

Balancing Connectivity with Function in Silver(I) networks of Pyridyltriazole (tzpa) Ligands Results in the Formation of a Metallogel

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Supporting Information

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Table S1 Crystal and refinement parameters for structures **4**, **1** and $\{[Ag_2(\mathbf{1})_2](CF_3SO_3)_2\}_n$

Identification code	4	1	$\{[Ag_2(\mathbf{1})_2](CF_3SO_3)_2\}_n$
Empirical formula	C ₁₈ H ₂₀ N ₂ O ₅ Si	C ₂₁ H ₁₈ N ₆ O	C ₂₂ H ₁₈ AgF ₃ N ₆ O ₄ S
Formula weight	308.45	370.41	627.35
Temperature/K	100(2)	100(2)	100(2)
Crystal system	triclinic	orthorhombic	monoclinic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ 2 ₁ 2	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> /Å	5.8838(2)	14.781(2)	17.0839(18)
<i>b</i> /Å	11.1708(4)	19.903(2)	9.8330(11)
<i>c</i> /Å	13.3912(5)	6.1151(6)	27.626(3)
α /°	84.6200(10)	90	90
β /°	80.2820(10)	90	92.821(2)
γ /°	77.1310(10)	90	90
Volume/Å ³	844.29(5)	1798.9(4)	4635.1(9)
<i>Z</i>	2	4	8
$\rho_{\text{calc}}/\text{cm}^3$	1.213	1.368	1.798
μ/mm^{-1}	0.142	0.721	1.028
<i>F</i> (000)	328.0	776.0	2512.0
Crystal size/mm ³	0.28 × 0.2 × 0.07	0.22 × 0.06 × 0.05	0.4 × 0.07 × 0.06
Radiation	MoK α (λ = 0.71073)	CuK α (λ = 1.54178)	MoK α (λ = 0.71073)
2 θ range for data collection/°	3.746 to 55.302	10.718 to 136.618	2.744 to 52.186
Index ranges	-7 ≤ <i>h</i> ≤ 7, -14 ≤ <i>k</i> ≤ 14, -17 ≤ <i>l</i> ≤ 17	-16 ≤ <i>h</i> ≤ 17, -22 ≤ <i>k</i> ≤ 23, -7 ≤ <i>l</i> ≤ 5	-16 ≤ <i>h</i> ≤ 21, -12 ≤ <i>k</i> ≤ 12, -34 ≤ <i>l</i> ≤ 34
Reflections collected	10456	10412	39534
Independent reflections	3925 [<i>R</i> _{int} = 0.0194, <i>R</i> _{sigma} = 0.0219]	3248 [<i>R</i> _{int} = 0.1015, <i>R</i> _{sigma} = 0.0898]	9198 [<i>R</i> _{int} = 0.0647, <i>R</i> _{sigma} = 0.0607]
Data/restraints/parameters	3925/0/202	3248/65/320	9198/2/673
Goodness-of-fit on <i>F</i> ²	1.038	1.056	1.009
Final <i>R</i> indexes [<i>I</i> >= 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0317, <i>wR</i> ₂ = 0.0776	<i>R</i> ₁ = 0.0823, <i>wR</i> ₂ = 0.2140	<i>R</i> ₁ = 0.0545, <i>wR</i> ₂ = 0.1191
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0392, <i>wR</i> ₂ = 0.0817	<i>R</i> ₁ = 0.1011, <i>wR</i> ₂ = 0.2264	<i>R</i> ₁ = 0.0918, <i>wR</i> ₂ = 0.1355
Largest diff. peak/hole / e Å ⁻³	0.31/-0.24	0.23/-0.25	2.01/-0.88
Flack parameter	n/a	0.1(12)	n/a
CCDC No.	1994746	1994747	1994748

X-Ray Powder Diffraction

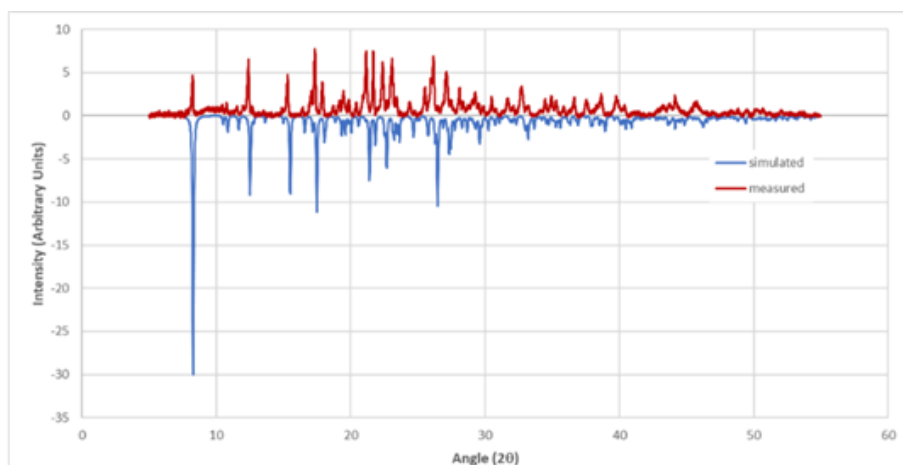


Figure S1 X-ray diffraction pattern for $\{[Ag_2(I)_2](CF_3SO_3)_2\}_n$ measured at (100 K) (blue) compared to the pattern simulated from the single crystal X-ray data obtained at (100K) (red)

Thermogravimetric Analysis

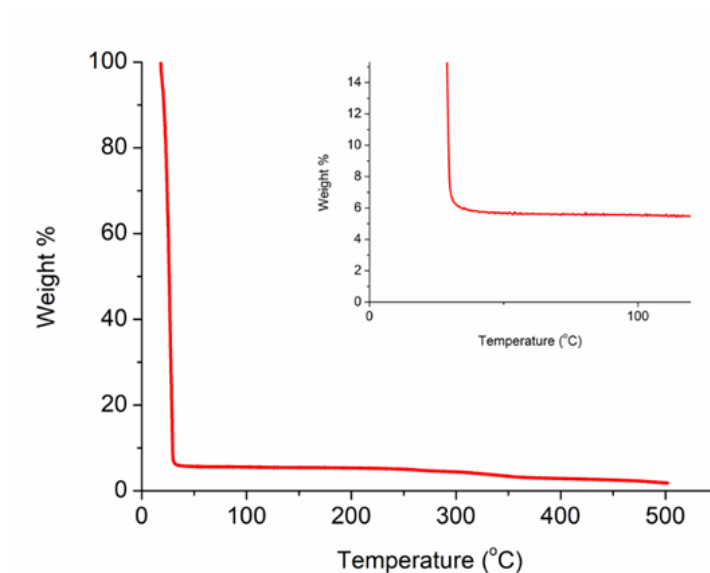


Figure S2 TGA thermograph of **2**. $AgBF_4$ gel showing weight loss of 5.5% before 50 °C.

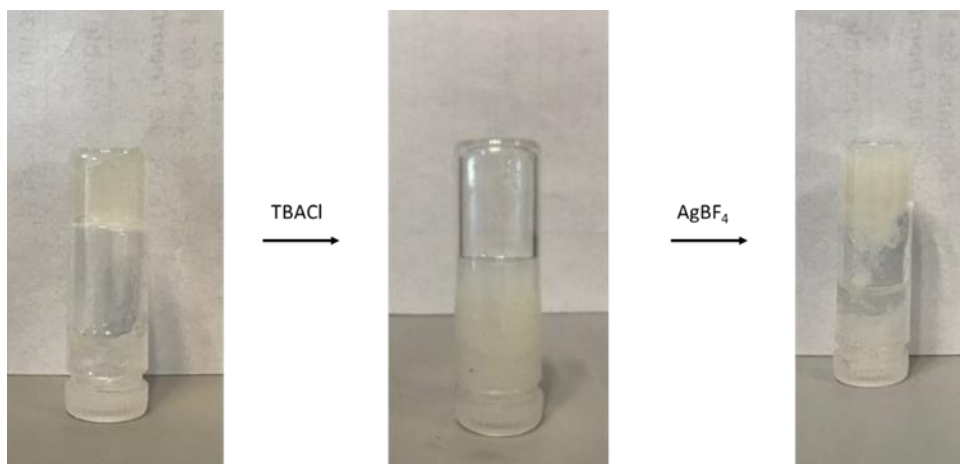


Figure S3 (Left) Inversion test of AgBF_4 gel of **2** in CH_3CN in 1:1 molar ratio. (Middle) Addition of TBACl resulting in destruction of the gel network. (Right) Addition of AgBF_4 to re-form the AgBF_4 gel of **2** demonstrating chemoreversibility of the system.

NMR Spectra

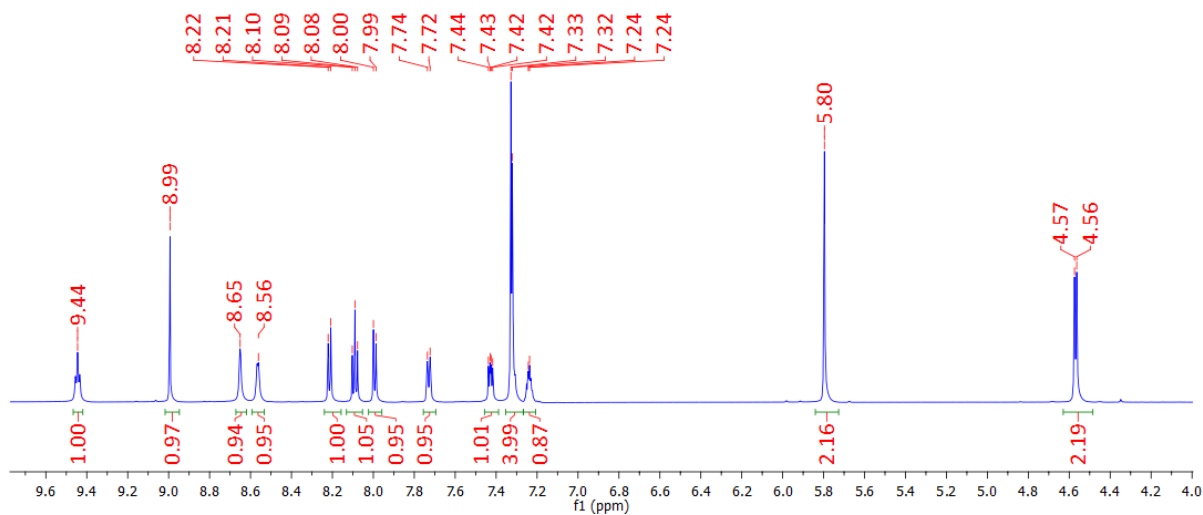


Figure S4 ^1H NMR spectrum (600 MHz, DMSO) of **1**.

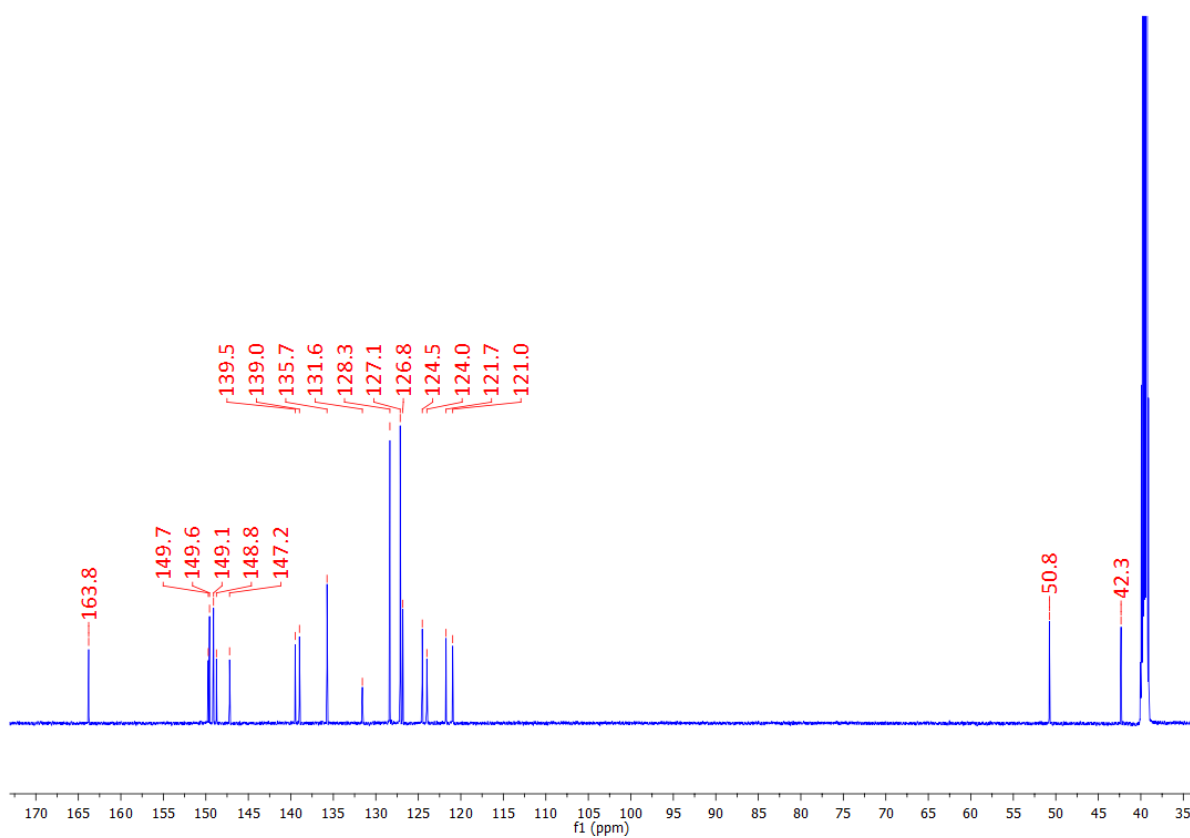


Figure S5 ^{13}C NMR spectrum (150 MHz, DMSO) of **1**.

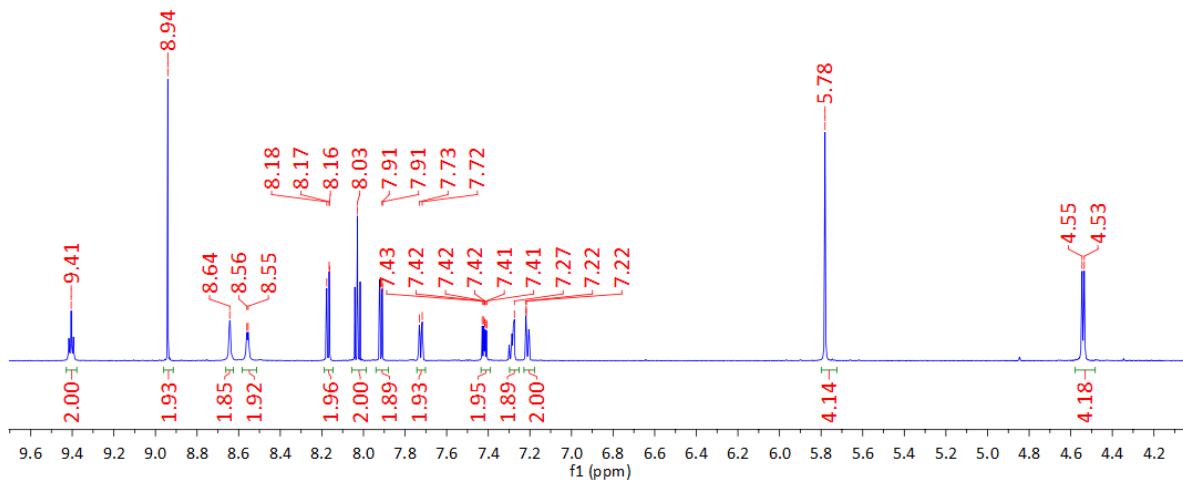


Figure S6 ^1H NMR spectrum (600 MHz, DMSO) of **2**.

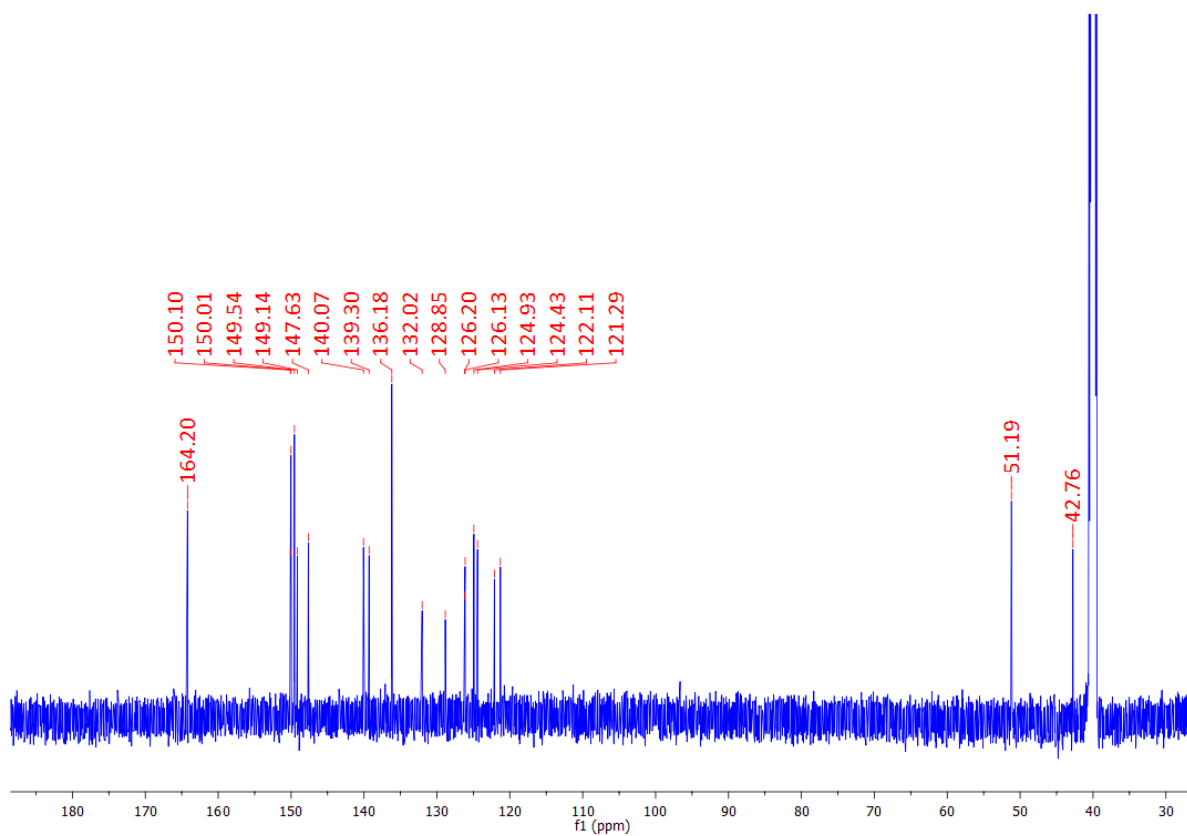


Figure S7 ^{13}C NMR spectrum (150 MHz, DMSO) of **2**.