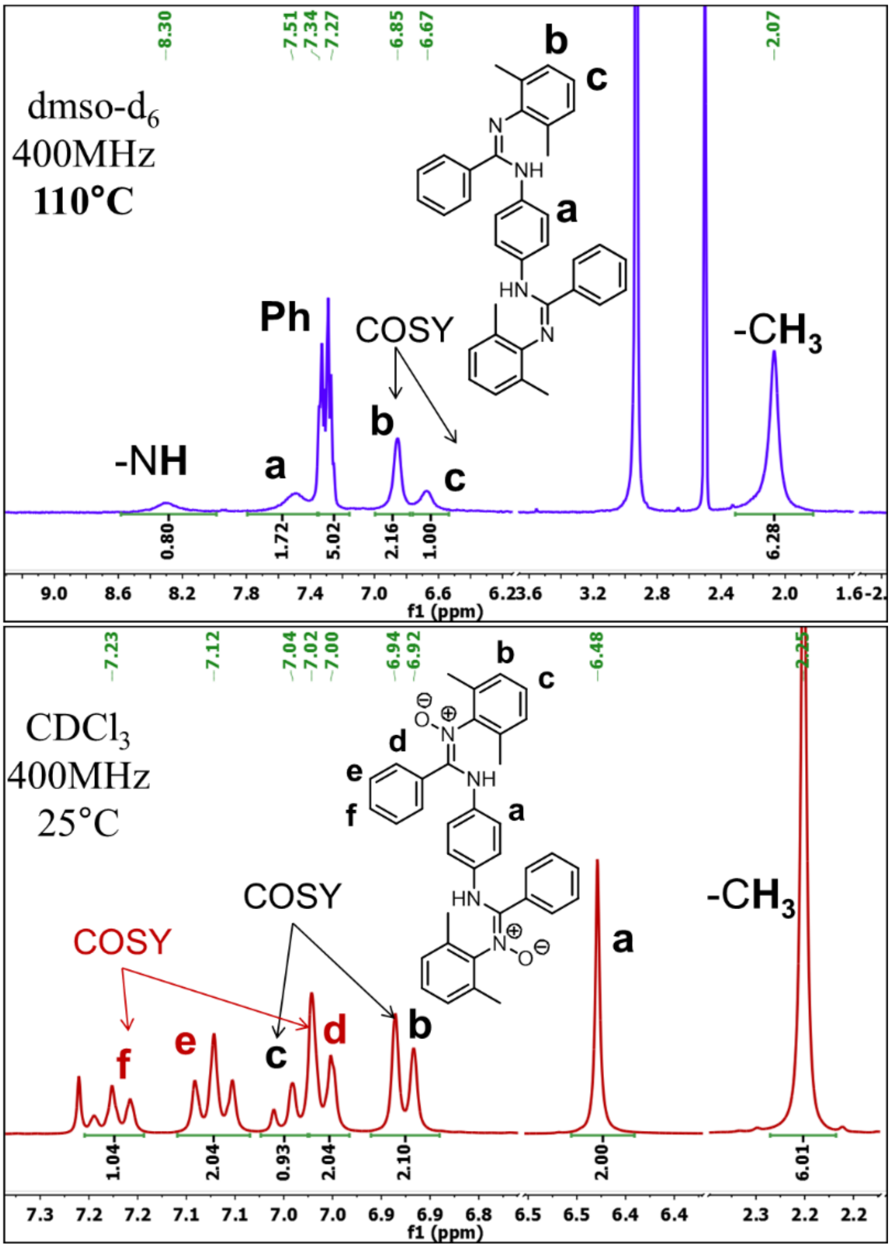


Fig. S14. ^{1}H NMR spectrum (400 MHz) of **bis-amidine (2)** in DMSO-d_6 at 110 °C (top) and **bis-AMOX (3)** in $CDCl_3$ at 25 °C (bottom) with proton resonance assignments.

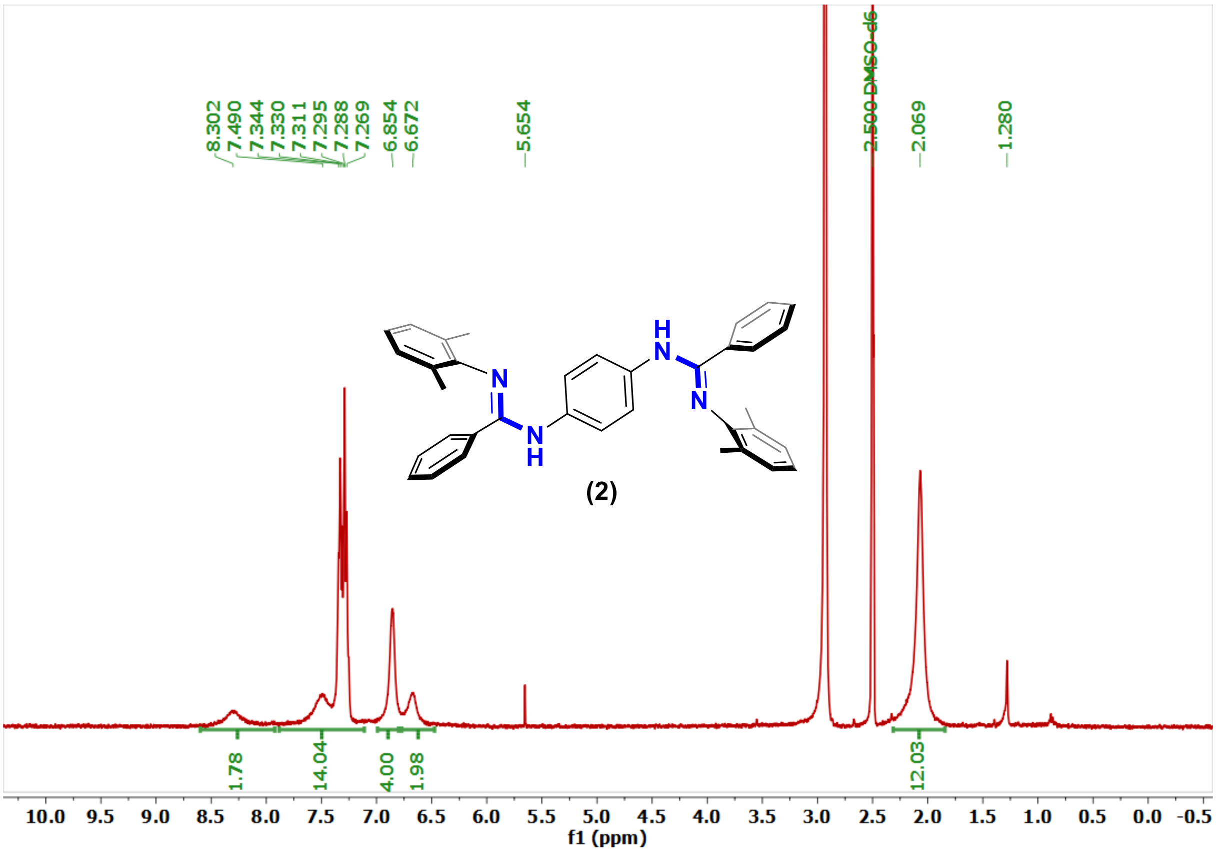


Fig. S15. ^{1}H NMR spectrum (400 MHz) of **bis-amidine (2)** in DMSO-d_6 at 110 °C.

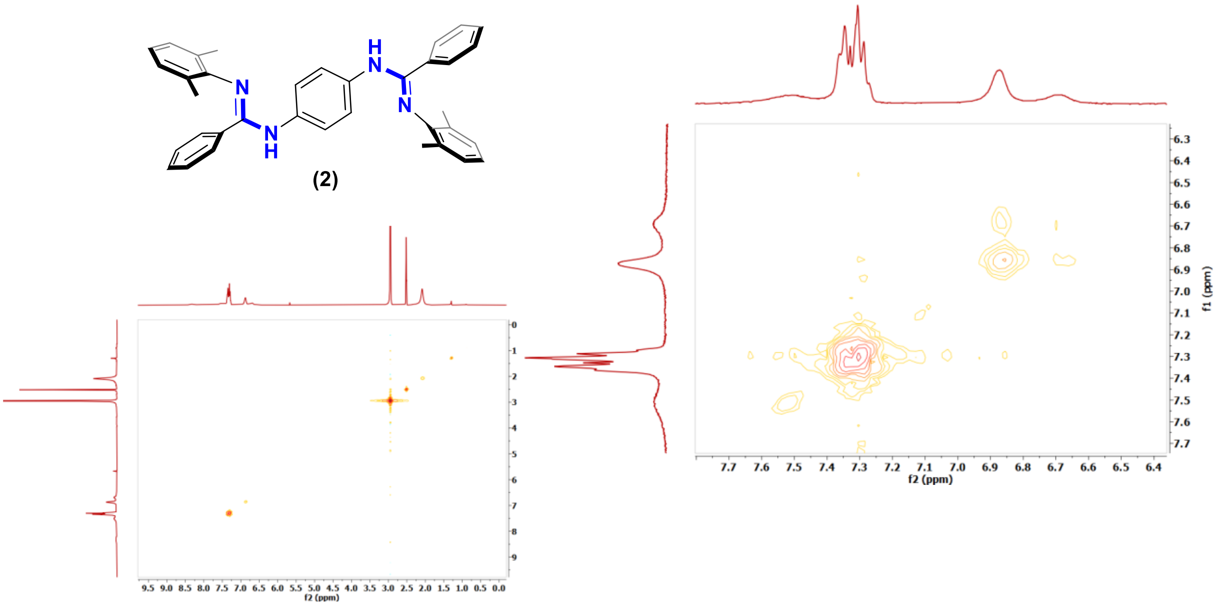


Fig. S16. COSY NMR spectrum (400 MHz) of **bis-amidine (2)** in DMSO-d_6 at 110 °C.

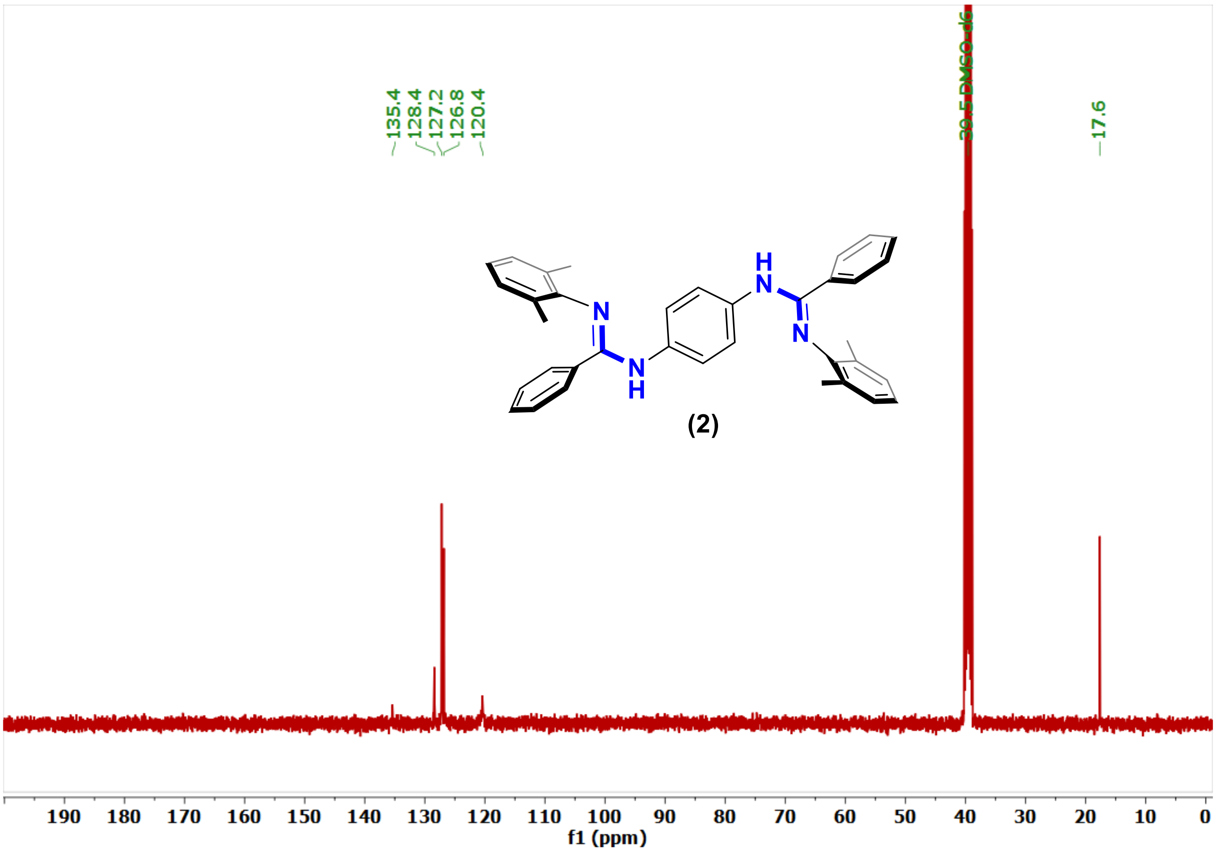


Fig. S17. ^{13}C NMR spectrum (101 MHz) of **bis-amidine (2)** in DMSO-d_6 at 110 °C.

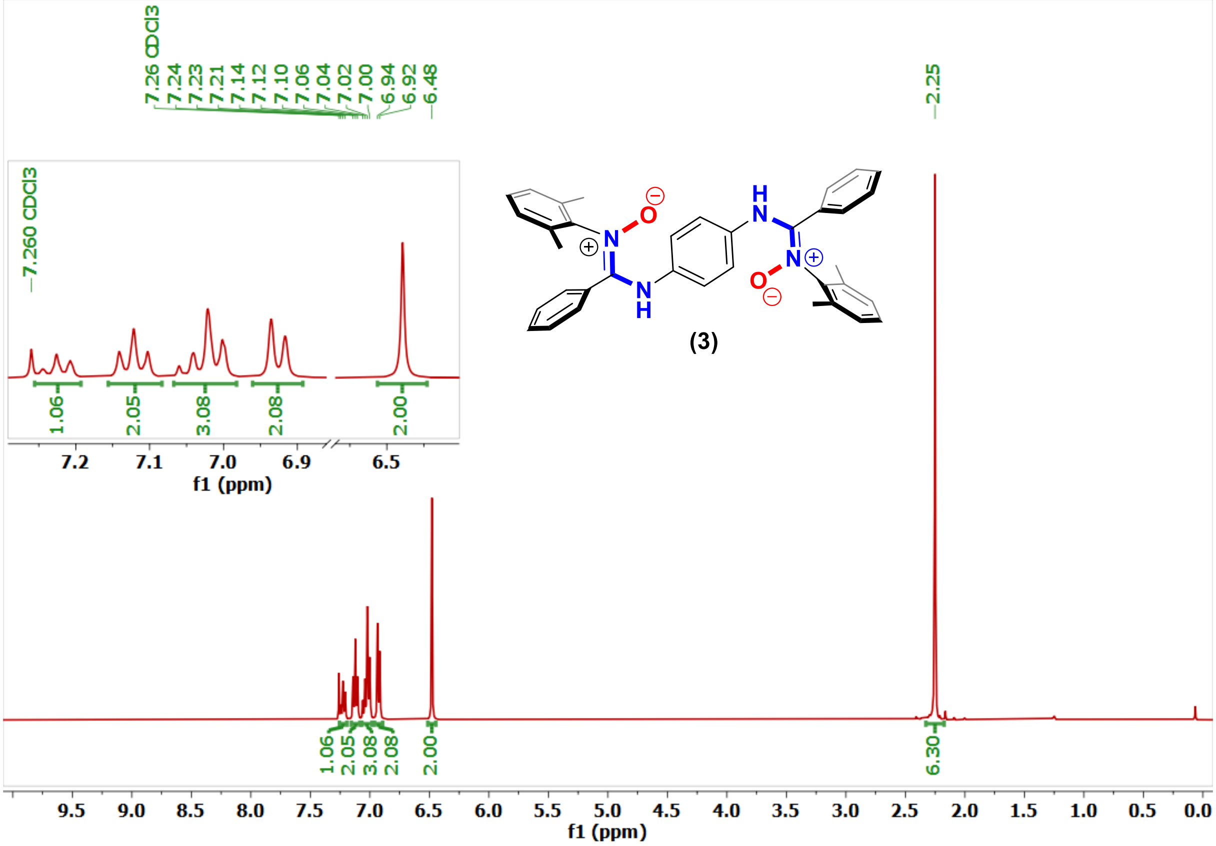


Fig. S18. ^{1}H NMR spectrum (400 MHz) of **bis-AMOX (3)** in $CDCl_3$ at 25 °C.

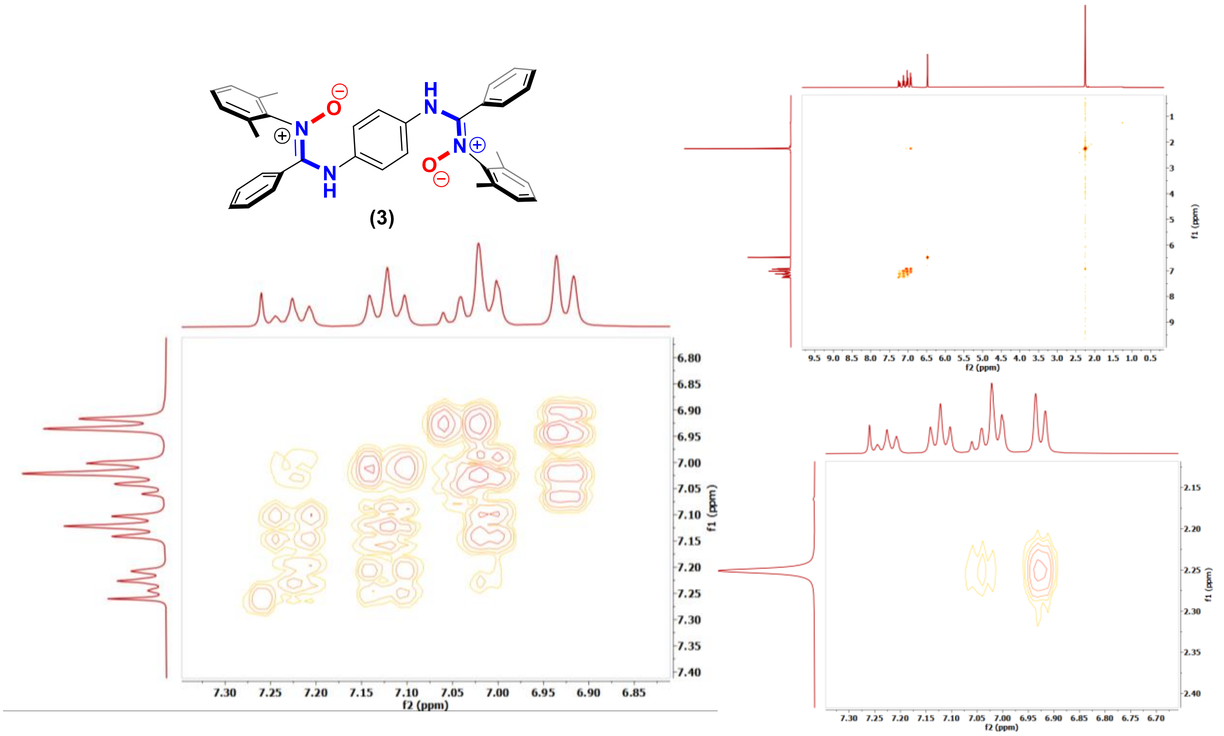


Fig. S19. COSY NMR spectrum (400 MHz) of **bis-AMOX (3)** in $CDCl_3$ at 25 °C.

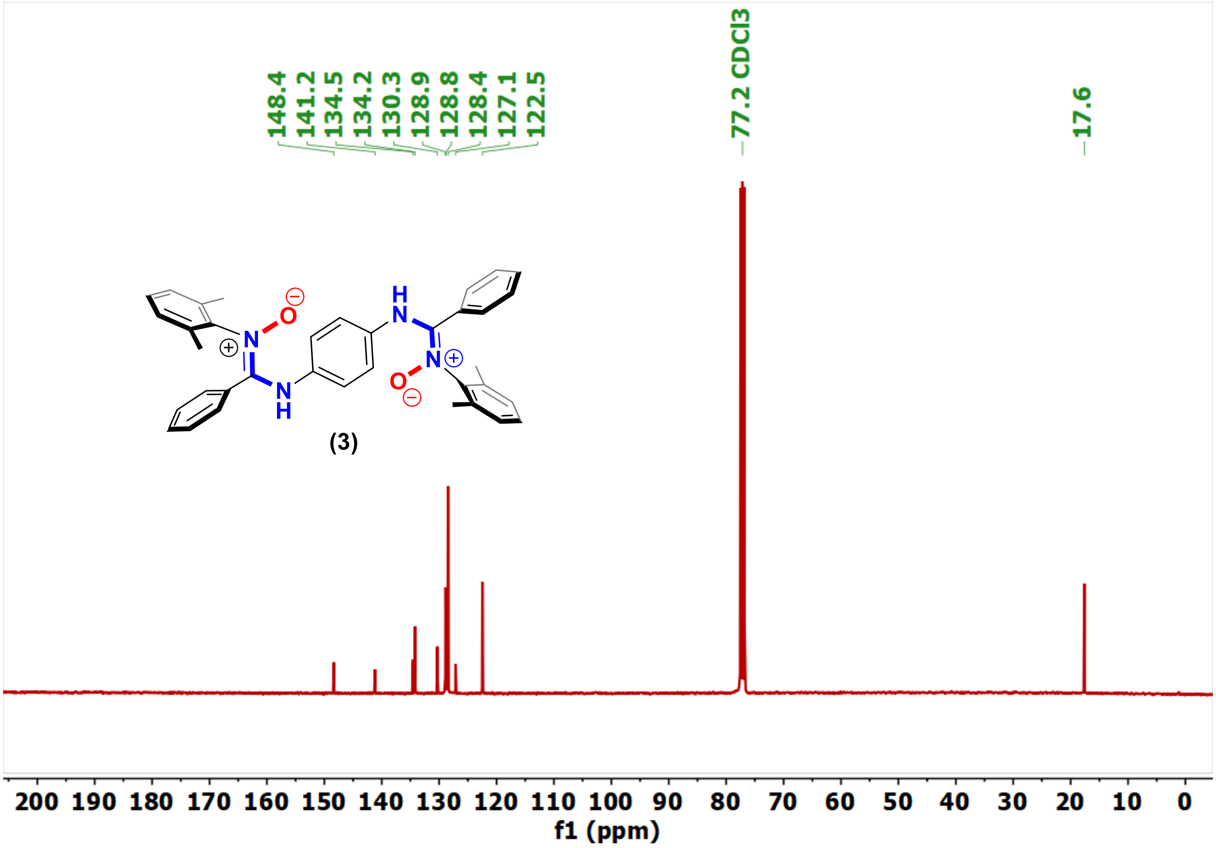


Fig. S20. ^{13}C NMR spectrum (101 MHz) of **bis-AMOX (3)** in $CDCl_3$ at 25 °C.

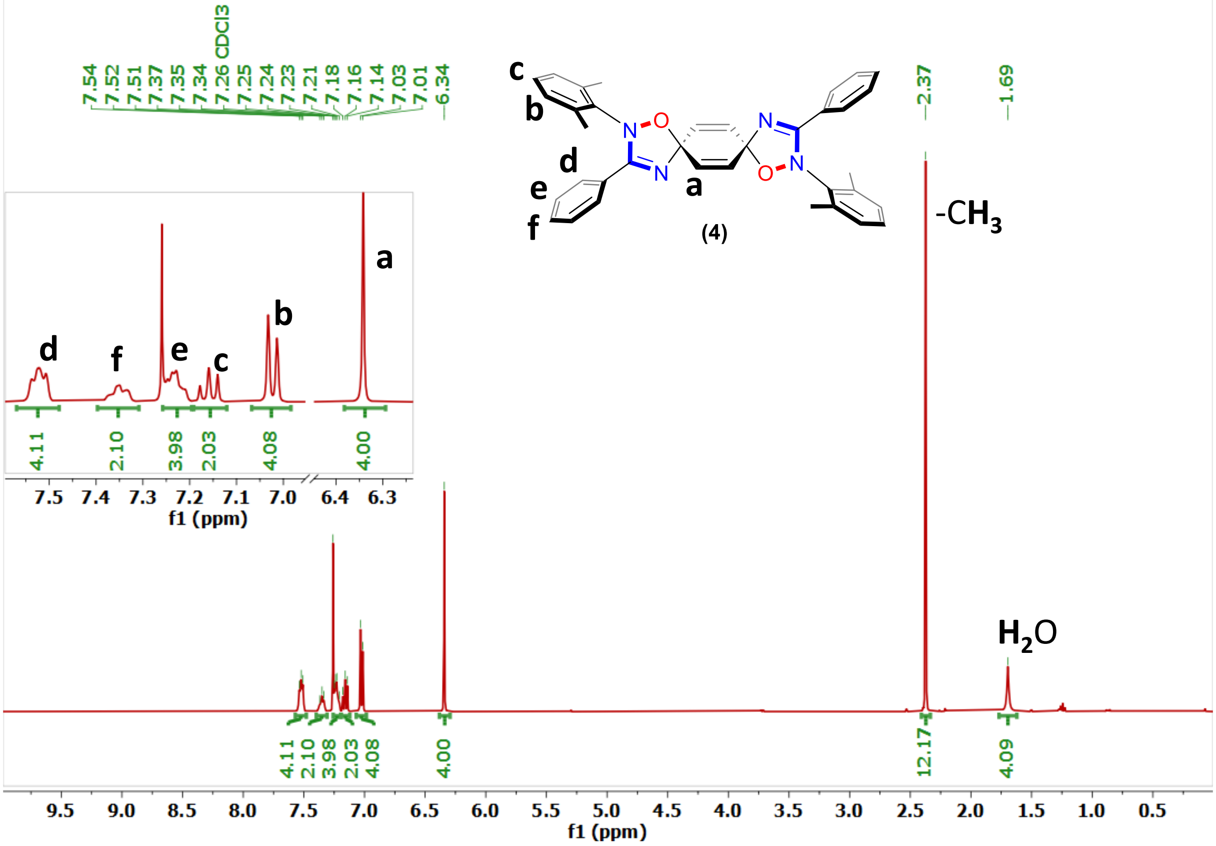


Fig. S21. ^{1}H NMR spectrum (400 MHz) of **oxidized bis-AMOX (4)** in $CDCl_3$ at 25 °C with proton resonances assignment. The presence of signals corresponding to water proton resonances at 1.69 ppm and the value of their integration (4H) confirm the results obtained by C/H/N elemental analysis indicating the formula **4**·$2H_2O$.

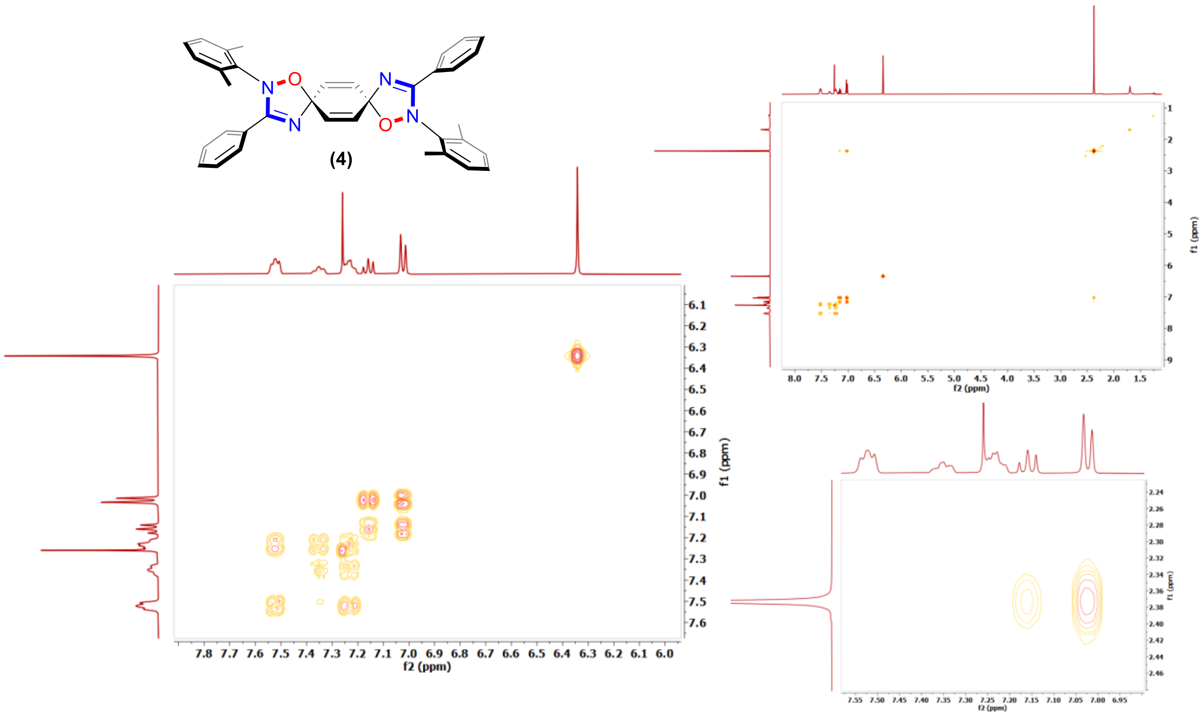


Fig. S22. COSY NMR spectrum (400 MHz) of **oxidized bis-AMOX (4)** in $CDCl_3$ at 25 °C.

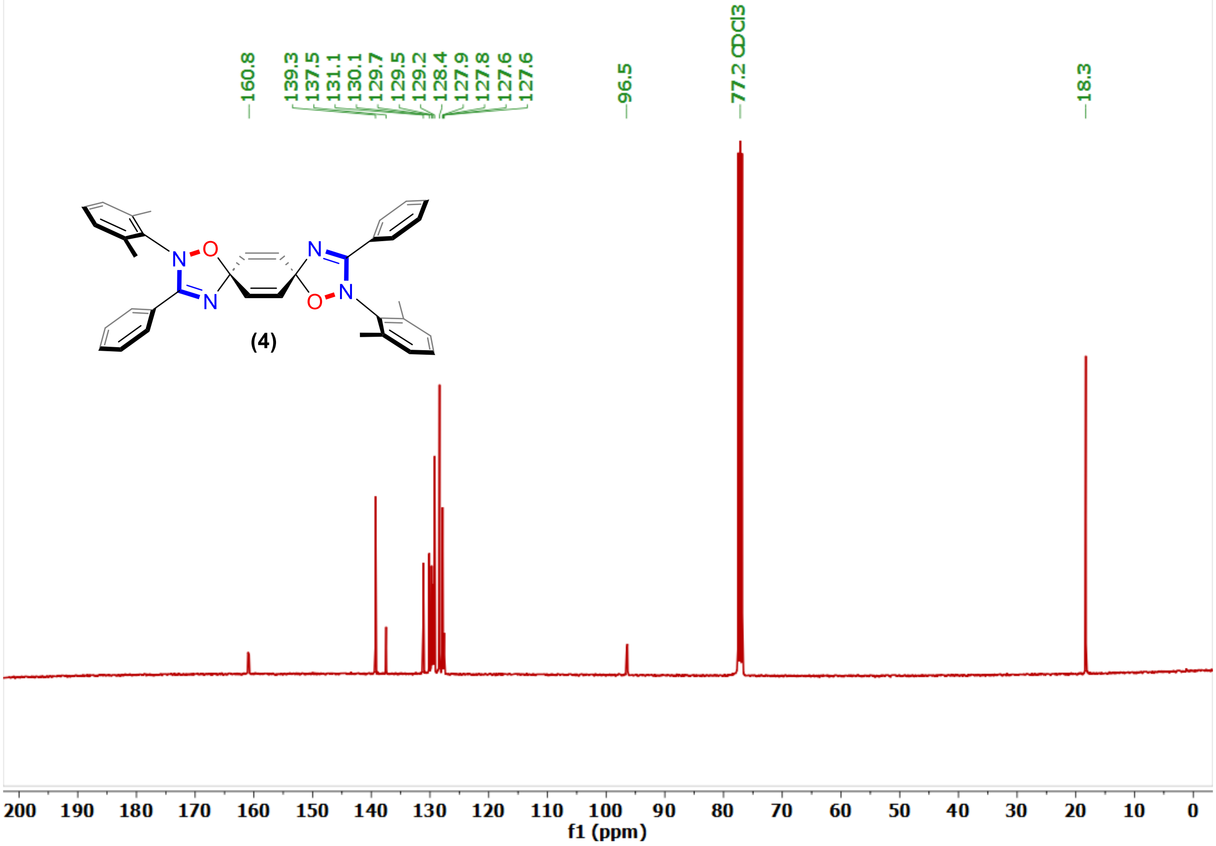


Fig. S23. ^{13}C NMR spectrum (101 MHz) of **oxidized bis-AMOX (4)** in CDCl$_3$ at 25 °C.

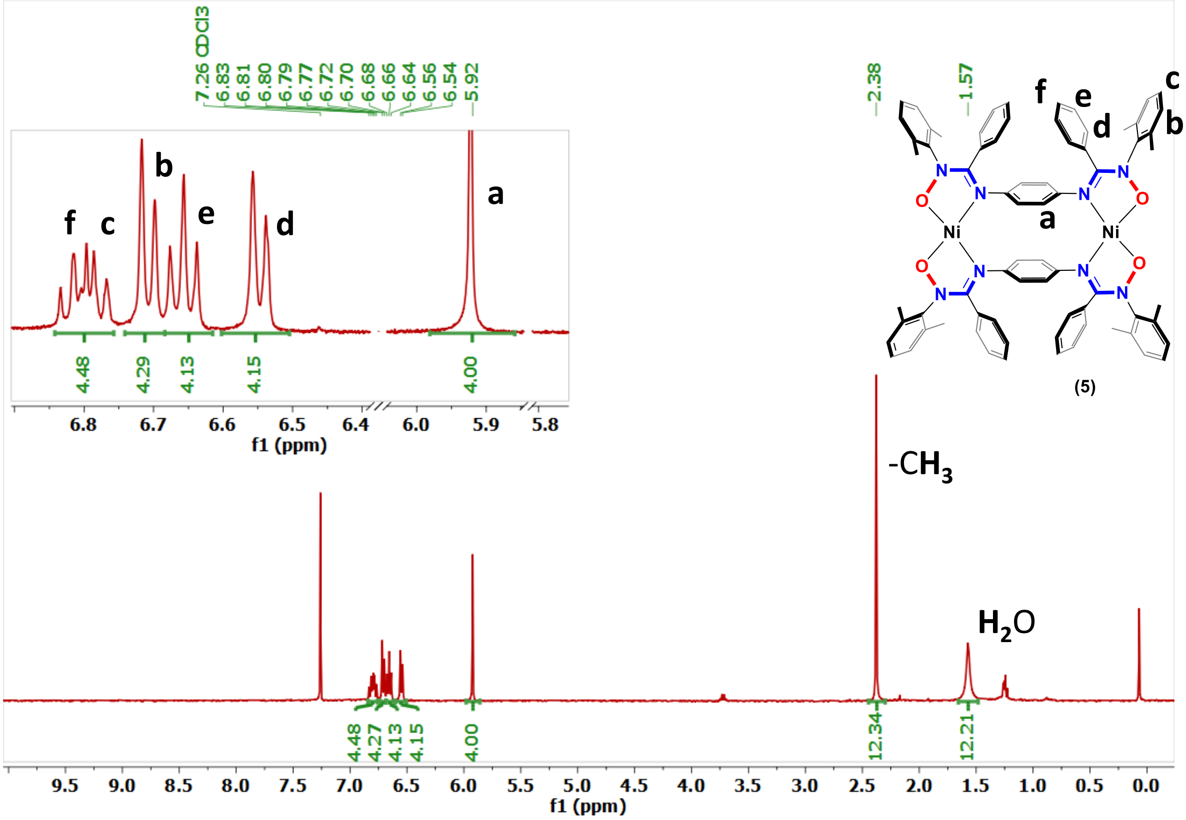


Fig. S24. ^{1}H NMR spectrum (400 MHz) of **Ni(II) bis-AMOX coordination dimer (5)** in CDCl$_3$ at 25 °C with proton resonances assignment.

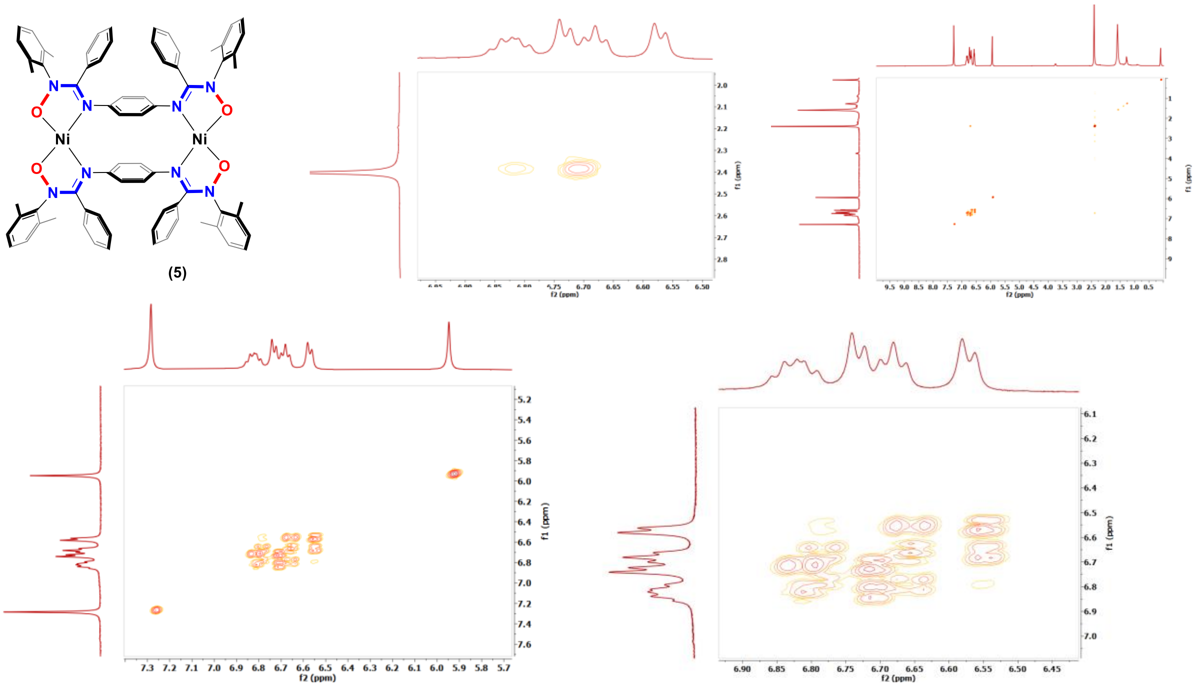


Fig. S25. COSY NMR spectrum (400 MHz) of **Ni(II) bis-AMOX coordination dimer (5)** in $CDCl_3$ at 25 °C.

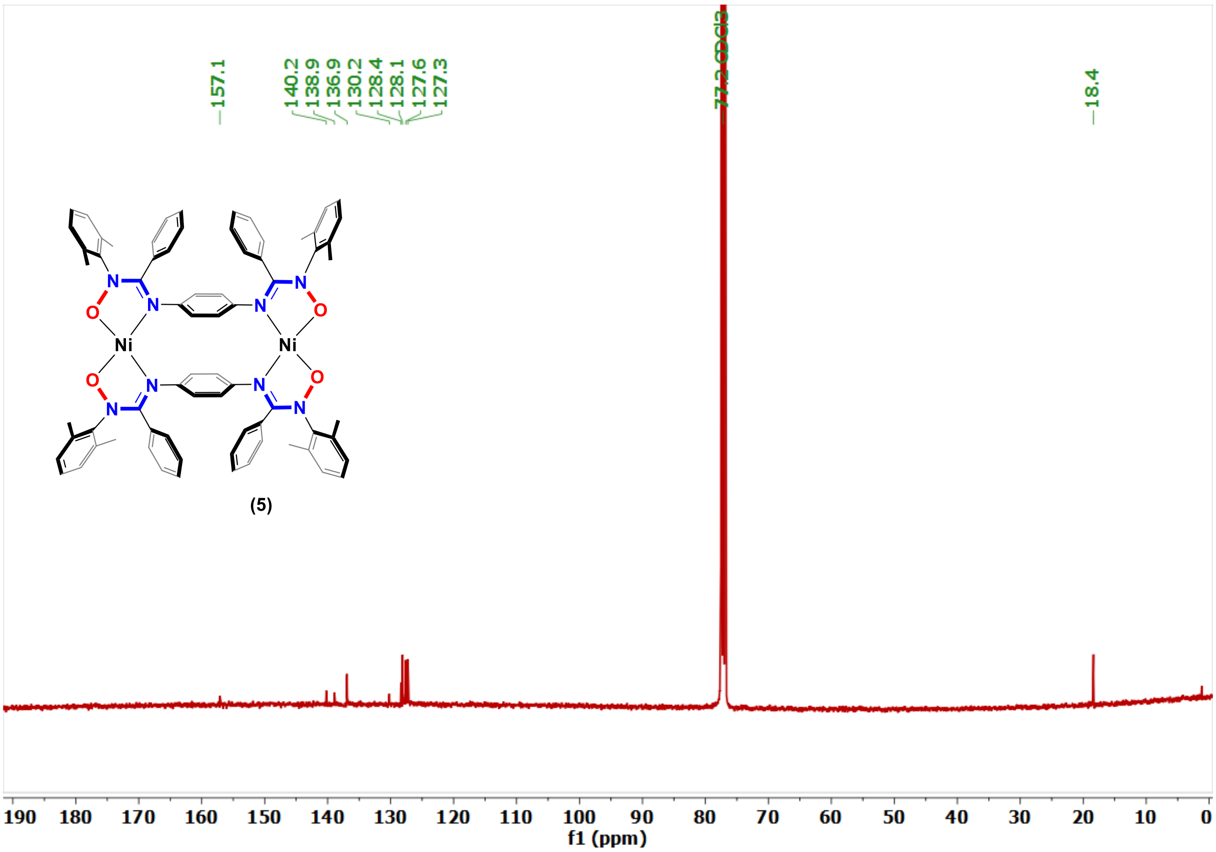


Fig. S26. ^{13}C NMR spectrum (101 MHz) of **Ni(II) bis-AMOX coordination dimer (5)** in $CDCl_3$ at 25 °C.

6. X-ray Diffraction Measurements and the Solid State Structure Determination

Crystallographic data for **3** and **4** were collected at 150 K from single crystals mounted on a loop fiber. Data were collected using a Bruker Microstar diffractometer equipped with a Platinum 135 CCD Detector, a Helios optics and a Kappa goniometer. The crystal-to-detector distance was 3.8 cm, and the data collection was carried out in 512 x 512 pixel mode. The initial unit cell parameters were determined by a least-squares fit of the angular setting of strong reflections, collected by a 110.0 degree scan in 110 frames over three different parts of the reciprocal space. Crystallographic data for **5** were collected at 100 K, using a Bruker Venture diffractometer equipped with a Photon 100 CMOS Detector, a Helios MX optics and a Kappa goniometer. The crystal-to-detector distance was 4.0 cm, and the data collection was carried out in 1024 x 1024 pixel mode. Crystallographic data for **6** were collected at 100 K, using a Bruker smart diffractometer equipped with an APEX II CCD Detector, an Incoatec IMuS source and a Quazar MX mirror. The crystal-to-detector distance was 4.0 cm, and the data collection was carried out in 512 x 512 pixel mode. The initial unit cell parameters were determined by a least-squares fit of the angular setting of strong reflections, collected by a 180.0 degree scan in 180 frames over three different parts of the reciprocal space. For data collection, determination of cell parameters, cell refinement, and data reduction, *APEX2* and *SAINT* (Bruker, 2009 and Bruker, 2013) were used.[9] Absorption corrections were applied using *SADABS* (Bruker 2014).[10] Employing *OLEX2* (Dolomanov *et al.*, 2009),[11] the structure solutions were performed using direct methods with *SHELXS97* ot *SHELXT* Intrinsic Phasing (Sheldrick, 2008; Sheldrick, 2015)[12] and refined on F^2 by full-matrix least squares using *SHELXL2014* (Sheldrick, 2008; Sheldrick, 2015).[12] *OLEX2* (Dolomanov *et al.*, 2009),[11] *ORTEP-3 for Windows* (Farrugia, 2012),[13] Mercury,[14] and POV-ray (2013)[15] were used for molecular graphics. The material was prepared for publication using *PLATON* (Spek, 2009),[16] Mercury,[14] and *publCIF* (Westrip, 2010).[17]

For all the structures presented herein, unless otherwise stated, all non-H atoms were refined by full-matrix least-squares with anisotropic displacement parameters. The H-atoms were included in calculated positions and treated as riding atoms: aromatic C–H 0.95 Å, methyl C–H 0.98 Å, with $U_{iso}(H) = k \times U_{eq}$ (parent C-atom), where k = 1.2 for the aromatic H-atoms and 1.5 for the methyl H-atoms. Unless mentioned differently, all the H-atoms connected to heteroatoms (N and O atoms) were located from the difference Fourier map and they were freely refined.

Crystal data and structure refinement details for compounds **3**, **4**, **5**, and **6** are summarized in Table S1. Their solid-state structures are illustrated in Figures 2 and 3 (article) and Fig. S27-S30. Crystallographic data for **3**, **4**, **5**, and **6** were deposited in CCDC.[18] The corresponding CCDC numbers are given in Table S1. Validation of the crystallographic information files (cifs) with the checkCIF/ PLATON routine was performed, returning only level C and G alerts. The comments to these alerts are included in the CIFs of the corresponding compounds.

Bis-AMOX (3). X-ray quality yellow crystals (plates) were obtained by slow diffusion of hexane into a DCM solution of the compound at r. t. A large K value in the Analysis of Variance is obtained for this structure (2.71). However, the place for the high values of K is in the lowest-intensity bin in the table. Therefore, large K value is most probably due to overestimated F_o, as most of area detector integration programs are slightly underestimating the background.

Oxidized bis-AMOX (4). X-ray quality pale yellow/colourless single crystals (blocks) of **4** were formed at r. t., by diffusion of hexane into a DCM solution of the compound. There aren't any specific comments regarding the resolution and the refinement of this structure.

Ni(II) bis-AMOX coordination dimer (5). X-ray quality yellow/brown single crystals (needles) of **5** were formed in aqueous EtOH, at 4 ºC. Its solid-state structure contains co-crystallized EtOH molecules (2.5 ethanol molecules for one molecule of compound). PART -1 instruction was used to model the solvent molecules disordered over a symmetry element and AFIX 83 was used for calculating the position of H-atom part of the -OH group in the disordered co-crystalized EtOH. The H-atoms connected to the N atoms and those part of the -OH group in EtOH molecules which don't present disorder were located from the difference Fourier map and they were freely refined. SADI/ SIMU were also employed in modelling the disordered atoms. The weight second parameter is unusually large for **5** (16.56), which can indicate twinning. No twin law was detected with TwinRotMat routine from *PLATON* (Spek, 2009),[16] nor was identified upon inspection of the diffraction pattern in *RLATT* (Bruker, 2013)[9] or upon checking for non-merohedral twinning using *CELL_NOW* (Bruker 2014).[10]

Zn(II) bis-AMOX coordination polymer (6). Single crystals (very fine yellow needles) were formed by slow evaporation of a hot toluene solution of **6**. Its solid-state structure was obtained from the best available crystal, which unfortunately was poor quality, resulting in mediocre overall quality of the data set. Co-crystallized disordered solvent molecules (toluene) are also present in the structure. They were modeled using DFIX/ DANG/ FLAT/ SADI/ DELU/ SIMU/ RIGU instructions. The weight first parameter is unusually large for **6** (0.15), which can indicate twinning. No twin law was detected with TwinRotMat routine from *PLATON* (Spek, 2009),[16] nor was identified upon inspection of the diffraction pattern in *RLATT* (Bruker, 2013)[9] or upon checking for non-merohedral twinning using *CELL_NOW* (Bruker 2014).[10]

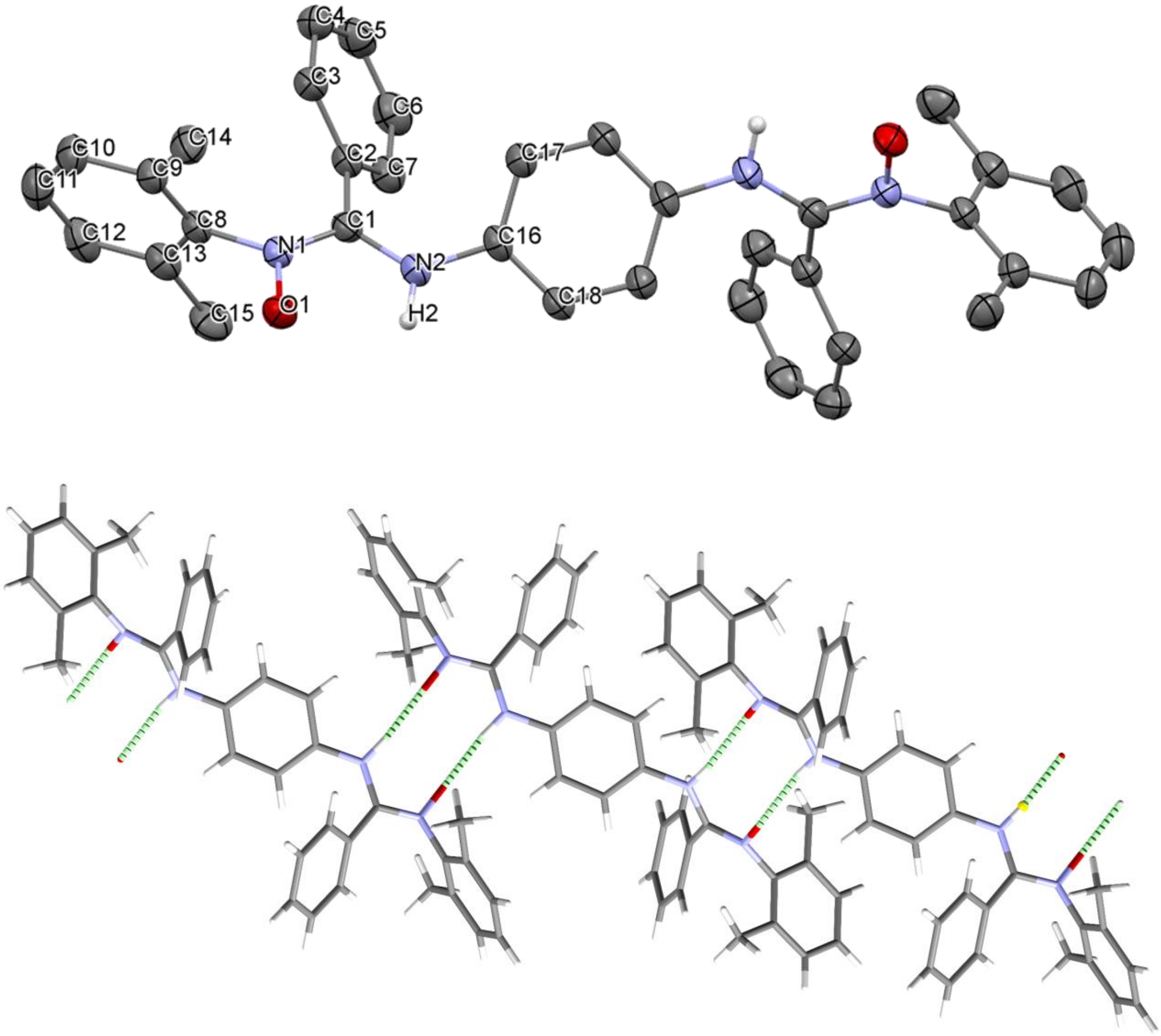


Fig. S27. The solid-state structure of **bis-AMOX (3)**: ORTEP view (ellipsoids at 50% probability level) with labelled atoms (symmetry code: 3/2-x, +y, 3/2-z) – C–*H* atoms were removed for clarity (top); H-bonding pattern (bottom) – cyclic dimers *via* N-H···O (*d* = 1.90(3) Å) bonds.

Table S1. Crystal data and structure refinement details for compounds **bis-AMOX (3)**, **oxidized bis-AMOX (4)**, **Ni(II) bis-AMOX coordination dimer (5)**, and **Zn(II) bis-AMOX coordination polymer (6)**

Compound	**3**	**4**	**5**	**6**
CCDC no.	2322646	2322647	2322741	2322755
Empirical formula	$C_{36}H_{34}N_4O_2$	$C_{36}H_{32}N_4O_2$	$C_{72}H_{64}N_8Ni_2O_4$ • 2.5(CH_3CH_2O)	$C_{36}H_{32}N_4O_2Zn$ • 2(CH_3CH_2O)
Formula weight	554.67	552.65	1337.90	802.29
Temperature/K	100	150	105	100
Crystal system	Monoclinic	Monoclinic	Trigonal	Monoclinic
Space group	P2/n	$P2_1/n$	R-3	$P2_1/n$
a/Å	13.9746(11)	15.1954(10)	38.0510(13)	9.5906(6)
b/Å	6.6772(6)	6.3722(4)	38.0510(13)	22.2020(11)
c/Å	17.1658(14)	15.5411(10)	12.1896(5)	20.2657(12)
α/°	90	90	90	90
β/°	108.555(3)	101.589(3)	90	99.741(4)
γ/°	90	90	120	90
Volume/Å^3	1518.5(2)	1474.14(16)	15284.5(12)	4253.0(4)
Z	2	2	9	4
ρ_{calc}g/cm^3	1.213	1.245	1.308	1.253
μ/mm^{-1}	0.600	0.618	3.409	1.140
F(000)	588.0	584.0	6345.0	1688
Crystal size/mm^3	0.130 × 0.104 × 0.026	0.18 × 0.08 × 0.08	0.12 × 0.06 × 0.04	0.210 x 0.042 x 0.021
Radiation	CuKα (λ = 1.54178)	CuKα (λ = 1.54178)	GaKα (λ = 1.34139)	CuKα (λ = 1.54178)
2θ range for data collection/°	7.138 to 139.554	7.424 to 139.478	6.726 to 121.426	5.952 to 142.516
Index ranges	$-16 \leq h \leq 16$, $-7 \leq k \leq 8$, $-20 \leq l \leq 20$	$-18 \leq h \leq 15$, $-7 \leq k \leq 7$, $-18 \leq l \leq 18$	$-49 \leq h \leq 48$, $-49 \leq k \leq 48$, $-15 \leq l \leq 15$	$-11 \leq h \leq 10$, $-26 \leq k \leq 27$, $-24 \leq l \leq 24$
Reflections collected	62523	31255	97569	56416
Independent reflections	2867 [R_{int} = 0.0574, R_{sigma} = 0.0185]	2771 [R_{int} = 0.0482, R_{sigma} = 0.0240]	7814 [R_{int} = 0.1004, R_{sigma} = 0.0496]	8189 [R_{int} = 0.1054, R_{sigma} = 0.0656]
Data/restraints/parameters	2867/0/196	2771/0/192	7814/14/449	8189 / 165 / 520
Goodness-of-fit on F^2	1.071	1.044	1.023	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0547, wR_2 = 0.1588	R_1 = 0.0360, wR_2 = 0.0992	R_1 = 0.0387, wR_2 = 0.0899	R_1 = 0.0742, wR_2 = 0.1925
Final R indexes [all data]	R_1 = 0.0581, wR_2 = 0.1627	R_1 = 0.0384, wR_2 = 0.1018	R_1 = 0.0602, wR_2 = 0.0995	R_1 = 0.1143, wR_2 = 0.2256
Largest diff. peak/hole / e Å^{-3}	0.44/-0.21	0.19/-0.17	0.36/-0.22	1.17/-1.23

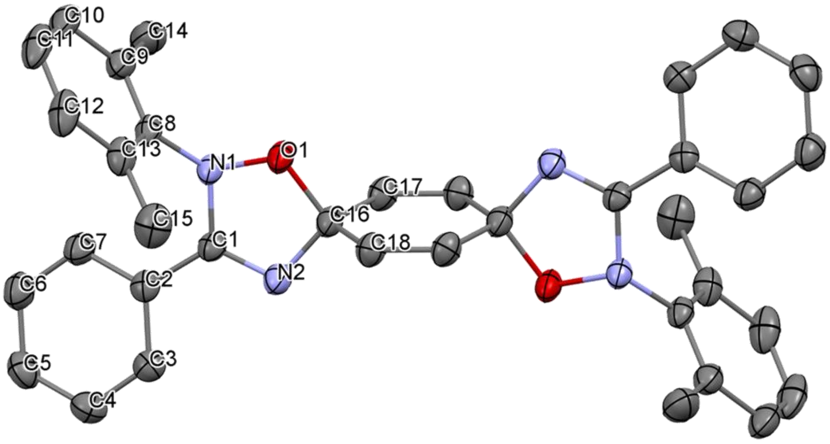


Fig. S28. The solid-state structure of **oxidized bis-AMOX (4)**: ORTEP view (ellipsoids at 50% probability level) with labelled atoms (symmetry code: -x,-y,-z). Hydrogen atoms were removed for clarity.

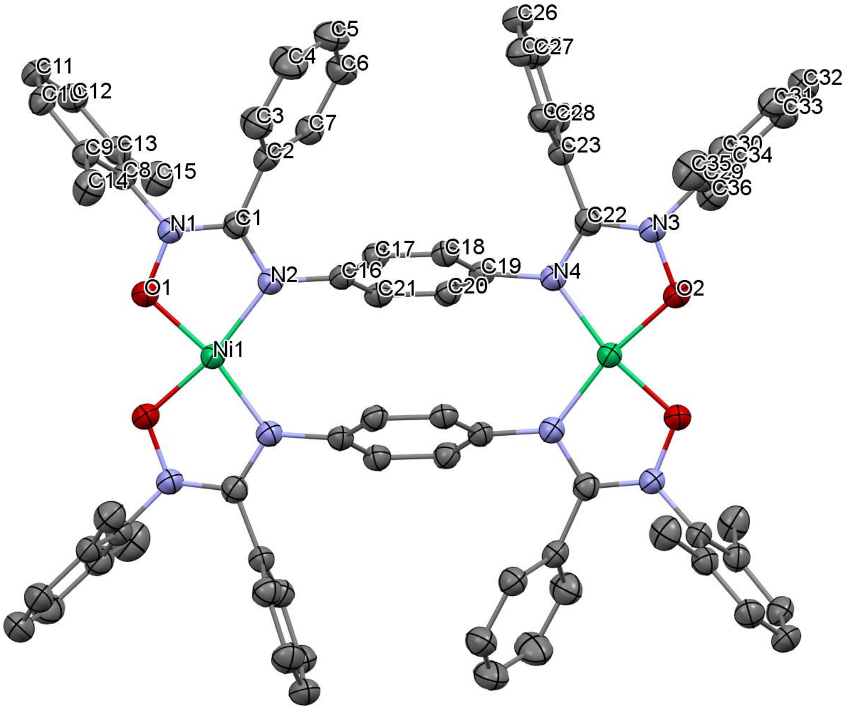


Fig. S29. The solid-state structure of **Ni(II) bis-AMOX coordination dimer (5)**: ORTEP view (ellipsoids at 50% probability level) with labelled atoms (symmetry code: 1-x, 1-y, 1-z). Hydrogen atoms and co-crystallized solvent were removed for clarity.

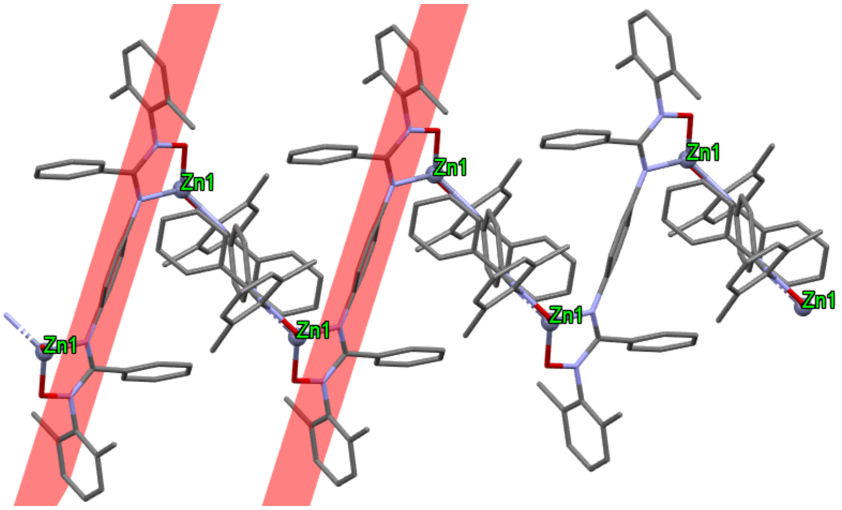
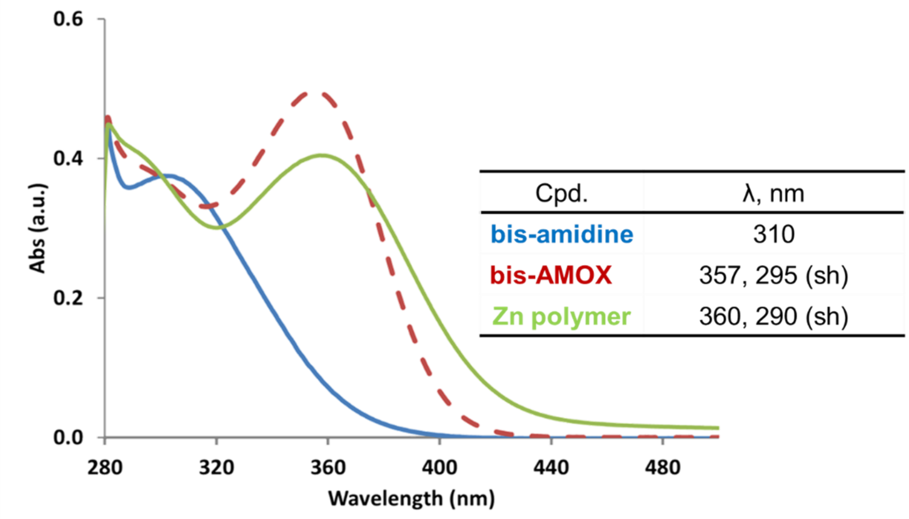


Fig. S30. The solid-state structure of **Zn(II) bis-AMOX coordination polymer (6)**: wireframe view. Hydrogen atoms and co-crystallized solvent were removed for clarity.

7. Electronic Spectra



Cpd.	λ, nm
bis-amidine	310
bis-AMOX	357, 295 (sh)
Zn polymer	360, 290 (sh)

Fig. S31. Electronic spectra of the **Zn(II) metallopolymer (6)** (green), the *N*-bridged **bis-AMOX** ligand **(3)** (red), and the *N*-bridged **bis-amidine** precursor **(2)** (blue) (in toluene at r. t.).

8. Thermogravimetric Analysis

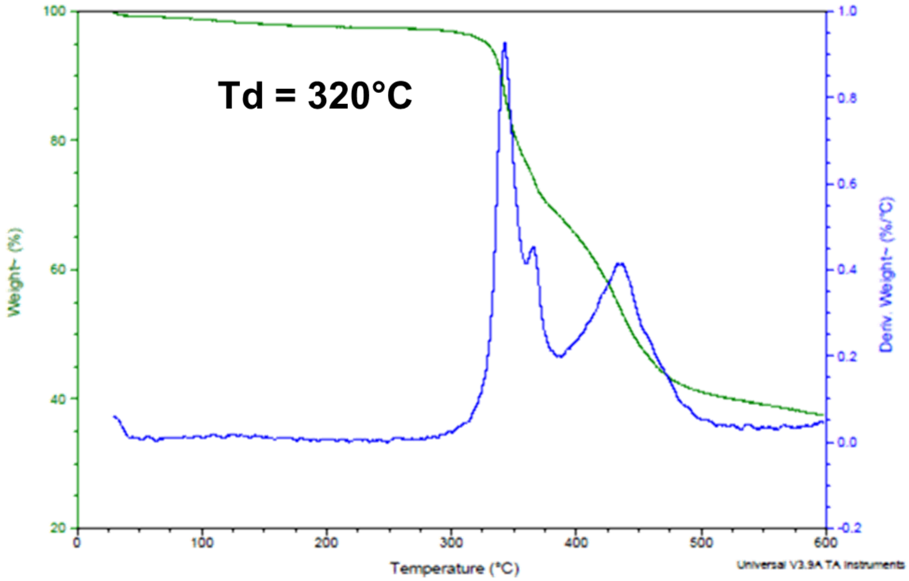


Fig. S32. TGA profile for the **Zn(II) metallopolymer (6)** (T_d calculated at 5% weight loss).

9. Atomic Coordinates Tables for DFT Optimized Structures

Table S2. Atomic coordinates for DFT optimization of **dimer** structure (theory level: B3LYP/ 6,31-g(d,p), gas phase)

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.421624   -1.832448    0.555619
      2          6           0       -0.693380   -2.622227   -0.350251
      3          6           0        0.693411   -2.622250   -0.350194
      4          6           0        1.421602   -1.832500    0.555744
      5          6           0        0.697107   -1.065987    1.480742
      6          6           0       -0.697189   -1.065960    1.480681
      7          7           0       -2.827139   -1.698953    0.449111
      8          7           0        2.827138   -1.699031    0.449399
      9          6           0        3.595252   -2.749374    0.122717
     10          7           0        4.726049   -2.487713   -0.550625
     11          6           0        3.286937   -4.145814    0.541202
     12          6           0       -3.595246   -2.749311    0.122491
     13          7           0       -4.725967   -2.487683   -0.551003
     14          6           0       -3.287068   -4.145693    0.541244
```

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20	6	0	-2.551483	-5.656290	2.295952
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22	6	0	-3.110257	-6.528788	0.115872
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24	6	0	3.411133	-5.241196	-0.325338
25	6	0	3.109840	-6.528789	0.115306
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27	6	0	2.551075	-5.656685	2.295550
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35	6	0	7.769394	-4.541586	0.070170
36	6	0	8.045985	-4.989877	-1.218018
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39	6	0	-6.419261	-3.179727	1.715877
40	6	0	-5.258805	-3.328229	-3.225675
41	6	0	5.259116	-3.327786	-3.225436
42	6	0	6.419021	-3.180409	1.716305
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44	30	0	3.773876	-0.000056	-0.000132
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48	6	0	-1.421566	1.832560	-0.555750
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52	7	0	-2.827098	1.699075	-0.449338
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72	6	0	-3.411012	5.241034	0.326238
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76	6	0	7.769468	4.541530	-0.070299
77	6	0	6.672297	3.709463	-0.326329
78	6	0	-6.672162	3.709696	-0.326327
79	6	0	-7.769318	4.541780	-0.070283
80	6	0	-8.046086	4.989759	1.217977
81	6	0	-7.234337	4.598443	2.282307
82	6	0	-6.124215	3.776333	2.073635
83	6	0	5.259447	3.327285	3.225340
84	6	0	6.418992	3.180520	-1.716494
85	6	0	-5.259634	3.326984	3.225410
86	6	0	-6.418745	3.180955	-1.716549
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88	1	0	1.222574	-3.199308	-1.101226
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98	1	0	2.452089	-7.746035	1.768747
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110	1	0	-5.691872	-3.637361	-4.180207
111	1	0	-5.148214	-2.240964	-3.212658
112	1	0	-4.247679	-3.750191	-3.165238
113	1	0	5.692338	-3.636663	-4.179981
114	1	0	4.248008	-3.749832	-3.165255
115	1	0	5.148462	-2.240533	-3.212156
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121	1	0	-1.237272	0.441043	-2.186161
122	1	0	1.237220	0.440995	-2.186226
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125	1	0	2.452025	7.746143	-1.768079
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    134          1           0         8.906073    5.628549    1.397363
    135          1           0         8.421124    4.820443   -0.893800
    136          1           0        -8.420895    4.820825   -0.893801
    137          1           0        -8.905996    5.628663    1.397422
    138          1           0        -7.464683    4.928017    3.291733
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    140          1           0         5.148771    2.240036    3.211897
    141          1           0         5.692764    3.635998    4.179894
    142          1           0         7.314228    3.289903   -2.333954
    143          1           0         6.150417    2.120456   -1.692354
    144          1           0         5.604822    3.719218   -2.214173
    145          1           0        -5.693111    3.635438    4.179975
    146          1           0        -5.148869    2.239747    3.211731
    147          1           0        -4.248560    3.749168    3.165638
    148          1           0        -5.604606    3.719805   -2.214115
    149          1           0        -6.150066    2.120916   -1.692542
    150          1           0        -7.313963    3.290331   -2.334036
 ---------------------------------------------------------------------
```

Table S3. Atomic coordinates for DFT optimization of **grid** structure (theory level: B3LYP/ 6,31-g(d,p) PCM: CH_2Cl_2)

```
                          Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        -1.354459    4.118025   -0.922689
      2          6           0        -0.313417    3.201487   -1.146473
      3          6           0         0.833661    3.216279   -0.355199
      4          6           0         0.985922    4.134298    0.696506
      5          6           0        -0.057521    5.049887    0.920549
      6          6           0        -1.205189    5.032696    0.132908
      7          7           0        -2.573304    4.115634   -1.642980
      8          7           0         2.203169    4.160121    1.416690
      9          6           0         2.253863    4.328461    2.741156
     10          7           0         3.442876    4.661067    3.268113
     11          6           0         1.111374    4.048629    3.660760
     12          6           0        -2.646511    4.097783   -2.972463
     13          7           0        -3.867976    3.955827   -3.514236
     14          6           0        -1.482420    4.306530   -3.883673
     15          8           0        -4.966075    3.826255   -2.696820
     16          6           0         3.789344    4.736964    4.661284
     17          8           0         4.519886    4.852195    2.441233
     18          6           0        -4.219491    4.084127   -4.902146
     19          6           0        -0.727006    5.483400   -3.763157
     20          6           0         0.349436    5.719228   -4.616664
     21          6           0         0.696876    4.775233   -5.586079
     22          6           0        -0.035761    3.592020   -5.695491
     23          6           0        -1.121383    3.359298   -4.851254
```

24	6	0	0.667560	4.971952	4.617289
25	6	0	-0.384172	4.648822	5.474647
26	6	0	-1.002270	3.399684	5.390031
27	6	0	-0.573073	2.477548	4.432309
28	6	0	0.471652	2.801379	3.568170
29	6	0	-4.557941	2.916728	-5.611412
30	6	0	-4.945094	3.051993	-6.948587
31	6	0	-5.010324	4.307778	-7.551798
32	6	0	-4.714126	5.452532	-6.815488
33	6	0	-4.328612	5.365024	-5.471685
34	6	0	3.978812	6.012959	5.224990
35	6	0	4.364109	6.085047	6.567090
36	6	0	4.572144	4.926155	7.315519
37	6	0	4.420008	3.675204	6.722364
38	6	0	4.040235	3.555588	5.379110
39	6	0	-4.511195	1.559065	-4.953492
40	6	0	-4.058622	6.613929	-4.669333
41	6	0	3.925928	2.198789	4.730374
42	6	0	3.783347	7.264363	4.404339
43	30	0	-4.408308	3.971610	-0.827951
44	30	0	4.039764	4.306664	0.616662
45	6	0	-5.021009	-1.479569	-0.120516
46	6	0	-4.050546	-0.635505	-0.678314
47	6	0	-4.017289	0.720306	-0.365647
48	6	0	-4.963175	1.301775	0.499893
49	6	0	-5.930388	0.448818	1.064208
50	6	0	-5.939399	-0.915125	0.774689
51	7	0	-5.028599	-2.878282	-0.387205
52	7	0	-4.926037	2.705236	0.648672
53	6	0	-5.405853	3.384863	1.694190
54	7	0	-5.526884	4.714876	1.549948
55	6	0	-5.695004	2.794331	3.035878
56	6	0	-5.610158	-3.386465	-1.470209
57	7	0	-5.457691	-4.704276	-1.691343
58	6	0	-6.395812	-2.587515	-2.458585
59	8	0	-4.701597	-5.454858	-0.816964
60	6	0	-5.966298	5.660712	2.540687
61	8	0	-5.182086	5.312768	0.364605
62	6	0	-6.187551	-5.506721	-2.634311
63	6	0	-7.545847	-1.888843	-2.059555
64	6	0	-8.271429	-1.137846	-2.983893
65	6	0	-7.853958	-1.066607	-4.314232
66	6	0	-6.703815	-1.748545	-4.716141
67	6	0	-5.978067	-2.502577	-3.794210
68	6	0	-6.960954	2.867777	3.633060
69	6	0	-7.180153	2.305742	4.890876
70	6	0	-6.136533	1.673742	5.569508
71	6	0	-4.872862	1.595536	4.979475
72	6	0	-4.653951	2.143472	3.715982
73	6	0	-5.486704	-6.062969	-3.721173
74	6	0	-6.191671	-6.880165	-4.610137
75	6	0	-7.545961	-7.150892	-4.414928
76	6	0	-8.207595	-6.627805	-3.307078
77	6	0	-7.538732	-5.810426	-2.386270
78	6	0	-7.270448	6.179109	2.420465
79	6	0	-7.680333	7.141340	3.348057
80	6	0	-6.815802	7.585078	4.349159

81	6	0	-5.518004	7.085845	4.422389
82	6	0	-5.061767	6.124284	3.510758
83	6	0	-4.015471	-5.798134	-3.921905
84	6	0	-8.259440	-5.297461	-1.163856
85	6	0	-3.642679	5.620074	3.578654
86	6	0	-8.198162	5.716391	1.323309
87	30	0	-4.039814	-4.306781	0.616686
88	6	0	5.021001	1.479464	-0.120550
89	6	0	4.050593	0.635382	-0.678423
90	6	0	4.017338	-0.720434	-0.365769
91	6	0	4.963174	-1.301888	0.499838
92	6	0	5.930334	-0.448917	1.064216
93	6	0	5.939336	0.915031	0.774715
94	7	0	5.028581	2.878187	-0.387199
95	7	0	4.926105	-2.705351	0.648587
96	6	0	5.405912	-3.384960	1.694117
97	7	0	5.527000	-4.714971	1.549881
98	6	0	5.695015	-2.794412	3.035815
99	6	0	5.610158	3.386402	-1.470189
100	7	0	5.457654	4.704209	-1.691312
101	6	0	6.395941	2.587512	-2.458509
102	8	0	4.701501	5.454752	-0.816961
103	6	0	5.966341	-5.660818	2.540643
104	8	0	5.182144	-5.312905	0.364565
105	6	0	6.187502	5.506704	-2.634254
106	6	0	7.545957	1.888868	-2.059361
107	6	0	8.271697	1.137954	-2.983640
108	6	0	7.854413	1.066775	-4.314041
109	6	0	6.704295	1.748685	-4.716069
110	6	0	5.978385	2.502631	-3.794194
111	6	0	6.960950	-2.867810	3.633035
112	6	0	7.180095	-2.305759	4.890852
113	6	0	6.136440	-1.673771	5.569444
114	6	0	4.872788	-1.595607	4.979373
115	6	0	4.653928	-2.143575	3.715884
116	6	0	5.486686	6.062799	-3.721207
117	6	0	6.191633	6.880032	-4.610157
118	6	0	7.545867	7.150945	-4.414834
119	6	0	8.207466	6.628010	-3.306887
120	6	0	7.538623	5.810597	-2.386099
121	6	0	7.270449	-6.179321	2.420422
122	6	0	7.680273	-7.141552	3.348040
123	6	0	6.815715	-7.585195	4.349160
124	6	0	5.517951	-7.085875	4.422383
125	6	0	5.061778	-6.124310	3.510726
126	6	0	4.015509	5.797751	-3.922054
127	6	0	8.259278	5.297783	-1.163591
128	6	0	3.642727	-5.619997	3.578598
129	6	0	8.198171	-5.716733	1.323211
130	30	0	4.408352	-3.971789	-0.827989
131	6	0	1.354433	-4.118097	-0.922714
132	6	0	0.313368	-3.201594	-1.146504
133	6	0	-0.833704	-3.216412	-0.355217
134	6	0	-0.985939	-4.134420	0.696497
135	6	0	0.057523	-5.049994	0.920536
136	6	0	1.205183	-5.032775	0.132887
137	7	0	2.573280	-4.115698	-1.642998

138	7	0	-2.203191	-4.160248	1.416681
139	6	0	-2.253908	-4.328477	2.741162
140	7	0	-3.442941	-4.660974	3.268141
141	6	0	-1.111410	-4.048604	3.660749
142	6	0	2.646493	-4.097775	-2.972467
143	7	0	3.867991	-3.955964	-3.514227
144	6	0	1.482407	-4.306304	-3.883726
145	8	0	4.966112	-3.826593	-2.696794
146	6	0	-3.789361	-4.736867	4.661317
147	8	0	-4.519953	-4.852155	2.441256
148	6	0	4.219486	-4.084126	-4.902149
149	6	0	0.726910	-5.483134	-3.763385
150	6	0	-0.349602	-5.718722	-4.616870
151	6	0	-0.697042	-4.774513	-5.586074
152	6	0	0.035694	-3.591344	-5.695322
153	6	0	1.121392	-3.358864	-4.851114
154	6	0	-0.667604	-4.971876	4.617331
155	6	0	0.384166	-4.648731	5.474635
156	6	0	1.002323	-3.399631	5.389902
157	6	0	0.573133	-2.477544	4.432130
158	6	0	-0.471644	-2.801385	3.568058
159	6	0	4.558095	-2.916686	-5.611271
160	6	0	4.945223	-3.051841	-6.948465
161	6	0	5.010266	-4.307561	-7.551838
162	6	0	4.713900	-5.452361	-6.815669
163	6	0	4.328409	-5.364962	-5.471851
164	6	0	-3.978964	-6.012849	5.225007
165	6	0	-4.364194	-6.084913	6.567127
166	6	0	-4.572035	-4.926009	7.315591
167	6	0	-4.419784	-3.675065	6.722454
168	6	0	-4.040079	-3.555472	5.379177
169	6	0	4.511538	-1.559094	-4.953192
170	6	0	4.058221	-6.613928	-4.669659
171	6	0	-3.925626	-2.198675	4.730463
172	6	0	-3.783734	-7.264257	4.404308
173	1	0	-0.406344	2.466197	-1.939031
174	1	0	1.623572	2.493245	-0.534102
175	1	0	0.038117	5.792427	1.705474
176	1	0	-1.997874	5.752684	0.314959
177	1	0	-0.987972	6.212851	-3.003735
178	1	0	0.916106	6.640024	-4.522619
179	1	0	1.535980	4.960008	-6.249762
180	1	0	0.234587	2.849297	-6.439839
181	1	0	-1.683888	2.436982	-4.939096
182	1	0	1.137559	5.945702	4.689231
183	1	0	-0.718381	5.373989	6.210172
184	1	0	-1.815875	3.148112	6.063391
185	1	0	-1.047818	1.503667	4.359696
186	1	0	0.800866	2.087167	2.820830
187	1	0	-5.204810	2.162752	-7.516308
188	1	0	-5.314140	4.394998	-8.590916
189	1	0	-4.798000	6.432304	-7.277446
190	1	0	4.508075	7.060193	7.023793
191	1	0	4.872677	4.999784	8.356600
192	1	0	4.613871	2.774377	7.298030
193	1	0	-4.889598	1.607995	-3.930253
194	1	0	-5.112125	0.838966	-5.513613

195	1	0	-3.489170	1.162770	-4.907750
196	1	0	-2.986388	6.832704	-4.614778
197	1	0	-4.547763	7.476510	-5.128830
198	1	0	-4.427314	6.514563	-3.644849
199	1	0	4.489814	1.454505	5.297237
200	1	0	2.884183	1.861449	4.681688
201	1	0	4.313934	2.212523	3.708291
202	1	0	2.725782	7.443728	4.175733
203	1	0	4.158036	8.140111	4.939390
204	1	0	4.306248	7.179611	3.448375
205	1	0	-3.321993	-1.047270	-1.370284
206	1	0	-3.251644	1.352813	-0.804671
207	1	0	-6.696648	0.847546	1.716658
208	1	0	-6.692374	-1.552984	1.228433
209	1	0	-7.874874	-1.936742	-1.028159
210	1	0	-9.162700	-0.607795	-2.662658
211	1	0	-8.419696	-0.480748	-5.032186
212	1	0	-6.370291	-1.696096	-5.748108
213	1	0	-5.079091	-3.020203	-4.109045
214	1	0	-7.778191	3.352824	3.111823
215	1	0	-8.166650	2.364328	5.340207
216	1	0	-6.307275	1.243636	6.551684
217	1	0	-4.055555	1.108348	5.502256
218	1	0	-3.673156	2.079180	3.256169
219	1	0	-5.667886	-7.312620	-5.458148
220	1	0	-8.078667	-7.788392	-5.114542
221	1	0	-9.253336	-6.867842	-3.135728
222	1	0	-8.684590	7.549527	3.277030
223	1	0	-7.149562	8.334850	5.060538
224	1	0	-4.836740	7.454277	5.184361
225	1	0	-3.480336	-5.846001	-2.971055
226	1	0	-3.586315	-6.531490	-4.609137
227	1	0	-3.832065	-4.805419	-4.349850
228	1	0	-8.666591	-4.293895	-1.329740
229	1	0	-9.097222	-5.953076	-0.912758
230	1	0	-7.593127	-5.245513	-0.299005
231	1	0	-3.576043	4.678987	4.134915
232	1	0	-3.232908	5.436584	2.582283
233	1	0	-3.001656	6.345159	4.086186
234	1	0	-7.670295	5.667641	0.367927
235	1	0	-8.600200	4.715542	1.523114
236	1	0	-9.048217	6.395911	1.225480
237	1	0	3.322076	1.047140	-1.370435
238	1	0	3.251738	-1.352954	-0.804856
239	1	0	6.696576	-0.847627	1.716697
240	1	0	6.692274	1.552891	1.228518
241	1	0	7.874837	1.936730	-1.027917
242	1	0	9.162946	0.607923	-2.662313
243	1	0	8.420279	0.480988	-5.031954
244	1	0	6.370917	1.696281	-5.748086
245	1	0	5.079431	3.020235	-4.109126
246	1	0	7.778215	-3.352836	3.111829
247	1	0	8.166576	-2.364318	5.340220
248	1	0	6.307151	-1.243644	6.551617
249	1	0	4.055458	-1.108408	5.502109
250	1	0	3.673139	-2.079316	3.256053
251	1	0	5.667871	7.312363	-5.458245

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    252          1           0        8.078557    7.788472   -5.114435
    253          1           0        9.253159    6.868196   -3.135454
    254          1           0        8.684491   -7.549830    3.277008
    255          1           0        7.149422   -8.334977    5.060554
    256          1           0        4.836666   -7.454242    5.184369
    257          1           0        3.480293    5.845529   -2.971244
    258          1           0        3.586280    6.531050   -4.609301
    259          1           0        3.832281    4.805013   -4.350026
    260          1           0        9.096983    5.953486   -0.912469
    261          1           0        7.592899    5.245833   -0.298792
    262          1           0        8.666527    4.294240   -1.329379
    263          1           0        3.576157   -4.678908    4.134861
    264          1           0        3.232997   -5.436475    2.582218
    265          1           0        3.001635   -6.345031    4.086112
    266          1           0        8.600541   -4.716034    1.523099
    267          1           0        9.048012   -6.396494    1.225195
    268          1           0        7.670222   -5.667718    0.367889
    269          1           0        0.406265   -2.466302   -1.939064
    270          1           0       -1.623641   -2.493406   -0.534115
    271          1           0       -0.038090   -5.792528    1.705467
    272          1           0        1.997890   -5.752742    0.314919
    273          1           0        0.987862   -6.212746   -3.004112
    274          1           0       -0.916328   -6.639496   -4.522954
    275          1           0       -1.536231   -4.959078   -6.249710
    276          1           0       -0.234643   -2.848462   -6.439515
    277          1           0        1.683968   -2.436579   -4.938828
    278          1           0       -1.137641   -5.945600    4.689361
    279          1           0        0.718367   -5.373860    6.210201
    280          1           0        1.815979   -3.148061    6.063201
    281          1           0        1.047934   -1.503696    4.359424
    282          1           0       -0.800857   -2.087208    2.820684
    283          1           0        5.205063   -2.162566   -7.516075
    284          1           0        5.314057   -4.394694   -8.590970
    285          1           0        4.797615   -6.432090   -7.277749
    286          1           0       -4.508277   -7.060047    7.023820
    287          1           0       -4.872522   -4.999626    8.356686
    288          1           0       -4.613501   -2.774225    7.298148
    289          1           0        4.889903   -1.608199   -3.929947
    290          1           0        5.112592   -0.839024   -5.513212
    291          1           0        3.489574   -1.162644   -4.907438
    292          1           0        2.985955   -6.832561   -4.615144
    293          1           0        4.547247   -7.476521   -5.129256
    294          1           0        4.426914   -6.514741   -3.645158
    295          1           0       -4.489391   -1.454322    5.297357
    296          1           0       -2.883836   -1.861474    4.681748
    297          1           0       -4.313663   -2.212341    3.708392
    298          1           0       -2.726169   -7.443989    4.175982
    299          1           0       -4.158870   -8.139911    4.939201
    300          1           0       -4.306362   -7.179260    3.448218
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10. References

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