

Supplementary Information

Table S1 Dispersive difference maps summary showing peak heights in electrons, peak heights / r.m.s (metal atom assignment), calculated with coefficients $|F_{\text{ref}} - F_{Z_{\text{nf}}}^{\pm}|$, where $F_{Z_{\text{nf}}^{\pm}}$ is data set 3 and F_{ref} are the reference data sets 11, 1, 2, 4, 5, 6 and 7. The values of $Zn? f'$ and $Ga? f'$ are estimated from Sasaki , 1989 (Table 1).

$\lambda 11-\lambda 3$ ($Zn? f'=11.3$ $Ga? f'=2.2e$)	$\lambda 1-\lambda 3$ ($Zn? f'=6.6$ $Ga? f'=0e$)	$\lambda 2-\lambda 3$ ($Zn? f'=5.8$ $Ga? f'=0e$)	$\lambda 4-\lambda 3$ ($Zn? f'=6.1$ $Ga? f'=0e$)	$\lambda 5-\lambda 3$ ($Zn? f'=6.8$ $Ga? f'=0e$)	$\lambda 6-\lambda 3$ ($Zn? f'=7.4$ $Ga? f'=0e$)	$\lambda 7-\lambda 3$ ($Zn? f'=9.1$ $Ga? f'=0e$)
4.41, 17.9 (M1)	1.11, 18.0 (M1)	1.08, 15.7 (M1)	0.95, 14.6 (M1)	1.16, 18.6 (M1)	1.36, 19.4 (M1)	1.58, 19.1 (M1)
4.29, 17.4 (M3)	0.73, 11.7 (M3)	0.82, 12.0 (M3)	0.87, 13.3 (M3)	0.98, 15.7 (M3)	1.15, 16.3 (M3)	1.12, 13.5 (M3)
3.63, 14.8 (M4)	0.27, 4.4	0.30, 4.4	0.24, 3.6	0.25, 4.0	0.36, 5.1 (M7?)	0.51, 6.1 (M4?)
3.48, 14.1 (M7)	0.24, 3.9	0.26, 3.7	0.24, 3.6	0.25, 4.0	0.29, 4.1	0.48, 5.8
3.44, 14.0 (M6)						0.47, 5.7
3.08, 12.5 (M8)						
2.69, 10.9 (M5)						
1.95, 7.9 (M2)						
1.11, 4.5						

Table S2 Dispersive difference maps summary showing peak heights in electrons, peak heights / r.m.s (metal atom assignment), calculated with coefficients $|F_{\text{ref}} - F_{G_{\text{af}}}^{\pm}|$, where $F_{G_{\text{af}}^{\pm}}$ is data set 9 and F_{ref} are the reference data sets 7, 8, 10, and 11. The values of $Zn? f'$ and $Ga? f'$ are estimated from Sasaki , 1989 (Table 1).

$\lambda 7-\lambda 9$ ($Zn? f'=0.6$ $Ga? f'=7.2e$)	$\lambda 8-\lambda 9$ ($Zn? f'=0$ $Ga? f'=2.7e$)	$\lambda 10-\lambda 9$ ($Zn? f'=0.1$ $Ga? f'=5.9e$)	$\lambda 11-\lambda 9$ ($Zn? f'=1.6$ $Ga? f'=10.2e$)
10.22, 21.2 (M7)	3.05, 23.8 (M7)	10.42, 23.3 (M7)	14.90, 21.3 (M7)
9.97, 20.7 (M6)	2.71, 21.1 (M6)	9.54, 21.4 (M4)	14.79, 21.1 (M4)
9.91, 20.6 (M4)	2.67, 20.8 (M4)	9.43, 21.1 (M8)	14.65, 20.9 (M6)
9.40, 19.5 (M8)	2.64, 20.6 (M8)	9.37, 21.0 (M6)	13.62, 19.4 (M8)
8.10, 16.8 (M5)	2.12, 16.6 (M5)	8.01, 17.9 (M5)	11.8, 16.9 (M5)
6.83, 14.2 (M3)	2.06, 16.0 (M3)	6.80, 15.2 (M3)	10.43, 14.9 (M3)
5.42, 11.3 (M1)	1.66, 12.9 (M1)	5.55, 12.4 (M1)	8.69, 12.4 (M1)
4.97, 10.3 (M2)	1.33, 10.4 (M2)	4.75, 10.6 (M2)	7.32, 10.5 (M2)

1.62, 3.4	0.52, 4.1	1.55, 3.5	2.49, 3.7
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Table S3 Peaks heights for anomalous difference maps, showing peak heights in electrons, peak heights / r.m.s (metal atom assignment), calculated for data set 1, 2, 3 and 7, where there is a significant anomalous difference for Zn. The values of Znf " and Gaf " are from Sasaki , 1989 (Table 1).

$\lambda 1$ (Znf"=3.9, Gaf"=0.5e)	$\lambda 2$ (Znf"=3.9, Gaf"=0.6e)	$\lambda 3$ (Znf"=2, Gaf"=0.6e)	$\lambda 7$ (Znf"=3.6, Gaf"=0.5e)
1.72, 18.7 (M1)	1.71, 17.5 (M1)	1.30, 13.5 (M1)	1.65, 19.8 (M1)
1.18, 12.8 (M3)	1.09, 11.2 (M3)	1.08, 11.3 (M3)	1.16, 13.9 (M3)
0.38, 4.1	0.39, 4.0	0.39, 4.1	0.36, 4.3

Table S4 Peaks heights for anomalous difference maps, showing peak heights in electrons, peak heights / r.m.s (metal atom assignment), calculated for data sets 8, 9 and 10, where there is a significant anomalous difference for both Ga and Zn, which is reduced for Ga for data set 9. The values of Znf " and Gaf " are from Sasaki , 1989 (Table 1). Those peaks marked (?) are at positions which cannot be related to one of the eight metal atom sites.

$\lambda 8$ (Znf"=3.4, Gaf"=3.9e)	$\lambda 9$ (Znf"=3.4, Gaf"=2e)	$\lambda 10$ (Znf"=3.3, Gaf"=3.8e)
4.01, 12.2 (M7)	1.88, 9.4 (M1)	4.94, 9.8 (M7)
3.86, 11.7 (M8)	1.74, 8.7 (M3)	4.84, 9.7 (M4)
2.47, 7.5 (M4)	1.50, 7.5 (M6)	4.77, 9.5 (M6)
2.41, 7.3 (M6)	1.48, 7.4 (M4)	4.62, 9.2 (M8)
2.06, 6.3 (M3)	1.44, 7.2 (M7)	3.37, 6.8 (M3)

2.05, 6.2 (?)	1.39, 7.0 (M8)	3.08, 6.2 (?)
1.91, 5.8 (M1)	1.09, 5.5 (?)	2.85, 5.7 (M5)
1.72, 5.2 (M5)	1.03, 5.2 (M5)	2.8, 5.7 (M1)
1.63, 5.0 (?)	0.93, 4.6 (?)	2.45, 4.9 (?)
1.25, 3.8 (M2) Peak 20	0.84, 4.2 (M2) peak 15	2.45, 4.9 (M2) Peak 10

Table S5 SCALEIT summary of the 11 data sets scaled to Fo of the final refinement of the structure using data set 11 in SHELXL, i.e. placing all the data sets on an approximately absolute scale (a) shows RMS differences, where RMSiso is the dispersive difference for the derivative versus Fo and RMSano is the anomalous difference for each derivative, in arbitrary units. (b) Shows the R values of the derivatives as a fraction of Fo versus Fo and one with another.

(a)

RMS differences	RMSiso	RMSano
F_1	6.34	2.69
F_2	6.35	2.86
F_3	6.70	2.82
F_4	6.05	2.11
F_5	6.11	2.30
F_6	6.05	2.55
F_7	7.18	2.40
F_8	17.13	9.45
F_9	19.27	5.74
F_10	8.92	14.32
F_11	0.8	3.41

(b)

Riso	Fo	F_1	F_2	F_3	F_4	F_5	F_6	F_7	F_8	F_9	F_10	F_11
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Fo	-	0.071	0.071	0.075	0.068	0.068	0.067	0.083	0.209	0.238	0.106	0.007
F_1	-	0.018	0.021	0.018	0.019	0.022	0.024	0.138	0.160	0.055	0.073	
F_2	-	0.022	0.017	0.019	0.021	0.025	0.138	0.161	0.063	0.073		
F_3	-	0.021	0.021	0.023	0.030	0.139	0.161	0.067	0.077			
F_4	-	0.017	0.019	0.024	0.140	0.162	0.054	0.070				
F_5	-	0.018	0.025	0.140	0.162	0.059	0.070					
F_6	-	0.027	0.141	0.163	0.066	0.069						
F_7	-	0.129	0.149	0.051	0.085							
F_8	-	0.040	0.111	0.206								
F_9	-	0.140	0.240									
F_10	-	-	0.104									
F_11	-	-	-									

Table S6 MLPHARE results. Isomorphous values in electrons, Di-j, and anomalous values in electrons, ANO*i*, for each metal atom site. The isomorphous values arise from the differences in f ' between the data sets i and j, measured at different wavelengths. The anomalous values arise from the f " value for data set i. Results are shown from data sets measured around (a) the Ga K absorption edge, (b) the Zn K absorption edge.

(a)

	D10-8	ANO8	D10-9	ANO9	ANO10	D7-8	D7-9	D7-10	D11-8	D11-9	D11-10
M1	-3.193	2.278	-3.712	1.610	4.125	-4.603	-5.123	-0.996	-7.335	-7.951	-4.028
M2	-4.413	1.997	-5.025	1.231	4.179	-5.833	-6.421	-1.181	-8.465	-9.329	-4.533
M3	-3.345	2.213	-3.900	1.525	4.122	-4.882	-5.426	-1.039	-7.503	-8.158	-4.090
M4	-4.123	2.007	-4.633	1.181	4.134	-5.875	-6.319	-1.391	-8.437	-8.902	-4.536
M5	-4.038	1.855	-4.600	1.072	3.740	-5.463	-6.075	-1.108	-8.248	-8.948	-4.380
M6	-4.132	2.007	-4.697	1.161	4.021	-5.729	-6.303	-1.291	-8.368	-8.806	-4.436
M7	-4.142	2.111	-4.724	1.040	4.042	-5.551	-6.178	-1.046	-8.343	-9.009	-4.326
M8	-4.176	2.064	-4.780	1.001	3.892	-5.517	-6.083	-0.999	-8.293	-8.974	-4.276

(b)

	ANO1	ANO2	ANO3	D4-3	D5-3	D6-3	D7-3	D11-3
M1	0.877	0.880	0.762	-0.435	-0.578	-0.735	-0.418	-3.636
M2	0.276	0.265	0.279	0.004	-0.125	-0.161	0.919	-2.919
M3	0.723	0.723	0.646	-0.319	-0.462	-0.741	-0.079	-3.378
M4	0.217	0.236	0.250	-0.018	-0.088	-0.195	0.823	-2.784
M5	0.210	0.207	0.217	-0.024	-0.098	-0.180	0.833	-2.802
M6	0.256	0.220	0.266	-0.020	-0.115	-0.148	0.880	-2.743
M7	0.272	0.282	0.284	-0.029	-0.112	-0.131	0.849	-2.832
M8	0.274	0.273	0.242	-0.002	-0.051	-0.163	0.845	-2.850

Table S7

MLPHARE, Model 1 and Model 2 values of Zn and Ga f' and f'' used in the JANA2006 multi-wavelength refinement of the metal atom occupancies. Values that are high-lighted in bold were determined using MLPHARE or JANA2006. Other values are from Sasaki, or input by JANA2006 for that wavelength (i.e. not refined). NB for Models 1 and 2, MLPHARE derived Ga occupancies of 0.78 and 0.82 for sites 1 and 3 were employed (with Zn occupancies of 0.22 and 0.18), and either 1.0 Ga and 0.0 Zn occupancies (Model 1) or 0.95 Ga and 0.05 Zn occupancies (Model 2), for the other metal atom sites

?	MLPHARE or Sasaki Zn f', f'' (e)	MLPHARE or Sasaki Ga f', f'' (e)	JANA2006 Model 1 Zn f , f'' (e)	JANA2006 Model 1 Ga f', f'' (e)	JANA2006 Model 2 Zn f , f'' (e)	JANA2006 Model 2 Ga f', f'' (e)
1	-4.882, 3.877	-2.529, 0.547	-4.0(2), 2.8(2)	-2.467, 0.564	-5.0(2), 2.7(2)	-2.467, 0.564
2	-5.660, 3.887	-2.422, 0.555	-3.8(2), 2.8(2)	-2.430, 0.567	-4.8(2), 2.7(2)	-2.430, 0.567
3	-7.3, 2.5	-2.422, 0.555	-6.2(2), 2.2(2)	-2.395, 0.569	-7.1(2), 2.1(2)	-2.395, 0.569
4	-5.391, 0.489	-2.422, 0.555	-4.0(2), 0.489	-2.350 0.573	-4.6(2), 0.489	-2.350 0.573
6	-4.015, 0.498	-2.246, 0.571	-2.8(2), 0.498	-2.212 0.585	-3.6(2), 0.498	-2.212 0.585
7	-2.394, 3.578	-3.223, 0.516	-1.9(1), 2.5(2)	-3.51(2), 0.51	-1.4(2), 2.7(2)	-3.58(2), 0.51
8	-1.648, 3.395	-8.7, 1.75	-1.648, 3.395	-8.42(2), 2.53(2)	-1.648, 3.395	-8.61(2), 2.49(2)
9	-1.654, 3.397	-9.2, 1.0	-1.654, 3.397	-8.86(2), 1.23(2)	-1.654, 3.397	-9.14(2), 1.22(2)
10	-1.555, 3.361	-4.531, 3.837	-1.555, 3.361	-4.84(2), 4.29(2)	-1.555, 3.361	-4.91(2), 4.35(2)

11	0.219, 1.328	0.172, 1.495	0.219, 1.328	0.172, 1.495	0.219, 1.328	0.172, 1.495
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Note Wavelength 5 was not used in the multi-wavelength JANA2006 refinements as ten wavelengths were the maximum allowed for JANA2006. This wavelength was at the base of the absorption edge and wavelengths 4 and 6 were likewise.

Table S8 Input coordinates file for MLPHARE for the eight metal atom sites, with starting values of the occupancy and anomalous occupancies of -1 and 2, and B factors taken from the refined structure. Note that the input atom types are given as ‘Ano’ so that the refined occupancies should indicate the number of electrons.

		x	y	z				
ATOM	Ano	0.437709	0.917631	0.114078	-1	2	bfac	1.96
ATOM	Ano	0.159325	0.654872	0.083927	-1	2	bfac	4.79
ATOM	Ano	0.559369	0.928979	0.380720	-1	2	bfac	1.79
ATOM	Ano	0.263207	0.586365	0.398302	-1	2	bfac	1.2
ATOM	Ano	0.345537	0.829479	0.591931	-1	2	bfac	2.02
ATOM	Ano	0.259018	0.395410	0.102087	-1	2	bfac	1.18
ATOM	Ano	0.225136	0.205603	0.079635	-1	2	bfac	1.33
ATOM	Ano	0.230917	0.775143	0.422913	-1	2	bfac	1.34

Figure S1 The whole framework structure determined from the ‘best phases’ derived from the MAD signals for Ga and Zn by MLPHARE.

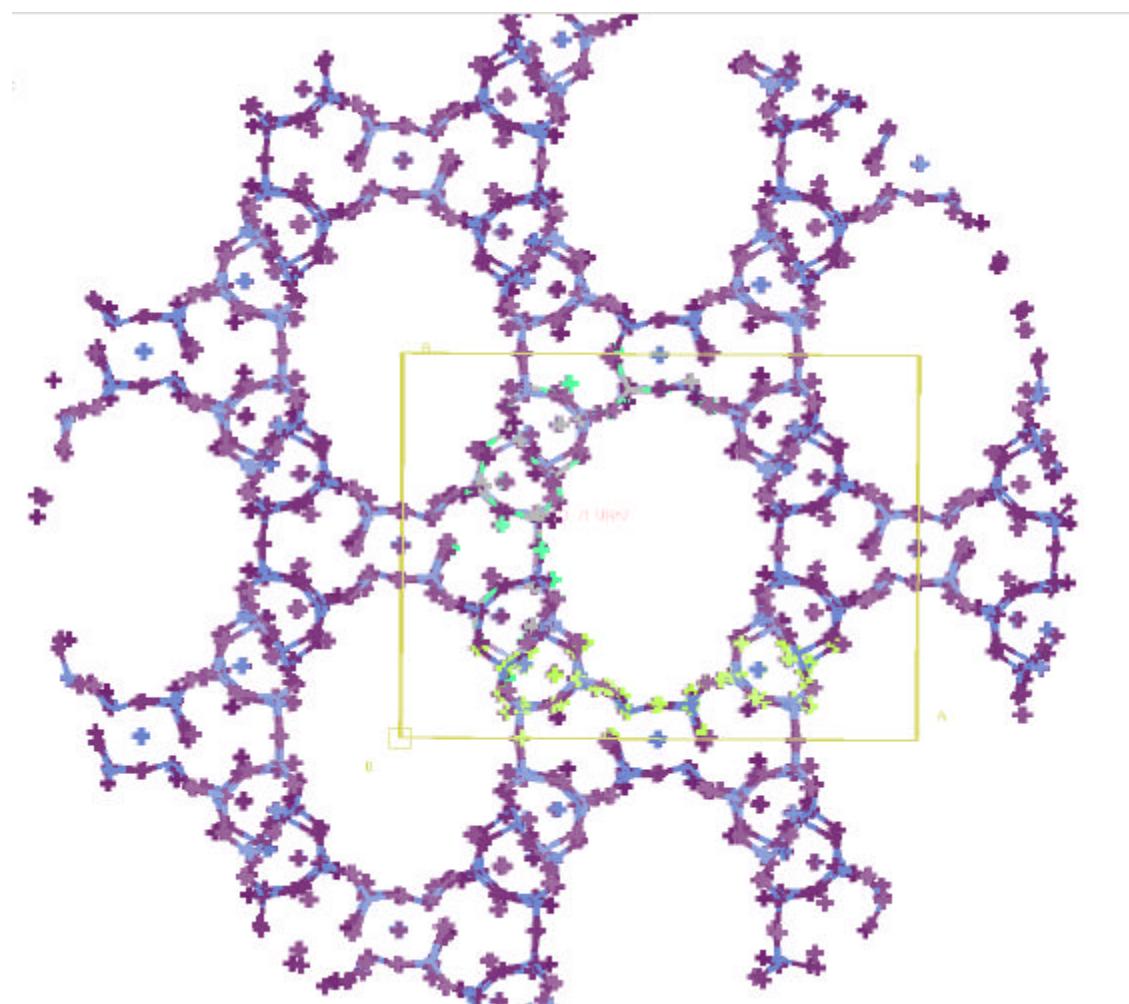


Figure S2 A close in view of a tetrahedral phosphate group of the framework, from the ‘best phases’ derived from the MAD signals for Ga and Zn in MLPHARE again nicely illustrating that the phasing quality is high.

