Data Article

Chemical and structural data of (1,2,3-triazol-4-yl)pyridine-containing coordination compounds

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A R T I C L E  I N F O

Article history:
Received 31 March 2018
Accepted 24 August 2018
Available online 30 August 2018

A B S T R A C T

The data presented in this paper are related to the research article entitled “Novel dichloro(bis{2-[1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl-κN3]pyridine-κN})metal(II) coordination compounds of seven transition metals (Mn, Fe, Co, Ni, Cu, Zn and Cd)” (Conradie et al., 2018) [1]. This paper presents characterization and structural data of the 2-{1-(4-methyl-phenyl)-1H-1,2,3-triazol-1-yl}pyridine ligand (L2) (Tawfiq et al., 2014) [2] as well as seven dichloro(bis{2-[1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl-κN3]pyridine-κN})metal (II) coordination compounds, [M(L2)2Cl2], all containing the same ligand but coordinated to different metal ions. The data illustrate the shift in IR, UV/VIS, and NMR (for diamagnetic complexes) peaks when L is coordinated to the metals, as well as the influence of the different metals on the peak positions. Solid state structural data is presented for M = Ni and Zn, while density functional theory calculated energies, structures and optimized coordinates

DOI of original article: https://doi.org/10.1016/j.poly.2018.03.026
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https://doi.org/10.1016/j.dib.2018.08.125
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are provided for the lowest energy cis and trans conformations for L² as well as [M(L²)₂Cl₂] with M = Mn, Fe, Co, Ni, Cu, Zn and Cd.

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Specifications table

| Subject area                  | Chemistry                     |
|-------------------------------|-------------------------------|
| More specific subject area    | Coordination compounds        |
| Type of data                  | Table, text file, graph, figure |
| How data was acquired         | IR on Thermo-Nicolet FT-IR Spectrometer (AVATAR 320). Mass spectra on WATERS LCT premier mass spectrometer. Magnetic susceptibility with a Gouy magnetic susceptibility balance. X-ray structure on Rigaku SPIDER RAXIS image plate detector and Rigaku AFC12 goniometer equipped with an enhanced sensitivity (HG) Saturn724+ detector mounted at the window of an FR-E+ SuperBright molybdenum rotating anode generator with HF Varimax optics (100 μm focus). NMR on an ECS-400 MHz, JEOL multi nuclear FT spectrometer. UV–vis spectra on a PerkinElmer Lambda 40 UV/Vis spectrometer. Electronic structure calculations using the Gaussian 09 package [3]. |
| Data format                   | Raw, calculated, analyzed. |
| Experimental factors          | –                             |
| Experimental features         | –                             |
| Data source location          | Division of Chemistry and Environmental Science, Manchester Metropolitan University, Manchester, M1 5GD, UK. Department of Chemistry, University of the Free State, Nelson Mandela Street, Bloemfontein, South Africa (DFT). Crystallographic data is held at the NCS University of Southampton. University of Sheffield (MS). |
| Data accessibility            | Data is with article.         |
| Related research article      | J. Conradie, M.M. Conradie, K.M. Tawfqi, M.J. Al-Jeboori, S.J. Coles C. Wilson, J.H. Potgieter, Novel dichloro(bis[2-{1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl-κN3]pyridine-κN})metal(II) coordination compounds of seven transition metals (Mn, Fe, Co, Ni, Cu, Zn and Cd), Polyhedron, 2018, 151 (2018) 243-254. http://dx.doi.org/10.1016/j.poly.2018.03.026. |

Value of the data

- This data would be valuable for the further characterization and structural studies of (1,2,3-triazol-4-yl)pyridine-containing coordination compounds.
- This data provide NMR, IR, UV/VIS and magnetic moment data for (1,2,3-triazol-4-yl)pyridine-containing coordination compounds.
- MS fragmentation data for 2-{1-(4-methyl-phenyl)-1H-1,2,3-triazol-1-yl}pyridine ligand and seven dichloro(bis[2-{1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl-κN3]pyridine-κN})metal(II) coordination compounds.
- This data provide solid state structures for two (1,2,3-triazol-4-yl)pyridine-containing coordination compounds.
- This data provide DFT optimized structures and coordinates for the lowest energy cis and trans isomers of the 2-{1-(4-methyl-phenyl)-1H-1,2,3-triazol-1-yl}pyridine ligand and seven (1,2,3-triazol-4-yl)pyridine-containing coordination compounds.
1. Data

1.1. Structural data

The \([\text{M}(L^2)\text{Cl}_2]\) compounds with \(L^2 = 2-(1-(4\text{-methyl-phenyl})-1\text{H}-1,2,3\text{-triazol-1-yl})\text{pyridine}\), all have the same chemical formula \(\text{C}_{28}\text{H}_{24}\text{Cl}_2\text{N}_8\text{M}\) with \(\text{M} = \text{Mn, Fe, Co, Ni, Cu, Zn and Cd}\). The X-ray solid state crystal structure of \([\text{Ni}(L^2)\text{Cl}_2]\) in Fig. 1 shows the coordination environment of the nickel metal ion with two \(2-(1-(4\text{-methyl-phenyl})-1\text{H}-1,2,3\text{-triazol-1-yl})\text{pyridine}\) ligands \(L\) and two chlorides. A list of bond lengths and angles for the ligand \(L^2\) (that crystallized together with \([\text{Zn}(L^2)\text{Cl}_2]\), \([\text{Zn}(L^2)\text{Cl}_2]\) and \([\text{Ni}(L^2)\text{Cl}_2]\) are listed in Table 1. The obtained geometrical parameters are in the

![Fig. 1. View of \([\text{Ni}(L^2)\text{Cl}_2]\) showing the coordination environment Ni with two \(2-(1-(4\text{-methyl-phenyl})-1\text{H}-1,2,3\text{-triazol-1-yl})\text{pyridine}\) pyridine ligands \(L^2\) and two chlorides, as well as the atom labelling scheme used in Table 1.](image)

| \(\text{Ni}(L^2)\text{Cl}_2\) | \(\text{Zn}(L^2)\text{Cl}_2\) | \(L^2\) (co-crystallize with \([\text{Zn}(L^2)\text{Cl}_2]\)) |
|-----------------|-----------------|------------------|
| \(\text{Ni}1\)–\(\text{N}1\) | 2.1015(19) | \(\text{Zn}1\)–\(\text{N}1\) | 2.144(3) |
| \(\text{Ni}1\)–\(\text{N}8\) | 2.0739(19) | \(\text{Zn}1\)–\(\text{N}8\) | 2.191(4) |
| \(\text{Ni}1\)–\(\text{Cl}1\) | 2.4123(6) | \(\text{Zn}1\)–\(\text{Cl}1\) | 2.4615(14) |
| \(\text{N}1\)–\(\text{C}2\) | 1.341(3) | \(\text{N}1\)–\(\text{C}2\) | 1.341(5) |
| \(\text{N}1\)–\(\text{C}6\) | 1.352(3) | \(\text{N}1\)–\(\text{C}6\) | 1.346(5) |
| \(\text{N}8\)–\(\text{N}9\) | 1.316(3) | \(\text{N}8\)–\(\text{N}9\) | 1.316(5) |
| \(\text{N}9\)–\(\text{N}10\) | 1.352(3) | \(\text{N}9\)–\(\text{N}10\) | 1.364(5) |
| \(\text{N}10\)–\(\text{C}11\) | 1.353(3) | \(\text{N}10\)–\(\text{C}11\) | 1.352(5) |
| \(\text{N}10\)–\(\text{C}12\) | 1.428(3) | \(\text{N}10\)–\(\text{C}12\) | 1.434(5) |
| \(\text{C}2\)–\(\text{C}3\) | 1.383(3) | \(\text{C}2\)–\(\text{C}3\) | 1.385(6) |
| \(\text{C}2\)–\(\text{H}2\) | 0.9300 | \(\text{C}2\)–\(\text{H}2\) | 0.930 |
| \(\text{C}3\)–\(\text{C}4\) | 1.385(3) | \(\text{C}3\)–\(\text{C}4\) | 1.381(6) |
| \(\text{C}3\)–\(\text{H}3\) | 0.9300 | \(\text{C}3\)–\(\text{H}3\) | 0.930 |
| \(\text{C}4\)–\(\text{C}5\) | 1.381(3) | \(\text{C}4\)–\(\text{C}5\) | 1.378(6) |
| \(\text{C}4\)–\(\text{H}4\) | 0.9300 | \(\text{C}4\)–\(\text{H}4\) | 0.930 |
| \(\text{C}5\)–\(\text{C}6\) | 1.388(3) | \(\text{C}5\)–\(\text{C}6\) | 1.403(6) |
| [Ni(L²)₂Cl₂]       | [Zn(L²)₂Cl₂]       | L² (co-crystallize with [Zn(L²)₂Cl₂]) |
|--------------------|--------------------|--------------------------------------|
| C5–H5               | 0.9300             | C5–H5                               |
| C6–C7               | 1.460(3)           | C6–C7                               |
| C7–C11              | 1.363(3)           | C7–C11                             |
| C11–H11             | 0.9300             | C11–H11                             |
| C12–C13             | 1.383(3)           | C12–C13                             |
| C12–C17             | 1.384(3)           | C12–C17                             |
| C13–C14             | 1.386(3)           | C13–C14                             |
| C13–H13             | 0.9300             | C13–H13                             |
| C14–C15             | 1.385(4)           | C14–C15                             |
| C14–H14             | 0.9300             | C14–H14                             |
| C15–C16             | 1.389(4)           | C15–C16                             |
| C15–C18             | 1.508(3)           | C15–C18                             |
| C16–C17             | 1.379(4)           | C16–C17                             |
| C16–H16             | 0.9300             | C16–H16                             |
| C17–H17             | 0.9300             | C17–H17                             |
| C18–H18A            | 0.9600             | C18–H18A                            |
| C18–H18B            | 0.9600             | C18–H18B                            |
| C18–H18C            | 0.9600             | C18–H18C                            |
| N8i–N11–N8i–N11     | 180.0              | N1–Zn1–N1i                         |
| N8–N11–N1i–N1i      | 100.4(8)           | N1–Zn1–N8i                            |
| N8–N11–N1i–N1i–N1i  | 79.59(8)           | N1i–Zn1–N8i–N8                      |
| N1–N11–N1–N1        | 180.0              | N8–Zn1–N8                          |
| N8i–N11–C1i–C1i     | 90.20(6)           | N1–Zn1–C1i                           |
| N8–Ni–C1i–C1i       | 89.80(6)           | N1i–Zn1–C1i                          |
| N1–N11–C1i–C1i      | 89.38(6)           | N8i–Zn1–C1i                          |
| N1–N11–C1i–C1i      | 90.62(6)           | N8–Zn1–C1i                          |
| N8i–N11–C1i–C1i     | 89.80(6)           | N1–Zn1–C1i                          |
| N8–N11–C1i–C1i      | 90.20(6)           | N1–Zn1–C1i                          |
| N1–N11–C1i–C1i      | 90.62(6)           | N8–Zn1–C1i                          |
| N1–N11–C1i–C1i      | 89.38(6)           | N8–Zn1–C1i                          |
| C11–N11–C1i–C1i     | 180.00(2)          | C11–Zn1–C1i                           |
| C2–N1–N1–C1i        | 127.46(16)         | C2–N1–Zn1                           |
| C6–N1–N1–C1i        | 114.55(15)         | C6–N1–Zn1                           |
| N8–N11–N1i–N1i–N1i  | 137.61(16)         | N9–N8–Zn1                           |
| C7–N8–N11–C1i–C1i   | 112.60(15)         | C7–N8–Zn1                           |
| C2–C3–C4            | 119.2(2)           | C4–C3–C2                           |
| C2–C3–H3            | 120.4              | C4–C3–H3                           |
| C2–N1–C6            | 117.9(2)           | C2–N1–C6                           |
| C3–C2–H2            | 118.8              | C3–C2–H2                           |
| C3–C4–H4            | 120.4              | C3–C4–H4                           |
| C4–C3–H3            | 120.4              | C4–C3–H3                           |
| C5–C5–C6            | 118.4(2)           | C5–C5–C6                           |
| C5–C4–C3            | 120.8              | C5–C4–C3                           |
| C5–C4–H4            | 120.4              | C5–C4–H4                           |
| C6–C6–C7            | 123.0(2)           | C5–C6–C7                           |
| C6–C5–H5            | 120.8              | C6–C5–H5                           |
| C7–C11–H11          | 127.7              | C7–C11–H11                          |
| C11–C7–C6           | 132.6(2)           | C11–C7–C6                          |
| C11–N10–C12         | 127.9(2)           | C11–N10–C12                         |
| C12–C13–C14         | 118.7(2)           | C12–C13–C14                         |
| C12–C13–H13         | 120.6              | C12–C13–H13                         |
| C12–C17–H17         | 120.3              | C12–C17–H17                         |
| C13–C12–C17         | 120.6(2)           | C13–C12–C17                         |
| C13–C12–N10         | 119.2(2)           | C13–C12–N10                         |
| C13–C14–H14         | 119                | C13–C14–H14                         |
| C14–C13–C13         | 120.6              | C14–C13–C13                         |
| C14–C15–C16         | 117.8(2)           | C14–C15–C16                         |
| C14–C15–C18         | 121.4(2)           | C14–C15–C18                         |
| C15–C14–C13         | 121.9(2)           | C15–C14–C13                         |

**Table 1 (continued)**
same range as reported for related complexes \([M(L_1)_2Cl_2]\) with \(L_1 = 2-(1-(4\text{-methoxyphenyl})-1H-1,2,3\text{-triazol-1-yl})\text{pyridine}\) and \(M = \text{Co and Ni}\) [4] and \([\text{Ni}(L)_2\text{Br}_2]\) with \(L = 1-(\text{cyclohexyl})-4-(2\text{-pyridyl})-1,2,3\text{-triazole}\) [5] (Fig. 2). The obtained geometrical parameters for ligand \(L_2\), that crystallized together with \([\text{Zn}(L_2)_2\text{Cl}_2]\), are in the same range as reported for ligand \(L_2\), isolated alone [2].

1.2. Spectroscopic data

The UV/vis spectra of \(L_2^\text{2}\) and the \([M(L_2)_2\text{Cl}_2]\) compounds are shown in Fig. 3 and characteristic data is summarized in Table 2. The IR spectra of \(L_2^\text{2}\) and the \([M(L_2)_2\text{Cl}_2]\) compounds are shown in
Fig. 3. UV–vis spectra of L² and [M(L²)₂Cl₂] in DMSO solutions.
Table 2
UV–vis spectral data and assignments of \(L^2\) and [M(\(L^2\))\(_2\)Cl\(_2\)] in DMSO solutions.

| Compound       | Band Position | \(\lambda_{\text{max}}\) nm | Wave number (cm\(^{-1}\)) | Extinction coefficient \(\varepsilon_{\text{max}}\) (dm\(^3\)/mol\(^{-1}\) cm\(^{-1}\)) | Assignment |
|----------------|---------------|-----------------------------|---------------------------|------------------------------------------------------------------------------------|------------|
| \(L^2\)        | 258, 287      | 38759, 34843                | 19740, 17200 (4 \times 10^{-5} M) | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |
| [Mn(\(L^2\))\(_2\)Cl\(_2\)] | 280, 284      | 35714, 35211                | 3165, 3124 (1 \times 10^{-4} M) | \(^5\)A\(_{1g}\) \(\rightarrow^4\)T\(_{1g}\) (4G)                                  |
| [Fe(\(L^2\))\(_2\)Cl\(_2\)]   | 682           | 14662                       | 13                          | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |
| [Co(\(L^2\))\(_2\)Cl\(_2\)]   | 284           | 35211                       | 29513 (1.2 \times 10^{-4} M) | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\) CT                    |
| [Ni(\(L^2\))\(_2\)Cl\(_2\)]   | 280, 286, 298 | 35714, 34965, 33557         | 3672, 3347, 3240 (1 \times 10^{-3} M) | \(^4\)T\(_{1g}\) \(\rightarrow^4\)T\(_{1g}\) \(^{(4G)}\) \(\rightarrow^4\)A\(_{2g}\) (F) |
| [Cu(\(L^2\))\(_2\)Cl\(_2\)]   | 615           | 1620                        | 56                          | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |
| [Zn(\(L^2\))\(_2\)Cl\(_2\)]   | 677           | 14970                       | 89                          | \(^4\)T\(_{1g}\) \(\rightarrow^4\)T\(_{1g}\) (F) \(\rightarrow^4\)A\(_{2g}\) (F)  |
| [Cd(\(L^2\))\(_2\)Cl\(_2\)]   | 278, 282, 300 | 35971, 35460, 33333         | 3602, 3653, 3656 (1 \times 10^{-3} M) | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |
| \(\[\text{Zn}(L^2)\text{Cl}_2]\) | 408           | 24509                       | 20                          | \(^3\)A\(_{2g}\) \(\rightarrow^3\)T\(_{1g}\) \(^{(p)}\) \(\rightarrow^3\)A\(_{2g}\) (F) |
| \(\[\text{Cd}(L^2)\text{Cl}_2]\) | 668           | 14970                       | 8                           | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |
| \(\[\text{Zn}(L^2)\text{Cl}_2]\) | 279, 284      | 35842,35211                 | 3507, 3603 (1 \times 10^{-3} M) | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |
| \(\[\text{Zn}(L^2)\text{Cl}_2]\) | 310           | 32258                       | 3696                        | \(^2\)B\(_{1g}\) \(\rightarrow^2\)B\(_{2g}\) g                                       |
| \(\[\text{Cd}(L^2)\text{Cl}_2]\) | 259, 287      | 38461, 35843                | 3220, 3067 (4 \times 10^{-5} M) | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |
| \(\[\text{Ni}(L^2)\text{Cl}_2]\) | 260, 287      | 38759, 34843                | 28005, 25695 (4 \times 10^{-5} M) | Intra-ligand \(\pi \rightarrow \pi^*\), \(n \rightarrow \pi^*\)                      |

Fig. 4. Selected characteristic IR bands of \(L^2\) and the [M(\(L^2\))\(_2\)Cl\(_2\)] compounds are listed and compared in reference [1]. The ionization data of the TOFMS-ES (+) mass spectra of \(L^2\) and the [M \((\text{L}^2)\text{Cl}_2\) ] compounds given are summarized in Table 3. The TOFMS-ES (+) mass spectra are provided in the Supplementary material. The \(^1\)H and \(^{13}\)C NMR spectra of \(L^2\) and the diamagnetic [M(\(L^2\))\(_2\)Cl\(_2\)] compounds (M = Zn or Cd) are shown in Fig. 5, while data to determine the spin state (amount of unpaired d-electrons) for the paramagnetic [M(\(L^2\))\(_2\)Cl\(_2\)] compounds (M = Mn, Fe, Co, Ni and Cu) are summarized in Table 4. More NMR spectra are provided in the Supplementary material.

1.3. DFT data

Both \(L^2\) and the [M(\(L^2\))\(_2\)Cl\(_2\)] complexes may have different stereoisomers. The density functional theory calculated lowest energy \(\text{cis}\) and \(\text{trans}\) isomers, as well as the relative energies of the isomers, are shown in Fig. 6. The data associated with the geometry of the optimized geometries (Cartesian coordinates) of the compounds shown are provided in the Supplementary material.
Fig. 4. FT-IR absorption spectra of L² and [M(L²)₂Cl₂] compounds.
2. Experimental design, materials, and methods

Density functional theory (DFT) calculations were performed in the gas phase on the neutral compounds, using the B3LYP functional and the triple-ζ basis set 6–311 G(d,p) on all atoms except for Cd where the Stuttgart/Dresden (SDD) pseudopotential was used to describe the metal electronic core, while the metal valence electrons were described using the def2-TZVPP basis set [7]. The Gaussian 09 package [3] were used to optimize the compounds. The multiplicity used for L² and the [M(L²)₂Cl₂] compounds is singlet ([L²] and [Zn(L²)₂Cl₂] and [Cd(L²)₂Cl₂]), doublet ([Cu(L²)₂Cl₂]), triplet ([Ni(L²)₂Cl₂]), quartet ([Co(L²)₂Cl₂]), quintet ([Fe(L²)₂Cl₂]) and sextet ([Mn(L²)₂Cl₂]).

| L² or coordination compound | Formula | MW | Fragmentation, m/z (%) |
|-----------------------------|---------|----|------------------------|
| L²                          | C₁₄H₁₂N₄ | 236.3 | 209 [M-Ν₂]⁺ 22%, 237 [M+H]⁺ 100%, 259 [M+Na]⁺ 7%, 495 [M+Na]⁺ 18% (consistent with literature [6]) |
| [Mn(L²)₂Cl₂]               | C₂₈H₂₄Cl₂MnN₈ | 598.4 | 562.1 [M-Cl]⁺ 90%, calculated for ([C₂₈H₂₄N₈MnCl])⁺, 237.1 [L²]⁺ 70%, calculated for ([C₁₄H₁₂N₂])⁺, 209.1 [L²-N₂]⁺ calculated for ([C₁₄H₁₂N₂])⁺ 100% |
| [Fe(L²)₂Cl₂]               | C₂₈H₂₄Cl₂FeN₈ | 599.3 | 563.1 [M-Cl]⁺ 90%, calculated for ([C₂₈H₂₄N₈FeCl])⁺, 237.1 [L²]⁺ 70%, calculated for ([C₁₄H₁₂N₂])⁺, 209.1 [L²-N₂]⁺ calculated for ([C₁₄H₁₂N₂])⁺ 100% |
| [Co(L²)₂Cl₂]               | C₂₈H₂₄Cl₂CoN₈ | 602.4 | 566.1 [M-Cl]⁺ 40%, calculated for ([C₂₈H₂₄N₈CoCl])⁺, 531 [M-Cl]⁺ 5%, calculated for ([C₂₈H₂₄CoN₈])⁺ |
| [Ni(L²)₂Cl₂]               | C₂₈H₂₄Cl₂NiN₈ | 602.1 | 565.1 [M-Cl]⁺ 40%, calculated for ([C₂₈H₂₄N₈NiCl])⁺, 265 [M-Cl-L²+N₂]⁺ 50%, calculated for ([C₁₄H₁₀N₂Ni])⁺, 209.1 [L²-N₂]⁺ (10%), calculated for ([C₁₄H₁₂N₂])⁺ |
| [Cu(L²)₂Cl₂]               | C₂₈H₂₄Cl₂CuN₈ | 607.0 | 594.1 [M-Cl]⁺ 45%, calculated for ([C₂₈H₂₄N₈CuCl])⁺, 535.1 [Cu (L²)]⁺ 30%, calculated for ([C₂₈H₂₄CuN₈])⁺ 30%, 358 [CuL²]⁺, calculated for ([C₁₄H₁₂N₄CuCH₃COO⁻])⁺ 100%, 237 [L²]⁺ calculated for ([C₁₄H₁₂N₄])⁺ 40%, 209 [L²-N₂]⁺ 15%, calculated for ([C₁₄H₁₂N₂])⁺ |
| [Zn(L²)₂Cl₂]               | C₂₈H₂₄Cl₂ZnN₈ | 608.8 | 571.2 [M-Cl]⁺ (80%), calculated for ([C₂₈H₂₄N₈ZnCl])⁺, 33 [M-Cl-L²]⁺ 5%, 237.1 [L²]⁺, calculated for ([C₁₄H₁₂N₂Zn])⁺ 30%, 209.1 [L²-N₂]⁺ calculated for ([C₁₄H₁₂N₂])⁺ 90% |
| [Cd(L²)₂Cl₂]               | C₂₈H₂₄Cl₂CdN₈ | 655.9 | 621.2 [M-Cl]⁺ (100%), calculated for ([C₂₈H₂₄N₈CdCl])⁺, 237.1 [L²]⁺ (20%), calculated for ([C₁₄H₁₂N₂CdCl⁺), 209.1 [L²-N₂]⁺ calculated for ([C₁₄H₁₂N₂])⁺ 50% |
Fig. 5. $^1$H and $^{13}$C NMR spectrum of L$^2$ in CD$_2$Cl$_2$, [Zn(L$^2$)$_2$Cl$_2$] and [Cd(L$^2$)$_2$Cl$_2$] in DMSO-d$_6$.

Table 4
Data for determination of the spin state of paramagnetic [M(L$^2$)$_2$Cl$_2$] complexes, $\mu_{\text{eff}}$ = effective magnetic moment.

| Compound     | amount of d electrons | $\mu_{\text{eff}}$ measured (B.M) | $\mu_{\text{eff}}$ calculated (B.M) | $S$  |
|--------------|-----------------------|-----------------------------------|-------------------------------------|------|
| [Mn(L$^2$)$_2$Cl$_2$] | 5                     | 5.62                              | 5.92                                | 5/2  |
| [Fe(L$^2$)$_2$Cl$_2$] | 6                     | 5.26                              | 4.90                                | 2    |
| [Co(L$^2$)$_2$Cl$_2$] | 7                     | 3.98                              | 3.87                                | 3/2  |
| [Ni(L$^2$)$_2$Cl$_2$] | 8                     | 3.00                              | 2.83                                | 1    |
| [Cu L$^2$)$_2$Cl$_2$] | 9                     | 1.70                              | 1.73                                | 1/2  |
Fig. 6. Density functional theory calculated optimized geometries of the lowest energy cis and trans isomers of L2 and the [M(L2)2Cl2]. The relative energies of the isomers, ΔE in eV, is also shown; the energy of the lowest energy isomer is indicated as 0 eV.

Acknowledgements

The National Mass Spectroscopy Centre at the University of Wales, Swansea is thanked for supplying the mass spectrometry data. XRD data and structures were supplied by the National Crystallography Service at the University of Southampton. KT expresses his gratitude to the Iraqi Government for financial support to conduct the research reported in the UK. This work has received support from the South African National Research Foundation (Grant numbers 113327 and 96111) and the Central Research Fund of the University of the Free State, Bloemfontein, South Africa. The High Performance Computing facility of the University of the Free State and the Centre for High Performance Computing CHPC of South Africa are gratefully acknowledged for computer time.

Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.08.125.
Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at https://dx.doi.org/10.1016/j.dib.2018.08.125. CCDC 1813109 and 1813110 contains the supplementary crystallographic data for the crystals of this study. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

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