Supporting Information

Self-Assembly of a Rare High Spin Fe^{II}/Pd^{II} Tetradecanuclear Cubic Cage Constructed via the Metalloligand Approach

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Figure S9. Schematic highlighting of the bonding axes of the i^{th} and j^{th} pyridine moieties in the metalloligand (**3**).

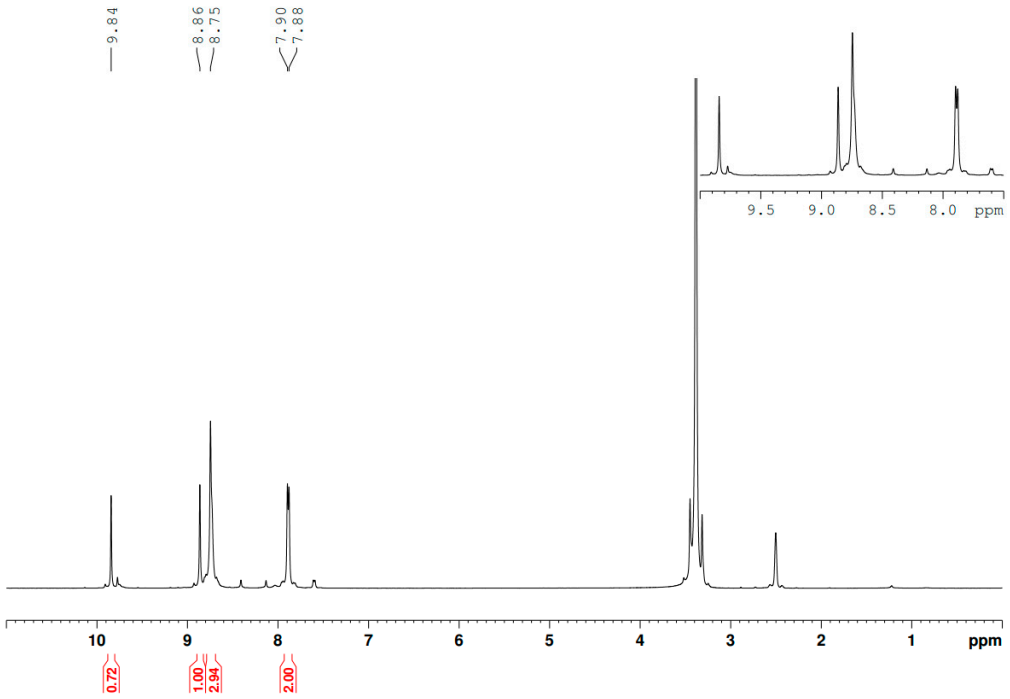

Figure S1. [1]H NMR spectrum of 1-(pyridine-4-yl)-1*H*-imidazole-4-carbaldehyde.

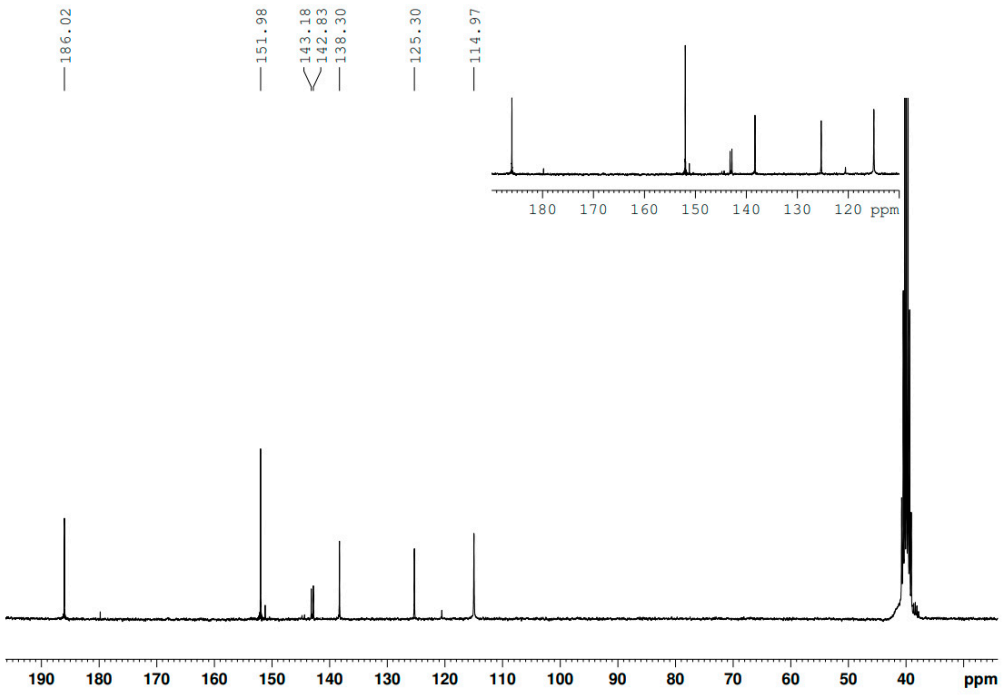

Figure S2. [13]C NMR spectrum (DMSO-d_6, 75MHz) of 1-(pyridine-4-yl)-1*H*-imidazole-4-carbaldehyde.

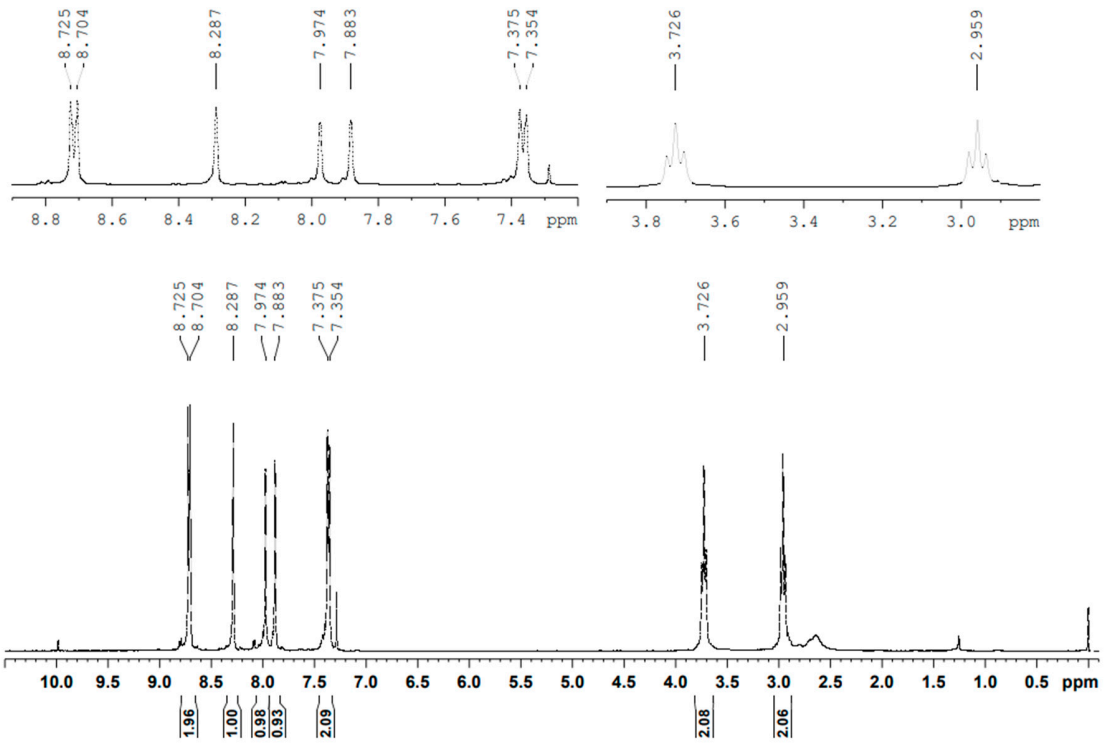

Figure S3. ^{1}H NMR spectrum of ligand **2** ($CDCl_3$, 300MHz)

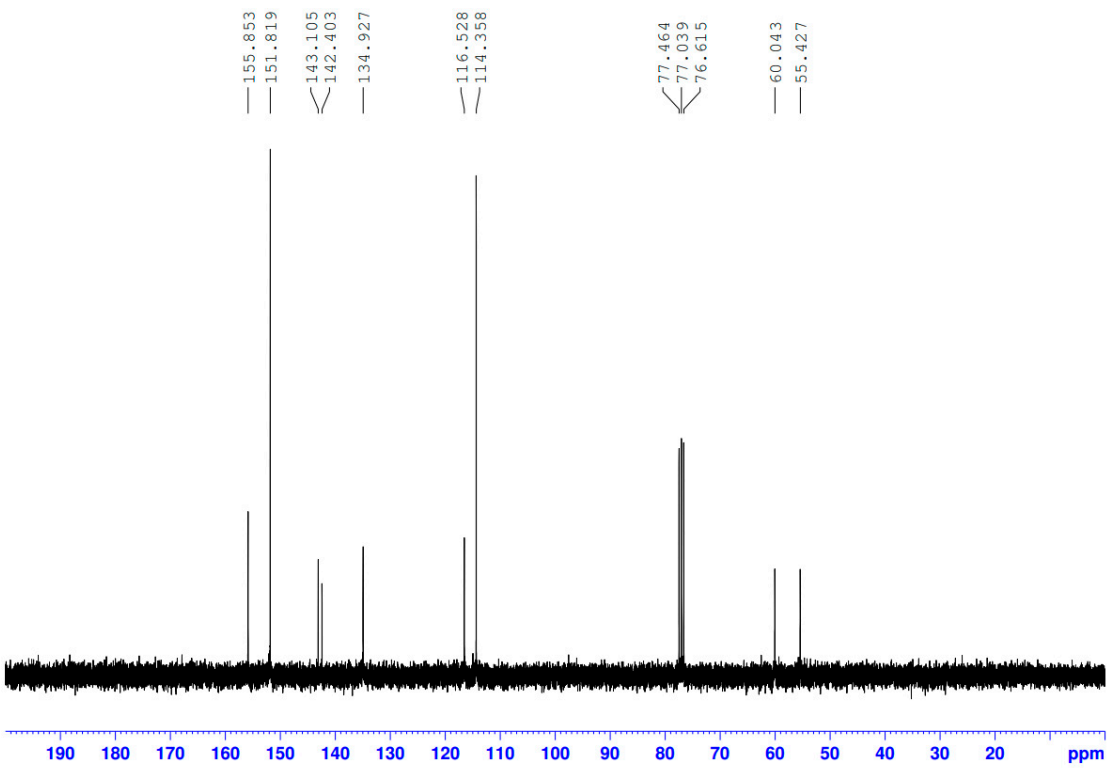

Figure S4. ^{13}C NMR spectrum of ligand **2** ($CDCl_3$, 75MHz)

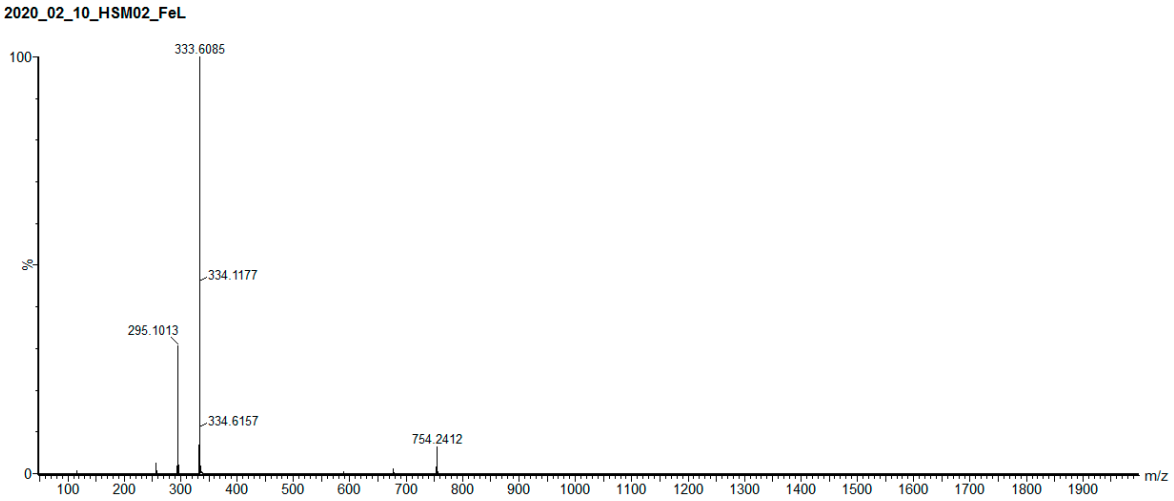

Figure S5. HR ESI-MS spectrum of Fe**L**$(BF_4)_2$ **(3)** in acetonitrile.

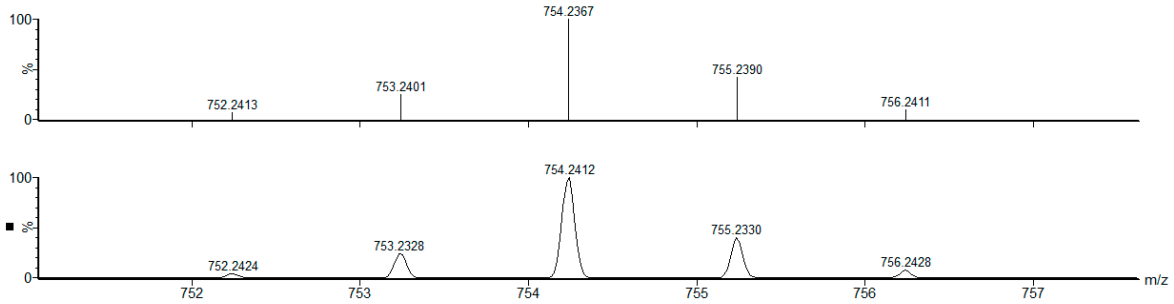

Figure S6. Isotopic pattern of $[Fe\mathbf{L}(BF_4)]^{1+}$ (bottom) and simulated distribution (top).

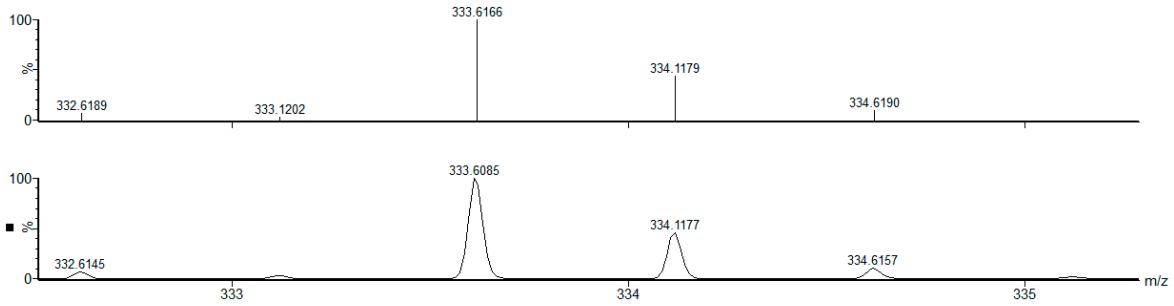

Figure S7. Isotopic pattern of $[Fe\mathbf{L}]^{2+}$ (bottom) and simulated distribution (top).

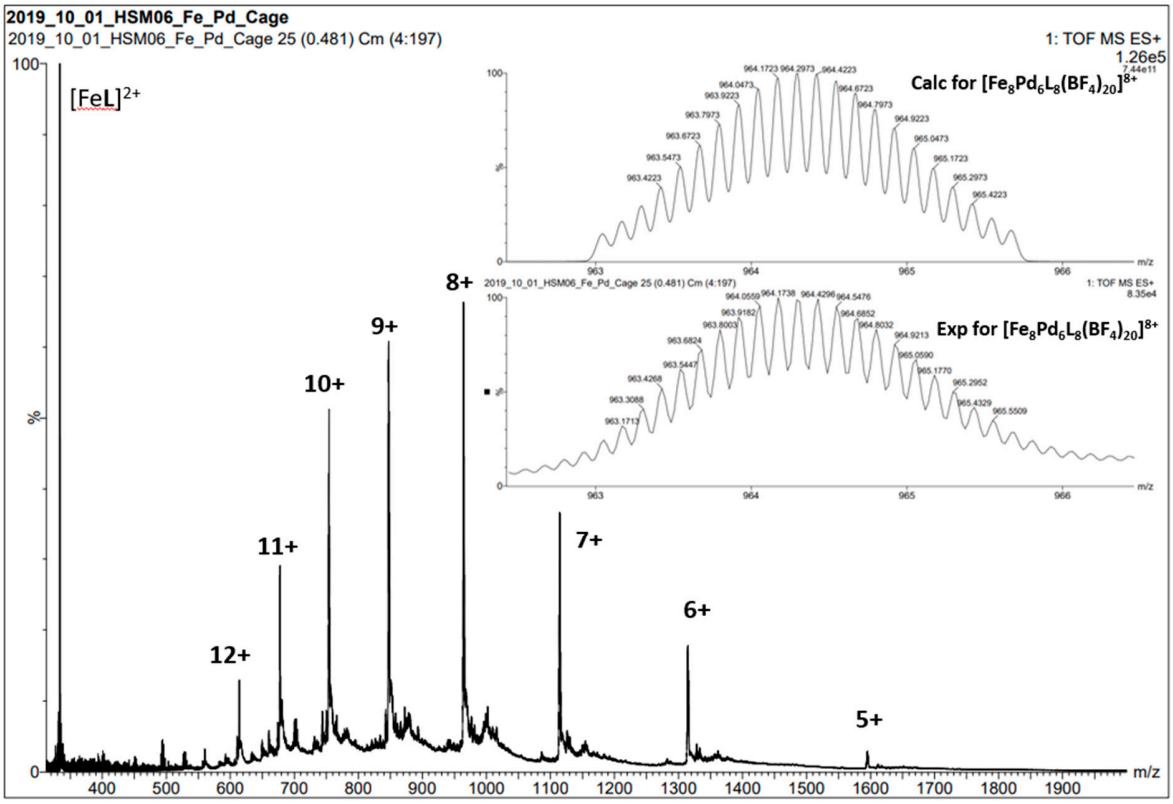

Figure S8. HR-ESI-MS spectra of [Fe$_8$Pd$_6$**L**$_8$(BF$_4$)$_{28}$] (**1**) in acetonitrile. The inset shows the isotopic pattern for [Fe$_8$Pd$_6$**L**$_8$(BF$_4$)$_{20}$]$^{8+}$ (bottom) with simulated pattern (top).

Calculation of mutual secondary bonding axis angles

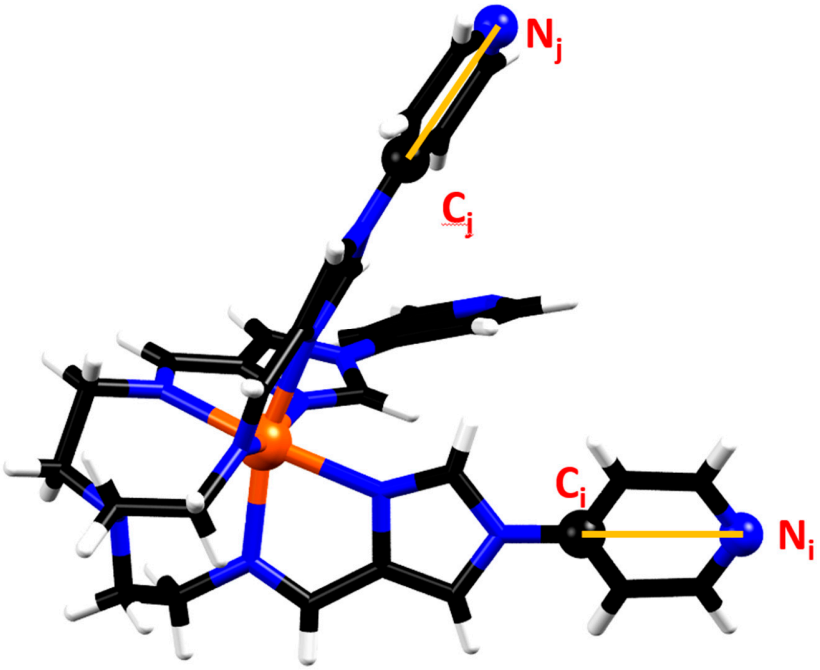

Figure S9. Schematic highlighting of the bonding axes of the i^{th} and j^{th} pyridine moieties in the metalloligand (**3**).

For each given angle, the coordinates of four atoms were selected, the i^{th} secondary N atom and the opposite C in the same pyridine (N_i and C_i), as well as the equivalent atoms in the j^{th} pyridine (N_j and C_j).

This system of coordinates was subjected to several translations and reorientations for the calculation of the given angle as follows.

- All four points were translated by the same distance, such that C_i occupied the origin of the Cartesian system.
- Both reference atoms in the j^{th} pyridine were translated, such that C_j occupied the origin.
- All coordinates were rotated about the z axis, such that the N_i sat in the xz plane.
- All coordinates were rotated about the y axis, such that the N_i sat in the x axis.
- All coordinates were rotated about the x axis, such that N_j sat in the xy plane.

The angle between bonding axes was then calculated using the N_j coordinates by arctan(y/x).