Supplementary Information (SI) for Chemical Science.
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Electronic Supplementary Information (ESI) for

Role of Ancillary Ligands in *S*-nitrosothiol and NO Generation from Nitrite-Thiol Interactions at Mononuclear Zinc(II) Sites

Balakrishnan S. Anju,[a] Neeraja R. Nair,[a] Janavi Rajput,[b] Jeffery A. Bertke,[c] Bhaskar Mondal,*[b] and Subrata Kundu*[a]

[a]School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram (IISER–TVM), Thiruvananthapuram 695551, India

[b]School of Chemical Sciences, Indian Institute of Technology Mandi, Kamand, Himachal Pradesh 175075, India

[c]Department of Chemistry, Georgetown University, Box 571227-1227, Washington, D. C. 20057, United States

*Corresponding authors email:
skundu@iisertvm.ac.in, skundu.chem@gmail.com (SK)
bhaskarmondal@iitmandi.ac.in (BM)

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1. General Instrumentation and Physical Methods

Air-sensitive chemicals were prepared and handled under dry argon/ nitrogen atmosphere by utilizing standard Schlenk techniques and/or a MBraun Glovebox with <0.1 ppm O_2 and H_2O. More specifically, apart from the preparations of the metal nitrite complexes, all the reactions and NMR sample preparations were exclusively carried out in the glovebox.

***NMR Spectroscopic Studies*:** ^{1}H and ^{13}C NMR spectra were recorded on Bruker Avance III 500 MHz NMR spectrometer at room temperature unless otherwise noted. The proton chemical shift (δ) values are expressed in ppm relative to tetramethylsilane, whereas the residual ^{1}H, ^{13}C signals of the deuterated solvent served as an internal standard. The ^{31}P and ^{15}N chemical shift (δ) values are reported in ppm relative to H_3PO_4 (85% solution) and liquid NH_3, respectively.

***CHNS Analyses*:** Elemental analyses were performed on an Elementar Vario Micro Cube CHNS analyzer.

***UV–vis Spectroscopic Studies*:** UV-vis spectra were recorded on an Agilent 8454 Diode Array spectrometer equipped with stirrer and Unisoku USP-203 cryostats for variable temperature (–105 °C to 90 °C) experiments. Solutions for UV-vis analysis were prepared freshly by dissolving analytically pure compounds in anhydrous solvents.

***Infrared (IR) Spectroscopic Studies*:** FTIR spectra (with the spectral resolution of 4 cm^{-1}) were collected on a Shimadzu IRPrestige-21 FTIR spectrometer by using KBr pellet method. The intensity of the vibrational bands are abbreviated as s=strong, m=medium, w=weak, and br=broad.

Electrospray Ionization – Mass Spectrometric (ESI–MS) Analyses: High-resolution mass spectra (HRMS) were recorded on Thermo Scientific™ Q Exactive™ Hybrid Quadrupole-Orbitrap Mass Spectrometer using electrospray ionization (ESI) technique. For the preparations of samples, the crude reaction mixtures were diluted with acetonitrile.

GCMS: GC-MS analyses of the reaction mixtures were performed on an Agilent 5977C GC/MSD system. Identification of the organic products were carried out by comparing their retention times, electron ionization (EI) mass spectra, and NMR spectra with those of the authentic and/or previously reported compounds.

***Single Crystal X-ray Diffraction (SCXRD) Analysis*:** Single crystals of [(**Me$_2$PzPy**)$_2$Zn^{II}(OClO$_3$)](ClO$_4$) (**1-Py**) (CCDC 2355797), [(**Me$_4$PzPz**)$_2$Zn^{II}(OClO$_3$)](ClO$_4$) (**1-Pz**) (CCDC 2355798), [{(**Me$_2$PzQu**)$_2$Zn^{II}}$_2$(μ–OH)](ClO$_4$)$_3$ (**2-Qu**) (CCDC 2355799), [(**Me$_2$PzPy**)$_2$Zn^{II}(OTf)](OTf) (**3-Py**) (CCDC 2355800), [(**Me$_4$PzPz**)$_2$Zn^{II}(OTf)](OTf) (**3-Pz**)

(CCDC 2355801), [(**Me$_2$PzQu**)$_2$Zn^{II}(OTf)](OTf) (**3-Qu**) (CCDC 2355802), [(**Me$_2$PzPy**)$_2$Zn^{II}(OPEt$_3$)](ClO$_4$)$_2$ (**4-Py**) (CCDC 2355803), [(**Me$_4$PzPz**)$_2$Zn^{II}(OPEt$_3$)](ClO$_4$)$_2$ (**4-Pz**) (CCDC 2355804), [(**Me$_2$PzPy**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Py**) (CCDC 2355805), [(**Me$_4$PzPz**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Pz**) (CCDC 2355806), [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Qu**) (CCDC 2355807) were mounted under mineral oil on a glass capillary. Data for all the complexes were collected at 150 K on a Bruker Kappa diffractometer equipped with an APEXII CCD detector and Mo fine focus sealed tube source employing graphite monochromated Mo K_α radiation (λ = 0.7107 Å). The data sets were processed using APEX II software. Integration of the data sets were carried out with the Bruker SAINT program. Structure solutions were performed using the SHELXTL/PC suite.[1] Intensities were corrected for Lorentz and polarization effects and an empirical absorption correction was applied using Blessing's method as incorporated into the program SADABS.[2] Non-hydrogen atoms were refined with anisotropic thermal parameters and hydrogen atoms were included in idealized positions. The molecular structures were rendered using MERCURY 3.10.3 software.[3]

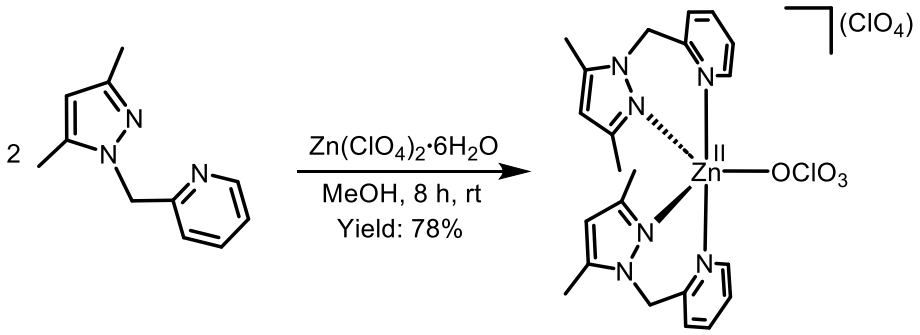
2. Materials

All chemicals were purchased from standard vendors (e.g., Sigma-Aldrich, Spectrochem, Strem Chemicals, TCI) and used without further purification unless otherwise mentioned. Molecular sieves (4Å, 4–8 mesh beads) were activated in *vacuo* at 220 °C for 24 h. Anhydrous solvents were sparged with nitrogen and stored over activated molecular sieves under nitrogen atmosphere.

2-(3,5-dimethylpyrazol-1-ylmethyl)pyridine (**Me$_2$PzPy**),[4] 2-(3,5-dimethylpyrazol-1-ylmethyl)quinoline (**Me$_2$PzQu**),[4] bis(3,5-dimethyl-1-pyrazolyl) methane (**Me$_4$PzPz**)[5] tetraphenylporphyrin cobalt(II) [(TPP)Co^{II}][6] were synthesized and characterized according to the previously reported literature procedures.

Caution! *While we did not encounter any problem, metal perchlorate complexes with organic ligands are potentially explosive. They should be prepared and handled with care and only used in small quantities at a time.*

3. Synthesis and Characterization of $[(Me_2PzPy)_2Zn^{II}(OClO_3)](ClO_4)$

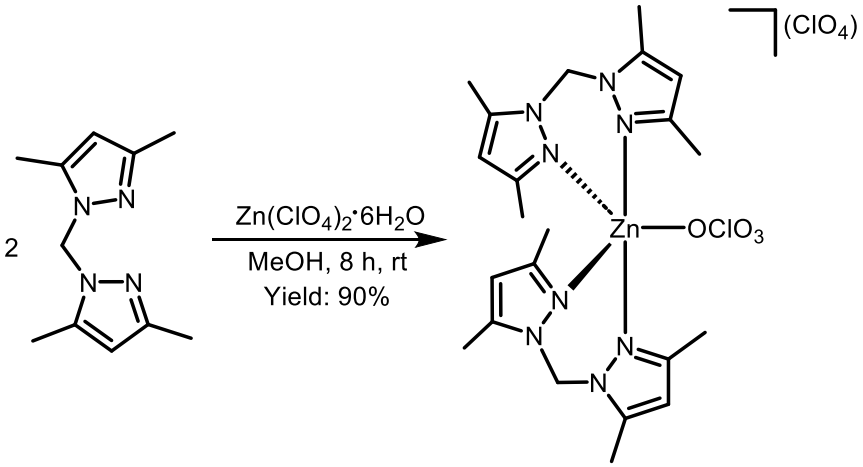


Scheme S1. Synthesis of $[(\mathbf{Me_2PzPy})_2Zn^{II}(OClO_3)](ClO_4)$ (**1-Py**).

To a solution of $Zn(ClO_4)_2{\cdot}6H_2O$ (0.298 g, 0.801 mmol) in methanol (~2 mL), a solution of **Me_2PzPy** (0.300 g, 1.602 mmol) in methanol (~2 mL) was added dropwise under N_2 atmosphere. The resultant clear solution was stirred at room temperature for 8 h to obtain a clear solution with a white precipitate. The reaction mixture was filtered, and the filtrate was washed with methanol and diethyl ether to afford $[(\mathbf{Me_2PzPy})_2Zn^{II}(OClO_3)](ClO_4)$ (**1-Py**) (0.399 g, 0.624 mmol) as a colorless solid in 78% yield. ^{1}H NMR (500 MHz, DMSO): δ 8.52 (d, J = 4.7 Hz, 1H), 7.76 (t, J = 7.7 Hz, 1H), 7.33 – 7.26 (m, 1H), 6.92 (d, J = 7.8 Hz, 1H), 5.87 (s, 1H), 5.26 (s, 2H), 2.19 (s, 3H), 2.09 (s, 3H) (Figure S1). ^{13}C NMR (126 MHz, DMSO): δ 157.11, 149.20, 146.51, 139.43, 137.30, 122.67, 121.34, 105.15, 53.33, 13.37, 10.72 (Figure S2).

Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **1-Py** in acetonitrile at room temperature (Figure S4). *Anal. % Calcd for* $C_{22}H_{26}Cl_2ZnN_6O_8{\cdot}(CH_4O)_{0.55}$: C, 41.26; H, 4.33; N, 12.80. Found: C, 41.32; H, 4.11; N, 12.58. FTIR (KBr pellet, cm^{-1}): 2922(w,br), 2015(w), 1604(m), 1550(m), 1477(s), 1435(s), 1390(m), 1311(m), 1087(s, ν_{ClO4}), 947(w), 839(m), 771(s), 684(m), 626(s, ν_{ClO4}), 480(w), 422(w) (Figure S3).

4. Synthesis and Characterization of $[(Me_4PzPz)_2Zn^{II}(OClO_3)](ClO_4)$

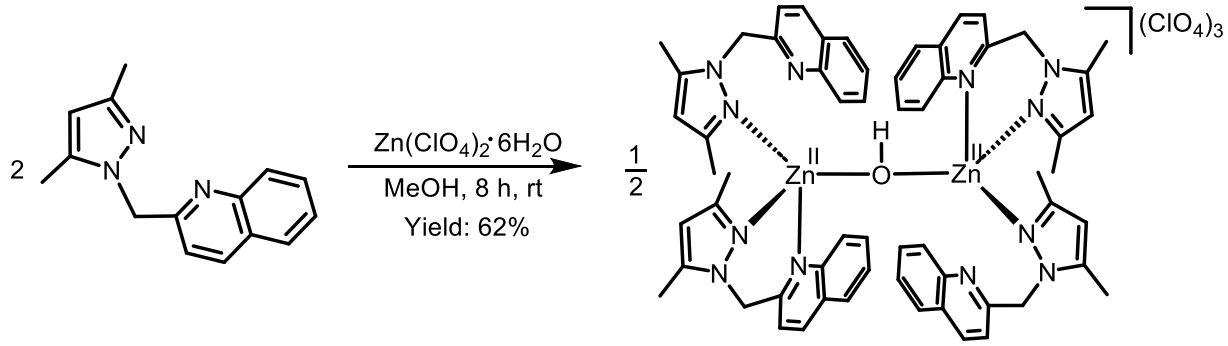


Scheme S2. Synthesis of $[(\mathbf{Me_4PzPz})_2Zn^{II}(OClO_3)](ClO_4)$ (**1-Pz**).

To a solution of $Zn(ClO_4)_2{\cdot}6H_2O$ (0.272 g, 0.974 mmol) in methanol (~2 mL), a solution of **Me$_4$PzPz** (0.300 g, 1.461 mmol) in methanol (~2 mL) was added dropwise under N_2 atmosphere. The resultant pale-yellow solution was stirred at room temperature for 8 h to obtain a clear solution with a yellow-white precipitate. The reaction mixture was filtered, and the filtrate was washed with methanol and diethyl ether to obtain $[(\mathbf{Me_4PzPz})_2Zn^{II}(OClO_3)](ClO_4)$ (**1-Pz**) (0.447 g, 0.664 mmol) as a colorless solid in 90% yield. ^{1}H NMR (500 MHz, DMSO): δ 6.01 (s, 2H), 5.80 (s, 2H), 2.38 (s, 6H), 2.04 (s, 6H) (Figure S5). ^{13}C NMR (126 MHz, DMSO): δ 147.11, 140.02, 105.58, 58.83, 13.33, 10.73 (Figure S6). *Anal. % Calcd for* $C_{22}H_{32}Cl_2ZnN_8O_8{\cdot}(H_2O)_2$: C, 37.28; H, 5.12; N, 15.81. Found: C, 36.76; H, 4.80; N, 15.81.

Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **1-Pz** in acetonitrile at room temperature (Figure S8). FTIR (KBr pellet, cm^{-1}): 3506(m,br), 3018(w), 2962(w), 2872(w), 2015(w), 1627(m), 1558(m), 1467(m), 1386(m), 1282(m), 1143(s, ν_{ClO4}), 1080(s, ν_{ClO4}), 808(w), 682(w), 628(s, ν_{ClO4}), 482(w) (Figure S7).

5. Synthesis and Characterization of $[\{(Me_2PzQu)_2Zn^{II}\}_2(\mu\text{–}OH)](ClO_4)_3$

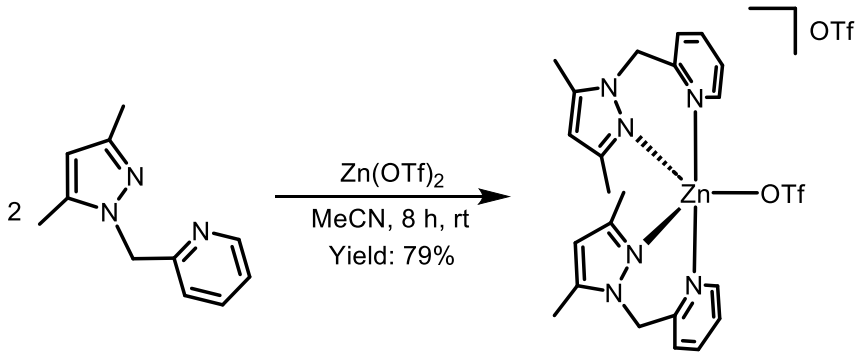


Scheme S3. Synthesis of $[\{(\mathbf{Me_2PzQu})_2Zn^{II}\}_2(\mu\text{–}OH)](ClO_4)_3$ (**2-Qu**).

To a solution of $Zn(ClO_4)_2{\cdot}6H_2O$ (0.235 g, 0.632 mmol) in methanol (~2 mL), a solution of **Me₂PzQu** (0.300 g, 1.264 mmol) in methanol (~2 mL) was added dropwise under N_2 atmosphere. The resultant pale-yellow solution was stirred at room temperature for 8 h to obtain a clear solution with a yellow-white precipitate. The reaction mixture was filtered, and the filtrate was washed with methanol and diethyl ether to obtain $[\{(\mathbf{Me_2PzQu})_2Zn^{II}\}_2(\mu\text{–}OH)](ClO_4)_3$ (**2-Qu**) (0.274 g, 0.316 mmol) as an off-white solid in 62% yield. ^{1}H NMR (500 MHz, DMSO): δ 8.32 (d, J = 8.5 Hz, 1H), 7.96 (dd, J = 16.0, 8.3 Hz, 2H), 7.76 (t, J = 7.6 Hz, 1H), 7.59 (t, J = 7.5 Hz, 1H), 7.00 (d, J = 8.5 Hz, 1H), 5.90 (s, 1H), 5.45 (s, 2H), 2.21 (s, 3H), 2.10 (s, 3H) (Figure S9). ^{13}C NMR (126 MHz, DMSO): δ 157.90, 146.96, 146.57, 139.55, 137.24, 129.93, 128.56, 127.92, 126.94, 126.52, 119.23, 105.31, 54.28, 13.38, 10.77 (Figure S10). *Anal. % Calcd for* $C_{60}H_{61}Cl_2Zn_2N_{12}O_{13}{\cdot}(CH_3CN)_{0.2}$: C, 51.69; H, 4.42; N, 12.17 Found: C, 51.97; H, 4.70; N, 11.89.

Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **2-Qu** in acetonitrile at room temperature (Figure 12). FTIR (KBr pellet, cm^{-1}): 3645(m, ν_{OH}), 3408(w,br), 3064(w), 2924(w), 1597(m) 1554(m), 1508(m), 1467(m), 1429(m), 1386(m), 1298(m), 1143(s, ν_{ClO4}), 1087(s, ν_{ClO4}), 979(w), 900(w), 771(s), 704(w), 628(s, ν_{ClO4}) (Figure S11).

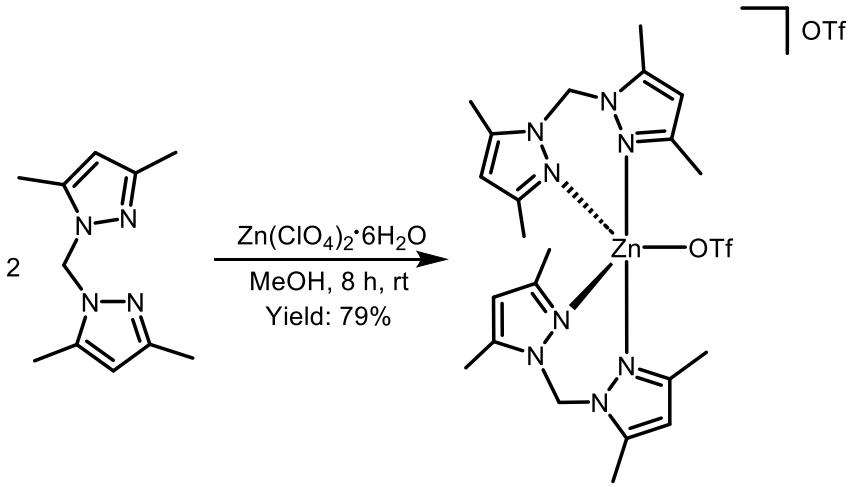
6. Synthesis and Characterization of $[(Me_2PzPy)_2Zn^{II}(OTf)](OTf)$



Scheme S4. Synthesis of $[(\mathbf{Me_2PzPy})_2Zn_2^{II}(OTf)](OTf)$ (**3-Py**).

A solution of **Me₂PzPy** (0.100 g, 0.534 mmol) in acetonitrile (~2 mL) was added dropwise to a solution of $Zn(OTf)_2$ (0.097 g, 0.267 mmol) in acetonitrile (~2 mL) under an inert atmosphere of a glovebox. The resultant solution was stirred for 8 h at room temperature. The reaction mixture was then filtered and the filtrate was dried under vacuum. Subsequent recrystallization of the crude from MeCN/Et_2O at −35 °C afforded a colorless powder of $[(\mathbf{Me_2PzPy})_2Zn^{II}(OTf)](OTf)$ (**3-Py**) (0.155 g, 0.210 mmol) in 79% yield. Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **3-Py** in acetonitrile at room temperature (Figure S16). *Anal. % Calcd for* $C_{24}H_{26}F_6N_6O_6S_2Zn\cdot(C_4H_{10}O)_{0.1}$: C, 39.32; H, 3.65; N, 11.27; S, 8.60 Found: C, 38.92; H, 3.79; N, 10.84; S, 8.67. ^{1}H NMR (500 MHz, CD_3CN): δ 8.46 (d, J = 5.3 Hz, 1H), 8.17 (t, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.62 (t, 1H), 6.09 (s, 1H), 5.55 (s, 2H), 2.46 (s, 3H), 2.44 (s, 3H) (Figure S13). ^{13}C NMR (126 MHz, CD_3CN): δ 153.88, 151.83, 150.29, 145.22, 142.94, 126.87, 126.62, 122.90, 120.35, 118.17, 108.28, 51.02, 12.40, 11.31 (Figure S14). ^{19}F NMR (471 MHz, 298 K, CD_3CN): δ −79.43. FTIR (KBr pellet, cm^{-1}): 3522(w,br), 1609(m), 1549(m), 1481(m) 1440(m), 1276(m), 1172(s), 1034(s), 802(m), 760(s), 646(s), 523(m) (Figure S15).

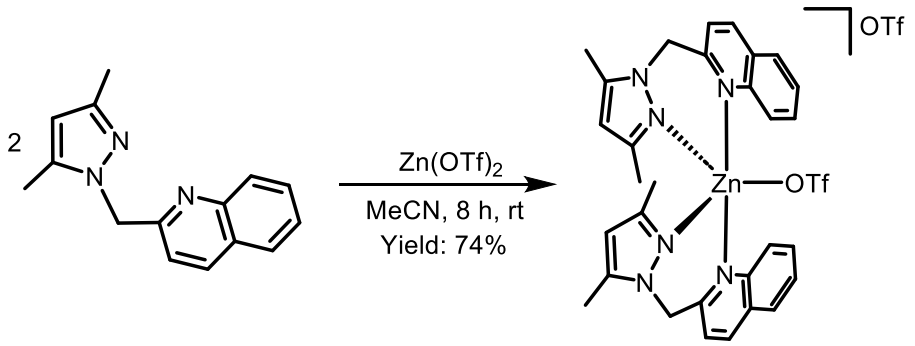
7. Synthesis and Characterization of $[(Me_4PzPz)_2Zn^{II}(OTf)](OTf)$



Scheme S5. Synthesis of $[(\mathbf{Me_4PzPz})_2Zn_2^{II}(OTf)](OTf)$ (**3-Pz**).

A solution of **Me$_4$PzPz** (0.100 g, 0.489 mmol) in acetonitrile (~2 mL) was added dropwise to a solution of $Zn(OTf)_2$ (0.089 g, 0.244 mmol) in acetonitrile (~2 mL) under an inert atmosphere of a glovebox. The resultant solution was stirred for 8 h at room temperature. The reaction mixture was filtered, and the filtrate was dried under vacuum. Subsequent recrystallization from MeCN/Et_2O at –35 °C afforded a colorless powder of $[(\mathbf{Me_4PzPz})_2Zn^{II}(OTf)](OTf)$ (**3-Pz**) (0.148 g, 0.192 mmol) in 79 % yield. Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **3-Pz** in acetonitrile at room temperature (Figure S20). *Anal. % Calcd for* $C_{24}H_{32}F_6N_8O_6S_2Zn\cdot(C_4H_{10}O)_{0.45}$: C, 38.48; H, 4.57; N, 13.91; S, 7.96 Found: C, 38.86; H, 4.26; N, 14.31; S, 8.01. ^{1}H NMR (500 MHz, CD_3CN): δ 6.31 (s, 2H), 6.13 (s, 2H), 2.48 (s, 6H), 1.72 (s, 6H) (Figure S17). ^{13}C NMR (126 MHz, CD_3CN): δ 153.13, 145.06, 108.27, 57.42, 12.19, 10.89 (Figure S18). FTIR (KBr pellet, cm^{-1}): 3526(w, br), 1639(w), 1560(s), 1461(s) 1420(m), 1380(m), 1352(m), 1267(m), 1172(s), 1030(s), 969(w), 808(m), 780(m), 674(s), 641(s), 574(w), 520(m) (Figure S19).

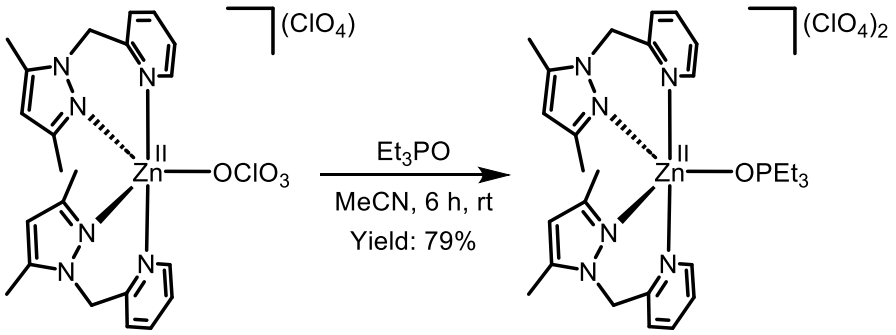
8. Synthesis and Characterization of $[(Me_2PzQu)_2Zn^{II}(OTf)](OTf)$



Scheme S6. Synthesis of $[(\mathbf{Me_2PzQu})_2Zn_2^{II}(OTf)](OTf)$ (**3-Qu**).

A solution of **Me₂PzQu** (0.100 g, 0.421 mmol) in acetonitrile (~2 mL) was added dropwise to a solution of $Zn(OTf)_2$ (0.076 g, 0.210 mmol) in acetonitrile (~2 mL) under an inert atmosphere of a glovebox. The resultant solution was stirred for 8 h at room temperature. The reaction mixture was filtered, and the filtrate was dried under vacuum. Subsequent recrystallization from $MeCN/Et_2O$ at –35 °C afforded a white powder of $[(\mathbf{Me_2PzQu})_2Zn^{II}(OTf)](OTf)$ (**3-Qu**) (0.115 g, 0.155 mmol) in 74 % yield. Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **3-Qu** in acetonitrile at room temperature (Figure S24). *Anal. % Calcd for* $C_{32}H_{30}F_6N_6O_6S_2Zn\cdot(CH_3CN)_{0.20}$: C, 45.98; H, 3.64; N, 10.26; S, 7.58 Found: C, 45.86; H, 3.77; N, 10.35; S, 7.56. ^{1}H NMR (500 MHz, CD_3CN): δ 8.84 (d, J = 8.4 Hz, 1H), 8.12 (dd, J = 12.7, 8.2 Hz, 2H), 7.62 (t, J = 7.5 Hz, 1H), 7.52 – 7.26 (m, 2H), 6.11 (s, 1H), 5.91 (s, 2H), 2.59 (s, 3H), 2.53 (s, 3H) (Figure S21). ^{13}C NMR (126 MHz, CD_3CN): δ 156.44, 152.13, 146.36, 145.49, 144.18, 133.35, 129.92, 129.18, 125.31, 124.19, 122.78, 120.24, 108.52, 52.43, 30.48, 11.93, 11.31 (Figure S22). ^{19}F NMR (471 MHz, 298 K, CD_3CN): δ –79.35. FTIR (KBr pellet, cm^{-1}): 3501(w,br), 1598(m), 1555(m), 1481(m) 1385(m), 1276(m), 1157(m) 1034(s), 1014(s), 823(s), 760(s), 642(s), 518(m) (Figure S23).

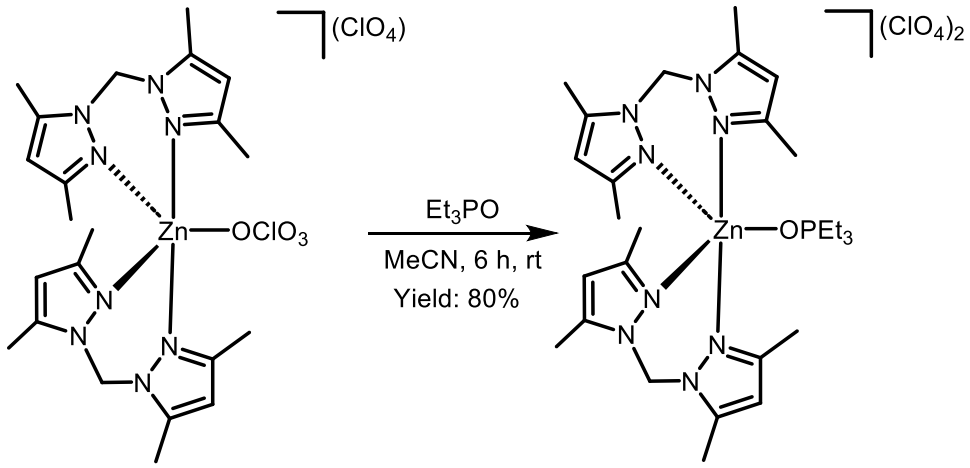
9. Synthesis and Characterization of $[(Me_2PzPy)_2Zn^{II}(OPEt_3)](ClO_4)_2$



Scheme S7. Synthesis of $[(\mathbf{Me_2PzPy})_2Zn_2^{II}(OPEt_3)](ClO_4)_2$ (**4-Py**).

To a solution of $[(\mathbf{Me_2PzPy})_2Zn^{II}(OClO_3)](ClO_4)$ (0.050 g, 0.078 mmol) in acetonitrile (~2 mL), a solution of Et_3PO (0.011 g, 0.078 mmol) in acetonitrile (~2 mL) was added dropwise under N_2 atmosphere. The resultant clear solution was stirred at room temperature for 6 h. The reaction mixture was filtered, and the filtrate dried under vacuum. Subsequent recrystallization from $MeCN/Et_2O$ at −35 °C afforded a colorless powder of $[(\mathbf{Me_2PzPy})_2Zn(OPEt_3)](ClO_4)_2$ (**4-Py**) (0.048 g, 0.062 mmol) in 79% yield. ^1H NMR (500 MHz, CD_3CN): δ 8.38 (d, J = 5.3 Hz, 1H), 8.13 (t, J = 7.8 Hz, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.57 (t, J = 6.5 Hz, 1H), 6.07 (s, 1H), 5.52 (s, 2H), 2.44 (s, 5H), 1.61 (dd, J = 12.3, 7.5 Hz, 6H), 0.95 (dt, J = 16.2, 7.6 Hz, 9H). (Figure S25). $^{31}P\{^1H\}$ NMR (202 MHz, CD_3CN): δ 67.12 (Figure S26). Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **4-Py** in acetonitrile at room temperature(Figure S27).

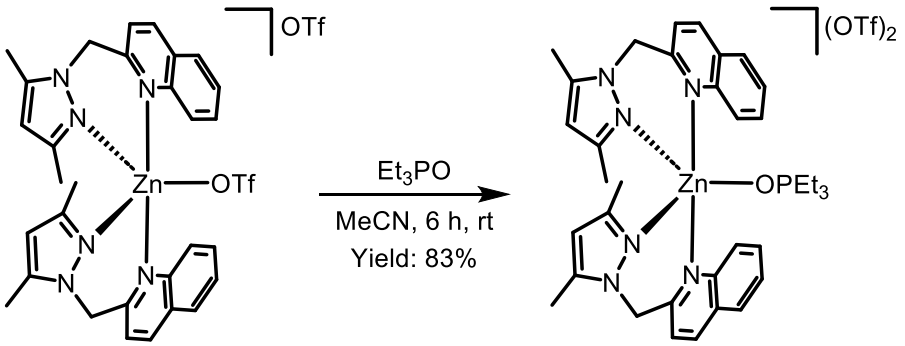
10. Synthesis and Characterization of $[(Me_4PzPz)_2Zn^{II}(OPEt_3)](ClO_4)_2$



Scheme S8. Synthesis of $[(\mathbf{Me_4PzPz})_2Zn_2^{II}(OPEt_3)](ClO_4)_2$ (**4-Pz**).

To a solution of $[(\mathbf{Me_4PzPz})_2Zn^{II}(OClO_3)](ClO_4)$ (0.050 g, 0.074 mmol) in acetonitrile (~2 mL), a solution of Et_3PO (0.010 g, 0.074 mmol) in acetonitrile (~2 mL) was added dropwise under N_2 atmosphere. The resultant clear solution was stirred at room temperature for 6 h. The reaction mixture was filtered and the filtrate dried under vacuum. Subsequent recrystallisation from $MeCN/Et_2O$ at –35 °C afforded a colorless powder of $[(\mathbf{Me_4PzPz})_2Zn(OPEt_3)](ClO_4)_2$ (**4-Pz**) (0.045 g, 0.056 mmol) in 80% yield. ^1H NMR (500 MHz, CD_3CN): δ 6.23 (s, 2H), 6.10 (s, 2H), 2.47 (s, 9H), 1.86 – 1.79 (m, 6H), 1.05 (dt, J = 16.2, 7.7 Hz, 9H). (Figure S28). $^{31}P\{^1H\}$ NMR (202 MHz, CD_3CN): δ 69.88 (Figure S29). Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **4-Pz** in acetonitrile at room temperature (Figure S30).

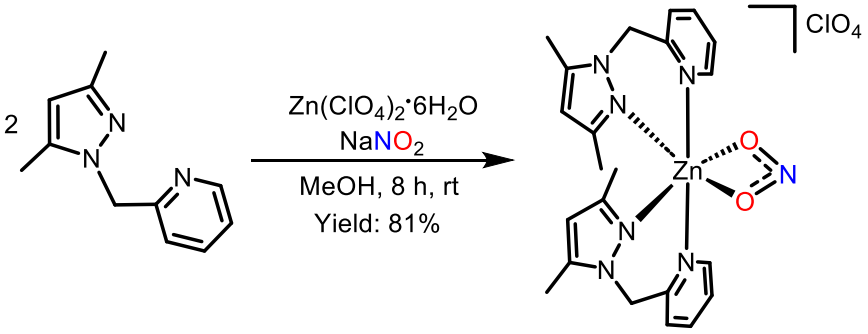
11. Synthesis and Characterization of $[(Me_2PzQu)_2Zn^{II}(OPEt_3)](OTf)_2$



Scheme S9. Synthesis of $[(\mathbf{Me_2PzQu})_2Zn(OPEt_3)](OTf)_2$ (**4-Qu**).

To a solution of $[(\mathbf{Me_2PzQu})_2Zn^{II}(OTf)](OTf)$ (0.050 g, 0.067 mmol) in acetonitrile (~2 mL), a solution of Et_3PO (0.009 g, 0 067mmol) in acetonitrile (~2 mL) was added dropwise under N_2 atmosphere. The resultant clear solution was stirred at room temperature for 6 h to obtain a clear solution. The reaction mixture was filtered, and the filtrate was dried under vacuum. Off-white sticky material thus obtained was washed with diethyl ether to afford $[(\mathbf{Me_2PzQu})_2Zn(OPEt_3)](OTf)_2$ (**4-Qu**) (0.049 g, 0.056 mmol) in 83% yield. ^{1}H NMR (500 MHz, CD_3CN): δ 8.53 (d, J = 8.4 Hz, 1H), 8.02 (d, J = 8.1 Hz, 1H), 7.87 (d, J = 8.6 Hz, 1H), 7.74 (t, J = 7.7 Hz, 1H), 7.69 – 7.56 (m, 2H), 6.05 (s, 1H), 5.63 (s, 2H), 2.41 (s, 3H), 2.37 (s, 3H), 1.80 – 1.75 (m, 8H), 0.98 (dt, J = 16.4, 7.7 Hz, 9H). (Figure S31). ^{31}P NMR (202 MHz, CD_3CN): δ 72.68 (Figure S32). Several attempts to grow X-ray quality single crystals of **4-Qu** were unsuccessful.

12. Synthesis and Characterization of $[(Me_2PzPy)_2Zn^{II}(ONO)](ClO_4)$



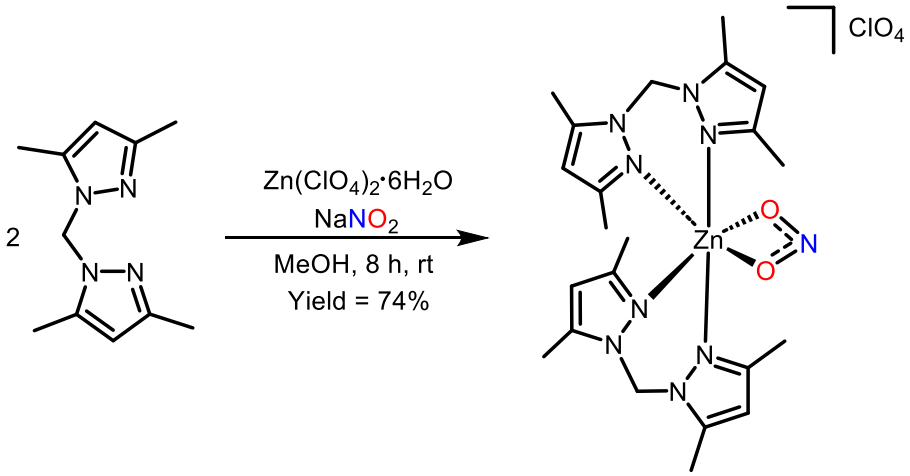
Scheme S10. Synthesis of complexes $[(\mathbf{Me_2PzPy})_2Zn^{II}(ONO)](ClO_4)$ (**5-Py**).

To a solution of $Zn(ClO_4)_2{\cdot}6H_2O$ (0.298g, 0.801 mmol) and $NaNO_2$ (0.055 g, 0.801 mmol) in methanol (~3 mL), a solution of **Me_2PzPy** (0.300 g, 1.602 mmol) in methanol (~3 mL)

was added dropwise under N_2 atmosphere. The resultant clear solution was stirred at room temperature for 8 h to obtain a clear solution with a white precipitate. The reaction mixture was filtered and subsequently washed with methanol and diethyl ether to obtain [(**Me$_2$PzPy**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Py**) (0.383 g, 0.654 mmol) in 81% yield. A similar synthetic protocol using Na^{15}NO$_2$ (instead of NaNO$_2$) provided ^{15}N-enriched [(**Me$_2$PzPy**)$_2$Zn^{II}(O^{15}NO)](ClO$_4$) (**5-Py-^{15}N**). ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.49 (d, J = 4.7 Hz, 1H), 7.83 (t, J = 7.6 Hz, 1H), 7.40 – 7.32 (m, 1H), 7.13 (d, J = 7.2 Hz, 1H), 5.91 (s, 1H), 5.30 (s, 2H), 2.23 (s, 3H), 2.09 (s, 3H) (Figure S33). ^{13}C NMR (126 MHz, DMSO-d_6): δ 156.17, 149.15, 147.18, 140.06, 138.09, 123.18, 122.14, 105.16, 52.52, 13.19, 10.69 (Figure S34). ^{15}N NMR (51 MHz, DMSO-d_6): δ 590.71 (Figure S35).

Anal. % Calcd for $C_{22}H_{26}ZnClN_7O_6$: C,45.14; H, 4.48; N, 16.75. Found: C, 45.54; H, 4.52; N, 16.79. Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **5-Py** in acetonitrile at room temperature (Figure S38). HRMS(+): *m/z calcd for* $[C_{22}H_{26}N_7O_2Zn]^+$: 484.1434; found: 484.1432 (Figure S36). FTIR (KBr pellet, cm^{-1}): 3408(m,br), 3014(w), 2929(w), 1602(s), 1550(s), 1475(s), 1435(s), **1273/1244(ν_{14NO2^-}/ν_{15NO2^-})**, 1145(s, ν_{ClO4}), 1085(s, ν_{ClO4}), 840(m), 771(s), 678(m), 630(s), 476(m), 416(m) (Figure S37).

13. Synthesis and Characterization of [(Me$_4$PzPz)$_2$Zn^{II}(ONO)](ClO$_4$)



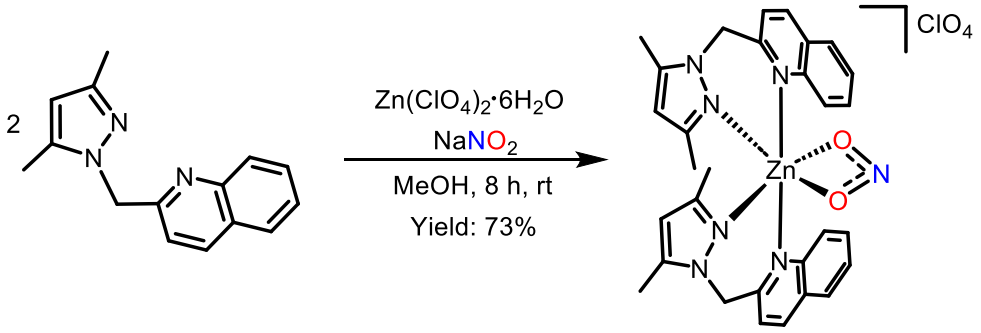
Scheme S11. Synthesis of [(**Me$_4$PzPz**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Pz**).

To a solution of Zn(ClO$_4$)$_2$·6H$_2$O (0.272 g, 0.731 mmol) and NaNO$_2$ (0.050 g, 0.731 mmol) in methanol (~3 mL), a solution of **Me$_4$PzPz** (0.300 g, 1.461 mmol) in methanol (~3 mL) was added dropwise under N_2 atmosphere. The resultant clear solution was stirred at room temperature for 8 h to obtain an off-white solution with a white-colored precipitate. The reaction

mixture was filtered, and the filtrate was washed with methanol and diethyl ether to obtain [(**Me$_4$PzPz**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Pz**) (0.334 g, 0.54 mmol) in 74% yield. A similar synthetic protocol using Na^{15}NO$_2$ instead of NaNO$_2$ provided ^{15}N-enriched [(**Me$_4$PzPz**)$_2$Zn^{II}(O^{15}NO)](ClO$_4$) (**5-Pz-^{15}N**). ^{1}H NMR (500 MHz, DMSO-*d*$_6$): δ 6.05 (s, 2H), 5.83 (s, 2H), 3.40 (s, 4H), 2.41 (s, 6H), 2.07 (s, 6H) (Figure S39). ^{13}C NMR (126 MHz, DMSO-*d*$_6$): δ 147.19, 140.06, 105.60, 58.75, 39.52, 13.32, 10.73 (Figure S40). ^{15}N NMR (51 MHz, DMSO-*d*$_6$): δ 589.66 (Figure S41).

Anal. % Calcd for $C_{22}H_{32}ClZnN_9O_6$ $(H_2O)_{0.45}$: C, 42.112; H, 5.28; N, 20.09. Found: C, 42.31; H, 5.23; N, 19.83. Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of **5-Pz** in acetonitrile at room temperature (Figure S44). HRMS(+): *m/z calcd for* $[C_{22}H_{32}N_9O_2Zn]^+$: 518.1965; found: 518.1962 (Figure S42). FTIR (KBr pellet, cm^{-1}): 3782(w), 3134(m), 3022(w), 2966(w), 2929(w), 1556(s), 1463(s), 1381(s), 1282(s), **1203/1180(ν_{14NO2^-}/ν_{15NO2^-})**, 1105(s, ν_{ClO4}), 1070(s, ν_{ClO4}), 827(s), 675(m), 624(s), 480(w) (Figure S43).

14. Synthesis and Characterization of [(Me$_2$PzQu)$_2$Zn^{II}(ONO)](ClO$_4$)



Scheme S12. Synthesis of [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Qu**).

To a solution of Zn(ClO$_4$)$_2$·6H$_2$O (0.235 g, 0.632 mmol) and NaNO$_2$ (0.044 g, 0.632 mmol) in methanol (~3 mL), a solution of **Me$_2$PzQu** (0.300 g, 1.264 mmol) in methanol (~3 mL) was added dropwise under N$_2$ atmosphere. The resultant clear solution was stirred at room temperature for 8 h to obtain an off-white solution with a yellow-white colored precipitate. The reaction mixture was filtered, and the filtrate was washed with methanol and diethyl ether to obtain [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Qu**) (0.317 g, 0.462 mmol) in 73% yield. A similar synthetic protocol using Na^{15}NO$_2$ instead of NaNO$_2$ provided ^{15}N-enriched [(**Me$_2$PzQu**)$_2$Zn^{II}(O^{15}NO)](ClO$_4$) (**5-Qu-^{15}N**). ^{1}H NMR (500 MHz, DMSO-*d*$_6$): δ 8.31 (d, *J* = 8.5 Hz, 1H), 7.96 (dd, *J* = 19.2, 8.3 Hz, 2H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H),

7.00 (d, J = 8.5 Hz, 1H), 5.90 (s, 1H), 5.45 (s, 2H), 2.21 (s, 3H), 2.10 (s, 3H). (Figure S45). ^{13}C NMR (126 MHz, DMSO-d_6): δ 157.88, 146.97, 146.62, 139.59, 137.26, 129.94, 128.57, 127.93, 126.96, 126.53, 119.26, 105.34, 54.28, 13.38, 10.78 (Figure S46). ^{15}N NMR (51 MHz, DMSO-d_6): δ 589.57 (Figure S47).

Colorless crystals suitable for single crystal X-ray diffraction were grown from the vapor diffusion of diethyl ether to a concentrated solution of [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)](ClO$_4$) in acetonitrile at room temperature (Figure S50). HRMS(+): *m/z calcd for* [$C_{30}H_{30}N_7O_2Zn$]$^+$: 584.1747; found: 584.1744 (Figure S48). FTIR (KBr pellet, cm^{-1}): 3398(m,br), 3064(w), 2926(w), 1598(m), 1552(m), 1510(m), 1469(m), 1429(m), **1269/1242**(ν_{14NO2}–/ν_{15NO2}–), 1143(s, ν_{ClO4}), 1118(s, ν_{ClO4}), 1082(s, ν_{ClO4}), 972(w), 902(w), 813(m), 704(w), 630(s), 536(w) (Figure S49).

15. Reactions of [L$_2$Zn^{II}(ONO)]ClO$_4$ (5-Py/ 5-Pz/ 5-Qu) with ^{t}BuBnSH

See **Section 18** for the analysis of headspace on the reactions of [**L**$_2$Zn^{II}(ONO)]ClO$_4$ (**5-Py/ 5-Pz/ 5-Qu**) and 4-*tert*-butylbenzyl thiol (^{t}BuBnSH).

The % amounts of unreacted thiol and thiol-derived products (RSNO and RSSR) were determined from the relative integrations of the benzylic-proton resonances of ^{t}BuBnSH, ^{t}BuBnSNO, and (^{t}BuBnS)$_2$ at 3.72 (2H), 4.65 (2H) and 3.59 (4H) ppm, respectively. These chemical shifts are comparable with the previous literature.[8]

(a) Reactivity of [(Me$_2$PzPy)$_2$Zn^{II}(ONO)]ClO$_4$ (5-Py) with 1 equivalent of ^{t}BuBnSH

Under an inert atmosphere of a glovebox, a solution of [(**Me$_2$PzPy**)$_2$Zn^{II}(ONO)]ClO$_4$ (0.020 g, 0.034 mmol) in anhydrous acetonitrile (~3 mL) was taken in a vial. Subsequently, a solution of ^{t}BuBnSH (0.006 g, 0.034 mmol) in acetonitrile (~0.2 mL) was added to the vial. Stirring the reaction mixture at room temperature resulted in a faintly pink solution. After 12 h, solvent from the crude reaction mixture was removed in vacuo and the crude residue thus obtained was analysed by ^{1}H NMR and FTIR spectroscopy. ^{1}H NMR of the crude reaction mixture showed 17% of ^{t}BuBnSNO along with disulfide and unreacted thiol (Figure S51). The FTIR analysis of the crude end product shows the band at 1269 cm^{-1}, thereby indicating that nitrite in complex **5-Py** was not consumed completely (Figure S53).

(b) Reactivity of [(Me$_4$PzPz)$_2$Zn^{II}(ONO)]ClO$_4$ (5-Pz) with 1 equivalent of ^{t}BuBnSH

Under an inert atmosphere of a glovebox, a solution of [(**Me$_4$PzPz**)$_2$Zn^{II}(ONO)]ClO$_4$ (**5-Pz**) (0.020 g, 0.032 mmol) in anhydrous acetonitrile (~3 mL) was taken in a vial. Subsequently, a solution of ^{t}BuBnSH (0.011 g, 0.064 mmol) in acetonitrile (~0.2 mL) was added to the vial. Stirring the reaction mixture at room temperature resulted in a faintly pink solution. After 12 h, solvent from the crude reaction mixture was removed in vacuo and the crude residue thus obtained was analysed by ^{1}H NMR and FTIR spectroscopy. ^{1}H NMR of the crude reaction mixture showed 19% of ^{t}BuBnSNO along with disulfide and unreacted thiol (Figure S55). The FTIR analysis of the crude end product shows the band at 1203 cm^{-1}, thereby indicating that nitrite in complex **5-Pz** was not consumed completely (Figure S53).

(c) Reactivity of [(Me$_2$PzQu)$_2$Zn^{II}(ONO)]ClO$_4$ (5-Qu) with 1 equivalent of ^{t}BuBnSH

Under an inert atmosphere of a glovebox, a solution of [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)]ClO$_4$ (**5-Qu**) (0.020 g, 0.029 mmol) in anhydrous acetonitrile (~3 mL) was taken in a vial. Subsequently, a solution of ^{t}BuBnSH (0.010 g, 0.058 mmol) in acetonitrile (~0.2 mL) was added to the vial. Stirring the reaction mixture for 12 h at room temperature resulted in a pink solution. The solvent from the crude reaction mixture was removed in vacuo and the crude residue thus obtained was analysed by ^{1}H NMR and FTIR spectroscopy. ^{1}H NMR of the crude reaction mixture showed 40% of ^{t}BuBnSNO along with disulfide and unreacted thiol (Figure S57). The FTIR analysis of the crude end product shows a very weak band at 1269 cm^{-1}, thus indicating near complete consumption of nitrite anion in **5-Qu** (Figure S53). The recrystallisation of the end product shows the formation of **2-Qu** in 88% yield (0.018 g, 0.013 mmol).

(d) Reactivity of [(Me$_2$PzPy)$_2$Zn^{II}(ONO)]ClO$_4$ with 2 equivalents of ^{t}BuBnSH

Under an inert atmosphere of a glovebox, a solution of [(**Me$_2$PzPy**)$_2$Zn^{II}(ONO)]ClO$_4$ (**5-Py**) (0.020 g, 0.034 mmol) in anhydrous acetonitrile (~3 mL) was taken in a vial. Subsequently, a solution of ^{t}BuBnSH (0.012 g, 0.068 mmol) in acetonitrile (~0.2 mL) was added to the vial. Stirring the reaction mixture at room temperature resulted in a faintly pink solution. After 12 h, solvent from crude the reaction mixture was removed in vacuo and the crude residue thus obtained was analyzed by ^{1}H NMR and FTIR spectroscopy. ^{1}H NMR of the crude reaction mixture showed 17% of ^{t}BuBnSNO along with disulfide and unreacted thiol (Figure S59). The FTIR analysis of the crude end product shows the band at 1272 cm^{-1}, thereby indicating that nitrite in complex **5-Py** was not consumed completely (Figure S60).

An analogous reaction using two equivalents of 4-methylthiophenol (4-Me-C_6H_4SH) and **5-Py** was carried out. The GCMS analysis of the end product shows the generation of corresponding disulfide (4-Me-$C_6H_4S)_2$ in near quantitative yield.

(e) Reactivity of [(Me$_4$PzPz)$_2$Zn^{II}(ONO)]ClO$_4$ with 2 equivalents of ^{t}BuBnSH

Under an inert atmosphere of a glovebox, a solution of [(**Me$_4$PzPz**)$_2$Zn^{II}(ONO)]ClO_4 (**5-Pz**) (0.020 g, 0.032 mmol) in anhydrous acetonitrile (~3 mL) was taken in a vial. Subsequently, a solution of ^{t}BuBnSH (0.011 g, 0.064 mmol) in acetonitrile (~0.2 mL) was added to the vial. Stirring the reaction mixture at room temperature resulted in a faintly pink solution. After 12 h, solvent from the crude reaction mixture was removed in vacuo and the crude residue thus obtained was analyzed by ^{1}H NMR and FTIR spectroscopy. ^{1}H NMR of the crude reaction mixture showed 22% of ^{t}BuBnSNO along with disulfide and unreacted thiol (Figure S62). The FTIR analysis of the crude end product shows the band at 1203 cm^{-1}, thereby indicating that nitrite in complex **5-Pz** was not consumed completely (Figure S63).

An analogous reaction using two equivalents of 4-Me-C_6H_4SH and **5-Pz** was carried out. The GCMS analysis of the end product shows the generation of (4-Me-$C_6H_4S)_2$ in near quantitative yield.

(f) Reactivity of [(Me$_2$PzQu)$_2$ Zn^{II}(ONO)]ClO$_4$ with 2 equivalents of ^{t}BuBnSH

Under an inert atmosphere of a glovebox, a solution of [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)]ClO_4 (**5-Qu**) (0.020 g, 0.029 mmol) in anhydrous acetonitrile (~3 mL), was taken in a vial. Subsequently, a solution of ^{t}BuBnSH (0.010 g, 0.058 mmol) in acetonitrile (~0.2 mL) was added to the vial. Stirring the reaction mixture at room temperature resulted in a pink solution. After 12 h, solvent from the crude reaction mixture was removed in vacuo and the crude residue thus obtained was analysed by ^{1}H NMR and FTIR spectroscopy. ^{1}H NMR of the crude reaction mixture showed 34% of ^{t}BuBnSNO, along with disulfide and unreacted thiol (Figure S65). The FTIR analysis of the crude end product shows the disappearance of the band at 1269 cm^{-1}, and thus indicating complete consumption of nitrite anion in **5-Qu** (Figure S66).

An analogous reaction using two equivalents of 4-Me-C_6H_4SH and [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)]ClO_4 (**5-Qu**) was carried out. The GCMS analysis of the end product shows the generation of (4-Me-$C_6H_4S)_2$ in near quantitative yield.

(g) UV-vis Monitoring of the Reaction of Complexes 5-Py/ 5-Pz/ 5-Qu with ^{t}BuBnSH

A 10 mM stock solution of [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)]ClO$_4$) (**5-Qu**) was prepared by dissolving a 0.034 g of **5-Qu** in 5 mL dry acetonitrile. Then, an aliquot of the stock solution (2.0 mL, 10 mM, 0.02 mmol) was taken in a quartz cuvette (path length 1.0 cm) and equipped with a magnetic stirring bar. The cuvette was capped with a rubber septum and placed in a Unisoku cryostat preset at 25 °C. ^{t}BuBnSH (8.0 μL, 0.04 mmol) was directly added to the cuvette. Subsequently, the reaction was followed by collecting the UV-vis spectrum at a time interval of 1 s, and the changes in the absorption features were monitored during the course of the reaction (Figure S68). Upon the addition of ^{t}BuBnSH, a fingers-like feature appeared in the range of 350-400 nm, while a new band around 550 nm developed subsequently. The appearance of a distinct band at 550 nm indicates the formation of ^{t}BuBnSNO. The observed changes in the absorption features are consistent with those reported previously.[7]

Analogous UV-vis experiments were performed for monitoring the reactions between **5-Pz** or **5-Py** and ^{t}BuBnSH (Figure S67-S69).

16. Catalytic Reactions of [(Me$_2$PzPy)$_2$Zn^{II}(OTf)]OTf (3-Py) with ^{t}BuBnSH

Under an inert atmosphere of a glovebox, a solution of [(**Me$_2$PzPy**)$_2$Zn(OTf)]OTf (**3-Py**) (0.005 g, 0.0067 mmol, 10 mol%) in anhydrous acetonitrile (~3 mL) was taken in a vial. Subsequently, a solution of ^{t}BuBnSH (0.024 g, 0.135 mmol) in acetonitrile (~0.2 mL) and *n*-tetrabutylammonium nitrite [TBA$^+$][NO$_2^-$] (0.019 g, 0.067 mmol) were added to the vial. The resultant pink solution was stirred for 12 h. The solvent from the crude reaction mixture was removed in vacuo, and the crude residue thus obtained was analysed by ^{1}H NMR and GCMS analysis. ^{1}H NMR of the crude reaction mixture showed 12% of ^{t}BuBnSNO along with disulfide and unreacted thiol (Figure S71).

The headspace on the catalytic reaction of **3-Py**, [TBA$^+$][NO$_2^-$], and ^{t}BuBnSH were analyzed for the quantification of NO gas as described in Section 18 (Figure S70 and Table S1).

The analogous reaction using NaNO$_2$ (instead of using [TBA$^+$][NO$_2^-$]) was also carried out following a similar procedure.

17. Catalytic Reactions of [(Me$_2$PzQu)$_2$Zn^{II}(OTf)]OTf with ^{t}BuBnSH

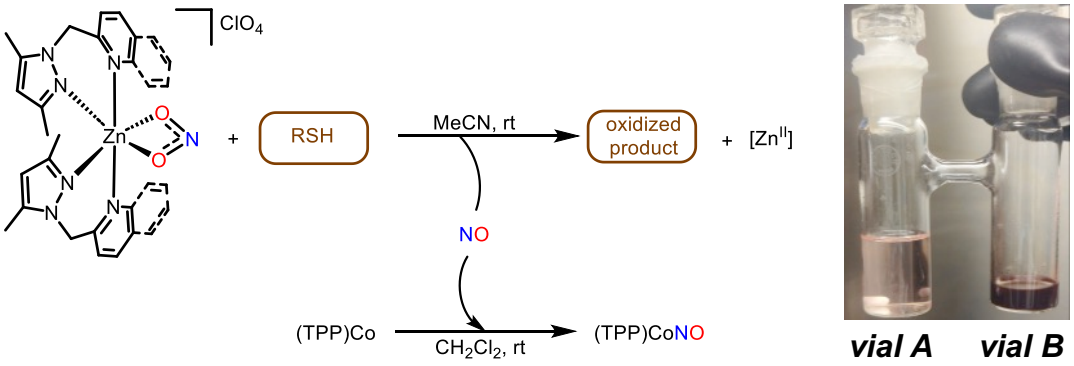
Under an inert atmosphere of a glovebox, a solution of [(**Me$_2$PzQu**)$_2$Zn^{II}(OTf)]OTf (**3-Qu**) (0.005 g, 0.006 mmol) in anhydrous acetonitrile (~3 mL), was taken in a vial. Subsequently, a solution of ^{t}BuBnSH, (0.021 g, 0.120 mmol) in acetonitrile (~0.2 mL) and [TBA$^+$][NO$_2^-$] (0.017 g, 0.060 mmol) were added to the vial. The resultant pink solution was stirred for 12 h.

The solvent from the crude reaction mixture was removed in vacuo and the crude residue thus obtained was analyzed by ^{1}H NMR and GCMS analysis. ^{1}H NMR of the crude reaction mixture showed the formation of 46% of ^{t}BuBnSNO along with disulfide and unreacted thiol (Figure S72).

The headspace on the catalytic reaction of **3-Qu**, [TBA$^+$][NO_2^-], and ^{t}BuBnSH was analyzed for the quantification of NO gas as described in Section 18 (Figure S73 and Table S1).

Following a similar protocol, the reaction of **2-Qu** (0.005 g, 0.005 mmol) with [TBA$^+$][NO_2^-] (0.015 g, 0.050 mmol) was performed (Table S1).The analogous reaction using $NaNO_2$ (instead of using [TBA$^+$][NO_2^-] was carried out following a similar procedure (Table S1).

18. Analysis of the Headspace for NO Trapping and Quantification



Scheme S13. Left: A representative scheme showing NO generation (in vial **A**) and NO trapping (in vial **B**). Right: A pictorial demonstration of "H-setup" utilized for the NO trapping experiments.

A "H-setup", as described elsewhere, was used for the trapping of NO using (TPP)Co^{II} complex under a N_2 atmosphere of glovebox (Scheme S13). Vial **A** of the "H-setup" was loaded with a solution of zinc(II)-nitrite complex **5-Qu** (0.020 g, 0.029 mmol) in acetonitrile (~2 mL). Vial **B** was charged with (TPP)Co^{II} (0.019 g, 0.029 mmol) solution in dichloromethane (~2 mL). Both the vials were equipped with magnetic stirrer bars and vial **B** was sealed with a glass stopcock. ^{t}BuBnSH (0.006 g, 6 μL, 0.029 mmol) was added to vial **A** and immediately sealed with a glass stopcock. The reaction mixtures in both vials were stirred at room temperature for 12 h. Then, the resultant solution in vial **B** was transferred to a round bottom flask and the solvent was evaporated under a reduced pressure. The crude residue, thus obtained, was analyzed by ^{1}H NMR (Figure S56). ^{1}H NMR of (TPP)Co(NO) (500 MHz, $CDCl_3$): δ 8.91 (s, 8H), 8.17 (d, J = 6.2 Hz, 8H), 7.73 (d, J = 7.2 Hz, 12H). ^{1}H NMR of (TPP)Co^{II} (500 MHz, $CDCl_3$): δ 15.95 (s, 8H), 13.16 (s, 8H), 9.94 (s, 8H), 9.74 (s, 4H). The yield of NO was calculated from the relative

integrals of the proton resonances of unreacted (TPP)Co^{II} and (TPP)Co(NO) and unreacted at δ = 15.95 and δ = 8.92 ppm, respectively.[9]

The analogous reactions of zinc(II)-nitrite complex **5-Py/ 5-Pz** (in 0.034/ 0.032 mmol scale) were performed and (TPP)Co^{II} (0.034/ 0.032 mmol) was used for trapping NO gas following a similar procedure as described above. In all cases, including the catalytic reaction of **3-Py**/ **3-Qu**, NO trapping experiments were conducted using the same equivalent of (TPP)Co^{II} with respect to the limiting reagent, namely nitrite anion. The yields of NO gas generated from the various reactions of zinc(II)-nitrite complexes are summarized in Table S1.

19. Computational Details

All calculations were performed using the Gaussian 16 suite of quantum chemical programs.[10] Geometry optimizations were carried out with the B3LYP[11] density functional by including the D3BJ (Grimme's D3 correction with Becke-Johnson damping)[12] dispersion corrections. Pople's double-ζ basis set 6-31G(d)[13] was used to describe the main group elements and the LANL2DZ[14] basis set and associated effective core potential (ECP) was used for the transition metal (Zn). All stationary points were verified to be local minima by all positive frequencies and transition states were verified to be first-order saddle points with one imaginary frequency corresponding to the reaction coordinate. Furthermore, transition states are confirmed to connect the right minima by the intrinsic reaction coordinate (IRC) analysis. To include the effect of solvation and find the more accurate electronic energy, single point energy calculations were performed at a higher level of theory including 6-311++G(d,p)[13] basis set for main group elements and LANL2TZ[15] basis set for the transition metal. The implicit solvation model based on density (SMD)[16] mimicking the solvation effect due to acetonitrile was employed.

To investigate the electron donation ability of the ligand in the metal complexes, solvent-phase geometry optimizations using the SMD(acetonitrile) solvent model were performed at the DFT-B3LYP level discussed above. Single point energy calculations were performed on optimized geometry with the B3LYP-D3BJ method and a combination of 6-311++G(d,p) and LANL2TZ basis set by using the NBO7 program, and the charge transfer donations were visualized by the NBOPro program.[17]

Metal Ligand Coordination

To verify the computational method, all three [$\mathbf{L}_2Zn^{II}(\kappa^2$-nitrite)]$^+$ (**L** = **Me_4PzPz**/ **Me_2PzPy**/ **Me_2PzQu**) complexes were optimized and their geometrical parameters were compared with the respective crystal structures (Table S2). The close correlation between the

bond length parameter obtained from the crystal structure and optimized geometries verified the reliability of the employed computational method.

To investigate the σ-donation ability of the ligand, natural bond orbital (NBO) analyses were performed for all three $[\mathbf{L}_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ complexes. The second-order perturbation energies (E_2, kcal/mol) due to the charge transfer interactions were obtained from NBO analysis, which quantifies the electron donation ability of the ligands and overall stabilization caused by the electron donation. As such, a higher value of E_2 signifies more stabilization due to the electron pair donation. Herein, a lone pair (LP) of nitrogen or oxygen atoms donates its electron density to the lone vacant (LV) orbital of the metal (Zn), the latter might be the 4*s* orbital of zinc. The charge-transfer donations can be visualized through NBO plots shown in Figure S74. From this analysis, it has been observed that $[(\mathbf{Me_4PzPz})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$, $[(\mathbf{Me_2PzPy})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$, and $[(\mathbf{Me_2PzQu})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ complexes experience 139.3, 127.5, and 119.4 kcal/mol, respectively stabilization energy due to the nitrogen lone pair to the lone vacant orbital of zinc metal centre (LP → LV). Additionally, the NO_2^- binding with the metal centre demonstrates that metal-oxygen stabilization energy does not change significantly by changing the heterocyclic ring ligands, which are 59.0, 53.5, and 56.8 kcal/mol for the $[(\mathbf{Me_4PzPz})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$, $[(\mathbf{Me_2PzPy})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$, and $[(\mathbf{Me_2PzQu})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ complexes respectively. Therefore, based on the bond length parameter and NBO analysis, it may be concluded that $[(\mathbf{Me_4PzPz})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ complex has the highest σ-donation ability. In contrast, the ligand in the $[(\mathbf{Me_2PzQu})_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ complex has the lowest σ-donation ability towards the zinc metal centre.

Mechanism of Thiol-Nitrite Interaction at Zinc(II)

We pursued two possible mechanistic scenarios for the formation of ^{t}BuBnSNO; the first mechanism is concerted transnitrosation and the second is the acid-base exchange mechanism. The separated complex $[\mathbf{L}_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ and ^{t}BuBnSH are used as the reference point, i.e., ΔG = 0.0 kcal/mol. In the first step, $[\mathbf{L}_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ coordinate with the ^{t}BuBnSH, leading to a coordinated reaction complex **(RC)**. Subsequently, **RC** can follow two possible mechanisms. In the concerted transnitrosation mechanism, **RC** undergoes a four-membered transition state with a free energy barrier of 31.2 kcal/mol (**TS-1**'), 38.7 kcal/mol (**TS-1**"), and 29.6 kcal/mol (**TS-1**) for **5-Pz**, **5-Py**, and **5-Qu**, respectively (Figure S75). This highly inaccessible transition state barrier of ~ 30 kcal/mol for the concerted transnitrosation mechanism makes this process redundant.

On the other hand, in the acid-base exchange mechanism, the reaction complex **(RC)** forms an intermediate **Int-1**, wherein the thiol S-atom of ^{t}BuBnSH is coordinated with the zinc(II) site of $[\mathbf{L}_2Zn^{II}(\kappa^2\text{-nitrite})]^+$. Intermediate, **Int-1**, then undergoes an intramolecular proton-transfer from the coordinated thiol to nitrite to generate **Int-2**, and HNO_2 is liberated. This process possesses a six-membered transition state (**TS-2**) with a free energy barrier of 25.2 kcal/mol, 22.7 kcal/mol, and 17.7 kcal/mol for **5-Pz**, **5-Py**, and **5-Qu**, respectively. Among the three complexes, **5-Qu** has the lowest transition state barrier of 17.7 kcal/mol, which highlights the role of the donation ability of the heterocyclic ring to the zinc metal centre and its effect on the reactivity. In the subsequent step, HNO_2 then reacts with the metal-bound sulfur to undergo *S*-nitrosation resulting in ^{t}BuBnSNO as a product and mononuclear zinc-hydroxo intermediate (**Int-4**), which rapidly dimerize to give highly thermodynamically stable product $[Zn_2^{II}(\mu\text{–}OH)]^{3+}$. Among both mechanisms, concerted transnitrosation suffers ~10 kcal/mol higher Gibbs free energy state barrier than the acid-base exchange mechanism. Therefore, a lower transition state barrier along with UV visible experimental verified the acid-base exchange mechanism as the most favourable mechanistic route. This combination of experimental and computational study highlights the role of ancillary ligands in the reactivity of *S*-nitrosation.

20. Figures

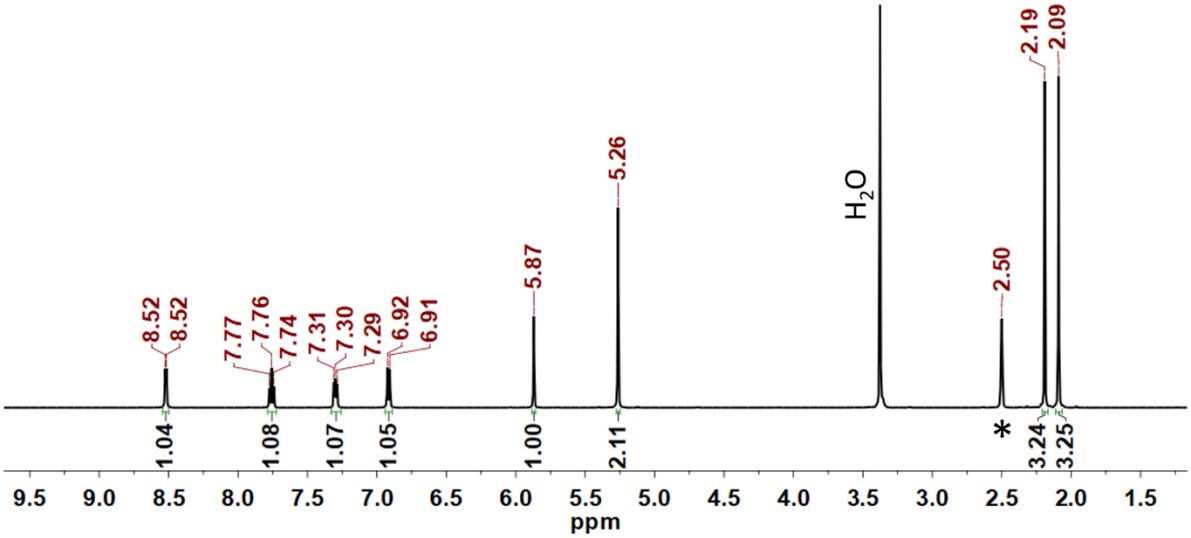


Figure S1. ^{1}H NMR spectrum (500 MHz, 298 K, DMSO-d_6) of [(**Me$_2$PzPy**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Py**). The resonance marked with * originates from DMSO-d_6.

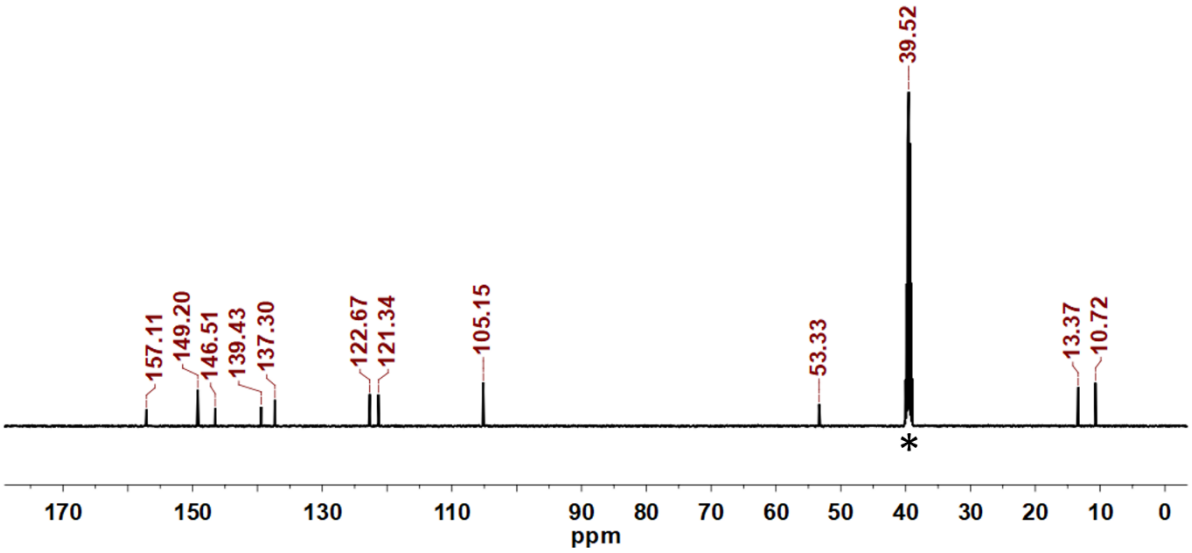


Figure S2. ^{13}C NMR spectrum (125 MHz, 298 K, DMSO-d_6) of [(**Me$_2$PzPy**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Py**). The resonance marked with * originate from DMSO-d_6.

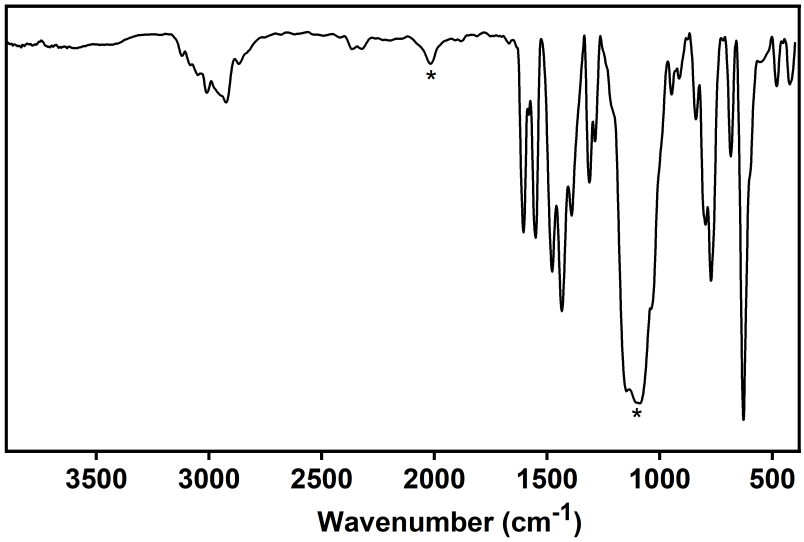


Figure S3. FTIR spectrum of [(**Me$_2$PzPy**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Py**). Asterisks indicate the vibrational features for perchlorate counterion (ν_{ClO4} = ~1087, 2015 cm^{-1}).

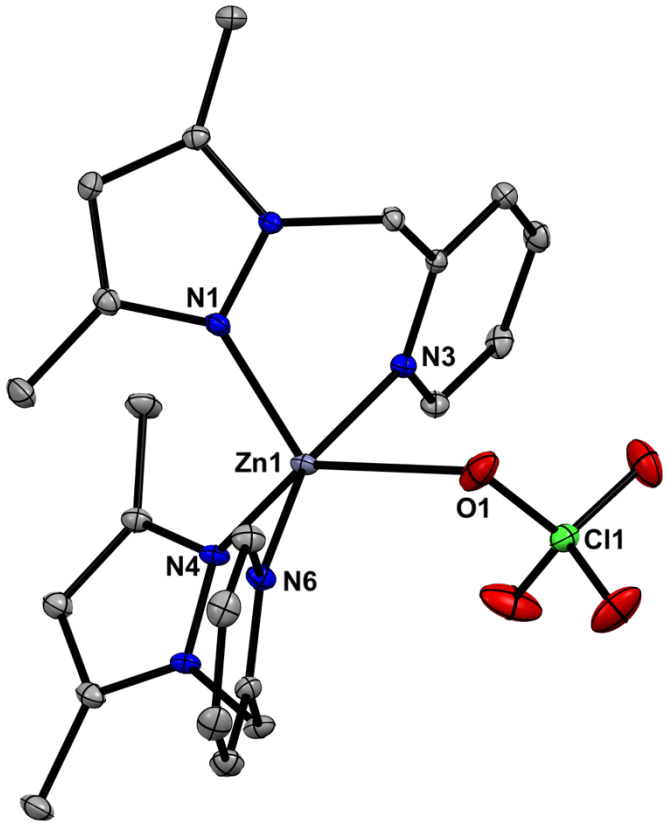


Figure S4. X-ray crystal structure of [(**Me$_2$PzPy**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Py**). Thermal ellipsoid plots are drawn at 30% probability level. One perchlorate anion and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-N1 2.052(1), Zn1-N3 2.065(1), Zn1-N4 2.051(1), Zn1-N6 2.072(1), Zn1-O1 2.450(2), N1-Zn1-N3 90.33(6), N1-Zn1-N4 111.56(7), N1-Zn1-N6 100.41(7), N1-Zn1-O1 106.95(6), N4-Zn1-N6 90.71(6), N4-Zn1-N3 101.33(6), N4-Zn1-O1 141.33(6), N3-Zn1-N6 159.74(7), N6-Zn1-O1 78.84(6), N3-Zn1-O1 81.62(6).

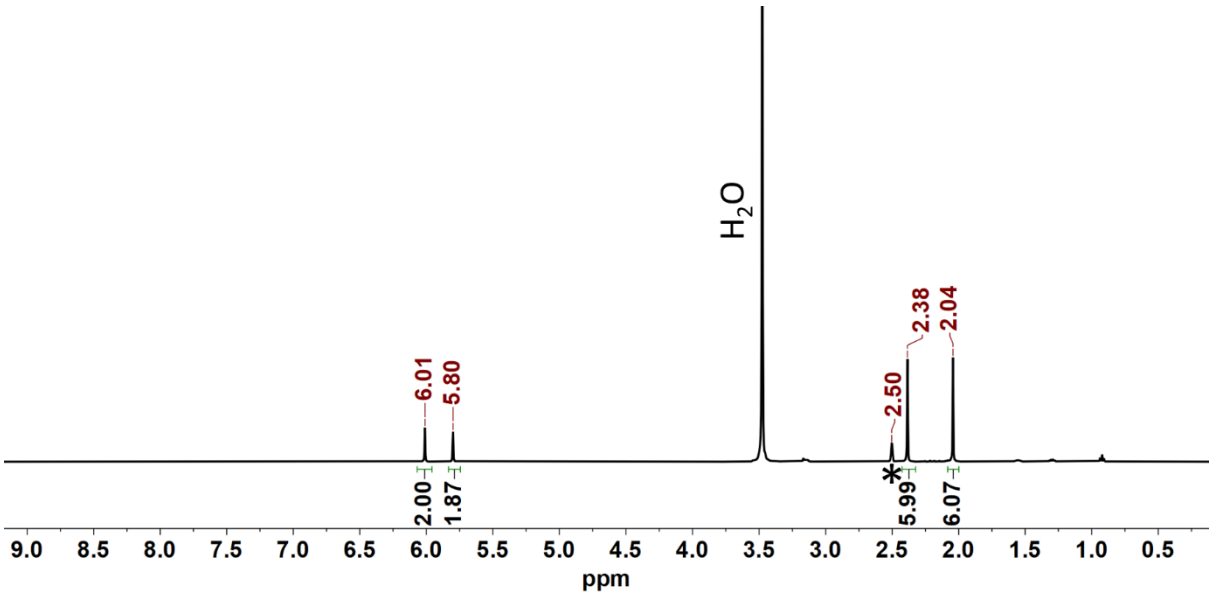


Figure S5. ^{1}H NMR spectrum (500 MHz, 298 K, DMSO-*d*$_6$) of [(**Me$_4$PzPz**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Pz**). The resonance marked with * originates from DMSO-*d*$_6$.

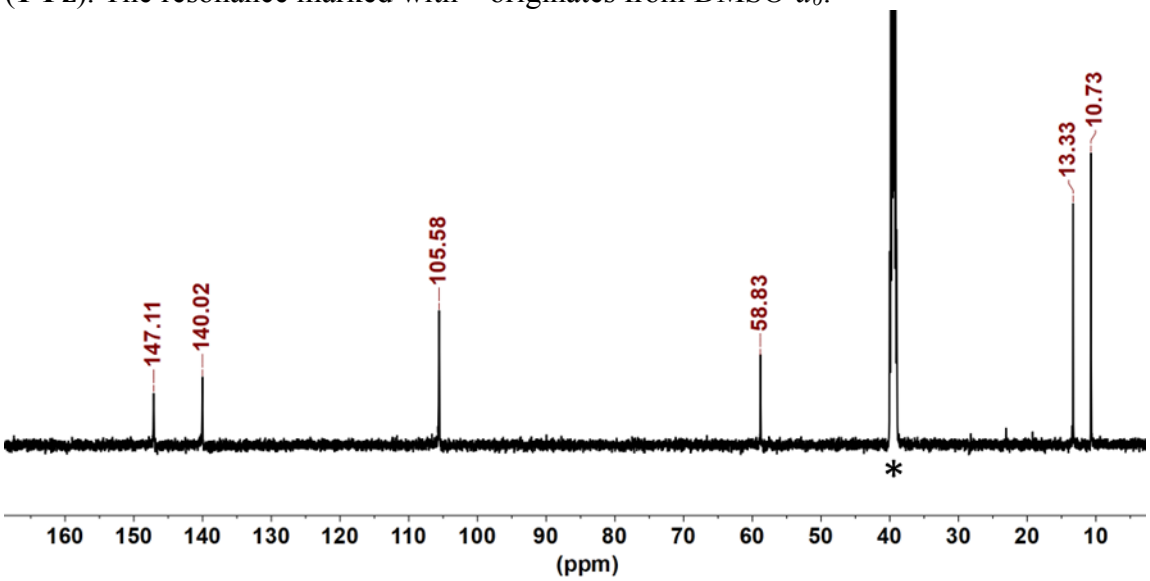


Figure S6. ^{13}C NMR spectrum (125 MHz, 298 K, DMSO-*d*$_6$) of [(**Me$_4$PzPz**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Pz**). The resonance marked with * originates from DMSO-d$_6$.

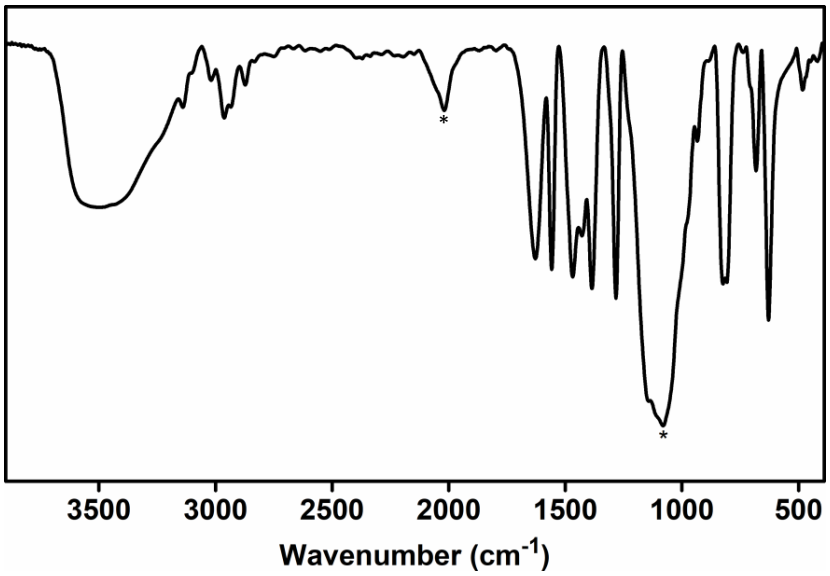


Figure S7. FTIR spectrum of [(**Me$_4$PzPz**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Pz**). Asterisks indicate the vibrational features for perchlorate counterion (ν_{ClO4} = ~1087, 2015 cm^{-1}).

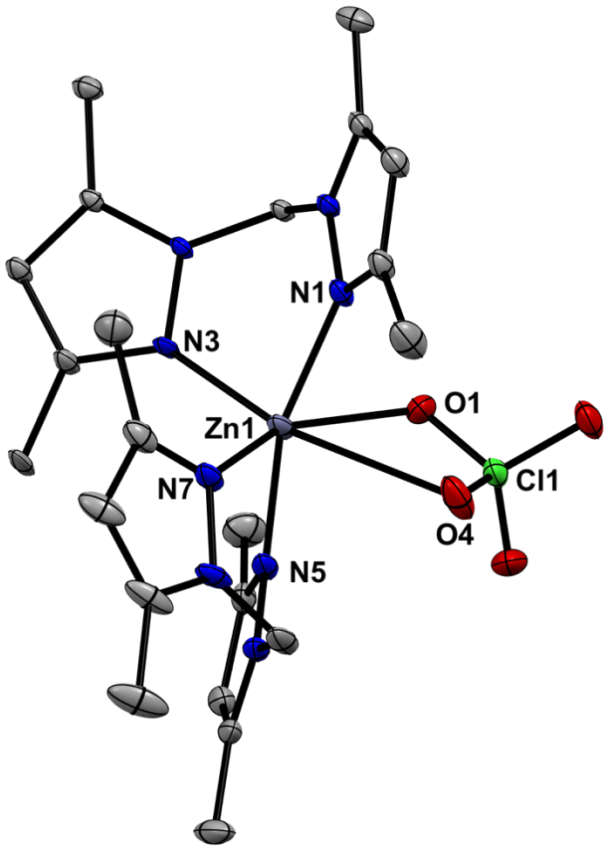


Figure S8. X-ray crystal structure of [(**Me$_4$PzPz**)$_2$Zn(OClO$_3$)](ClO$_4$) (**1-Pz**). Thermal ellipsoid plots are drawn at 30% probability level. One perchlorate anion, hydrogen atoms, and co-crystallized acetonitrile molecule are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-N1 2.088(6), Zn1-N3 2.084(7), Zn1-N5 2.055(4), Zn1-N7 2.078(4), Zn1-O1 2.474(3), Zn1-O4 2.548(4), N1-Zn1-N3 90.6(3), N1-Zn1-N5 163.1(4), N1-Zn1-N7 99.1(3), N3-Zn1-N5 101.0(3), N3-Zn1-N7 101.8(4), N5-Zn1-N7 90.49(4), N1-Zn1-O1 82.0(4), N3-Zn-O1 101.8(4), N5-Zn1-O1 83.70(12), N7-Zn1-N3 156.38(12), O1-Zn1-O4 55.03.

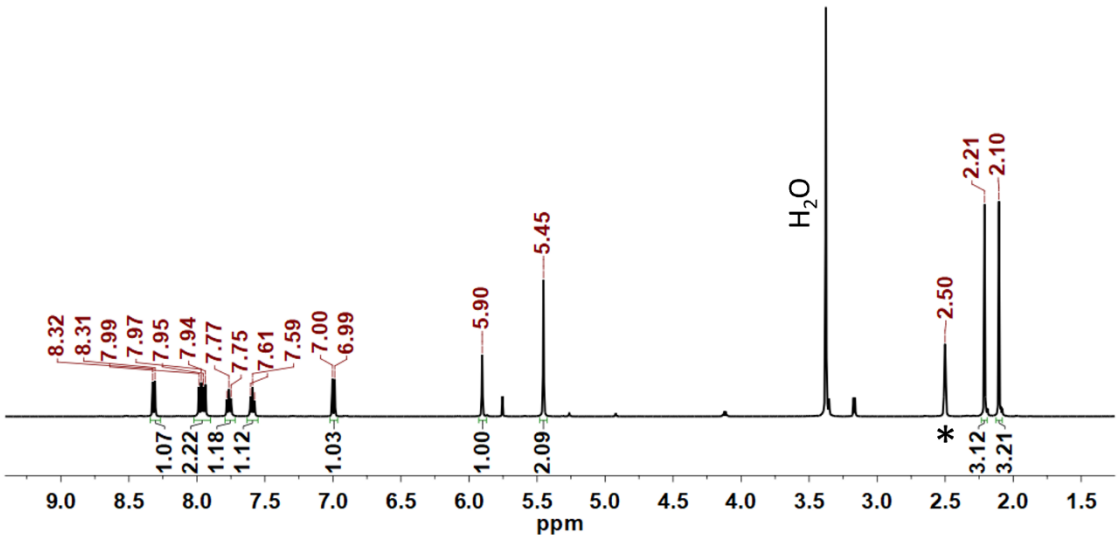


Figure S9. ^{1}H NMR spectrum (500 MHz, 298 K, DMSO-d_6) of [{(**Me$_2$PzQu**)$_2$Zn^{II}}$_2$(μ–OH)](ClO$_4$)$_3$ (**2-Qu**). The resonance marked with * originates from DMSO-d_6.

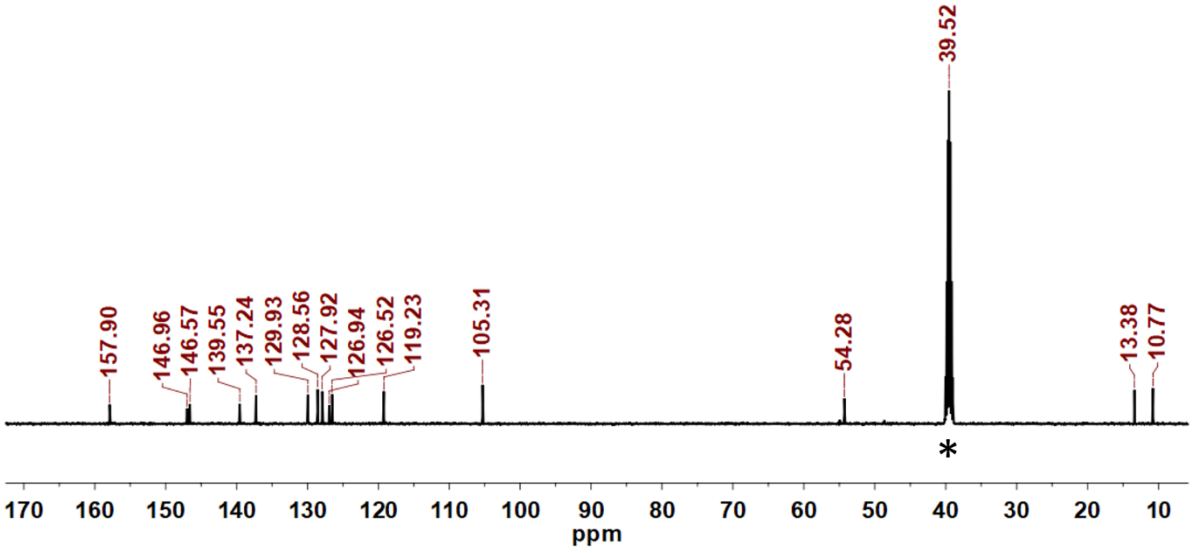


Figure S10. ^{13}C NMR spectrum (125 MHz, 298 K, DMSO-d_6) of [{(**Me$_2$PzQu**)$_2$Zn^{II}}$_2$(μ–OH)](ClO$_4$)$_3$ (**2-Qu**). The resonance marked with * originates from DMSO-d_6.

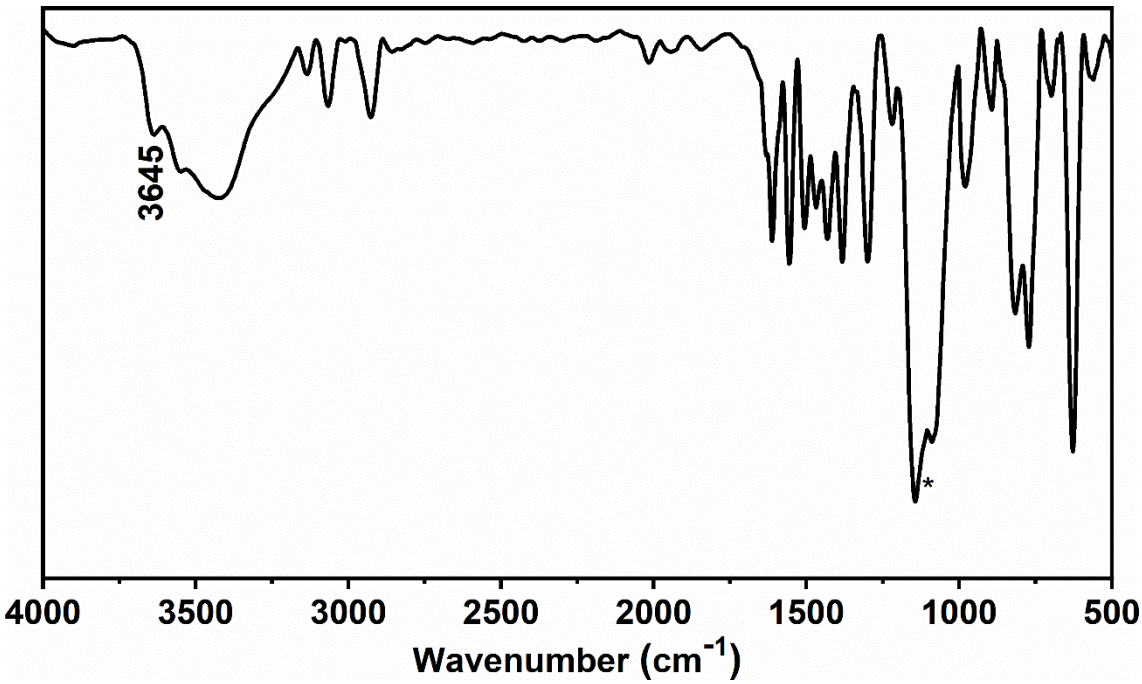


Figure S11. FTIR spectrum of [{(**Me$_2$PzQu**)$_2$Zn^{II}}$_2$(μ–OH)](ClO$_4$)$_3$ (**2-Qu**). Asterisks indicate the vibrational features for perchlorate counterion (ν_{ClO4} = ~1087 cm^{-1}).

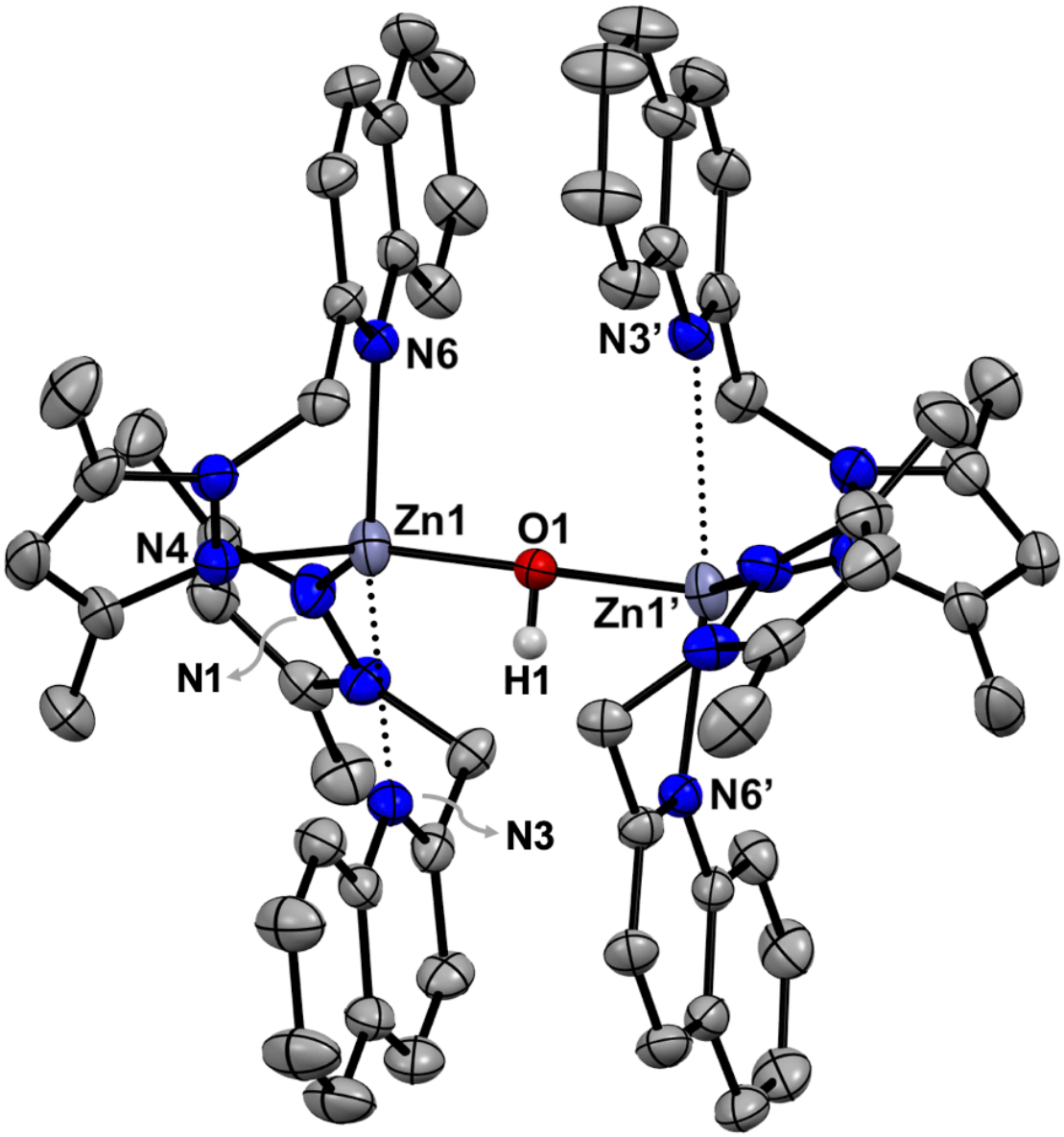


Figure S12. X-ray crystal structure of [{(**Me$_2$PzQu**)$_2$Zn^{II}}$_2$(μ–OH)](ClO$_4$)$_3$ (**2-Qu**). Thermal ellipsoid plots are drawn at 30% probability level. Perchlorate counter anions, co-crystallized solvent, and hydrogen atoms (except OH) are omitted for clarity. The atom sites labelled with prime are symmetry generated. While O1-H1 is shown, symmetry generated H1' is not shown for clarity. Selected bond distances (Å) and angles (°): Zn1-O1 1.889(2), Zn1-N1 1.964(4), Zn1···N3 2.720(9), Zn1-N4 2.062(5), Zn1-N6 2.212(9), O1-Zn1-N1 124.84(2), O1-Zn1-N4 120.99(3), N1-Zn1-N4 108.0(2), O1-Zn1-N6 92.3(2), N1-Zn1-N6 112.4(4), N4-Zn1-N6 90.3(2), Zn1-O1-Zn1 174.86(3).

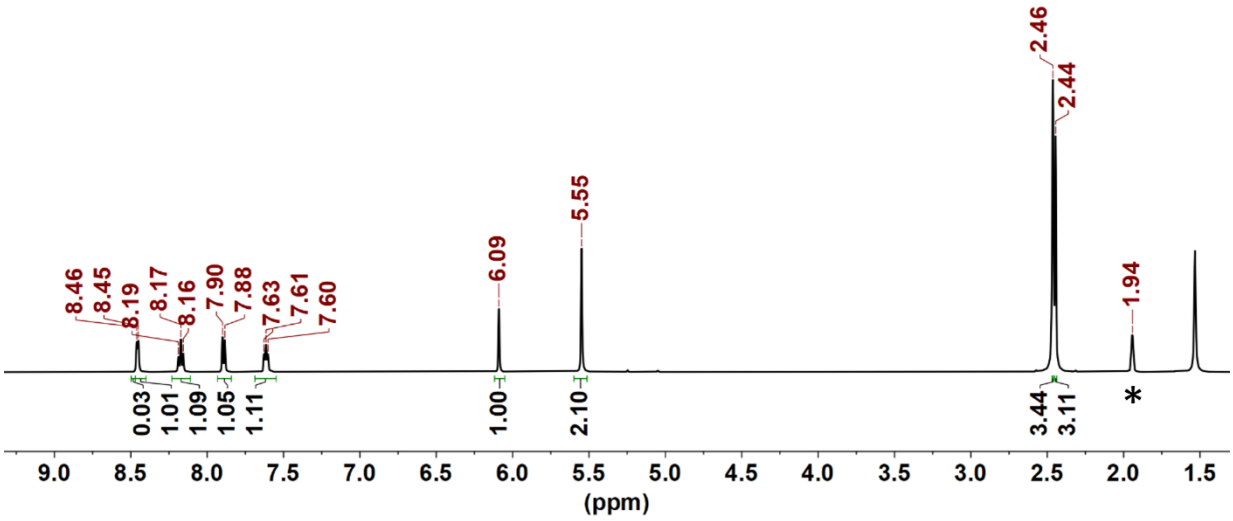


Figure S13. ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) of [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) (**3-Py**). The resonance marked with * originates from CD_3CN.

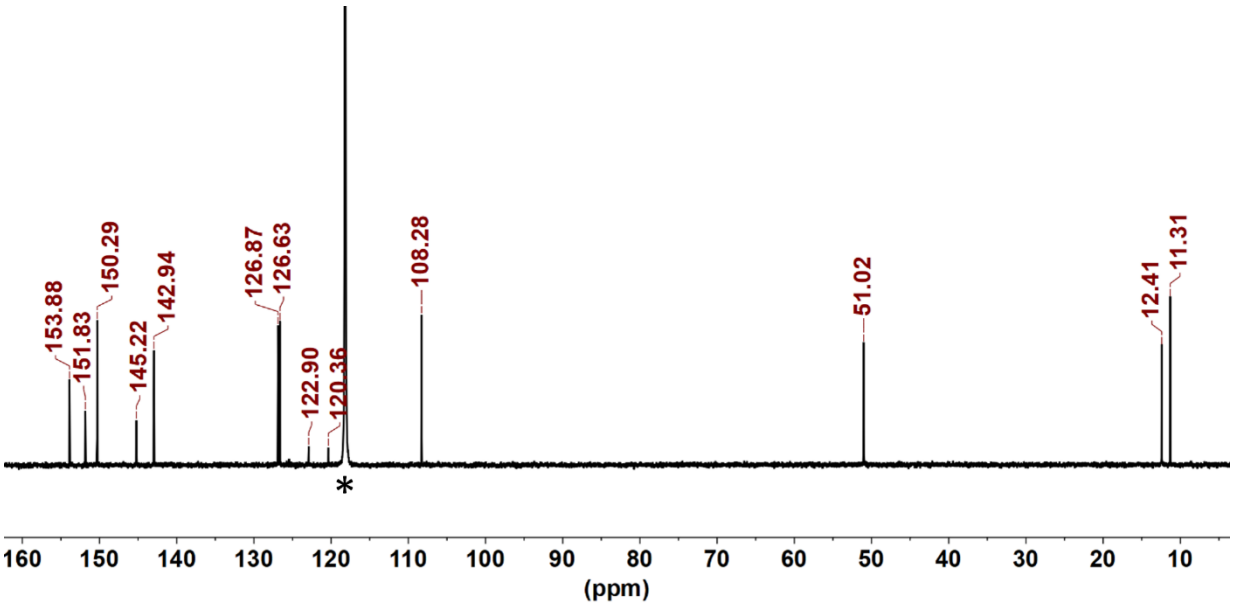


Figure S14. ^{13}C NMR spectrum (125 MHz, 298 K, CD_3CN) of [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) (**3-Py**). The resonance marked with * originates from CD_3CN.

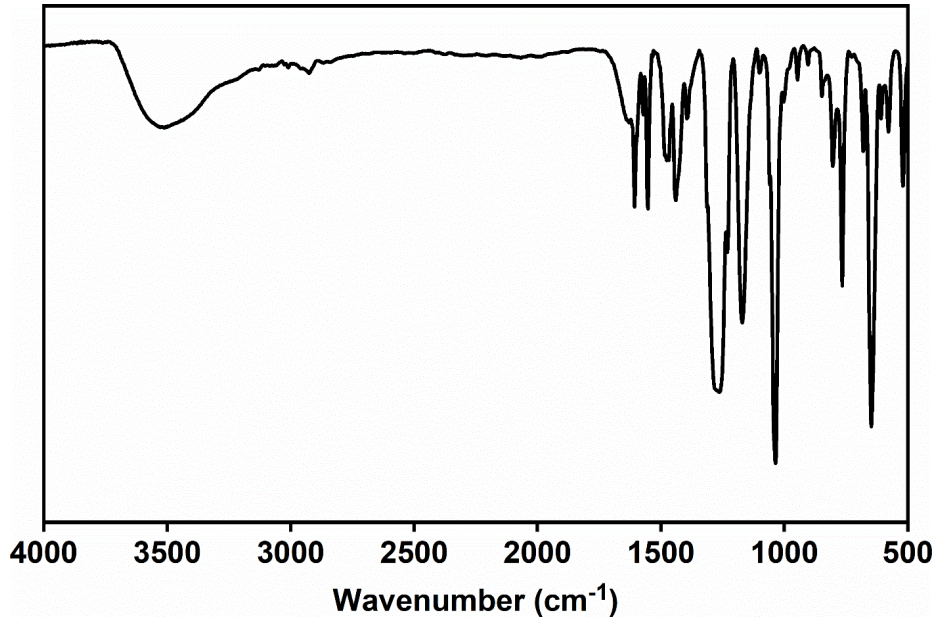


Figure S15. FTIR spectrum of [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) (**3-Py**).

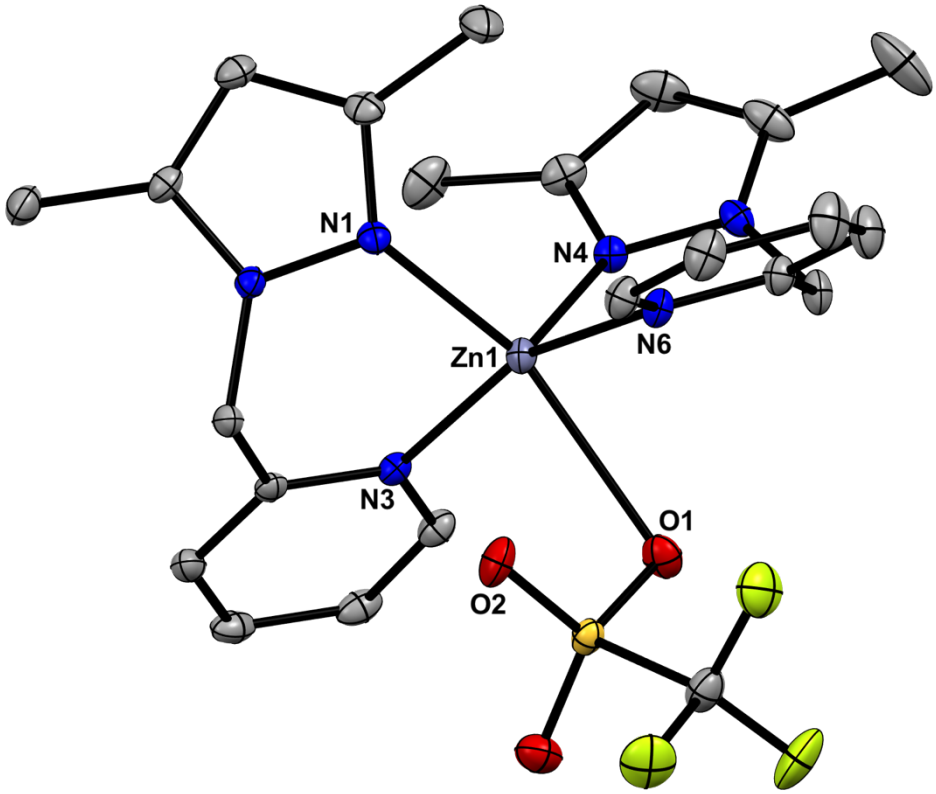


Figure S16. X-ray crystal structure of [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) (**3-Py**). Thermal ellipsoid plots are drawn at 30% probability level. One triflate anion and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-N1 2.058(2), Zn1-N3 2.069(2), Zn1-N4 2.031(2), Zn1-N6 2.056(2), Zn1-O1 2.542(2), Zn1-O2 2.621(2), N4-Zn1-N1 104.81(6), N4-Zn1-N6 93.56(6), N1-Zn1-N6 98.81(6), N4-Zn1-N3 101.48(6), N1-Zn1-N3 91.64(6), N6- Zn1-N3 158.89(6). N1-Zn1-O1 158.60(6), N3-Zn1-O1 82.33(5), N4-Zn1-O1 96.52(6), N6-Zn1-O1 81.31(6)

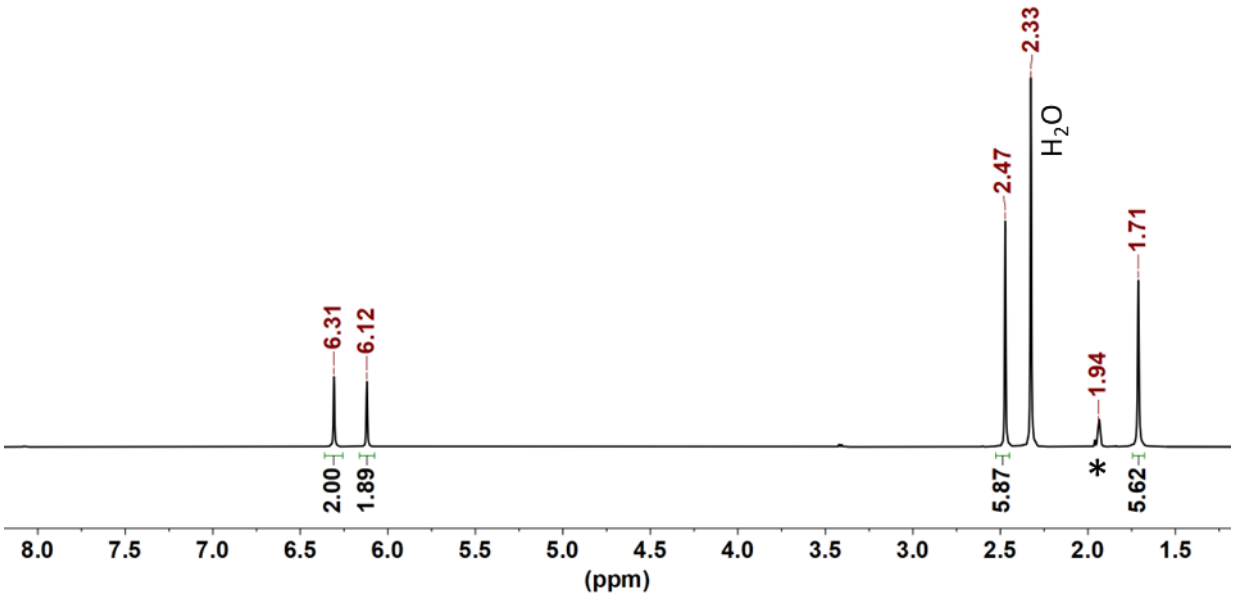


Figure S17. ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) of [(**Me$_4$PzPz**)$_2$Zn(OTf)](OTf) (**3-Pz**). The resonance marked with * originates from CD_3CN.

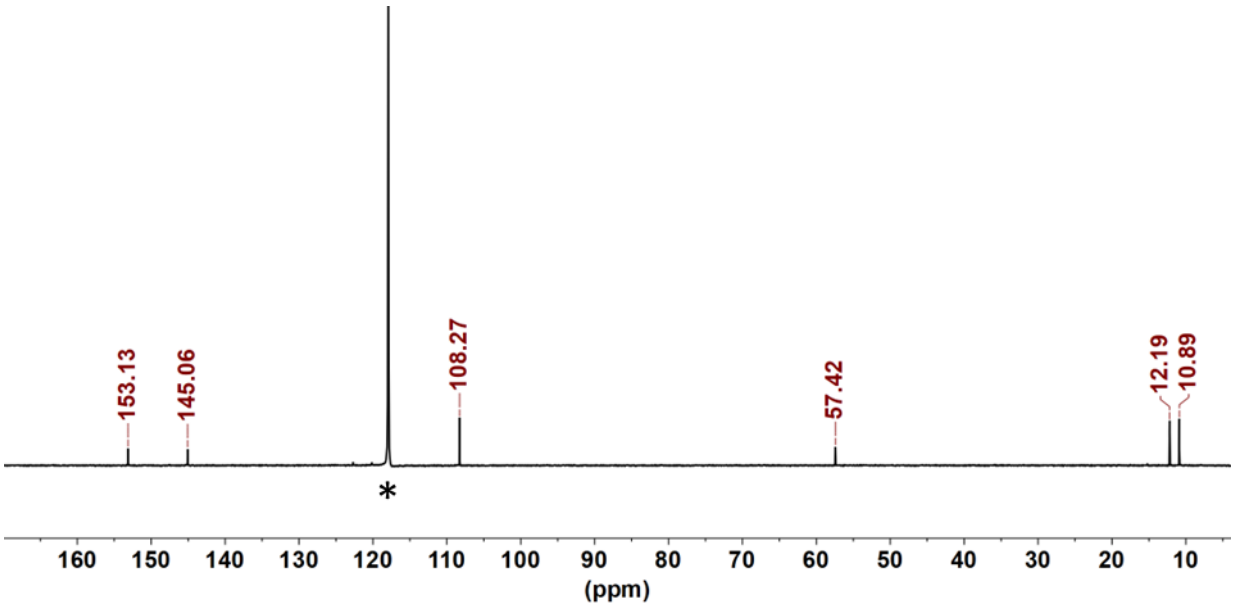


Figure S18. ^{13}C NMR spectrum (125 MHz, 298 K, CD_3CN) of [(**Me$_4$PzPz**)$_2$Zn(OTf)](OTf) (**3-Pz**). The resonance marked with * originates from CD_3CN.

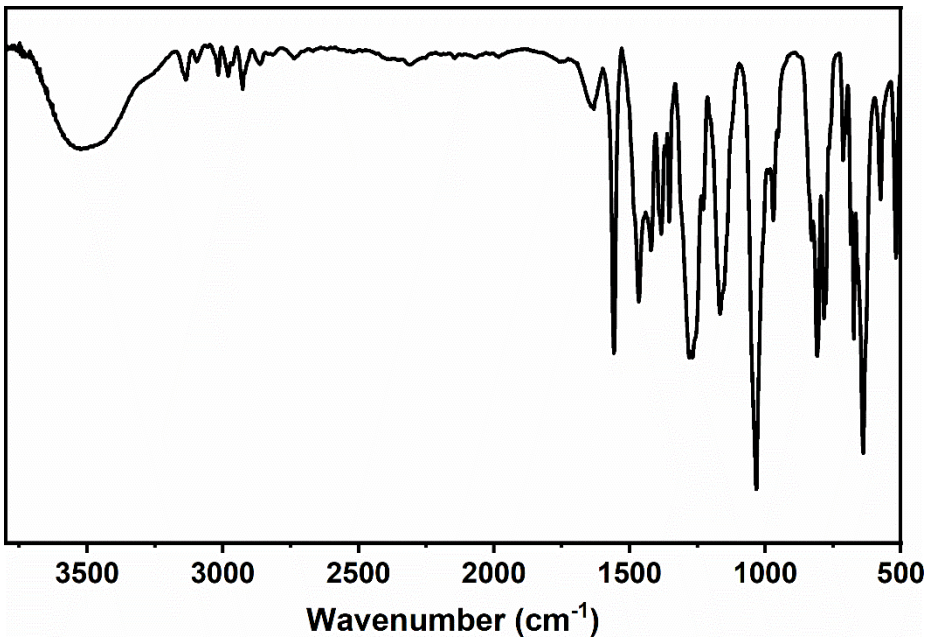


Figure S19. FTIR spectrum of [(**Me$_4$PzPz**)$_2$Zn(OTf)](OTf) (**3-Pz**).

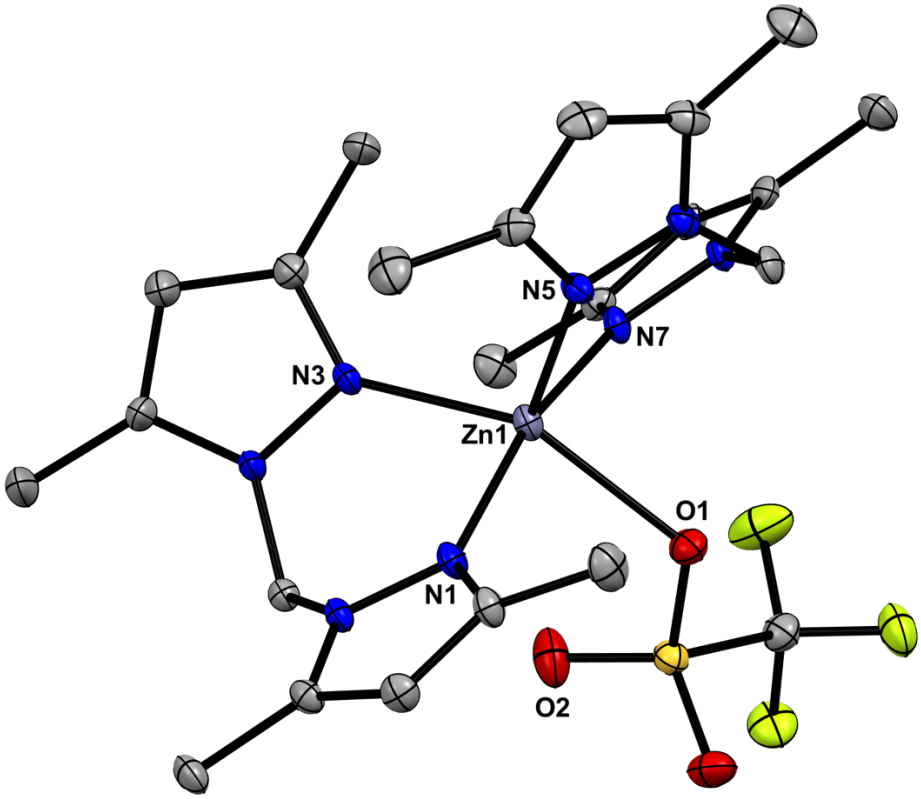


Figure S20. X-ray crystal structure of [(**Me$_4$PzPz**)$_2$Zn(OTf)](OTf) (**3-Pz**). Thermal ellipsoid plots are drawn at 30% probability level. One triflate anion and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-N1 2.096(5), Zn1-N3 2.082(4), Zn1-N4 2.057(4), Zn1-N7 2.080(4), Zn1-O1 2.178(4), N5-Zn1-N1 101.46(17), N3-Zn1-N1 88.34(17), N7-Zn1-N1 165.39(16), N7-Zn1-N3 95.93(16), N5-Zn1-N3 105.94(17), N5-Zn1-N7 90.82(16), N1-Zn1-O1 84.71(16), N3-Zn1-O1 148.86(15), N5-Zn1-O1 105.18(16), N7-Zn1-O1 84.44(16).

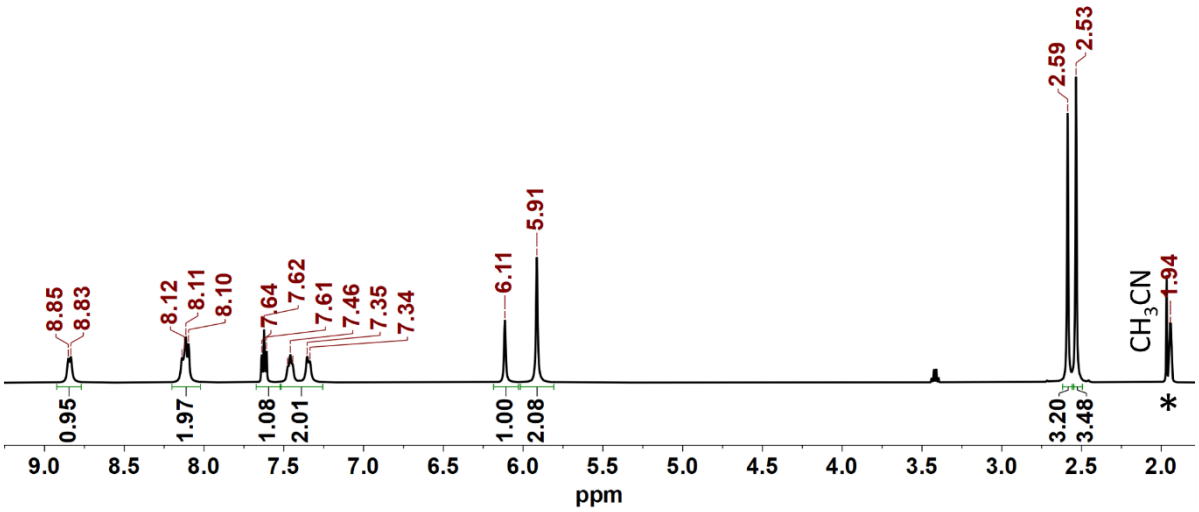


Figure S21. ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) of [(**Me$_2$PzQu**)$_2$Zn(OTf)](OTf) (**3-Qu**). The resonance marked with * originates from CD_3CN.

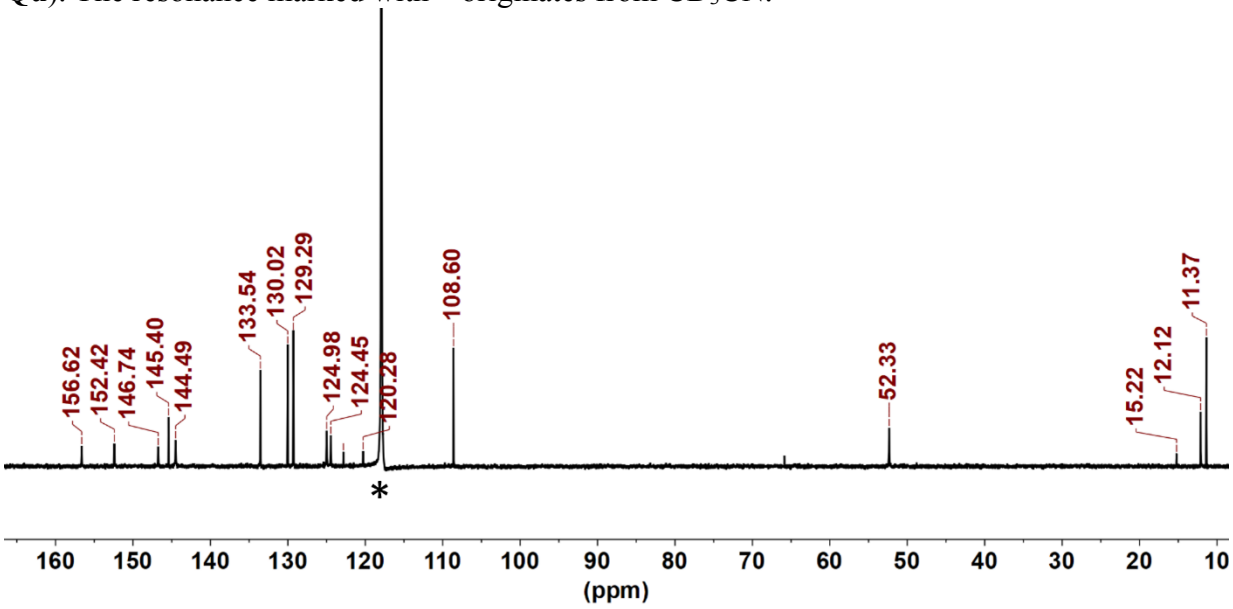


Figure S22. ^{13}C NMR spectrum (126 MHz, 298 K, CD_3CN) of [(**Me$_2$PzQu**)$_2$Zn(OTf)](OTf) (**3-Qu**). The resonance marked with * originates from CD_3CN.

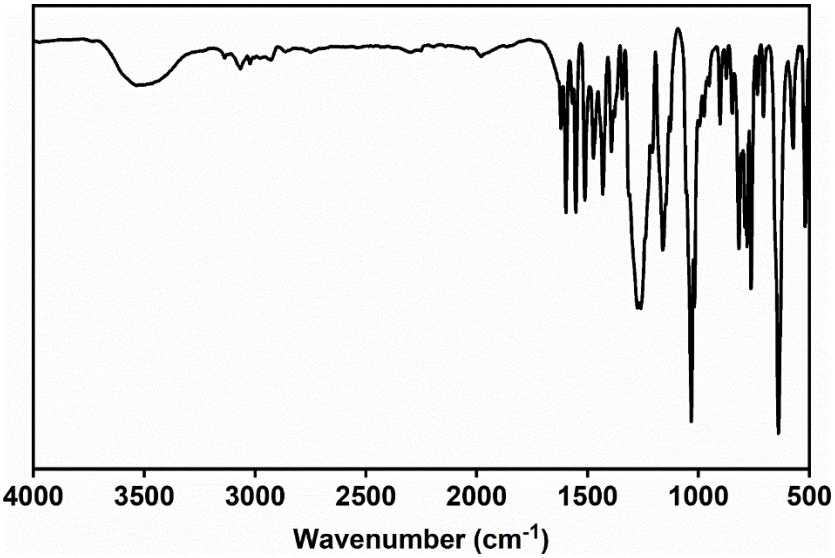


Figure S23. FTIR spectrum of [(**Me$_2$PzQu**)$_2$Zn(OTf)](OTf) (**3-Qu**).

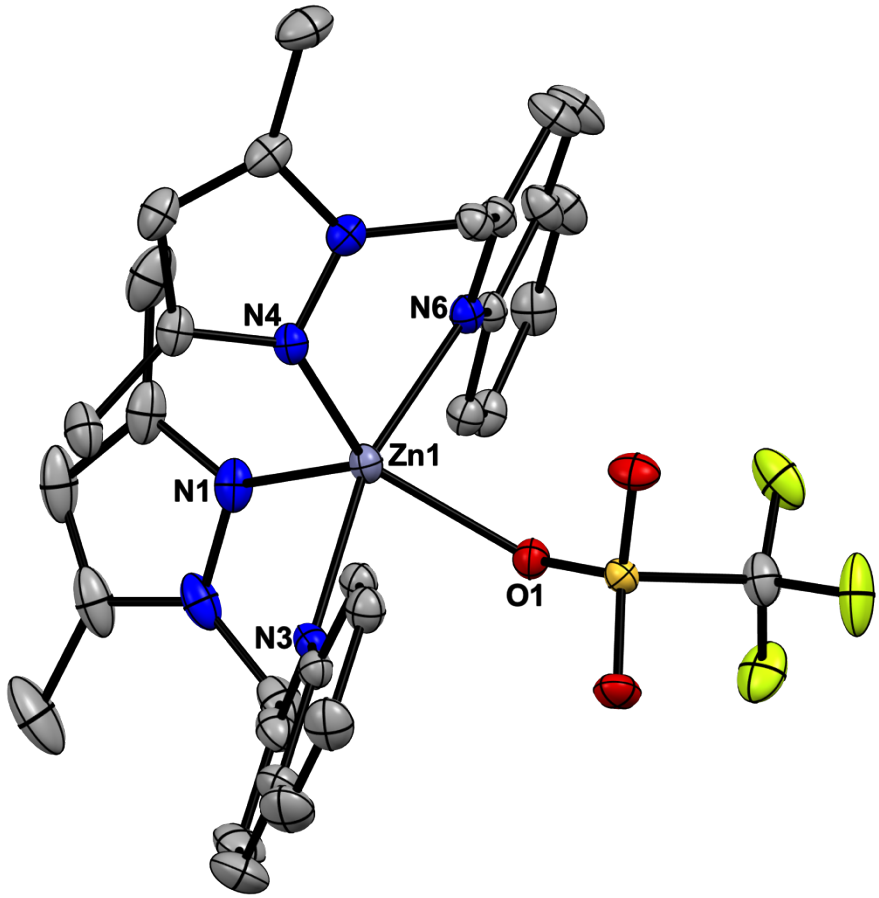


Figure S24. X-ray crystal structure of [(**Me$_2$PzQu**)$_2$Zn(OTf)](OTf) (**3-Qu**). Thermal ellipsoid plots are drawn at 30% probability level. One triflate anion and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-N1 2.039(2), Zn1-N3 2.245(2), Zn1-N4 2.025(2), Zn1-N6 2.212(2), Zn1-O1 2.098(2), N4-Zn1-N1 103.32(8), N4-Zn1-O1 136.76(8), N1-Zn1-O1 119.92(9), N4- Zn1-N6 90.63(7), N1-Zn1-N6 97.73(8), O1-Zn1-N6 84.29(8), N4-Zn1-N3 101.28(7), N1-Zn1-N3 89.28(8), O1-Zn1-N3 80.19(8), N6- Zn1-N3 164.45(7).

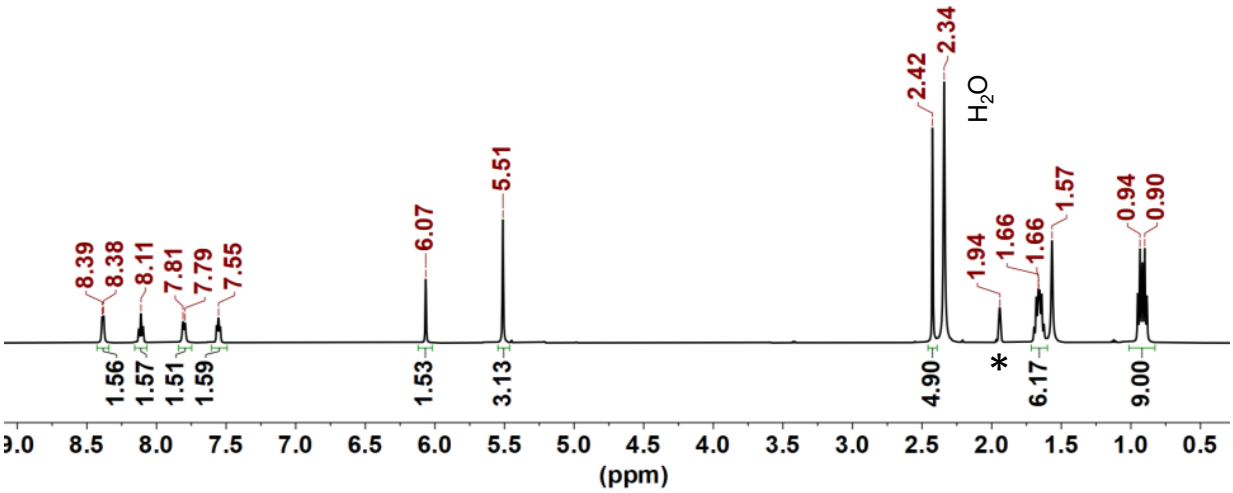


Figure S25. ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) of [(**Me$_2$PzPy**)$_2$Zn(OPEt$_3$)](ClO$_4$)$_2$ (**4-Py**) The resonance marked with * originates from CD_3CN.

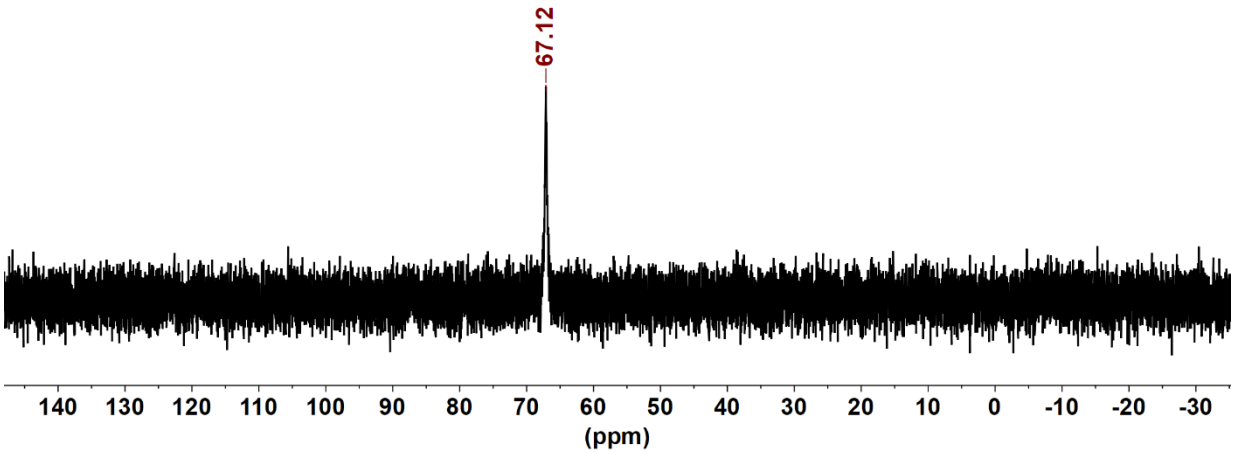


Figure S26. ^{31}P{^{1}H} NMR spectrum (202 MHz, 298 K, CD_3CN) of **4-Py**.

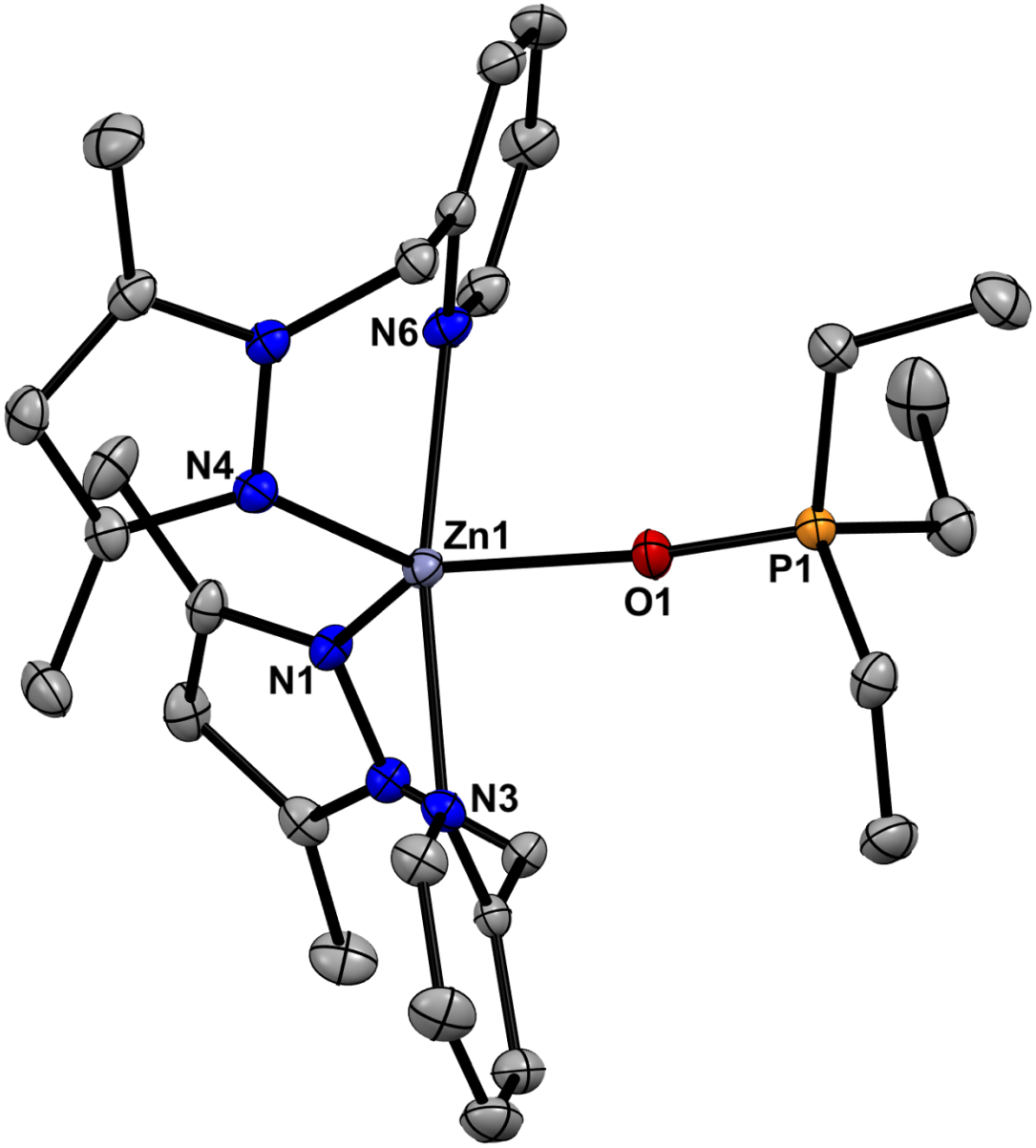


Figure S27. X-ray crystal structure of [(**Me$_2$PzPy**)$_2$Zn(OPEt$_3$)](ClO$_4$)$_2$ (**4-Py**). Thermal ellipsoid plots are drawn at 30% probability level. Two perchlorate anions and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn-O1 1.990(2), Zn-N1 2.040(2), Zn-N4 2.042(2), Zn-N3 2.157(2), Zn-N6 2.174(2), O1-P1 1.504(19), O1-Zn-N1 122.70(8), O1-Zn-N4 124.97(8), N1-Zn-N4 112.15(9), O1-Zn-N3 86.39(8), N1-Zn-N3 86.35(8), N4-Zn-N3 101.72(9), O1-Zn-N6 84.10(8), N1-Zn-N6 95.47(8), N4-Zn-N6 87.02(8), N3-Zn1-N6 169.70(8).

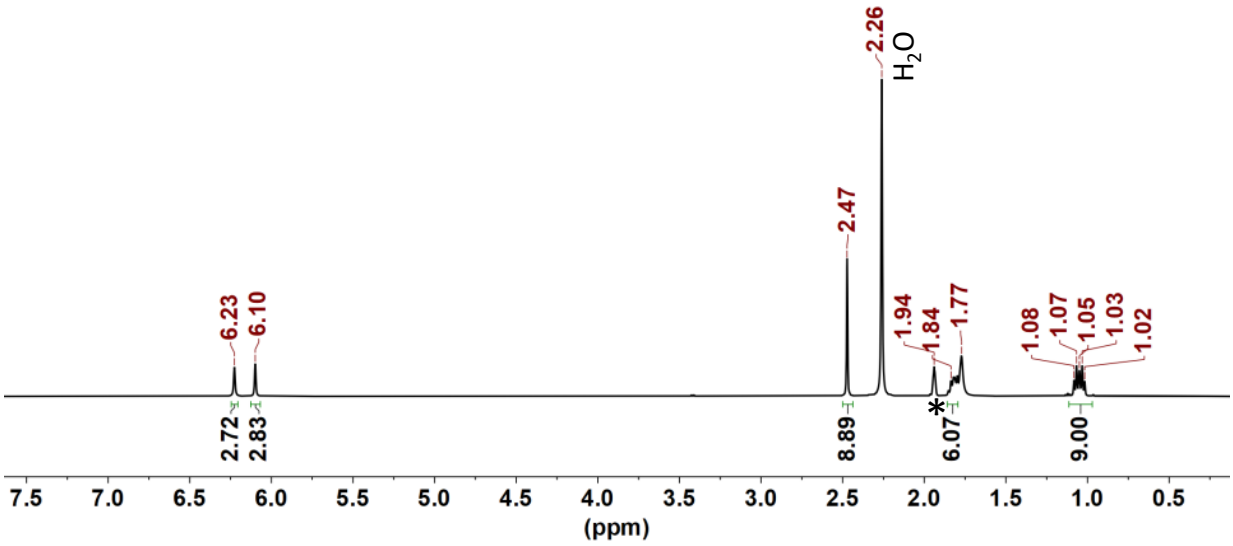


Figure S28. ^{1}H NMR spectrum (500 MHz, 298 K, CD_3CN) of [(**Me$_4$PzPz**)$_2$Zn(OPEt$_3$)](ClO$_4$)$_2$ (**4-Pz**). The resonance marked with * originates from CD_3CN.

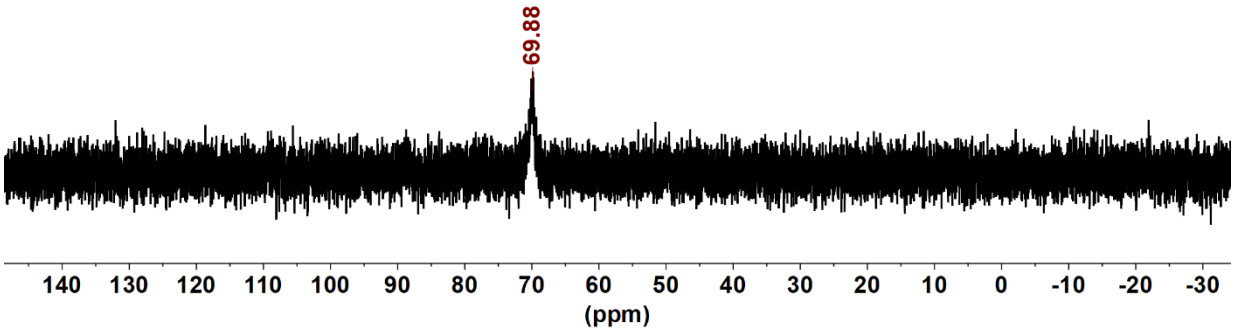


Figure S29. ^{31}P{^{1}H} NMR spectrum (202 MHz, 298 K, CD_3CN) of **4-Pz**.

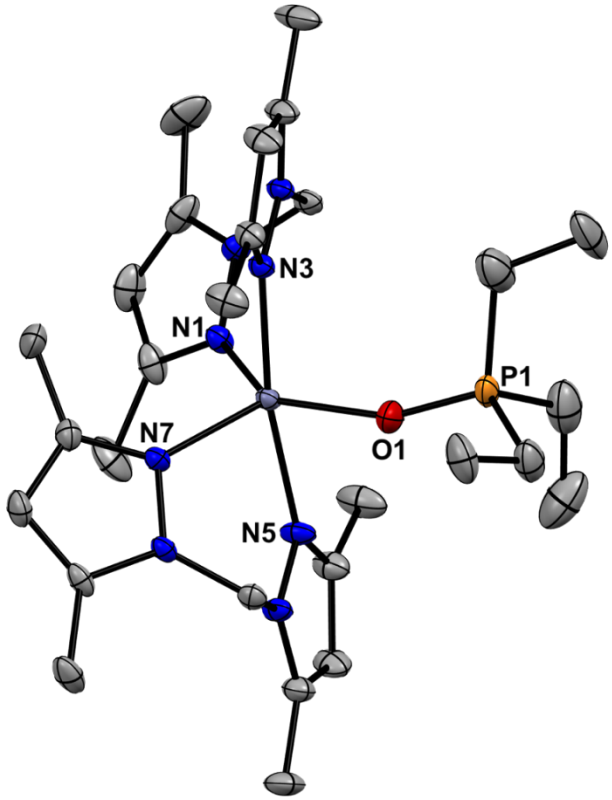


Figure S30. X-ray crystal structure of [(**Me$_4$PzPz**)$_2$Zn(OPEt$_3$)](ClO$_4$)$_2$ (**4-Pz**). Thermal ellipsoid plots are drawn at 30% probability level. Two perchlorate anions and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-O1 1.982(3), Zn1-N1 2.060(2), Zn1-N3 2.118(2), Zn1-N5 2.149(2), Zn1-N7 2.050(2), O1-Zn1-N7 114.86(15), O1-Zn1-N1 137.04(15), N7-Zn1-N1 108.04(10), O1-Zn1-N3 87.93(11), N7-Zn1-N3 98.43(9), N1-Zn1-N3 88.10(10), O1-Zn1-N5 83.38(12), N7-Zn1-N5 87.79(9), N1-Zn1-N5 96.35(10), N3-Zn1-N5 170.88(10).

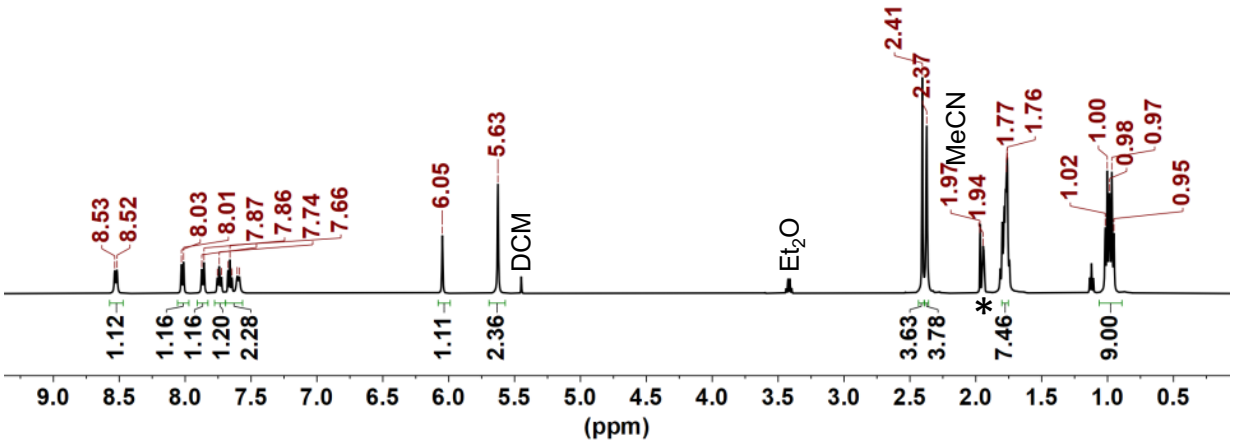


Figure S31. ^{1}H NMR spectrum (500 MHz, 298 K, CD$_3$CN) of [(**Me$_2$PzQu**)$_2$Zn(OPEt$_3$)](ClO$_4$)$_2$ (**4-Qu**). The resonance marked with * originates from CD$_3$CN. The proton resonances of CH$_2$Cl$_2$, Et$_2$O, and CH$_3$CN are likely originating from the glovebox atmosphere.

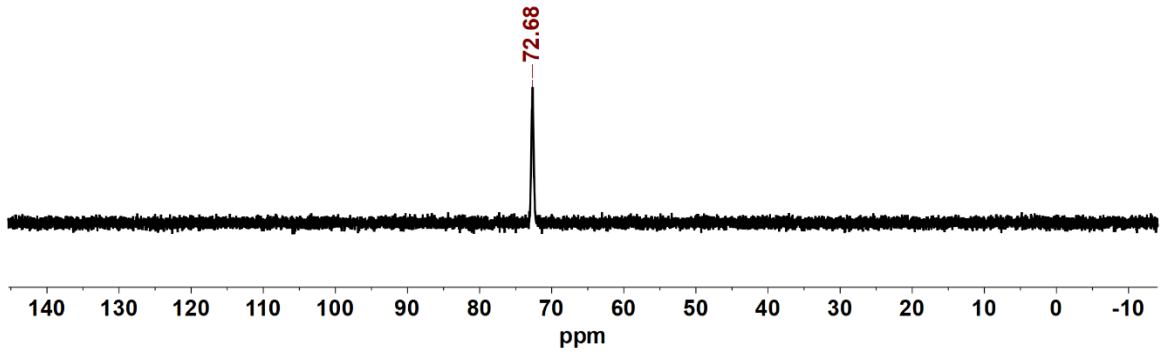


Figure S32. $^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, 298 K, CD_3CN) **4-Qu**.

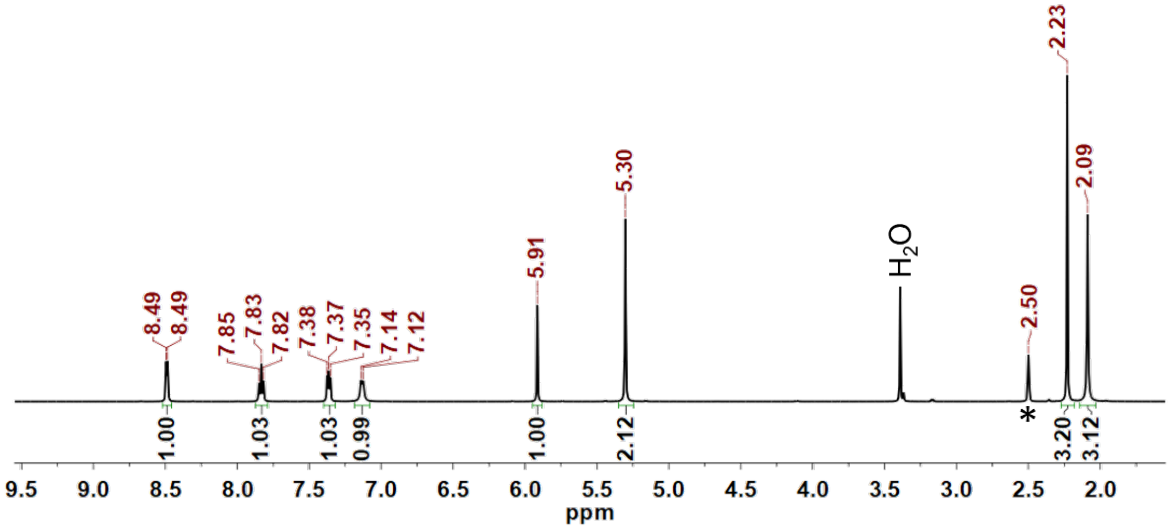


Figure S33. ^{1}H NMR spectrum (500 MHz, 298 K, DMSO-d_6) of [(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO_4) (**5-Py**). The resonance marked with * originates from DMSO-d_6.

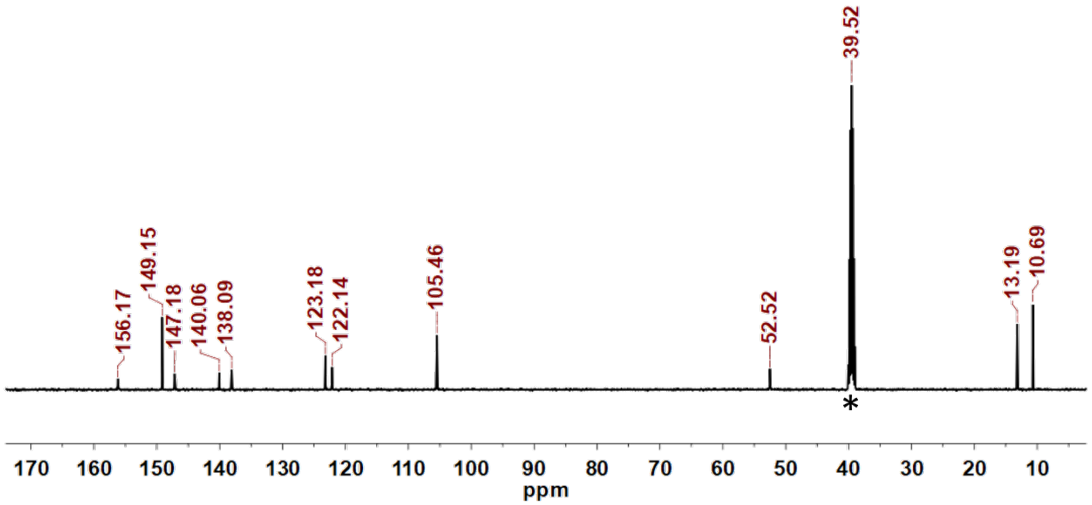


Figure S34. ^{13}C NMR spectrum (125 MHz, 298 K, DMSO-d_6) of [(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO_4) (**5-Py**). The resonance marked with * originates from DMSO-d_6.

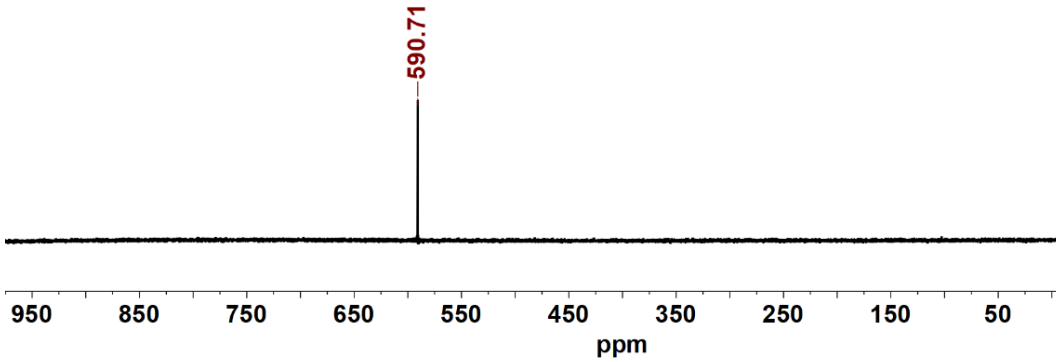


Figure S35. ^{15}N NMR spectrum (51 MHz, 298 K, DMSO-d_6) of [(**Me$_2$PzPy**)$_2$Zn(O^{15}NO)](ClO$_4$) (**5-Py-^{15}N**).

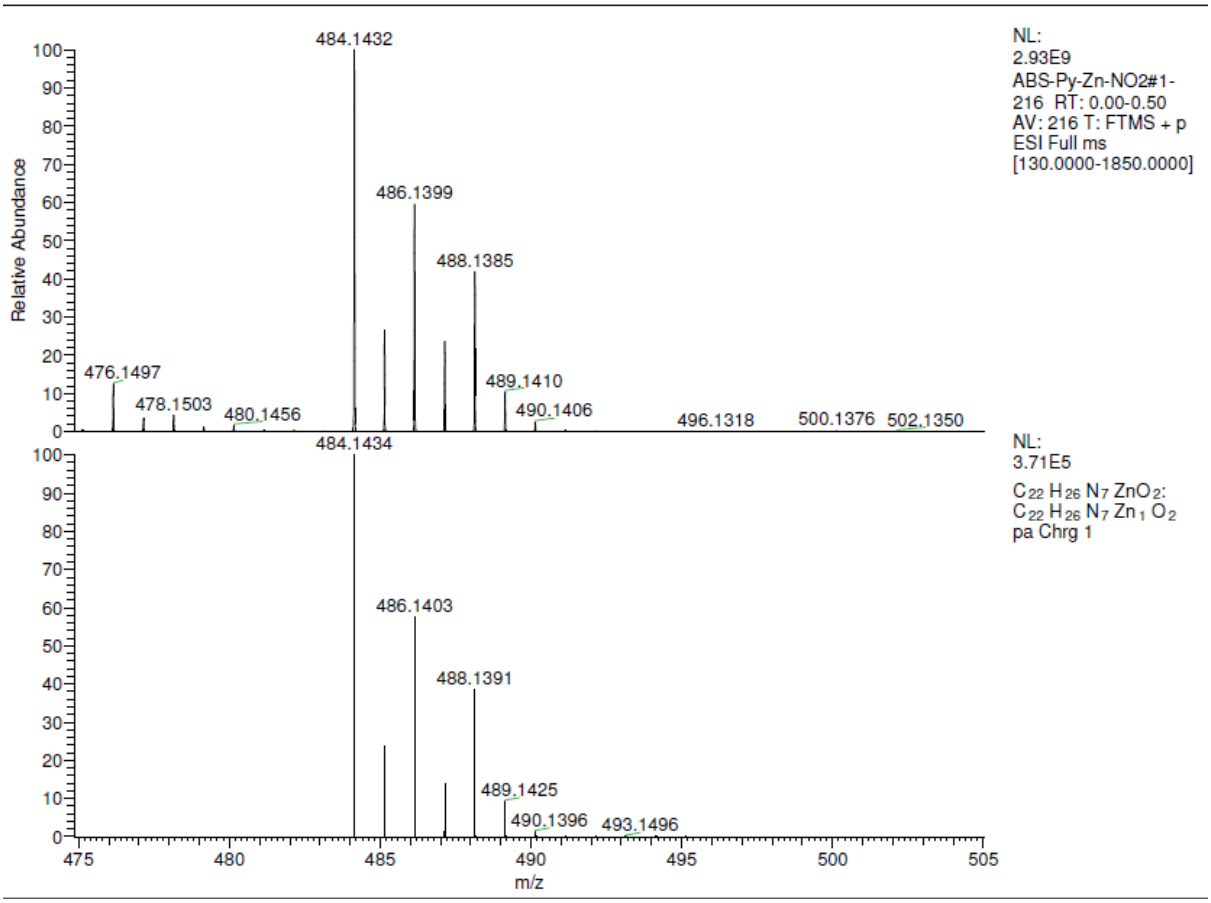


Figure S36. High resolution ESI-MS (+) spectrum of [(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO$_4$) (**5-Py**). The *m/z* peak at 484.1432 (*calc. m/z* 484.1434) originates from $[C_{22}H_{26}N_7O_2Zn]^+$.

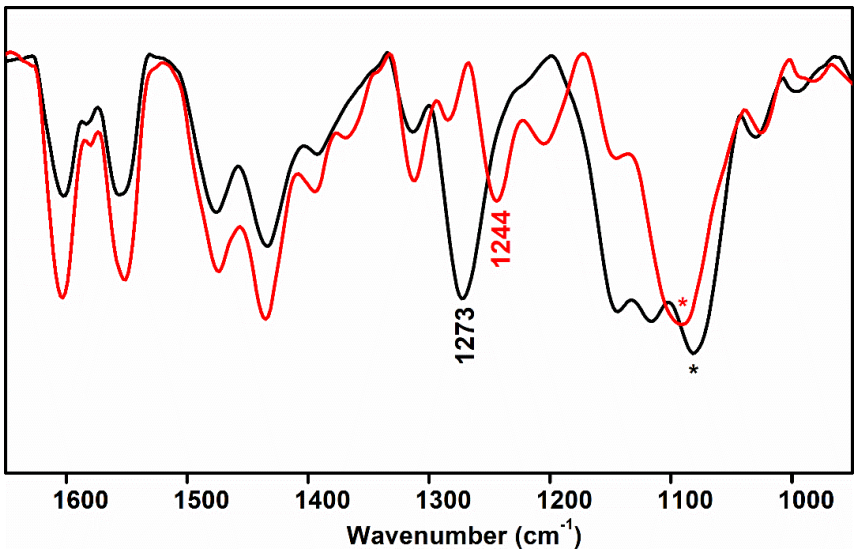


Figure S37. FTIR (KBr pellet) spectra of [(**Me$_2$PzPy**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Py**) (black trace) and [(**Me$_2$PzPy**)$_2$Zn^{II}(O^{15}NO)](ClO$_4$) (**5-Py-^{15}N**) (red trace). Asterisks indicate the vibrational features for perchlorate counterion.

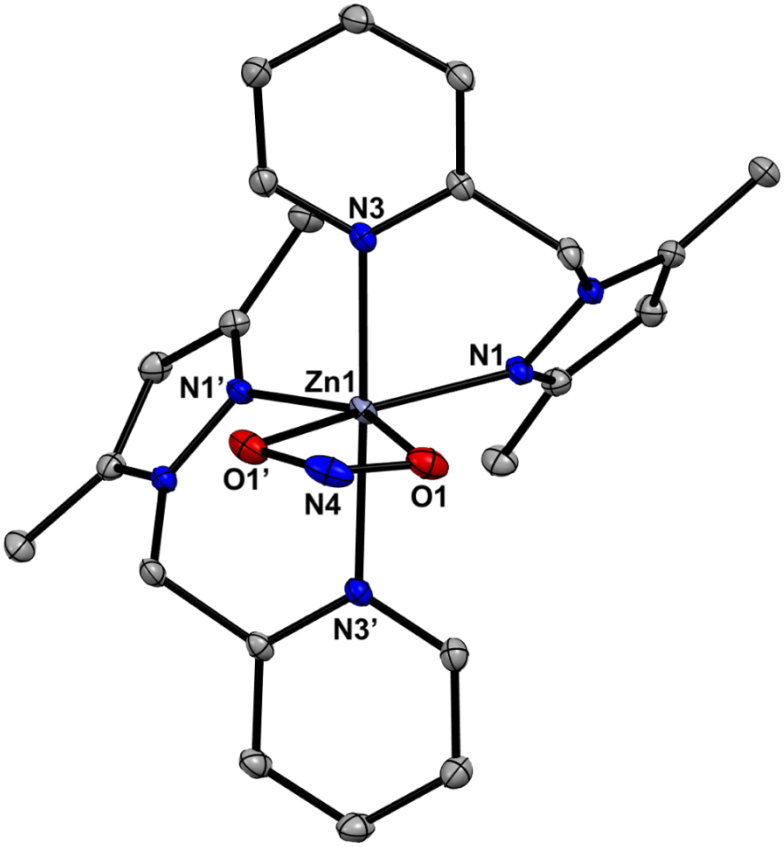


Figure S38. X-ray crystal structure of [(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO$_4$) (**5-Py**). Thermal ellipsoid plots are drawn at 30% probability level. One perchlorate anion and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn-N1 2.085(1), Zn-N3 2.156(1), Zn-O1 2.229(1), O1-Zn-N1 154.85(5), N1-Zn-N1' 105.17(8), O1-Zn-N3 84.21(5), N1-Zn-N3 87.37(5), N3-Zn-N1' 101.72(9), O1-Zn-N6 84.10(8), N1-Zn-N3 99.18(5), N3-Zn-N3' 169.28(8).

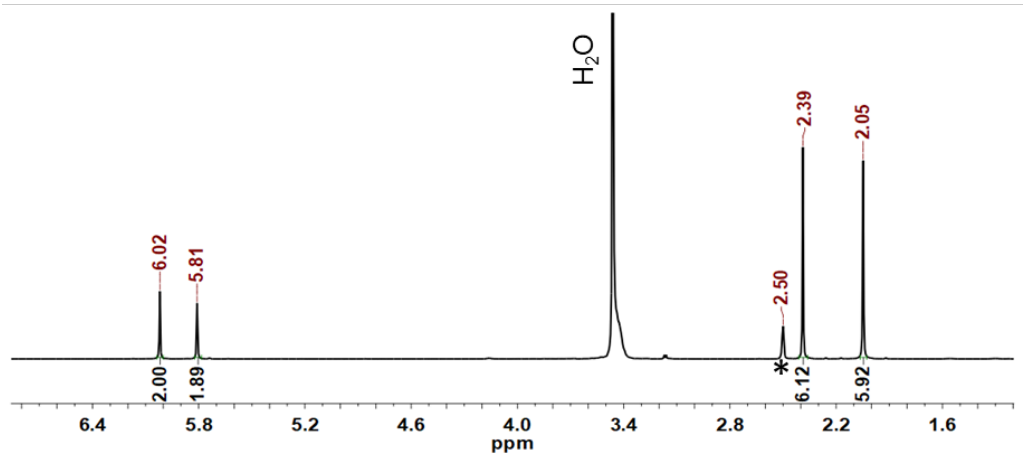


Figure S39. ^{1}H NMR spectrum (500 MHz, 298 K, DMSO-d_6) of [(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) (**5-Pz**). The resonance marked with * originates from DMSO-d_6.

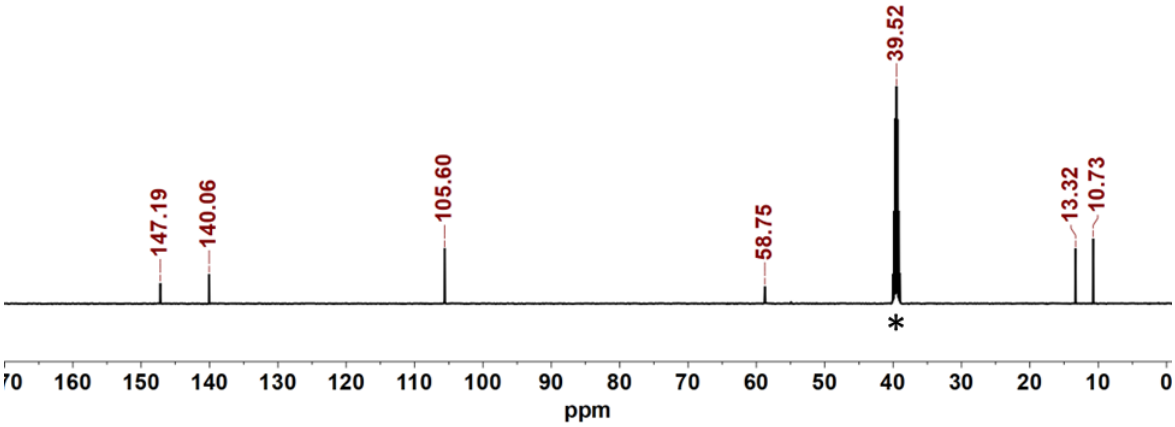


Figure S40. ^{13}C NMR spectrum (500 MHz, 298 K, DMSO-d$_6$) of [(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) (**5-Pz**). The resonance marked with * originates from DMSO-d$_6$.

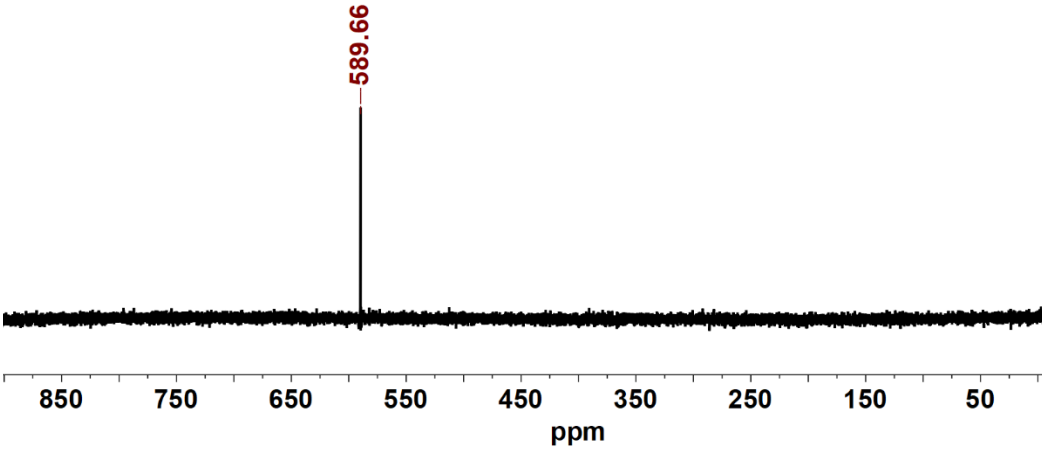


Figure S41. ^{15}N NMR spectrum (51 MHz, 298 K, DMSO-d_6) of [(**Me$_4$PzPz**)$_2$Zn(O^{15}NO)](ClO$_4$) (**5-Pz-^{15}N**).

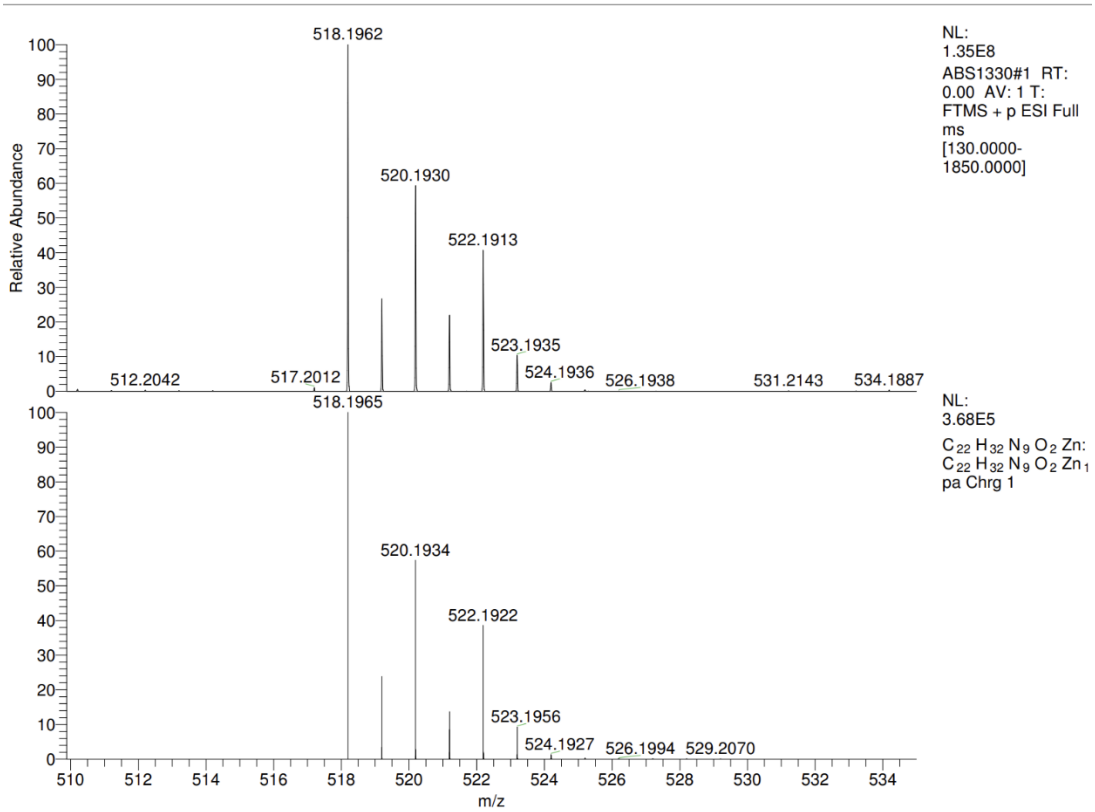


Figure S42. High resolution ESI-MS (+) spectrum of [(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) (**5-Pz**). The *m/z* peak at 518.1962 (*calc. m/z* 518.1965) originates from $[C_{22}H_{32}N_9O_2Zn]^+$.

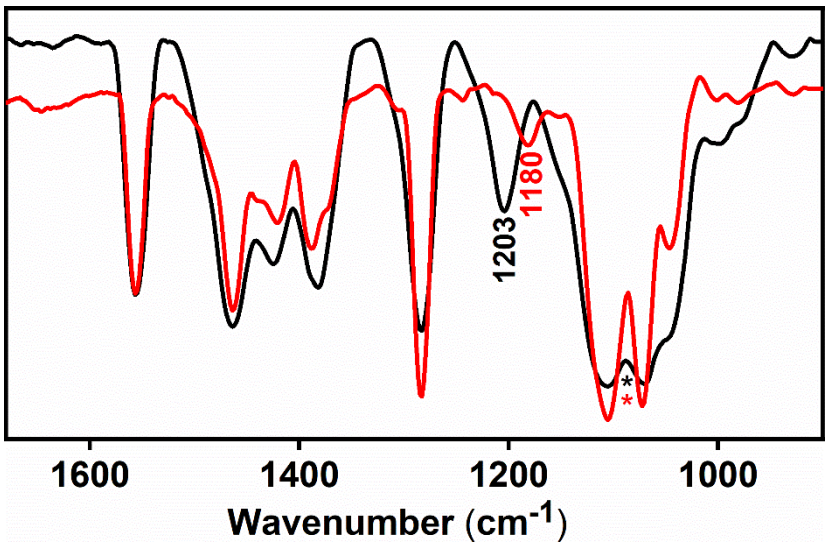


Figure S43. FTIR (KBr pellet) spectra of [(**Me$_4$PzPz**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Pz**) (black trace) and [(**Me$_4$PzPz**)$_2$Cu^{II}(O^{15}NO)](ClO$_4$) (**5-Pz-^{15}N**) (red trace). Asterisks indicate the vibrational features of perchlorate counterion.

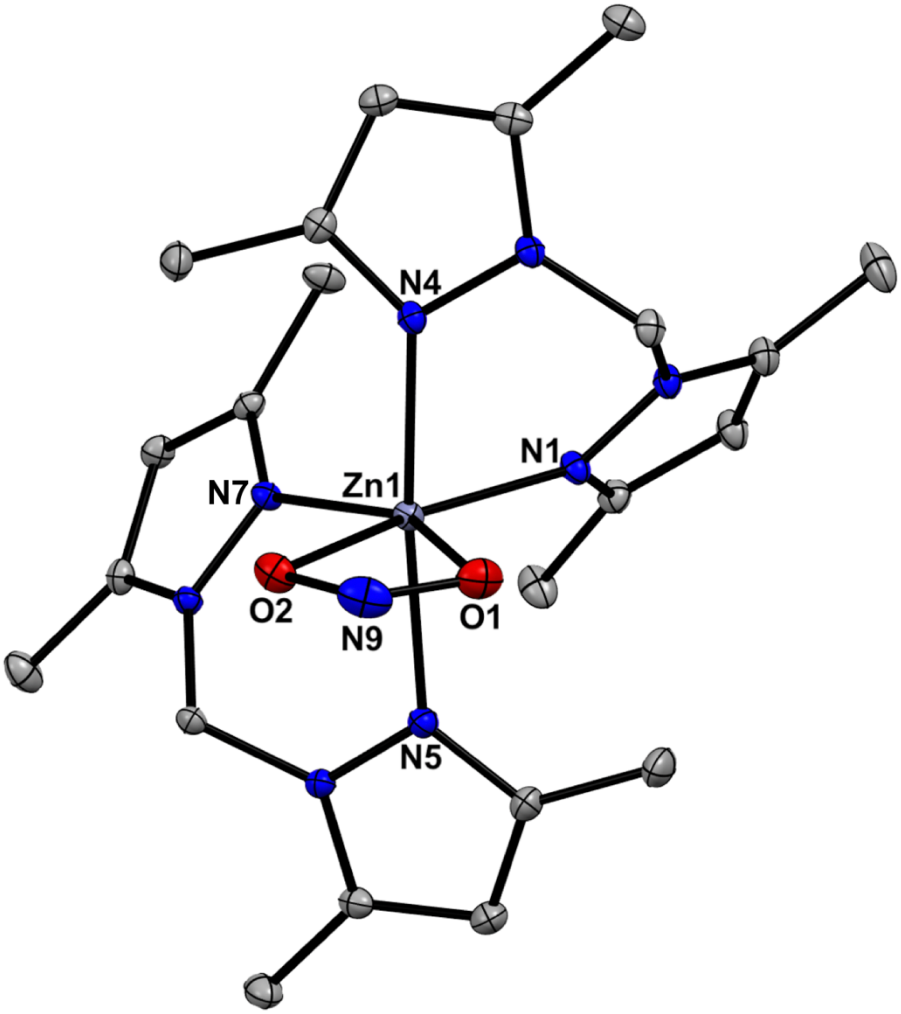


Figure S44. X-ray crystal structure of [(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) (**5-Pz**). Thermal ellipsoid plots are drawn at 30% probability level. One perchlorate anion and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-N1 2.114(2), Zn1-N3 2.134(2), Zn1-N5 2.155(2), Zn1-N7 2.101(2), Zn1-O1 2.226(2), Zn1-O2 2.167(1), N7-Zn1-N1 96.78(6), N7-Zn1-N3 100.14(6), N1-Zn1-N3 88.03(6), N7-Zn1-N5 88.07(6), N1-Zn1-N5 91.98(6), N3-Zn1-N5 171.73(6), N7-Zn1-O2 97.96(6), N1-Zn1-O2 165.24(6), N3-Zn1-O2 90.05(6), N5-Zn1-O2 87.83(6), N7-Zn1-O1 154.44(6), N1-Zn1-O1 108.09(6), N3-Zn1-O1 86.85(6), N5-Zn1-O1 85.28(6), O2-Zn1-O1 57.18(6).

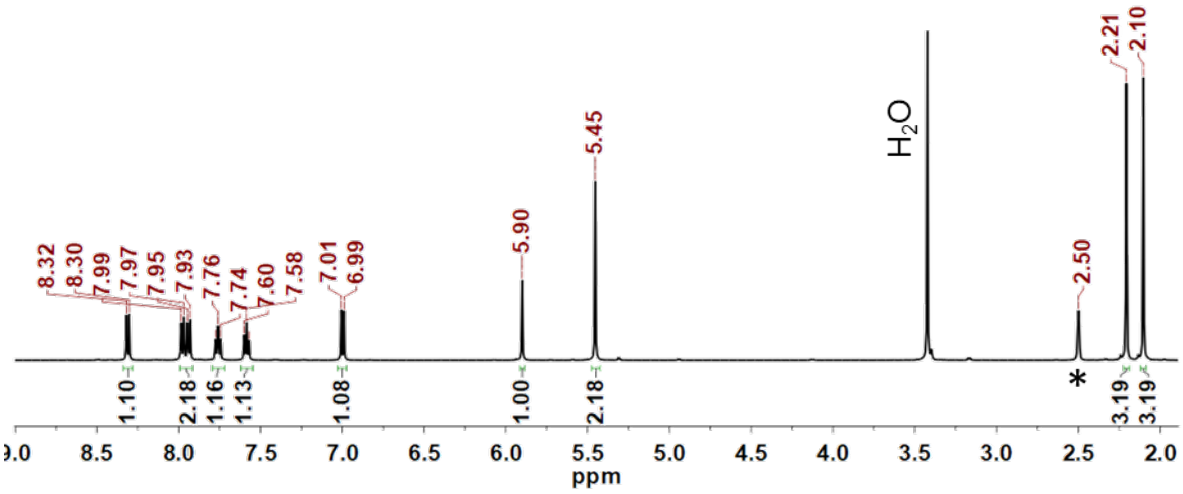


Figure S45. ^{1}H NMR spectrum (500 MHz, 298 K, DMSO-*d*$_6$) of [(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) (**5-Qu**). The resonance marked with * originates from DMSO-*d*$_6$.

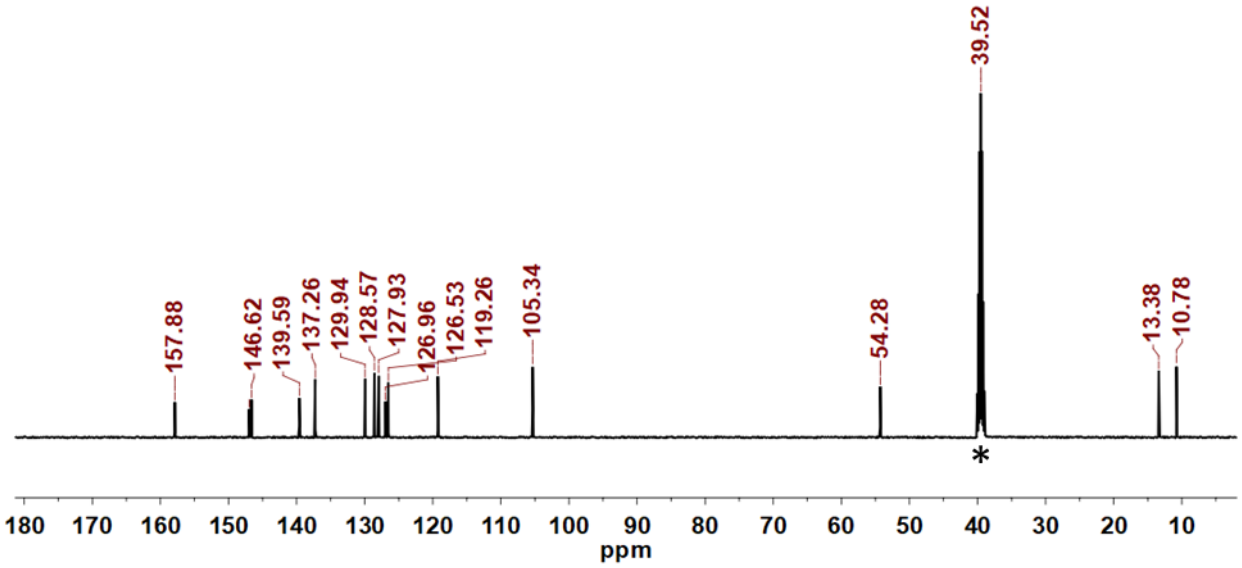


Figure S46. ^{13}C NMR spectrum (125 MHz, 298 K, DMSO-*d*$_6$) of [(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) (**5-Qu**). The resonance marked with * originates from DMSO-*d*$_6$.

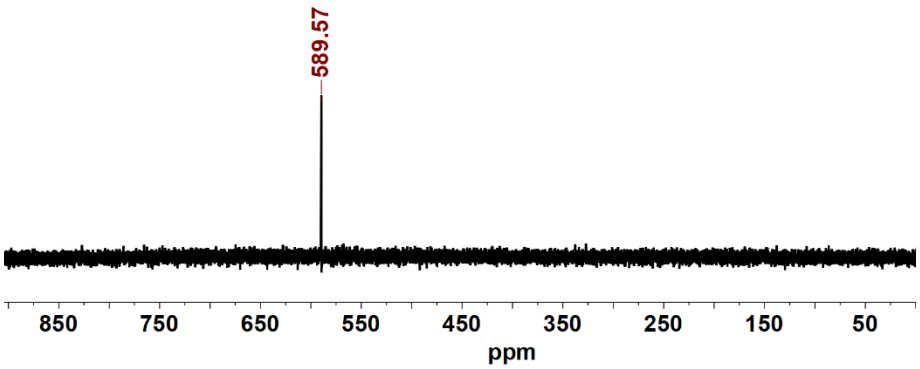


Figure S47. ^{15}N NMR spectrum (51 MHz, 298 K, DMSO-d$_6$) of [(**Me$_2$PzQu**)$_2$Zn(O^{15}NO)](ClO$_4$) (**5-Qu-^{15}N**).

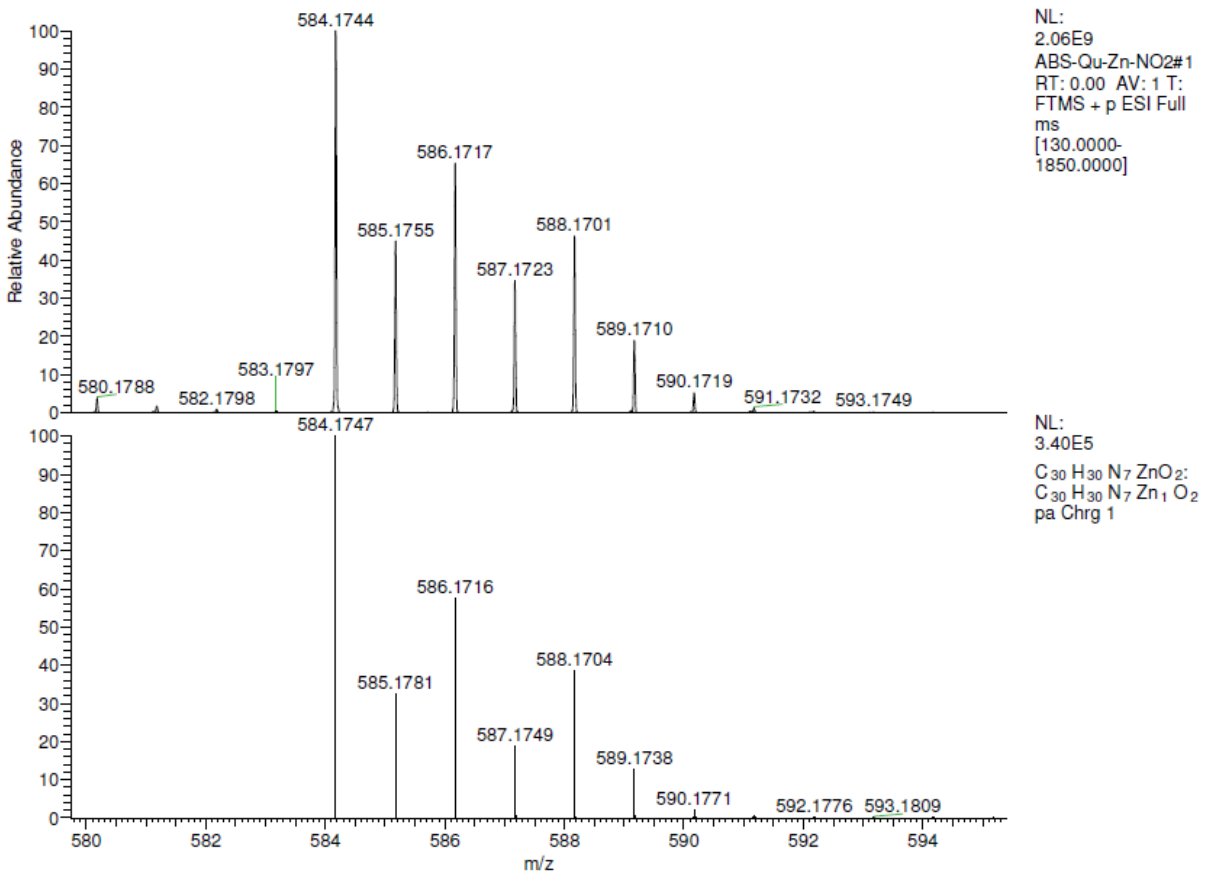


Figure S48. High resolution ESI-MS (+) spectrum of [(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) (**5-Qu**). The *m/z* peak at 584.1744 (*Calc. m/z* 584.1747) originates from $[C_{30}H_{30}N_7O_2Zn]^+$.

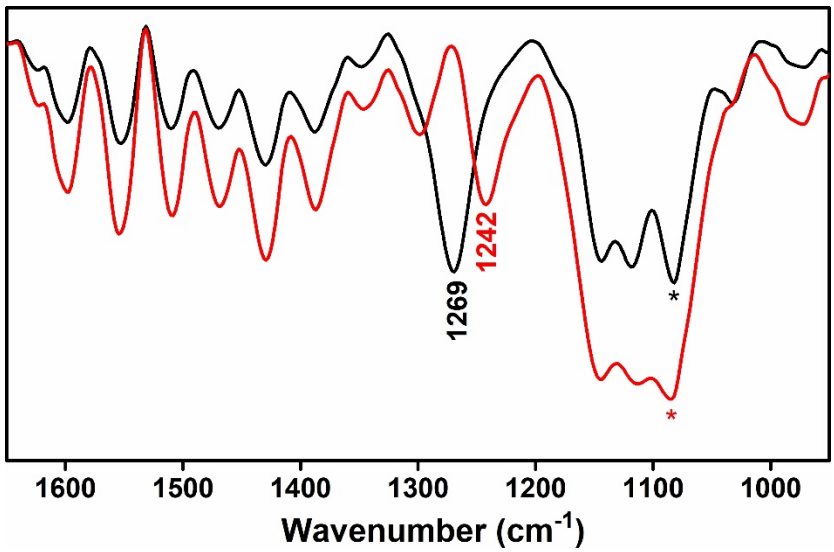


Figure S49. FTIR (KBr pellet) spectra of [(**Me$_2$PzQu**)$_2$Zn^{II}(ONO)](ClO$_4$) (**5-Qu**) (black trace) and [(**Me$_2$PzQu**)$_2$Cu^{II}(O^{15}NO)](ClO$_4$) (**5-Qu-^{15}N**) (red trace). Asterisks indicate the vibrational features for perchlorate counterion.

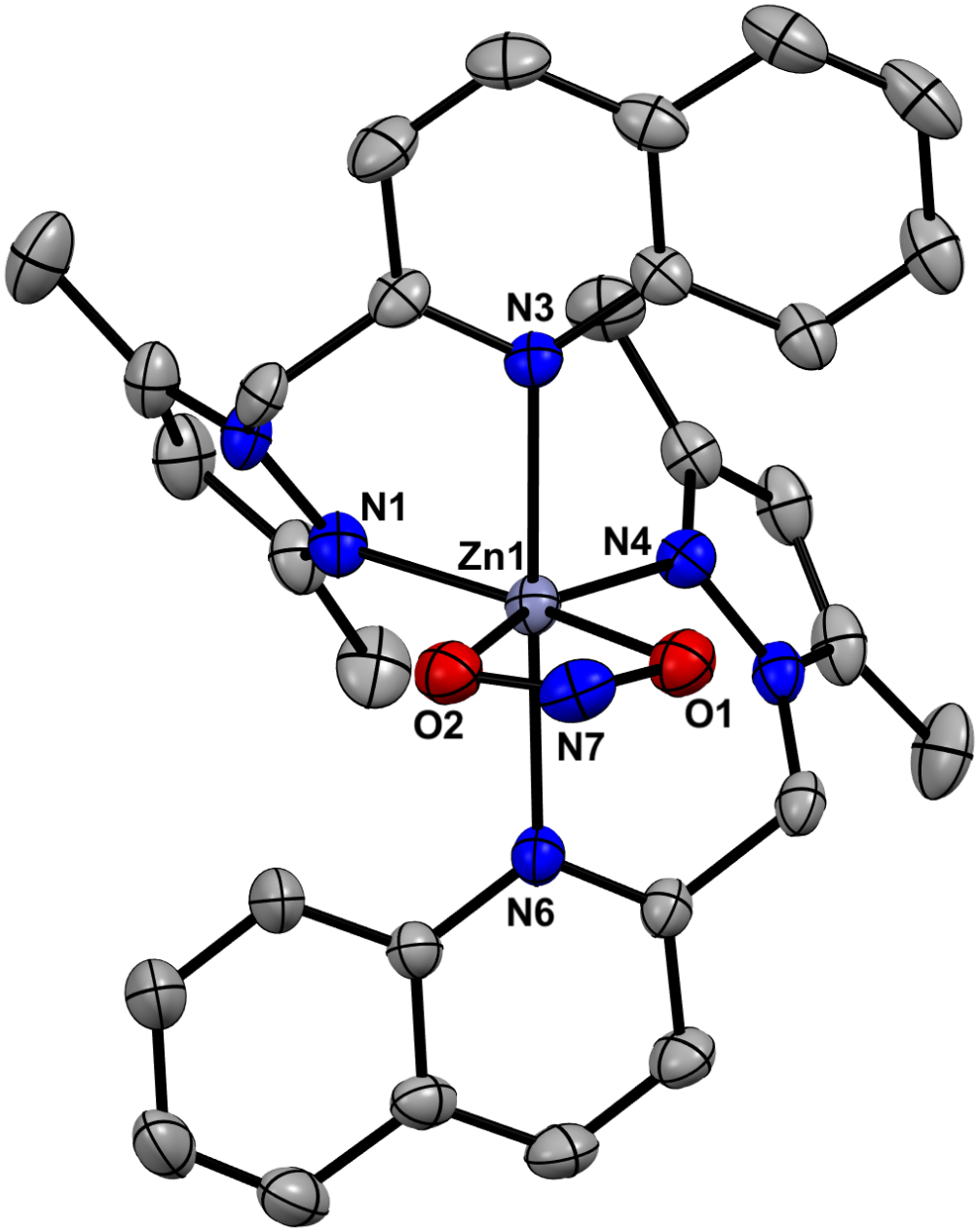


Figure S50. X-ray crystal structure of [(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) (**5-Qu**). Thermal ellipsoid plots are drawn at 30% probability level. One perchlorate anion and hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (°): Zn1-N1 2.065(3), Zn1-N3 2.334(3), Zn1-N4 2.064(3), Zn1-N6 2.278(3), Zn1-O1 2.213(3), Zn1-O2 2.186(3), O1-Zn1-O2 56.29(11), N1-Zn1-N3 87.25(11), N1-Zn1-N4 97.66(12), N1-Zn1-N6 98.14(11), N1-Zn1-O1 158.86(12), N1-Zn1-O2 103.37(12), N4-Zn1-N6 89.61(11), N4-Zn1-N3 95.45(11), N4-Zn1-O1 102.69(12), N4-Zn1-O2 158.94(12), N3-Zn1-N6 172.07(11), N6-Zn1-O1 87.75(10), N6-Zn1-O2 88.41(10).

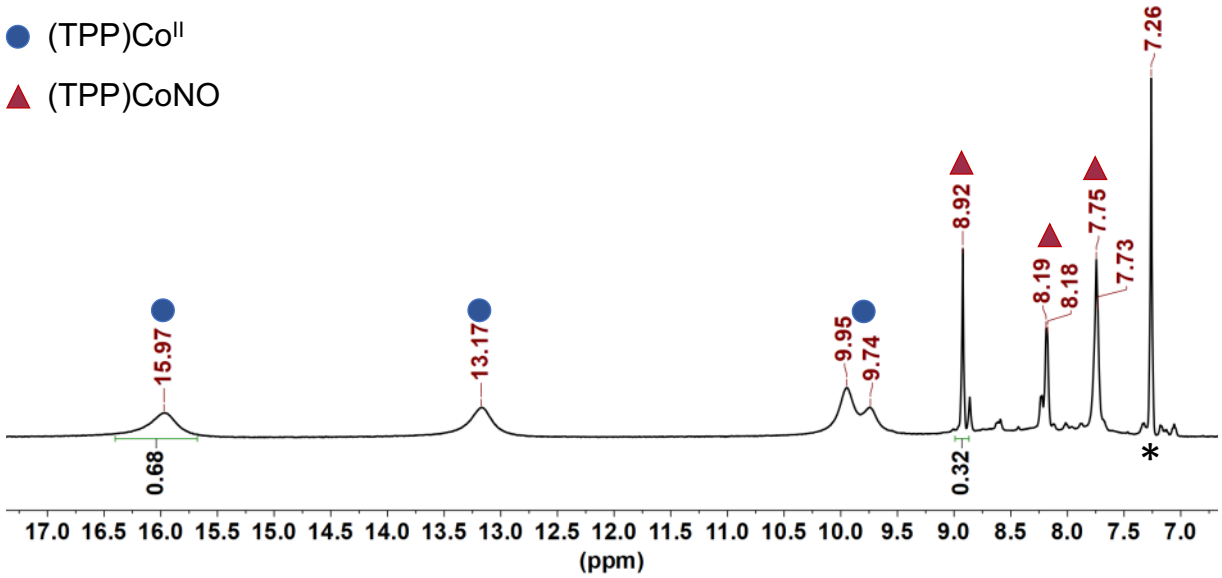


Figure S51. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of (TPP)Co^{II} solution after the NO–trapping experiments performed for the reaction of **5-Py** with ^{t}BuBnSH (1.0 equiv.). The resonance marked with * originates from $CDCl_3$.

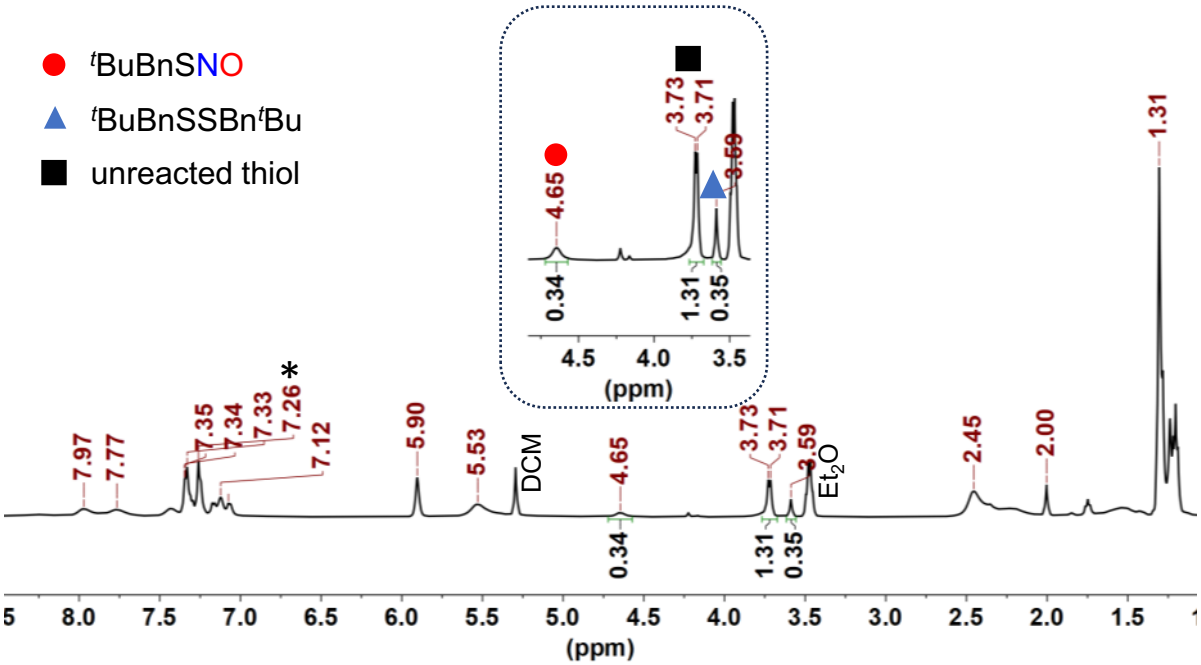


Figure S52. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the crude sample obtained from the reaction of **5-Py** with ^{t}BuBnSH (1.0 equiv.) showing signals for ^{t}BuBnSNO (0.17 equiv., 17% yield), (^{t}BuBnS)$_2$ (0.08 equiv.), and unreacted ^{t}BuBnSH (0.65 equiv.). The resonance marked with * originates from $CDCl_3$. The proton resonances of CH_2Cl_2 and Et_2O are likely originating from the glovebox atmosphere.

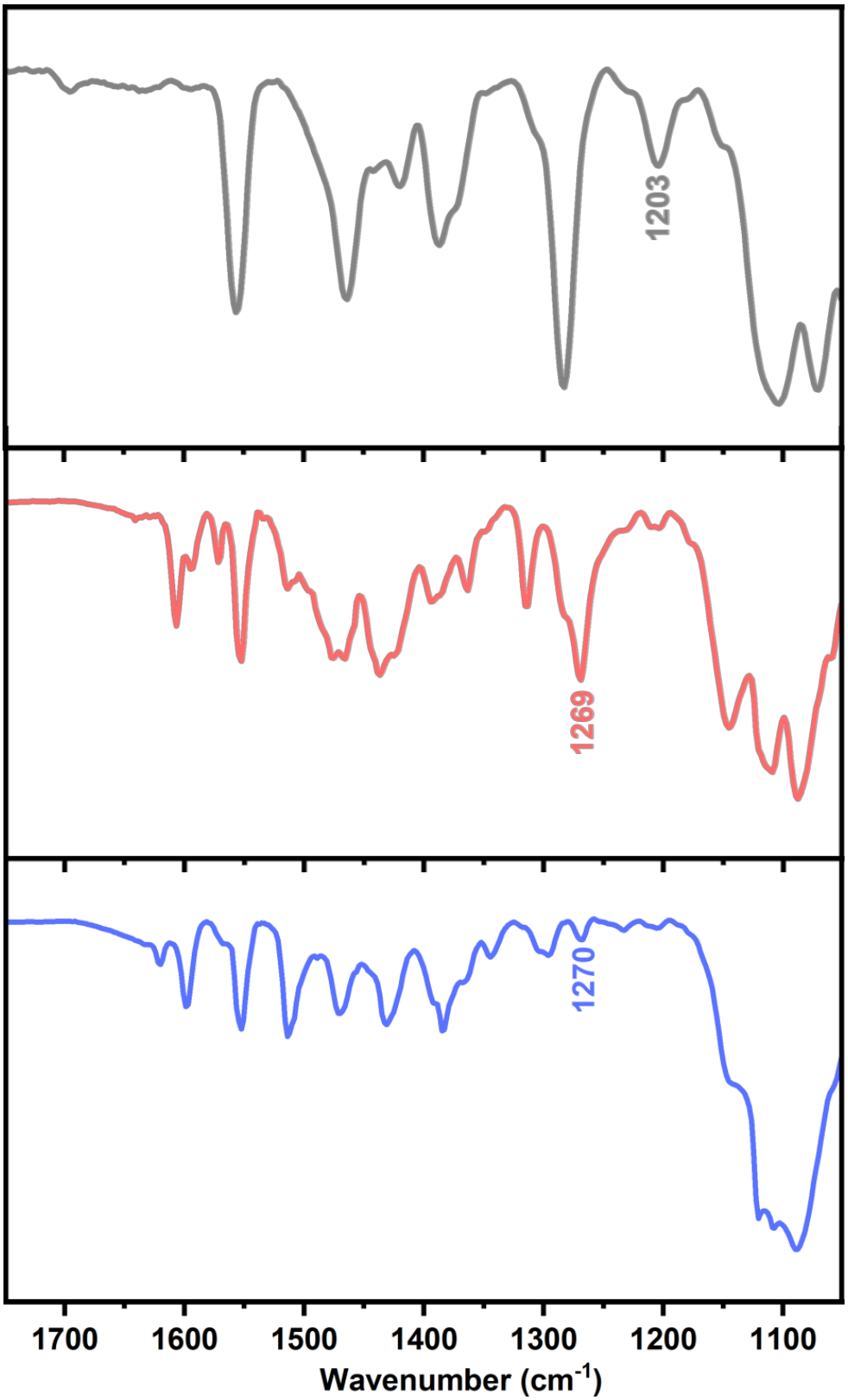


Figure S53. FTIR spectrum of the crude end product obtained from the reaction of 1.0 equivalent of ^{t}BuBnSH with **5-Pz** (grey trace), **5-Py** (red trace), and **5-Qu** (blue trace). The band at 1203/ 1269/ 1270 cm^{-1} shows the presence of unreacted zinc(II)-nitrite.

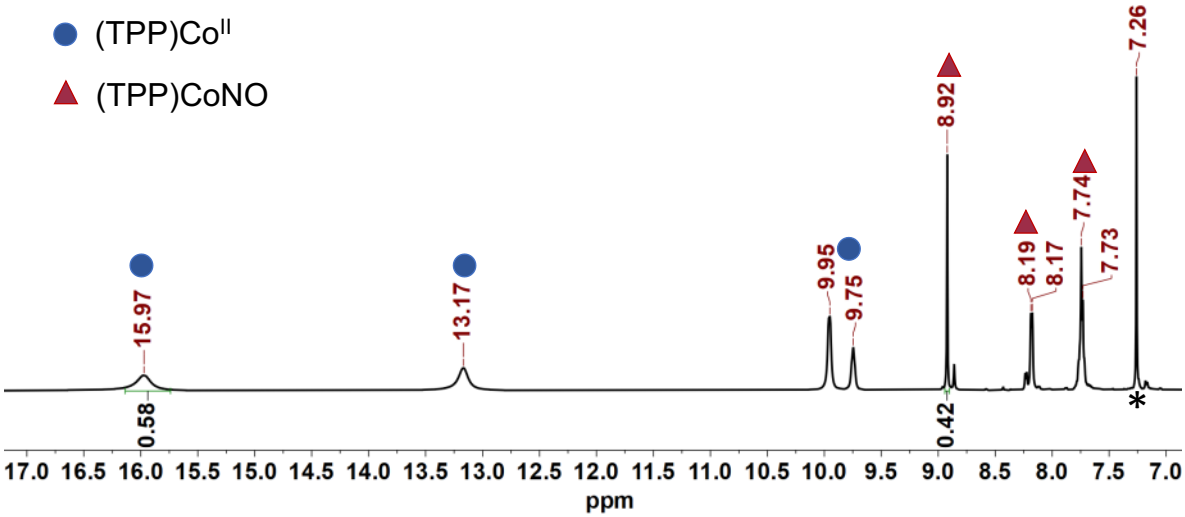


Figure S54. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of $(TPP)Co^{II}$ solution after the NO–trapping experiments performed for the reaction of **5-Pz** with ^{t}BuBnSH (1.0 equiv.). The resonance marked with * originates from $CDCl_3$.

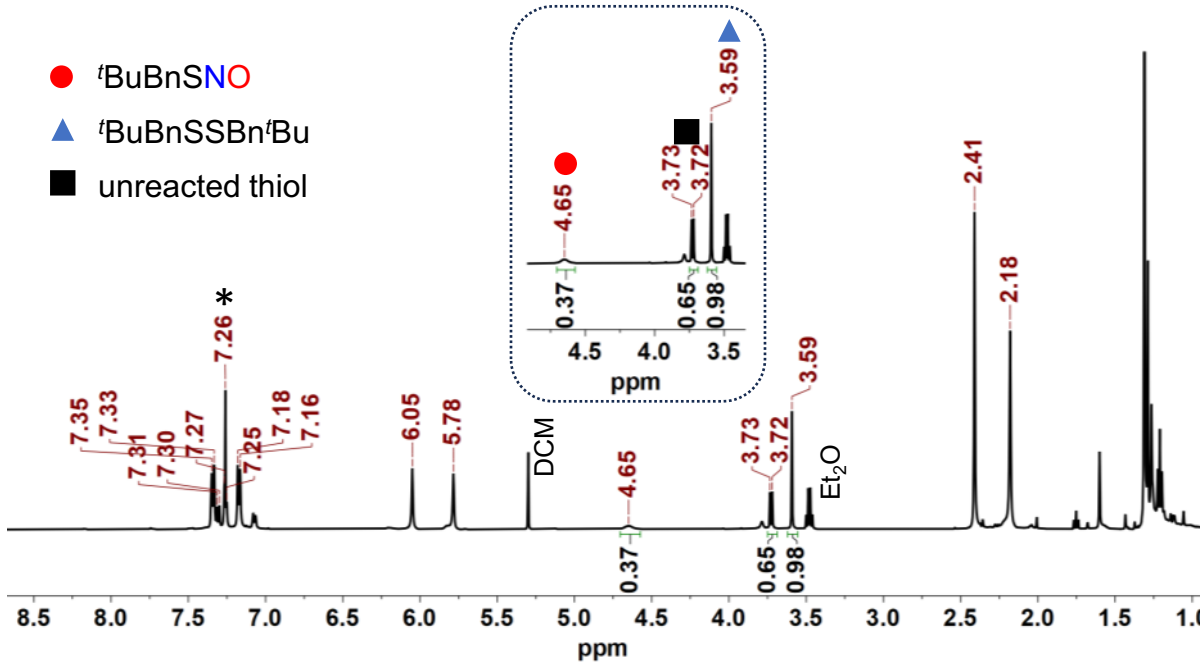


Figure S55. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the crude sample obtained from the reaction of **5-Pz** with ^{t}BuBnSH (1.0 equiv.) showing signals for ^{t}BuBnSNO (0.19 equiv., 19% yield), $(^t$BuBnS$)_2$ (0.25 equiv.), and unreacted ^{t}BuBnSH (0.32 equiv.). The resonance marked with * originates from $CDCl_3$. The proton resonances of CH_2Cl_2 and Et_2O are likely originating from the glovebox atmosphere.

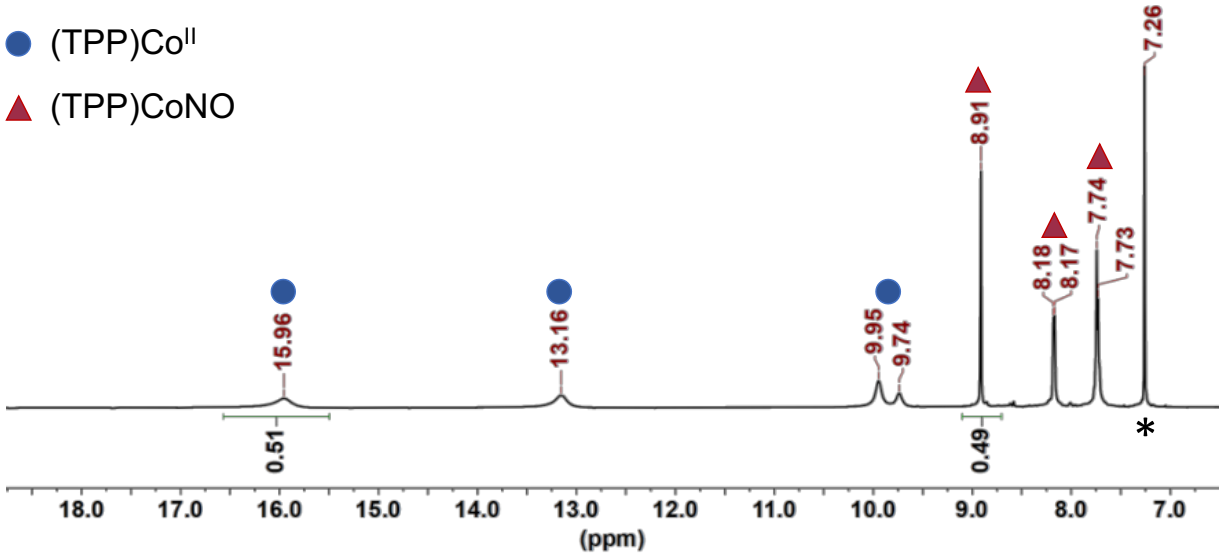


Figure S56. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of (TPP)Co^{II} solution after the NO–trapping experiments performed for the reaction of **5-Qu** with ^{t}BuBnSH (1.0 equiv.). The resonance marked with * originates from $CDCl_3$.

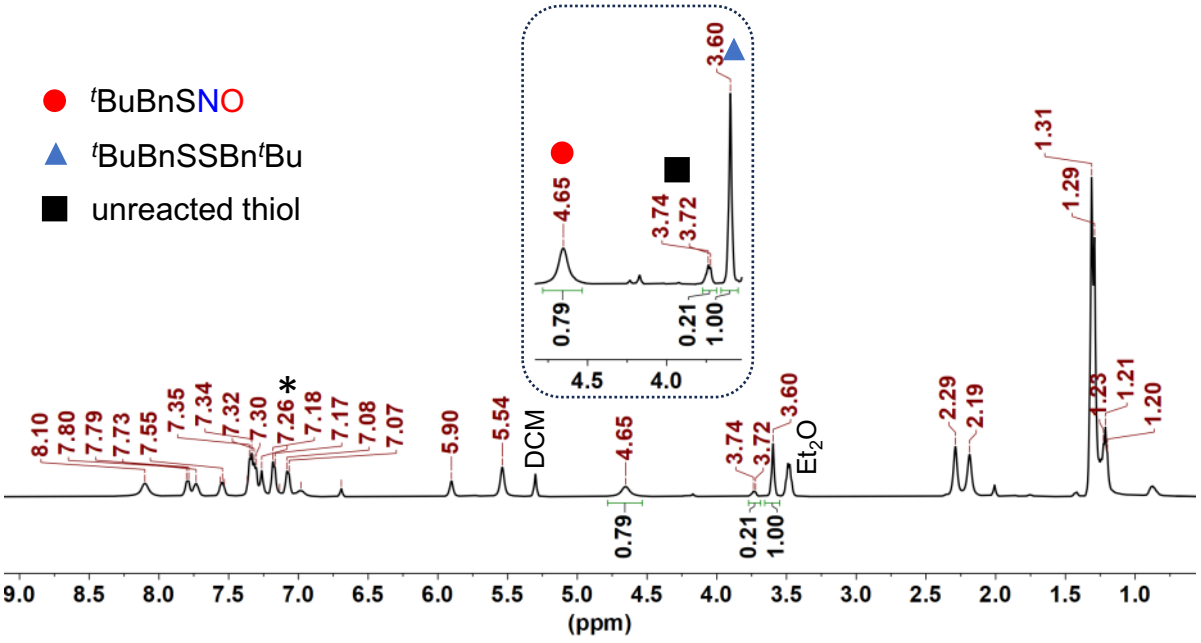


Figure S57. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the samples obtained from the reaction of **5-Qu** with ^{t}BuBnSH (1.0 equiv) showing signals for ^{t}BuBnSNO (0.40 equiv., 40% yield), (^{t}BuBnS)$_2$ (0.20 equiv.), and unreacted ^{t}BuBnSH (0.19 equiv.). The resonance marked with * originates from $CDCl_3$. The proton resonances of CH_2Cl_2 and Et_2O are likely originating from the glovebox atmosphere.

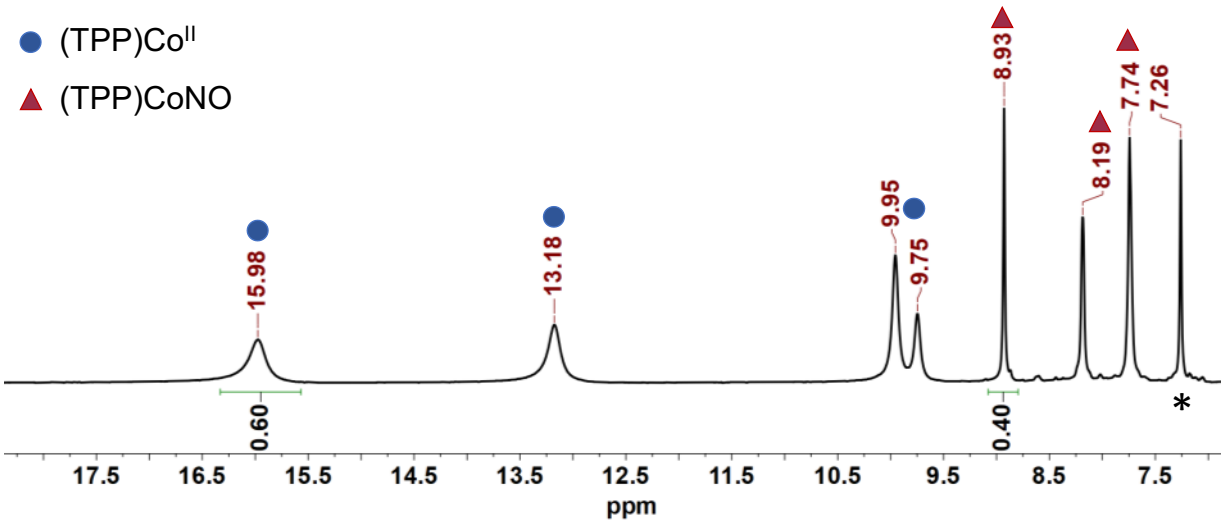


Figure S58. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of $(TPP)Co^{II}$ solution after the NO–trapping experiments performed for the reaction of **5-Py** with ^{t}BuBnSH (2.0 equiv.). The resonance marked with * originates from $CDCl_3$.

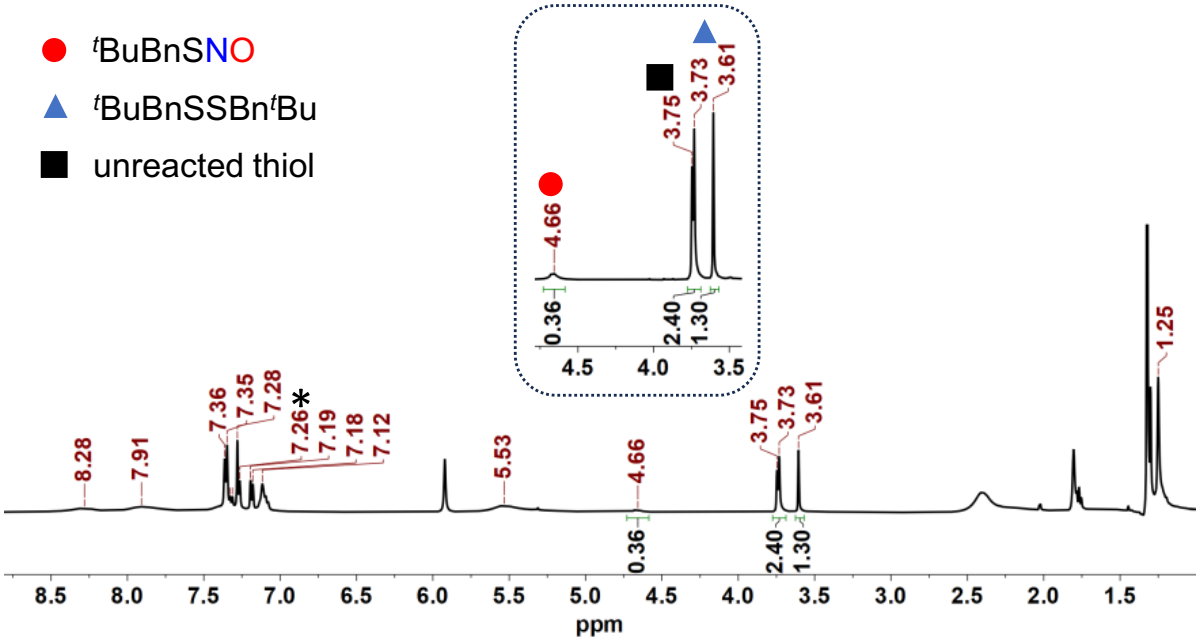


Figure S59. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the crude sample obtained from the reaction of **5-Py** with ^{t}BuBnSH (2.0 equiv.) showing signals for ^{t}BuBnSNO (0.17 equiv., 17% yield), $(^{t}BuBnS)_2$ (0.32 equiv.), and unreacted ^{t}BuBnSH (1.19 equiv.). The resonance marked with * originates from $CDCl_3$.

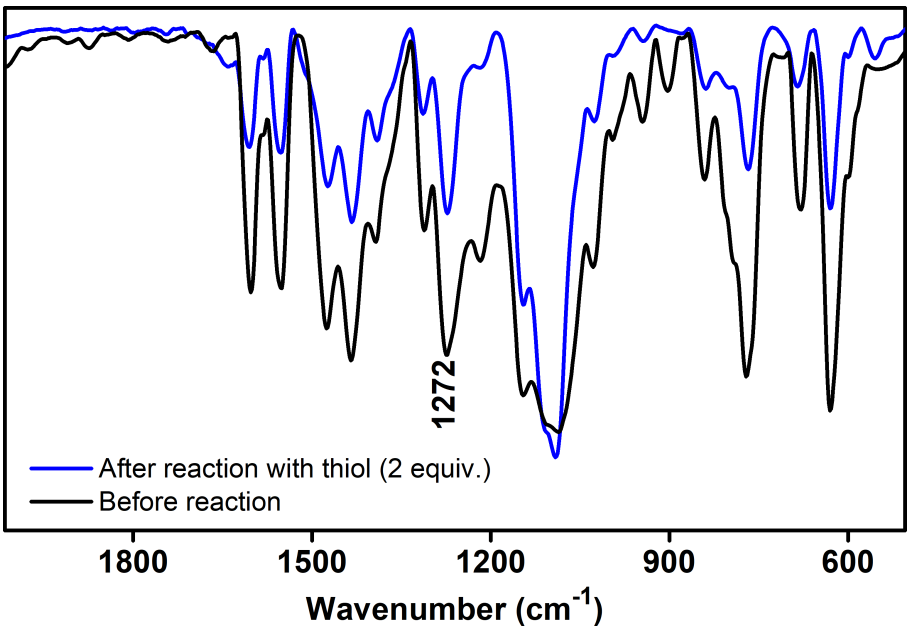


Figure S60. FTIR spectrum of the inorganic end product obtained from the reaction of **5-Py** with 2.0 equivalents of ^{t}BuBnSH (blue trace) and the **5-Py** (black trace). The band at 1272 cm^{-1} shows the presence of unreacted nitrite.

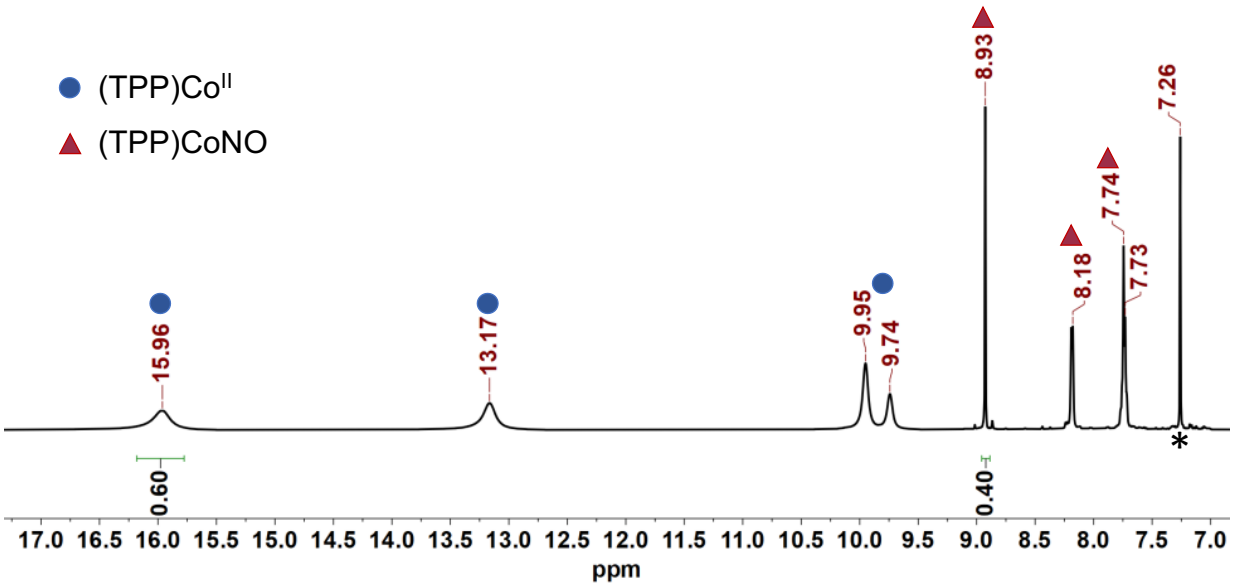


Figure S61. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of (TPP)Co^{II} solution after the NO–trapping experiment performed for the reaction of **5-Pz** with ^{t}BuBnSH (2.0 equiv.). The resonance marked with * originates from $CDCl_3$.

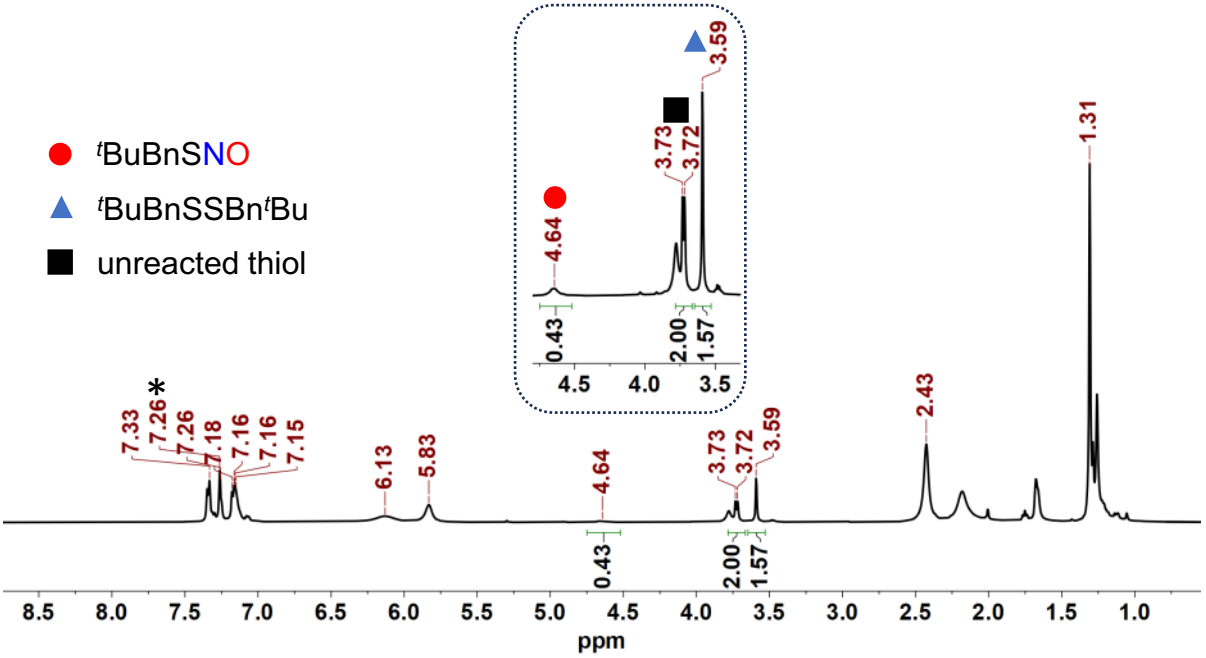


Figure S62. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the crude samples obtained from the reaction of **5-Pz** with ^{t}BuBnSH (2.0 equiv.) showing signals for ^{t}BuBnSNO (0.22 equiv., 22% yield), $(^{t}BuBnS)_2$ (0.39 equiv.), and unreacted ^{t}BuBnSH (1.00 equiv.). The resonance marked with * originates from $CDCl_3$.

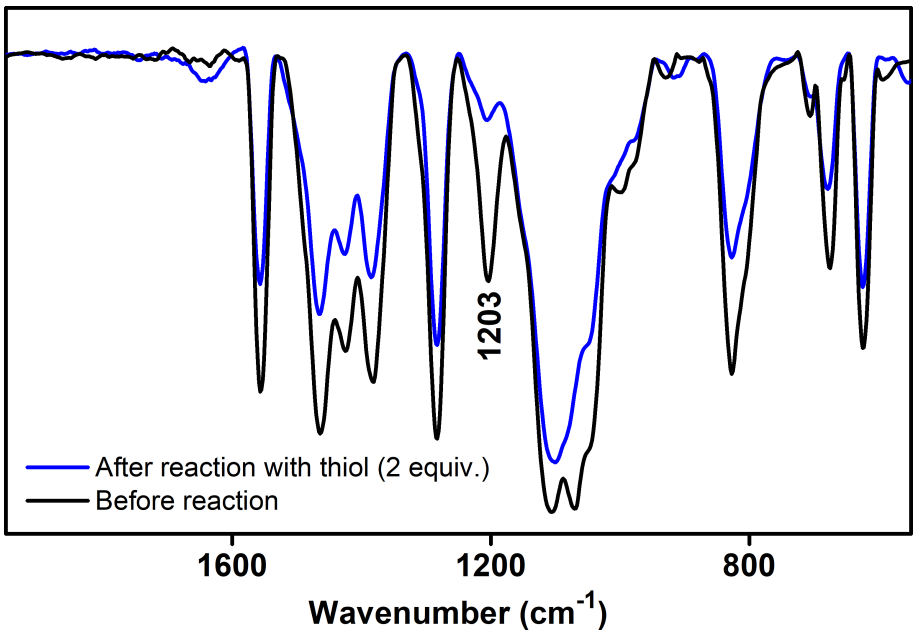


Figure S63. FTIR spectrum of the inorganic end product obtained from the reaction of **5-Pz** with 2.0 equivalents of ^{t}BuBnSH (blue trace) and the **5-Pz** (black trace). The peak at 1203 cm^{-1} shows the presence of unreacted nitrite.

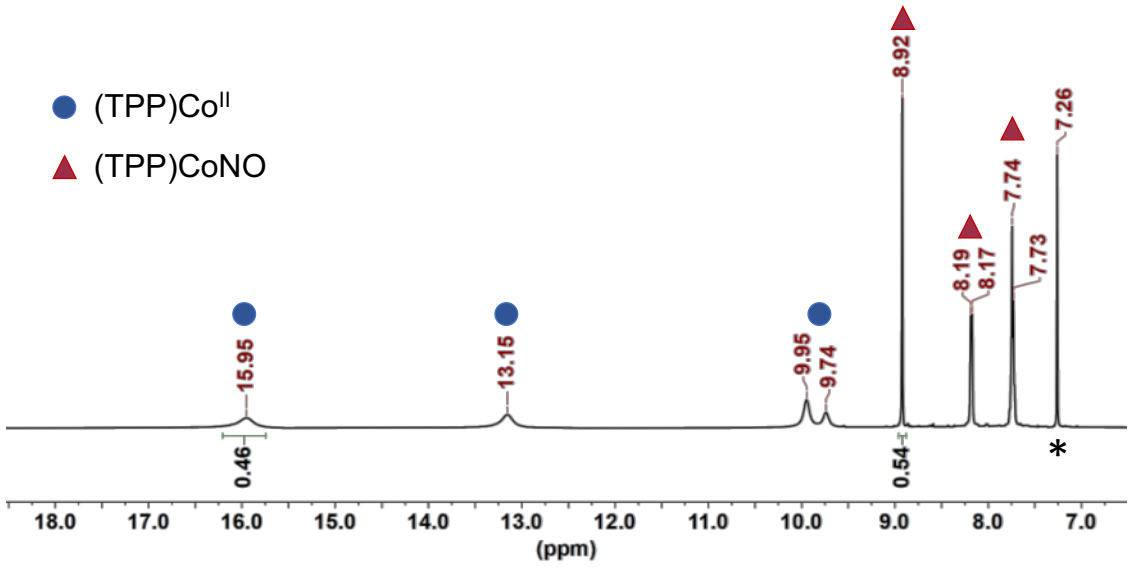


Figure S64. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of (TPP)Co^{II} solution after the NO–trapping experiment performed for the reaction of **5-Qu** with ^{t}BuBnSH (2.0 equiv.). The resonance marked with * originates from $CDCl_3$.

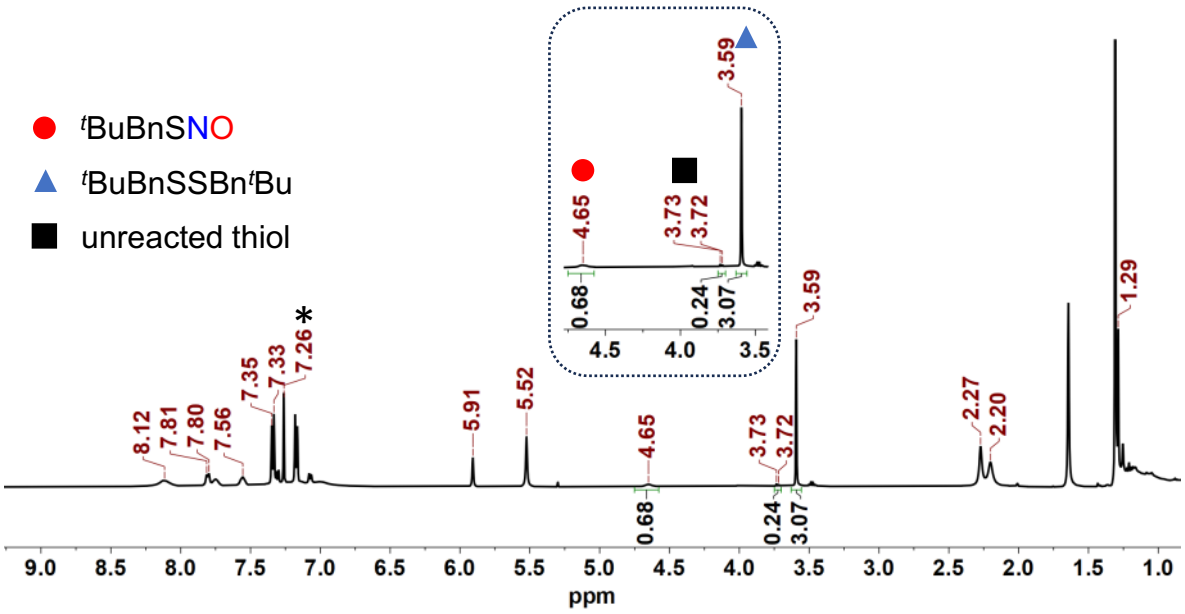


Figure S65. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the crude sample obtained from the reaction of **5-Qu** with ^{t}BuBnSH (2.0 equiv.) showing signals for ^{t}BuBnSNO (0.34 equiv., 34% yield), (^{t}BuBnS)$_2$ (0.77 equiv.), and unreacted ^{t}BuBnSH (0.12 equiv.). The resonance marked with * originates from $CDCl_3$.

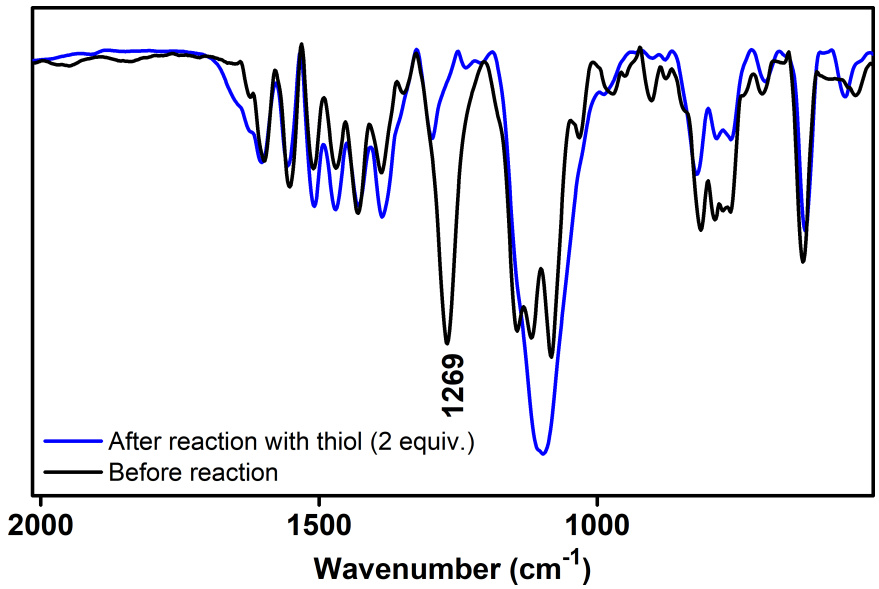


Figure S66. FTIR spectrum of the inorganic end product obtained from the reaction of **5-Qu** with 2.0 equivalents of ^{t}BuBnSH (blue trace) and the **5-Qu** (black trace).

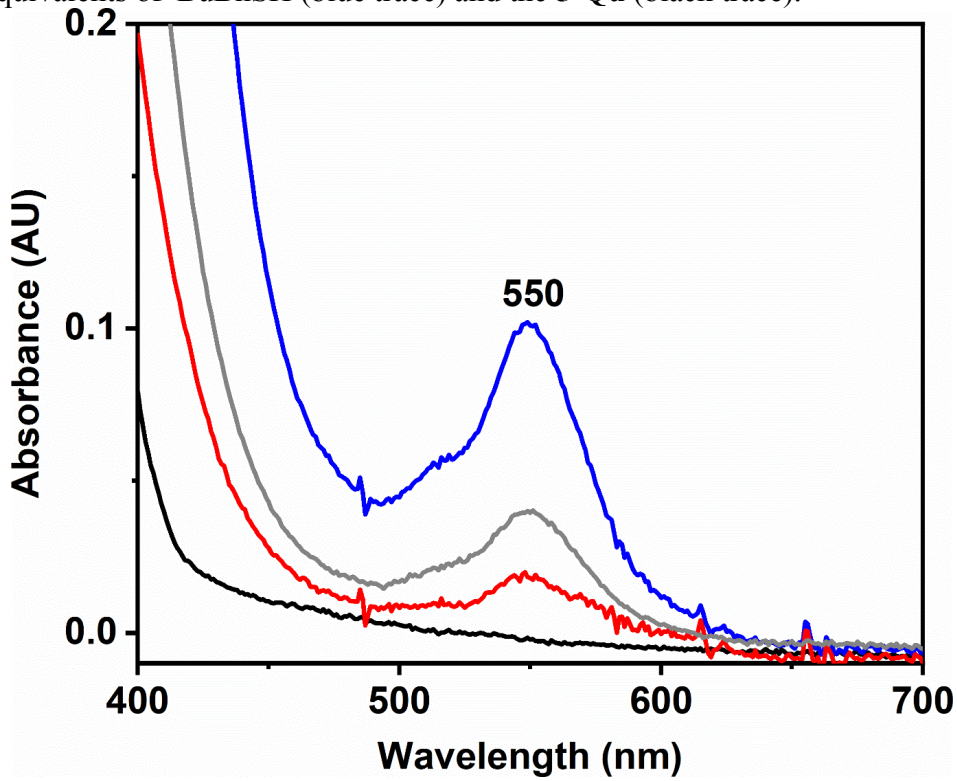


Figure S67. UV-vis spectra showing the formation of ^{t}BuBnSNO as obtained from the reactions of **5-Qu** (blue trace), **5-Pz** (grey trace), **5-Py** (red trace) with ^{t}BuBnSH (2.0 equiv.). The black trace shows the spectrum obtained for the control reaction of [TBA^{+}][NO_2^{-}] with ^{t}BuBnSH (2.0 equiv.) under comparable conditions. In all the cases, the reactants were allowed to stir for 12 h at room temperature in acetonitrile under an inert atmosphere. Subsequently, the UV-vis samples were prepared by diluting an aliquot of the crude reaction mixture to a 2.0 mM concentration in acetonitrile at 25 °C.

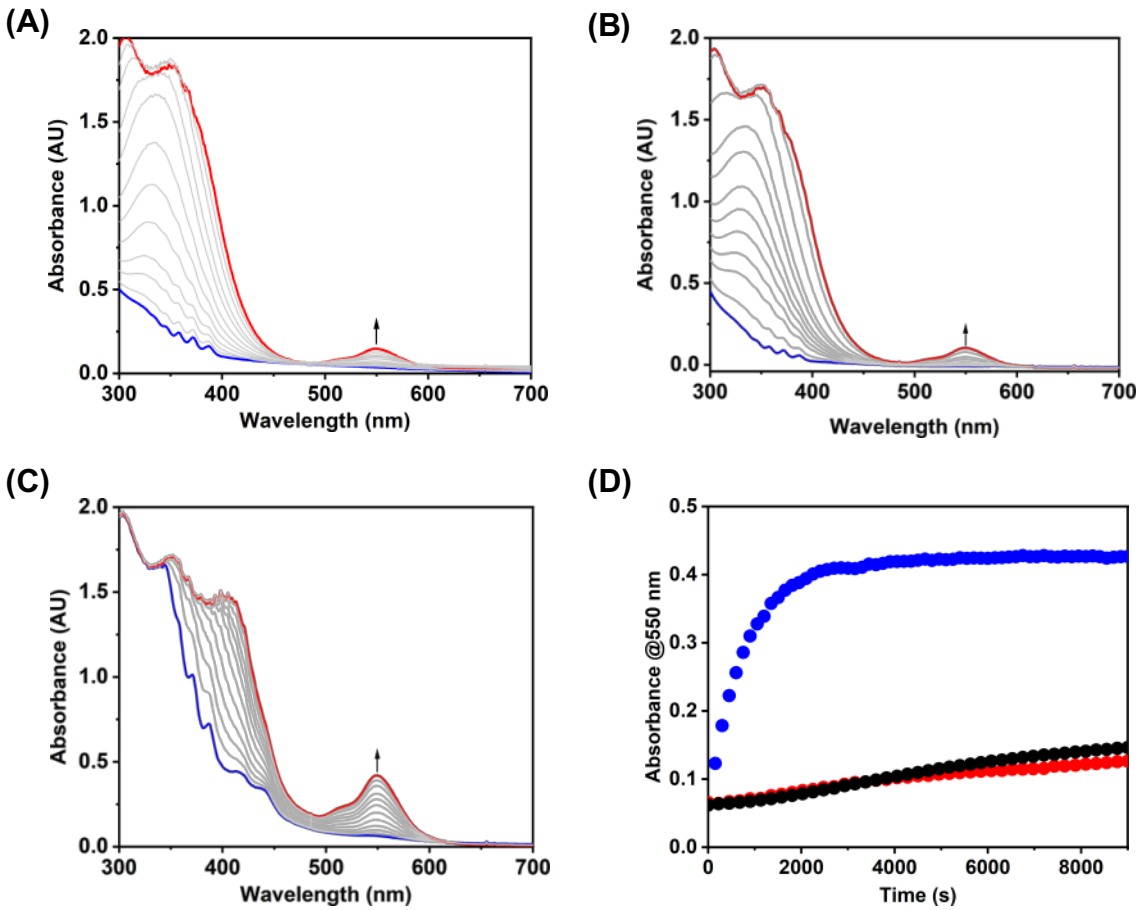


Figure S68. Changes in the UV-vis spectra (10 mM, in acetonitrile, at 25 °C) during the reaction of ^{t}BuBnSH (2.0 equiv.) with (**A**) [(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) (**5-Pz**) (**B**) [(**Me$_4$PzPy**)$_2$Zn(ONO)](ClO$_4$) (**5-Py**) (**C**) [(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) (**5-Qu**) (**D**) The time trace monitored at 550 nm (originating from ^{t}BuBnSNO) during the reactions of [(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) (black trace), [(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO$_4$) (red trace) and [(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) (blue trace) with ^{t}BuBnSH (2.0 equiv.).

Comment: *A single wavelength background correction at 700 nm (using Agilent 8454 data analysis software) was performed for the time trace corresponding to the reaction of* ***5-Pz*** *and thiol.*

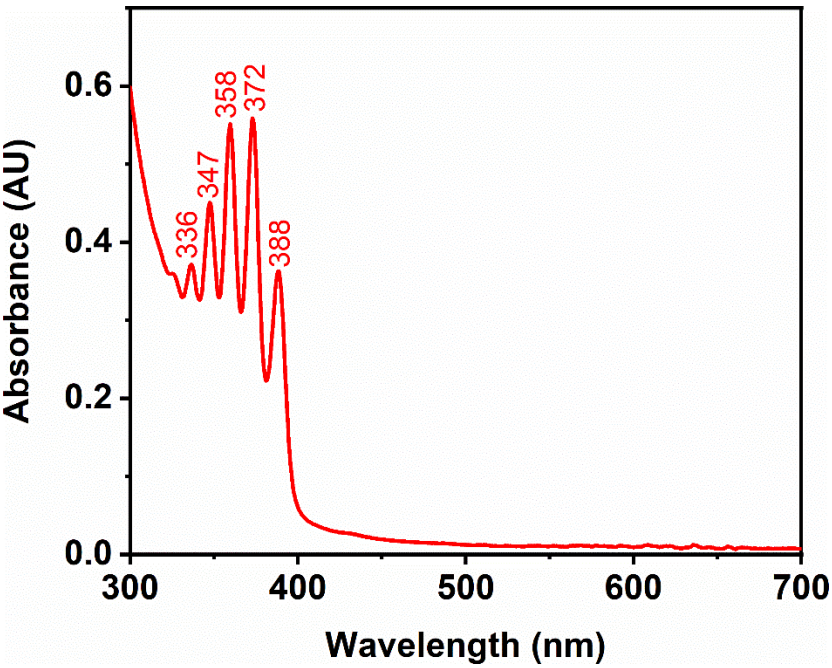


Figure S69. The UV-vis spectrum of an authentic sample of HNO_2 generated from the reaction $[NO^+][BF_4^-]$ (1 mM, in acetonitrile at 25 °C) with deionized water (50 μL).

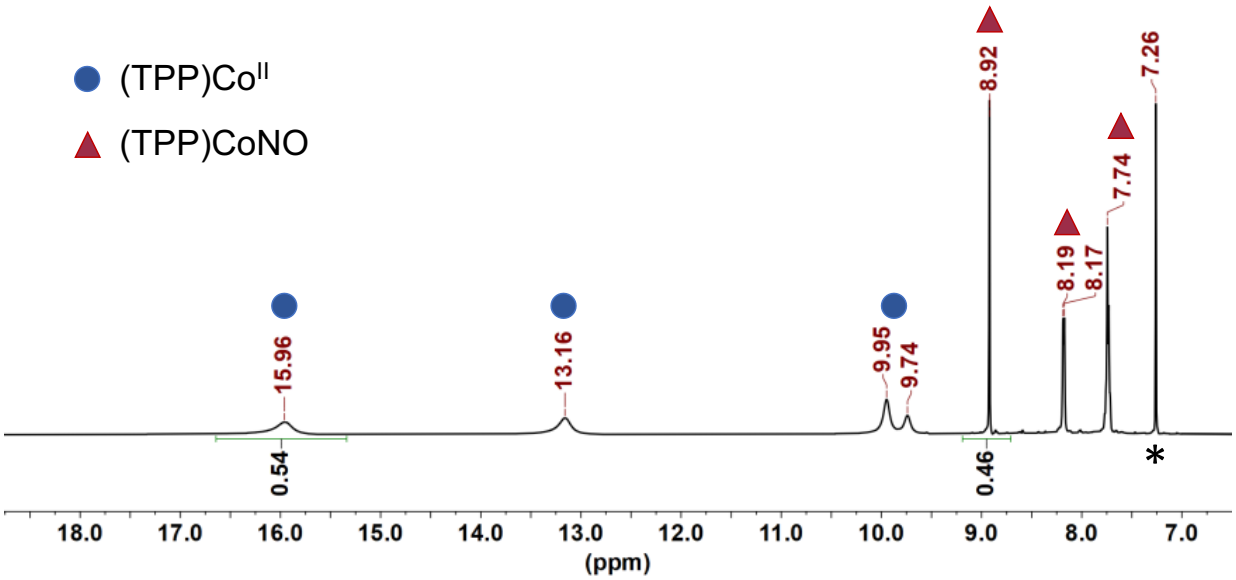


Figure S70. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of (TPP)Co^{II} solution after the NO–trapping experiment performed for the catalytic reaction of [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) (**3-Py**) (10 mol%) with $[TBA^+][NO_2^-]$ and ^{t}BuBnSH. The resonance marked with * originates from $CDCl_3$.

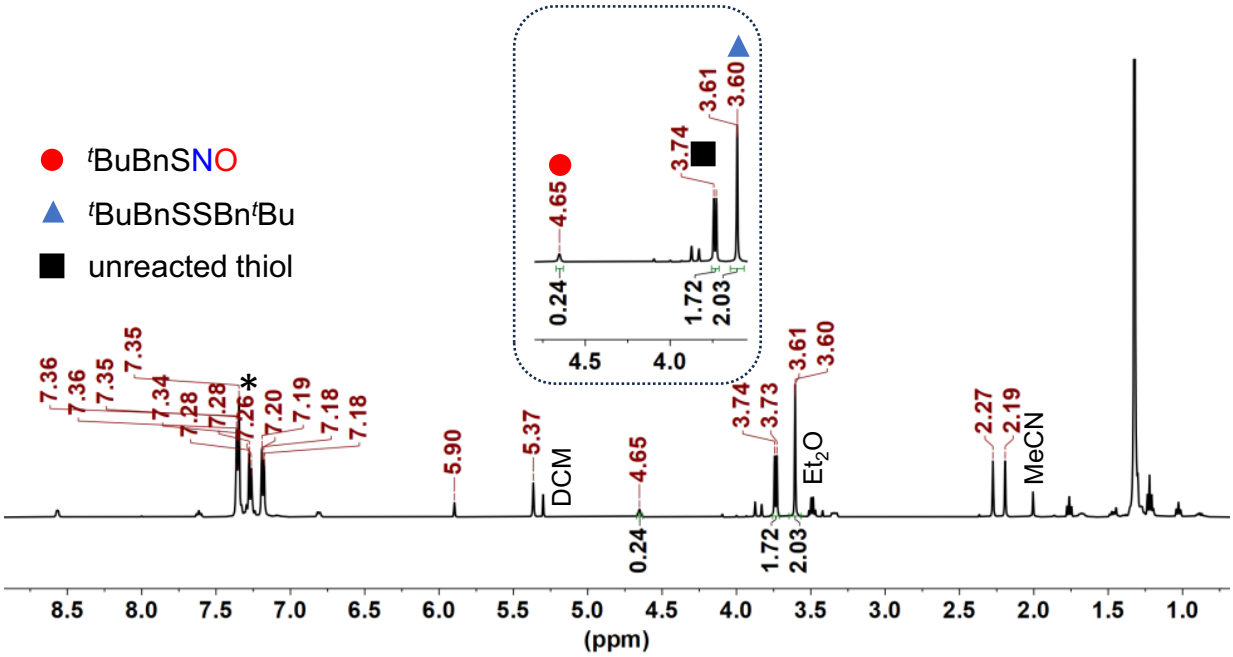


Figure S71. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the sample obtained from the reaction of the catalytic reaction of [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) (**3-Py**) (10 mol%) with [TBA$^+$][NO_2^-] and ^{t}BuBnSH showing signals for ^{t}BuBnSNO (0.12 equiv., 12% yield), (^{t}BuBnS)$_2$ (0.51 equiv.), and unreacted ^{t}BuBnSH (0.86 equiv.). The resonance marked with * originates from $CDCl_3$. The proton resonances of CH_2Cl_2 and Et_2O are likely originating from the glovebox atmosphere.

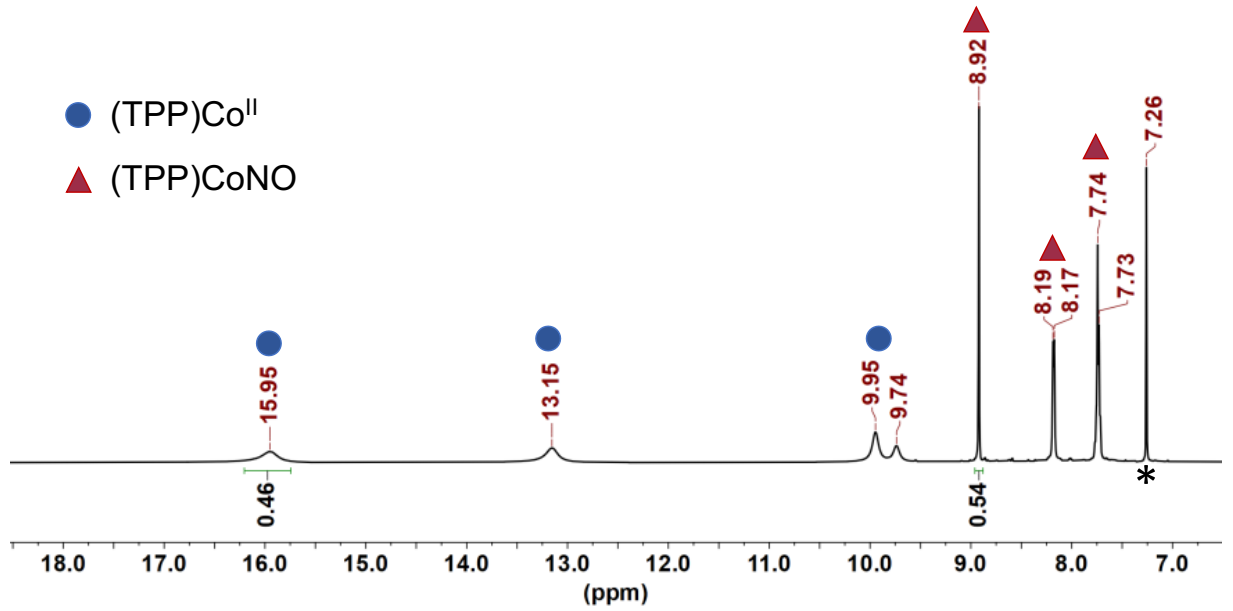


Figure S72. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of (TPP)Co^{II} solution after the NO–trapping experiment performed for the catalytic reaction of [(**Me$_2$PzQu**)$_2$Zn(OTf)](OTf) (**3-Qu**) (10 mol%) with [TBA$^+$][NO_2^-] and ^{t}BuBnSH. The resonance marked with * originates from $CDCl_3$.

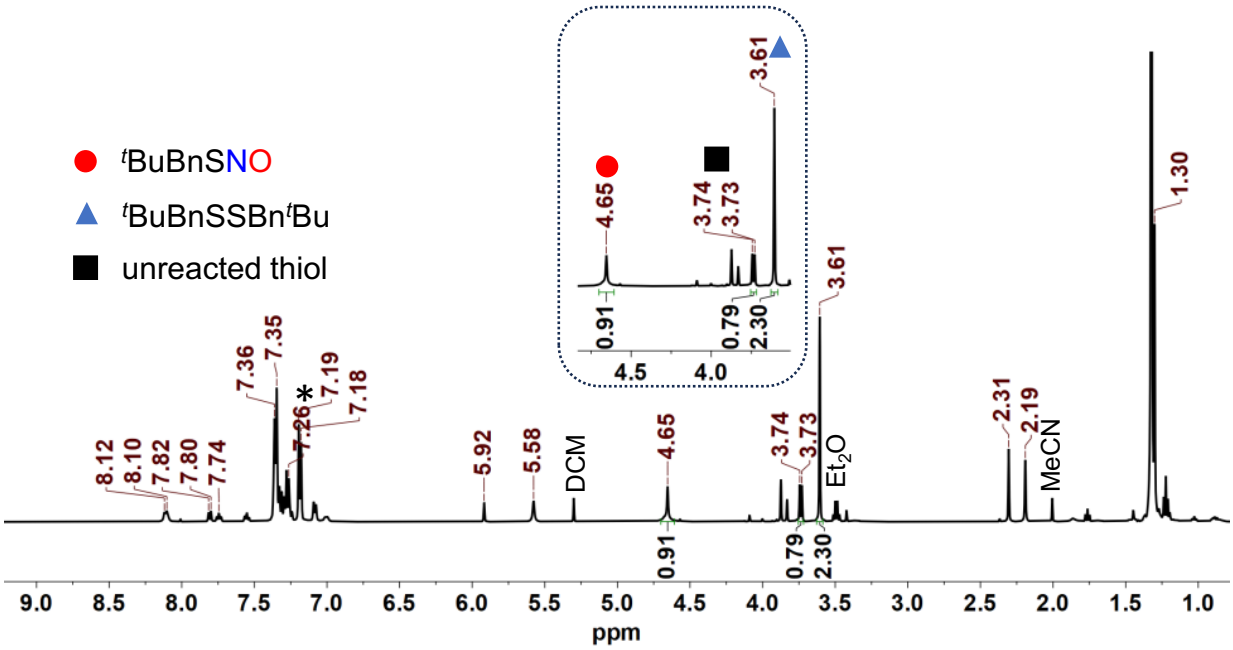


Figure S73. ^{1}H NMR spectrum (500 MHz, 298 K, $CDCl_3$) of the sample obtained from the reaction of the catalytic reaction of [(**Me$_2$PzQu**)$_2$Zn(OTf)](OTf) (**3-Qu**) (10 mol%) with [TBA$^+$][NO_2^-] and ^{t}BuBnSH showing signals for ^{t}BuBnSNO (0.46 equiv., 46% yield), (^{t}BuBnS)$_2$ (0.58 equiv.), and unreacted ^{t}BuBnSH (0.40 equiv.). The resonance marked with * originates from $CDCl_3$. The proton resonances of CH_2Cl_2 and Et_2O are likely originating from the glovebox atmosphere.

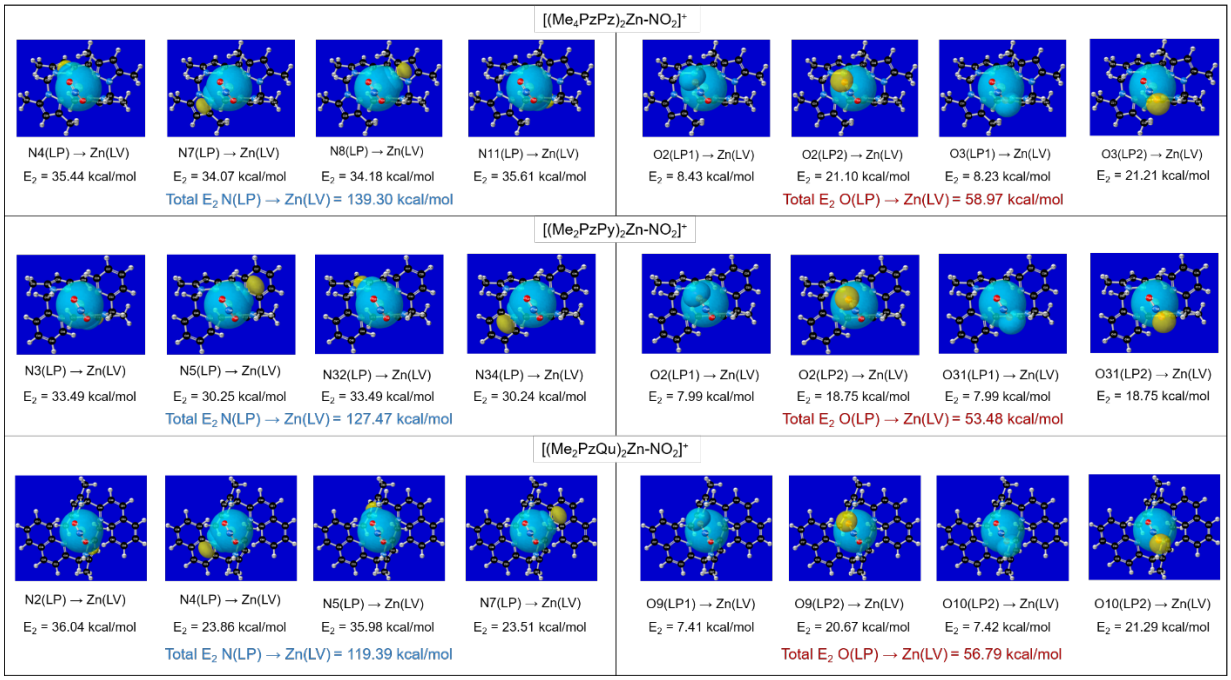


Figure S74. Second-order perturbation energy (E_2, kcal/mol) for the charge-transfer interaction between the ligand and the lone vacant (LV) orbital of Zn for all the nitrite-bound complexes, **5-Pz**, **5-Py**, and **5-Qu** obtained from the NBO analysis.

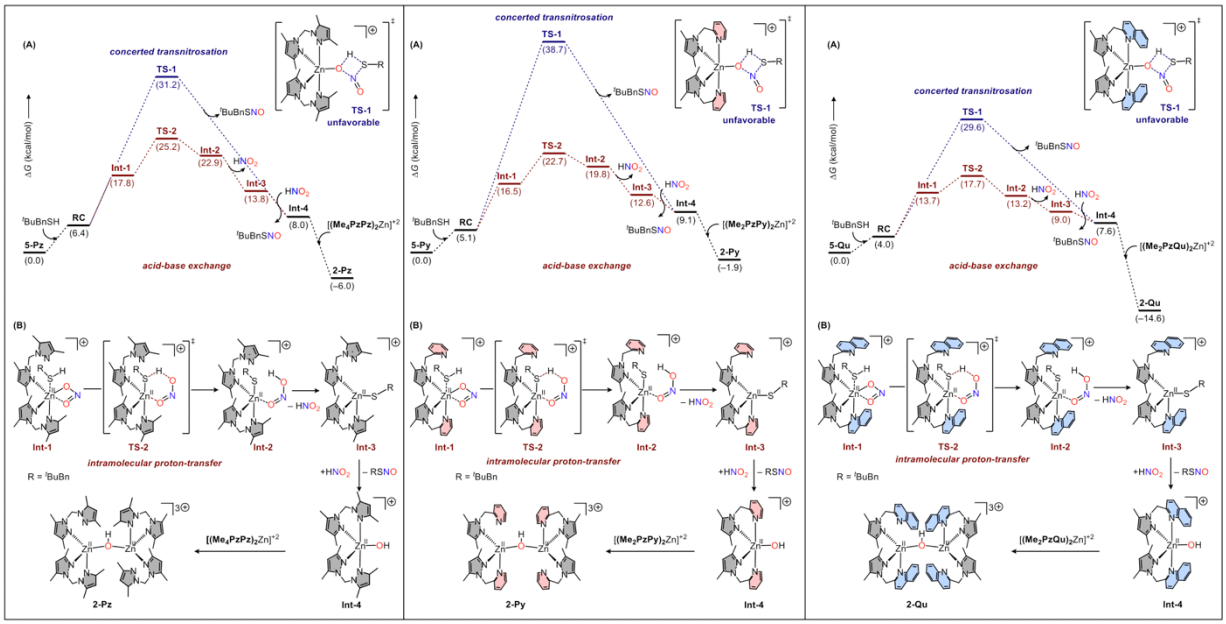
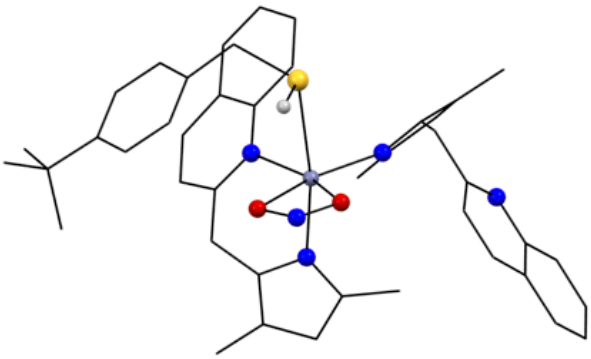
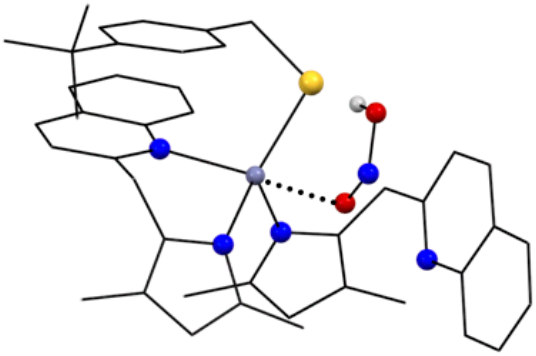


Figure S75. (A) Gibbs free energy profile (ΔG, kcal/mol) for the concerted transnitrosation and acid-base exchange routes for the reactions of $[\mathbf{L}_2Zn^{II}(\kappa^2\text{-nitrite})]^+$ and ^{t}BuBnSH calculated at B3LYP-D3BJ/[6-311++G(d,p)+LANL2TZ]/SMD(MeCN)//B3LYP-D3BJ[6-31G(d)+LANL2DZ] level of theory. (B) Schematic representations of the key intermediates and the transition state proposed for the acid-base exchange route.

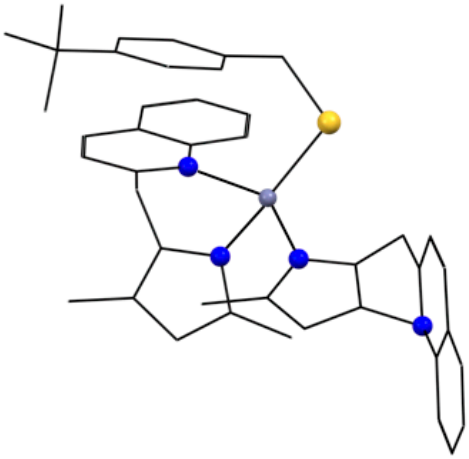
Comment: While **2-Qu** has been observed experimentally, the analogous complexes **2-Pz** and **2-Py** are not observed experimentally. **2-Pz** and **2-Py** are computationally considered for a comparison with the reaction profile of **5-Qu**.



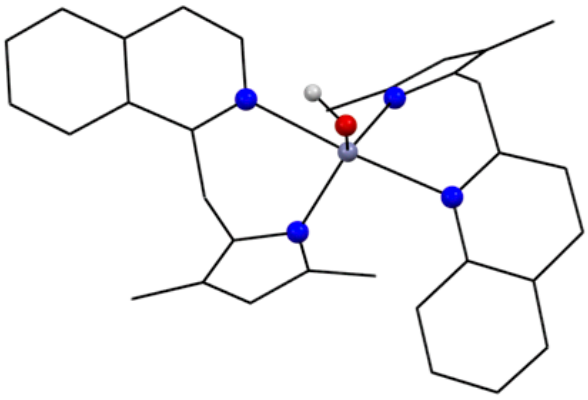
Int-1	distances in Å
Zn–N_{Pz}	2.133, 2.141
Zn–N_{Qu}	2.234, 4.661
Zn–O	2.153, 2.264
Zn–S	2.893
N–O	1.257, 1.271



Int-2	distances in Å
Zn–N_{Pz}	2.103, 2.130
Zn–N_{Qu}	2.200, 4.139
Zn–O	3.063, 4.132
Zn–S	2.342
N–O	1.355, 1.204
S–H	2.144

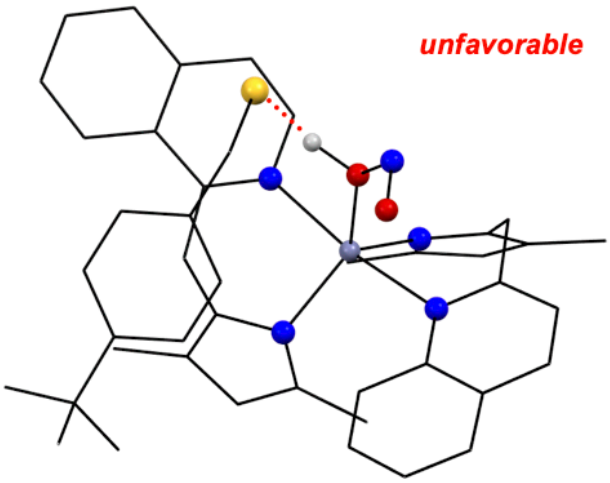


Int-3	distances in Å
Zn–N_{Pz}	2.127, 2.108
Zn–N_{Qu}	2.173, 4.574
Zn–S	2.308

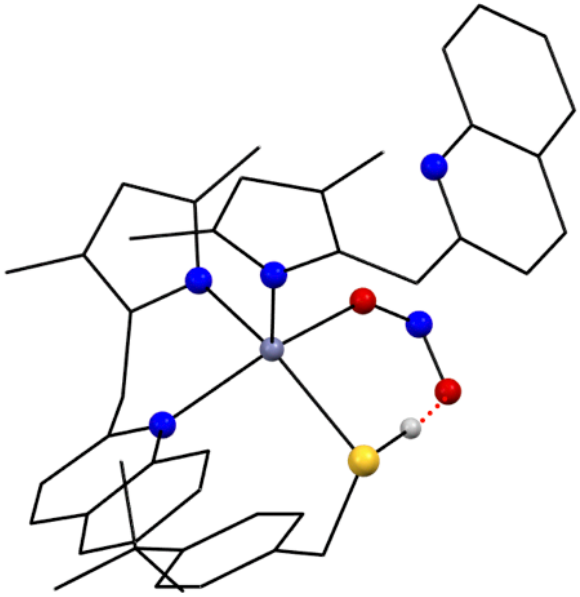


Int-4	distances in Å
Zn–N_{Pz}	2.143, 2.141
Zn–N_{Qu}	2.268, 2.312
Zn–O	1.900

Figure S76. DFT optimized structures of **Int-1**, **Int-2**, **Int-3**, and **Int-4** for the reaction of **5-Qu** and ^{t}BuBnSH in Figures 8 and S75.



TS-1	distances in Å
Zn–N_{Pz}	2.108, 2.125
Zn–N_{Qu}	2.280, 2.250
Zn–O	1.987, 3.619
Zn–S	4.384
S–N	2.987
N–O	1.603, 1.166
S–H	1.761
O–H	1.109



TS-2	distances in Å
Zn–N_{Pz}	2.132, 2.115
Zn–N_{Qu}	2.300, 4.198
Zn–O	2.211, 3.558
Zn–S	2.483
N–O	1.259, 1.269
S–H	1.524
O–H	1.382

Figure S77. DFT optimized structures of **TS-1** and **TS-2** for the reaction of **5-Qu** and ^{t}BuBnSH in Figures 8 and S75. The tables indicate the interatomic distances between the pair of atoms.

21. Tables

Table S1. Summary of yields obtained from various reactions of nitrite at zinc(II).

Entry	Reaction	% yield of RSNO	% yield of NO
1	[(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO$_4$) + ^{t}BuBnSH	17	32
2	[(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) + ^{t}BuBnSH	19	42
3	[(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) + ^{t}BuBnSH	41	49
4	[(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO$_4$) + ^{t}BuBnSH (2 equiv.)	17	40
5	[(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) + ^{t}BuBnSH (2 equiv.)	22	40
6	[(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) + ^{t}BuBnSH (2 equiv.)	34	54
7	[(**Me$_2$PzPy**)$_2$Zn(ONO)](ClO$_4$) + 4-Me-C$_6$H$_4$-SH (2 equiv.)	NA$^\blacklozenge$	82
8	[(**Me$_4$PzPz**)$_2$Zn(ONO)](ClO$_4$) + 4-Me-C$_6$H$_4$-SH (2 equiv.)	NA$^\blacklozenge$	74
9	[(**Me$_2$PzQu**)$_2$Zn(ONO)](ClO$_4$) + 4-Me-C$_6$H$_4$-SH (2 equiv.)	NA$^\blacklozenge$	100
10	10 mol% [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) + ^{t}BuBnSH + [TBA$^+$][NO$_2^-$]	12	46
11	10 mol% [(**Me$_2$PzQu**)$_2$Zn(OTf)](OTf) + ^{t}BuBnSH + [TBA$^+$][NO$_2^-$]	46	54
12	10 mol% [{(**Me$_2$PzQu**)$_2$Zn}$_2$(μ–OH)](ClO$_4$)$_3$ + ^{t}BuBnSH + [TBA$^+$][NO$_2^-$]	26	72
13	^{t}BuBnSH + [TBA$^+$][NO$_2^-$]	0	-
13	10 mol% [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) + ^{t}BuBnSH + NaNO$_2$	8	26
14	10 mol% [(**Me$_2$PzPy**)$_2$Zn(OTf)](OTf) + ^{t}BuBnSH + NaNO$_2$	9	40

$^\blacklozenge$ 4-Me-C$_6$H$_4$-SNO is not observed under the present experimental conditions, as the *S*-nitrosothiol derivatives of thiophenols contain extremely weak S–N bond. Consequently, 4-Me-C$_6$H$_4$-SNO rapidly transforms to NO and corresponding disulfide.[7b]

Table S2. Comparison of the bond length parameter (in Å) between the crystal structure and DFT-optimized structures. Bond lengths are obtained at the B3LYP-D3BJ/[6-31G(d)+LANL2DZ]/SMD(acetonitrile) level of theory.

Bond	Crystal Structure (Å)	Optimized Structure (Å)
N4-Zn$_{[(Me4PzPz)2Zn-NO2]+}$	2.11373	2.17265
N7-Zn$_{[(Me4PzPz)2Zn-NO2]+}$	2.13438	2.19989
N11-Zn$_{[(Me4PzPz)2Zn-NO2]+}$	2.10082	2.17301
N8-Zn$_{[(Me4PzPz)2Zn-NO2]+}$	2.15462	2.20256
O3-Zn$_{[(Me4PzPz)2Zn-NO2]+}$	2.22563	2.23324
O2-Zn$_{[(Me4PzPz)2Zn-NO2]+}$	2.16714	2.23328
N3-Zn$_{[(Me2PzPy)2Zn-NO2]+}$	2.08513	2.16379
N5-Zn$_{[(Me2PzPy)2Zn-NO2]+}$	2.15554	2.20916
N32-Zn$_{[(Me2PzPy)2Zn-NO2]+}$	2.08513	2.16368
N34-Zn$_{[(Me2PzPy)2Zn-NO2]+}$	2.15554	2.20949
O2-Zn$_{[(Me2PzPy)2Zn-NO2]+}$	2.22879	2.25141
O31-Zn$_{[(Me2PzPy)2Zn-NO2]+}$	2.22879	2.25150
N2-Zn$_{[(Me2PzQu)2Zn-NO2]+}$	2.06486	2.14534
N4-Zn$_{[(Me2PzQu)2Zn-NO2]+}$	2.33385	2.33899
N5-Zn$_{[(Me2PzQu)2Zn-NO2]+}$	2.06431	2.14525
N7-Zn$_{[(Me2PzQu)2Zn-NO2]+}$	2.27836	2.33958

O10-Zn$_{[(Me2PzQu)2Zn-NO2]+}$	2.18674	2.23502
O9-Zn$_{[(Me2PzQu)2Zn-NO2]+}$	2.21287	2.25139

Table S3. Optimized Cartesian Coordinates.

^{t}BuBnSH

C	-2.681085000	-0.011714000	0.156011000
C	-3.295463000	1.388699000	0.315457000
C	-2.950043000	-0.807911000	1.451784000
H	-2.571802000	-1.832808000	1.383535000
H	-2.466187000	-0.328683000	2.309930000
H	-4.027294000	-0.860096000	1.650125000
H	-2.859358000	1.928850000	1.163012000
H	-4.372084000	1.299638000	0.497065000
H	-3.159990000	1.996357000	-0.586139000
C	-3.377337000	-0.712572000	-1.031083000
H	-3.011576000	-1.734987000	-1.169237000
H	-4.459599000	-0.763434000	-0.861876000
H	-3.201867000	-0.164649000	-1.963531000
C	-1.169420000	0.040678000	-0.101107000
C	-0.451117000	1.239890000	-0.176699000
C	-0.448375000	-1.152944000	-0.271418000
C	0.924669000	1.248198000	-0.411626000
C	0.922287000	-1.148428000	-0.506001000
C	1.631190000	0.056534000	-0.584826000
H	-0.959244000	2.188981000	-0.052295000
H	-0.965075000	-2.106720000	-0.220561000
H	1.454834000	2.196251000	-0.459131000
H	1.452354000	-2.089829000	-0.627639000
C	3.117538000	0.063487000	-0.814880000
H	3.419545000	-0.783164000	-1.436844000
H	3.431116000	0.990011000	-1.302372000
S	3.982143000	-0.068695000	0.823944000
H	5.244877000	-0.060107000	0.339171000

^{t}BuBnSNO

O	3.963210000	-1.561722000	-0.539634000
N	4.246342000	-1.017891000	0.482640000
C	-3.247382000	-0.226765000	0.143035000
C	-4.102020000	1.044644000	0.273529000
C	-3.400439000	-1.047769000	1.442258000
H	-2.846427000	-1.990561000	1.393881000
H	-3.028070000	-0.484029000	2.304677000
H	-4.455761000	-1.287544000	1.618752000
H	-3.785572000	1.660807000	1.122411000
H	-5.149514000	0.768592000	0.436046000
H	-4.057476000	1.658449000	-0.632960000
C	-3.782301000	-1.048922000	-1.050015000
H	-3.238568000	-1.991458000	-1.169009000
H	-4.841887000	-1.289229000	-0.902131000
H	-3.685958000	-0.485753000	-1.984867000
C	-1.763570000	0.089336000	-0.084410000
C	-1.267104000	1.394873000	-0.166692000
C	-0.838687000	-0.960539000	-0.221282000
C	0.091330000	1.643666000	-0.374884000
C	0.513692000	-0.718416000	-0.429167000
C	0.999297000	0.593505000	-0.510704000
H	-1.937526000	2.240721000	-0.069206000
H	-1.180513000	-1.989794000	-0.166735000
H	0.444149000	2.670793000	-0.432645000
H	1.204700000	-1.551061000	-0.531029000
C	2.465131000	0.852440000	-0.723250000
H	2.893451000	0.143233000	-1.443967000
H	2.656345000	1.867898000	-1.079121000
S	3.473180000	0.623851000	0.792749000

5-Qu

Zn	-0.000092000	0.000023000	-0.702300000
N	0.360387000	-1.590842000	0.697482000
N	-0.289896000	-2.776645000	0.528776000
N	-2.196336000	-0.741907000	-0.721473000
N	-0.360839000	1.590730000	0.697428000
N	0.289782000	2.776394000	0.529186000
N	2.196314000	0.741938000	-0.720871000
N	0.000521000	0.000309000	-3.311770000
O	-0.289758000	1.012247000	-2.608779000
O	0.290468000	-1.011819000	-2.608991000
C	1.033518000	-1.690483000	1.855704000
C	0.797054000	-2.952792000	2.429399000
H	1.200547000	-3.332602000	3.356485000
C	-0.056972000	-3.623775000	1.565965000
C	1.903290000	-0.590588000	2.374402000
H	2.939451000	-0.727147000	2.045376000
H	1.562227000	0.384620000	2.023449000
H	1.897796000	-0.589501000	3.467936000
C	-1.188389000	-2.946141000	-0.607584000
H	-0.638864000	-2.731980000	-1.527926000
H	-1.497030000	-3.990994000	-0.625339000
C	-2.398035000	-2.037830000	-0.510883000
C	-3.665153000	-2.576853000	-0.197901000
H	-3.770789000	-3.644679000	-0.038603000
C	-4.744708000	-1.730827000	-0.093123000
H	-5.728853000	-2.112298000	0.164420000
C	-5.649301000	0.577429000	-0.264754000
H	-6.637500000	0.214294000	0.002282000
C	-5.436063000	1.907862000	-0.539246000
H	-6.257651000	2.614902000	-0.485654000
C	-4.146622000	2.357979000	-0.916033000
H	-3.999316000	3.405082000	-1.161808000
C	-3.082999000	1.487066000	-0.989985000
H	-2.108426000	1.825607000	-1.311774000
C	-3.266331000	0.115505000	-0.682541000
C	-4.576917000	-0.349210000	-0.338488000
C	-1.034077000	1.690189000	1.855615000
C	-0.797325000	2.952238000	2.429741000
H	-1.200742000	3.331829000	3.356952000
C	0.056990000	3.623262000	1.566629000
C	-1.904101000	0.590315000	2.373940000
H	-1.898306000	0.588647000	3.467479000
H	-2.940311000	0.727373000	2.045297000
H	-1.563446000	-0.384816000	2.022405000
C	1.188310000	2.946183000	-0.607103000
H	0.638817000	2.732254000	-1.527511000
H	1.496918000	3.991042000	-0.624547000
C	2.398002000	2.037902000	-0.510625000
C	3.665196000	2.577103000	-0.198191000
H	3.770791000	3.644971000	-0.039155000
C	4.744846000	1.731195000	-0.093597000
H	5.729062000	2.112789000	0.163492000
C	4.577058000	0.349497000	-0.338543000
C	5.649542000	-0.577030000	-0.264946000
H	6.637806000	-0.213750000	0.001652000
C	5.436331000	-1.907552000	-0.539038000
H	6.257999000	-2.614506000	-0.485537000
C	4.146799000	-2.357870000	-0.915251000
H	3.999488000	-3.405049000	-1.160695000
C	3.083082000	-1.487056000	-0.989061000
H	2.108422000	-1.825787000	-1.310358000
C	3.266391000	-0.115400000	-0.682041000
C	-0.657261000	-4.988537000	1.658740000
H	-0.374340000	-5.617501000	0.806809000
H	-0.306390000	-5.481114000	2.567886000
H	-1.752077000	-4.949596000	1.701080000
C	0.657568000	4.987865000	1.659847000
H	0.375036000	5.617062000	0.807960000
H	0.306538000	5.480348000	2.568983000
H	1.752362000	4.948653000	1.702506000

RC			
Zn	1.355381000	0.306038000	-0.460403000
N	2.662488000	1.777163000	0.396713000
N	3.974194000	1.783267000	0.028068000
N	3.204920000	-1.089069000	-0.492892000
N	0.530166000	-0.489493000	1.348067000
N	-0.814891000	-0.691569000	1.424979000
N	-0.490330000	1.667733000	-0.514220000
N	0.967315000	-0.297297000	-2.994538000
O	0.432369000	-0.915980000	-2.025427000
O	1.716576000	0.641909000	-2.610491000
C	2.565509000	2.591129000	1.461216000
C	3.835283000	3.109697000	1.773205000
H	4.080460000	3.794989000	2.571201000
C	4.718084000	2.572889000	0.846956000
C	1.262182000	2.871758000	2.137981000
H	0.750524000	3.715118000	1.661097000
H	0.598795000	2.006034000	2.095980000
H	1.431093000	3.131577000	3.186448000
C	4.417394000	0.939073000	-1.073087000
H	3.772604000	1.123145000	-1.936267000
H	5.430023000	1.246742000	-1.332459000
C	4.391259000	-0.535839000	-0.721988000
C	5.601902000	-1.259662000	-0.662755000
H	6.540478000	-0.753317000	-0.861298000
C	5.567193000	-2.599542000	-0.354185000
H	6.482485000	-3.181826000	-0.294197000
C	4.218100000	-4.610995000	0.190799000
H	5.126148000	-5.203452000	0.255981000
C	2.984948000	-5.182706000	0.396815000
H	2.904372000	-6.239373000	0.630668000
C	1.812028000	-4.395754000	0.292103000
H	0.839675000	-4.855077000	0.435629000
C	1.882546000	-3.053568000	-0.005713000
H	0.979958000	-2.468096000	-0.091883000
C	3.138949000	-2.431373000	-0.210758000
C	4.325388000	-3.230324000	-0.120390000
C	1.042457000	-0.901133000	2.520865000
C	0.005000000	-1.365636000	3.347236000
H	0.097187000	-1.762152000	4.347630000
C	-1.171368000	-1.219343000	2.623033000
C	2.509516000	-0.866827000	2.808080000
H	2.682203000	-0.683859000	3.872344000
H	2.976544000	-1.824827000	2.553422000
H	3.009160000	-0.084325000	2.234780000
C	-1.666772000	-0.297519000	0.309820000
H	-1.363832000	-0.851416000	-0.579073000
H	-2.685236000	-0.594273000	0.550615000
C	-1.595434000	1.191736000	0.049596000
C	-2.680355000	2.016502000	0.417403000
H	-3.553864000	1.565790000	0.868286000
C	-2.603372000	3.370376000	0.195516000
H	-3.416674000	4.029871000	0.486258000
C	-1.458302000	3.910862000	-0.433498000
C	-1.317076000	5.295244000	-0.710387000
H	-2.116605000	5.970928000	-0.420386000
C	-0.190135000	5.765103000	-1.343505000
H	-0.084839000	6.824028000	-1.556746000
C	0.829138000	4.864798000	-1.739208000
H	1.699528000	5.243979000	-2.265786000
C	0.726632000	3.516432000	-1.479316000
H	1.489031000	2.826623000	-1.812390000
C	-0.410034000	3.007757000	-0.802598000
C	6.192267000	2.754471000	0.688534000
H	6.447270000	3.191804000	-0.283888000
H	6.563424000	3.427805000	1.463880000
H	6.730950000	1.804441000	0.783433000
C	-2.584463000	-1.541055000	2.982032000
H	-3.030917000	-2.235236000	2.262950000
H	-2.614996000	-2.000810000	3.972107000
H	-3.213710000	-0.643783000	3.006115000
S	-1.303928000	-3.762441000	-1.425917000

C	-2.987592000	-3.490545000	-2.154004000
H	-2.863237000	-3.249922000	-3.211988000
H	-3.468822000	-4.470418000	-2.095184000
C	-3.816401000	-2.452455000	-1.447762000
C	-4.456535000	-2.755057000	-0.237901000
C	-3.991348000	-1.171373000	-1.975488000
C	-5.262524000	-1.817891000	0.399743000
C	-4.799985000	-0.228952000	-1.330590000
C	-5.467426000	-0.533382000	-0.136950000
H	-4.335944000	-3.744575000	0.196673000
H	-3.505272000	-0.905249000	-2.911131000
H	-5.767700000	-2.104808000	1.317094000
H	-4.919762000	0.746180000	-1.788216000
C	-6.453611000	0.427102000	0.543614000
C	-6.492849000	1.806722000	-0.135520000
C	-6.085641000	0.619254000	2.031223000
H	-6.077933000	-0.329001000	2.577322000
H	-5.097642000	1.080638000	2.149128000
H	-6.815450000	1.274652000	2.518942000
H	-5.512817000	2.296422000	-0.136968000
H	-7.191196000	2.459572000	0.398114000
H	-6.836084000	1.736285000	-1.172736000
C	-7.869011000	-0.189835000	0.457795000
H	-7.917923000	-1.157121000	0.967749000
H	-8.603817000	0.475891000	0.924787000
H	-8.161150000	-0.345116000	-0.585949000
H	-0.696923000	-2.699965000	-1.998991000

TS-1

Zn	1.142066000	-0.603368000	0.017536000
O	1.221554000	0.827659000	-3.305799000
O	0.851789000	-0.962339000	-1.915434000
N	0.247203000	0.362742000	1.663339000
N	-1.043243000	0.016289000	1.934535000
C	-1.745128000	-1.762569000	0.358484000
N	-0.482903000	-2.145889000	0.228779000
N	2.824113000	0.830288000	-0.542798000
C	3.939805000	0.271981000	-1.005358000
N	3.864346000	-1.838350000	0.286266000
N	2.633369000	-1.855759000	0.867616000
N	1.253609000	-0.337546000	-3.335500000
C	0.803935000	0.707341000	2.840600000
C	-0.148801000	0.577475000	3.862997000
H	-0.010597000	0.788474000	4.913173000
C	-1.318234000	0.128971000	3.256650000
C	2.229355000	1.150126000	2.936975000
H	2.902075000	0.438155000	2.449240000
H	2.370457000	2.123386000	2.455023000
H	2.525100000	1.241545000	3.984657000
C	-1.941967000	-0.344607000	0.850312000
H	-1.770197000	0.353575000	0.027916000
C	4.008960000	-1.244112000	-1.032892000
H	3.208944000	-1.637784000	-1.669472000
H	4.963251000	-1.571441000	-1.444872000
C	2.785979000	-2.441109000	2.066823000
C	4.136581000	-2.794606000	2.244994000
H	4.573432000	-3.291436000	3.098766000
C	4.804263000	-2.393744000	1.095431000
C	1.633231000	-2.629369000	3.000589000
H	0.683766000	-2.496414000	2.478891000
H	1.655820000	-3.632284000	3.437609000
H	1.671818000	-1.907976000	3.824008000
C	6.242394000	-2.511036000	0.709960000
H	6.686323000	-1.531439000	0.498459000
H	6.806050000	-2.965074000	1.527416000
H	6.374598000	-3.141343000	-0.177428000
C	-2.660473000	-0.184053000	3.831486000
H	-2.993178000	-1.190010000	3.553120000
H	-2.617166000	-0.129164000	4.921112000
H	-3.420374000	0.529246000	3.490902000
H	-2.953271000	-0.168618000	1.199958000
C	-3.826423000	3.413294000	1.095646000
C	-5.080059000	2.817675000	1.759247000
C	-4.160786000	4.838010000	0.600410000
H	-3.285289000	5.312757000	0.144791000
H	-4.955680000	4.811046000	-0.152107000
H	-4.496078000	5.467947000	1.432758000
H	-5.942456000	2.822707000	1.085329000
H	-5.351167000	3.407731000	2.640732000
H	-4.913434000	1.783262000	2.086468000
C	-2.714937000	3.500871000	2.164175000
H	-1.819287000	4.004902000	1.787989000
H	-3.068499000	4.070176000	3.030879000
H	-2.412245000	2.507151000	2.510249000
C	-3.355592000	2.576682000	-0.101031000
C	-4.150038000	1.588876000	-0.704486000
C	-2.095350000	2.808988000	-0.670961000
C	-3.703445000	0.867563000	-1.812998000
C	-1.645041000	2.090800000	-1.779074000
C	-2.444359000	1.107939000	-2.377712000
H	-5.140662000	1.376831000	-0.316363000
H	-1.453983000	3.580261000	-0.258605000
H	-4.339756000	0.103549000	-2.251263000
H	-0.666167000	2.308366000	-2.197087000
C	-1.981961000	0.373791000	-3.608763000
H	-2.773982000	0.393260000	-4.363551000
H	-1.119001000	0.903095000	-4.032760000
S	-1.538024000	-1.399115000	-3.359710000
H	-0.154681000	-1.249693000	-2.280856000
C	5.026622000	1.024662000	-1.498370000

H	5.910567000	0.513831000	-1.864604000
C	4.941644000	2.397411000	-1.511435000
H	5.762637000	3.003105000	-1.884549000
C	2.706855000	2.197966000	-0.558594000
C	3.769695000	3.028580000	-1.039607000
C	-0.200399000	-3.392559000	-0.246887000
H	0.853303000	-3.635740000	-0.321902000
C	-1.178726000	-4.275080000	-0.616802000
H	-0.917330000	-5.255340000	-1.001599000
C	-2.841748000	-2.590478000	-0.006272000
C	-2.539259000	-3.893317000	-0.518051000
C	-3.597247000	-4.747770000	-0.914916000
H	-3.358142000	-5.732170000	-1.305579000
C	-4.903247000	-4.326452000	-0.819475000
H	-5.710217000	-4.981104000	-1.133306000
C	-4.201496000	-2.186694000	0.081707000
C	-5.205804000	-3.036541000	-0.319790000
H	-6.241098000	-2.716110000	-0.259450000
H	-4.457414000	-1.193929000	0.431229000
C	1.512046000	2.811546000	-0.105913000
H	0.695952000	2.193040000	0.244134000
C	1.394947000	4.183954000	-0.113183000
H	0.478489000	4.644905000	0.241810000
C	3.613113000	4.439118000	-1.035928000
H	4.427592000	5.055859000	-1.404324000
C	2.448679000	5.007876000	-0.577681000
H	2.329875000	6.086423000	-0.575286000

Int-1

Zn	0.209114000	-0.078047000	0.520781000
N	0.504727000	-1.864571000	-0.607305000
N	-0.592056000	-2.531670000	-1.056873000
C	-2.261430000	-0.717563000	-1.195089000
N	-1.579034000	0.335829000	-0.752030000
N	4.790365000	0.713431000	0.191146000
C	4.120025000	0.715718000	1.323828000
N	2.436189000	2.074128000	0.150885000
N	1.632635000	1.161735000	-0.489498000
C	1.575196000	-2.512673000	-1.089581000
C	1.144668000	-3.606245000	-1.864754000
H	1.766697000	-4.322553000	-2.380918000
C	-0.243361000	-3.596873000	-1.826870000
C	2.964514000	-2.054776000	-0.780681000
H	3.696726000	-2.773528000	-1.155303000
H	3.175937000	-1.080795000	-1.231710000
H	3.105149000	-1.945968000	0.299012000
C	-1.911729000	-2.083045000	-0.636626000
H	-1.946471000	-2.062852000	0.455481000
C	3.001208000	1.740420000	1.449980000
H	2.213037000	1.362713000	2.099027000
H	3.371080000	2.669815000	1.893078000
C	1.657733000	1.490456000	-1.793602000
C	2.490110000	2.605454000	-1.987913000
H	2.711493000	3.096550000	-2.924053000
C	2.998556000	2.932355000	-0.742935000
C	0.893000000	0.745705000	-2.841597000
H	0.554074000	-0.223998000	-2.477996000
H	0.020666000	1.316569000	-3.177279000
H	1.533215000	0.581373000	-3.713953000
C	4.006656000	3.959339000	-0.351015000
H	4.938607000	3.472025000	-0.044884000
H	4.222984000	4.609244000	-1.201676000
H	3.654660000	4.586606000	0.475301000
C	-1.242876000	-4.518434000	-2.445873000
H	-1.929597000	-3.986767000	-3.115100000
H	-0.724740000	-5.277623000	-3.035364000
H	-1.842604000	-5.036555000	-1.688147000
H	-2.634816000	-2.819543000	-0.982300000
C	-6.217555000	-1.570377000	0.560204000
C	-5.525814000	-2.875310000	0.111281000
C	-7.068586000	-1.054827000	-0.612035000
H	-7.647565000	-0.167568000	-0.335600000
H	-6.449862000	-0.803779000	-1.481846000
H	-7.779502000	-1.828053000	-0.920724000
H	-4.906220000	-2.700080000	-0.775690000
H	-6.274926000	-3.630359000	-0.150830000
H	-4.889050000	-3.296676000	0.895124000
C	-7.155249000	-1.878840000	1.749212000
H	-7.656983000	-0.968421000	2.093371000
H	-7.923000000	-2.602111000	1.451649000
H	-6.605239000	-2.299938000	2.596740000
C	-5.172820000	-0.543082000	1.015743000
C	-4.257437000	-0.872215000	2.030460000
C	-5.107931000	0.754631000	0.495426000
C	-3.333591000	0.050618000	2.509167000
C	-4.177803000	1.681758000	0.967753000
C	-3.279139000	1.346156000	1.982058000
H	-4.271941000	-1.863482000	2.472839000
H	-5.787822000	1.062348000	-0.289794000
H	-2.642523000	-0.255272000	3.287076000
H	-4.156150000	2.679990000	0.537961000
C	-2.321742000	2.381619000	2.506154000
H	-2.376257000	3.294635000	1.909348000
H	-2.537992000	2.655144000	3.542772000
S	-0.521773000	1.924509000	2.476151000
C	4.388176000	-0.168923000	2.399380000
H	3.778082000	-0.136218000	3.294266000
C	5.400042000	-1.087843000	2.255990000
H	5.630272000	-1.790022000	3.052806000
C	5.792065000	-0.198032000	0.026090000

C	6.139631000	-1.137162000	1.047628000
C	-3.280362000	-0.611110000	-2.167605000
H	-3.791311000	-1.506491000	-2.502181000
C	-3.614841000	0.623593000	-2.665077000
C	-1.893654000	1.585490000	-1.232261000
C	-2.936260000	1.769361000	-2.194867000
C	7.181015000	-2.069156000	0.805744000
H	7.442650000	-2.780085000	1.584840000
C	7.847487000	-2.069069000	-0.399104000
H	8.644798000	-2.783479000	-0.579527000
C	6.495069000	-0.221197000	-1.204777000
H	6.211853000	0.500678000	-1.964017000
C	7.501205000	-1.138544000	-1.410672000
H	8.038493000	-1.152658000	-2.354244000
C	-3.257850000	3.076871000	-2.641883000
H	-4.058440000	3.197636000	-3.365894000
C	-2.567485000	4.166810000	-2.165458000
H	-2.816997000	5.166166000	-2.506722000
H	-4.400364000	0.733019000	-3.407506000
C	-1.183449000	2.725350000	-0.780275000
H	-0.365851000	2.601173000	-0.085739000
C	-1.517269000	3.982044000	-1.234702000
H	-0.961506000	4.843039000	-0.876554000
N	0.438034000	-1.471303000	2.753488000
O	-0.652404000	-1.417801000	2.129840000
O	1.335635000	-0.736272000	2.233294000
H	-0.548416000	1.034232000	3.484172000

TS-2

Zn	-0.231177000	0.429773000	-0.133455000
N	0.093483000	-0.572235000	1.700834000
N	1.343903000	-0.633527000	2.235925000
C	2.698273000	0.986150000	0.935339000
N	1.708156000	1.591444000	0.288198000
N	-4.395271000	-0.104776000	-0.122636000
C	-3.897395000	0.219935000	-1.295553000
N	-2.868761000	2.143122000	-0.119166000
N	-1.679025000	1.862736000	0.495609000
C	-0.758385000	-0.942500000	2.672791000
C	-0.026898000	-1.241384000	3.838406000
H	-0.425538000	-1.575111000	4.785054000
C	1.311806000	-1.045388000	3.530490000
C	-2.235981000	-0.998096000	2.462353000
H	-2.466465000	-1.503884000	1.523523000
H	-2.710115000	-1.534866000	3.287592000
H	-2.676461000	0.002717000	2.404931000
C	2.487738000	-0.448689000	1.363369000
H	2.351932000	-1.080677000	0.481019000
C	-3.217307000	1.574376000	-1.405346000
H	-2.312859000	1.514746000	-2.014778000
H	-3.877885000	2.287681000	-1.909328000
C	-1.723747000	2.485502000	1.691913000
C	-2.958288000	3.133899000	1.840523000
H	-3.288076000	3.717933000	2.686951000
C	-3.673885000	2.884214000	0.678348000
C	-0.597242000	2.458480000	2.676585000
H	0.367815000	2.340012000	2.184094000
H	-0.583409000	3.392715000	3.244790000
H	-0.711209000	1.635406000	3.390281000
C	-5.058296000	3.274998000	0.284332000
H	-5.672420000	2.382030000	0.126593000
H	-5.513102000	3.873318000	1.076420000
H	-5.071805000	3.869932000	-0.636442000
C	2.543271000	-1.243588000	4.352079000
H	3.156182000	-0.336080000	4.395024000
H	2.263628000	-1.507951000	5.373932000
H	3.166789000	-2.055347000	3.957454000
H	3.369901000	-0.813973000	1.885601000
C	5.209844000	-3.285642000	-0.138999000
C	4.435668000	-3.832250000	1.081246000
C	6.515402000	-2.649470000	0.364997000
H	7.131674000	-2.276396000	-0.459783000
H	6.324251000	-1.817915000	1.054411000
H	7.104937000	-3.396530000	0.905834000
H	4.201549000	-3.027989000	1.789987000
H	5.039582000	-4.577384000	1.610422000
H	3.494443000	-4.309140000	0.791534000
C	5.567834000	-4.456099000	-1.081532000
H	6.115352000	-4.095145000	-1.958506000
H	6.198738000	-5.184045000	-0.559437000
H	4.674191000	-4.979675000	-1.435091000
C	4.330698000	-2.283436000	-0.897142000
C	3.082600000	-2.687451000	-1.404726000
C	4.706250000	-0.953335000	-1.118709000
C	2.250206000	-1.809476000	-2.093929000
C	3.873641000	-0.067144000	-1.807855000
C	2.634917000	-0.476201000	-2.304609000
H	2.749261000	-3.711044000	-1.265510000
H	5.659066000	-0.587008000	-0.754824000
H	1.301011000	-2.171959000	-2.475417000
H	4.197198000	0.960042000	-1.955605000
C	1.794526000	0.487436000	-3.100818000
H	2.217337000	1.493626000	-3.053644000
H	1.756824000	0.196937000	-4.155129000
S	0.023094000	0.667654000	-2.591762000
C	-3.980059000	-0.599642000	-2.448681000
H	-3.541705000	-0.272128000	-3.386314000
C	-4.587469000	-1.826108000	-2.336851000
H	-4.650854000	-2.496164000	-3.189513000
C	-5.005344000	-1.319183000	0.006828000

C	-5.118028000	-2.233447000	-1.087426000
C	3.941748000	1.605104000	1.190131000
H	4.708101000	1.058361000	1.728226000
C	4.166431000	2.877928000	0.725980000
C	1.896769000	2.876724000	-0.167837000
C	3.144811000	3.553704000	0.020022000
C	-5.744707000	-3.488253000	-0.879883000
H	-5.823686000	-4.180890000	-1.713240000
C	-6.243213000	-3.819467000	0.360033000
H	-6.722131000	-4.781356000	0.514573000
C	-5.533266000	-1.684051000	1.270484000
H	-5.444997000	-0.970530000	2.083339000
C	-6.138285000	-2.909473000	1.441062000
H	-6.541915000	-3.185242000	2.410766000
C	3.313702000	4.867546000	-0.487717000
H	4.267234000	5.365888000	-0.338972000
C	2.284877000	5.494994000	-1.150413000
H	2.416151000	6.499387000	-1.539570000
H	5.118067000	3.374383000	0.894211000
C	0.849278000	3.556234000	-0.837134000
H	-0.106739000	3.068240000	-0.957336000
C	1.045768000	4.832428000	-1.318305000
H	0.235048000	5.339011000	-1.832561000
N	-1.453922000	-2.328282000	-1.411237000
O	-1.364637000	-1.424464000	-0.538997000
O	-1.027968000	-2.036626000	-2.570969000
H	-0.507754000	-0.759508000	-2.659754000

Int-2

Zn	-0.243467000	0.586332000	-0.162510000
N	-0.037767000	-0.392127000	1.687104000
N	1.219110000	-0.523195000	2.202119000
C	2.624701000	1.025725000	0.862479000
N	1.688415000	1.600693000	0.115442000
N	-4.337673000	-0.023188000	-0.181661000
C	-3.785117000	0.301693000	-1.331633000
N	-2.866590000	2.293180000	-0.171775000
N	-1.641687000	2.089911000	0.402732000
C	-0.891155000	-0.648870000	2.693853000
C	-0.158121000	-0.943829000	3.858985000
H	-0.558941000	-1.198213000	4.829056000
C	1.183575000	-0.862006000	3.517013000
C	-2.373613000	-0.630542000	2.525723000
H	-2.741088000	-1.637972000	2.307585000
H	-2.851985000	-0.283013000	3.446165000
H	-2.695277000	0.008807000	1.703171000
C	2.370568000	-0.391254000	1.327670000
H	2.220597000	-1.037654000	0.458043000
C	-3.209870000	1.703279000	-1.452402000
H	-2.317051000	1.697042000	-2.082018000
H	-3.938383000	2.365939000	-1.930465000
C	-1.666255000	2.756804000	1.575898000
C	-2.918991000	3.359935000	1.749493000
H	-3.240101000	3.964569000	2.584712000
C	-3.668966000	3.035274000	0.626168000
C	-0.494389000	2.809297000	2.505571000
H	0.446988000	2.892352000	1.958641000
H	-0.585835000	3.678318000	3.162202000
H	-0.439635000	1.916406000	3.137253000
C	-5.080895000	3.358203000	0.269789000
H	-5.656539000	2.436098000	0.136773000
H	-5.539827000	3.943119000	1.069505000
H	-5.147964000	3.943254000	-0.655090000
C	2.414274000	-1.096578000	4.330234000
H	3.070473000	-0.218693000	4.340491000
H	2.134588000	-1.317564000	5.362272000
H	2.992960000	-1.947786000	3.951626000
H	3.238568000	-0.769836000	1.863094000
C	5.430754000	-3.037747000	-0.030542000
C	4.801880000	-3.521577000	1.295177000
C	6.695677000	-2.230950000	0.304540000
H	7.210544000	-1.888411000	-0.599211000
H	6.467649000	-1.354165000	0.922939000
H	7.395422000	-2.857650000	0.866638000
H	4.547745000	-2.670931000	1.940686000
H	5.508592000	-4.154262000	1.843366000
H	3.890198000	-4.103550000	1.128468000
C	5.843047000	-4.263237000	-0.875621000
H	6.287603000	-3.947456000	-1.825212000
H	6.581340000	-4.866213000	-0.335192000
H	4.987107000	-4.906217000	-1.102811000
C	4.403487000	-2.209124000	-0.812236000
C	3.179642000	-2.786355000	-1.196670000
C	4.616110000	-0.873723000	-1.173416000
C	2.213265000	-2.063885000	-1.891471000
C	3.650330000	-0.147164000	-1.875944000
C	2.431256000	-0.721837000	-2.240290000
H	2.970927000	-3.822525000	-0.948412000
H	5.542831000	-0.377467000	-0.909839000
H	1.279876000	-2.547822000	-2.160260000
H	3.849903000	0.890332000	-2.133397000
C	1.421031000	0.083526000	-3.018277000
H	1.721573000	1.134310000	-3.043071000
H	1.376041000	-0.263050000	-4.056041000
S	-0.333216000	-0.006917000	-2.426820000
C	-3.730898000	-0.562009000	-2.455292000
H	-3.253208000	-0.232451000	-3.371409000
C	-4.264505000	-1.822948000	-2.339847000
H	-4.223500000	-2.523093000	-3.169286000
C	-4.874829000	-1.271529000	-0.049293000

C	-4.852592000	-2.225233000	-1.115269000
C	3.844330000	1.663250000	1.173719000
H	4.572444000	1.149240000	1.791368000
C	4.094197000	2.918369000	0.670946000
C	1.919333000	2.842126000	-0.425141000
C	3.137340000	3.544887000	-0.160841000
C	-5.398886000	-3.516232000	-0.902299000
H	-5.371325000	-4.239062000	-1.712882000
C	-5.951932000	-3.844198000	0.315063000
H	-6.368119000	-4.833965000	0.474620000
C	-5.460266000	-1.633154000	1.189547000
H	-5.480399000	-0.889545000	1.979636000
C	-5.985816000	-2.894152000	1.365767000
H	-6.433374000	-3.167252000	2.316711000
C	3.343314000	4.823505000	-0.740086000
H	4.269959000	5.349687000	-0.530337000
C	2.386006000	5.378312000	-1.557260000
H	2.547139000	6.354517000	-2.002770000
H	5.024764000	3.432570000	0.894465000
C	0.952597000	3.433964000	-1.274304000
H	0.039884000	2.895457000	-1.496356000
C	1.188014000	4.673401000	-1.827750000
H	0.446040000	5.115262000	-2.485375000
N	-1.623120000	-3.146998000	-0.679974000
O	-1.675139000	-2.118955000	-0.055434000
O	-1.226326000	-2.998320000	-1.967219000
H	-1.002643000	-2.020979000	-2.122812000

Int-3

Zn	-0.222165000	0.314439000	-0.402132000
N	-0.177940000	-1.121475000	1.140667000
N	0.976971000	-1.244824000	1.854181000
C	2.421961000	0.643672000	1.115789000
N	1.555644000	1.306011000	0.357484000
N	-4.785903000	0.016848000	-0.483011000
C	-3.880532000	0.100753000	-1.438678000
N	-2.842482000	2.026223000	-0.308862000
N	-1.745228000	1.579367000	0.375985000
C	-1.157661000	-1.629957000	1.906818000
C	-0.610935000	-2.086330000	3.119500000
H	-1.139911000	-2.556762000	3.935119000
C	0.753350000	-1.831034000	3.059140000
C	-2.577885000	-1.634842000	1.446281000
H	-2.641112000	-1.881459000	0.383085000
H	-3.161383000	-2.371443000	2.003473000
H	-3.046682000	-0.655305000	1.584503000
C	2.237664000	-0.853660000	1.245382000
H	2.295133000	-1.310054000	0.252732000
C	-3.197530000	1.449472000	-1.597427000
H	-2.294138000	1.366316000	-2.206457000
H	-3.868119000	2.157574000	-2.091695000
C	-1.812480000	2.143870000	1.598383000
C	-2.969442000	2.929912000	1.691633000
H	-3.296750000	3.506501000	2.544107000
C	-3.617513000	2.820830000	0.468176000
C	-0.762870000	1.946617000	2.647424000
H	0.160154000	2.478123000	2.393930000
H	-1.122735000	2.338923000	3.601735000
H	-0.518625000	0.890576000	2.786348000
C	-4.918813000	3.385779000	0.006028000
H	-5.618224000	2.574952000	-0.221772000
H	-5.349474000	4.010108000	0.791771000
H	-4.801082000	4.005846000	-0.890145000
C	1.845060000	-2.121184000	4.036373000
H	2.386661000	-1.212493000	4.323197000
H	1.420266000	-2.558182000	4.942303000
H	2.572387000	-2.834557000	3.630362000
H	3.040926000	-1.277725000	1.844540000
C	5.798804000	-2.635401000	-0.272513000
C	5.154943000	-3.444068000	0.875564000
C	6.896842000	-1.742802000	0.328285000
H	7.423569000	-1.171511000	-0.443244000
H	6.490165000	-1.035129000	1.061111000
H	7.636908000	-2.363344000	0.843846000
H	4.732458000	-2.774961000	1.636235000
H	5.906075000	-4.071841000	1.367571000
H	4.353951000	-4.098263000	0.517525000
C	6.456231000	-3.610384000	-1.274244000
H	6.916996000	-3.062108000	-2.102545000
H	7.235396000	-4.199117000	-0.777023000
H	5.727552000	-4.308355000	-1.698103000
C	4.720306000	-1.820946000	-0.998697000
C	3.627458000	-2.475231000	-1.597337000
C	4.761899000	-0.426217000	-1.107078000
C	2.621847000	-1.771362000	-2.253987000
C	3.760103000	0.282060000	-1.777722000
C	2.670511000	-0.372016000	-2.354863000
H	3.555901000	-3.557735000	-1.548044000
H	5.581904000	0.131289000	-0.669800000
H	1.780942000	-2.303168000	-2.688993000
H	3.827293000	1.365643000	-1.840896000
C	1.608779000	0.410638000	-3.087617000
H	1.758748000	1.481408000	-2.923022000
H	1.690841000	0.237782000	-4.165957000
S	-0.143980000	-0.045225000	-2.680949000
C	-3.533205000	-0.976610000	-2.291940000
H	-2.772199000	-0.845312000	-3.053761000
C	-4.169810000	-2.184790000	-2.115642000
H	-3.927368000	-3.036579000	-2.745503000
C	-5.421898000	-1.173183000	-0.290559000

C	-5.141603000	-2.324502000	-1.095323000
C	3.522372000	1.275261000	1.732838000
H	4.199249000	0.690070000	2.345425000
C	3.724945000	2.620824000	1.532695000
C	1.748449000	2.642063000	0.109746000
C	2.844644000	3.347980000	0.698078000
C	-5.827729000	-3.538351000	-0.831313000
H	-5.613239000	-4.408175000	-1.446264000
C	-6.749685000	-3.607159000	0.187966000
H	-7.273605000	-4.537150000	0.385851000
C	-6.377384000	-1.274945000	0.753034000
H	-6.573603000	-0.390137000	1.349833000
C	-7.025193000	-2.466990000	0.985242000
H	-7.757198000	-2.540116000	1.783934000
C	3.012838000	4.728924000	0.418980000
H	3.845993000	5.257012000	0.873364000
C	2.138250000	5.379352000	-0.420172000
H	2.271359000	6.434340000	-0.636238000
H	4.562903000	3.132358000	1.997934000
C	0.868359000	3.333305000	-0.758948000
H	0.055042000	2.796582000	-1.233798000
C	1.065674000	4.672132000	-1.016204000
H	0.393155000	5.192089000	-1.6910880006

Int-4

Zn	0.018522000	-0.022076000	-0.612016000
O	0.129273000	-0.052535000	-2.508383000
N	-0.175864000	1.730422000	0.606196000
N	-1.147341000	2.613686000	0.238823000
C	-2.867172000	1.236167000	-0.834445000
N	-2.291837000	0.029659000	-0.533217000
N	2.282888000	-0.027697000	-0.489577000
C	2.885971000	-1.212217000	-0.818898000
N	1.175071000	-2.650500000	0.200395000
N	0.169607000	-1.804195000	0.565078000
C	0.177160000	2.054350000	1.859871000
C	-0.587171000	3.153656000	2.295289000
H	-0.526855000	3.653166000	3.251128000
C	-1.436039000	3.479059000	1.246858000
C	1.241812000	1.303290000	2.596102000
H	1.364929000	0.295403000	2.193765000
H	2.210162000	1.812590000	2.525416000
H	0.988078000	1.228217000	3.657454000
C	-1.887128000	2.376719000	-0.997949000
H	-1.160233000	2.127820000	-1.781198000
C	-3.062898000	-1.031105000	-0.392364000
C	-4.224032000	1.383183000	-0.980983000
C	3.024415000	1.052771000	-0.350557000
C	1.934777000	-2.370164000	-1.017710000
H	1.224513000	-2.106248000	-1.811631000
H	2.467545000	-3.277600000	-1.302255000
C	-0.196470000	-2.160532000	1.806291000
C	0.590240000	-3.245401000	2.236276000
H	0.527651000	-3.764322000	3.181600000
C	1.468520000	-3.525349000	1.198086000
C	-1.290334000	-1.444251000	2.534855000
H	-1.456000000	-0.449221000	2.115486000
H	-2.236649000	-1.995311000	2.478873000
H	-1.036740000	-1.338669000	3.593797000
C	2.557002000	-4.541819000	1.087577000
H	3.536175000	-4.066946000	0.954413000
H	2.595338000	-5.142643000	1.998537000
H	2.394422000	-5.221104000	0.242813000
C	4.244286000	-1.320414000	-0.981100000
C	5.070768000	-0.176544000	-0.825204000
C	-2.490421000	4.530530000	1.133698000
H	-3.482292000	4.089405000	0.979457000
H	-2.524156000	5.119628000	2.052439000
H	-2.292979000	5.216323000	0.301692000
H	-2.395964000	3.300515000	-1.273874000
C	-4.472357000	-0.997424000	-0.525498000
H	-0.702042000	-0.277778000	-2.950138000
C	-5.079803000	0.259902000	-0.830367000
H	-4.648282000	2.354262000	-1.219593000
H	-2.557731000	-1.967032000	-0.163142000
C	-6.487928000	0.325536000	-0.967136000
H	-6.955280000	1.277694000	-1.200370000
C	-7.250112000	-0.811677000	-0.807473000
H	-8.329046000	-0.757297000	-0.914701000
C	-5.279362000	-2.151754000	-0.367411000
H	-4.806472000	-3.102842000	-0.139198000
C	-6.645648000	-2.057692000	-0.506236000
H	-7.268371000	-2.938471000	-0.387099000
C	4.432334000	1.059983000	-0.502097000
H	4.691309000	-2.275473000	-1.241473000
H	2.497419000	1.973310000	-0.110070000
C	6.478694000	-0.201383000	-0.977760000
H	6.969540000	-1.137897000	-1.225758000
C	7.210692000	0.955151000	-0.816528000
H	8.289427000	0.931971000	-0.936762000
C	5.208395000	2.235074000	-0.343099000
H	4.711276000	3.170622000	-0.102325000
C	6.575101000	2.181122000	-0.497911000
H	7.174041000	3.078274000	-0.378695000

2-Qu

Zn	0.171489000	-1.937724000	0.035305000
O	-0.198352000	0.000558000	-0.000693000
N	-0.056579000	-3.165587000	1.703625000
N	-1.102612000	-3.027759000	2.573808000
N	-2.418998000	-1.752436000	0.192567000
N	0.112347000	-3.194154000	-1.632791000
N	1.105971000	-3.063670000	-2.562811000
N	2.388303000	-1.727555000	-0.175039000
C	0.459708000	-4.392857000	1.924670000
C	-0.273692000	-5.033244000	2.934002000
H	-0.099082000	-6.019827000	3.337506000
C	-1.268534000	-4.146457000	3.328095000
C	1.653972000	-4.898728000	1.180287000
H	1.772176000	-5.971613000	1.346221000
H	2.567865000	-4.402653000	1.525283000
H	1.561881000	-4.728075000	0.103856000
C	-2.344280000	-4.284785000	4.354213000
H	-2.277101000	-5.266181000	4.827269000
H	-3.341280000	-4.195487000	3.907973000
H	-2.254043000	-3.528858000	5.143246000
C	-1.906093000	-1.816124000	2.554515000
H	-1.226360000	-0.965158000	2.449754000
H	-2.405663000	-1.728385000	3.519414000
C	-2.916044000	-1.797279000	1.423508000
C	-4.299393000	-1.811941000	1.700865000
H	-4.646050000	-1.844838000	2.727569000
C	-5.189043000	-1.766600000	0.651259000
H	-6.260279000	-1.776658000	0.830660000
C	-4.704275000	-1.696560000	-0.675206000
C	-5.561572000	-1.622877000	-1.804489000
H	-6.636420000	-1.642959000	-1.649584000
C	-5.036333000	-1.538461000	-3.073556000
H	-5.694436000	-1.493959000	-3.935179000
C	-3.631700000	-1.523446000	-3.261338000
H	-3.231673000	-1.470373000	-4.269648000
C	-2.772197000	-1.595582000	-2.185940000
H	-1.698097000	-1.614255000	-2.326411000
C	-3.285283000	-1.689422000	-0.867467000
C	-0.454270000	-4.397400000	-1.850992000
C	0.195137000	-5.030665000	-2.923914000
H	-0.034144000	-6.000629000	-3.340339000
C	1.189234000	-4.163907000	-3.358947000
C	-1.619664000	-4.886077000	-1.053196000
H	-1.589363000	-5.974992000	-0.964571000
H	-2.560244000	-4.618461000	-1.548149000
H	-1.631818000	-4.453313000	-0.051672000
C	2.190161000	-4.303127000	-4.458162000
H	3.217422000	-4.259281000	-4.078554000
H	2.072238000	-3.521425000	-5.217873000
H	2.059990000	-5.267126000	-4.953384000
C	1.915707000	-1.858936000	-2.558920000
H	1.242612000	-0.996881000	-2.506479000
H	2.447378000	-1.806760000	-3.508600000
C	2.897087000	-1.806319000	-1.403231000
C	4.282745000	-1.829824000	-1.659270000
H	4.639893000	-1.892777000	-2.680632000
C	5.161467000	-1.765819000	-0.602561000
H	6.234346000	-1.791447000	-0.770005000
C	4.663286000	-1.657814000	0.715236000
C	5.514994000	-1.569373000	1.847893000
H	6.590071000	-1.604240000	1.697906000
C	4.984899000	-1.455100000	3.112167000
H	5.637937000	-1.401661000	3.977032000
C	3.579888000	-1.420339000	3.288213000
H	3.171625000	-1.341970000	4.291466000
C	2.726151000	-1.504471000	2.208640000
H	1.653121000	-1.507290000	2.354806000
C	3.243356000	-1.633852000	0.895808000
H	-1.169926000	0.000982000	-0.000893000

Zn	0.173735000	1.938289000	-0.035095000
N	1.111449000	3.063602000	2.562241000
N	2.390340000	1.725339000	0.174372000
N	-0.053845000	3.166888000	-1.702947000
N	-1.100734000	3.030704000	-2.572365000
N	-2.417573000	1.755522000	-0.192052000
C	-0.448568000	4.398203000	1.851588000
C	0.202996000	5.031747000	2.923038000
H	-0.024766000	6.002280000	3.338968000
C	1.196879000	4.164391000	3.357374000
C	-1.614721000	4.887301000	1.055158000
H	-1.584821000	5.976305000	0.967614000
H	-2.554833000	4.618843000	1.550543000
H	-1.627537000	4.455537000	0.053203000
C	2.199348000	4.303421000	4.455205000
H	2.072315000	5.268905000	4.948347000
H	3.226090000	4.255875000	4.074665000
H	2.080030000	3.523790000	5.216837000
C	1.919763000	1.857933000	2.558621000
H	1.245578000	0.996641000	2.507535000
H	2.452172000	1.805914000	3.507900000
C	2.900148000	1.803160000	1.402182000
C	4.286031000	1.823726000	1.657284000
H	4.643997000	1.886003000	2.678401000
C	5.163903000	1.757747000	0.600000000
H	6.236946000	1.781060000	0.766719000
C	4.664591000	1.650825000	-0.717460000
C	5.515362000	1.560687000	-1.850683000
H	6.590606000	1.593292000	-1.701388000
C	4.984203000	1.447640000	-3.114620000
H	5.636552000	1.392958000	-3.979926000
C	3.579010000	1.415845000	-3.289721000
H	3.169903000	1.338446000	-4.292705000
C	2.726160000	1.501668000	-2.209575000
N	0.116631000	3.194234000	1.633533000
H	1.653053000	1.506812000	-2.355080000
C	3.244489000	1.629849000	-0.897071000
C	0.463203000	4.393985000	-1.923285000
C	-0.270530000	5.035856000	-2.931412000
H	-0.095474000	6.022675000	-3.334142000
C	-1.266391000	4.150197000	-3.325510000
C	1.658268000	4.898438000	-1.179205000
H	1.781318000	5.969946000	-1.350338000
H	2.570675000	4.396690000	-1.519838000
H	1.563356000	4.733748000	-0.102058000
C	-2.342802000	4.290208000	-4.350702000
H	-3.339518000	4.200735000	-3.903870000
H	-2.253399000	3.535215000	-5.140728000
H	-2.275570000	5.272151000	-4.822612000
C	-1.904811000	1.819451000	-2.554013000
H	-1.225442000	0.968096000	-2.450006000
H	-2.404480000	1.732746000	-3.518957000
C	-2.914694000	1.800169000	-1.422957000
C	-4.298059000	1.814086000	-1.700307000
H	-4.644743000	1.846827000	-2.727007000
C	-5.187668000	1.768223000	-0.650695000
H	-6.258909000	1.777668000	-0.830083000
C	-4.702829000	1.698602000	0.675771000
C	-5.560054000	1.624692000	1.805088000
H	-6.634914000	1.644198000	1.650202000
C	-5.034747000	1.540855000	3.074165000
H	-5.692810000	1.496177000	3.935811000
C	-3.630103000	1.526696000	3.261926000
H	-3.230025000	1.474213000	4.270246000
C	-2.770662000	1.599045000	2.186485000
H	-1.696555000	1.618510000	2.326902000
C	-3.283831000	1.692237000	0.868002000

$[(Me_2PzQu)_2Zn]^{+2}$

Zn	-0.000053000	-0.000206000	-0.062963000
N	-0.109646000	-1.632729000	1.183734000
N	-1.261363000	-2.370930000	1.182462000
N	-1.877736000	-0.264296000	-0.950891000
N	0.105483000	1.624426000	1.194299000
N	1.257267000	2.362560000	1.199736000
N	1.879455000	0.269998000	-0.944965000
C	0.447939000	-1.791677000	2.398281000
C	-0.347083000	-2.657683000	3.165863000
H	-0.158971000	-2.992427000	4.175429000
C	-1.424802000	-3.022385000	2.367294000
C	1.705137000	-1.074117000	2.771845000
H	1.484101000	-0.139522000	3.300594000
H	2.316531000	-1.692762000	3.433709000
H	2.298756000	-0.833845000	1.884498000
C	-2.563653000	-3.946970000	2.645164000
H	-2.520988000	-4.842099000	2.013231000
H	-2.522294000	-4.276016000	3.685155000
H	-3.532102000	-3.460389000	2.485436000
C	-1.983952000	-2.559097000	-0.066664000
H	-1.285985000	-2.966415000	-0.808202000
H	-2.743543000	-3.319282000	0.110747000
C	-2.647234000	-1.311635000	-0.626930000
C	-4.034512000	-1.316445000	-0.858763000
H	-4.621359000	-2.185429000	-0.583236000
C	-4.632435000	-0.213810000	-1.434017000
H	-5.704451000	-0.195938000	-1.607922000
C	-3.847789000	0.895771000	-1.813837000
C	-4.394377000	2.049598000	-2.435083000
H	-5.463860000	2.089190000	-2.617123000
C	-3.576811000	3.090919000	-2.807264000
H	-3.994164000	3.969841000	-3.286646000
C	-2.180136000	3.013698000	-2.582290000
H	-1.544018000	3.831073000	-2.906555000
C	-1.621257000	1.911319000	-1.972562000
H	-0.544217000	1.848017000	-1.842686000
C	-2.440429000	0.833545000	-1.563810000
C	-0.453157000	1.774094000	2.409557000
C	0.341290000	2.634036000	3.184504000
H	0.152246000	2.961169000	4.196389000
C	-1.710800000	1.053884000	2.776455000
H	-1.490419000	0.116658000	3.300789000
H	-2.324073000	1.668686000	3.440184000
H	-2.302235000	0.817958000	1.886503000
C	2.646805000	1.316996000	-0.614865000
C	4.634221000	0.228204000	-1.428694000
C	3.851899000	-0.880833000	-1.814821000
C	4.400950000	-2.029804000	-2.442842000
H	5.470472000	-2.065884000	-2.625383000
C	3.585684000	-3.070871000	-2.820726000
C	2.188938000	-2.998200000	-2.594754000
H	1.554615000	-3.815283000	-2.923233000
C	1.627696000	-1.900586000	-1.978622000
H	0.550607000	-1.840880000	-1.847623000
C	2.444453000	-0.823189000	-1.564121000
C	4.034055000	1.326104000	-0.846779000
H	5.706229000	0.213665000	-1.602945000
H	4.619095000	2.194644000	-0.566076000
H	4.004906000	-3.946085000	-3.305224000
C	1.981155000	2.559869000	-0.047187000
H	1.283490000	2.971136000	-0.786810000
H	2.739507000	3.319898000	0.136089000
C	1.419772000	3.004788000	2.389719000
C	2.558430000	3.927164000	2.675584000
H	3.526990000	3.441938000	2.512464000
H	2.515980000	4.827300000	2.050778000
H	2.516526000	4.247922000	3.718141000

5-Pz

Zn	-0.011150000	-0.029329000	-0.734340000
O	-0.559264000	0.827495000	-2.667321000
O	0.483386000	-1.007301000	-2.614167000
N	-0.922054000	1.376241000	0.657668000
N	-2.272640000	1.571943000	0.603505000
N	-3.104057000	-0.343036000	-0.581695000
N	-1.957607000	-1.062543000	-0.739275000
N	1.911617000	1.030236000	-0.845034000
N	3.070348000	0.342624000	-0.642042000
N	2.310330000	-1.564975000	0.599257000
N	0.966757000	-1.341959000	0.711992000
N	-0.044395000	-0.112808000	-3.341961000
C	-0.523483000	1.859976000	1.842472000
C	-1.635223000	2.364505000	2.548372000
H	-1.630383000	2.828831000	3.523596000
C	-2.741064000	2.161540000	1.738925000
C	0.910467000	1.845588000	2.271656000
H	1.481071000	2.637316000	1.774850000
H	0.979270000	2.007105000	3.350268000
H	1.389306000	0.894820000	2.029317000
C	-3.004563000	1.100936000	-0.555149000
H	-2.486145000	1.435544000	-1.456751000
C	-2.329704000	-2.342117000	-0.854257000
C	-4.208001000	-1.145170000	-0.600227000
C	2.254472000	2.314278000	-0.982943000
C	3.001989000	-1.102965000	-0.587571000
H	2.468296000	-1.461009000	-1.471008000
H	4.012870000	-1.504429000	-0.580472000
C	0.618618000	-1.779401000	1.930243000
C	1.752686000	-2.290544000	2.595058000
H	1.786187000	-2.728706000	3.581733000
C	2.820907000	-2.132669000	1.728680000
C	-0.779066000	-1.661148000	2.449739000
H	-1.503879000	-1.649446000	1.635056000
H	-1.008929000	-2.496152000	3.117228000
H	-0.902498000	-0.733535000	3.021063000
C	4.262123000	-2.492526000	1.885438000
H	4.910847000	-1.610212000	1.836600000
H	4.417106000	-2.964073000	2.857912000
H	4.592617000	-3.199478000	1.115717000
C	4.154635000	1.171872000	-0.649901000
C	3.655137000	2.446300000	-0.860118000
C	5.558657000	0.689620000	-0.483655000
H	6.242296000	1.540432000	-0.514677000
H	5.707558000	0.179096000	0.475047000
H	5.851940000	0.000253000	-1.284350000
C	1.226266000	3.370252000	-1.240275000
H	0.663689000	3.611651000	-0.331432000
H	1.703993000	4.285704000	-1.597366000
H	0.512571000	3.026300000	-1.994132000
H	4.232366000	3.356225000	-0.934432000
C	-4.181565000	2.490844000	1.956501000
H	-4.808743000	1.591676000	1.957349000
H	-4.302610000	2.980792000	2.924678000
H	-4.565861000	3.172214000	1.188535000
H	-4.007340000	1.521623000	-0.530574000
C	-3.735479000	-2.436304000	-0.766863000
H	-4.332694000	-3.333985000	-0.830532000
C	-5.603223000	-0.624384000	-0.481765000
H	-6.305762000	-1.460198000	-0.487688000
H	-5.757654000	-0.067613000	0.449995000
H	-5.865478000	0.034511000	-1.318085000
C	-1.319106000	-3.429100000	-1.038585000
H	-0.583502000	-3.138184000	-1.793835000
H	-0.782067000	-3.632619000	-0.105068000
H	-1.807880000	-4.352493000	-1.357997000

RC'

Zn	1.273735000	-0.196229000	-0.430956000
O	0.104305000	1.047881000	-1.820890000
O	1.078323000	-0.673140000	-2.558087000
N	0.960691000	0.768241000	1.487206000
N	-0.314662000	1.010603000	1.901897000
N	-1.426395000	-0.841890000	0.866450000
N	-0.520174000	-1.378574000	0.001608000
N	3.009699000	1.058660000	-0.945995000
N	4.188403000	0.465941000	-1.288013000
N	3.942386000	-1.752102000	-0.396956000
N	2.718249000	-1.695834000	0.206064000
N	0.342150000	0.318665000	-2.830429000
C	1.763083000	1.234429000	2.456841000
C	0.981883000	1.792604000	3.487810000
H	1.338035000	2.252542000	4.397852000
C	-0.342921000	1.637178000	3.106519000
C	3.254318000	1.137439000	2.375668000
H	3.683315000	1.997110000	1.849719000
H	3.682928000	1.112882000	3.381152000
H	3.562805000	0.235909000	1.842972000
C	-1.413103000	0.590105000	1.055216000
H	-1.313352000	1.054693000	0.078055000
C	-0.831142000	-2.673357000	-0.112576000
C	-2.314690000	-1.774130000	1.307843000
C	3.256682000	2.368975000	-0.858528000
C	4.176117000	-0.951741000	-1.582933000
H	3.380454000	-1.150468000	-2.304631000
H	5.137047000	-1.232843000	-2.008107000
C	2.817709000	-2.432308000	1.321645000
C	4.120312000	-2.962840000	1.425669000
H	4.500697000	-3.604017000	2.207223000
C	4.821407000	-2.505983000	0.322304000
C	1.670483000	-2.610107000	2.265644000
H	1.099157000	-1.685080000	2.367391000
H	0.982671000	-3.388119000	1.918395000
H	2.040392000	-2.904572000	3.251083000
C	6.236020000	-2.739581000	-0.096743000
H	6.812322000	-1.807599000	-0.128056000
H	6.723060000	-3.406058000	0.617906000
H	6.296992000	-3.209106000	-1.085334000
C	5.190363000	1.383484000	-1.425312000
C	4.618262000	2.613294000	-1.147749000
C	6.583738000	1.024437000	-1.826584000
H	7.196821000	1.927275000	-1.862101000
H	7.051287000	0.333590000	-1.115253000
H	6.617721000	0.562275000	-2.820429000
C	2.181168000	3.345592000	-0.500883000
H	2.003552000	3.372306000	0.579942000
H	2.460602000	4.352274000	-0.821029000
H	1.240553000	3.072587000	-0.984625000
H	5.117312000	3.571053000	-1.168482000
C	-1.611965000	2.050259000	3.775480000
H	-2.250001000	1.190709000	4.012544000
H	-1.384715000	2.564748000	4.711327000
H	-2.184201000	2.733417000	3.137805000
H	-2.351053000	0.915028000	1.494354000
C	-1.951535000	-2.964545000	0.696771000
H	-2.446411000	-3.918215000	0.806399000
C	-3.427588000	-1.440917000	2.244682000
H	-3.984339000	-2.345737000	2.496080000
H	-3.053024000	-1.008067000	3.179675000
H	-4.125721000	-0.729182000	1.789401000
C	-0.030833000	-3.584124000	-0.988786000
H	0.371351000	-3.032595000	-1.842474000
H	0.811564000	-4.025451000	-0.442833000
H	-0.653882000	-4.402778000	-1.358790000
C	-6.185542000	-1.354981000	-0.793380000
C	-7.163176000	-1.225224000	0.387128000
C	-5.465339000	-2.714122000	-0.672391000

H	-4.774812000	-2.893765000	-1.501394000
H	-6.201051000	-3.525840000	-0.674117000
H	-6.638706000	-1.195168000	1.349626000
H	-7.837159000	-2.087841000	0.403112000
H	-7.785462000	-0.327979000	0.307766000
C	-6.998340000	-1.333142000	-2.108616000
H	-6.348306000	-1.466114000	-2.979577000
H	-7.741345000	-2.139045000	-2.111814000
H	-7.525223000	-0.380138000	-2.224984000
C	-5.176833000	-0.198779000	-0.844992000
C	-5.326625000	0.972780000	-0.086299000
C	-4.095044000	-0.242828000	-1.737940000
C	-4.455464000	2.054563000	-0.232949000
C	-3.224370000	0.834344000	-1.887960000
C	-3.397421000	2.009938000	-1.145491000
H	-6.146380000	1.063249000	0.617321000
H	-3.932235000	-1.125527000	-2.347752000
H	-4.615101000	2.945946000	0.368676000
H	-2.402674000	0.764211000	-2.592997000
C	-2.468688000	3.179228000	-1.372167000
H	-1.622126000	2.865984000	-1.986497000
H	-2.972197000	3.999781000	-1.890916000
S	-1.682032000	3.896605000	0.148355000
H	-2.736555000	4.629352000	0.560983000
H	-4.893139000	-2.777974000	0.257772000

TS-1'

Zn	-1.056077000	-0.259292000	0.072258000
O	-0.811183000	1.320197000	3.280654000
O	-1.114751000	-0.602215000	2.052078000
N	0.268122000	0.266801000	-1.521490000
N	1.389287000	-0.502902000	-1.659019000
N	1.213967000	-2.350978000	-0.166339000
N	-0.135498000	-2.251181000	-0.000028000
N	-2.032396000	1.707176000	0.352457000
N	-3.351253000	1.694344000	0.709846000
N	-4.066302000	-0.322439000	-0.370469000
N	-2.902492000	-0.844526000	-0.855247000
N	-1.222356000	0.239685000	3.417386000
C	-0.041444000	0.696173000	-2.757052000
C	0.889588000	0.187796000	-3.682104000
H	0.914473000	0.368297000	-4.746704000
C	1.784547000	-0.584803000	-2.955032000
C	-1.212087000	1.590649000	-3.015507000
H	-2.050784000	1.351226000	-2.358455000
H	-0.946060000	2.640128000	-2.846491000
H	-1.539604000	1.493992000	-4.053798000
C	1.944868000	-1.145305000	-0.490627000
H	1.899506000	-0.442104000	0.341586000
C	-0.531562000	-3.427112000	0.513231000
C	1.689595000	-3.547150000	0.269478000
C	-1.670378000	2.993471000	0.318544000
C	-4.018090000	0.418905000	0.871673000
H	-3.474643000	-0.179034000	1.608592000
H	-5.033163000	0.595537000	1.220118000
C	-3.209128000	-1.439675000	-2.014821000
C	-4.589530000	-1.294084000	-2.268611000
H	-5.139784000	-1.677612000	-3.115212000
C	-5.112189000	-0.571304000	-1.208711000
C	-2.164713000	-2.113754000	-2.845986000
H	-1.290043000	-2.361899000	-2.240874000
H	-2.561729000	-3.032228000	-3.287848000
H	-1.838136000	-1.465208000	-3.666766000
C	-6.508024000	-0.121021000	-0.926979000
H	-6.579997000	0.971792000	-0.876284000
H	-7.170660000	-0.460295000	-1.725576000
H	-6.886576000	-0.531046000	0.016601000
C	-3.833069000	2.957928000	0.898647000
C	-2.772663000	3.810682000	0.651701000
C	-5.240959000	3.245025000	1.307529000
H	-5.387526000	4.324822000	1.375368000
H	-5.967134000	2.856555000	0.583716000
H	-5.476577000	2.816011000	2.288575000
C	-0.271966000	3.405634000	-0.007601000
H	-0.264428000	4.182564000	-0.779394000
H	0.220104000	3.821377000	0.878812000
H	0.315841000	2.555269000	-0.356624000
H	-2.789318000	4.888865000	0.713953000
C	2.973194000	-1.378878000	-3.384369000
H	2.867823000	-2.435188000	-3.111633000
H	3.086804000	-1.318543000	-4.468469000
H	3.895289000	-0.999845000	-2.929213000
H	2.987096000	-1.390870000	-0.670122000
C	0.580878000	-4.270476000	0.681984000
H	0.582545000	-5.272537000	1.084048000
C	3.144766000	-3.874333000	0.303914000
H	3.281794000	-4.915589000	0.601845000
H	3.625742000	-3.736753000	-0.671902000
H	3.660076000	-3.242248000	1.036300000
C	-1.961459000	-3.683207000	0.865989000
H	-2.288581000	-2.965403000	1.625358000
H	-2.617180000	-3.579891000	-0.004564000
H	-2.077247000	-4.691374000	1.269886000
C	4.967879000	1.977232000	-1.011451000
C	6.046326000	1.022897000	-1.552749000
C	5.656636000	3.277954000	-0.539404000

H	4.921868000	4.004222000	-0.176267000	H	6.356620000	3.072724000	0.277173000
H	6.214353000	3.739345000	-1.362827000				
H	6.835807000	0.836599000	-0.818059000				
H	6.520615000	1.460731000	-2.436980000				
H	5.622842000	0.053673000	-1.845109000				
C	4.000255000	2.314548000	-2.165600000				
H	3.252300000	3.058031000	-1.873899000				
H	4.557081000	2.728505000	-3.013430000				
H	3.464890000	1.425524000	-2.513414000				
C	4.208739000	1.375250000	0.178885000				
C	4.680722000	0.266556000	0.900689000				
C	3.031287000	1.979731000	0.645031000				
C	4.010745000	-0.209979000	2.028615000				
C	2.357214000	1.502053000	1.769089000				
C	2.835122000	0.398072000	2.487213000				
H	5.596301000	-0.228921000	0.596510000				
H	2.642762000	2.857249000	0.138694000				
H	4.407562000	-1.064885000	2.570414000				
H	1.452975000	2.000030000	2.108430000				
C	2.113793000	-0.109772000	3.706103000				
H	2.835923000	-0.321865000	4.500126000				
H	1.442874000	0.674460000	4.077692000				
S	1.152784000	-1.664669000	3.438452000				
H	-0.238402000	-1.144689000	2.411338000				

Int-1'

Zn	-0.767660000	0.583621000	-0.089044000
O	-0.499525000	-0.728064000	-1.784450000
O	0.841340000	0.885701000	-1.602556000
N	-2.227172000	-0.384275000	1.120635000
N	-2.255018000	-1.728485000	1.378049000
N	-2.469252000	-3.434100000	-0.286771000
N	-3.379390000	-2.765039000	-1.045514000
N	-2.059124000	1.928472000	-1.204844000
N	-1.689364000	3.231503000	-1.376817000
N	-0.255225000	3.554977000	0.521472000
N	-0.212111000	2.324468000	1.119252000
N	0.475447000	-0.103460000	-2.298423000
C	-3.156901000	0.168943000	1.916637000
C	-3.791254000	-0.833369000	2.673264000
H	-4.581319000	-0.699741000	3.397531000
C	-3.209200000	-2.031982000	2.300001000
C	-3.417998000	1.641772000	1.958677000
H	-2.897847000	2.115352000	2.798468000
H	-3.093384000	2.132126000	1.040624000
H	-4.488580000	1.823803000	2.090395000
C	-1.552643000	-2.671669000	0.518186000
H	-0.972380000	-3.363650000	1.131160000
C	-0.379570000	3.644535000	-0.920744000
H	0.375927000	3.004823000	-1.380489000
H	-0.216844000	4.677953000	-1.218089000
C	-0.144197000	2.556944000	2.438026000
C	-0.145836000	3.945205000	2.679572000
H	-0.088950000	4.438300000	3.638833000
C	-0.224760000	4.559563000	1.441444000
C	-0.068973000	1.452351000	3.444197000
H	0.966506000	1.130713000	3.603202000
H	-0.458783000	1.793967000	4.406887000
H	-0.643487000	0.579874000	3.125846000
C	-0.260252000	6.007447000	1.076133000
H	-1.190413000	6.275188000	0.561558000
H	-0.196106000	6.613793000	1.981829000
H	0.579007000	6.286743000	0.428626000
C	-3.512280000	-3.430414000	2.722582000
H	-2.604562000	-3.974014000	3.007644000
H	-4.181193000	-3.417536000	3.585584000
H	-3.999887000	-3.989014000	1.916082000
H	-0.879823000	-2.097510000	-0.115480000
C	7.879246000	-0.523035000	-0.452671000
C	8.171814000	0.490388000	-1.571325000
C	8.674696000	-1.814068000	-0.747136000
H	8.544326000	-2.561413000	0.041951000
H	8.352741000	-2.263352000	-1.692867000
H	9.744823000	-1.589902000	-0.821699000
H	7.881234000	0.105720000	-2.555073000
H	9.245726000	0.701182000	-1.603151000
H	7.652954000	1.441140000	-1.405003000
C	8.355999000	0.081308000	0.886570000
H	8.214145000	-0.613492000	1.720479000
H	9.423096000	0.324969000	0.832830000
H	7.806984000	1.001163000	1.117141000
C	6.387058000	-0.862415000	-0.350347000
C	5.419943000	-0.304035000	-1.195680000
C	5.943566000	-1.774114000	0.623419000
C	4.070037000	-0.638360000	-1.079653000
C	4.600796000	-2.111844000	0.746713000
C	3.645494000	-1.549604000	-0.108530000
H	5.711985000	0.399031000	-1.966511000
H	6.660352000	-2.233293000	1.296870000
H	3.343020000	-0.186751000	-1.749091000
H	4.290228000	-2.819364000	1.511864000
C	2.190795000	-1.882708000	0.026360000
H	1.667587000	-1.807785000	-0.926800000
H	2.038210000	-2.884007000	0.437072000
S	1.327972000	-0.749921000	1.243076000

H	2.093348000	0.331383000	1.002733000
C	-3.272321000	1.803344000	-1.756391000
C	-3.675439000	3.045890000	-2.292640000
C	-4.087356000	-3.714269000	-1.652664000
C	-2.582500000	-4.797849000	-0.401521000
C	-3.624946000	-5.005477000	-1.281454000
H	-3.999768000	-5.961661000	-1.617622000
H	-4.599196000	3.261070000	-2.809286000
C	-4.021912000	0.512133000	-1.720576000
H	-3.360367000	-0.354744000	-1.667560000
H	-4.681032000	0.470414000	-0.844804000
H	-4.650079000	0.417988000	-2.611241000
C	-2.505097000	5.383378000	-2.393995000
H	-3.406880000	5.724253000	-2.906561000
H	-2.369328000	6.013852000	-1.507409000
H	-1.656081000	5.555784000	-3.065997000
C	-1.690470000	-5.765515000	0.307031000
H	-0.640647000	-5.649440000	0.011360000
H	-1.744644000	-5.663002000	1.398088000
H	-1.991117000	-6.785916000	0.059111000
C	-5.198236000	-3.360961000	-2.590949000
H	-6.142290000	-3.822853000	-2.280670000
H	-5.335639000	-2.277164000	-2.621333000
H	-4.982291000	-3.709628000	-3.607348000
C	-2.649482000	3.939359000	-2.039330000

TS-2'

Zn	-0.615204000	0.126568000	-0.348445000
N	0.143105000	0.940093000	1.506422000
N	1.408159000	1.448143000	1.585646000
N	2.086982000	1.663697000	-0.700868000
N	0.936526000	1.317078000	-1.340041000
N	-4.329054000	-0.668038000	1.076499000
N	-4.050001000	-1.185336000	-0.153864000
N	-3.577044000	1.044937000	-0.869806000
N	-2.284094000	1.435685000	-0.635435000
C	-0.495969000	1.346153000	2.612900000
C	0.383083000	2.116329000	3.406118000
H	0.162738000	2.571974000	4.360272000
C	1.591140000	2.161799000	2.732399000
C	-1.931431000	1.023100000	2.866434000
H	-2.199066000	0.059625000	2.432328000
H	-2.125407000	1.000329000	3.942327000
H	-2.590778000	1.777977000	2.422936000
C	2.370325000	1.060476000	0.583332000
H	2.357049000	-0.024737000	0.478298000
C	-3.913754000	-0.291032000	-1.289160000
H	-3.140172000	-0.661347000	-1.964501000
H	-4.850727000	-0.226314000	-1.850997000
C	-2.359117000	2.718098000	-0.228637000
C	-3.702997000	3.125736000	-0.179367000
H	-4.076255000	4.098502000	0.104660000
C	-4.458590000	2.035963000	-0.575292000
C	-1.161448000	3.551515000	0.104500000
H	-0.261651000	3.178008000	-0.382398000
H	-1.330807000	4.582288000	-0.220127000
H	-0.980427000	3.569942000	1.184554000
C	-5.936001000	1.854113000	-0.661553000
H	-6.251893000	1.045842000	0.006945000
H	-6.438263000	2.774385000	-0.356863000
H	-6.264897000	1.613215000	-1.679180000
C	2.893207000	2.796875000	3.096192000
H	3.232038000	3.503221000	2.329234000
H	2.782467000	3.349330000	4.031396000
H	3.682865000	2.050004000	3.243332000
H	3.361770000	1.368995000	0.901593000
C	5.556555000	-1.598269000	1.009869000
C	5.046526000	-1.090135000	2.377044000
C	6.699513000	-0.678486000	0.550722000
H	7.129163000	-1.005922000	-0.401734000
H	6.367845000	0.361575000	0.438709000
H	7.501862000	-0.687384000	1.295135000
H	4.680803000	-0.057926000	2.300575000
H	5.857768000	-1.100722000	3.112961000
H	4.231856000	-1.707240000	2.767758000
C	6.116868000	-3.028479000	1.174560000
H	6.482679000	-3.414548000	0.217428000
H	6.950397000	-3.029680000	1.885618000
H	5.356641000	-3.721279000	1.548228000
C	4.394281000	-1.626255000	0.009534000
C	3.252050000	-2.401089000	0.280982000
C	4.400499000	-0.902970000	-1.189624000
C	2.172231000	-2.451908000	-0.597239000
C	3.315996000	-0.942887000	-2.070339000
C	2.186902000	-1.717156000	-1.792990000
H	3.201913000	-2.987424000	1.193075000
H	5.261597000	-0.302725000	-1.460259000
H	1.322191000	-3.081043000	-0.353237000
H	3.355221000	-0.361413000	-2.987614000
C	1.080741000	-1.815738000	-2.811583000
H	1.250732000	-1.103759000	-3.622223000
H	1.055200000	-2.814277000	-3.258266000
S	-0.651897000	-1.514006000	-2.223839000
C	-4.136836000	-2.551869000	-0.187022000
C	-4.543556000	-1.730827000	1.852020000
C	-4.438490000	-2.931755000	1.106333000

C	2.871155000	2.464003000	-1.472033000
N	-1.211664000	-2.732246000	1.065838000
O	-1.188324000	-1.474956000	1.001829000
O	-0.978223000	-3.358574000	-0.014759000
H	-0.795577000	-2.544296000	-1.096397000
H	-4.551248000	-3.944474000	1.465538000
C	2.174580000	2.653047000	-2.656051000
H	2.490976000	3.250008000	-3.498774000
C	4.206601000	2.964105000	-1.029390000
H	4.136896000	3.562874000	-0.113731000
H	4.901603000	2.137270000	-0.842108000
H	4.639421000	3.596147000	-1.807349000
C	-0.149326000	1.804846000	-3.515876000
H	-0.082134000	0.871932000	-4.086411000
H	-1.115788000	1.808608000	-3.005493000
H	-0.122271000	2.635530000	-4.225506000
C	-3.949445000	-3.357215000	-1.430639000
H	-3.013086000	-3.118026000	-1.945125000
H	-3.922160000	-4.418708000	-1.176183000
H	-4.770575000	-3.203066000	-2.142701000
C	-4.817122000	-1.561086000	3.313213000
H	-5.706542000	-2.122278000	3.619301000
H	-3.976150000	-1.926399000	3.914795000
H	-4.974796000	-0.504646000	3.546600000
C	0.972731000	1.925873000	-2.534182000

Int2'

Zn	0.615349000	-0.223876000	-0.386121000
N	-0.110209000	-0.628775000	1.588752000
N	-1.380587000	-1.114843000	1.748418000
N	-2.056004000	-1.792938000	-0.449989000
N	-0.906720000	-1.564029000	-1.140792000
N	4.330835000	0.736386000	0.883149000
N	4.017445000	1.127723000	-0.386287000
N	3.565874000	-1.169607000	-0.853383000
N	2.302609000	-1.516647000	-0.454079000
C	0.530667000	-0.872073000	2.743229000
C	-0.347128000	-1.515844000	3.641314000
H	-0.123188000	-1.828946000	4.650434000
C	-1.556661000	-1.657462000	2.984802000
C	1.953190000	-0.489395000	2.988290000
H	2.551750000	-0.458143000	2.077039000
H	2.003244000	0.509911000	3.432555000
H	2.410720000	-1.194943000	3.687986000
C	-2.343529000	-0.943573000	0.687051000
H	-2.335221000	0.098309000	0.366266000
C	3.859059000	0.119272000	-1.424261000
H	3.052178000	0.409517000	-2.100482000
H	4.779801000	0.013436000	-2.005136000
C	2.415549000	-2.734570000	0.107190000
C	3.758709000	-3.146831000	0.084745000
H	4.158844000	-4.077473000	0.458871000
C	4.472951000	-2.122633000	-0.511749000
C	1.250111000	-3.492177000	0.661570000
H	0.320432000	-3.225638000	0.158057000
H	1.416739000	-4.566161000	0.540599000
H	1.122823000	-3.293979000	1.731253000
C	5.937396000	-1.965050000	-0.745574000
H	6.312959000	-1.088598000	-0.205869000
H	6.465023000	-2.847888000	-0.379187000
H	6.177381000	-1.847341000	-1.808574000
C	-2.854581000	-2.240147000	3.439497000
H	-3.182630000	-3.061735000	2.791987000
H	-2.743389000	-2.637070000	4.450466000
H	-3.651140000	-1.486761000	3.463194000
H	-3.332612000	-1.186087000	1.063839000
C	-5.725674000	1.639022000	0.651997000
C	-5.284015000	1.281508000	2.089022000
C	-6.852980000	0.677657000	0.241756000
H	-7.225132000	0.893138000	-0.765278000
H	-6.529024000	-0.370183000	0.271443000
H	-7.694534000	0.778861000	0.934350000
H	-4.925837000	0.244724000	2.140614000
H	-6.126820000	1.375778000	2.782464000
H	-4.481145000	1.934480000	2.445123000
C	-6.283744000	3.079080000	0.632991000
H	-6.599127000	3.359289000	-0.377419000
H	-7.151624000	3.158197000	1.297022000
H	-5.539679000	3.808534000	0.967203000
C	-4.514554000	1.550440000	-0.285016000
C	-3.394977000	2.373462000	-0.067339000
C	-4.449130000	0.664628000	-1.367638000
C	-2.266147000	2.308055000	-0.880949000
C	-3.315839000	0.591918000	-2.182681000
C	-2.204389000	1.407732000	-1.955488000
H	-3.400011000	3.084352000	0.753190000
H	-5.290462000	0.020501000	-1.596697000
H	-1.427100000	2.965974000	-0.678467000
H	-3.298294000	-0.117499000	-3.005861000
C	-1.023305000	1.339389000	-2.892218000
H	-1.093539000	0.438745000	-3.507131000
H	-1.033718000	2.195443000	-3.575136000
S	0.654942000	1.382182000	-2.115746000
C	4.142039000	2.480029000	-0.567616000
C	4.602584000	1.867690000	1.533487000
C	4.501696000	2.985373000	0.667758000

C	-2.857911000	-2.683768000	-1.095299000
N	1.340883000	3.005227000	1.166453000
O	1.335646000	1.795458000	1.131669000
O	1.047761000	3.608029000	0.002037000
H	0.883012000	2.896891000	-0.712034000
H	4.660098000	4.026168000	0.911260000
C	-2.168803000	-3.060108000	-2.238903000
H	-2.501078000	-3.768041000	-2.983912000
C	-4.204663000	-3.079583000	-0.586795000
H	-4.150756000	-3.520017000	0.415626000
H	-4.882940000	-2.219438000	-0.544157000
H	-4.646490000	-3.823027000	-1.253210000
C	0.185836000	-2.383125000	-3.194960000
H	0.646196000	-1.395093000	-3.294690000
H	0.961374000	-3.077449000	-2.850950000
H	-0.154137000	-2.717003000	-4.178434000
C	3.935570000	3.155657000	-1.883730000
H	2.971321000	2.897138000	-2.333668000
H	3.963355000	4.238657000	-1.745451000
H	4.721940000	2.890490000	-2.602421000
C	4.923006000	1.846340000	2.994721000
H	5.842319000	2.402220000	3.208039000
H	4.119139000	2.308859000	3.580257000
H	5.051865000	0.816416000	3.337975000
C	-0.955094000	-2.341163000	-2.229655000

Int-3'

Zn	0.588059000	-0.060488000	-0.545948000	H	-2.481181000	-1.549490000	3.951348000
N	0.065189000	0.465053000	1.450279000	H	-1.952566000	-0.442291000	5.223701000
N	-1.097751000	-0.032442000	1.971376000	H	-3.107446000	0.110302000	4.005274000
N	-1.896214000	-1.606336000	0.337865000	H	-3.082861000	-0.530169000	1.651364000
N	-0.863634000	-1.602821000	-0.546838000	C	-5.911362000	1.452648000	0.229697000
N	5.057940000	0.799134000	0.454339000	C	-5.459926000	1.637012000	1.696050000
N	4.249740000	1.195229000	-0.570741000	C	-6.897251000	0.274516000	0.173147000
N	3.510049000	-1.047516000	-0.892085000	H	-7.264476000	0.100966000	-0.843665000
N	2.344985000	-1.172413000	-0.181552000	H	-6.446544000	-0.656784000	0.537961000
C	0.850603000	0.763741000	2.495637000	H	-7.763632000	0.486981000	0.807614000
C	0.172972000	0.460247000	3.694233000	H	-4.982870000	0.723493000	2.075800000
H	0.538266000	0.604593000	4.700259000	H	-6.321328000	1.850514000	2.338467000
C	-1.065948000	-0.045115000	3.332794000	H	-4.747828000	2.461468000	1.802956000
C	2.229425000	1.304916000	2.306500000	C	-6.652659000	2.724459000	-0.238300000
H	2.937546000	0.517773000	2.027540000	H	-6.975687000	2.623149000	-1.279552000
H	2.259134000	2.059532000	1.515096000	H	-7.540359000	2.895464000	0.380796000
H	2.584849000	1.767825000	3.230182000	H	-6.020274000	3.614608000	-0.168061000
C	-2.173898000	-0.387454000	1.074665000	C	-4.679022000	1.226542000	-0.656052000
H	-2.325702000	0.429661000	0.369306000	C	-3.695644000	2.227815000	-0.761140000
C	3.844482000	0.200498000	-1.545443000	C	-4.462089000	0.046276000	-1.377617000
H	2.982905000	0.563437000	-2.109322000	C	-2.555343000	2.057819000	-1.542172000
H	4.654995000	-0.014974000	-2.246508000	C	-3.318426000	-0.127165000	-2.163565000
C	2.473278000	-2.290685000	0.553441000	C	-2.346195000	0.871302000	-2.261965000
C	3.732817000	-2.869289000	0.320834000	H	-3.819922000	3.162405000	-0.222498000
H	4.127967000	-3.767860000	0.771027000	H	-5.191078000	-0.755597000	-1.345320000
C	4.384071000	-2.043709000	-0.579693000	H	-1.809988000	2.845666000	-1.594656000
C	1.396320000	-2.798139000	1.461650000	H	-3.183516000	-1.060204000	-2.704680000
H	0.636701000	-3.365019000	0.913392000	C	-1.146135000	0.680453000	-3.157976000
H	1.834734000	-3.463412000	2.209893000	H	-1.084489000	-0.364864000	-3.472390000
H	0.894000000	-1.981340000	1.984311000	H	-1.261585000	1.279871000	-4.067245000
C	5.774603000	-2.103730000	-1.115199000	S	0.486503000	1.221466000	-2.458279000
H	6.347591000	-1.242925000	-0.754126000	C	4.105449000	2.558741000	-0.632448000
H	6.262591000	-3.016661000	-0.767683000	C	5.400218000	1.924440000	1.080599000
H	5.795197000	-2.105455000	-2.210635000	C	4.829429000	3.052144000	0.437143000
C	-2.215892000	-0.507642000	4.166214000	C	-2.655309000	-2.728979000	0.206976000

C	-0.936829000	-2.749431000	-1.231326000
H	4.933778000	4.092323000	0.711559000
C	-2.053447000	-3.487567000	-0.787026000
H	-2.383051000	-4.451776000	-1.145048000
C	-3.890911000	-2.970607000	1.009074000
H	-3.692020000	-2.945093000	2.086693000
H	-4.660681000	-2.222266000	0.787278000
H	-4.300031000	-3.953944000	0.768997000
C	0.096528000	-3.093448000	-2.256053000
H	0.488110000	-2.189015000	-2.732622000
H	0.942080000	-3.621750000	-1.799419000
H	-0.325454000	-3.740887000	-3.028884000
C	3.327947000	3.272930000	-1.689752000
H	2.259653000	3.031395000	-1.664974000
H	3.433186000	4.350927000	-1.546641000
H	3.689617000	3.034111000	-2.696754000
C	6.268209000	1.883236000	2.299140000
H	7.173216000	2.485325000	2.161206000
H	5.744098000	2.281758000	3.175998000
H	6.566017000	0.853528000	2.512668000

Int-4'

Zn	0.032041000	-0.045282000	-0.925485000
O	0.624903000	-0.816309000	-2.570410000
N	-1.011390000	1.456310000	0.326401000
N	-2.368366000	1.628916000	0.247728000
N	-3.154979000	-0.344423000	-0.856869000
N	-1.984159000	-1.028365000	-0.965111000
N	1.960045000	1.111418000	-0.871480000
N	3.072362000	0.334974000	-0.732636000
N	2.231026000	-1.523589000	0.531291000
N	0.903369000	-1.240586000	0.666059000
C	-0.651837000	1.948250000	1.523348000
C	-1.788823000	2.428244000	2.205976000
H	-1.811075000	2.891703000	3.181371000
C	-2.872115000	2.204604000	1.376345000
C	0.762385000	1.975234000	2.009697000
H	1.300878000	1.070296000	1.728740000
H	1.306354000	2.827499000	1.589968000
H	0.774333000	2.072768000	3.098399000
C	-3.085285000	1.097838000	-0.889619000
H	-2.570328000	1.412513000	-1.801684000
C	-2.304834000	-2.326184000	-0.960598000
C	-4.228901000	-1.186405000	-0.785468000
C	2.396995000	2.362940000	-1.022782000
C	2.903998000	-1.106180000	-0.687884000
H	2.284096000	-1.398083000	-1.547774000
H	3.883178000	-1.577562000	-0.728552000
C	0.550380000	-1.653104000	1.888405000
C	1.669707000	-2.208927000	2.542724000
H	1.700982000	-2.640632000	3.532424000
C	2.731322000	-2.103960000	1.657487000
C	-0.845173000	-1.471095000	2.395561000
H	-1.525864000	-1.237143000	1.575172000
H	-1.197940000	-2.377205000	2.897594000
H	-0.893766000	-0.650930000	3.121118000
C	4.159098000	-2.519998000	1.796306000
H	4.839425000	-1.662449000	1.737440000
H	4.309548000	-2.997595000	2.766635000
H	4.452258000	-3.237477000	1.021314000
C	4.214799000	1.078621000	-0.793341000
C	3.808687000	2.389328000	-0.972027000
C	5.583903000	0.488620000	-0.696242000
H	6.329106000	1.285159000	-0.747782000
H	5.735825000	-0.047988000	0.247605000
H	5.786344000	-0.208687000	-1.517858000
C	1.448497000	3.498217000	-1.244387000
H	1.704772000	4.356819000	-0.614907000
H	1.487779000	3.833662000	-2.287080000
H	0.422846000	3.194826000	-1.021870000
H	4.450959000	3.252684000	-1.066823000
C	-4.323230000	2.501152000	1.569038000
H	-4.926061000	1.585829000	1.593784000
H	-4.466844000	3.017735000	2.520126000
H	-4.718655000	3.147422000	0.776831000
H	-4.094774000	1.503885000	-0.892465000
C	-3.706922000	-2.467309000	-0.846634000
H	-4.270155000	-3.388804000	-0.825560000
C	-5.641888000	-0.710441000	-0.691274000
H	-6.314183000	-1.569943000	-0.652999000
H	-5.816740000	-0.113147000	0.211279000
H	-5.928139000	-0.104294000	-1.558998000
C	-1.242182000	-3.374241000	-1.057611000
H	-0.371218000	-2.971527000	-1.582720000
H	-0.918770000	-3.699049000	-0.061661000
H	-1.614725000	-4.252319000	-1.592235000
H	-0.056748000	-1.262822000	-3.090777000

2-Pz

Zn	1.966822000	-0.099950000	-0.049827000
O	-0.003270000	-0.432895000	0.232953000
N	3.898368000	-0.077562000	0.918709000
N	4.341474000	-1.106147000	1.710867000
N	2.084599000	-2.341270000	0.140691000
N	2.537369000	0.216156000	-2.070295000
N	2.153133000	1.377711000	-2.690100000
N	1.731742000	2.066517000	0.225891000
C	4.991183000	0.655342000	0.630154000
C	6.122462000	0.089552000	1.247588000
H	7.136255000	0.460215000	1.205840000
C	5.687708000	-1.035043000	1.926957000
C	4.957851000	1.892522000	-0.210892000
H	5.934360000	2.047449000	-0.676019000
H	4.738788000	2.777693000	0.396143000
H	4.206890000	1.830989000	-0.998140000
C	6.442977000	-2.017973000	2.759893000
H	7.493030000	-1.723618000	2.807777000
H	6.403030000	-3.028569000	2.337846000
H	6.064400000	-2.059988000	3.787707000
C	3.407347000	-2.114940000	2.148521000
H	2.557007000	-1.627410000	2.635121000
H	3.902800000	-2.760047000	2.871021000
N	2.914842000	-2.925219000	1.055665000
C	3.095676000	-4.255136000	0.798517000
C	2.342095000	-4.528794000	-0.332102000
H	2.248101000	-5.488902000	-0.818313000
C	1.731217000	-3.316861000	-0.711121000
C	3.571106000	-0.261638000	-2.783438000
C	3.837848000	0.597928000	-3.866124000
H	4.599372000	0.472248000	-4.621913000
C	2.928330000	1.639452000	-3.783563000
C	4.280174000	-1.525445000	-2.413484000
H	5.280618000	-1.535887000	-2.852085000
H	3.745642000	-2.404546000	-2.789599000
H	4.374569000	-1.627437000	-1.329958000
C	2.744065000	2.836507000	-4.656843000
H	2.983153000	3.766068000	-4.127755000
H	1.719900000	2.912801000	-5.039586000
H	3.412631000	2.767793000	-5.517034000
C	1.086181000	2.156300000	-2.103774000
H	0.256908000	1.489239000	-1.867183000
H	0.757401000	2.904567000	-2.821272000
N	1.481495000	2.827294000	-0.880184000
C	1.638039000	4.158209000	-0.622377000
C	2.004707000	4.246012000	0.712557000
H	2.224030000	5.153590000	1.256679000
C	2.059413000	2.923470000	1.201305000
H	0.035998000	-1.390079000	0.378268000
Zn	-2.005165000	-0.165121000	0.158664000
N	-2.673163000	0.324486000	2.109887000
N	-2.252780000	1.506314000	2.662961000
N	-1.781311000	1.980015000	-0.304870000
N	-3.847381000	-0.233580000	-0.962559000
N	-4.175472000	-1.303599000	-1.754505000
N	-2.103767000	-2.398822000	0.081298000
C	-3.711060000	-0.089951000	2.853937000
C	-3.947444000	0.832414000	3.891518000
H	-4.704833000	0.766933000	4.659024000
C	-3.012165000	1.843928000	3.747245000
C	-4.439558000	-1.360746000	2.555215000
H	-5.499511000	-1.257905000	2.801764000
H	-4.043245000	-2.187839000	3.155564000
H	-4.350121000	-1.633281000	1.501565000
C	-2.788315000	3.076658000	4.559664000
H	-3.445341000	3.063501000	5.431338000
H	-3.014359000	3.986041000	3.991586000
H	-1.757097000	3.146995000	4.923963000
C	-1.166360000	2.218524000	2.026030000

H	-0.354687000	1.515932000	1.834404000
H	-0.823733000	3.008556000	2.690210000
N	-1.548956000	2.809513000	0.756816000
C	-1.753347000	4.117595000	0.427675000
C	-2.126303000	4.120624000	-0.908362000
C	-2.140588000	2.772730000	-1.323647000
C	-4.992822000	0.447649000	-0.775882000
C	-6.046061000	-0.194980000	-1.455246000
H	-7.078162000	0.121157000	-1.497868000
C	-5.505053000	-1.312258000	-2.066848000
C	-5.074373000	1.711629000	0.020570000
H	-6.050038000	1.781942000	0.508305000
H	-4.969088000	2.589381000	-0.627016000
H	-4.300104000	1.762265000	0.785343000
C	-6.144000000	-2.360989000	-2.916423000
H	-6.089260000	-3.351636000	-2.450578000
H	-5.683034000	-2.421847000	-3.909078000
H	-7.199811000	-2.122695000	-3.057917000
C	-3.155890000	-2.265583000	-2.091012000
H	-2.290157000	-1.736667000	-2.502606000
H	-3.545388000	-2.941839000	-2.849133000
N	-2.730582000	-3.042584000	-0.947006000
C	-2.826104000	-4.386803000	-0.720901000
C	-2.226458000	-4.607019000	0.509006000
C	-1.794435000	-3.349746000	0.976310000
H	-2.125885000	-5.559273000	1.009082000
H	-2.374308000	4.989749000	-1.500859000
C	3.947803000	-5.148630000	1.638656000
H	3.903850000	-6.167938000	1.250474000
H	4.998120000	-4.836437000	1.626498000
H	3.611969000	-5.176448000	2.681781000
C	0.815536000	-3.052138000	-1.864560000
H	0.374436000	-2.056437000	-1.784086000
H	1.350616000	-3.119975000	-2.817966000
H	0.011414000	-3.794930000	-1.884622000
C	1.407866000	5.227375000	-1.638255000
H	1.585377000	6.205995000	-1.188032000
H	2.083841000	5.132866000	-2.494749000
H	0.377284000	5.210156000	-2.010234000
C	2.440410000	2.449117000	2.568069000
H	2.017640000	1.462732000	2.779281000
H	3.528459000	2.368276000	2.667146000
H	2.095694000	3.150373000	3.333436000
C	-1.067916000	-3.027171000	2.244555000
H	-1.429748000	-3.654116000	3.064131000
H	0.006144000	-3.223694000	2.134835000
H	-1.201627000	-1.979018000	2.524696000
C	-3.470987000	-5.339189000	-1.674173000
H	-2.988841000	-5.328050000	-2.658567000
H	-3.397693000	-6.355214000	-1.281767000
H	-4.534964000	-5.116847000	-1.813677000
C	-1.562003000	5.248816000	1.382519000
H	-2.262836000	5.198815000	2.222568000
H	-0.543212000	5.266092000	1.785017000
H	-1.735560000	6.196218000	0.868453000
C	-2.498622000	2.220106000	-2.667310000
H	-2.138742000	2.876480000	-3.465137000
H	-2.075389000	1.222749000	-2.814338000
H	-3.584536000	2.134898000	-2.782122000

[($Me_4PzPz)_2Zn]^{+2}$

Zn	0.000084000	0.000365000	-0.493284000
N	1.662689000	0.856831000	-1.349801000
N	2.448575000	-1.323684000	0.608111000
N	2.912557000	0.388247000	-1.027289000
N	-1.080670000	1.315229000	0.689108000
N	-2.449180000	1.323437000	0.608041000
N	1.080036000	-1.315680000	0.688530000
N	-2.912049000	-0.387653000	-1.028527000
N	-1.662019000	-0.855455000	-1.351584000
C	-3.076215000	1.003455000	-0.658980000
H	-2.641528000	1.634840000	-1.439681000
H	-4.139899000	1.217768000	-0.584189000
C	-0.769955000	1.779028000	1.912822000
C	0.660707000	2.972472000	-2.152935000
H	-0.085918000	2.386270000	-2.700065000
H	0.979033000	3.795241000	-2.796812000
H	0.180999000	3.406484000	-1.267430000
C	-3.864811000	-1.334787000	-1.263682000
C	-1.949581000	2.102693000	2.605688000
H	-2.027990000	2.513497000	3.601595000
C	5.324844000	1.098881000	-1.050985000
H	5.543949000	0.789176000	-0.022909000
H	5.875219000	2.021575000	-1.243646000
H	5.714416000	0.333386000	-1.732453000
C	1.830580000	2.126025000	-1.766526000
C	-3.193246000	-2.455501000	-1.731866000
H	-3.641682000	-3.394631000	-2.020633000
C	-1.829354000	-2.124671000	-1.768469000
C	3.194667000	2.456073000	-1.730333000
H	3.643521000	3.395044000	-2.018966000
C	-3.006297000	1.810818000	1.753967000
C	3.076193000	-1.003127000	-0.658496000
H	2.641646000	-1.634008000	-1.439684000
H	4.139791000	-1.217737000	-0.583399000
C	3.865766000	1.334899000	-1.262582000
C	3.005214000	-1.811682000	1.754011000
C	0.768779000	-1.780291000	1.911821000
C	1.948109000	-2.104213000	2.605048000
H	2.026105000	-2.515587000	3.600755000
C	-0.653934000	-1.865523000	2.364270000
H	-1.334071000	-1.947442000	1.510661000
H	-0.800914000	-2.739693000	3.003699000
H	-0.938735000	-0.980041000	2.944739000
C	-0.659170000	-2.970418000	-2.155464000
H	-0.178961000	-3.404394000	-1.270207000
H	-0.977285000	-3.793199000	-2.799429000
H	0.086973000	-2.383697000	-2.702702000
C	-5.323937000	-1.099600000	-1.051506000
H	-5.714032000	-0.333652000	-1.732163000
H	-5.873970000	-2.022353000	-1.244863000
H	-5.542887000	-0.790931000	-0.023083000
C	-4.477683000	1.981514000	1.941198000
H	-4.889990000	2.728454000	1.252553000
H	-5.019284000	1.040494000	1.793017000
H	-4.679758000	2.324338000	2.957590000
C	0.652526000	1.863797000	2.366090000
H	0.936990000	0.977745000	2.945856000
H	1.333128000	1.946511000	1.512930000
H	0.799177000	2.737344000	3.006440000
C	4.476527000	-1.982328000	1.941814000
H	4.678206000	-2.325423000	2.958194000
H	4.889157000	-2.729064000	1.253137000
H	5.018130000	-1.041236000	1.794121000

5-Py

Zn	-0.000039000	-0.000120000	-0.708545000
O	0.454367000	-0.952613000	-2.621628000
N	0.896996000	-1.427516000	0.640938000
N	2.242936000	-1.633195000	0.541480000
N	1.984852000	0.993295000	-0.760085000
N	0.000081000	-0.000413000	-3.322674000
C	0.546035000	-1.840744000	1.871420000
C	1.681444000	-2.308441000	2.555643000
H	1.718526000	-2.713456000	3.556197000
C	2.753397000	-2.158417000	1.685950000
C	-0.868310000	-1.784448000	2.358017000
H	-1.325933000	-0.814203000	2.148768000
H	-1.484259000	-2.553600000	1.879459000
H	-0.898270000	-1.953663000	3.437070000
C	4.201294000	-2.480769000	1.861374000
H	4.833155000	-1.594431000	1.732313000
H	4.371028000	-2.869486000	2.867478000
H	4.537431000	-3.242554000	1.148108000
C	2.953854000	-1.232982000	-0.666200000
H	3.926305000	-1.725101000	-0.658621000
H	2.390648000	-1.597444000	-1.530798000
C	3.118830000	0.269386000	-0.772478000
C	4.368035000	0.868783000	-0.912324000
H	5.266186000	0.259917000	-0.918914000
C	4.440711000	2.255371000	-1.054275000
H	5.402953000	2.744459000	-1.168616000
C	3.262095000	2.998911000	-1.051007000
H	3.273462000	4.076830000	-1.167636000
C	2.053257000	2.324608000	-0.901306000
H	1.103507000	2.850080000	-0.896292000
O	-0.454276000	0.951943000	-2.621895000
N	-0.896945000	1.427585000	0.640751000
N	-2.242883000	1.633253000	0.541281000
N	-1.984930000	-0.993388000	-0.759965000
C	-0.545952000	1.841070000	1.871139000
C	-1.681344000	2.308916000	2.555287000
H	-1.718405000	2.714155000	3.555751000
C	-2.753318000	2.158731000	1.685643000
C	0.868393000	1.784820000	2.357739000
H	1.325998000	0.814542000	2.148605000
H	1.484354000	2.553903000	1.879084000
H	0.898355000	1.954162000	3.436772000
C	-2.953808000	1.232937000	-0.666367000
H	-2.390550000	1.597242000	-1.530997000
C	-3.118880000	-0.269434000	-0.772431000
C	-2.053390000	-2.324724000	-0.900964000
H	-3.926221000	1.725131000	-0.658875000
C	-4.368113000	-0.868801000	-0.912132000
H	-5.266238000	-0.259898000	-0.918798000
C	-4.440849000	-2.255411000	-1.053843000
H	-5.403115000	-2.744481000	-1.168063000
C	-3.262264000	-2.999000000	-1.050497000
H	-1.103660000	-2.850231000	-0.895920000
H	-3.273683000	-4.076938000	-1.166940000
C	-4.201205000	2.481145000	1.861027000
H	-4.370960000	2.869799000	2.867153000
H	-4.537273000	3.243001000	1.147803000
H	-4.833109000	1.594852000	1.731876000

RC''

Zn	-1.597759000	-0.157788000	-0.588507000
O	-0.553612000	1.167244000	-1.990779000
N	-0.521453000	0.050247000	1.260004000
N	0.792569000	-0.315633000	1.257738000
N	-0.113466000	-1.686440000	-1.152341000
N	-1.250959000	0.854433000	-3.004762000
C	-0.931061000	-0.034100000	2.538532000
C	0.135179000	-0.460107000	3.348490000
H	0.120490000	-0.613639000	4.417484000
C	1.223816000	-0.636668000	2.503309000
C	-2.327796000	0.304715000	2.956693000
H	-3.069371000	-0.166967000	2.307365000
H	-2.498602000	1.386375000	2.927334000
H	-2.502311000	-0.035214000	3.980444000
C	2.619899000	-1.079362000	2.790522000
H	2.875435000	-1.992455000	2.239851000
H	2.728997000	-1.286764000	3.857110000
H	3.346680000	-0.309657000	2.511691000
C	1.543119000	-0.326039000	0.011315000
H	2.604586000	-0.329705000	0.253317000
H	1.335913000	0.612285000	-0.508442000
C	1.190379000	-1.503337000	-0.872565000
C	2.172550000	-2.335755000	-1.403815000
H	3.213514000	-2.157889000	-1.165225000
C	1.792763000	-3.383665000	-2.242386000
H	2.542681000	-4.044069000	-2.666795000
C	0.440831000	-3.569866000	-2.525986000
H	0.103036000	-4.368968000	-3.176360000
C	-0.479555000	-2.692532000	-1.960709000
H	-1.543570000	-2.777799000	-2.157747000
O	-2.134546000	-0.005197000	-2.738291000
N	-3.189402000	-1.509270000	-0.043948000
N	-4.472347000	-1.057741000	-0.163799000
N	-3.003419000	1.485384000	-0.124283000
C	-3.230318000	-2.522176000	0.838688000
C	-4.551074000	-2.711491000	1.281277000
H	-4.903569000	-3.454084000	1.981851000
C	-5.323480000	-1.758551000	0.630586000
C	-2.001798000	-3.278277000	1.238193000
H	-1.231382000	-2.609227000	1.632691000
H	-1.571169000	-3.816946000	0.388095000
H	-2.249515000	-4.008544000	2.012160000
C	-4.769792000	0.079011000	-1.026888000
H	-4.270755000	-0.082701000	-1.986851000
C	-4.309859000	1.395416000	-0.433678000
H	-5.846138000	0.093518000	-1.197833000
C	-6.789208000	-1.479833000	0.702692000
H	-7.254802000	-2.151910000	1.426406000
H	-6.991891000	-0.450645000	1.020761000
H	-7.281341000	-1.637997000	-0.264248000
C	-5.180972000	2.464834000	-0.241772000
C	-4.680422000	3.661719000	0.273912000
C	-2.522929000	2.631462000	0.379824000
C	-3.326524000	3.748410000	0.591540000
H	-6.230366000	2.364440000	-0.499116000
H	-5.339932000	4.510546000	0.425062000
H	-1.464414000	2.639852000	0.620045000
H	-2.893221000	4.658955000	0.989735000
S	0.946961000	3.547130000	-0.283054000
H	0.592341000	2.793769000	-1.346660000
C	2.736748000	3.759832000	-0.718042000
H	2.795025000	4.058007000	-1.767178000
H	3.059421000	4.612997000	-0.115831000
C	3.599809000	2.559243000	-0.439075000
C	3.973165000	1.674818000	-1.458468000
C	4.079659000	2.309920000	0.850099000
C	4.816994000	0.595364000	-1.196934000
C	4.932613000	1.236242000	1.106859000
C	5.331434000	0.356694000	0.088934000
H	3.617127000	1.842752000	-2.472168000
H	3.802663000	2.977673000	1.662035000

H	5.104822000	-0.049823000	-2.021896000
H	5.313534000	1.109901000	2.113753000
C	6.336104000	-0.780201000	0.324966000
C	6.734218000	-0.911716000	1.804686000
C	7.611112000	-0.491941000	-0.499212000
H	7.394554000	-0.435124000	-1.570748000
H	8.061121000	0.459395000	-0.197041000
H	8.351407000	-1.285289000	-0.345658000
H	7.226462000	-0.007082000	2.176049000
H	7.439389000	-1.740676000	1.922891000
H	5.868556000	-1.120335000	2.444344000
C	5.734215000	-2.126618000	-0.127937000
H	5.470273000	-2.117393000	-1.190905000
H	6.456128000	-2.936688000	0.022527000
H	4.835276000	-2.369246000	0.452161000

TS-1''

Zn	1.446396000	-0.116290000	-0.272674000
O	1.160974000	-0.638686000	-2.653831000
O	0.930264000	-2.013313000	-0.951502000
N	1.965581000	1.958607000	-0.578609000
N	1.021867000	2.810074000	-1.076009000
C	-1.085142000	1.678643000	-0.508437000
N	-0.597008000	0.572517000	0.092308000
N	3.544719000	-0.755805000	-0.765254000
C	4.104333000	-1.781265000	-0.095657000
N	2.927465000	-1.398160000	2.042833000
N	1.981729000	-0.449143000	1.777520000
N	1.088111000	-1.827372000	-2.437335000
C	2.924974000	2.737114000	-0.043747000
C	2.578515000	4.089993000	-0.203815000
H	3.151426000	4.949615000	0.111402000
C	1.353839000	4.108816000	-0.856410000
C	4.156593000	2.180587000	0.598696000
H	4.917463000	1.931618000	-0.149322000
H	4.586844000	2.921635000	1.277165000
H	3.939687000	1.274914000	1.167731000
C	-0.225149000	2.269489000	-1.603387000
H	0.020300000	1.503669000	-2.345128000
C	3.281215000	-2.380723000	1.025357000
H	2.357604000	-2.789400000	0.604095000
H	3.827616000	-3.185865000	1.516035000
C	1.947198000	0.356884000	2.854250000
C	2.879124000	-0.087925000	3.807020000
H	3.075892000	0.344573000	4.776926000
C	3.497712000	-1.204657000	3.260399000
C	1.027078000	1.533931000	2.942275000
H	1.014843000	2.101890000	2.008322000
H	-0.001097000	1.223419000	3.156454000
H	1.350747000	2.199897000	3.745854000
C	4.570930000	-2.087591000	3.807705000
H	5.456413000	-2.097582000	3.161696000
H	4.877566000	-1.725697000	4.791122000
H	4.225785000	-3.121533000	3.924532000
C	0.493743000	5.254729000	-1.278456000
H	-0.484604000	5.231088000	-0.784415000
H	0.979826000	6.195244000	-1.011513000
H	0.326200000	5.260216000	-2.361648000
H	-0.749553000	3.078127000	-2.111814000
C	-6.873056000	-0.316197000	1.030236000
C	-7.059595000	-1.334595000	2.166847000
C	-8.134621000	-0.346962000	0.139625000
H	-8.085410000	0.397671000	-0.661131000
H	-8.256191000	-1.331025000	-0.324904000
H	-9.028550000	-0.137246000	0.738128000
H	-7.202632000	-2.349490000	1.781465000
H	-7.946766000	-1.074511000	2.753544000
H	-6.202354000	-1.344762000	2.850179000
C	-6.728662000	1.086233000	1.660789000
H	-6.602853000	1.863586000	0.899291000
H	-7.619899000	1.337444000	2.246708000
H	-5.865483000	1.123161000	2.337493000
C	-5.639094000	-0.622226000	0.171072000
C	-4.796614000	-1.713366000	0.405551000
C	-5.323482000	0.200400000	-0.925164000
C	-3.688961000	-1.973012000	-0.407848000
C	-4.224113000	-0.058555000	-1.736962000
C	-3.378854000	-1.149870000	-1.490628000
H	-5.002063000	-2.393383000	1.224595000
H	-5.957816000	1.050284000	-1.161337000
H	-3.068707000	-2.842699000	-0.215549000
H	-4.022190000	0.593164000	-2.584970000
C	-2.193972000	-1.386885000	-2.410496000
H	-2.541623000	-1.328031000	-3.447633000
H	-1.467312000	-0.569716000	-2.283342000
S	-1.316415000	-2.978949000	-2.229529000
H	-0.083518000	-2.510515000	-1.089348000
C	5.355884000	-2.285878000	-0.440021000

H	5.780000000	-3.113809000	0.118598000
C	6.042374000	-1.720587000	-1.515312000
H	7.016374000	-2.101721000	-1.805461000
C	4.205951000	-0.212513000	-1.797572000
C	5.456574000	-0.664050000	-2.209551000
C	-2.302874000	2.233109000	-0.139604000
H	-2.671921000	3.118567000	-0.646505000
C	-3.049727000	1.624719000	0.872885000
H	-4.006526000	2.034906000	1.172358000
C	-1.326942000	-0.025471000	1.044275000
C	-2.555181000	0.472120000	1.472094000
H	3.704002000	0.606382000	-2.302456000
H	5.950803000	-0.200094000	-3.055801000
H	-3.118858000	-0.053657000	2.232060000
H	-0.899828000	-0.924124000	1.477634000

Int-1''

Zn	0.846625000	-0.396692000	0.007498000
O	0.576974000	1.220013000	-1.423308000
O	-0.643237000	-0.480947000	-1.653980000
N	2.343842000	0.360937000	1.335156000
N	2.472949000	1.676903000	1.679685000
C	2.468339000	3.343131000	-0.153004000
N	3.433142000	2.614178000	-0.723508000
N	2.334000000	-1.314498000	-1.339909000
C	2.128083000	-2.524455000	-1.893604000
N	0.693187000	-3.436986000	-0.095269000
N	0.457414000	-2.387680000	0.748085000
N	-0.317524000	0.648747000	-2.114613000
C	3.347902000	-0.287038000	1.954843000
C	4.126365000	0.629563000	2.681758000
H	4.996609000	0.410464000	3.282736000
C	3.556120000	1.874513000	2.474173000
C	3.550090000	-1.767127000	1.864801000
H	3.051199000	-2.290215000	2.687543000
H	3.164647000	-2.174344000	0.929947000
H	4.617573000	-1.996433000	1.928792000
C	1.715578000	2.715463000	1.009057000
H	1.447187000	3.476652000	1.747265000
C	0.830081000	-3.215699000	-1.530440000
H	-0.014493000	-2.607148000	-1.865716000
H	0.767956000	-4.187602000	-2.019372000
C	0.401915000	-2.908301000	1.985516000
C	0.604310000	-4.297617000	1.925493000
H	0.608461000	-4.991948000	2.752756000
C	0.793490000	-4.608570000	0.586442000
C	0.164372000	-2.061246000	3.195816000
H	-0.901139000	-1.844521000	3.332129000
H	0.510448000	-2.582497000	4.092251000
H	0.692160000	-1.106223000	3.125549000
C	1.049278000	-5.921575000	-0.078294000
H	1.988812000	-5.915450000	-0.642793000
H	1.117946000	-6.706661000	0.677436000
H	0.241398000	-6.192603000	-0.768233000
C	3.964351000	3.230140000	2.945723000
H	3.170513000	3.714196000	3.526613000
H	4.846843000	3.150432000	3.583611000
H	4.210073000	3.884876000	2.101836000
H	0.788039000	2.272931000	0.645010000
C	-7.772301000	0.222160000	-0.424361000
C	-7.970149000	-0.602147000	-1.707109000
C	-8.639346000	1.496389000	-0.527588000
H	-8.577160000	2.105530000	0.379722000
H	-8.321501000	2.117118000	-1.372364000
H	-9.690884000	1.226760000	-0.677748000
H	-7.677763000	-0.040313000	-2.601026000
H	-9.027467000	-0.865672000	-1.813801000
H	-7.397374000	-1.536007000	-1.683146000
C	-8.245795000	-0.626959000	0.776052000
H	-8.171255000	-0.076294000	1.719164000
H	-9.293348000	-0.919674000	0.642225000
H	-7.645785000	-1.538991000	0.869937000
C	-6.307755000	0.624556000	-0.211070000
C	-5.284603000	0.272783000	-1.100807000
C	-5.949171000	1.382323000	0.917157000
C	-3.962020000	0.658855000	-0.880014000
C	-4.633831000	1.769861000	1.145995000
C	-3.622291000	1.415364000	0.245450000
H	-5.510774000	-0.306073000	-1.988213000
H	-6.711357000	1.679470000	1.630534000
H	-3.189825000	0.367534000	-1.586932000
H	-4.389221000	2.354288000	2.029743000
C	-2.195708000	1.802640000	0.490055000
H	-1.646787000	1.945323000	-0.440363000
H	-2.116417000	2.710363000	1.093159000
S	-1.287494000	0.504646000	1.492130000
H	-1.990957000	-0.548474000	1.033655000
C	3.049432000	-3.093283000	-2.768373000

H	2.858998000	-4.070382000	-3.200208000
C	4.210768000	-2.384123000	-3.080905000
H	4.942853000	-2.806829000	-3.761991000
C	3.449329000	-0.627853000	-1.636544000
C	4.413836000	-1.131561000	-2.506578000
C	4.077612000	3.143809000	-1.771636000
H	4.858666000	2.527283000	-2.211884000
C	3.794567000	4.403364000	-2.295197000
H	4.348361000	4.781233000	-3.147953000
C	2.118472000	4.621233000	-0.593753000
C	2.790295000	5.157788000	-1.689327000
H	1.335380000	5.180966000	-0.090584000
H	2.539260000	6.147335000	-2.058553000
H	5.302061000	-0.549299000	-2.725896000
H	3.550550000	0.345327000	-1.161296000

TS-2''

Zn	0.697473000	-0.071968000	-0.277206000
N	-0.067339000	-0.912587000	1.524244000
N	-1.273488000	-1.548219000	1.557940000
C	-1.897386000	-1.812053000	-0.826049000
N	-0.741750000	-1.377304000	-1.359929000
N	4.380769000	0.982905000	0.986177000
C	4.069802000	1.446082000	-0.229449000
N	3.662356000	-0.922079000	-0.843766000
N	2.393174000	-1.352897000	-0.566919000
C	0.572838000	-1.249436000	2.657310000
C	-0.248337000	-2.101726000	3.419737000
H	-0.017564000	-2.534111000	4.382143000
C	-1.422477000	-2.270250000	2.700097000
C	1.956089000	-0.773854000	2.963396000
H	2.200206000	-0.985471000	4.007342000
H	2.700039000	-1.270121000	2.330506000
H	2.039188000	0.298728000	2.779246000
C	-2.261974000	-1.260409000	0.531675000
H	-2.379580000	-0.175933000	0.463905000
C	3.924774000	0.415428000	-1.336123000
H	3.131405000	0.689639000	-2.034661000
H	4.848830000	0.364596000	-1.920290000
C	2.526722000	-2.622776000	-0.123118000
C	3.883196000	-2.975662000	-0.097471000
H	4.302038000	-3.924456000	0.203712000
C	4.584880000	-1.866822000	-0.548139000
C	1.376838000	-3.497692000	0.268385000
H	0.461621000	-3.229920000	-0.258014000
H	1.616416000	-4.538818000	0.034108000
H	1.175432000	-3.438074000	1.342882000
C	6.051246000	-1.638988000	-0.699973000
H	6.369872000	-0.790971000	-0.084499000
H	6.597900000	-2.526684000	-0.375326000
H	6.330763000	-1.434759000	-1.740316000
C	-2.663848000	-3.034439000	3.026025000
H	-2.914030000	-3.761043000	2.244627000
H	-2.521512000	-3.582679000	3.959513000
H	-3.525750000	-2.369170000	3.159296000
H	-3.214949000	-1.671387000	0.860546000
C	-5.601709000	1.232713000	0.842933000
C	-5.108301000	0.758503000	2.228224000
C	-6.656148000	0.233659000	0.339846000
H	-7.078439000	0.537516000	-0.623766000
H	-6.241674000	-0.776034000	0.230314000
H	-7.480609000	0.175216000	1.057442000
H	-4.661962000	-0.241793000	2.165010000
H	-5.946962000	0.705625000	2.930876000
H	-4.359511000	1.434401000	2.652183000
C	-6.269272000	2.618490000	0.986949000
H	-6.626300000	2.980402000	0.017073000
H	-7.126546000	2.557560000	1.666542000
H	-5.574988000	3.362916000	1.388967000
C	-4.409422000	1.349879000	-0.114684000
C	-3.331062000	2.194062000	0.206777000
C	-4.327553000	0.646818000	-1.322775000
C	-2.228233000	2.329762000	-0.632389000
C	-3.221361000	0.777248000	-2.166887000
C	-2.155581000	1.618329000	-1.839714000
H	-3.350884000	2.767223000	1.128333000
H	-5.131360000	-0.014335000	-1.625001000
H	-1.430435000	3.009583000	-0.351437000
H	-3.193162000	0.213994000	-3.096436000
C	-1.019792000	1.801858000	-2.812153000
H	-1.123749000	1.109909000	-3.650996000
H	-1.022528000	2.814756000	-3.225998000
S	0.702634000	1.559282000	-2.165079000
C	3.925539000	2.803330000	-0.522163000
H	3.662923000	3.127160000	-1.524789000
C	4.102277000	3.724843000	0.507177000
H	3.980003000	4.786891000	0.320714000
C	4.540945000	1.878496000	1.968217000

C	4.410496000	3.254617000	1.782709000
C	-2.734846000	-2.687543000	-1.513751000
H	-3.660422000	-3.021133000	-1.056713000
C	-2.374313000	-3.107875000	-2.793314000
C	-0.390465000	-1.785574000	-2.589254000
C	-1.180432000	-2.644939000	-3.345946000
H	-3.015147000	-3.784860000	-3.349483000
N	1.043347000	2.837272000	1.131060000
O	1.161676000	1.586766000	1.070239000
O	0.826667000	3.438507000	0.032641000
H	0.769889000	2.610769000	-1.034612000
H	-0.862093000	-2.945380000	-4.337932000
H	0.554290000	-1.403196000	-2.963050000
H	4.543796000	3.935212000	2.616695000
H	4.784180000	1.472472000	2.947446000

Int-2''

Zn	0.714772000	-0.207002000	-0.389510000
N	0.038455000	-0.666844000	1.556577000
N	-1.191740000	-1.239985000	1.716679000
C	-1.889216000	-1.924516000	-0.566096000
N	-0.730870000	-1.647091000	-1.191638000
N	4.397472000	1.090587000	0.746217000
C	4.034321000	1.402252000	-0.503211000
N	3.692594000	-1.030581000	-0.841131000
N	2.446048000	-1.451390000	-0.465527000
C	0.703973000	-0.867706000	2.708007000
C	-0.121402000	-1.569519000	3.606138000
H	0.126994000	-1.872395000	4.612616000
C	-1.324098000	-1.790397000	2.951734000
C	2.101924000	-0.391243000	2.935629000
H	2.591225000	-1.022858000	3.682216000
H	2.702168000	-0.400566000	2.023971000
H	2.096480000	0.638873000	3.304632000
C	-2.196016000	-1.114304000	0.672174000
H	-2.280140000	-0.058117000	0.403056000
C	3.896610000	0.251624000	-1.486752000
H	3.071901000	0.427700000	-2.181544000
H	4.807983000	0.166857000	-2.086489000
C	2.625910000	-2.646905000	0.137055000
C	3.990509000	-2.965052000	0.158004000
H	4.444589000	-3.856026000	0.565819000
C	4.648089000	-1.908747000	-0.457365000
C	1.503719000	-3.469924000	0.688076000
H	0.568748000	-3.290876000	0.156810000
H	1.750307000	-4.531956000	0.602823000
H	1.332347000	-3.252519000	1.747589000
C	6.102572000	-1.669662000	-0.686830000
H	6.420189000	-0.747734000	-0.188020000
H	6.682042000	-2.500247000	-0.278697000
H	6.342351000	-1.584840000	-1.753231000
C	-2.576202000	-2.459801000	3.415598000
H	-2.863753000	-3.288821000	2.758928000
H	-2.424941000	-2.864043000	4.418514000
H	-3.416832000	-1.756941000	3.462711000
H	-3.152643000	-1.417435000	1.093239000
C	-5.743953000	1.244807000	0.593075000
C	-5.300828000	0.926282000	2.038658000
C	-6.775743000	0.189825000	0.162387000
H	-7.152986000	0.379109000	-0.848112000
H	-6.358109000	-0.824017000	0.188914000
H	-7.631749000	0.210938000	0.844337000
H	-4.853425000	-0.074222000	2.098746000
H	-6.162831000	0.946660000	2.714427000
H	-4.566095000	1.647158000	2.410444000
C	-6.422389000	2.632095000	0.561392000
H	-6.741772000	2.884606000	-0.455114000
H	-7.306040000	2.636944000	1.209236000
H	-5.749130000	3.422145000	0.908137000
C	-4.514144000	1.262743000	-0.323230000
C	-3.466066000	2.167496000	-0.074900000
C	-4.363635000	0.403145000	-1.417639000
C	-2.323281000	2.203870000	-0.869603000
C	-3.218465000	0.438637000	-2.218520000
C	-2.176424000	1.331646000	-1.959001000
H	-3.539396000	2.861652000	0.756589000
H	-5.141991000	-0.310446000	-1.662184000
H	-1.542285000	2.921436000	-0.641018000
H	-3.135965000	-0.248381000	-3.057338000
C	-0.975889000	1.369112000	-2.871534000
H	-0.988269000	0.499499000	-3.533715000
H	-1.013500000	2.257262000	-3.511058000
S	0.686921000	1.456321000	-2.059666000
C	3.833907000	2.714912000	-0.938273000
H	3.520928000	2.913426000	-1.958262000
C	4.027226000	3.751729000	-0.028204000
H	3.869434000	4.782643000	-0.328472000
C	4.573562000	2.096164000	1.613288000

C	4.404721000	3.438668000	1.277484000
C	-2.780565000	-2.867824000	-1.071562000
H	-3.706764000	-3.072920000	-0.545412000
C	-2.474244000	-3.518626000	-2.266098000
C	-0.432612000	-2.272953000	-2.341219000
C	-1.280818000	-3.211337000	-2.919736000
H	-3.158234000	-4.251862000	-2.681794000
N	1.037995000	3.116541000	1.267900000
O	1.263395000	1.929797000	1.210473000
O	0.745399000	3.692156000	0.089100000
H	0.751504000	2.976036000	-0.641035000
H	-1.007890000	-3.689823000	-3.853590000
H	0.516028000	-2.002955000	-2.795404000
H	4.558779000	4.213591000	2.020697000
H	4.860475000	1.809146000	2.622301000

Int-3''

Zn	0.737658000	-0.014595000	-0.506846000	H	-2.353220000	-2.215127000	3.649213000
N	0.215764000	0.159492000	1.530268000	H	-1.816396000	-1.343699000	5.091471000
N	-0.944059000	-0.421609000	1.953007000	H	-2.966339000	-0.584723000	3.984040000
C	-1.777114000	-1.738817000	0.014121000	H	-2.933808000	-0.839047000	1.581270000
N	-0.682690000	-1.625260000	-0.761309000	C	-5.859443000	1.131668000	0.360894000
N	5.075408000	1.249953000	0.365369000	C	-5.439712000	1.166565000	1.847431000
C	4.178786000	1.528788000	-0.592380000	C	-6.744760000	-0.105749000	0.141408000
N	3.708091000	-0.866549000	-0.925695000	H	-7.106127000	-0.168881000	-0.890356000
N	2.511318000	-1.163167000	-0.331441000	H	-6.211231000	-1.035166000	0.375515000
C	0.990484000	0.303171000	2.617981000	H	-7.620465000	-0.054729000	0.796352000
C	0.306878000	-0.184564000	3.745914000	H	-4.892155000	0.255188000	2.120699000
H	0.659562000	-0.195719000	4.766625000	H	-6.323562000	1.227797000	2.491899000
C	-0.926143000	-0.637906000	3.294644000	H	-4.800320000	2.025811000	2.072548000
C	2.365600000	0.878671000	2.519170000	C	-6.693449000	2.391139000	0.038040000
H	2.695090000	1.246013000	3.494056000	H	-6.999885000	2.393931000	-1.013181000
H	3.087917000	0.130199000	2.176444000	H	-7.596291000	2.418424000	0.658430000
H	2.393713000	1.711616000	1.811237000	H	-6.130030000	3.310374000	0.225882000
C	-2.032283000	-0.628667000	1.009214000	C	-4.607339000	1.115296000	-0.525293000
H	-2.198592000	0.308894000	0.471606000	C	-3.679253000	2.171176000	-0.451837000
C	3.910606000	0.414848000	-1.589276000	C	-4.322930000	0.082130000	-1.425099000
H	3.035936000	0.633731000	-2.206291000	C	-2.522942000	2.186224000	-1.226337000
H	4.767734000	0.293944000	-2.256794000	C	-3.166020000	0.098820000	-2.210852000
C	2.713251000	-2.300691000	0.366494000	C	-2.244350000	1.143616000	-2.124229000
C	4.045457000	-2.710695000	0.223370000	H	-3.859908000	2.999406000	0.226805000
H	4.507460000	-3.583847000	0.659804000	H	-5.004245000	-0.754387000	-1.528913000
C	4.661642000	-1.768891000	-0.590996000	H	-1.817674000	3.006734000	-1.134636000
C	1.633680000	-2.991439000	1.141200000	H	-2.979418000	-0.722959000	-2.898544000
H	0.954381000	-3.543065000	0.482346000	C	-1.018182000	1.156464000	-3.003138000
H	2.083891000	-3.710820000	1.829782000	H	-0.916346000	0.193498000	-3.511221000
H	1.037832000	-2.288855000	1.727557000	H	-1.124131000	1.917741000	-3.783287000
C	6.079346000	-1.659008000	-1.042779000	S	0.574667000	1.590099000	-2.155953000
H	6.524564000	-0.736967000	-0.655945000	C	3.535161000	2.763221000	-0.699176000
H	6.652046000	-2.510026000	-0.668194000	H	2.811492000	2.941921000	-1.487509000
H	6.159726000	-1.653646000	-2.135931000	C	3.841663000	3.754408000	0.236016000
C	-2.079528000	-1.227716000	4.038196000	H	3.358104000	4.725073000	0.182102000

C	5.360565000	2.207248000	1.253838000
C	4.771946000	3.474199000	1.234239000
C	-2.667034000	-2.799489000	-0.139397000
H	-3.540764000	-2.866889000	0.499862000
C	-2.431304000	-3.747964000	-1.133240000
C	-0.450870000	-2.540243000	-1.716914000
C	-1.304316000	-3.614095000	-1.944484000
H	-3.117641000	-4.577011000	-1.274034000
H	-1.085777000	-4.325979000	-2.732464000
H	0.450649000	-2.396896000	-2.305134000
H	5.040938000	4.214597000	1.980407000
H	6.093497000	1.949486000	2.015239000

Int-4''

Zn	0.018153000	-0.004837000	-0.713950000
O	0.125469000	0.026842000	-2.610565000
N	-1.108182000	1.358824000	0.479044000
N	-2.393778000	1.585125000	0.085149000
C	-3.074362000	-0.514909000	-0.985309000
N	-1.970748000	-1.212793000	-0.656078000
N	1.934592000	1.222382000	-0.610428000
C	3.052840000	0.563421000	-0.965774000
N	2.421071000	-1.582672000	0.057703000
N	1.123633000	-1.412674000	0.443154000
C	-1.002418000	1.840524000	1.726826000
C	-2.240787000	2.374269000	2.131903000
H	-2.471045000	2.845822000	3.075993000
C	-3.114808000	2.183334000	1.071454000
C	0.286413000	1.778376000	2.484523000
H	0.810744000	2.740675000	2.456302000
H	0.098949000	1.539262000	3.535472000
H	0.953397000	1.020360000	2.067678000
C	-2.870141000	0.978260000	-1.152562000
H	-2.115693000	1.153781000	-1.930077000
C	2.892692000	-0.930632000	-1.161212000
H	2.148747000	-1.092621000	-1.952107000
H	3.833674000	-1.396586000	-1.453614000
C	1.022173000	-1.927399000	1.678166000
C	2.273126000	-2.429144000	2.083372000
H	2.510865000	-2.915613000	3.018019000
C	3.150665000	-2.180831000	1.036871000
C	-0.275871000	-1.916139000	2.422974000
H	-0.972534000	-1.196309000	1.986691000
H	-0.753702000	-2.902705000	2.407800000
H	-0.112172000	-1.649981000	3.471556000
C	4.611041000	-2.462432000	0.901190000
H	5.188853000	-1.539695000	0.772087000
H	4.975113000	-2.963033000	1.800654000
H	4.820923000	-3.114309000	0.045337000
C	-4.562514000	2.520202000	0.926752000
H	-5.172995000	1.621938000	0.776399000
H	-4.917027000	3.017957000	1.831572000
H	-4.739784000	3.194720000	0.081120000
H	-3.795567000	1.475738000	-1.443093000
H	-0.431336000	-0.629500000	-3.053393000
C	4.262442000	1.221225000	-1.170854000
H	5.146624000	0.660441000	-1.456175000
C	4.310346000	2.607820000	-1.016530000
H	5.240076000	3.145243000	-1.174950000
C	1.980771000	2.552331000	-0.469653000
C	3.147905000	3.288723000	-0.662287000
C	-4.309228000	-1.131104000	-1.170639000
H	-5.179773000	-0.540047000	-1.436343000
C	-4.401076000	-2.515982000	-1.017133000
H	-5.351274000	-3.021273000	-1.158778000
C	-2.061161000	-2.540884000	-0.510437000
C	-3.256637000	-3.236574000	-0.681571000
H	1.044581000	3.032590000	-0.201895000
H	3.138777000	4.366431000	-0.542339000
H	-3.283658000	-4.313602000	-0.557800000
H	-1.137683000	-3.051384000	-0.253330000

2-Py

Zn	1.956184000	-0.120928000	-0.207607000
O	0.039482000	-0.231182000	-0.812014000
N	2.570579000	-0.171971000	1.808080000
N	2.082462000	-1.139654000	2.650385000
N	1.812418000	-2.424810000	-0.014921000
N	3.501562000	-0.210121000	-1.625243000
N	3.456656000	0.673792000	-2.669726000
N	2.003203000	2.089583000	-0.506355000
C	3.722931000	0.258450000	2.362966000
C	3.959803000	-0.437473000	3.559912000
H	4.795049000	-0.306512000	4.232400000
C	2.913512000	-1.334723000	3.712923000
C	4.574744000	1.314809000	1.733250000
H	5.625570000	1.135962000	1.975020000
H	4.321948000	2.312384000	2.109953000
H	4.469825000	1.325658000	0.645823000
C	2.656804000	-2.352389000	4.775118000
H	3.422690000	-2.276529000	5.549160000
H	2.690863000	-3.371930000	4.373614000
H	1.682171000	-2.206659000	5.254906000
C	0.973629000	-1.978646000	2.222116000
H	0.172401000	-1.330365000	1.852732000
H	0.595545000	-2.502771000	3.100331000
C	1.377419000	-2.963165000	1.142483000
C	1.302027000	-4.340082000	1.334956000
H	0.961662000	-4.741573000	2.284238000
C	1.680672000	-5.191489000	0.293485000
H	1.638840000	-6.268588000	0.421792000
C	2.123782000	-4.634614000	-0.904671000
C	2.179277000	-3.246164000	-1.012151000
C	4.763954000	-0.680563000	-1.583974000
C	5.519751000	-0.087512000	-2.608639000
H	6.558485000	-0.272042000	-2.840802000
C	4.670130000	0.782699000	-3.278173000
C	5.202249000	-1.691913000	-0.572787000
H	6.242748000	-1.514452000	-0.288253000
H	5.146629000	-2.708427000	-0.979244000
H	4.585742000	-1.654328000	0.328730000
C	4.924729000	1.689124000	-4.437031000
H	4.781230000	2.741902000	-4.167363000
H	4.268106000	1.459828000	-5.284138000
H	5.955823000	1.571638000	-4.775402000
C	2.266030000	1.491272000	-2.851550000
H	1.390443000	0.833310000	-2.827573000
H	2.320874000	1.952055000	-3.837791000
C	2.143634000	2.546046000	-1.769077000
C	2.200122000	3.907878000	-2.055366000
H	2.319801000	4.244014000	-3.080080000
C	2.116017000	4.826889000	-1.007842000
H	2.170871000	5.892496000	-1.207116000
C	1.976440000	4.351804000	0.294955000
C	1.925198000	2.976003000	0.497075000
H	-0.042789000	-1.154767000	-1.094637000
Zn	-1.828918000	0.168446000	-0.192353000
N	-2.517461000	-0.156120000	1.787465000
N	-2.025588000	0.606141000	2.817780000
N	-1.407039000	2.277020000	0.375819000
N	-3.475487000	0.620328000	-1.422079000
N	-3.716262000	-0.127102000	-2.544773000
N	-2.165889000	-2.039601000	-0.895954000
C	-3.691811000	-0.657516000	2.226916000
C	-3.935136000	-0.213940000	3.536929000
H	-4.787434000	-0.455514000	4.155138000
C	-2.870020000	0.601896000	3.887093000
C	-4.566140000	-1.538434000	1.392100000
H	-5.603758000	-1.444432000	1.721553000
H	-4.286860000	-2.593091000	1.492424000
H	-4.515088000	-1.273847000	0.334125000
C	-2.609719000	1.367888000	5.142455000
H	-3.392157000	1.151430000	5.872172000
H	-2.613280000	2.449769000	4.965313000

H	-1.648632000	1.098882000	5.595419000
C	-0.866246000	1.456742000	2.601213000
H	-0.049469000	0.846566000	2.201733000
H	-0.547302000	1.830760000	3.574226000
C	-1.153853000	2.607600000	1.658786000
C	-1.149690000	3.930940000	2.091042000
H	-0.962029000	4.163492000	3.134343000
C	-1.391757000	4.948079000	1.164886000
H	-1.402725000	5.986775000	1.480182000
C	-1.617436000	4.606036000	-0.167034000
C	-1.626797000	3.257283000	-0.514957000
C	-4.639477000	1.239879000	-1.131738000
C	-5.613379000	0.879970000	-2.075608000
H	-6.636721000	1.223389000	-2.116090000
C	-5.005553000	0.000158000	-2.961068000
C	-4.792176000	2.167995000	0.031773000
H	-5.842890000	2.225457000	0.325685000
H	-4.467516000	3.182791000	-0.223998000
H	-4.212966000	1.834853000	0.896400000
C	-5.553287000	-0.708455000	-4.155770000
H	-5.506504000	-1.797296000	-4.039119000
H	-5.013512000	-0.438379000	-5.070849000
H	-6.600460000	-0.434492000	-4.296429000
C	-2.691129000	-1.027942000	-3.044063000
H	-1.744960000	-0.475908000	-3.082474000
H	-2.954761000	-1.306071000	-4.064562000
C	-2.535631000	-2.261259000	-2.174615000
C	-2.752222000	-3.546424000	-2.666917000
H	-3.056937000	-3.692184000	-3.698099000
C	-2.570512000	-4.638339000	-1.815306000
H	-2.737307000	-5.648385000	-2.176031000
C	-2.178973000	-4.408168000	-0.496718000
C	-1.994712000	-3.092682000	-0.081070000
H	2.537808000	-2.762757000	-1.916049000
H	2.432153000	-5.258097000	-1.736716000
H	1.831514000	2.556143000	1.493168000
H	1.918301000	5.029350000	1.139087000
H	-2.030049000	-5.227216000	0.198044000
H	-1.711279000	-2.858694000	0.940608000
H	-1.802593000	5.363339000	-0.920831000
H	-1.838188000	2.939293000	-1.530942000

$[(Me_2PzPy)_2Zn]^{+2}$

Zn	-0.000030000	0.000221000	-0.146350000
N	-1.355230000	-1.285528000	-1.112648000
N	2.740741000	-1.008450000	0.262578000
N	1.355247000	1.285691000	-1.112928000
N	1.468787000	-1.090679000	0.767591000
N	-1.468799000	1.091747000	0.766961000
N	-2.740819000	1.008692000	0.262249000
C	2.624497000	0.879935000	-1.357347000
C	3.652738000	-1.454195000	1.169093000
C	-2.624384000	-0.879788000	-1.357578000
C	2.934894000	-1.823286000	2.300596000
H	3.347648000	-2.223628000	3.214869000
C	1.023190000	2.574779000	-1.325367000
H	0.000663000	2.851808000	-1.088448000
C	-1.023029000	-2.574577000	-1.325131000
H	-0.000600000	-2.851607000	-1.087779000
C	1.582673000	-1.583256000	2.017786000
C	2.944507000	-0.583130000	-1.116125000
H	2.328276000	-1.215270000	-1.768456000
C	-2.944602000	0.583250000	-1.116389000
H	-3.985294000	0.781569000	-1.370790000
H	-2.328495000	1.215457000	-1.768768000
C	3.584868000	1.763548000	-1.837396000
H	4.594308000	1.415328000	-2.028229000
C	1.930228000	3.509326000	-1.811251000
H	1.617683000	4.534339000	-1.975452000
C	3.234859000	3.095270000	-2.073370000
H	3.972319000	3.795996000	-2.451486000
C	-1.582821000	1.583542000	2.017474000
C	-1.929803000	-3.509088000	-1.811563000
H	-1.617139000	-4.534063000	-1.975776000
C	-3.652990000	1.453050000	1.169250000
C	-3.584505000	-1.763379000	-1.838180000
H	-4.593881000	-1.415175000	-2.029385000
C	0.380830000	-1.813538000	2.876119000
H	-0.519242000	-1.369500000	2.438799000
H	0.199578000	-2.885765000	3.008628000
H	0.526358000	-1.383087000	3.871346000
C	-3.234336000	-3.095046000	-2.074208000
H	-3.971595000	-3.795746000	-2.452761000
C	-0.380945000	1.814631000	2.875542000
H	-0.200326000	2.886984000	3.007905000
H	-0.526010000	1.384185000	3.870834000
H	0.519321000	1.371130000	2.438074000
C	-2.935175000	1.822232000	2.300751000
H	-3.348047000	2.221856000	3.215286000
C	-5.119767000	1.505583000	0.896454000
H	-5.521043000	0.518410000	0.641643000
H	-5.644512000	1.859416000	1.785720000
H	-5.354569000	2.194594000	0.076557000
H	3.985159000	-0.781619000	-1.370547000
C	5.119397000	-1.507903000	0.895878000
H	5.644133000	-1.861887000	1.785088000
H	5.353434000	-2.197325000	0.076106000
H	5.521342000	-0.521108000	0.640682000

Optimized cartesian coordinates for NBO Analysis

5-Qu

Zn	0.052186000	0.076396000	-0.539759000
N	-0.159529000	-1.477360000	0.924318000
N	0.628321000	-2.586141000	0.848565000
N	2.297640000	-0.574978000	-0.606937000
N	0.118819000	1.790301000	0.748719000
N	-0.832507000	2.755180000	0.613846000
N	-2.243966000	0.473867000	-0.747889000
N	0.067222000	0.018286000	-3.211139000
O	0.256288000	1.075421000	-2.547012000
O	-0.117549000	-1.001708000	-2.490193000
C	-0.752335000	-1.513514000	2.128982000
C	-0.328628000	-2.661414000	2.824269000
H	-0.631945000	-2.974237000	3.813130000
C	0.557363000	-3.325405000	1.985577000
C	-1.695606000	-0.449193000	2.588452000
H	-2.589716000	-0.901354000	3.030466000
H	-2.003201000	0.195309000	1.764976000
H	-1.229057000	0.179138000	3.355534000
C	1.416675000	-2.829086000	-0.349483000
H	0.761158000	-2.740185000	-1.219570000
H	1.781770000	-3.853514000	-0.304270000
C	2.579376000	-1.866550000	-0.473718000
C	3.901042000	-2.366153000	-0.444298000
H	4.062325000	-3.432504000	-0.331307000
C	4.952617000	-1.488149000	-0.554780000
H	5.980350000	-1.839069000	-0.530344000
C	5.732240000	0.856193000	-0.815482000
H	6.762531000	0.512801000	-0.792294000
C	5.431555000	2.191805000	-0.952662000
H	6.226597000	2.926054000	-1.039933000
C	4.079766000	2.614760000	-0.982425000
H	3.852546000	3.671081000	-1.091904000
C	3.049632000	1.706293000	-0.874485000
H	2.020374000	2.038292000	-0.892556000
C	3.328849000	0.323650000	-0.726006000
C	4.694142000	-0.105158000	-0.699313000
C	0.665657000	1.960519000	1.963707000
C	0.043346000	3.044905000	2.607926000
H	0.262634000	3.432354000	3.592481000
C	-0.914881000	3.530263000	1.725076000
C	1.779711000	1.094342000	2.455058000
H	1.759681000	1.036555000	3.547114000
H	2.751634000	1.505603000	2.157180000
H	1.705761000	0.083879000	2.048367000
C	-1.618283000	2.824539000	-0.608500000
H	-0.934928000	2.745970000	-1.457504000
H	-2.091833000	3.804413000	-0.641353000
C	-2.666767000	1.733028000	-0.683040000
C	-4.034640000	2.088013000	-0.677178000
H	-4.311701000	3.134775000	-0.620796000
C	-4.984399000	1.096908000	-0.735187000
H	-6.044332000	1.334691000	-0.723558000
C	-4.577353000	-0.255132000	-0.810957000
C	-5.509014000	-1.324209000	-0.877519000
H	-6.569514000	-1.089137000	-0.865424000
C	-5.070117000	-2.625557000	-0.957206000
H	-5.783170000	-3.442794000	-1.007611000
C	-3.681452000	-2.903064000	-0.980017000
H	-3.343189000	-3.932635000	-1.050748000
C	-2.752387000	-1.887782000	-0.916466000
H	-1.696674000	-2.113708000	-0.938956000
C	-3.173411000	-0.536266000	-0.823561000
C	-1.885559000	4.654618000	1.860280000
H	-1.760750000	5.128907000	2.836465000
H	-1.730264000	5.414928000	1.085947000
H	-2.919367000	4.300175000	1.777637000
C	1.323281000	-4.590163000	2.183449000
H	1.059436000	-5.341783000	1.430283000
H	2.403607000	-4.416961000	2.118980000

H	1.099227000	-5.000954000	3.170644000

5-Pz

Zn	-0.007349000	0.039372000	-0.772268000
O	0.456962000	1.033480000	-2.717447000
O	-0.515269000	-0.846265000	-2.758479000
N	0.922798000	1.414593000	0.629161000
N	2.277507000	1.597451000	0.604772000
N	3.087506000	-0.284794000	-0.640731000
N	1.941248000	-0.971185000	-0.918014000
N	-1.988302000	0.999638000	-0.843002000
N	-3.107985000	0.259942000	-0.595386000
N	-2.217497000	-1.622013000	0.595891000
N	-0.868518000	-1.400704000	0.608505000
N	-0.034039000	0.112163000	-3.430276000
C	0.511561000	1.838519000	1.834393000
C	1.616561000	2.297456000	2.577759000
H	1.603424000	2.707437000	3.577344000
C	2.733025000	2.126235000	1.772964000
C	-0.925566000	1.809540000	2.244144000
H	-1.459613000	2.688026000	1.864197000
H	-1.000596000	1.816069000	3.335069000
H	-1.432838000	0.921189000	1.863028000
C	4.170806000	2.426394000	2.028827000
H	4.773276000	1.511238000	2.040515000
H	4.272335000	2.915779000	3.000177000
H	4.585367000	3.091039000	1.262561000
C	3.026972000	1.160352000	-0.554134000
H	2.538889000	1.544269000	-1.450995000
H	4.037908000	1.553039000	-0.486114000
C	2.286530000	-2.261696000	-0.992614000
C	3.672351000	-2.396380000	-0.765175000
H	4.249144000	-3.310147000	-0.772106000
C	4.161420000	-1.117599000	-0.542978000
C	1.273779000	-3.330443000	-1.249773000
H	0.796986000	-3.650329000	-0.316025000
H	1.752902000	-4.204480000	-1.700385000
H	0.490411000	-2.970007000	-1.921400000
C	5.549997000	-0.642070000	-0.275533000
H	5.886019000	0.068252000	-1.039755000
H	6.231706000	-1.495762000	-0.278511000
H	5.625613000	-0.146042000	0.698418000
C	-2.382889000	2.277507000	-0.871782000
C	-2.990528000	-1.183585000	-0.546511000
H	-2.493724000	-1.525155000	-1.455557000
H	-3.985674000	-1.615925000	-0.485654000
C	-0.429118000	-1.848943000	1.794431000
C	-1.511049000	-2.361814000	2.537531000
H	-1.472457000	-2.800810000	3.524065000
C	-2.642974000	-2.198209000	1.753302000
C	1.011824000	-1.795892000	2.189554000
H	1.490402000	-0.878714000	1.842009000
H	1.566117000	-2.641945000	1.767806000
H	1.099404000	-1.845220000	3.278428000
C	-4.068870000	-2.543439000	2.020836000
H	-4.694608000	-1.645267000	2.067783000
H	-4.142663000	-3.062977000	2.978953000
H	-4.477987000	-3.196576000	1.241865000
C	-4.212028000	1.047563000	-0.463686000
C	-3.772173000	2.351291000	-0.637784000
C	-5.579272000	0.511424000	-0.200463000
H	-6.293118000	1.338077000	-0.175318000
H	-5.893720000	-0.190001000	-0.981843000
H	-5.628236000	-0.013517000	0.760013000
C	-1.420557000	3.390404000	-1.137126000
H	-0.433873000	3.164126000	-0.725664000
H	-1.304610000	3.556782000	-2.214718000
H	-1.785066000	4.320590000	-0.691705000
H	-4.382035000	3.242757000	-0.604563000

5-Py

Zn	0.000054000	-0.000134000	-0.664495000
O	0.429648000	0.966294000	-2.652032000
N	0.928909000	1.503960000	0.583262000
N	2.282508000	1.662043000	0.497344000
N	1.975227000	-0.983376000	-0.775459000
N	-0.000218000	-0.000103000	-3.344299000
C	0.586325000	1.886533000	1.826639000
C	1.733571000	2.295947000	2.528465000
H	1.780725000	2.666769000	3.542297000
C	2.805244000	2.132192000	1.658147000
C	-0.828900000	1.845227000	2.307584000
H	-1.316352000	0.906432000	2.030885000
H	-1.419515000	2.664886000	1.882697000
H	-0.853141000	1.940636000	3.396515000
C	4.263060000	2.383967000	1.849207000
H	4.847082000	1.466178000	1.715642000
H	4.439087000	2.759822000	2.859800000
H	4.639359000	3.126275000	1.135667000
C	2.991455000	1.230871000	-0.698960000
H	3.976607000	1.695374000	-0.692253000
H	2.442350000	1.600598000	-1.568990000
C	3.121397000	-0.275872000	-0.776448000
C	4.364666000	-0.898375000	-0.863471000
H	5.268234000	-0.298443000	-0.855737000
C	4.420325000	-2.288955000	-0.961686000
H	5.378175000	-2.795108000	-1.030661000
C	3.230906000	-3.015609000	-0.966760000
H	3.227508000	-4.097379000	-1.042385000
C	2.029026000	-2.320999000	-0.869326000
H	1.075221000	-2.838439000	-0.858380000
O	-0.429931000	-0.966565000	-2.652049000
N	-0.928248000	-1.503380000	0.584516000
N	-2.281815000	-1.661965000	0.498890000
N	-1.975911000	0.982166000	-0.776232000
C	-0.585534000	-1.884137000	1.828430000
C	-1.732657000	-2.292775000	2.530895000
H	-1.779638000	-2.662094000	3.545284000
C	-2.804412000	-2.130513000	1.660395000
C	0.829638000	-1.841843000	2.309429000
H	1.315534000	-0.901462000	2.035284000
H	1.421621000	-2.659322000	1.882308000
H	0.854012000	-1.940122000	3.398092000
C	-2.990885000	-1.232539000	-0.697970000
H	-2.441354000	-1.602735000	-1.567513000
C	-3.121701000	0.274061000	-0.776699000
C	-2.030401000	2.319708000	-0.870669000
C	-4.365309000	0.895865000	-0.863830000
C	-3.232672000	3.013644000	-0.968220000
C	-4.421697000	2.286370000	-0.962681000
H	-5.268594000	0.295520000	-0.855667000
H	-5.379827000	2.791979000	-1.031785000
H	-3.229882000	4.095379000	-1.044322000
H	-1.076860000	2.837653000	-0.860100000
C	-4.262166000	-2.382246000	1.851882000
H	-4.438065000	-2.756977000	2.862916000
H	-4.846314000	-1.464683000	1.717324000
H	-4.638451000	-3.125425000	1.139237000
H	-3.975730000	-1.697678000	-0.690934000

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