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Supporting Information for:

Multiple Coordination Modes of a New Ditopic Bis(pyrazolyl)methane Ligand

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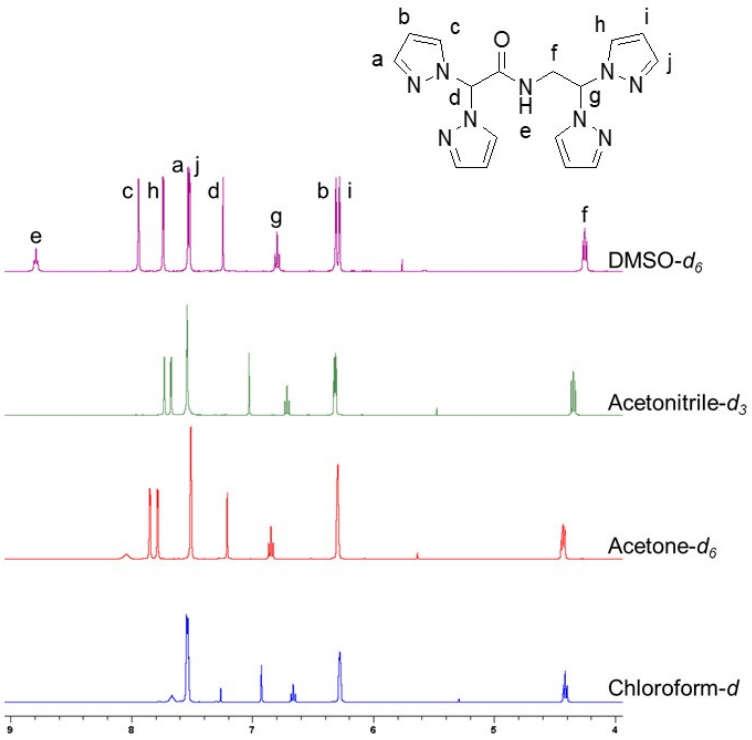

Figure S1. ^{1}H-NMR spectra of **L4Pz** in various solvents.

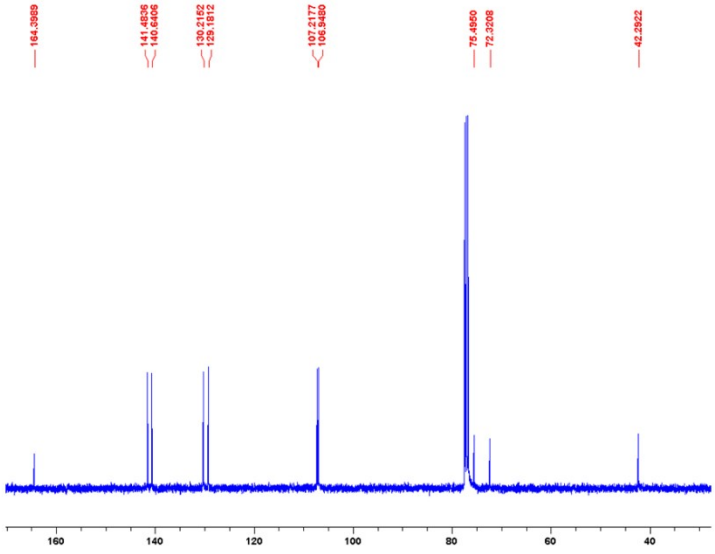

Figure S2. ^{13}C-NMR spectrum of **L4Pz** in $CDCl_3$.

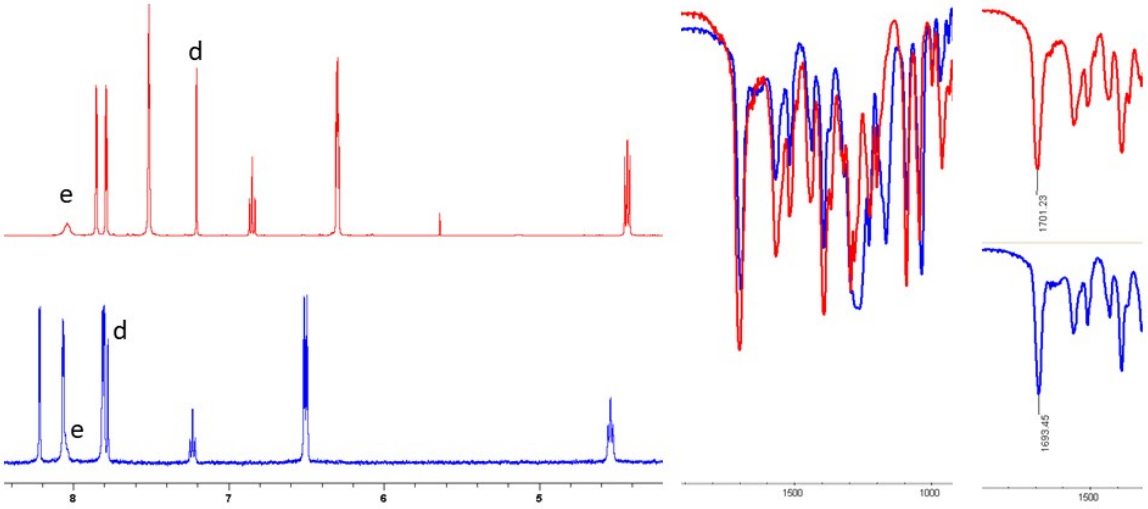

Figure S3. Spectral characterization (^{1}H-NMR – left and IR – right) of $\{[Ag(\mathbf{L4Pz})](O_3SCF_3)\}_n$; red lines – the free ligand, blue lines – the complex.

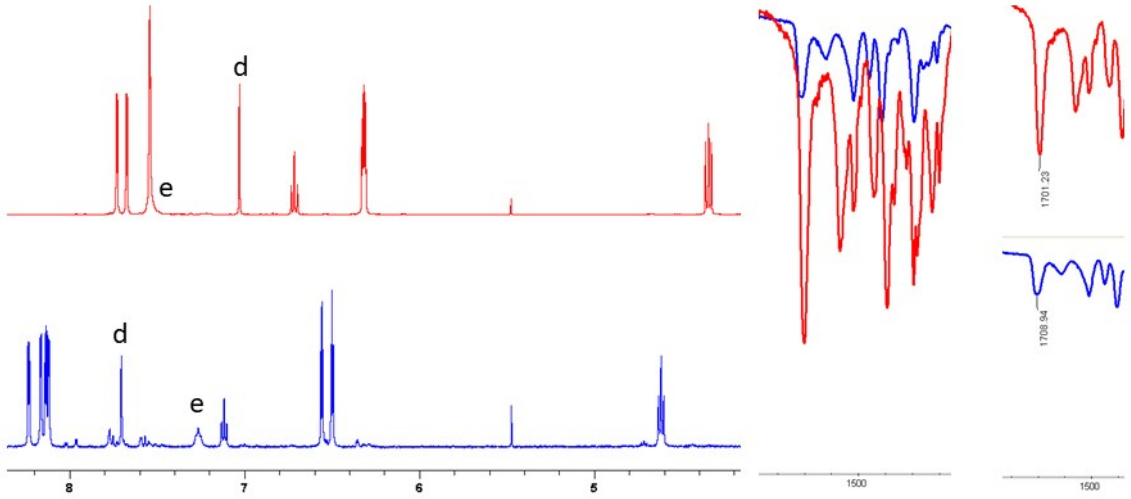

Figure S4. Spectral characterization (^{1}H-NMR – left and IR – right) of $[(\mathbf{L4Pz})(PdCl_2)_2]$; red lines – the free ligand, blue lines – the complex.

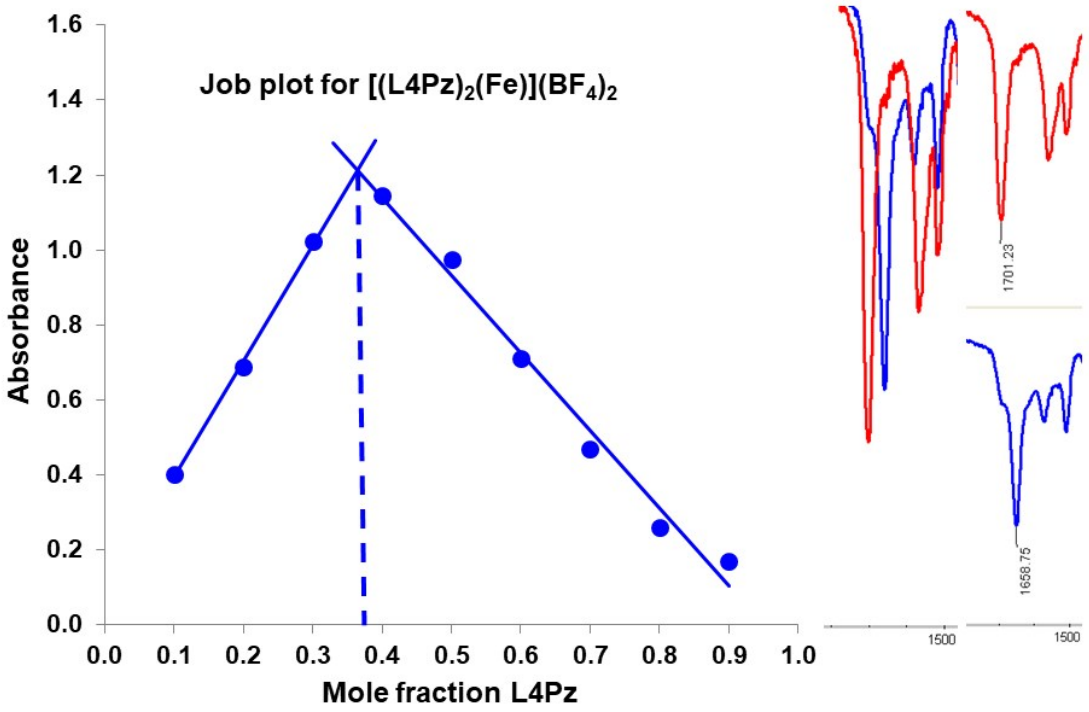

Figure S5. Job plot (left) and IR spectrum (right) of [(**L4Pz**)$_2$Fe](BF$_4$)$_2$; red line – the free ligand, blue line – the complex.

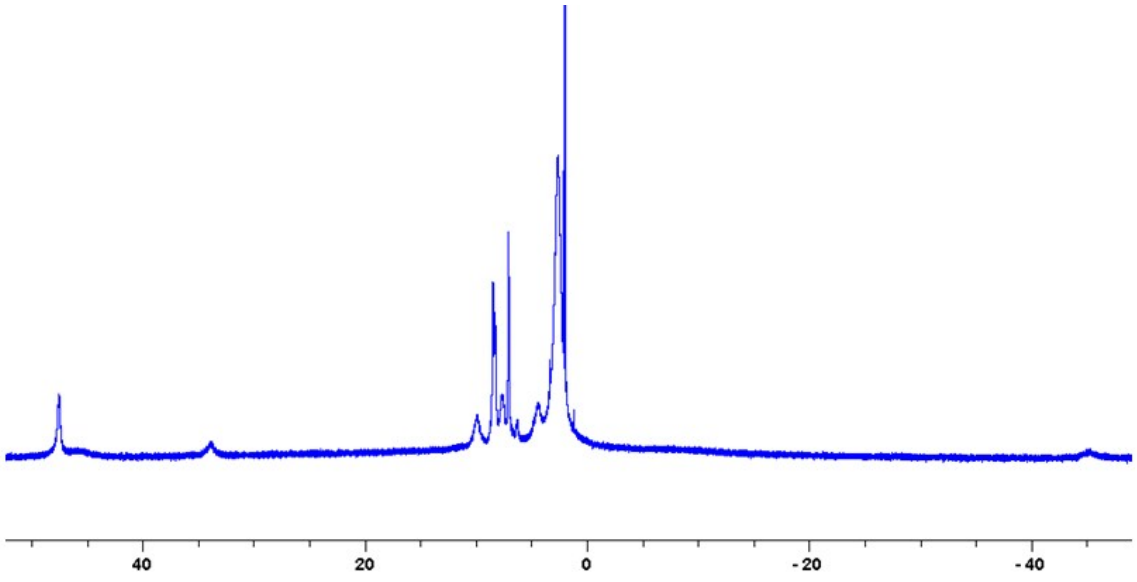

Figure S6. ^{1}H-NMR spectrum of [(**L4Pz**)$_2$Fe](BF$_4$)$_2$.

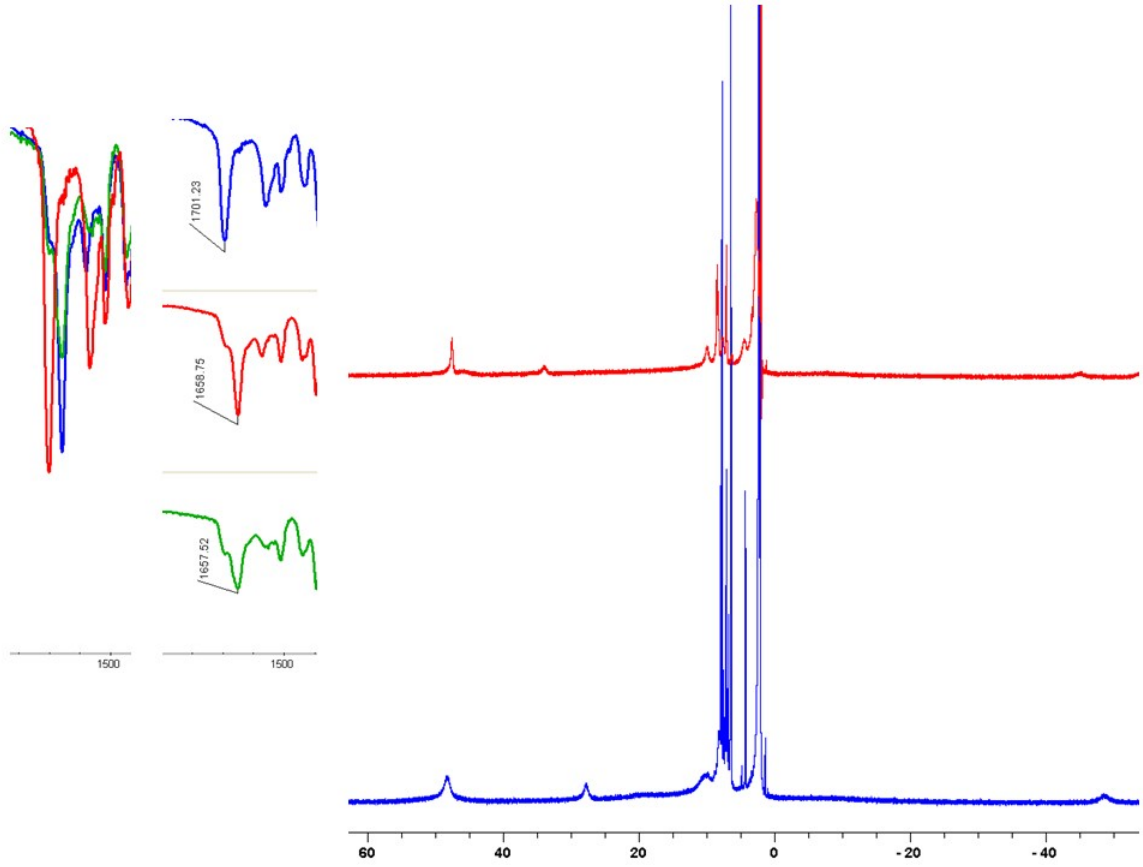

Figure S7. Spectral characterization of [(**L4Pz**)$_2$FeAg](BF$_4$)$_3$; left: IR spectra of **L4Pz** (blue line), [(**L4Pz**)$_2$Fe](BF$_4$)$_2$ (red line), and [(**L4Pz**)$_2$FeAg](BF$_4$)$_3$ (green line); right: ^{1}H-NMR spectrum of [(**L4Pz**)$_2$Fe](BF$_4$)$_2$ (red line) and [(**L4Pz**)$_2$FeAg](BF$_4$)$_3$ (blue line).

Table S1. Crystal data and structure refinement for **{[(L4Pz)Ag](O$_3$SCF$_3$)}$_n$, (1); [(L4Pz)(PdCl$_2$)$_2$], (2)**; **{(L4Pz)[Re(CO)$_3$][Re(CO)$_3$Br]}Br, (3)**; **[(L4Pz)$_2$Fe](BF$_4$)$_2$, (4); [(L4Pz)$_2$FeAg](BF$_4$)$_3$, (5).**

Compound	**1**	**2**	**3**	**4**	**5**
Chemical formula	$C_{16.50}H_{17}AgF_{1.50}N_9O_{2.50}S_{0.50}$	$C_{16}H_{17}Cl_4N_9OPd_2 \cdot C_2H_6OS$	$C_{22}H_{17}Br_2N_9O_7Re_2$	$C_{16}H_{17}Fe_{0.50}N_9O \cdot BF_4$	$C_{32}H_{34}AgB_3F_{12}FeN_{18}O_2$
FW	533.79	784.11	1051.66	466.12	1126.92
Crystal system, space group	Monoclinic, *Cm*	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$
Temperature (K)	100	100	100	100	100
a, b, c (Å)	12.2382 (4), 27.6761 (10), 7.7791 (3)	8.1580 (2), 11.6246 (3), 15.2480 (4)	10.4206 (4), 13.4302 (5), 13.6824 (6)	7.7191 (2), 11.2092 (3), 11.6297 (3)	11.9228 (5), 13.0749 (5), 14.3672 (6)
α, β, γ (°)	90.00, 113.565 (2), 90.00	99.275 (1), 104.487 (2), 100.988 (2)	63.050 (2), 78.311 (2), 71.078 (2)	75.435 (2), 89.899 (2), 86.181 (2)	78.345 (2), 84.386 (2), 81.075 (2)
V (Å3)	2415.10 (15)	1340.78 (6)	1611.16 (12)	971.64 (4)	2161.84 (15)
Z	4	2	2	2	2
μ (mm^{-1})	7.49	15.53	17.84	3.98	7.3
R_{int}	0.077	0.044	0.034	0.05	0.045
R[F2 > 2σ(F2)], wR(F2), S	0.043, 0.098, 1.01	0.025, 0.065, 1.09	0.022, 0.053, 1.12	0.037, 0.102, 1.05	0.026, 0.066, 1.03
No. of reflections	4075	4780	5772	3476	7737
No. of parameters	290	331	382	302	628
No. of restraints	3	1	1	9	2