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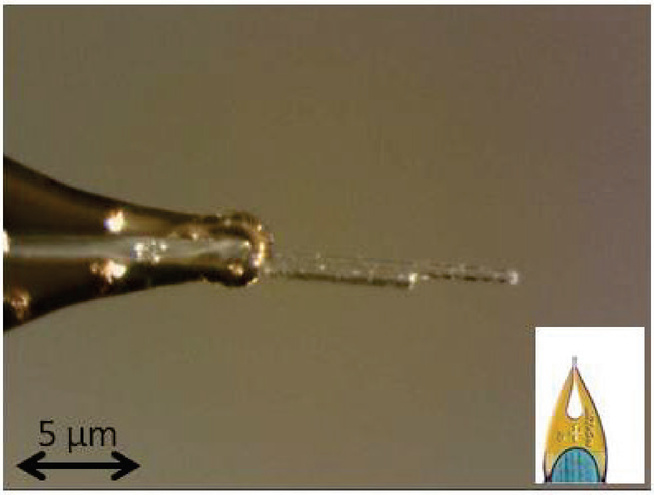
Supporting information for article:

Depicting the crystal structure of fibrous ferrierite from British Columbia using a combined synchrotron techniques approach

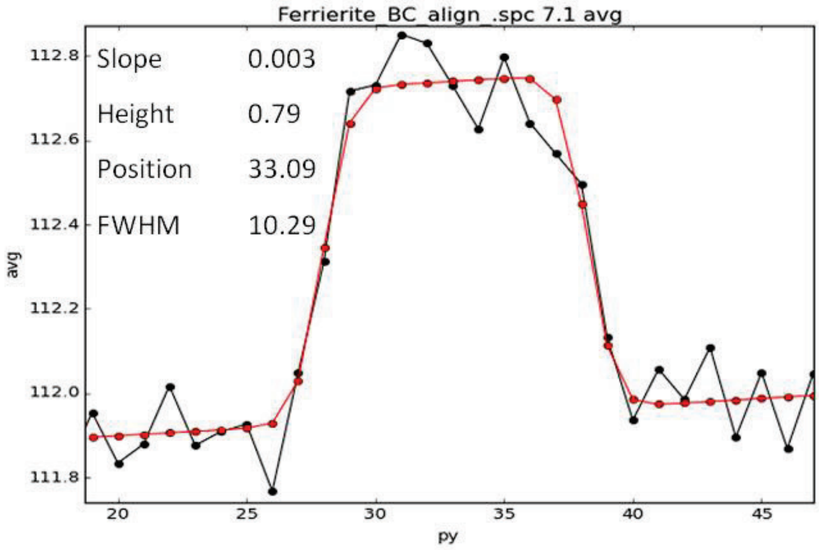
Carlotta Giacobbe, Jonathan Wright, Catherine Dejoie, Paul Tafforeau, Camille Berruyer, Ruggero Vigliaturo, Reto Gieré and Alessandro F. Gualtieri

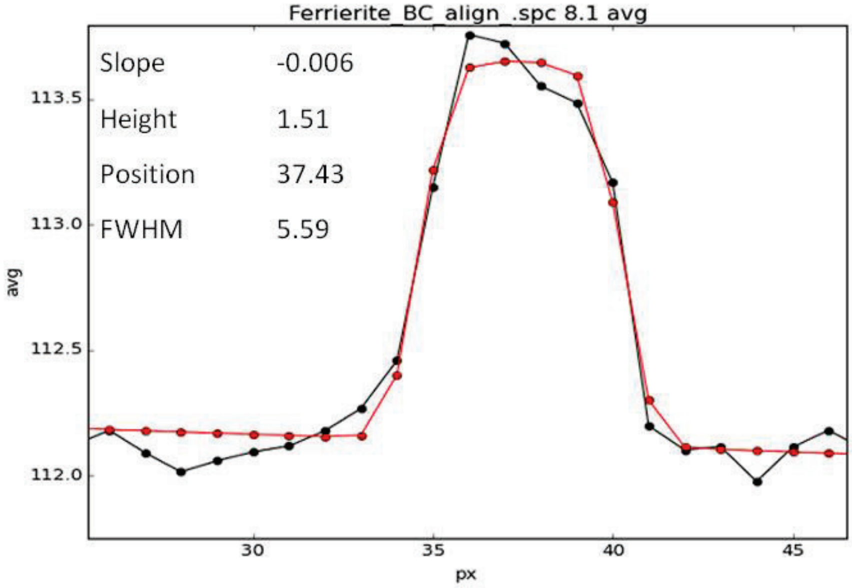
Supporting Information for article

Depicting the crystal structure of fibrous ferrierite from British Columbia using a combined synchrotron technique approach.

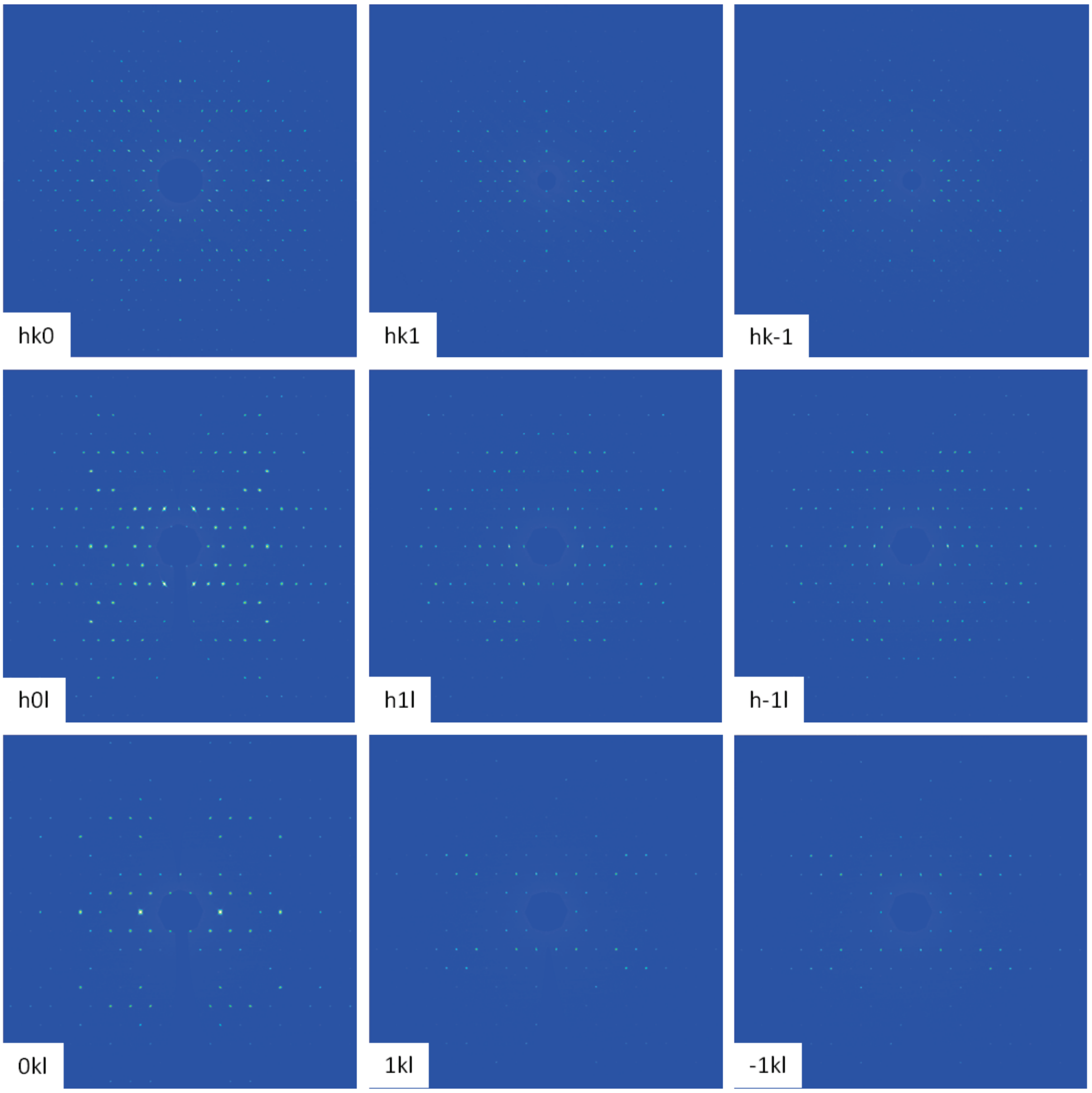


S1. A prismatic fibre of ferrierite glued on a MiTeGen microloop. A precise estimation of the size of the fibre has been accomplished during the alignment phase using the nano X-ray beam (see S2. for further description).

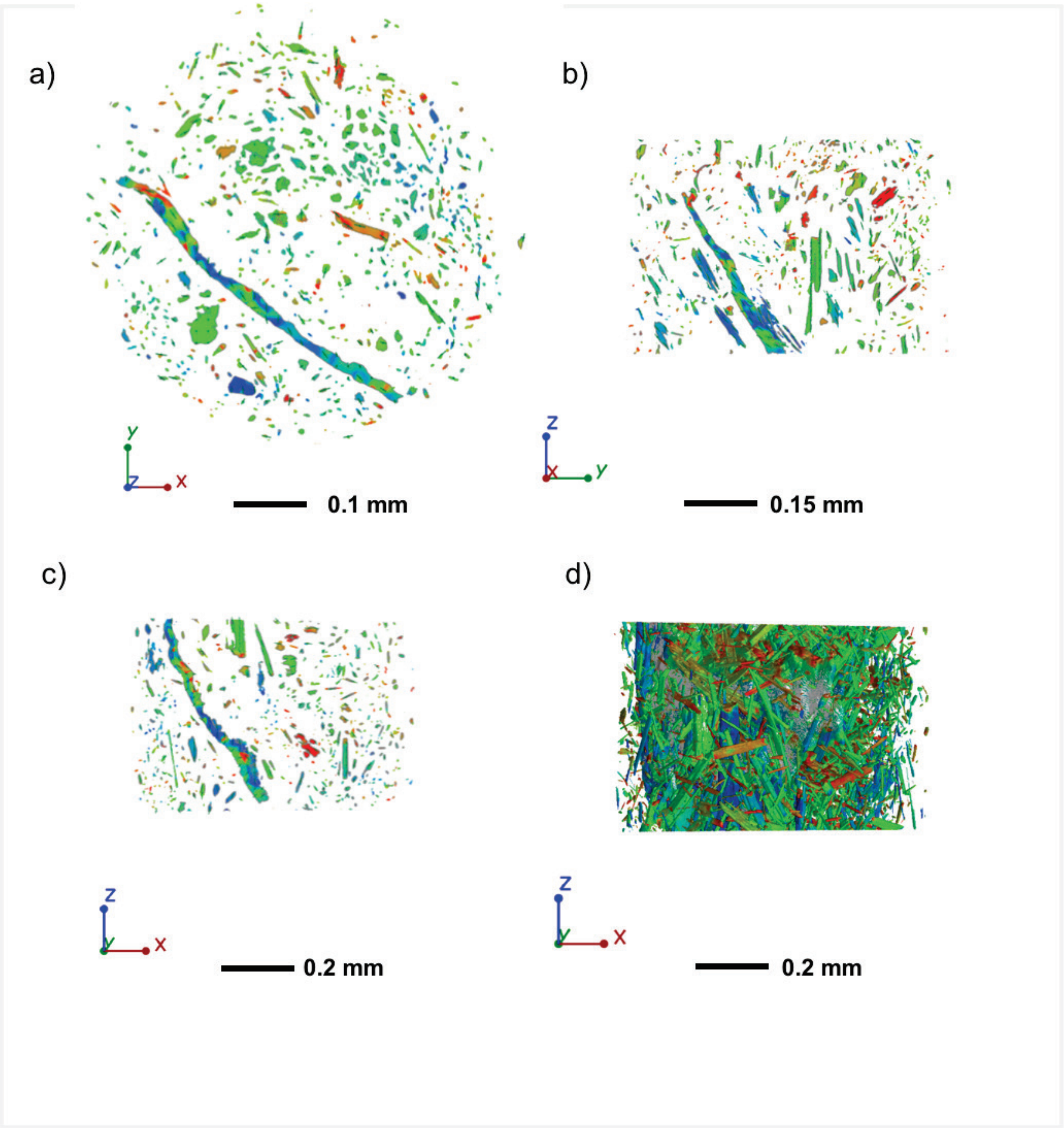




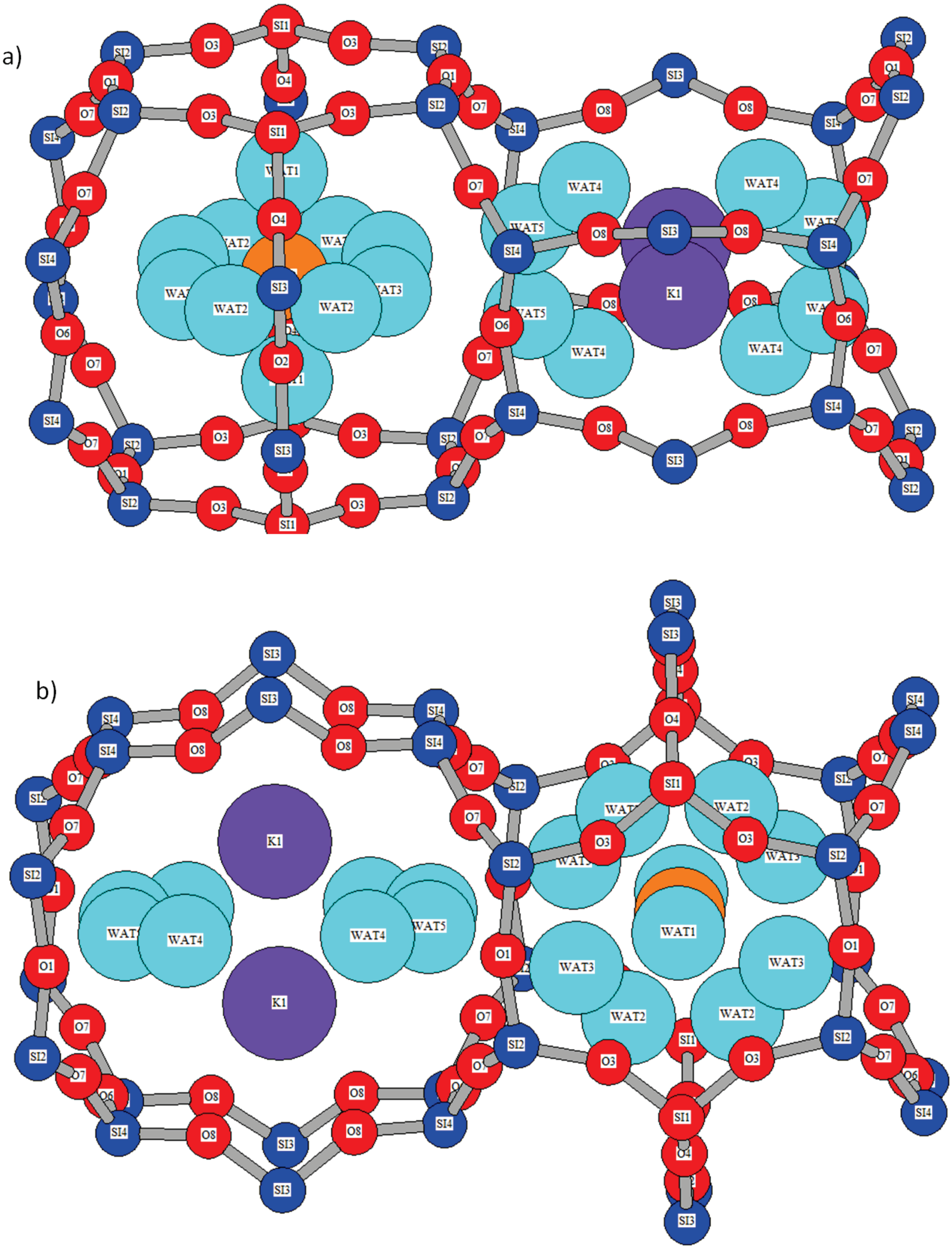
S2. Alignment scan of the ferrierite fibre reported in this study. The first picture is relative to the fit of the crystal size of the amphibole fibre by scanning the motor “px” across the beam (x dimension of the fibre). b. Fit of the crystal size of the amphibole fibre by scanning the motor “py” across the beam, after a rotation at 90° on z (y dimension of the fibre).



S3. Unwarped pictures of the single crystal experiment of the single fibre of ferrierite from British Columbia. No low symmetry (monoclinic) spots are present. Streaking, indicating disorder or faults, is also absent in this specific crystal.



S4. Tomography of the portion of the capillary analized by HR-PXRD. a) segmentation of the capillary viewed along the length of the capillary (z direction, xy-section); b) segmentation of the capillary viewed along the x direction (yz-section); c) segmentation of the capillary viewed along y direction (xz-section); d) full reconstruction of the capillary volume. The big fibres show a preferential orientation (green component) along the length of the capillary. A packing fraction of 49% has been estimated by the software VGStudio Max 3.2. The Cartesian coordinate system, in this picture, does not correspond to the unit cell axis system.High-resolution synchrotron powder diffraction.



S5. The Mg site is bonded to two W1, two W2 and two W3 water molecules, in a slightly distorted octahedron.

site	ss	x/a	y/b	z/c	B_{eq}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
K1	mm2	0.4251(3)	0	0	0.0500(17)	0.063(3)	0.045(2)	0.042(3)	0	0	0
Mg1	mmm	0	0	0.5	0.0265(9)	0.0181(10)	0.0385(13)	0.0228(12)	0	0	0
Si1	mm2	0.1550(5)	0	0	0.0203(7)	0.0224(7)	0.0183(7)	0.0202(8)	0	0	0
Al1	mm2	0.1550(5)	0	0							
Si2	m..	0.08419(3)	0.20274(4)	0	0.0183(7)	0.0187(7)	0.0177(7)	0.0184(7)	0.00028(17)	0	0
Al2	m..	0.08419(3)	0.20274(4)	0							
Si3	.m.	0.27227(4)	0	0.29217(9)	0.0245(7)	0.0208(7)	0.0238(7)	0.0291(8)	0	0.0039(2)	0
Si4	1	0.32301(3)	0.20235(3)	0.20618(6)	0.0207(7)	0.0171(7)	0.0210(7)	0.0239(7)	0.00099(13)	0.00054(12)	-0.00156(12)
O1	m2m	0	0.2163(3)	0	0.0393(10)	0.055(2)	0.0431(17)	0.0196(14)	0	0	0
O2	mm2	0.2494(3)	0	0.5	0.0434(11)	0.0231(13)	0.0413(17)	0.066(3)	0	0	0
O3	m..	0.89814(19)	0.0889(2)	0	0.0647(13)	0.120(3)	0.0310(13)	0.0435(17)	-0.0131(11)	0	0
O4	.m.	0.2014(2)	0	0.1804(5)	0.0775(15)	0.0500(18)	0.136(4)	0.047(2)	0	0.0260(15)	0
O5	-1	0.25	0.25	0.25	0.0555(10)	0.071(2)	0.0596(18)	0.0363(15)	-0.0177(13)	-0.0074(13)	-0.0078(16)
O6	m..	0.15730(17)	0.2810(2)	0.5	0.0453(9)	0.0201(10)	0.0586(17)	0.0572(18)	0.0070(13)	0	0
O7	1	0.11562(3)	0.25080(19)	0.1808(11)	0.0566(9)	0.0422(11)	0.0882(18)	0.0394(12)	0.0098(10)	0.0087(7)	-0.0323(11)
O8	1	0.32130(13)	0.09061(13)	0.24720(4)	0.0542(9)	0.0758(17)	0.0269(10)	0.0599(15)	-0.0001(7)	-0.0124(11)	0.0130(9)
WAT1	2mm	0	0	0.2347(4)	0.0410(10)	0.0212(12)	0.070(3)	0.0321(17)	0	0	0
WAT2	m..	0.0963(4)	0.0676(8)	0.5	0.063(3)	0.052(4)	0.108(8)	0.031(3)	-0.020(4)	0	0
WAT3	m..	0.0493(8)	0.1303(8)	0.5	0.083(6)	0.047(8)	0.043(7)	0.056(10)	0	-0.002(6)	0
WAT4	..m	0	0.3828(2)	0.2890(4)	0.39(2)	0.59(4)	0.51(4)	0.074(8)	0	0	0.35(3)
WAT5	.m.	0	0.3110(4)	0.3910(2)	0.048(5)	0.044(4)	0.080(7)	0.124(12)	-0.073(8)	0	0

Table 1. Final atomic coordinates, occupancies, and atomic displacement parameters (Å^2). Numbers in parentheses are estimated standard deviations in the least significant digits.

The cif file has been transformed to the above atomic coordinates for better comparison to the not standard settings reported in literature (e.g. Vaughan, 1966). The transformation to an equivalent structure has been made using the bilbao crystallographic application at the page: - http://www.cryst.ehu.es/cgi-bin/cryst/programs/nph-equivstru

Normalizer coset representative: x+1/2,y,z

Matrix form:

$$(P, p) = \begin{array}{lccccr} [& 0 & 0 & 1\,] & [& 0] \\ [& 0 & 1 & 0\,] & [& 0] \\ [& 1 & 0 & 0\,] & [& 0] \end{array}$$

Table2 .Selected geometric parameters (Å)

K1—WAT4^{i}	2.71 (2)	Mg1—WAT2^{vii}	2.075 (7)
K1—WAT4^{ii}	2.705 (19)	Si1—O4	1.619 (3)
K1—WAT4	2.705 (19)	Si1—O4^{viii}	1.619 (3)
K1—K1^{ii}	2.870 (12)	Si1—O3^{ix}	1.622 (3)
K1—WAT5^{iii}	3.01 (8)	Si1—O3^{x}	1.622 (3)
K1—WAT5^{ii}	3.01 (8)	Si2—O1	1.6305 (8)
K1—WAT5^{i}	3.01 (8)	Si2—O7	1.6342 (18)
K1—WAT5	3.01 (8)	Si2—O7^{xi}	1.6342 (18)
K1—O8	3.017 (5)	Si2—O3	1.642 (3)
K1—O8^{iii}	3.017 (5)	Si3—O4	1.601 (4)
K1—O8^{iv}	3.017 (5)	Si3—O2	1.6211 (16)
Mg1—WAT1	1.994 (3)	Si3—O8^{iii}	1.628 (2)
Mg1—WAT1^{v}	1.994 (3)	Si3—O8	1.628 (2)
Mg1—WAT3^{v}	2.064 (8)	Si4—O5	1.5921 (5)
Mg1—WAT3^{vi}	2.064 (8)	Si4—O7	1.5979 (19)
Mg1—WAT3^{vii}	2.064 (8)	Si4—O8	1.6085 (19)
Mg1—WAT3	2.064 (8)	Si4—O6	1.6112 (10)
Mg1—WAT2	2.075 (7)	WAT2—WAT3	1.280 (16)
Mg1—WAT2^{v}	2.075 (7)	WAT4—WAT5	1.33 (6)
Mg1—WAT2^{vi}	2.075 (7)	WAT5—WAT5^{i}	1.32 (10)

Symmetry code(s): (i) $-x+1, y, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x, -y+2, z$; (iv) $-x+1, y, z$; (v) $-x+1, -y+1, -z+1$; (vi) $x, y, -z+1$; (vii) $-x+1, -y+1, z$; (viii) $-x+1, -y+2, z$; (ix) $-x+1/2, -y+3/2, -z+1/2$; (x) $x+1/2, y+1/2, -z+1/2$; (xi) $-x, y, z$.

Selected geometric parameters (Å, º)

K1—WAT4^{i}	2.71 (2)	Mg1—WAT2^{vii}	2.075 (7)

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K1—WAT4	2.705 (19)	Si1—O4^{viii}	1.619 (3)
K1—K1^{ii}	2.870 (12)	Si1—O3^{ix}	1.622 (3)
K1—WAT5^{iii}	3.01 (8)	Si1—O3^{x}	1.622 (3)
K1—WAT5^{ii}	3.01 (8)	Si2—O1	1.6305 (8)
K1—WAT5^{i}	3.01 (8)	Si2—O7	1.6342 (18)
K1—WAT5	3.01 (8)	Si2—O7^{xi}	1.6342 (18)
K1—O8	3.017 (5)	Si2—O3	1.642 (3)
K1—O8^{iii}	3.017 (5)	Si3—O4	1.601 (4)
K1—O8^{iv}	3.017 (5)	Si3—O2	1.6211 (16)
Mg1—WAT1	1.994 (3)	Si3—O8^{iii}	1.628 (2)
Mg1—WAT1^{v}	1.994 (3)	Si3—O8	1.628 (2)
Mg1—WAT3^{v}	2.064 (8)	Si4—O5	1.5921 (5)
Mg1—WAT3^{vi}	2.064 (8)	Si4—O7	1.5979 (19)
Mg1—WAT3^{vii}	2.064 (8)	Si4—O8	1.6085 (19)
Mg1—WAT3	2.064 (8)	Si4—O6	1.6112 (10)
Mg1—WAT2	2.075 (7)	WAT2—WAT3	1.280 (16)
Mg1—WAT2^{v}	2.075 (7)	WAT4—WAT5	1.33 (6)
Mg1—WAT2^{vi}	2.075 (7)	WAT5—WAT5^{i}	1.32 (10)
WAT4^{iii}—K1—WAT4^{ii}	73 (2)	WAT5^{ii}—K1—O8^{iii}	79.6 (7)
WAT4^{i}—K1—WAT4^{ii}	74.4 (17)	WAT5^{i}—K1—O8^{iii}	122.9 (8)
WAT4^{iii}—K1—WAT4	74.4 (17)	WAT5—K1—O8^{iii}	144.4 (12)
WAT4^{i}—K1—WAT4	73 (2)	O8—K1—O8^{iii}	50.32 (10)
WAT4^{ii}—K1—WAT4	115.9 (5)	WAT4^{iii}—K1—O8^{iv}	104.1 (9)
WAT4^{iii}—K1—K1^{ii}	58.0 (3)	WAT4^{i}—K1—O8^{iv}	117.4 (8)
WAT4^{i}—K1—K1^{ii}	58.0 (3)	WAT4^{ii}—K1—O8^{iv}	167.1 (6)
WAT4^{ii}—K1—K1^{ii}	58.0 (3)	WAT4—K1—O8^{iv}	74.3 (4)
WAT4—K1—K1^{ii}	58.0 (3)	K1^{ii}—K1—O8^{iv}	131.58 (10)
WAT4^{iii}—K1—WAT5^{iii}	26.1 (9)	WAT5^{iii}—K1—O8^{iv}	122.9 (8)
WAT4^{i}—K1—WAT5^{iii}	113.1 (9)	WAT5^{ii}—K1—O8^{iv}	144.4 (12)
WAT4^{ii}—K1—WAT5^{iii}	50.4 (17)	WAT5^{i}—K1—O8^{iv}	95.1 (11)

WAT4—K1—WAT5$^{\rm iii}$	97.6 (17)	WAT5—K1—O8$^{\rm iv}$	79.6 (7)
K1$^{\rm ii}$—K1—WAT5$^{\rm iii}$	61.5 (8)	O8—K1—O8$^{\rm iv}$	75.98 (16)
WAT4$^{\rm iii}$—K1—WAT5$^{\rm ii}$	50.4 (17)	O8$^{\rm iii}$—K1—O8$^{\rm iv}$	96.8 (2)
WAT4$^{\rm i}$—K1—WAT5$^{\rm ii}$	97.6 (17)	WAT1—Mg1—WAT1$^{\rm v}$	180.0
WAT4$^{\rm ii}$—K1—WAT5$^{\rm ii}$	26.1 (9)	WAT1—Mg1—WAT3$^{\rm v}$	90.000 (1)
WAT4—K1—WAT5$^{\rm ii}$	113.1 (9)	WAT1$^{\rm v}$—Mg1—WAT3$^{\rm v}$	90.000 (2)
K1$^{\rm ii}$—K1—WAT5$^{\rm ii}$	61.5 (8)	WAT1—Mg1—WAT3$^{\rm vi}$	90.000 (4)
WAT5$^{\rm iii}$—K1—WAT5$^{\rm ii}$	25 (2)	WAT1$^{\rm v}$—Mg1—WAT3$^{\rm vi}$	90.000 (1)
WAT4$^{\rm iii}$—K1—WAT5$^{\rm i}$	113.1 (9)	WAT3$^{\rm v}$—Mg1—WAT3$^{\rm vi}$	124.8 (9)
WAT4$^{\rm i}$—K1—WAT5$^{\rm i}$	26.1 (9)	WAT1—Mg1—WAT3$^{\rm vii}$	90.000 (1)
WAT4$^{\rm ii}$—K1—WAT5$^{\rm i}$	97.6 (17)	WAT1$^{\rm v}$—Mg1—WAT3$^{\rm vii}$	90.000 (4)
WAT4—K1—WAT5$^{\rm i}$	50.4 (17)	WAT3$^{\rm v}$—Mg1—WAT3$^{\rm vii}$	55.2 (9)
K1$^{\rm ii}$—K1—WAT5$^{\rm i}$	61.5 (8)	WAT3$^{\rm vi}$—Mg1—WAT3$^{\rm vii}$	180.0 (7)
WAT5$^{\rm iii}$—K1—WAT5$^{\rm i}$	123.1 (17)	WAT1—Mg1—WAT3	90.000 (2)
WAT5$^{\rm ii}$—K1—WAT5$^{\rm i}$	117 (2)	WAT1$^{\rm v}$—Mg1—WAT3	90.000 (1)
WAT4$^{\rm iii}$—K1—WAT5	97.6 (17)	WAT3$^{\rm v}$—Mg1—WAT3	180.0
WAT4$^{\rm i}$—K1—WAT5	50.4 (17)	WAT3$^{\rm vi}$—Mg1—WAT3	55.2 (9)
WAT4$^{\rm ii}$—K1—WAT5	113.1 (9)	WAT3$^{\rm vii}$—Mg1—WAT3	124.8 (9)
WAT4—K1—WAT5	26.1 (9)	WAT1—Mg1—WAT2	90.000 (2)
K1$^{\rm ii}$—K1—WAT5	61.5 (8)	WAT1$^{\rm v}$—Mg1—WAT2	90.000 (1)
WAT5$^{\rm iii}$—K1—WAT5	117 (2)	WAT3$^{\rm v}$—Mg1—WAT2	144.0 (5)
WAT5$^{\rm ii}$—K1—WAT5	123.1 (17)	WAT3$^{\rm vi}$—Mg1—WAT2	91.2 (7)
WAT5$^{\rm i}$—K1—WAT5	25 (2)	WAT3$^{\rm vii}$—Mg1—WAT2	88.8 (7)
WAT4$^{\rm iii}$—K1—O8	167.1 (6)	WAT3—Mg1—WAT2	36.0 (5)
WAT4$^{\rm i}$—K1—O8	74.3 (4)	WAT1—Mg1—WAT2$^{\rm v}$	90.000 (1)
WAT4$^{\rm ii}$—K1—O8	104.1 (9)	WAT1$^{\rm v}$—Mg1—WAT2$^{\rm v}$	90.000 (2)
WAT4—K1—O8	117.4 (8)	WAT3$^{\rm v}$—Mg1—WAT2$^{\rm v}$	36.0 (5)
K1$^{\rm ii}$—K1—O8	131.57 (10)	WAT3$^{\rm vi}$—Mg1—WAT2$^{\rm v}$	88.8 (7)
WAT5$^{\rm iii}$—K1—O8	144.4 (12)	WAT3$^{\rm vii}$—Mg1—WAT2$^{\rm v}$	91.2 (7)
WAT5$^{\rm ii}$—K1—O8	122.9 (8)	WAT3—Mg1—WAT2$^{\rm v}$	144.0 (5)
WAT5$^{\rm i}$—K1—O8	79.6 (7)	WAT2—Mg1—WAT2$^{\rm v}$	180.0

WAT5—K1—O8	95.1 (11)	WAT1—Mg1—WAT2^{vi}	90.000 (2)
WAT4^{iii}—K1—O8^{iii}	117.4 (8)	WAT1^{v}—Mg1—WAT2^{vi}	90.000 (2)
WAT4^{i}—K1—O8^{iii}	104.1 (9)	WAT3^{v}—Mg1—WAT2^{vi}	88.8 (7)
WAT4^{ii}—K1—O8^{iii}	74.3 (4)	WAT3^{vi}—Mg1—WAT2^{vi}	36.0 (5)
WAT4—K1—O8^{iii}	167.1 (6)	WAT3^{vii}—Mg1—WAT2^{vi}	144.0 (5)
K1^{ii}—K1—O8^{iii}	131.58 (10)	WAT3—Mg1—WAT2^{vi}	91.2 (7)
WAT5^{iii}—K1—O8^{iii}	95.1 (11)	WAT2—Mg1—WAT2^{vi}	127.2 (8)

Symmetry code(s): (i) −*x*+1, *y*, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) *x*, −*y*+2, *z*; (iv) −*x*+1, *y*, *z*; (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*, *y*, −*z*+1; (vii) −*x*+1, −*y*+1, *z*; (viii) −*x*+1, −*y*+2, *z*; (ix) −*x*+1/2, −*y*+3/2, −*z*+1/2; (x) *x*+1/2, *y*+1/2, −*z*+1/2; (xi) −*x*, *y*, *z*.

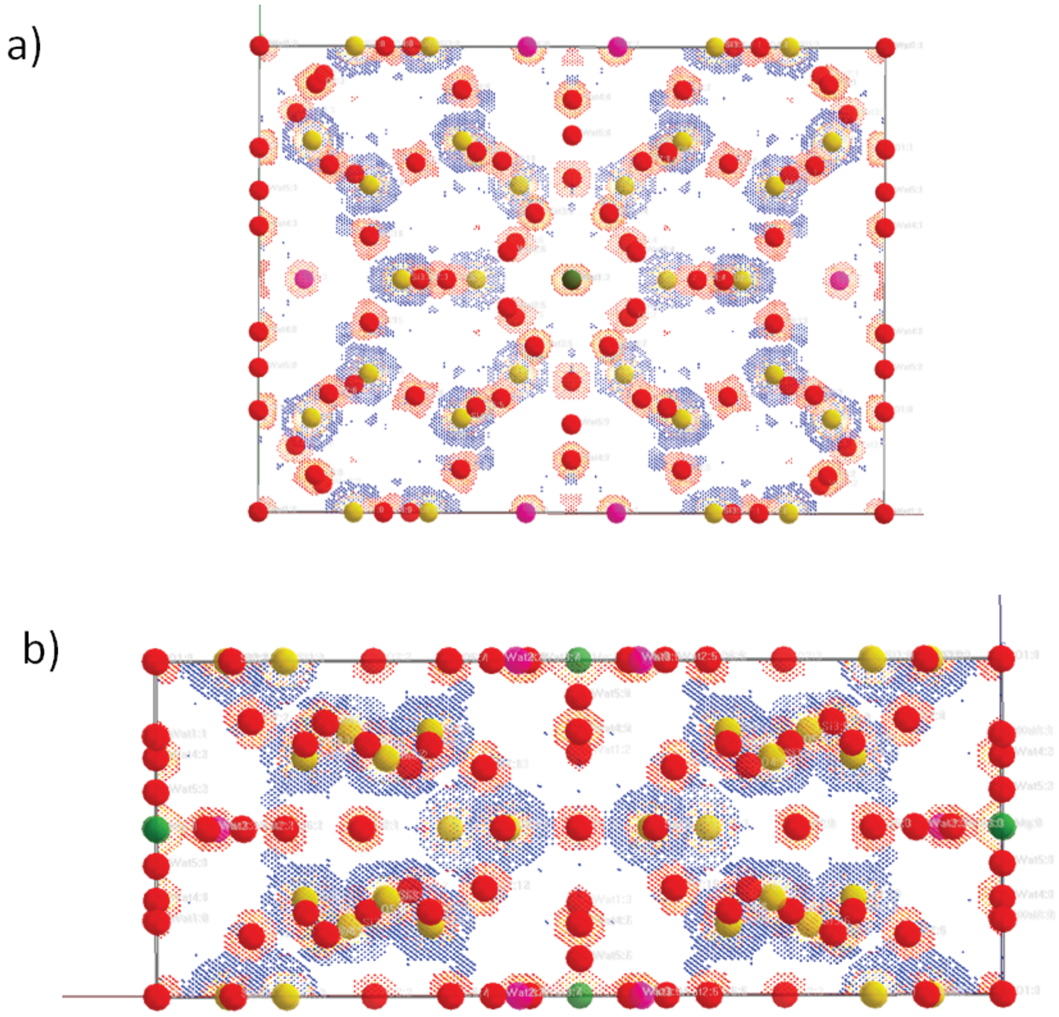
Selected geometric parameters (Å, º)

K1—WAT4^{i}	2.71 (2)	Mg1—WAT2^{vii}	2.075 (7)
K1—WAT4^{ii}	2.705 (19)	Si1—O4	1.619 (3)
K1—WAT4	2.705 (19)	Si1—O4^{viii}	1.619 (3)
K1—K1^{ii}	2.870 (12)	Si1—O3^{ix}	1.622 (3)
K1—WAT5^{iii}	3.01 (8)	Si1—O3^{x}	1.622 (3)
K1—WAT5^{ii}	3.01 (8)	Si2—O1	1.6305 (8)
K1—WAT5^{i}	3.01 (8)	Si2—O7	1.6342 (18)
K1—WAT5	3.01 (8)	Si2—O7^{xi}	1.6342 (18)
K1—O8	3.017 (5)	Si2—O3	1.642 (3)
K1—O8^{iii}	3.017 (5)	Si3—O4	1.601 (4)
K1—O8^{iv}	3.017 (5)	Si3—O2	1.6211 (16)
Mg1—WAT1	1.994 (3)	Si3—O8^{iii}	1.628 (2)
Mg1—WAT1^{v}	1.994 (3)	Si3—O8	1.628 (2)
Mg1—WAT3^{v}	2.064 (8)	Si4—O5	1.5921 (5)
Mg1—WAT3^{vi}	2.064 (8)	Si4—O7	1.5979 (19)
Mg1—WAT3^{vii}	2.064 (8)	Si4—O8	1.6085 (19)
Mg1—WAT3	2.064 (8)	Si4—O6	1.6112 (10)
Mg1—WAT2	2.075 (7)	WAT2—WAT3	1.280 (16)

Mg1—WAT2^{v}	2.075 (7)	WAT4—WAT5	1.33 (6)
Mg1—WAT2^{vi}	2.075 (7)	WAT5—WAT5^{i}	1.32 (10)
WAT4^{iii}—K1—WAT4^{ii}	73 (2)	WAT5^{ii}—K1—O8^{iii}	79.6 (7)
WAT4^{i}—K1—WAT4^{ii}	74.4 (17)	WAT5^{i}—K1—O8^{iii}	122.9 (8)
WAT4^{iii}—K1—WAT4	74.4 (17)	WAT5—K1—O8^{iii}	144.4 (12)
WAT4^{i}—K1—WAT4	73 (2)	O8—K1—O8^{iii}	50.32 (10)
WAT4^{ii}—K1—WAT4	115.9 (5)	WAT4^{iii}—K1—O8^{iv}	104.1 (9)
WAT4^{iii}—K1—K1^{ii}	58.0 (3)	WAT4^{i}—K1—O8^{iv}	117.4 (8)
WAT4^{i}—K1—K1^{ii}	58.0 (3)	WAT4^{ii}—K1—O8^{iv}	167.1 (6)
WAT4^{ii}—K1—K1^{ii}	58.0 (3)	WAT4—K1—O8^{iv}	74.3 (4)
WAT4—K1—K1^{ii}	58.0 (3)	K1^{ii}—K1—O8^{iv}	131.58 (10)
WAT4^{iii}—K1—WAT5^{iii}	26.1 (9)	WAT5^{iii}—K1—O8^{iv}	122.9 (8)
WAT4^{i}—K1—WAT5^{iii}	113.1 (9)	WAT5^{ii}—K1—O8^{iv}	144.4 (12)
WAT4^{ii}—K1—WAT5^{iii}	50.4 (17)	WAT5^{i}—K1—O8^{iv}	95.1 (11)
WAT4—K1—WAT5^{iii}	97.6 (17)	WAT5—K1—O8^{iv}	79.6 (7)
K1^{ii}—K1—WAT5^{iii}	61.5 (8)	O8—K1—O8^{iv}	75.98 (16)
WAT4^{iii}—K1—WAT5^{ii}	50.4 (17)	O8^{iii}—K1—O8^{iv}	96.8 (2)
WAT4^{i}—K1—WAT5^{ii}	97.6 (17)	WAT1—Mg1—WAT1^{v}	180.0
WAT4^{ii}—K1—WAT5^{ii}	26.1 (9)	WAT1—Mg1—WAT3^{v}	90.000 (1)
WAT4—K1—WAT5^{ii}	113.1 (9)	WAT1^{v}—Mg1—WAT3^{v}	90.000 (2)
K1^{ii}—K1—WAT5^{ii}	61.5 (8)	WAT1—Mg1—WAT3^{vi}	90.000 (4)
WAT5^{iii}—K1—WAT5^{ii}	25 (2)	WAT1^{v}—Mg1—WAT3^{vi}	90.000 (1)
WAT4^{iii}—K1—WAT5^{i}	113.1 (9)	WAT3^{v}—Mg1—WAT3^{vi}	124.8 (9)
WAT4^{i}—K1—WAT5^{i}	26.1 (9)	WAT1—Mg1—WAT3^{vii}	90.000 (1)
WAT4^{ii}—K1—WAT5^{i}	97.6 (17)	WAT1^{v}—Mg1—WAT3^{vii}	90.000 (4)
WAT4—K1—WAT5^{i}	50.4 (17)	WAT3^{v}—Mg1—WAT3^{vii}	55.2 (9)
K1^{ii}—K1—WAT5^{i}	61.5 (8)	WAT3^{vi}—Mg1—WAT3^{vii}	180.0 (7)
WAT5^{iii}—K1—WAT5^{i}	123.1 (17)	WAT1—Mg1—WAT3	90.000 (2)
WAT5^{ii}—K1—WAT5^{i}	117 (2)	WAT1^{v}—Mg1—WAT3	90.000 (1)
WAT4^{iii}—K1—WAT5	97.6 (17)	WAT3^{v}—Mg1—WAT3	180.0
WAT4^{i}—K1—WAT5	50.4 (17)	WAT3^{vi}—Mg1—WAT3	55.2 (9)

WAT4$^{\mathrm{ii}}$—K1—WAT5	113.1 (9)	WAT3$^{\mathrm{vii}}$—Mg1—WAT3	124.8 (9)
WAT4—K1—WAT5	26.1 (9)	WAT1—Mg1—WAT2	90.000 (2)
K1$^{\mathrm{ii}}$—K1—WAT5	61.5 (8)	WAT1$^{\mathrm{v}}$—Mg1—WAT2	90.000 (1)
WAT5$^{\mathrm{iii}}$—K1—WAT5	117 (2)	WAT3$^{\mathrm{v}}$—Mg1—WAT2	144.0 (5)
WAT5$^{\mathrm{ii}}$—K1—WAT5	123.1 (17)	WAT3$^{\mathrm{vi}}$—Mg1—WAT2	91.2 (7)
WAT5$^{\mathrm{i}}$—K1—WAT5	25 (2)	WAT3$^{\mathrm{vii}}$—Mg1—WAT2	88.8 (7)
WAT4$^{\mathrm{iii}}$—K1—O8	167.1 (6)	WAT3—Mg1—WAT2	36.0 (5)
WAT4$^{\mathrm{i}}$—K1—O8	74.3 (4)	WAT1—Mg1—WAT2$^{\mathrm{v}}$	90.000 (1)
WAT4$^{\mathrm{ii}}$—K1—O8	104.1 (9)	WAT1$^{\mathrm{v}}$—Mg1—WAT2$^{\mathrm{v}}$	90.000 (2)
WAT4—K1—O8	117.4 (8)	WAT3$^{\mathrm{v}}$—Mg1—WAT2$^{\mathrm{v}}$	36.0 (5)
K1$^{\mathrm{ii}}$—K1—O8	131.57 (10)	WAT3$^{\mathrm{vi}}$—Mg1—WAT2$^{\mathrm{v}}$	88.8 (7)
WAT5$^{\mathrm{iii}}$—K1—O8	144.4 (12)	WAT3$^{\mathrm{vii}}$—Mg1—WAT2$^{\mathrm{v}}$	91.2 (7)
WAT5$^{\mathrm{ii}}$—K1—O8	122.9 (8)	WAT3—Mg1—WAT2$^{\mathrm{v}}$	144.0 (5)
WAT5$^{\mathrm{i}}$—K1—O8	79.6 (7)	WAT2—Mg1—WAT2$^{\mathrm{v}}$	180.0
WAT5—K1—O8	95.1 (11)	WAT1—Mg1—WAT2$^{\mathrm{vi}}$	90.000 (2)
WAT4$^{\mathrm{iii}}$—K1—O8$^{\mathrm{iii}}$	117.4 (8)	WAT1$^{\mathrm{v}}$—Mg1—WAT2$^{\mathrm{vi}}$	90.000 (2)
WAT4$^{\mathrm{i}}$—K1—O8$^{\mathrm{iii}}$	104.1 (9)	WAT3$^{\mathrm{v}}$—Mg1—WAT2$^{\mathrm{vi}}$	88.8 (7)
WAT4$^{\mathrm{ii}}$—K1—O8$^{\mathrm{iii}}$	74.3 (4)	WAT3$^{\mathrm{vi}}$—Mg1—WAT2$^{\mathrm{vi}}$	36.0 (5)
WAT4—K1—O8$^{\mathrm{iii}}$	167.1 (6)	WAT3$^{\mathrm{vii}}$—Mg1—WAT2$^{\mathrm{vi}}$	144.0 (5)
K1$^{\mathrm{ii}}$—K1—O8$^{\mathrm{iii}}$	131.58 (10)	WAT3—Mg1—WAT2$^{\mathrm{vi}}$	91.2 (7)
WAT5$^{\mathrm{iii}}$—K1—O8$^{\mathrm{iii}}$	95.1 (11)	WAT2—Mg1—WAT2$^{\mathrm{vi}}$	127.2 (8)

Symmetry code(s): (i) $-x+1, y, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x, -y+2, z$; (iv) $-x+1, y, z$; (v) $-x+1, -y+1, -z+1$; (vi) $x, y, -z+1$; (vii) $-x+1, -y+1, z$; (viii) $-x+1, -y+2, z$; (ix) $-x+1/2, -y+3/2, -z+1/2$; (x) $x+1/2, y+1/2, -z+1/2$; (xi) $-x, y, z$.



S6. Difference Fourier analysis obtained after the Rietveld refinement of the data collected at ID22 using Topas6. Projection along the c axis (a) and b axis (b).

fourier_map_formula = 2 Fobs - Fcalc;