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Supporting information for article:

Structural characterization of a hybrid terpyridine–pyrazine ligand and its one-dimensional Zn^{II} coordination polymer: a computational approach to *conventional* and *nonconventional* intermolecular interactions

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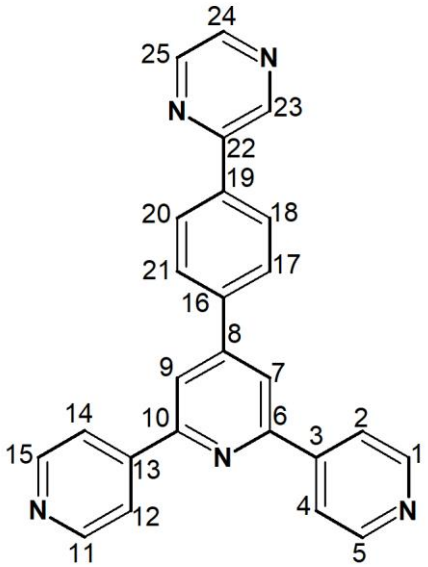
Sup. 1 (NMR spectra)

The NMR spectra of L2 (performed through Proton Noise Decoupled (PND), Distortionless Enhancement by Polarization Transfer (DEPT), Correlation Spectroscopy (COSY), Heteronuclear Single Quantum Coherence (HSQC) and Heteronuclear Multiple Bond Correlation (HMBC)).

The NMR results in $CDCl_3$ solution of 44-pyrazine are in good agreement with the expected molecular structure (Scheme 1). Thus, the ^{13}C-DEPT NMR spectrum shows seven signals exclusively for sp^2 methine groups. Additionally, in ^{13}C-PND we found five non-protonated carbons: 155.4 (C6/C10 [q]), 151.7 (C22 [q]), 150.4 (C1/C5/C11/C15 [d]), 150.4 (C8 [q]), 146.1 (C3/C13 [q]), 144.4 (C24 [d]), 143.6 (C25 [d]), 142.3 (C23 [d]), 139.2 (C16 [q]), 137.6 (C19 [q]), 127.9 (C17/18/20/21 [d]), 121.3 (C2/4/12/14[d]) and 119.0 (C7/9 [d]). The HMBC allows to identified C8, at the same chemical shift than the four methines C1/C5/C11/C15, by the coupling at ^{3}JC-H with H 17/21.

The ^{1}H-NMR is characterized for a low field doublet (9.13 ppm), a doublet of doublet (8.69 ppm) and a doublet (8.58 ppm) due to the pyrazine ring protons H23, H24 and H25, respectively. The four phenyl protons H17/21 (7.91 ppm) and H18/20 (8.25 ppm) form a AA´BB´pattern. The protons H7 and H9 of the central pyridine ring appear as a singlet (8.11 ppm). The eight protons of the two 4-pyridyl rings show an AA´BB´pattern involving the H1/H5/H11/H15 (8.82 ppm) and H2/H4/H12/H14 (8.13 ppm) protons.



Scheme 1. The sketch of the ligand **L2**. The numbering of carbon atoms (hydrogen atoms where correspond) for NMR spectroscopic assigments is indicated.

Sup. 2 (Complement to Figure 7).

The different moieties present in the asymmetric unit in the coordination polymer $[Zn(acac)_2(L2)]_n$ and showing the same orientation displayed in Fig.7 in the text.