supplementary materials

(I)

Crystal data

$Ga_4O_{19}Zn_{13}$	$F(000) = 2664$
$M_r = 1432.8$	$D_x = 5.671$ Mg m^{-3}
Monoclinic, $C2/m$	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Hall symbol: -C 2y	Cell parameters from 16 reflections
$a = 19.66$ (4) Å	$\theta = 20.1$–$21.0°$
$b = 3.2487$ (5) Å	$\mu = 24.61$ mm^{-1}
$c = 27.31$ (2) Å	$T = 295$ K
$\beta = 105.9$ (1)°	Plate, Colorless
$V = 1678$ (4) Å^3	0.12 × 0.10 × 0.02 mm
$Z = 4$	

Data collection

Four-circle diffractometer	4676 reflections with $I > 2\sigma(I)$
Radiation source: X-ray tube	$R_{int} = 0.088$
graphite	$\theta_{max} = 45.4°$, $\theta_{min} = 2.7°$
ω scans	$h = 0 \rightarrow 38$
Absorption correction: ψ scans ?	$k = -6 \rightarrow 6$
$T_{min} = 0.466$, $T_{max} = 0.996$	$l = -54 \rightarrow 52$
14188 measured reflections	3 standard reflections every 150 reflections
7763 independent reflections	intensity decay: 2.3%

Refinement

Refinement on F^2	111 constraints
$R[F^2 > 2\sigma(F^2)] = 0.061$	Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0001I^2)$
$wR(F^2) = 0.195$	$(\Delta/\sigma)_{max} = 0.012$
$S = 2.88$	$\Delta\rho_{max} = 3.59$ e Å^{-3}
7763 reflections	$\Delta\rho_{min} = -3.74$ e Å^{-3}
225 parameters	Extinction correction: B-C type 1 Gaussian isotropic (Becker & Coppens, 1974)
0 restraints	Extinction coefficient: 310 (20)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.21170 (5)	0	0.53326 (5)	0.0099 (3)	0.7647
Zn2	0.85726 (5)	0	0.59388 (5)	0.0108 (3)	0.7647
Zn3	0.50166 (6)	0	0.64777 (5)	0.0149 (3)	0.7647
Zn4	0.14303 (5)	0	0.70417 (4)	0.0099 (3)	0.7647
Zn5	0.62577 (6)	0	0.30013 (5)	0.0099 (3)	0.7647

Zn6	0.27143 (5)	0	0.36026 (5)	0.0103 (3)	0.7647
Zn7	0.91592 (5)	0	0.42068 (5)	0.0102 (3)	0.7647
Zn8	0.56414 (5)	0	0.47553 (5)	0.0097 (3)	0.7647
Zn9	0.18938 (6)	0	0.82541 (5)	0.0112 (3)	0.7647
Zn10	0.58810 (6)	0	0.88032 (6)	0.0159 (3)	0.7647
Zn11	0.98503 (6)	0	0.93459 (5)	0.0128 (3)	0.7647
Zn12	0.38574 (6)	0	0.99567 (5)	0.0100 (3)	0.7647
Zn13	0.77823 (6)	0	0.05097 (5)	0.0097 (3)	0.7647
Zn14	0.17650 (6)	0	0.11037 (5)	0.0108 (3)	0.7647
Zn15	0.57818 (5)	0	0.17262 (5)	0.0104 (3)	0.7647
Zn16	0.78535 (6)	0	0.76428 (4)	0.0094 (3)	0.7647
Zn17	0.97979 (17)	0	0.23583 (17)	0.0440 (16)	0.352 (3)
Zn18	0.95397 (10)	0.5	0.23574 (8)	0.0098 (5)	0.412 (3)
Ga1	0.21170 (5)	0	0.53326 (5)	0.0099 (3)	0.2353
Ga2	0.85726 (5)	0	0.59388 (5)	0.0108 (3)	0.2353
Ga3	0.50166 (6)	0	0.64777 (5)	0.0149 (3)	0.2353
Ga4	0.14303 (5)	0	0.70417 (4)	0.0099 (3)	0.2353
Ga5	0.62577 (6)	0	0.30013 (5)	0.0099 (3)	0.2353
Ga6	0.27143 (5)	0	0.36026 (5)	0.0103 (3)	0.2353
Ga7	0.91592 (5)	0	0.42068 (5)	0.0102 (3)	0.2353
Ga8	0.56414 (5)	0	0.47553 (5)	0.0097 (3)	0.2353
Ga9	0.18938 (6)	0	0.82541 (5)	0.0112 (3)	0.2353
Ga10	0.58810 (6)	0	0.88032 (6)	0.0159 (3)	0.2353
Ga11	0.98503 (6)	0	0.93459 (5)	0.0128 (3)	0.2353
Ga12	0.38574 (6)	0	0.99567 (5)	0.0100 (3)	0.2353
Ga13	0.77823 (6)	0	0.05097 (5)	0.0097 (3)	0.2353
Ga14	0.17650 (6)	0	0.11037 (5)	0.0108 (3)	0.2353
Ga15	0.57818 (5)	0	0.17262 (5)	0.0104 (3)	0.2353
Ga16	0.78535 (6)	0	0.76428 (4)	0.0094 (3)	0.2353
Ga17	0.97979 (17)	0	0.23583 (17)	0.0440 (16)	0.1084 (10)
Ga18	0.95397 (10)	0.5	0.23574 (8)	0.0098 (5)	0.1269 (10)
O1	0.5357 (4)	0	0.5535 (3)	0.020 (2)	
O2	0.1868 (3)	0	0.6049 (3)	0.0116 (17)	
O3	0.8319 (3)	0	0.6614 (2)	0.0096 (16)	
O4	0.4744 (4)	0	0.7066 (4)	0.054 (5)	
O5	0.2994 (3)	0	0.2959 (2)	0.0072 (15)	
O6	0.9417 (3)	0	0.3543 (3)	0.0116 (17)	
O7	0.5881 (3)	0	0.4040 (3)	0.0117 (17)	
O8	0.2351 (4)	0	0.4553 (3)	0.017 (2)	
O9	0.8873 (4)	0	0.5004 (3)	0.020 (2)	
O10	0.1093 (4)	0	0.7640 (3)	0.022 (2)	
O11	0.5142 (4)	0	0.8192 (3)	0.042 (4)	
O12	0.9070 (3)	0	0.8665 (3)	0.0127 (17)	
O13	0.3008 (4)	0	0.9228 (4)	0.024 (3)	
O14	0.6922 (4)	0	0.9760 (4)	0.033 (3)	
O15	0.0804 (5)	0	0.0222 (5)	0.044 (4)	
O16	0.4632 (4)	0	0.0664 (3)	0.0134 (18)	
O17	0.8561 (3)	0	0.1177 (3)	0.0133 (18)	
O18	0.2552 (3)	0	0.1759 (2)	0.0093 (16)	
O19	0.6568 (3)	0	0.2363 (2)	0.0095 (15)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0060 (3)	0.0045 (4)	0.0173 (5)	0	0.0003 (3)	0
Zn2	0.0069 (3)	0.0058 (4)	0.0178 (5)	0	0.0005 (3)	0
Zn3	0.0066 (4)	0.0086 (5)	0.0275 (6)	0	0.0014 (4)	0
Zn4	0.0079 (4)	0.0065 (4)	0.0140 (5)	0	0.0010 (3)	0
Zn5	0.0082 (4)	0.0079 (5)	0.0133 (4)	0	0.0023 (3)	0
Zn6	0.0073 (4)	0.0058 (4)	0.0158 (5)	0	−0.0002 (3)	0
Zn7	0.0063 (3)	0.0057 (4)	0.0168 (5)	0	0.0000 (3)	0
Zn8	0.0066 (3)	0.0048 (4)	0.0164 (5)	0	0.0007 (3)	0
Zn9	0.0116 (4)	0.0057 (4)	0.0174 (5)	0	0.0059 (4)	0
Zn10	0.0119 (4)	0.0078 (5)	0.0312 (7)	0	0.0114 (4)	0
Zn11	0.0115 (4)	0.0055 (4)	0.0243 (6)	0	0.0096 (4)	0
Zn12	0.0091 (3)	0.0047 (4)	0.0178 (5)	0	0.0064 (3)	0
Zn13	0.0098 (4)	0.0056 (4)	0.0149 (5)	0	0.0054 (3)	0
Zn14	0.0119 (4)	0.0050 (4)	0.0174 (5)	0	0.0068 (3)	0
Zn15	0.0090 (4)	0.0074 (4)	0.0144 (5)	0	0.0024 (3)	0
Zn16	0.0080 (4)	0.0061 (4)	0.0132 (5)	0	0.0015 (3)	0
Zn17	0.0147 (13)	0.070 (4)	0.051 (2)	0	0.0158 (14)	0
Zn18	0.0067 (7)	0.0118 (9)	0.0110 (8)	0	0.0025 (6)	0
Ga1	0.0060 (3)	0.0045 (4)	0.0173 (5)	0	0.0003 (3)	0
Ga2	0.0069 (3)	0.0058 (4)	0.0178 (5)	0	0.0005 (3)	0
Ga3	0.0066 (4)	0.0086 (5)	0.0275 (6)	0	0.0014 (4)	0
Ga4	0.0079 (4)	0.0065 (4)	0.0140 (5)	0	0.0010 (3)	0
Ga5	0.0082 (4)	0.0079 (5)	0.0133 (4)	0	0.0023 (3)	0
Ga6	0.0073 (4)	0.0058 (4)	0.0158 (5)	0	−0.0002 (3)	0
Ga7	0.0063 (3)	0.0057 (4)	0.0168 (5)	0	0.0000 (3)	0
Ga8	0.0066 (3)	0.0048 (4)	0.0164 (5)	0	0.0007 (3)	0
Ga9	0.0116 (4)	0.0057 (4)	0.0174 (5)	0	0.0059 (4)	0
Ga10	0.0119 (4)	0.0078 (5)	0.0312 (7)	0	0.0114 (4)	0
Ga11	0.0115 (4)	0.0055 (4)	0.0243 (6)	0	0.0096 (4)	0
Ga12	0.0091 (3)	0.0047 (4)	0.0178 (5)	0	0.0064 (3)	0
Ga13	0.0098 (4)	0.0056 (4)	0.0149 (5)	0	0.0054 (3)	0
Ga14	0.0119 (4)	0.0050 (4)	0.0174 (5)	0	0.0068 (3)	0
Ga15	0.0090 (4)	0.0074 (4)	0.0144 (5)	0	0.0024 (3)	0
Ga16	0.0080 (4)	0.0061 (4)	0.0132 (5)	0	0.0015 (3)	0
Ga17	0.0147 (13)	0.070 (4)	0.051 (2)	0	0.0158 (14)	0
Ga18	0.0067 (7)	0.0118 (9)	0.0110 (8)	0	0.0025 (6)	0
O1	0.013 (3)	0.007 (3)	0.034 (5)	0	−0.002 (3)	0
O2	0.010 (2)	0.009 (3)	0.015 (3)	0	0.003 (2)	0
O3	0.010 (2)	0.009 (3)	0.010 (3)	0	0.0041 (19)	0
O4	0.011 (3)	0.108 (13)	0.036 (6)	0	−0.004 (3)	0
O5	0.011 (2)	0.008 (3)	0.006 (2)	0	0.0070 (18)	0
O6	0.009 (2)	0.008 (3)	0.016 (3)	0	0.001 (2)	0
O7	0.010 (2)	0.009 (3)	0.015 (3)	0	0.001 (2)	0
O8	0.014 (3)	0.009 (3)	0.024 (4)	0	0.000 (3)	0
O9	0.012 (3)	0.010 (3)	0.033 (4)	0	−0.003 (3)	0
O10	0.022 (3)	0.041 (6)	0.006 (3)	0	0.011 (2)	0
O11	0.018 (3)	0.098 (11)	0.016 (3)	0	0.015 (3)	0
O12	0.012 (2)	0.010 (3)	0.016 (3)	0	0.004 (2)	0
O13	0.020 (3)	0.005 (3)	0.042 (5)	0	0.001 (3)	0

O14	0.019 (3)	0.004 (3)	0.067 (7)	0	−0.002 (4)	0
O15	0.029 (4)	0.005 (3)	0.106 (10)	0	0.029 (6)	0
O16	0.014 (3)	0.009 (3)	0.017 (3)	0	0.004 (2)	0
O17	0.011 (2)	0.018 (4)	0.012 (3)	0	0.005 (2)	0
O18	0.011 (2)	0.011 (3)	0.008 (2)	0	0.0064 (19)	0
O19	0.013 (2)	0.008 (3)	0.007 (2)	0	0.0025 (19)	0

Table *S*1 Correspondence between metal sites *Ps* for the idealized structure in Fig. 5 and *Mn* for the real structure in Fig. 1.

Ps	*Mn*
s = 1	*n*= 12
2	13
3	14
4	15
5	17
6	5
7	6
8	7
9	8
10	1
11	2
12	3
13	4
14	16
15	9
16	10
17	11