

Supporting Information for

From one-dimensional chains to three-dimensional networks:

solvothermal synthesis of thiogallates in ethylenediamine

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Table 1: Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2) for non-hydrogen atoms in [enH2][Ga4S7(en)2] (**1**).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
Ga(1)	0.32282(4)	0.22527(5)	0.76456(3)	0.0164
Ga(2)	0.56414(4)	0.01851(5)	0.78552(3)	0.0172
Ga(3)	0.81398(4)	0.01847(5)	0.72949(3)	0.0169
Ga(4)	1.04010(4)	0.22832(5)	0.70583(3)	0.0167
S(1)	0.44216(10)	0.09556(12)	0.85137(8)	0.0198
S(2)	0.59483(10)	-0.18516(12)	0.83065(8)	0.0219
S(3)	0.70728(10)	0.14208(13)	0.78976(9)	0.0265
S(4)	0.72163(9)	-0.13269(11)	0.64358(7)	0.0180
S(5)	0.88423(9)	0.14335(12)	0.63954(8)	0.0200
S(6)	1.18140(9)	0.10348(12)	0.70333(8)	0.0228
S(7)	1.05626(10)	0.43309(12)	0.66697(8)	0.0204
N(1)	0.4973(3)	0.0094(4)	0.6636(2)	0.0200
N(2)	0.4380(4)	-0.1689(5)	0.5109(3)	0.0381
N(3)	1.0384(3)	0.2310(4)	0.8268(2)	0.0193
N(4)	1.0848(5)	0.3391(6)	0.9902(3)	0.0530
N(5)	0.3125(4)	-0.1478(5)	0.9046(3)	0.0422
N(6)	0.1994(4)	0.1117(6)	1.0240(3)	0.0461
C(1)	0.3995(4)	-0.0718(6)	0.6403(3)	0.0273
C(2)	0.3637(5)	-0.0945(6)	0.5487(4)	0.0382
C(3)	0.9632(4)	0.3193(5)	0.8543(4)	0.0298
C(4)	0.9725(6)	0.3156(6)	0.9473(4)	0.0466
C(5)	0.2915(5)	-0.0742(7)	0.9783(4)	0.0442
C(6)	0.2186(5)	0.0354(6)	0.9521(4)	0.0445

Table 2: Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2) for non-hydrogen atoms in $[\text{M}(\text{en})_3]_{0.5}[\text{GaS}_2]$ ($\text{M} = \text{Mn, Co, Ni}$).

		$[\text{M}(\text{en})_3]_{0.5}[\text{GaS}_2]$		
		$\text{M} = \text{Mn (3)}$	$\text{M} = \text{Co (4)}$	$\text{M} = \text{Ni (5)}$
Ga(1)	x	0.0000	0.0000	0.0000
	y	0.00709(3)	0.00663(4)	0.00644(4)
	z	0.62414(4)	0.62416(4)	0.62410(4)
	U_{iso}	0.0090	0.0088	0.0094
S(1)	x	0.0000	0.0000	0.0000
	y	-0.10391(9)	-0.10359(11)	-0.10350(13)
	z	0.7500	0.7500	0.7500
	U_{iso}	0.0118	0.0120	0.0128
S(2)	x	0.0000	0.0000	0.0000
	y	0.12032(8)	0.11981(10)	0.11965(11)
	z	0.7500	0.7500	0.7500
	U_{iso}	0.0110	0.0108	0.0124
S(3)	x	0.17956(8)	0.18115(10)	0.18190(10)
	y	0.0000	0.0000	0.0000
	z	0.5000	0.5000	0.5000
	U_{iso}	0.0139	0.0141	0.0151
M(1)	x	0.0000	0.0000	0.0000
	y	0.39525(5)	0.39180(6)	0.39109(6)
	z	0.2500	0.2500	0.2500
	U_{iso}	0.0116	0.0088	0.0090
N(1)	x	0.1476(3)	0.1466(4)	0.1459(4)
	y	0.5136(2)	0.5022(3)	0.4980(3)
	z	0.2500	0.2500	0.2500
	U_{iso}	0.0176(6)	0.0131(7)	0.0135(7)
N(2)	x	0.0000	0.0000	0.0000
	y	0.3783(2)	0.3804(2)	0.3814(3)
	z	0.0651(3)	0.0726(3)	0.0760(3)
	U_{iso}	0.0224(7)	0.0154(8)	0.0152(8)
N(3)	x	0.1701(5)	0.1656(5)	0.1623(5)
	y	0.2933(3)	0.2944(3)	0.2954(3)
	z	0.2154(3)	0.2243(4)	0.2267(4)
	U_{iso}	0.0160(8)	0.0109(11)	0.0112(11)
	Occ^a	0.5	0.5	0.5
C(1)	x	0.0716(4)	0.0713(4)	0.0708(5)
	y	0.5967(3)	0.5856(4)	0.5811(4)
	z	0.2263(4)	0.2772(4)	0.2775(4)
	U_{iso}	0.0204(12)	0.0163(14)	0.0151(14)
	Occ^a	0.5	0.5	0.5
C(2)	x	0.0412(5)	0.0475(6)	0.0476(6)
	y	0.2860(3)	0.2903(4)	0.2915(4)
	z	0.0416(5)	0.0453(5)	0.0472(5)
	U_{iso}	0.0191(11)	0.0167(13)	0.0158(13)
	Occ^a	0.5	0.5	0.5
C(3)	x	0.1810(6)	0.1843(6)	0.1840(6)
	y	0.2746(3)	0.2760(4)	0.2772(4)
	z	0.0958(4)	0.1050(5)	0.1078(5)
	U_{iso}	0.0191(11)	0.0160(13)	0.0155(13)
	Occ^a	0.5	0.5	0.5

^a The site occupancy factors are 1.00 unless stated otherwise.

Table 3: Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2) for non-hydrogen atoms in $\text{Mn}(\text{en})_2\text{Ga}_2\text{S}_4$ (5).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
Ga(1)	0.050052(2)	0.01161(3)	0.87358(2)	0.0203
S(1)	0.5000	0.22815(10)	0.7500	0.0311
S(2)	0.62156(4)	-0.00322(7)	1.02578(4)	0.0245
S(3)	0.5000	-0.20462(9)	0.7500	0.0231
Mn(1)	0.7500	-0.2500	1.0	0.0328
N(1)	0.75927(14)	-0.1440(3)	0.83042(17)	0.0305
N(2)	0.85723(14)	-0.0445(3)	1.04684(17)	0.0296
C(1)	0.88670(17)	0.0172(3)	0.9425(2)	0.0311
C(2)	0.80181(19)	0.0250(3)	0.8488(2)	0.0316

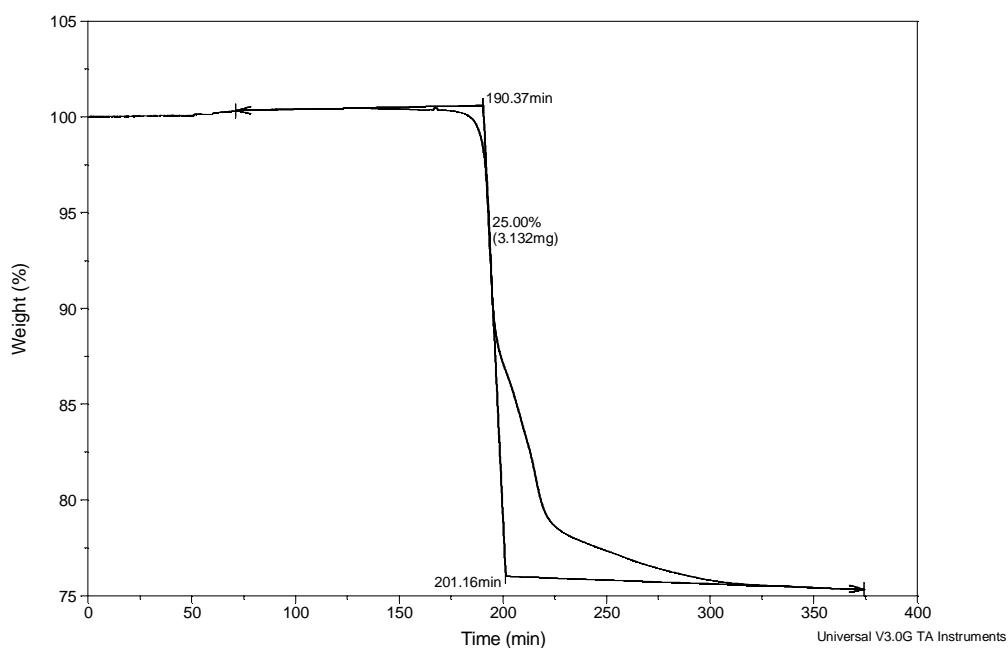


Figure 1: TGA curve for $[\text{enH}_2][\text{Ga}_4\text{S}_7(\text{en})_2]$ (**1**).

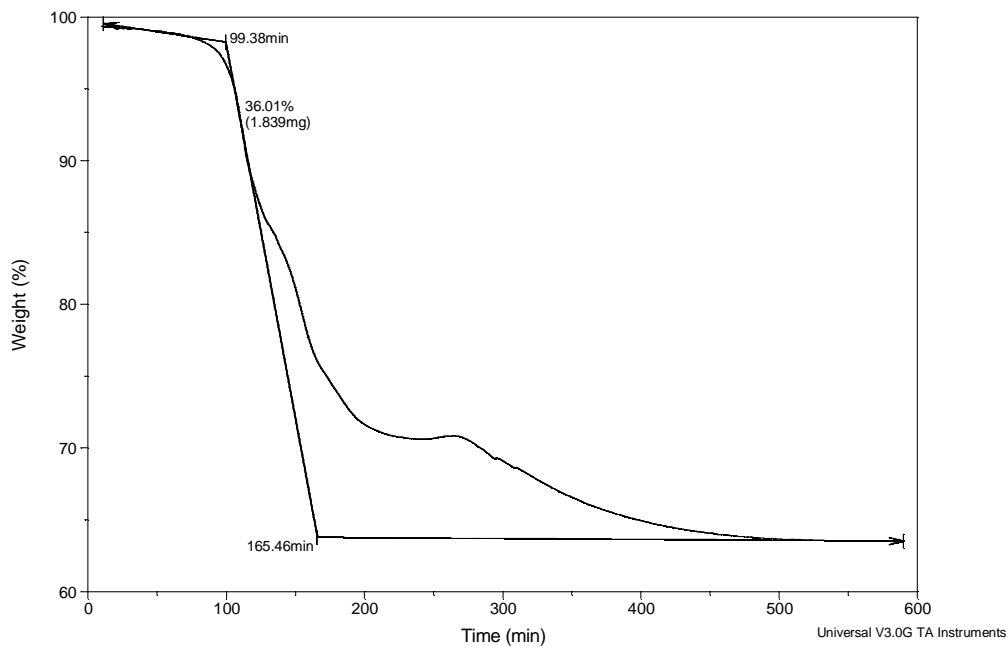


Figure 2: TGA curve for $[\text{Mn}(\text{en})_3]_{0.5}[\text{GaS}_2]$ (**2**).

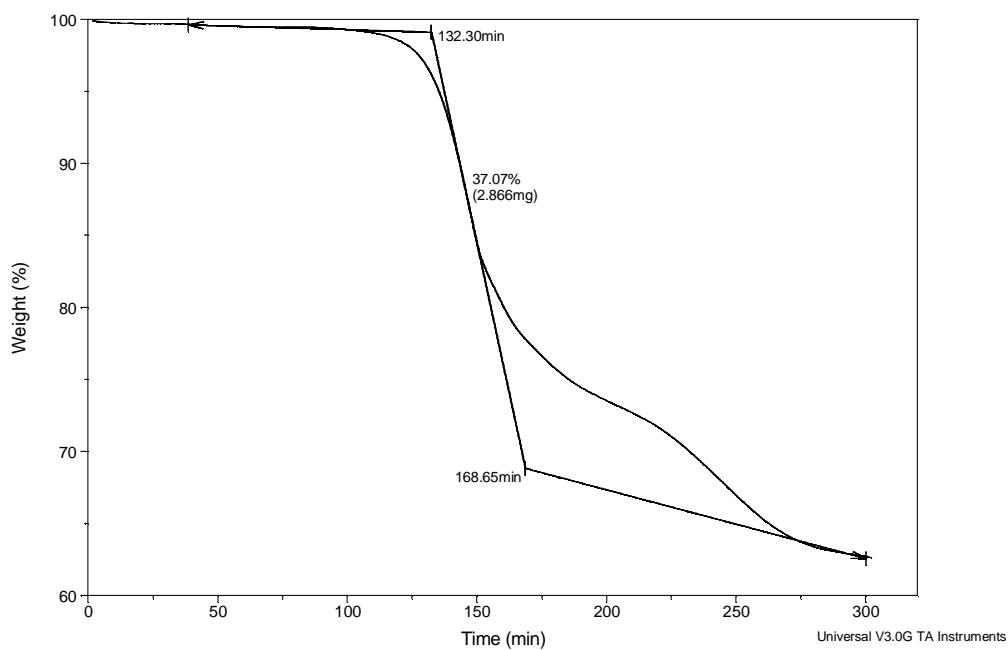


Figure 3: TGA curve for $[\text{Co}(\text{en})_3]_{0.5}[\text{GaS}_2]$ (**3**).

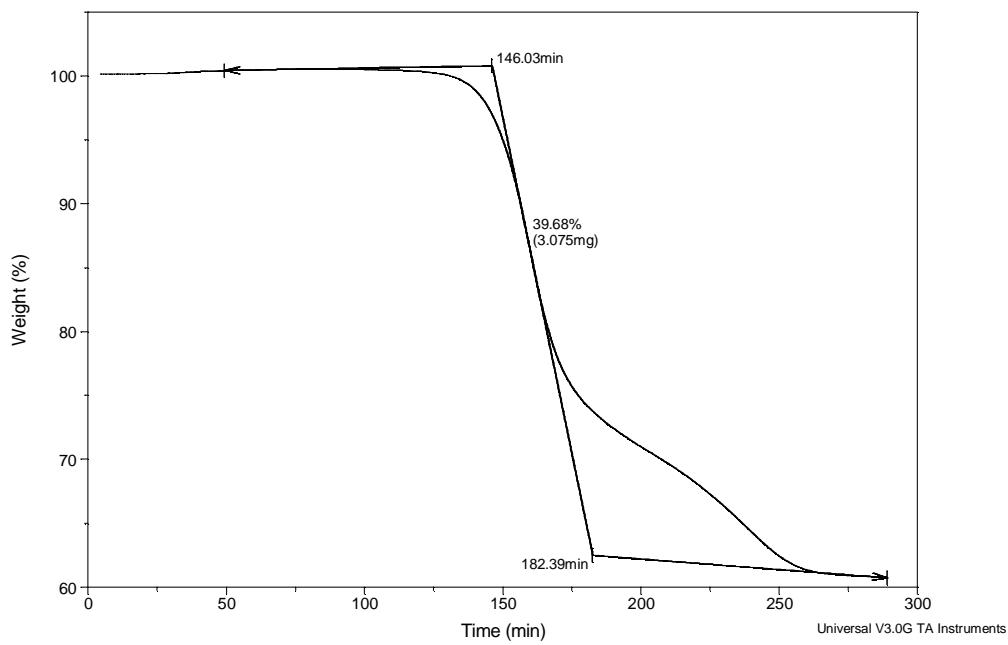


Figure 4: TGA curve for $[\text{Ni}(\text{en})_3]_{0.5}[\text{GaS}_2]$ (**4**).

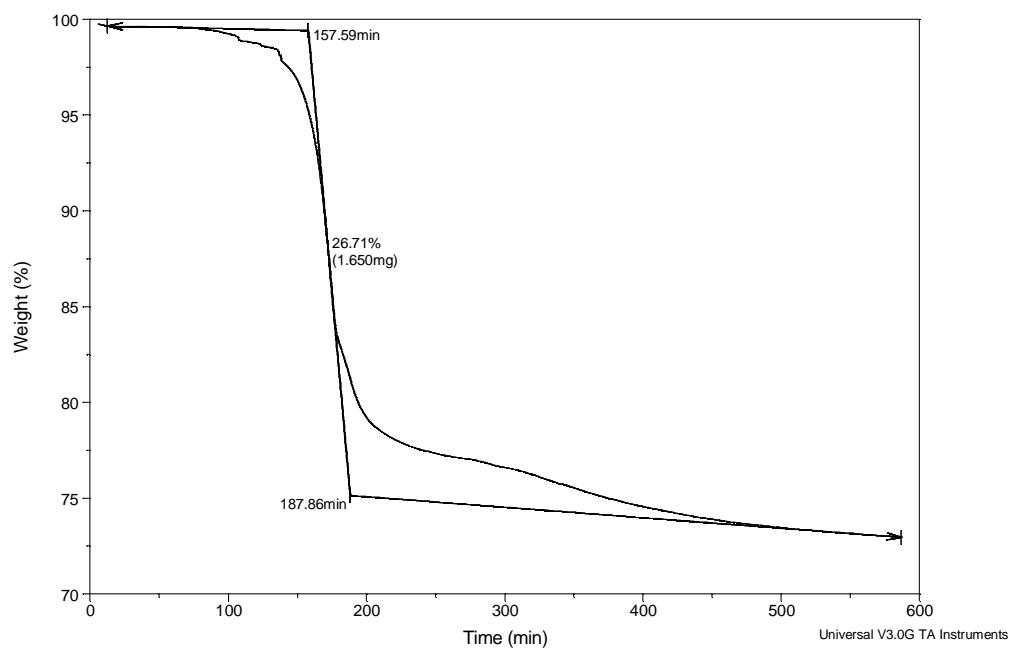


Figure 5: TGA curve for $\text{Mn}(\text{en})_2\text{Ga}_2\text{S}_4$ (**5**).

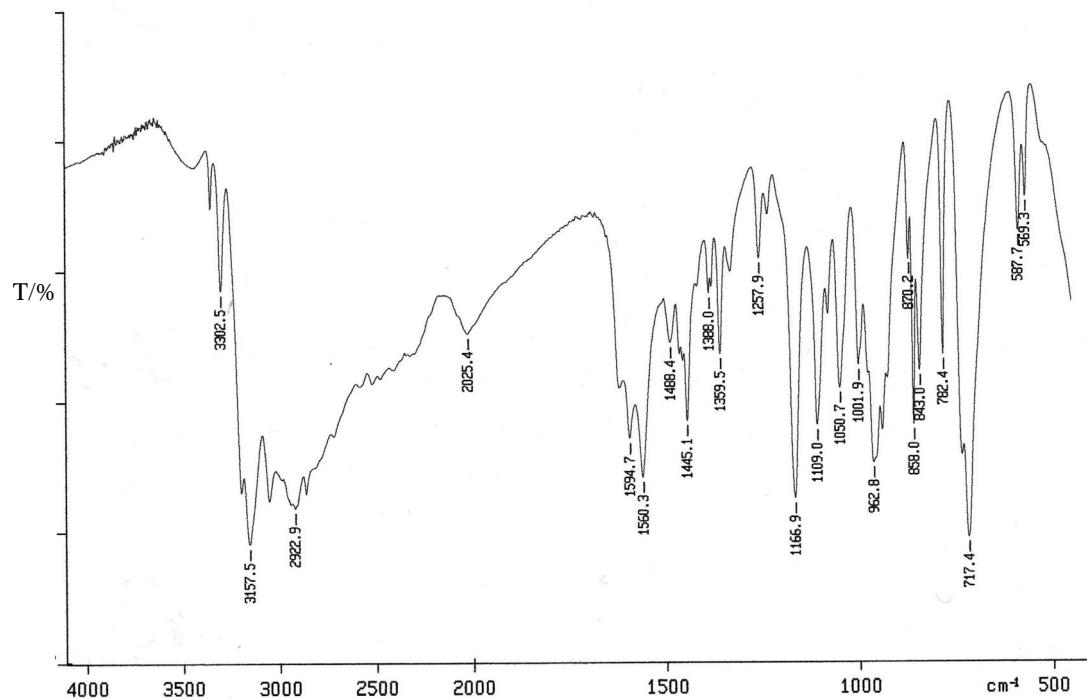


Figure 6: IR spectrum of $[\text{enH}_2][\text{Ga}_4\text{S}_7(\text{en})_2]$ (**1**).