

Magnetism and luminescence of a MOF with linear Mn₃ nodes derived from an emissive terthiophene-based imidazole linker.

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Table S1. Bond valance sum (BVS) method for Mn1 and Mn2 in **6**.

	Mn1*			
	Bond Distance (R _{ij} , Å)	s(Mn(II))	s(Mn(III))	s(Mn(IV))
O1	2.177	0.351	0.239	0.319
O4	2.192	0.338	0.224	0.307
O5	2.129	0.393	0.290	0.363
Total bond valence**		2.165	1.505	1.978
	Mn2*			
	Bond Distance	s(Mn(II))	s(Mn(III))	s(Mn(IV))
O2	2.100	0.422	0.326	0.392
O3	2.332	0.242	0.127	0.211
O4	2.242	0.300	0.183	0.268
O6	2.082	0.440	0.350	0.412
O7	2.234	0.306	0.189	0.274
O8	2.182	0.346	0.234	0.315
Total bond valence		2.056	1.410	1.872

* Parameter used [21]: Mn(II): R₀ = 1.740, B₀ = 0.417; Mn(III): R₀ = 1.823, B₀ = 0.247; Mn(IV): R₀ = 1.750, B₀ = 0.374. s(Mn(n)) = exp[(R₀ - R_{ij})/B₀].

** Due to the octahedral nature of Mn1, each of O1, O4 and O5 were counted twice.

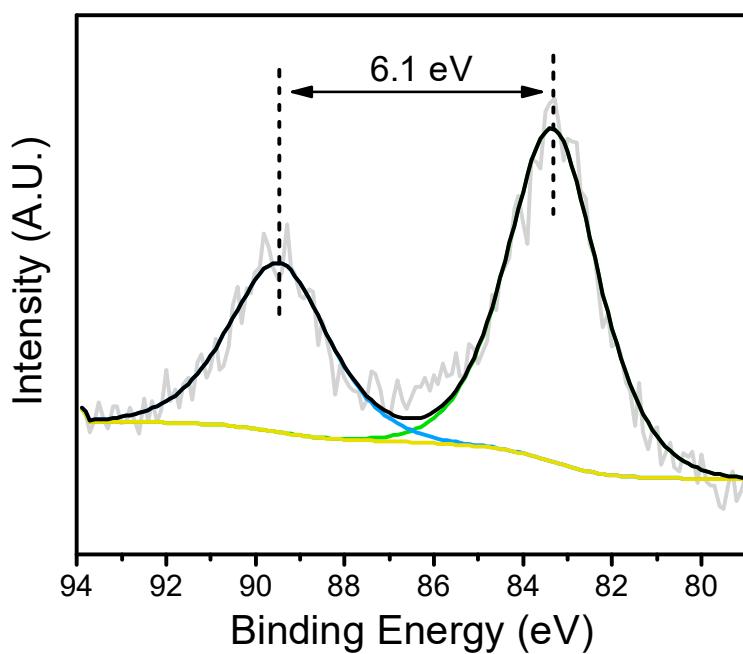


Fig. S1. Deconvoluted Mn 2s spectra of as-synthesized **6** polycrystals.

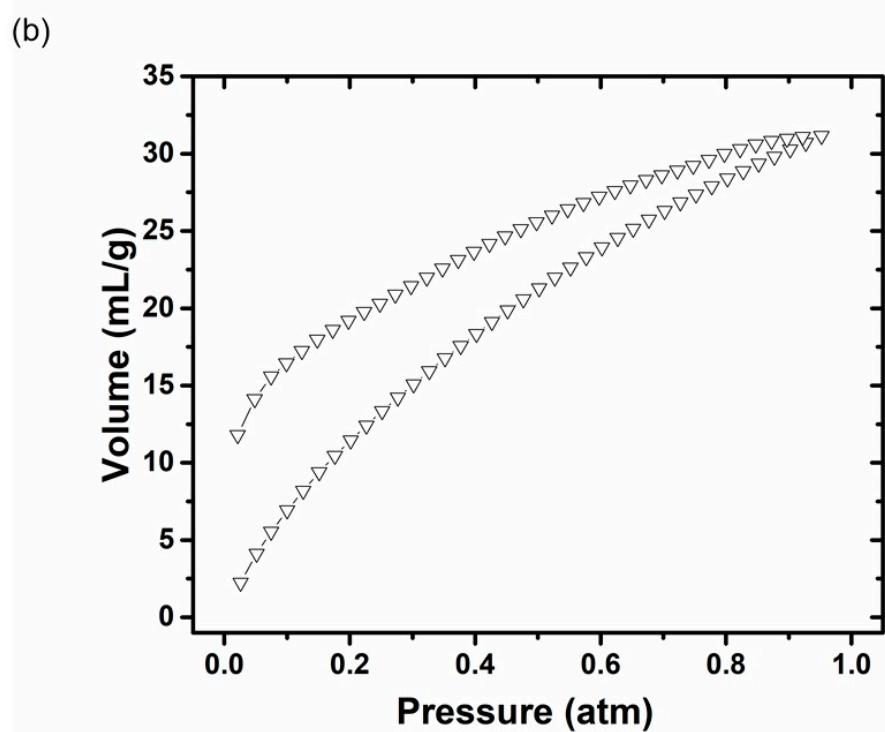
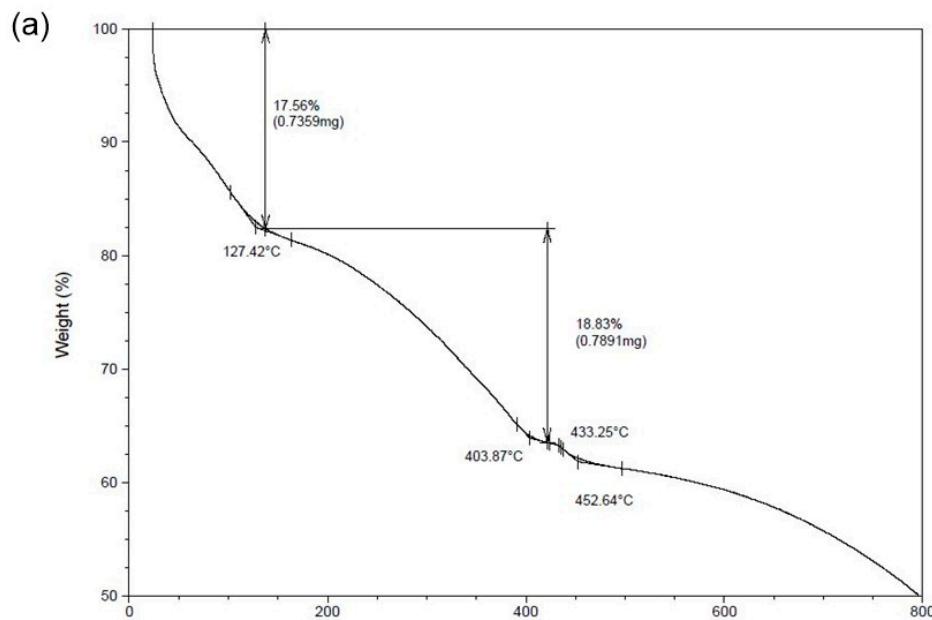


Fig. S2. (a). TGA profile of as-synthesized **6**, obtained at a heating rate of 3.5 °C from 23 °C to 500 °C and a heating rate of 5 °C from 500 °C to 800 °C. (b) adsorption isotherms of carbon dioxide for **6**.

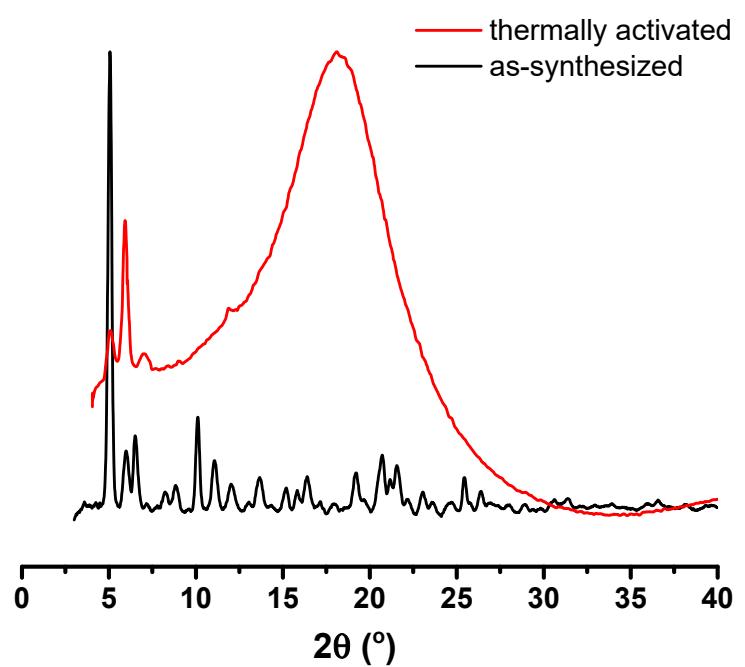


Fig. S3. Powder X-ray diffraction analysis of **6** heating at 100 °C under vacuum.

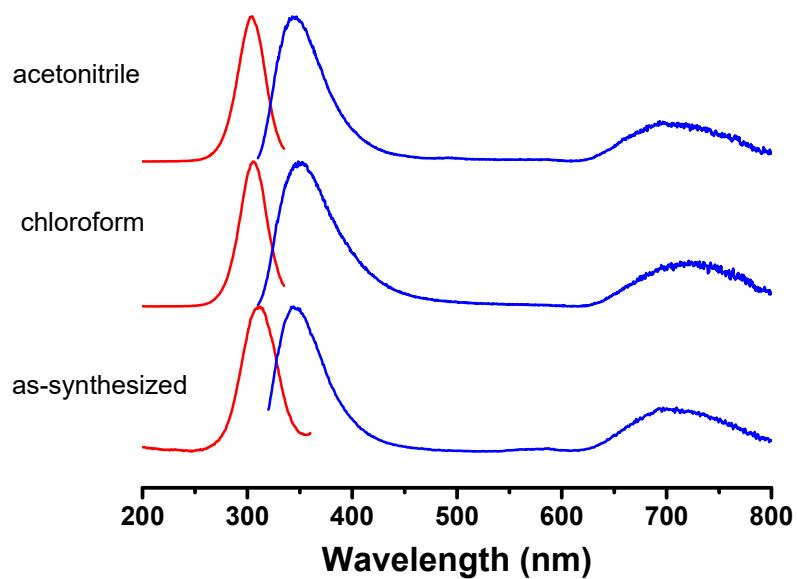


Fig. S4. Excitation (red) and emission (blue) profiles of solvent-exchanged and as-synthesized **6** poly crystalline sample.

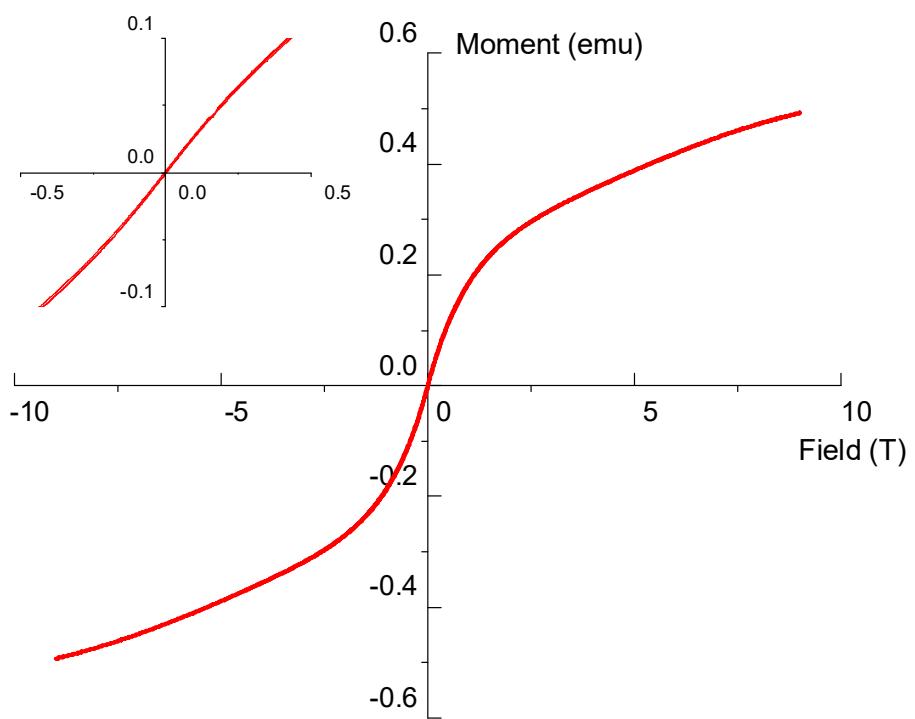


Fig. S5. Magnetic hysteresis curve of **6** (as-synthesized) at 2 K.

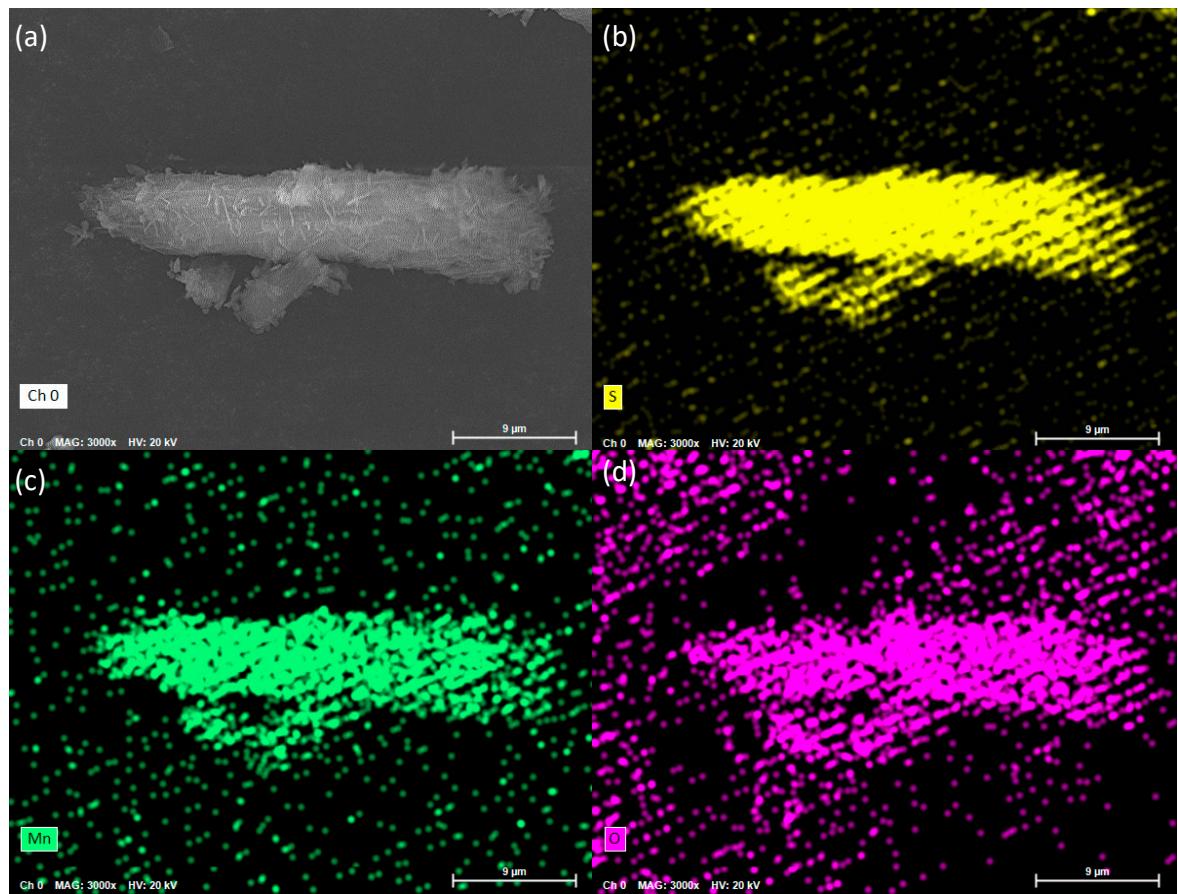


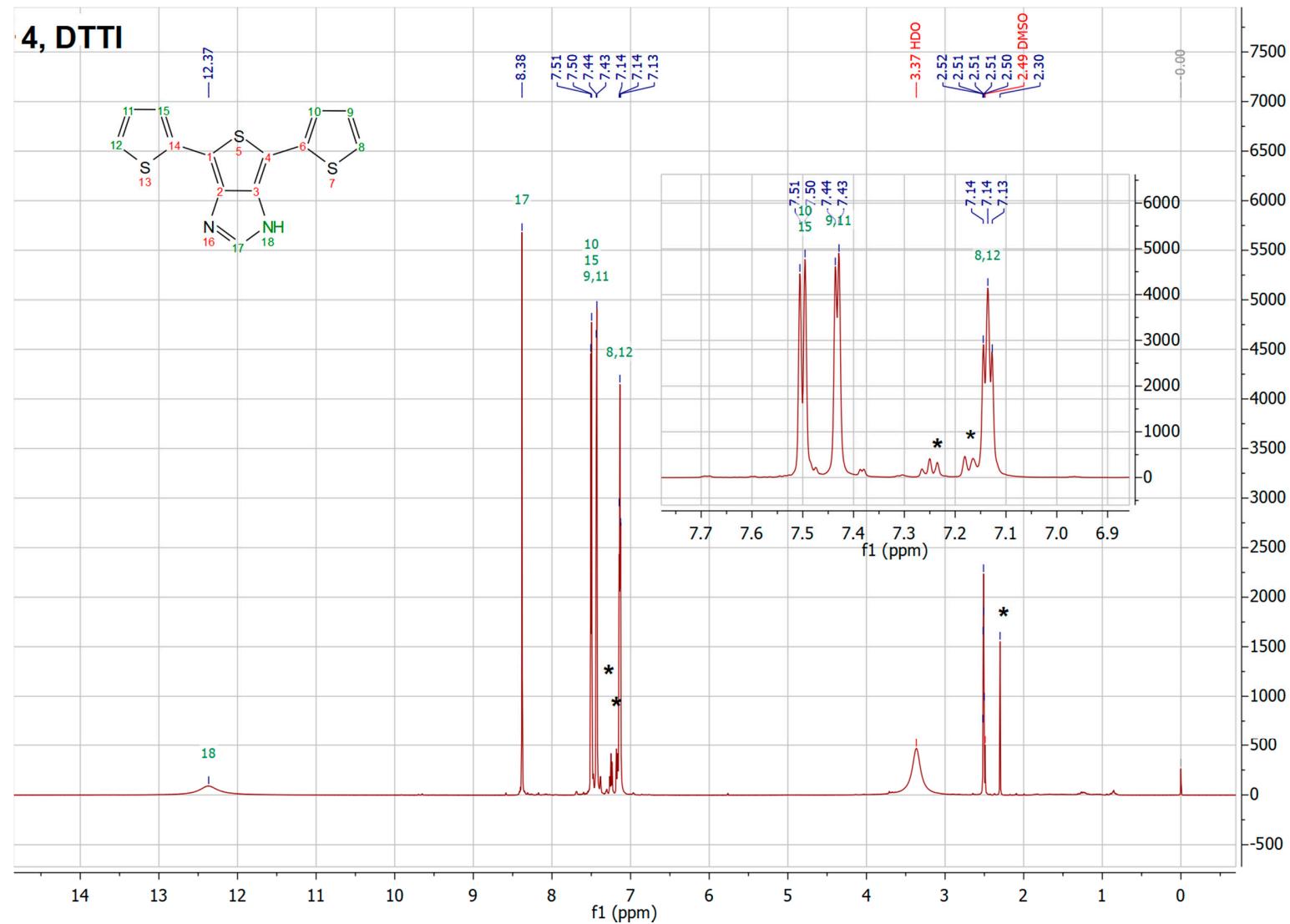
Fig. S6. The SEM image (a) and EDS spectra of S (b), Mn (c) and O (d) signal of as-synthesized 6.

Table S2. Crystal data and structure refinement for **4** and **6**.

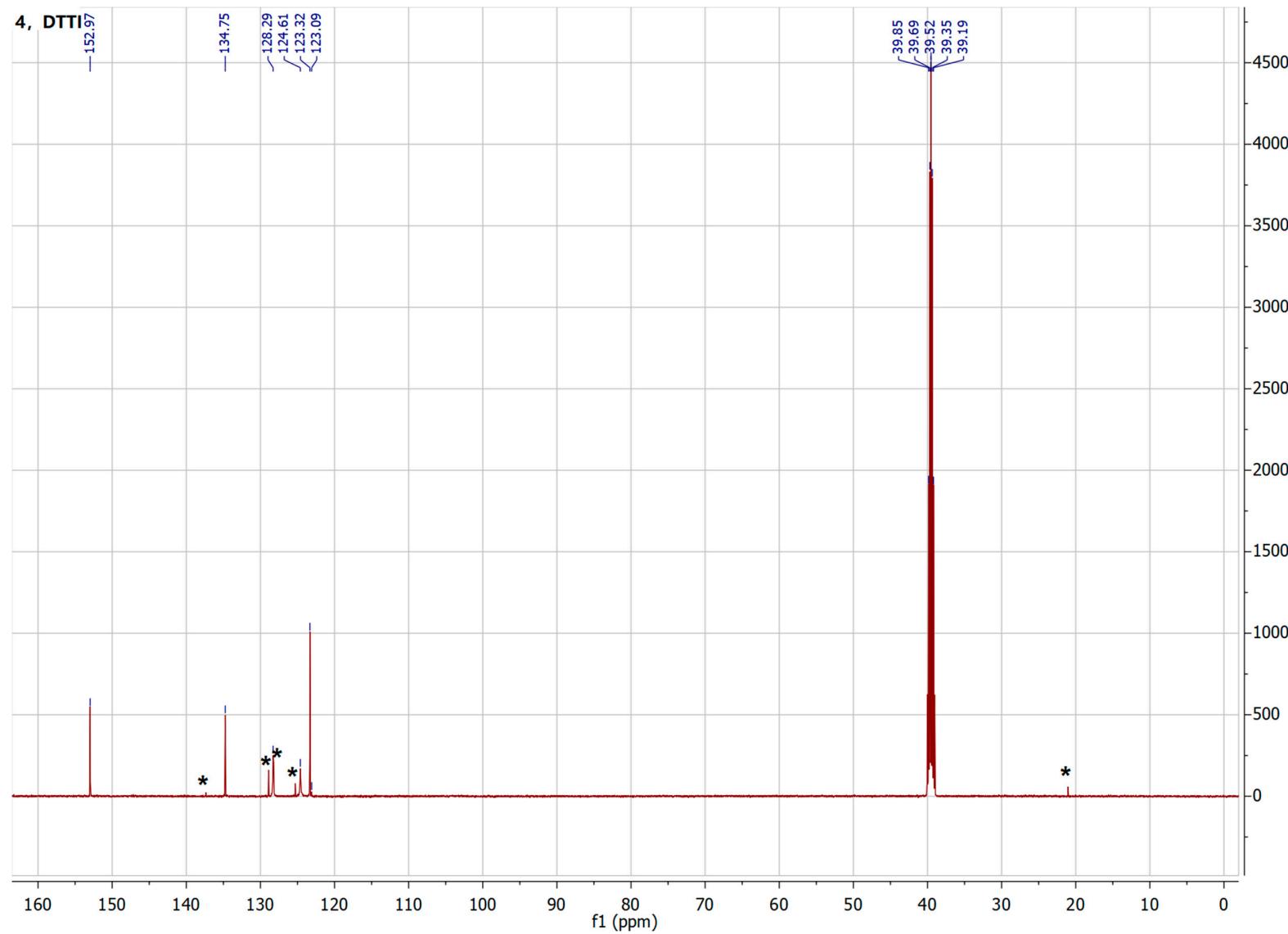
Identification code	4-DTTI	6
Empirical formula	C _{14.75} H ₁₀ N ₂ S ₃	C ₃₀ H ₁₃ Mn _{1.5} N ₄ O ₈ S ₆
Formula weight	311.43	832.21
Temperature/K	100.15	100.01(11)
Crystal system	monoclinic	orthorhombic
Space group	<i>P2₁/n</i>	<i>Pccca</i>
a/Å	9.2726(11)	29.5736(10)
b/Å	13.1237(16)	17.3377(8)
c/Å	23.051(3)	25.9995(9)
α/°	90	90
β/°	90.328(3)	90
γ/°	90	90
Volume/Å ³	2805.1(6)	13330.9(9)
Z	8	8
ρ _{calc} g/cm ³	1.475	0.829
μ/mm ⁻¹	0.517	4.354
F(000)	1284	3348
Crystal size/mm ³	0.24 × 0.09 × 0.06	0.188 × 0.071 × 0.05
Radiation	MoKα ($\lambda = 0.71075 \text{ \AA}$)	CuKα ($\lambda = 1.54184 \text{ \AA}$)
2Θ range for data collection/°	4.704 to 54.966	9.012 to 136.476

Index ranges	$-12 \leq h \leq 12, -17 \leq k \leq 17, -29 \leq l \leq 29$	$-20 \leq h \leq 35, -15 \leq k \leq 20, -31 \leq l \leq 21$
Reflections collected	43111	38321
Independent reflections	6413 [$R_{\text{int}} = 0.0718, R_{\text{sigma}} = 0.0520$]	12184 [$R_{\text{int}} = 0.1188, R_{\text{sigma}} = 0.1263$]
Data/restraints/parameters	6413/1231/544	12184/300/448
Goodness-of-fit on F^2	1.057	0.944
Final R indexes [$I >= 2\sigma(I)$]	$R_1 = 0.0536, wR_2 = 0.0992$	$R_1 = 0.0813, wR_2 = 0.2098$
Final R indexes [all data]	$R_1 = 0.0804, wR_2 = 0.1086$	$R_1 = 0.1294, wR_2 = 0.2421$
Largest diff. peak/hole / e Å ⁻³	0.34/-0.34	1.08/-0.66

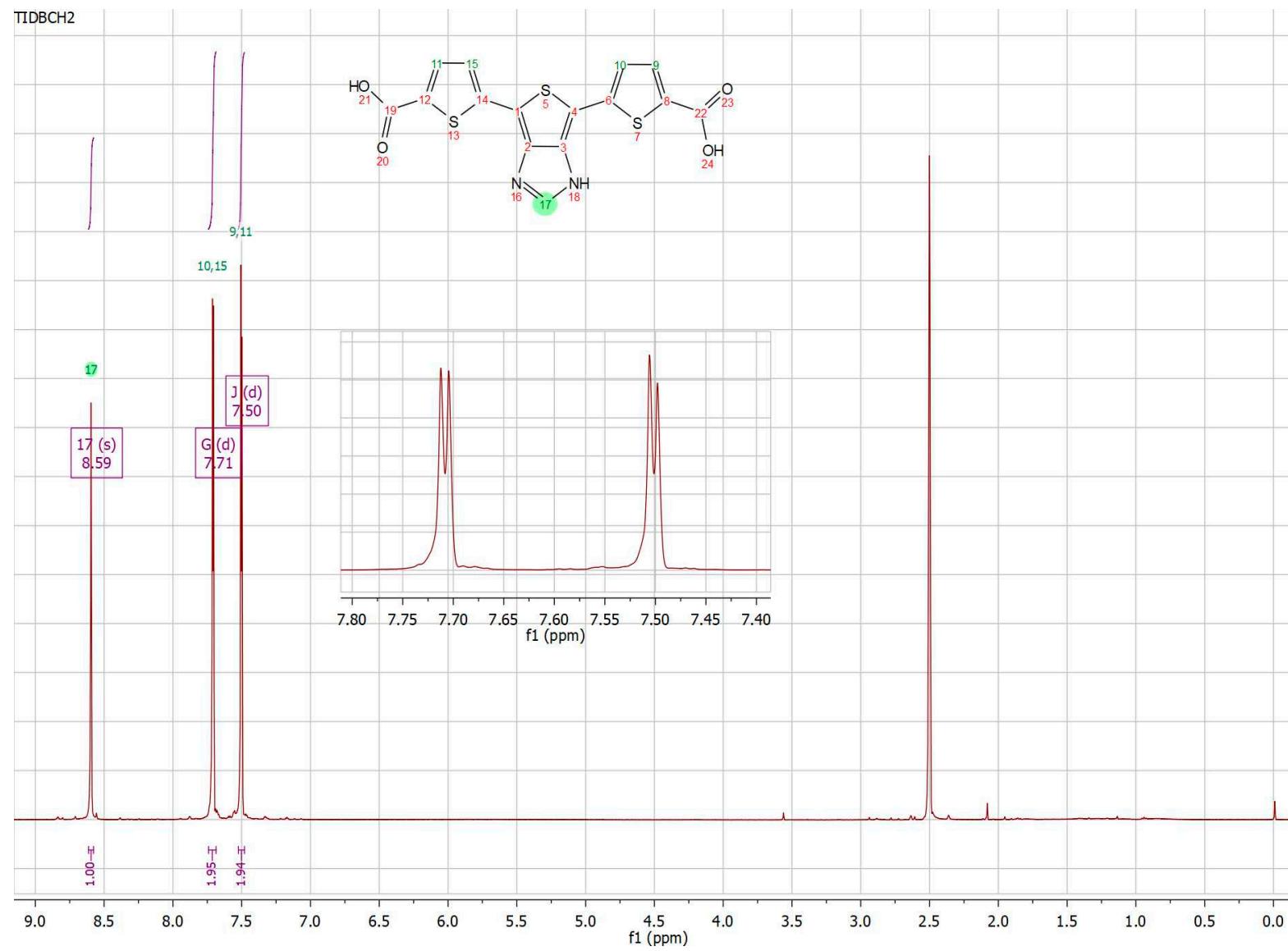
S1. ^1H -NMR of 4.



S2. ^{13}C -NMR of 4.



S3. ^1H -NMR of 5.



S4. ^{13}C -NMR of 5.

