Supplementary Materials: Three–D Mineralogical Mapping of the Kovdor Phoscorite–Carbonatite Complex, NW Russia: I. Forsterite

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1. X-Ray Supplementary Data for Forsterite_1

Table S1. Fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for Forsterite_1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}
Si1	4058.7(9)	7500	739.6(19)	3.2(3)
*M*2	2225.8(10)	7500	5100(2)	2.0(4)
Fe2	2225.8(10)	7500	5100(2)	2.0(4)
*M*1	5000	5000	5000	1.6(4)
Fe1	5000	5000	5000	1.6(4)
O1	4088(2)	7500	−2661(5)	3.7(5)
O2	3370.1(15)	5338(3)	2227(3)	4.3(4)
O3	5527(2)	7500	2212(5)	4.8(5)

Table S2. Anisotropic displacement parameters (Å^2 × 10^3) for Forsterite_1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a \times {}^2U_{11} + 2hka \times b \times U_{12} + \ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	4.2(5)	3.1(5)	2.4(5)	0	−0.2(3)	0
*M*2	2.7(6)	1.2(6)	2.1(6)	0	−0.5(4)	0
Fe2	2.7(6)	1.2(6)	2.1(6)	0	−0.5(4)	0
*M*1	3.0(6)	1.2(7)	0.7(6)	0.6(4)	0.6(4)	0.2(4)
Fe1	3.0(6)	1.2(7)	0.7(6)	0.6(4)	0.6(4)	0.2(4)
O1	5.9(10)	2.5(11)	2.7(10)	0	−0.1(8)	0
O2	4.9(8)	4.1(8)	4.0(8)	−0.2(7)	0.6(6)	0.0(7)
O3	5.5(11)	4.0(11)	5.0(11)	0	0.5(9)	0

Table S3. Bond lengths for Forsterite_1.

Atom	Atom	Length/Å
Si1	O1	1.612(3)
Si1	O2	1.6301(16)
Si1	$O2^4$	1.6301(16)
Si1	O3	1.651(2)
*M*2	$O1^6$	2.174(3)
*M*2	$O2^7$	2.0635(17)
*M*2	O2	2.2097(18)
*M*2	$O2^8$	2.0635(17)
*M*2	$O2^4$	2.2097(18)
*M*2	$O3^5$	2.049(2)
*M*1	$O1^{11}$	2.0792(17)
*M*1	$O1^6$	2.0792(17)
*M*1	O2	2.1278(16)

*M*1	O2[9]	2.1278(16)
*M*1	O3[9]	2.0650(16)
*M*1	O3	2.0650(16)

[1]1 − *X*, 1/2 + *Y*, −*Z*; [2]1 − *X*, 1/2 + *Y*, 1 − *Z*; [3]+*X*, +*Y*, −1 + *Z*; [4]+*X*, 3/2 − *Y*, +*Z*; [5]−1/2 + *X*, +*Y*, 1/2 − *Z*; [6]+*X*, +*Y*, 1 + *Z*; [7]1/2 − *X*, 1/2 + *Y*, 1/2 + *Z*; [8]1/2 − *X*, 1 − *Y*, 1/2 + *Z*; [9]1 − *X*, 1 − *Y*, 1 − *Z*; [10]1 − *X*, −1/2 + *Y*, 1 − *Z*; [11]1 − *X*, 1 − *Y*, −*Z*; [12]1/2 − *X*, 1 − *Y*, −1/2 + *Z*; [13]1/2 + *X*, +*Y*, 1/2 – *Z*.

Table S4. Atomic occupancy for Forsterite_1.

Atom	Occupancy
*M*2	0.965(5)
Fe1	0.020(4)
Fe2	0.035(5)
*M*1	0.980(4)

2. X-Ray Supplementary Data for Forsterite_2

Table S5. Fractional atomic coordinates (×10[4]) and equivalent isotropic displacement parameters (Å[2] × 10[3]) for Forsterite_2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U_{eq}
Si1	4058.6(8)	7500	733.7(17)	3.9(3)
*M*2	2226.2(9)	7500	5102.3(17)	2.7(3)
Fe2	2226.2(9)	7500	5102.3(17)	2.7(3)
*M*1	5000	5000	5000	2.7(3)
Mg1	5000	5000	5000	2.7(3)
O1	4087(2)	7500	−2661(4)	5.4(5)
O2	3368.5(14)	5335(2)	2223(3)	5.3(4)
O3	5526(2)	7500	2212(4)	5.0(4)

Table S6. Anisotropic displacement parameters (Å[2] × 10[3]) for Forsterite_2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a \times {}^2U_{11} + 2hka \times b \times U_{12} + \ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	5.9(4)	4.4(4)	1.4(4)	0	0.1(3)	0
*M*2	4.7(4)	3.0(4)	0.4(4)	0	0.1(2)	0
Fe2	4.7(4)	3.0(4)	0.4(4)	0	0.1(2)	0
*M*1	4.7(4)	3.0(4)	0.4(4)	0	0.1(2)	0
Mg1	4.7(4)	3.0(4)	0.4(4)	0	0.1(2)	0
O1	7.7(10)	7.6(10)	0.8(9)	0	0.2(7)	0
O2	8.1(7)	6.1(7)	1.8(7)	0.4(5)	0.0(5)	0.3(6)
O3	6.7(10)	5.7(10)	2.6(9)	0	0.3(8)	0

Table S7. Bond lengths for Forsterite_2.

Atom	Atom	Length/Å
Si1	O1	1.617(2)
Si1	O2[4]	1.6379(15)
Si1	O2	1.6379(15)
Si1	O3	1.656(2)
*M*2	O1[6]	2.179(2)
*M*2	O2[4]	2.2192(16)
*M*2	O2	2.2191(16)
*M*2	O2[7]	2.0671(15)

*M*2	O2[8]	2.0671(15)
*M*2	O3[5]	2.058(2)
*M*1	O1[6]	2.0867(15)
*M*1	O1[11]	2.0867(15)
*M*1	O2	2.1371(14)
*M*1	O2[9]	2.1371(14)
*M*1	O3	2.0721(14)
*M*1	O3[9]	2.0721(14)

[1]1 − *X*, 1/2 + *Y*, 1 − *Z*; [2]+X, +*Y*, −1 + *Z*; [3]1 − *X*, 1/2 + *Y*, −*Z*; [4]+*X*, 3/2 − *Y*, +*Z*; [5]−1/2 + *X*, +*Y*, 1/2 − *Z*; [6]+*X*, +*Y*, 1 + *Z*; [7]1/2 − *X*, 1/2 + *Y*, 1/2 + *Z*; [8]1/2 − *X*, 1−*Y*, 1/2 + *Z*; [9]1 − *X*, 1 − *Y*, 1 − *Z*; [10]1 − *X*, −1/2 + *Y*, 1 − *Z*; [11]1 − *X*, 1 − *Y*, −*Z*; [12]1/2 − *X*, 1 − *Y*, −1/2 + *Z*; [13]1/2 + X, +*Y*, 1/2 − *Z*.

Table S8. Atomic occupancy for Forsterite_2.

Atom	Occupancy
*M*2	0.932(4)
Mg1	0.941(3)
Fe2	0.068(4)
*M*1	0.059(3)

3. X-Ray Supplementary Data for Forsterite_3

Table S9. Fractional atomic coordinates (×10[4]) and equivalent isotropic displacement parameters (Å[2] × 10[3]) for Forsterite_3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U_{eq}
Si1	4058.3(10)	7500	733(2)	3.8(3)
*M*2	2223.9(10)	7500	5104(2)	2.7(4)
Fe2	2223.9(10)	7500	5104(2)	2.7(4)
*M*1	5000	5000	5000	3.1(4)
Mg1	5000	5000	5000	3.1(4)
O1	4085(2)	7500	−2664(5)	3.6(6)
O2	3369.0(16)	5335(3)	2218(4)	5.0(4)
O3	5523(2)	7500	2207(5)	3.9(6)

Table S10. Anisotropic displacement parameters (Å[2] × 10[3]) for Forsterite_3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a \times {}^2U_{11} + 2hka \times b \times U_{12} + \ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	3.3(5)	4.5(5)	3.6(6)	0	0.1(4)	0
*M*2	2.3(5)	2.8(6)	2.9(7)	0	−0.1(4)	0
Fe2	2.3(5)	2.8(6)	2.9(7)	0	−0.1(4)	0
*M*1	3.5(5)	3.0(6)	2.9(7)	0.1(4)	0.6(4)	0.3(4)
Mg1	3.5(5)	3.0(6)	2.9(7)	0.1(4)	0.6(4)	0.3(4)
O1	4.7(11)	4.0(11)	2.1(14)	0	−0.6(10)	0
O2	6.2(8)	4.9(8)	3.9(10)	0.1(7)	0.1(7)	−0.4(7)
O3	3.7(11)	3.9(12)	4.1(14)	0	0.8(10)	0

Table S11. Bond lengths for Forsterite_3.

Atom	Atom	Length/Å
Si1	O1	1.617(3)
Si1	O2[4]	1.6359(17)
Si1	O2	1.6359(17)

Si1	O3	1.652(3)
*M*2	O1[6]	2.177(3)
*M*2	O2[7]	2.0639(17)
*M*2	O2[4]	2.2214(19)
*M*2	O2	2.2215(19)
*M*2	O2[8]	2.0639(17)
*M*2	O3[5]	2.056(3)
*M*1	O1[6]	2.0855(17)
*M*1	O1[11]	2.0855(17)
*M*1	O2[9]	2.1369(17)
*M*1	O2	2.1369(17)
*M*1	O3[9]	2.0721(17)
*M*1	O3	2.0721(17)

[1]1/2 + *X*, +*Y*, 1/2 − *Z*; [2]1 − *X*, 1/2 + *Y*, 1 − *Z*; [3]+*X*, +*Y*, −1 + *Z*; [4]+*X*, 3/2 − *Y*, +*Z*; [5]−1/2 + *X*, +*Y*, 1/2 − *Z*; [6]+*X*, +*Y*, 1 + *Z*; [7]1/2 − *X*, 1/2 + *Y*, 1/2 + *Z*; [8]1/2 − *X*, 1 − *Y*, 1/2 + *Z*; [9]1 − *X*, 1 − *Y*, 1 − *Z*; [10]1 − *X*, −1/2 + *Y*, 1 − *Z*; [11]1 − *X*, 1 − *Y*, −*Z*; [12]1 −*X*, 1/2 + *Y*, −*Z*; [13]1/2 − *X*, 1 − *Y*, −1/2 + *Z*.

Table S12. Atomic occupancy for Forsterite_3.

Atom	Occupancy
*M*2	0.916(4)
Mg1	0.920(4)
Fe2	0.084(4)
*M*1	0.080(4)

4. X-Ray Supplementary Data for Forsterite_4

Table S13. Fractional atomic coordinates (×10[4]) and equivalent isotropic displacement parameters (Å[2] × 10[3]) for Forsterite_4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U_{eq}
Si1	4056.9(8)	7500	736.7(17)	3.6(2)
*M*2	2226.4(9)	7500	5101.5(19)	2.1(3)
Fe2	2226.4(9)	7500	5101.5(19)	2.1(3)
*M*1	5000	5000	5000	2.2(3)
Fe1	5000	5000	5000	2.2(3)
O1	4086(2)	7500	−2660(4)	4.7(5)
O2	3368.9(13)	5334(2)	2225(3)	4.5(3)
O3	5523.9(19)	7500	2213(4)	5.0(5)

Table S14. Anisotropic displacement parameters (Å[2] × 10[3]) for Forsterite_4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a \times {}^2U_{11} + 2hka \times b \times U_{12} + \ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	3.5(4)	3.4(4)	3.8(4)	0	−0.1(3)	0
*M*2	1.3(5)	1.8(5)	3.1(5)	0	−0.1(3)	0
Fe2	1.3(5)	1.8(5)	3.1(5)	0	−0.1(3)	0
*M*1	3.1(5)	1.3(5)	2.2(5)	0.1(3)	0.1(4)	0.9(4)
Fe1	3.1(5)	1.3(5)	2.2(5)	0.1(3)	0.1(4)	0.9(4)
O1	5.1(9)	6(1)	3(1)	0	−0.1(8)	0
O2	5.2(6)	5.3(7)	3.0(7)	0.0(6)	0.6(6)	0.5(6)
O3	5.1(9)	5(1)	4.8(9)	0	0.2(9)	0

Table S15. Bond lengths for Forsterite_4.

Atom	Atom	Length/Å
Si1	O1	1.615(2)
Si1	O2[4]	1.6339(15)
Si1	O2	1.6339(15)
Si1	O3	1.653(2)
*M*2	O1[6]	2.175(2)
*M*2	O2[7]	2.0635(15)
*M*2	O2[4]	2.2147(16)
*M*2	O2[8]	2.0635(15)
*M*2	O2	2.2147(16)
*M*2	O3[5]	2.056(2)
*M*1	O1[11]	2.0836(15)
*M*1	O1[6]	2.0836(15)
*M*1	O2	2.1330(14)
*M*1	O2[9]	2.1330(14)
*M*1	O3	2.0676(14)
*M*1	O3[9]	2.0676(14)

[1]1 − *X*, 1/2 + *Y*, −*Z*; [2]1 − *X*, 1/2 + *Y*, 1 − Z; [3]+*X*, +*Y*, −1 + *Z*; [4]+*X*, 3/2 − *Y*, +Z; [5]−1/2 + *X*, +*Y*, 1/2 − *Z*; [6]+*X*, +*Y*, 1 + *Z*; [7]1/2 − *X*, 1/2 + *Y*, 1/2 + *Z*; [8]1/2 − *X*, 1 − *Y*, 1/2 + *Z*; [9]1 − *X*, 1 − *Y*, 1 − *Z*; [10]1 − *X*, −1/2 + *Y*, 1 − *Z*; [11]1 − *X*, 1 − *Y*, −*Z*; [12]1/2 − *X*, 1 − *Y*, −1/2 + *Z*; [13]1/2 + *X*, +*Y*, 1/2 – *Z*.

Table S16. Atomic occupancy for Forsterite_4.

Atom	Occupancy
*M*2	0.943(4)
Fe1	0.048(3)
Fe2	0.057(4)
*M*1	0.952(3)

5. X-Ray Supplementary Data for Forsterite_5

Table S17. Fractional atomic coordinates (×10[4]) and equivalent isotropic displacement parameters (Å[2] × 10[3]) for Forsterite_5. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U^{eq}
Si1	4058.3(8)	7500	738.3(17)	3.3(3)
*M*2	2226.4(9)	7500	5099.9(18)	2.2(3)
Fe2	2226.4(9)	7500	5099.9(18)	2.2(3)
*M*1	5000	5000	5000	2.2(3)
Fe1	5000	5000	5000	2.2(3)
O1	4086(2)	7500	−2661(4)	4.3(5)
O2	3370.2(13)	5338(2)	2225(3)	4.4(3)
O3	5525(2)	7500	2207(4)	4.7(5)

Table S18. Anisotropic displacement parameters (Å[2] × 10[3]) for Forsterite_5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a \times {}^2U_{11} + 2hka \times b \times U_{12} + \ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	4.1(4)	2.5(4)	3.2(4)	0	0.2(3)	0
*M*2	2.3(5)	1.1(5)	3.1(5)	0	0.2(3)	0
Fe2	2.3(5)	1.1(5)	3.1(5)	0	0.2(3)	0
*M*1	3.0(5)	1.0(5)	2.5(5)	0.1(3)	0.2(3)	0.6(3)
Fe1	3.0(5)	1.0(5)	2.5(5)	0.1(3)	0.2(3)	0.6(3)

O1	4.8(10)	3.3(9)	4.7(10)	0	0.5(8)	0
O2	5.7(7)	3.6(6)	3.8(7)	0.2(5)	0.3(5)	−0.4(6)
O3	6.5(10)	4.0(9)	3.7(9)	0	−0.4(8)	0

Table S19. Bond lengths for Forsterite_5.

Atom	Atom	Length/Å
Si1	O1	1.616(2)
Si1	O2[4]	1.6323(14)
Si1	O2	1.6323(14)
Si1	O3	1.650(2)
*M*2	O1[6]	2.174(2)
*M*2	O2[7]	2.0669(15)
*M*2	O2[4]	2.2137(16)
*M*2	O2[8]	2.0669(15)
*M*2	O2	2.2137(16)
*M*2	O3[5]	2.053(2)
*M*1	O1[11]	2.0836(14)
*M*1	O1[6]	2.0836(14)
*M*1	O2	2.1316(14)
*M*1	O2[9]	2.1316(14)
*M*1	O3	2.0701(14)
*M*1	O3[9]	2.0701(14)

[1]1/2 + *X*, +*Y*, 1/2 − *Z*; [2]1 − *X*, 1/2 + *Y*, 1 − *Z*; [3]+X, +*Y*, −1 + *Z*; [4]+*X*, 3/2 − *Y*, +*Z*; [5]−1/2 + *X*, +*Y*, 1/2 − *Z*; [6]+*X*, +*Y*, 1 + *Z*; [7]1/2 − *X*, 1/2 + *Y*, 1/2 + *Z*; [8]1/2 − *X*, 1 − *Y*, 1/2 + *Z*; [9]1 − *X*, 1 − *Y*, 1 − *Z*; [10]1 − *X*, −1/2 + *Y*, 1 − *Z*; [11]1 − *X*, 1 − *Y*, −*Z*; [12]1 − *X*, 1/2 + *Y*, −*Z*; [13]1/2 − *X*, 1 − *Y*, −1/2 + *Z*.

Table S20. Atomic occupancy for Forsterite_5.

Atom	Occupancy
*M*2	0.946(4)
Fe1	0.040(4)
Fe2	0.054(4)
*M*1	0.960(4)