Supplementary material to "Perbøeite-(Ce) and alnaperbøeite-(Ce), two new members of the epidote - törnebohmite polysomatic series: chemistry, structure, dehydrogenation and clue for a sodian epidote end-member" by Paola Bonazzi et al. American Mineralogist, Jan 2014. AM-14-102. This document: 3 Supplementary figures and captions and deposit Table 3. Separate documents: CIF, table 4 (txt) and Table 7 (xls).

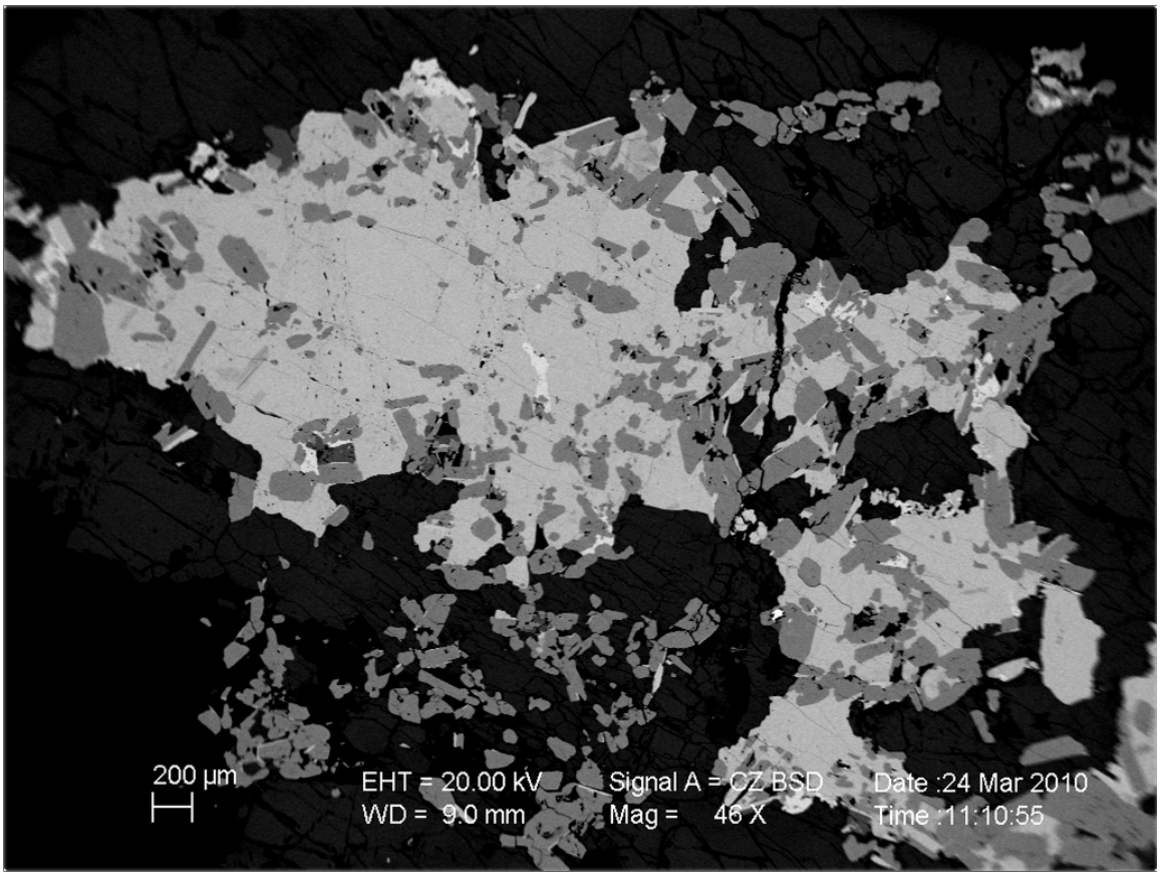

Figure S1.
Backscattered-electron image of a section showing the relations between crystals of perbøeite-(Ce) (medium gray), a fluorthalénite-(Y) aggregate (pale gray) and the matrix of yttrian fluorite (black). The few blebby, brighter inclusions in fluorthalénite-(Y) are bastnäsite-(Ce). White lamellae sharing a rational contact plane along some perbøeite-(Ce) prisms are törnebohmite-(Ce). Sample ST2, Stetind, a detail of which is shown in Figure S2.

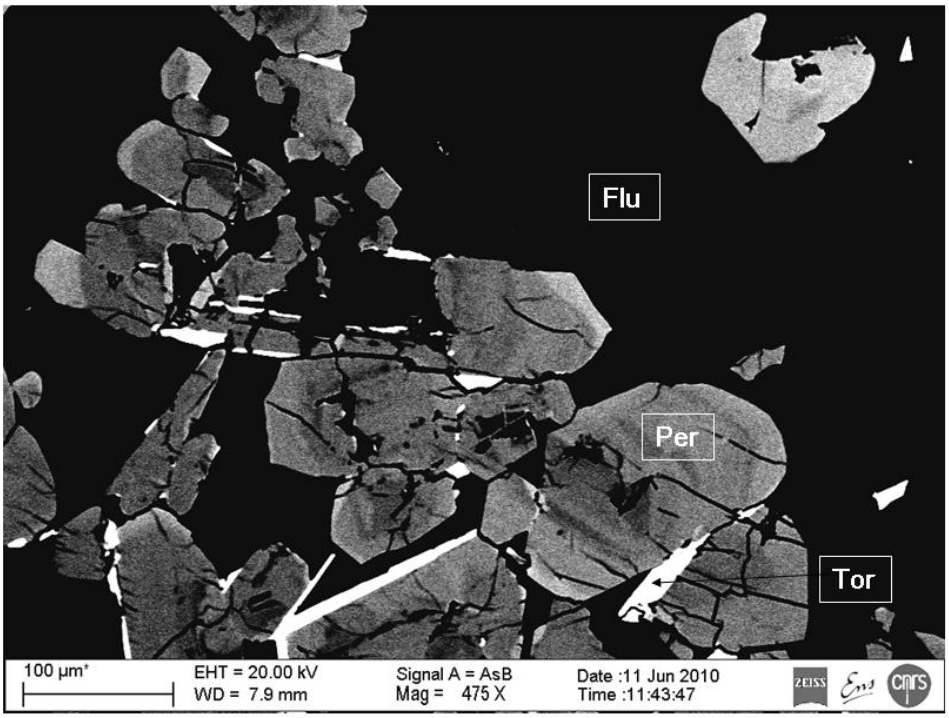

Figure S2.
Zoned crystals of perbøeite-(Ce) (shades of gray) with törnebohmite-(Ce) lamellae (white) in yttrian fluorite groundmass (black). High-contrast BSE image of sample ST2, Stetind.

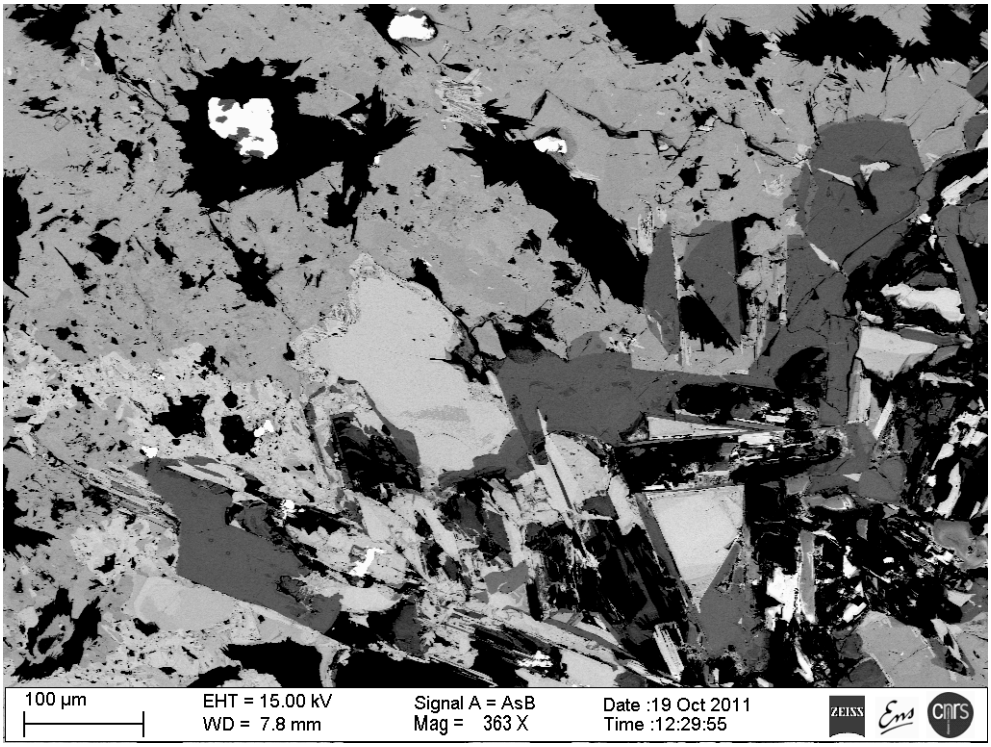

Figure S3
Large prisms of alnaperbøeite-(Ce) [(dark gray, with small lighter overgrowths of perbøeite-(Ce)] intergrown with massive fluorthalénite-(Y) and törnbohmite-(Ce) lamellae (both light gray) with minor fluorite (black) in kuliokite-(Y) (mottled medium gray, upper part of the picture), which includes radial aggregates of muscovite (black) with thorite (brightest grains, the largest of them including zircon, very dark gray). BSE image of sample ST4, Stetind.

TABLE 3– Fractional atomic coordinates, equivalent isotropic displacement parameters (Å^2) and anisotropic displacement parameters (Å^2) for all the investigated crystals (except for the alnaperbøeite-(Ce) and perbøeite-(Ce) holotype crystals given in Table 2)

ST4_09

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.7317 (2)	0.2500	0.41031 (10)	0.0253 (6)	0.947 (4)
A1CE	0.7317 (2)	0.2500	0.41031 (10)	0.0253 (6)	0.053 (4)
A2CE	0.88957 (6)	0.2500	0.24985 (3)	0.01981 (18)	0.922 (6)
A2CA	0.88957 (6)	0.2500	0.24985 (3)	0.01981 (18)	0.078 (6)
A3CE	0.73976 (8)	0.2500	0.01017 (3)	0.0362 (2)	0.913 (6)
A3CA	0.73976 (8)	0.2500	0.01017 (3)	0.0362 (2)	0.087 (6)
A4CE	0.08087 (7)	0.7500	0.16464 (3)	0.01985 (18)	0.887 (5)
A4CA	0.08087 (7)	0.7500	0.16464 (3)	0.01985 (18)	0.113 (5)
M1AL	0.5000	0.5000	0.5000	0.0150 (7)	0.979 (9)
M1FE	0.5000	0.5000	0.5000	0.0150 (7)	0.021 (9)
M2AL	0.48248 (19)	0.0002 (3)	0.20517 (10)	0.0150 (5)	0.951 (8)
M2FE	0.48248 (19)	0.0002 (3)	0.20517 (10)	0.0150 (5)	0.049 (8)
M3FE	0.1988 (2)	0.7500	0.37601 (11)	0.0217 (6)	0.448 (10)
M3AL	0.1988 (2)	0.7500	0.37601 (11)	0.0217 (6)	0.552 (10)
Si1	0.1620 (3)	0.2500	0.47562 (13)	0.0141 (5)	
Si2	0.8084 (3)	0.7500	0.33730 (13)	0.0131 (5)	
Si3	0.3069 (2)	0.2500	0.31357 (13)	0.0118 (4)	
Si4	0.6722 (3)	0.7500	0.10404 (14)	0.0158 (5)	
Si5	0.1561 (3)	0.2500	0.07737 (13)	0.0132 (5)	
O1	0.2651 (5)	0.4914 (7)	0.4776 (3)	0.0215 (9)	
O2	0.1839 (5)	0.4809 (7)	0.2917 (3)	0.0217 (9)	
O3	0.6983 (5)	0.9870 (6)	0.2967 (2)	0.0193 (9)	
O4	0.4416 (7)	0.7500	0.4243 (3)	0.0162 (11)	
O5	0.4524 (7)	0.2500	0.4137 (3)	0.0148 (11)	
O6	0.4198 (7)	0.2500	0.2601 (3)	0.0151 (11)	
O7	−0.0188 (7)	0.2500	0.3978 (4)	0.0227 (14)	
O8	−0.0304 (9)	0.7500	0.3217 (5)	0.0384 (18)	
O9	0.8647 (8)	0.7500	0.4388 (4)	0.0308 (15)	
O10	0.5572 (7)	0.2500	0.1628 (3)	0.0144 (11)	
O11	0.4062 (7)	0.7500	0.2478 (4)	0.0150 (12)	
O12	0.5402 (6)	0.7500	0.1475 (3)	0.0141 (11)	
O13	0.2700 (5)	0.4900 (6)	0.1105 (3)	0.0183 (9)	
O14	0.7965 (5)	−0.0232 (7)	0.1335 (3)	0.0250 (10)	

O15	0.5570 (11)	0.6808 (13)	0.0042 (5)	0.029 (3)	0.50
O16	0.0633 (11)	0.2500	−0.0236 (4)	0.051 (2)	
O17	0.0244 (8)	0.2500	0.1170 (5)	0.0411 (18)	
H1	0.416 (13)	0.7500	0.295 (6)	0.03 (3)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0282 (10)	0.0221 (9)	0.0263 (9)	0.000	0.0129 (7)	0.000
A1CE	0.0282 (10)	0.0221 (9)	0.0263 (9)	0.000	0.0129 (7)	0.000
A2CE	0.0159 (3)	0.0222 (3)	0.0176 (3)	0.000	0.0041 (2)	0.000
A2CA	0.0159 (3)	0.0222 (3)	0.0176 (3)	0.000	0.0041 (2)	0.000
A3CE	0.0262 (4)	0.0616 (5)	0.0149 (3)	0.000	0.0038 (2)	0.000
A3CA	0.0262 (4)	0.0616 (5)	0.0149 (3)	0.000	0.0038 (2)	0.000
A4CE	0.0154 (3)	0.0244 (3)	0.0167 (3)	0.000	0.0045 (2)	0.000
A4CA	0.0154 (3)	0.0244 (3)	0.0167 (3)	0.000	0.0045 (2)	0.000
M1AL	0.0111 (12)	0.0115 (12)	0.0200 (13)	−0.0001 (8)	0.0049 (9)	−0.0011 (8)
M1FE	0.0111 (12)	0.0115 (12)	0.0200 (13)	−0.0001 (8)	0.0049 (9)	−0.0011 (8)
M2AL	0.0097 (8)	0.0137 (8)	0.0194 (9)	0.0000 (5)	0.0046 (6)	0.0003 (6)
M2FE	0.0097 (8)	0.0137 (8)	0.0194 (9)	0.0000 (5)	0.0046 (6)	0.0003 (6)
M3FE	0.0188 (10)	0.0159 (9)	0.0284 (10)	0.000	0.0086 (8)	0.000
M3AL	0.0188 (10)	0.0159 (9)	0.0284 (10)	0.000	0.0086 (8)	0.000
Si1	0.0120 (10)	0.0122 (10)	0.0173 (10)	0.000	0.0058 (8)	0.000
Si2	0.0116 (10)	0.0112 (10)	0.0174 (10)	0.000	0.0073 (8)	0.000
Si3	0.0071 (10)	0.0141 (10)	0.0146 (10)	0.000	0.0053 (8)	0.000
Si4	0.0128 (11)	0.0180 (11)	0.0178 (10)	0.000	0.0078 (9)	0.000
Si5	0.0112 (10)	0.0109 (10)	0.0133 (9)	0.000	0.0018 (8)	0.000
O1	0.016 (2)	0.016 (2)	0.036 (2)	−0.0042 (15)	0.0148 (19)	−0.0079 (17)
O2	0.017 (2)	0.026 (2)	0.026 (2)	0.0095 (17)	0.0136 (18)	0.0058 (17)
O3	0.0119 (19)	0.0110 (18)	0.027 (2)	0.0003 (14)	0.0010 (16)	−0.0004 (16)
O4	0.013 (3)	0.016 (3)	0.018 (3)	0.000	0.006 (2)	0.000
O5	0.018 (3)	0.014 (3)	0.013 (2)	0.000	0.008 (2)	0.000
O6	0.016 (3)	0.013 (3)	0.022 (3)	0.000	0.014 (2)	0.000
O7	0.007 (3)	0.017 (3)	0.030 (3)	0.000	−0.004 (2)	0.000
O8	0.040 (4)	0.036 (4)	0.063 (5)	0.000	0.043 (4)	0.000
O9	0.031 (4)	0.043 (4)	0.021 (3)	0.000	0.013 (3)	0.000
O10	0.013 (3)	0.010 (3)	0.019 (3)	0.000	0.007 (2)	0.000
O11	0.009 (3)	0.012 (3)	0.020 (3)	0.000	0.003 (2)	0.000
O12	0.011 (3)	0.008 (2)	0.024 (3)	0.000	0.009 (2)	0.000
O13	0.0091 (18)	0.0112 (18)	0.027 (2)	−0.0011 (14)	0.0015 (16)	0.0009 (15)
O14	0.025 (2)	0.017 (2)	0.041 (3)	−0.0046 (17)	0.021 (2)	−0.0038 (18)
O15	0.033 (5)	0.035 (7)	0.022 (4)	−0.012 (4)	0.015 (4)	−0.006 (3)

O16	0.065 (6)	0.061 (5)	0.011 (3)	0.000	0.003 (3)	0.000
O17	0.019 (4)	0.060 (5)	0.052 (5)	0.000	0.023 (3)	0.000

ST3_01

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73172 (18)	0.2500	0.40975 (10)	0.0234 (5)	0.947 (3)
A1CE	0.73172 (18)	0.2500	0.40975 (10)	0.0234 (5)	0.053 (3)
A2CE	0.89009 (5)	0.2500	0.24994 (3)	0.02004 (16)	0.926 (6)
A2CA	0.89009 (5)	0.2500	0.24994 (3)	0.02004 (16)	0.074 (6)
A3CE	0.73994 (7)	0.2500	0.01007 (4)	0.0374 (2)	0.923 (6)
A3CA	0.73994 (7)	0.2500	0.01007 (4)	0.0374 (2)	0.077 (6)
A4CE	0.08081 (6)	0.7500	0.16486 (3)	0.01994 (17)	0.887 (5)
A4CA	0.08081 (6)	0.7500	0.16486 (3)	0.01994 (17)	0.113 (5)
M1AL	0.5000	0.5000	0.5000	0.0148 (7)	0.986 (9)
M1FE	0.5000	0.5000	0.5000	0.0148 (7)	0.014 (9)
M2AL	0.48239 (16)	−0.0001 (3)	0.20518 (10)	0.0141 (5)	0.972 (7)
M2FE	0.48239 (16)	−0.0001 (3)	0.20518 (10)	0.0141 (5)	0.028 (7)
M3FE	0.19783 (18)	0.7500	0.37592 (11)	0.0195 (5)	0.454 (10)
M3AL	0.19783 (18)	0.7500	0.37592 (11)	0.0195 (5)	0.546 (10)
Si1	0.1624 (2)	0.2500	0.47604 (13)	0.0140 (4)	
Si2	0.8076 (2)	0.7500	0.33676 (13)	0.0137 (4)	
Si3	0.3066 (2)	0.2500	0.31347 (13)	0.0133 (4)	
Si4	0.6722 (2)	0.7500	0.10419 (14)	0.0155 (4)	
Si5	0.1558 (2)	0.2500	0.07729 (13)	0.0132 (4)	
O1	0.2659 (4)	0.4905 (6)	0.4789 (3)	0.0211 (9)	
O2	0.1829 (4)	0.4798 (7)	0.2917 (3)	0.0217 (9)	
O3	0.6964 (4)	0.9878 (6)	0.2968 (3)	0.0196 (8)	
O4	0.4424 (6)	0.7500	0.4244 (3)	0.0146 (10)	
O5	0.4526 (6)	0.2500	0.4141 (3)	0.0149 (11)	
O6	0.4189 (6)	0.2500	0.2596 (3)	0.0152 (11)	
O7	−0.0175 (6)	0.2500	0.3972 (4)	0.0215 (12)	
O8	−0.0332 (8)	0.7500	0.3195 (5)	0.0385 (17)	
O9	0.8663 (7)	0.7500	0.4391 (4)	0.0319 (14)	
O10	0.5569 (5)	0.2500	0.1625 (3)	0.0128 (10)	
O11	0.4048 (6)	0.7500	0.2475 (4)	0.0174 (11)	
O12	0.5410 (5)	0.7500	0.1471 (3)	0.0144 (10)	
O13	0.2698 (4)	0.4909 (6)	0.1106 (3)	0.0187 (9)	
O14	0.7967 (5)	−0.0237 (7)	0.1337 (3)	0.0268 (10)	

O15	0.5547 (9)	0.6822 (13)	0.0040 (5)	0.031 (2)	0.50
O16	0.0623 (9)	0.2500	−0.0236 (4)	0.053 (2)	
O17	0.0246 (7)	0.2500	0.1176 (4)	0.0387 (17)	
H1	0.433 (12)	0.7500	0.309 (7)	0.04(3)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0285 (8)	0.0226 (8)	0.0209 (8)	0.000	0.0125 (6)	0.000
A1CE	0.0285 (8)	0.0226 (8)	0.0209 (8)	0.000	0.0125 (6)	0.000
A2CE	0.0175 (2)	0.0231 (3)	0.0148 (3)	0.000	0.00298 (17)	0.000
A2CA	0.0175 (2)	0.0231 (3)	0.0148 (3)	0.000	0.00298 (17)	0.000
A3CE	0.0302 (3)	0.0621 (5)	0.0126 (3)	0.000	0.0029 (2)	0.000
A3CA	0.0302 (3)	0.0621 (5)	0.0126 (3)	0.000	0.0029 (2)	0.000
A4CE	0.0171 (2)	0.0248 (3)	0.0141 (3)	0.000	0.00350 (17)	0.000
A4CA	0.0171 (2)	0.0248 (3)	0.0141 (3)	0.000	0.00350 (17)	0.000
M1AL	0.0134 (11)	0.0130 (11)	0.0150 (12)	0.0005 (8)	0.0036 (8)	0.0002 (9)
M1FE	0.0134 (11)	0.0130 (11)	0.0150 (12)	0.0005 (8)	0.0036 (8)	0.0002 (9)
M2AL	0.0105 (7)	0.0130 (8)	0.0153 (8)	−0.0002 (5)	0.0027 (6)	−0.0002 (6)
M2FE	0.0105 (7)	0.0130 (8)	0.0153 (8)	−0.0002 (5)	0.0027 (6)	−0.0002 (6)
M3FE	0.0184 (8)	0.0163 (8)	0.0188 (9)	0.000	0.0037 (6)	0.000
M3AL	0.0184 (8)	0.0163 (8)	0.0188 (9)	0.000	0.0037 (6)	0.000
Si1	0.0125 (9)	0.0137 (9)	0.0140 (10)	0.000	0.0043 (7)	0.000
Si2	0.0143 (9)	0.0108 (9)	0.0159 (10)	0.000	0.0065 (8)	0.000
Si3	0.0110 (8)	0.0150 (9)	0.0127 (10)	0.000	0.0043 (7)	0.000
Si4	0.0156 (9)	0.0154 (10)	0.0154 (10)	0.000	0.0066 (8)	0.000
Si5	0.0111 (8)	0.0103 (9)	0.0142 (10)	0.000	0.0021 (7)	0.000
O1	0.0176 (17)	0.0168 (18)	0.031 (2)	−0.0041 (14)	0.0122 (16)	−0.0064 (17)
O2	0.0198 (18)	0.028 (2)	0.019 (2)	0.0090 (16)	0.0104 (15)	0.0027 (17)
O3	0.0155 (17)	0.0137 (17)	0.022 (2)	−0.0016 (14)	0.0013 (14)	−0.0040 (16)
O4	0.014 (2)	0.015 (2)	0.015 (3)	0.000	0.0070 (19)	0.000
O5	0.015 (2)	0.015 (2)	0.013 (3)	0.000	0.0044 (19)	0.000
O6	0.013 (2)	0.017 (2)	0.017 (3)	0.000	0.008 (2)	0.000
O7	0.015 (2)	0.014 (2)	0.022 (3)	0.000	−0.004 (2)	0.000
O8	0.045 (4)	0.030 (3)	0.063 (5)	0.000	0.044 (4)	0.000
O9	0.034 (3)	0.040 (4)	0.019 (3)	0.000	0.010 (3)	0.000
O10	0.012 (2)	0.011 (2)	0.016 (3)	0.000	0.0067 (19)	0.000
O11	0.011 (2)	0.015 (3)	0.021 (3)	0.000	0.003 (2)	0.000
O12	0.011 (2)	0.013 (2)	0.019 (3)	0.000	0.0075 (19)	0.000
O13	0.0132 (16)	0.0118 (17)	0.022 (2)	−0.0025 (13)	0.0002 (14)	0.0024 (15)
O14	0.029 (2)	0.0178 (19)	0.040 (3)	−0.0053 (16)	0.021 (2)	−0.0024 (19)
O15	0.042 (4)	0.029 (6)	0.018 (4)	−0.006 (3)	0.009 (3)	−0.007 (3)

O16	0.065 (5)	0.062 (5)	0.012 (3)	0.000	−0.001 (3)	0.000
O17	0.024 (3)	0.061 (4)	0.038 (4)	0.000	0.020 (3)	0.000

NE_01

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.7321 (3)	0.2500	0.40986 (13)	0.0296 (7)	0.918 (4)
A1CE	0.7321 (3)	0.2500	0.40986 (13)	0.0296 (7)	0.082 (4)
A2CE	0.88953 (8)	0.2500	0.25023 (4)	0.0248 (2)	0.910 (6)
A2CA	0.88953 (8)	0.2500	0.25023 (4)	0.0248 (2)	0.090 (6)
A3CE	0.73973 (10)	0.2500	0.01002 (5)	0.0441 (3)	0.921 (7)
A3CA	0.73973 (10)	0.2500	0.01002 (5)	0.0441 (3)	0.079 (7)
A4CE	0.08213 (8)	0.7500	0.16457 (4)	0.0253 (2)	0.877 (6)
A4CA	0.08213 (8)	0.7500	0.16457 (4)	0.0253 (2)	0.123 (6)
M1AL	0.5000	0.5000	0.5000	0.0190 (9)	0.967 (11)
M1FE	0.5000	0.5000	0.5000	0.0190 (9)	0.033 (11)
M2AL	0.4823 (2)	−0.0004 (4)	0.20513 (13)	0.0186 (6)	0.950 (8)
M2FE	0.4823 (2)	−0.0004 (4)	0.20513 (13)	0.0186 (6)	0.050 (8)
M3FE	0.1979 (3)	0.7500	0.37598 (15)	0.0257 (7)	0.472 (11)
M3AL	0.1979 (3)	0.7500	0.37598 (15)	0.0257 (7)	0.528 (11)
Si1	0.1628 (3)	0.2500	0.47619 (18)	0.0166 (6)	
Si2	0.8078 (3)	0.7500	0.33724 (17)	0.0165 (6)	
Si3	0.3068 (3)	0.2500	0.31369 (17)	0.0154 (6)	
Si4	0.6728 (3)	0.7500	0.10417 (18)	0.0190 (6)	
Si5	0.1564 (3)	0.2500	0.07705 (18)	0.0160 (6)	
O1	0.2667 (6)	0.4902 (8)	0.4794 (3)	0.0259 (12)	
O2	0.1844 (6)	0.4794 (9)	0.2924 (3)	0.0249 (12)	
O3	0.6957 (5)	0.9875 (8)	0.2968 (3)	0.0219 (11)	
O4	0.4412 (8)	0.7500	0.4245 (4)	0.0175 (14)	
O5	0.4526 (8)	0.2500	0.4136 (4)	0.0212 (15)	
O6	0.4203 (8)	0.2500	0.2605 (4)	0.0166 (14)	
O7	−0.0163 (8)	0.2500	0.3983 (5)	0.0264 (18)	
O8	−0.0288 (10)	0.7500	0.3231 (6)	0.040 (2)	
O9	0.8643 (10)	0.7500	0.4383 (5)	0.036 (2)	
O10	0.5568 (8)	0.2500	0.1628 (4)	0.0172 (15)	
O11	0.4040 (8)	0.7500	0.2471 (4)	0.0181 (15)	
O12	0.5423 (7)	0.7500	0.1477 (4)	0.0205 (16)	

O13	0.2700 (6)	0.4898 (8)	0.1101 (3)	0.0215 (11)	
O14	0.7957 (6)	−0.0236 (8)	0.1333 (4)	0.0297 (13)	
O15	0.5539 (13)	0.6858 (16)	0.0030 (6)	0.034 (4)	0.50
O16	0.0633 (12)	0.2500	−0.0232 (5)	0.057 (3)	
O17	0.0262 (10)	0.2500	0.1159 (6)	0.046 (2)	
H1	0.438 (17)	0.7500	0.316 (10)	0.06 (4)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0344 (12)	0.0284 (12)	0.0296 (11)	0.000	0.0174 (9)	0.000
A1CE	0.0344 (12)	0.0284 (12)	0.0296 (11)	0.000	0.0174 (9)	0.000
A2CE	0.0217 (4)	0.0282 (4)	0.0203 (4)	0.000	0.0057 (3)	0.000
A2CA	0.0217 (4)	0.0282 (4)	0.0203 (4)	0.000	0.0057 (3)	0.000
A3CE	0.0364 (5)	0.0705 (7)	0.0176 (4)	0.000	0.0052 (3)	0.000
A3CA	0.0364 (5)	0.0705 (7)	0.0176 (4)	0.000	0.0052 (3)	0.000
A4CE	0.0205 (4)	0.0324 (4)	0.0184 (3)	0.000	0.0048 (3)	0.000
A4CA	0.0205 (4)	0.0324 (4)	0.0184 (3)	0.000	0.0048 (3)	0.000
M1AL	0.0150 (15)	0.0172 (16)	0.0233 (17)	0.0010 (11)	0.0072 (12)	−0.0016 (11)
M1FE	0.0150 (15)	0.0172 (16)	0.0233 (17)	0.0010 (11)	0.0072 (12)	−0.0016 (11)
M2AL	0.0138 (10)	0.0169 (10)	0.0221 (11)	0.0013 (7)	0.0055 (8)	0.0013 (7)
M2FE	0.0138 (10)	0.0169 (10)	0.0221 (11)	0.0013 (7)	0.0055 (8)	0.0013 (7)
M3FE	0.0260 (12)	0.0181 (11)	0.0296 (13)	0.000	0.0097 (10)	0.000
M3AL	0.0260 (12)	0.0181 (11)	0.0296 (13)	0.000	0.0097 (10)	0.000
Si1	0.0133 (12)	0.0167 (13)	0.0194 (14)	0.000	0.0069 (11)	0.000
Si2	0.0143 (13)	0.0171 (14)	0.0186 (14)	0.000	0.0078 (11)	0.000
Si3	0.0112 (12)	0.0177 (13)	0.0182 (13)	0.000	0.0075 (10)	0.000
Si4	0.0195 (14)	0.0206 (15)	0.0192 (14)	0.000	0.0108 (11)	0.000
Si5	0.0131 (12)	0.0119 (13)	0.0189 (13)	0.000	0.0036 (10)	0.000
O1	0.019 (2)	0.021 (3)	0.038 (3)	−0.001 (2)	0.012 (2)	−0.006 (2)
O2	0.019 (3)	0.033 (3)	0.026 (3)	0.008 (2)	0.014 (2)	0.003 (2)
O3	0.012 (2)	0.015 (2)	0.027 (3)	−0.0020 (18)	−0.001 (2)	−0.004 (2)
O4	0.016 (3)	0.020 (3)	0.019 (3)	0.000	0.010 (3)	0.000
O5	0.021 (4)	0.023 (4)	0.019 (4)	0.000	0.008 (3)	0.000
O6	0.018 (3)	0.014 (3)	0.023 (4)	0.000	0.014 (3)	0.000
O7	0.024 (4)	0.008 (3)	0.025 (4)	0.000	−0.008 (3)	0.000
O8	0.046 (5)	0.038 (5)	0.059 (6)	0.000	0.044 (5)	0.000
O9	0.043 (5)	0.049 (5)	0.022 (4)	0.000	0.019 (4)	0.000
O10	0.015 (3)	0.010 (3)	0.023 (4)	0.000	0.005 (3)	0.000
O11	0.013 (3)	0.017 (3)	0.021 (4)	0.000	0.005 (3)	0.000
O12	0.009 (3)	0.018 (3)	0.034 (4)	0.000	0.010 (3)	0.000
O13	0.015 (2)	0.014 (2)	0.027 (3)	−0.0014 (18)	0.001 (2)	−0.005 (2)

O14	0.027 (3)	0.025 (3)	0.048 (4)	−0.009 (2)	0.026 (3)	−0.002 (3)
O15	0.041 (6)	0.037 (10)	0.019 (5)	−0.013 (5)	0.009 (4)	−0.004 (4)
O16	0.078 (7)	0.051 (6)	0.018 (4)	0.000	0.001 (5)	0.000
O17	0.031 (5)	0.067 (6)	0.055 (6)	0.000	0.031 (5)	0.000

ST4_10

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73193 (18)	0.2500	0.40999 (8)	0.0233 (5)	0.936 (3)
A1CE	0.73193 (18)	0.2500	0.40999 (8)	0.0233 (5)	0.064 (3)
A2CE	0.88997 (6)	0.2500	0.24990 (2)	0.01881 (14)	0.943 (5)
A2CA	0.88997 (6)	0.2500	0.24990 (2)	0.01881 (14)	0.057 (5)
A3CE	0.73956 (7)	0.2500	0.01001 (3)	0.0360 (2)	0.941 (5)
A3CA	0.73956 (7)	0.2500	0.01001 (3)	0.0360 (2)	0.059 (5)
A4CE	0.08058 (6)	0.7500	0.16494 (2)	0.01876 (14)	0.906 (5)
A4CA	0.08058 (6)	0.7500	0.16494 (2)	0.01876 (14)	0.094 (5)
M1AL	0.5000	0.5000	0.5000	0.0146 (6)	0.982 (8)
M1FE	0.5000	0.5000	0.5000	0.0146 (6)	0.018 (8)
M2AL	0.48200 (17)	0.0000 (2)	0.20504 (8)	0.0124 (4)	0.978 (7)
M2FE	0.48200 (17)	0.0000 (2)	0.20504 (8)	0.0124 (4)	0.022 (7)
M3FE	0.19768 (19)	0.7500	0.37633 (8)	0.0204 (5)	0.520 (9)
M3AL	0.19768 (19)	0.7500	0.37633 (8)	0.0204 (5)	0.480 (9)
Si1	0.1622 (2)	0.2500	0.47608 (10)	0.0134 (4)	
Si2	0.8072 (2)	0.7500	0.33686 (10)	0.0129 (4)	
Si3	0.3063 (2)	0.2500	0.31346 (10)	0.0114 (4)	
Si4	0.6718 (2)	0.7500	0.10387 (11)	0.0144 (4)	
Si5	0.1562 (2)	0.2500	0.07744 (10)	0.0118 (4)	
O1	0.2660 (4)	0.4901 (6)	0.4789 (2)	0.0204 (8)	
O2	0.1824 (5)	0.4783 (6)	0.2918 (2)	0.0204 (7)	
O3	0.6963 (4)	0.9870 (5)	0.2972 (2)	0.0181 (7)	
O4	0.4421 (6)	0.7500	0.4245 (3)	0.0139 (9)	
O5	0.4512 (6)	0.2500	0.4138 (3)	0.0162 (10)	
O6	0.4201 (6)	0.2500	0.2602 (3)	0.0140 (9)	
O7	−0.0186 (6)	0.2500	0.3976 (3)	0.0190 (11)	
O8	−0.0352 (8)	0.7500	0.3183 (4)	0.0369 (15)	
O9	0.8649 (7)	0.7500	0.4387 (3)	0.0302 (13)	
O10	0.5570 (6)	0.2500	0.1622 (3)	0.0129 (9)	

O11	0.4048 (6)	0.7500	0.2480 (3)	0.0140 (9)	
O12	0.5404 (6)	0.7500	0.1474 (3)	0.0136 (9)	
O13	0.2695 (4)	0.4898 (5)	0.1104 (2)	0.0176 (7)	
O14	0.7949 (5)	−0.0242 (6)	0.1332 (2)	0.0225 (8)	
O15	0.5551 (9)	0.6839 (10)	0.0042 (4)	0.0242 (19)	0.50
O16	0.0628 (9)	0.2500	−0.0225 (3)	0.050 (2)	
O17	0.0241 (7)	0.2500	0.1168 (4)	0.0382 (14)	
H1	0.465 (11)	0.7500	0.332 (5)	0.03 (2)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0287 (8)	0.0224 (7)	0.0210 (6)	0.000	0.0130 (5)	0.000
A1CE	0.0287 (8)	0.0224 (7)	0.0210 (6)	0.000	0.0130 (5)	0.000
A2CE	0.0168 (2)	0.0230 (2)	0.01293 (17)	0.000	0.00328 (15)	0.000
A2CA	0.0168 (2)	0.0230 (2)	0.01293 (17)	0.000	0.00328 (15)	0.000
A3CE	0.0284 (3)	0.0624 (4)	0.01085 (19)	0.000	0.00317 (18)	0.000
A3CA	0.0284 (3)	0.0624 (4)	0.01085 (19)	0.000	0.00317 (18)	0.000
A4CE	0.0162 (2)	0.0249 (3)	0.01210 (18)	0.000	0.00360 (15)	0.000
A4CA	0.0162 (2)	0.0249 (3)	0.01210 (18)	0.000	0.00360 (15)	0.000
M1AL	0.0131 (10)	0.0148 (11)	0.0137 (9)	0.0001 (8)	0.0039 (7)	0.0004 (6)
M1FE	0.0131 (10)	0.0148 (11)	0.0137 (9)	0.0001 (8)	0.0039 (7)	0.0004 (6)
M2AL	0.0093 (7)	0.0124 (7)	0.0135 (6)	−0.0003 (5)	0.0031 (5)	−0.0003 (4)
M2FE	0.0093 (7)	0.0124 (7)	0.0135 (6)	−0.0003 (5)	0.0031 (5)	−0.0003 (4)
M3FE	0.0201 (8)	0.0166 (7)	0.0215 (7)	0.000	0.0065 (6)	0.000
M3AL	0.0201 (8)	0.0166 (7)	0.0215 (7)	0.000	0.0065 (6)	0.000
Si1	0.0118 (9)	0.0137 (8)	0.0121 (7)	0.000	0.0031 (7)	0.000
Si2	0.0122 (9)	0.0141 (8)	0.0125 (7)	0.000	0.0056 (7)	0.000
Si3	0.0095 (8)	0.0141 (8)	0.0098 (7)	0.000	0.0036 (6)	0.000
Si4	0.0126 (9)	0.0171 (9)	0.0149 (7)	0.000	0.0073 (7)	0.000
Si5	0.0096 (8)	0.0105 (8)	0.0114 (7)	0.000	0.0013 (6)	0.000
O1	0.0147 (17)	0.0172 (16)	0.0315 (18)	−0.0017 (14)	0.0123 (15)	−0.0062 (13)
O2	0.0200 (18)	0.0270 (18)	0.0178 (15)	0.0109 (15)	0.0116 (14)	0.0054 (13)
O3	0.0145 (17)	0.0114 (15)	0.0194 (15)	−0.0001 (13)	−0.0004 (13)	−0.0015 (12)
O4	0.013 (2)	0.014 (2)	0.0161 (19)	0.000	0.0072 (18)	0.000
O5	0.019 (3)	0.015 (2)	0.0128 (19)	0.000	0.0053 (18)	0.000
O6	0.013 (2)	0.015 (2)	0.0147 (19)	0.000	0.0069 (18)	0.000
O7	0.015 (2)	0.013 (2)	0.015 (2)	0.000	−0.0064 (18)	0.000
O8	0.037 (4)	0.035 (3)	0.057 (4)	0.000	0.037 (3)	0.000
O9	0.036 (3)	0.044 (3)	0.009 (2)	0.000	0.009 (2)	0.000
O10	0.011 (2)	0.013 (2)	0.0130 (18)	0.000	0.0037 (17)	0.000
O11	0.011 (2)	0.011 (2)	0.018 (2)	0.000	0.0048 (18)	0.000

O12	0.013 (2)	0.012 (2)	0.019 (2)	0.000	0.0096 (18)	0.000
O13	0.0117 (16)	0.0139 (15)	0.0207 (15)	−0.0009 (13)	0.0015 (13)	0.0000 (12)
O14	0.027 (2)	0.0159 (16)	0.0328 (19)	−0.0047 (15)	0.0205 (17)	−0.0041 (14)
O15	0.032 (4)	0.027 (5)	0.012 (3)	−0.007 (3)	0.009 (3)	−0.002 (2)
O16	0.064 (5)	0.055 (4)	0.011 (2)	0.000	−0.002 (3)	0.000
O17	0.020 (3)	0.063 (4)	0.034 (3)	0.000	0.015 (3)	0.000

ST4_02

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73232 (18)	0.2500	0.40993 (8)	0.0198 (5)	0.973 (3)
A1CE	0.73232 (18)	0.2500	0.40993 (8)	0.0198 (5)	0.027 (3)
A2CE	0.89058 (5)	0.2500	0.24976 (2)	0.01699 (15)	0.969 (5)
A2CA	0.89058 (5)	0.2500	0.24976 (2)	0.01699 (15)	0.031 (5)
A3CE	0.73944 (6)	0.2500	0.00990 (3)	0.03223 (19)	0.952 (5)
A3CA	0.73944 (6)	0.2500	0.00990 (3)	0.03223 (19)	0.048 (5)
A4CE	0.07896 (5)	0.7500	0.16537 (2)	0.01680 (15)	0.944 (5)
A4CA	0.07896 (5)	0.7500	0.16537 (2)	0.01680 (15)	0.056 (5)
M1AL	0.5000	0.5000	0.5000	0.0132 (7)	0.995 (8)
M1FE	0.5000	0.5000	0.5000	0.0132 (7)	0.005 (8)
M2AL	0.48144 (16)	−0.0001 (2)	0.20512 (8)	0.0119 (5)	0.985 (6)
M2FE	0.48144 (16)	−0.0001 (2)	0.20512 (8)	0.0119 (5)	0.015 (6)
M3FE	0.19617 (15)	0.7500	0.37628 (7)	0.0165 (4)	0.591 (9)
M3AL	0.19617 (15)	0.7500	0.37628 (7)	0.0165 (4)	0.409 (9)
Si1	0.1622 (2)	0.2500	0.47653 (11)	0.0129 (4)	
Si2	0.8064 (2)	0.7500	0.33609 (11)	0.0125 (4)	
Si3	0.3054 (2)	0.2500	0.31315 (11)	0.0118 (4)	
Si4	0.6702 (2)	0.7500	0.10339 (11)	0.0142 (4)	
Si5	0.1549 (2)	0.2500	0.07762 (11)	0.0110 (4)	
O1	0.2672 (4)	0.4909 (5)	0.4805 (2)	0.0187 (8)	
O2	0.1813 (4)	0.4762 (6)	0.2907 (2)	0.0201 (8)	
O3	0.6953 (4)	0.9866 (5)	0.2975 (2)	0.0169 (7)	
O4	0.4423 (6)	0.7500	0.4245 (3)	0.0156 (10)	
O5	0.4512 (6)	0.2500	0.4132 (3)	0.0134 (10)	
O6	0.4187 (5)	0.2500	0.2596 (3)	0.0130 (10)	
O7	−0.0164 (6)	0.2500	0.3972 (3)	0.0177 (11)	
O8	−0.0382 (7)	0.7500	0.3143 (4)	0.0319 (13)	

O9	0.8698 (7)	0.7500	0.4383 (3)	0.0279 (13)	
O10	0.5570 (5)	0.2500	0.1622 (3)	0.0109 (9)	
O11	0.4036 (5)	0.7500	0.2487 (3)	0.0138 (10)	
O12	0.5387 (5)	0.7500	0.1473 (3)	0.0114 (9)	
O13	0.2687 (4)	0.4903 (5)	0.1102 (2)	0.0172 (8)	
O14	0.7938 (4)	−0.0245 (6)	0.1328 (2)	0.0225 (8)	
O15	0.5539 (8)	0.6798 (10)	0.0045 (4)	0.026 (2)	0.50
O16	0.0626 (8)	0.2500	−0.0235 (3)	0.0491 (18)	
O17	0.0234 (6)	0.2500	0.1170 (3)	0.0331 (14)	
H1	0.438 (12)	0.7500	0.323 (7)	0.08 (3)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0233 (9)	0.0204 (8)	0.0180 (8)	0.000	0.0111 (6)	0.000
A1CE	0.0233 (9)	0.0204 (8)	0.0180 (8)	0.000	0.0111 (6)	0.000
A2CE	0.0134 (2)	0.0224 (3)	0.0129 (2)	0.000	0.00379 (16)	0.000
A2CA	0.0134 (2)	0.0224 (3)	0.0129 (2)	0.000	0.00379 (16)	0.000
A3CE	0.0221 (3)	0.0592 (4)	0.0115 (2)	0.000	0.00381 (18)	0.000
A3CA	0.0221 (3)	0.0592 (4)	0.0115 (2)	0.000	0.00381 (18)	0.000
A4CE	0.0130 (2)	0.0228 (3)	0.0129 (2)	0.000	0.00415 (16)	0.000
A4CA	0.0130 (2)	0.0228 (3)	0.0129 (2)	0.000	0.00415 (16)	0.000
M1AL	0.0117 (11)	0.0139 (11)	0.0139 (10)	−0.0002 (8)	0.0056 (8)	−0.0002 (7)
M1FE	0.0117 (11)	0.0139 (11)	0.0139 (10)	−0.0002 (8)	0.0056 (8)	−0.0002 (7)
M2AL	0.0075 (8)	0.0133 (7)	0.0138 (8)	0.0004 (5)	0.0038 (6)	−0.0002 (5)
M2FE	0.0075 (8)	0.0133 (7)	0.0138 (8)	0.0004 (5)	0.0038 (6)	−0.0002 (5)
M3FE	0.0140 (7)	0.0164 (7)	0.0163 (7)	0.000	0.0043 (5)	0.000
M3AL	0.0140 (7)	0.0164 (7)	0.0163 (7)	0.000	0.0043 (5)	0.000
Si1	0.0107 (9)	0.0152 (9)	0.0135 (9)	0.000	0.0058 (7)	0.000
Si2	0.0122 (10)	0.0126 (9)	0.0129 (9)	0.000	0.0059 (7)	0.000
Si3	0.0097 (9)	0.0159 (9)	0.0106 (8)	0.000	0.0053 (7)	0.000
Si4	0.0110 (9)	0.0172 (9)	0.0153 (9)	0.000	0.0067 (7)	0.000
Si5	0.0093 (9)	0.0092 (8)	0.0119 (8)	0.000	0.0023 (7)	0.000
O1	0.0138 (17)	0.0162 (16)	0.0270 (19)	−0.0012 (14)	0.0097 (14)	−0.0041 (14)
O2	0.0178 (19)	0.0259 (18)	0.0194 (18)	0.0078 (15)	0.0109 (14)	0.0055 (14)
O3	0.0151 (18)	0.0120 (15)	0.0172 (17)	−0.0016 (14)	0.0014 (13)	−0.0004 (13)
O4	0.014 (2)	0.017 (2)	0.015 (2)	0.000	0.0059 (18)	0.000
O5	0.013 (2)	0.014 (2)	0.015 (2)	0.000	0.0081 (18)	0.000
O6	0.013 (2)	0.012 (2)	0.015 (2)	0.000	0.0081 (18)	0.000
O7	0.012 (2)	0.017 (2)	0.018 (2)	0.000	0.0008 (18)	0.000
O8	0.033 (3)	0.034 (3)	0.044 (3)	0.000	0.030 (3)	0.000
O9	0.027 (3)	0.043 (3)	0.016 (3)	0.000	0.012 (2)	0.000

O10	0.006 (2)	0.012 (2)	0.012 (2)	0.000	0.0021 (17)	0.000
O11	0.007 (2)	0.012 (2)	0.018 (2)	0.000	0.0026 (18)	0.000
O12	0.009 (2)	0.013 (2)	0.017 (2)	0.000	0.0099 (18)	0.000
O13	0.0109 (16)	0.0120 (15)	0.0228 (18)	−0.0046 (14)	0.0020 (13)	−0.0019 (13)
O14	0.025 (2)	0.0188 (17)	0.034 (2)	−0.0048 (15)	0.0219 (17)	−0.0043 (15)
O15	0.028 (4)	0.025 (5)	0.021 (3)	−0.004 (3)	0.009 (3)	−0.004 (3)
O16	0.056 (4)	0.064 (4)	0.013 (3)	0.000	0.002 (3)	0.000
O17	0.017 (3)	0.056 (4)	0.035 (3)	0.000	0.020 (2)	0.000

ST2_01

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73250 (15)	0.2500	0.40977 (7)	0.0212 (4)	0.934 (3)
A1CE	0.73250 (15)	0.2500	0.40977 (7)	0.0212 (4)	0.066 (3)
A2CE	0.89117 (5)	0.2500	0.24969 (2)	0.01753 (12)	0.949 (5)
A2CA	0.89117 (5)	0.2500	0.24969 (2)	0.01753 (12)	0.051 (5)
A3CE	0.73982 (6)	0.2500	0.00977 (3)	0.03453 (18)	0.938 (5)
A3CA	0.73982 (6)	0.2500	0.00977 (3)	0.03453 (18)	0.062 (5)
A4CE	0.07940 (5)	0.7500	0.16531 (2)	0.01735 (13)	0.928 (5)
A4CA	0.07940 (5)	0.7500	0.16531 (2)	0.01735 (13)	0.072 (5)
M1AL	0.5000	0.5000	0.5000	0.0128 (5)	0.977 (8)
M1FE	0.5000	0.5000	0.5000	0.0128 (5)	0.023 (8)
M2AL	0.48129 (14)	0.0003 (2)	0.20515 (7)	0.0122 (4)	0.965 (6)
M2FE	0.48129 (14)	0.0003 (2)	0.20515 (7)	0.0122 (4)	0.035 (6)
M3FE	0.19507 (14)	0.7500	0.37608 (7)	0.0172 (4)	0.624 (9)
M3AL	0.19507 (14)	0.7500	0.37608 (7)	0.0172 (4)	0.376 (9)
Si1	0.1623 (2)	0.2500	0.47693 (10)	0.0117 (3)	
Si2	0.80604 (19)	0.7500	0.33625 (10)	0.0115 (3)	
Si3	0.30556 (19)	0.2500	0.31300 (10)	0.0109 (3)	
Si4	0.6712 (2)	0.7500	0.10376 (11)	0.0138 (3)	
Si5	0.15526 (19)	0.2500	0.07740 (10)	0.0112 (3)	
O1	0.2670 (4)	0.4902 (6)	0.4814 (2)	0.0198 (7)	
O2	0.1812 (4)	0.4776 (6)	0.29045 (19)	0.0177 (7)	
O3	0.6947 (4)	0.9865 (5)	0.29786 (19)	0.0170 (7)	
O4	0.4422 (5)	0.7500	0.4253 (3)	0.0140 (8)	
O5	0.4504 (5)	0.2500	0.4136 (3)	0.0147 (9)	
O6	0.4188 (5)	0.2500	0.2597 (2)	0.0127 (8)	

O7	−0.0157 (5)	0.2500	0.3967 (3)	0.0170 (9)	
O8	−0.0400 (6)	0.7500	0.3141 (4)	0.0345 (13)	
O9	0.8685 (6)	0.7500	0.4388 (3)	0.0260 (11)	
O10	0.5576 (5)	0.2500	0.1631 (2)	0.0118 (8)	
O11	0.4037 (5)	0.7500	0.2483 (3)	0.0143 (9)	
O12	0.5395 (5)	0.7500	0.1476 (3)	0.0127 (8)	
O13	0.2697 (4)	0.4898 (5)	0.1105 (2)	0.0168 (7)	
O14	0.7945 (4)	−0.0234 (6)	0.1327 (2)	0.0222 (7)	
O15	0.5533 (7)	0.6841 (10)	0.0047 (3)	0.0242 (16)	0.50
O16	0.0631 (8)	0.2500	−0.0230 (3)	0.0491 (17)	
O17	0.0235 (6)	0.2500	0.1167 (3)	0.0341 (13)	
H1	0.417 (10)	0.7500	0.328 (5)	0.05 (3)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0272 (7)	0.0187 (6)	0.0204 (6)	0.000	0.0131 (5)	0.000
A1CE	0.0272 (7)	0.0187 (6)	0.0204 (6)	0.000	0.0131 (5)	0.000
A2CE	0.01653 (19)	0.0191 (2)	0.01348 (18)	0.000	0.00352 (14)	0.000
A2CA	0.01653 (19)	0.0191 (2)	0.01348 (18)	0.000	0.00352 (14)	0.000
A3CE	0.0277 (3)	0.0586 (4)	0.0112 (2)	0.000	0.00324 (16)	0.000
A3CA	0.0277 (3)	0.0586 (4)	0.0112 (2)	0.000	0.00324 (16)	0.000
A4CE	0.01633 (19)	0.0196 (2)	0.01327 (18)	0.000	0.00401 (14)	0.000
A4CA	0.01633 (19)	0.0196 (2)	0.01327 (18)	0.000	0.00401 (14)	0.000
M1AL	0.0134 (9)	0.0095 (9)	0.0146 (9)	0.0007 (6)	0.0054 (7)	−0.0007 (7)
M1FE	0.0134 (9)	0.0095 (9)	0.0146 (9)	0.0007 (6)	0.0054 (7)	−0.0007 (7)
M2AL	0.0108 (6)	0.0089 (6)	0.0149 (6)	0.0005 (4)	0.0040 (5)	0.0003 (4)
M2FE	0.0108 (6)	0.0089 (6)	0.0149 (6)	0.0005 (4)	0.0040 (5)	0.0003 (4)
M3FE	0.0176 (6)	0.0129 (6)	0.0162 (6)	0.000	0.0032 (4)	0.000
M3AL	0.0176 (6)	0.0129 (6)	0.0162 (6)	0.000	0.0032 (4)	0.000
Si1	0.0126 (7)	0.0094 (7)	0.0119 (7)	0.000	0.0045 (6)	0.000
Si2	0.0125 (7)	0.0090 (7)	0.0133 (7)	0.000	0.0059 (6)	0.000
Si3	0.0117 (7)	0.0100 (7)	0.0112 (7)	0.000	0.0054 (6)	0.000
Si4	0.0136 (7)	0.0126 (8)	0.0159 (8)	0.000	0.0073 (6)	0.000
Si5	0.0103 (7)	0.0071 (7)	0.0120 (7)	0.000	0.0011 (6)	0.000
O1	0.0180 (14)	0.0137 (15)	0.0293 (17)	−0.0027 (12)	0.0121 (14)	−0.0055 (13)
O2	0.0163 (14)	0.0203 (16)	0.0179 (14)	0.0086 (12)	0.0089 (12)	0.0056 (13)
O3	0.0132 (13)	0.0106 (14)	0.0199 (15)	0.0013 (11)	0.0008 (12)	0.0003 (12)
O4	0.0115 (18)	0.013 (2)	0.0137 (19)	0.000	0.0026 (16)	0.000
O5	0.018 (2)	0.0101 (19)	0.0130 (19)	0.000	0.0047 (16)	0.000
O6	0.0143 (19)	0.0097 (19)	0.0144 (19)	0.000	0.0068 (16)	0.000
O7	0.014 (2)	0.014 (2)	0.0138 (19)	0.000	−0.0022 (16)	0.000

O8	0.032 (3)	0.038 (3)	0.051 (3)	0.000	0.033 (3)	0.000
O9	0.030 (3)	0.035 (3)	0.013 (2)	0.000	0.0096 (19)	0.000
O10	0.0100 (18)	0.0111 (19)	0.0128 (19)	0.000	0.0038 (15)	0.000
O11	0.0100 (18)	0.0083 (19)	0.021 (2)	0.000	0.0040 (16)	0.000
O12	0.0103 (18)	0.0101 (19)	0.017 (2)	0.000	0.0058 (16)	0.000
O13	0.0112 (13)	0.0090 (13)	0.0235 (16)	−0.0006 (11)	0.0016 (12)	−0.0017 (12)
O14	0.0254 (16)	0.0114 (15)	0.0369 (19)	−0.0029 (13)	0.0204 (15)	−0.0024 (14)
O15	0.035 (3)	0.022 (4)	0.015 (3)	−0.008 (3)	0.011 (2)	−0.001 (2)
O16	0.060 (4)	0.062 (4)	0.013 (2)	0.000	0.005 (2)	0.000
O17	0.019 (2)	0.051 (4)	0.036 (3)	0.000	0.016 (2)	0.000

ST2_03

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73229 (19)	0.2500	0.40997 (9)	0.0212 (5)	0.944 (3)
A1CE	0.73229 (19)	0.2500	0.40997 (9)	0.0212 (5)	0.056 (3)
A2CE	0.89122 (6)	0.2500	0.24965 (3)	0.01784 (16)	0.958 (5)
A2CA	0.89122 (6)	0.2500	0.24965 (3)	0.01784 (16)	0.042 (5)
A3CE	0.74003 (7)	0.2500	0.00973 (3)	0.0341 (2)	0.944 (5)
A3CA	0.74003 (7)	0.2500	0.00973 (3)	0.0341 (2)	0.056 (5)
A4CE	0.07929 (6)	0.7500	0.16549 (3)	0.01730 (16)	0.932 (5)
A4CA	0.07929 (6)	0.7500	0.16549 (3)	0.01730 (16)	0.068 (5)
M1AL	0.5000	0.5000	0.5000	0.0150 (7)	0.966 (8)
M1FE	0.5000	0.5000	0.5000	0.0150 (7)	0.034 (8)
M2AL	0.48153 (18)	0.0001 (3)	0.20524 (9)	0.0133 (5)	0.962 (6)
M2FE	0.48153 (18)	0.0001 (3)	0.20524 (9)	0.0133 (5)	0.038 (6)
M3FE	0.19482 (17)	0.7500	0.37633 (8)	0.0174 (4)	0.660 (9)
M3AL	0.19482 (17)	0.7500	0.37633 (8)	0.0174 (4)	0.340 (9)
Si1	0.1630 (3)	0.2500	0.47704 (12)	0.0115 (4)	
Si2	0.8060 (2)	0.7500	0.33628 (12)	0.0119 (5)	
Si3	0.3055 (2)	0.2500	0.31277 (12)	0.0113 (4)	
Si4	0.6713 (3)	0.7500	0.10365 (12)	0.0145 (5)	
Si5	0.1558 (2)	0.2500	0.07787 (11)	0.0110 (4)	
O1	0.2674 (4)	0.4895 (7)	0.4817 (2)	0.0185 (9)	
O2	0.1815 (4)	0.4754 (7)	0.2903 (2)	0.0180 (9)	
O3	0.6941 (4)	0.9870 (6)	0.2977 (2)	0.0173 (8)	
O4	0.4409 (6)	0.7500	0.4249 (3)	0.0152 (11)	

O5	0.4504 (6)	0.2500	0.4135 (3)	0.0130 (11)	
O6	0.4185 (6)	0.2500	0.2599 (3)	0.0139 (11)	
O7	−0.0161 (6)	0.2500	0.3973 (3)	0.0162 (11)	
O8	−0.0418 (8)	0.7500	0.3137 (4)	0.0338 (16)	
O9	0.8707 (7)	0.7500	0.4389 (3)	0.0266 (14)	
O10	0.5583 (6)	0.2500	0.1622 (3)	0.0108 (10)	
O11	0.4026 (6)	0.7500	0.2482 (3)	0.0144 (11)	
O12	0.5408 (6)	0.7500	0.1477 (3)	0.0139 (11)	
O13	0.2696 (4)	0.4904 (6)	0.1104 (2)	0.0174 (8)	
O14	0.7939 (5)	−0.0249 (6)	0.1324 (2)	0.0215 (9)	
O15	0.5524 (9)	0.6812 (13)	0.0043 (4)	0.027 (3)	0.50
O16	0.0630 (8)	0.2500	−0.0230 (3)	0.049 (2)	
O17	0.0241 (7)	0.2500	0.1166 (4)	0.0363 (16)	
H1	0.459 (14)	0.7500	0.332 (8)	0.09 (4)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0262 (9)	0.0207 (9)	0.0191 (7)	0.000	0.0122 (6)	0.000
A1CE	0.0262 (9)	0.0207 (9)	0.0191 (7)	0.000	0.0122 (6)	0.000
A2CE	0.0159 (3)	0.0219 (3)	0.0127 (2)	0.000	0.00363 (17)	0.000
A2CA	0.0159 (3)	0.0219 (3)	0.0127 (2)	0.000	0.00363 (17)	0.000
A3CE	0.0270 (3)	0.0588 (5)	0.0105 (2)	0.000	0.0030 (2)	0.000
A3CA	0.0270 (3)	0.0588 (5)	0.0105 (2)	0.000	0.0030 (2)	0.000
A4CE	0.0155 (3)	0.0213 (3)	0.0123 (2)	0.000	0.00367 (18)	0.000
A4CA	0.0155 (3)	0.0213 (3)	0.0123 (2)	0.000	0.00367 (18)	0.000
M1AL	0.0139 (13)	0.0128 (13)	0.0160 (11)	−0.0005 (9)	0.0045 (9)	−0.0010 (8)
M1FE	0.0139 (13)	0.0128 (13)	0.0160 (11)	−0.0005 (9)	0.0045 (9)	−0.0010 (8)
M2AL	0.0111 (8)	0.0114 (8)	0.0149 (7)	0.0004 (6)	0.0036 (6)	−0.0008 (6)
M2FE	0.0111 (8)	0.0114 (8)	0.0149 (7)	0.0004 (6)	0.0036 (6)	−0.0008 (6)
M3FE	0.0156 (8)	0.0149 (8)	0.0168 (7)	0.000	0.0028 (5)	0.000
M3AL	0.0156 (8)	0.0149 (8)	0.0168 (7)	0.000	0.0028 (5)	0.000
Si1	0.0140 (10)	0.0087 (10)	0.0116 (9)	0.000	0.0055 (8)	0.000
Si2	0.0121 (11)	0.0121 (11)	0.0121 (9)	0.000	0.0058 (8)	0.000
Si3	0.0092 (10)	0.0139 (11)	0.0102 (8)	0.000	0.0037 (7)	0.000
Si4	0.0133 (11)	0.0177 (12)	0.0133 (9)	0.000	0.0066 (8)	0.000
Si5	0.0108 (10)	0.0088 (10)	0.0100 (8)	0.000	0.0016 (7)	0.000
O1	0.014 (2)	0.016 (2)	0.028 (2)	−0.0002 (16)	0.0108 (17)	−0.0028 (16)
O2	0.018 (2)	0.023 (2)	0.0160 (17)	0.0080 (17)	0.0098 (15)	0.0037 (16)
O3	0.0148 (19)	0.012 (2)	0.0181 (18)	0.0009 (16)	0.0010 (15)	0.0000 (15)
O4	0.009 (3)	0.019 (3)	0.018 (2)	0.000	0.005 (2)	0.000
O5	0.012 (3)	0.012 (3)	0.012 (2)	0.000	0.003 (2)	0.000

O6	0.018 (3)	0.009 (3)	0.016 (2)	0.000	0.009 (2)	0.000
O7	0.015 (3)	0.009 (3)	0.015 (2)	0.000	−0.002 (2)	0.000
O8	0.032 (4)	0.040 (4)	0.043 (4)	0.000	0.029 (3)	0.000
O9	0.031 (3)	0.035 (4)	0.015 (3)	0.000	0.011 (2)	0.000
O10	0.011 (3)	0.003 (2)	0.016 (2)	0.000	0.003 (2)	0.000
O11	0.008 (3)	0.013 (3)	0.020 (3)	0.000	0.005 (2)	0.000
O12	0.012 (3)	0.012 (3)	0.019 (2)	0.000	0.007 (2)	0.000
O13	0.0140 (19)	0.0089 (19)	0.025 (2)	−0.0025 (15)	0.0043 (16)	−0.0020 (15)
O14	0.022 (2)	0.014 (2)	0.039 (2)	−0.0022 (17)	0.0230 (19)	−0.0027 (18)
O15	0.032 (4)	0.034 (7)	0.012 (3)	−0.007 (4)	0.008 (3)	0.001 (3)
O16	0.061 (5)	0.056 (5)	0.009 (3)	0.000	−0.004 (3)	0.000
O17	0.022 (3)	0.060 (5)	0.030 (3)	0.000	0.014 (3)	0.000

ST2_04

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73123 (19)	0.2500	0.41010 (10)	0.0219 (5)	0.942 (4)
A1CE	0.73123 (19)	0.2500	0.41010 (10)	0.0219 (5)	0.058 (4)
A2CE	0.89131 (5)	0.2500	0.24962 (3)	0.01652 (15)	0.973 (6)
A2CA	0.89131 (5)	0.2500	0.24962 (3)	0.01652 (15)	0.027 (6)
A3CE	0.73919 (7)	0.2500	0.00967 (3)	0.0312 (2)	0.945 (6)
A3CA	0.73919 (7)	0.2500	0.00967 (3)	0.0312 (2)	0.055 (6)
A4CE	0.07848 (5)	0.7500	0.16564 (3)	0.01576 (15)	0.945 (6)
A4CA	0.07848 (5)	0.7500	0.16564 (3)	0.01576 (15)	0.055 (6)
M1AL	0.5000	0.5000	0.5000	0.0120 (7)	0.993 (14)
M1FE	0.5000	0.5000	0.5000	0.0120 (7)	0.007 (14)
M2AL	0.48117 (17)	0.0005 (3)	0.20518 (10)	0.0115 (5)	0.968 (8)
M2FE	0.48117 (17)	0.0005 (3)	0.20518 (10)	0.0115 (5)	0.032 (8)
M3FE	0.19571 (17)	0.7500	0.37678 (9)	0.0188 (4)	0.732 (11)
M3AL	0.19571 (17)	0.7500	0.37678 (9)	0.0188 (4)	0.268 (11)
Si1	0.1618 (2)	0.2500	0.47706 (13)	0.0129 (4)	
Si2	0.8058 (2)	0.7500	0.33585 (13)	0.0114 (4)	
Si3	0.3047 (2)	0.2500	0.31268 (13)	0.0100 (4)	
Si4	0.6702 (2)	0.7500	0.10335 (13)	0.0121 (4)	
Si5	0.1553 (2)	0.2500	0.07728 (13)	0.0102 (4)	
O1	0.2679 (5)	0.4882 (7)	0.4819 (3)	0.0198 (9)	
O2	0.1794 (5)	0.4776 (7)	0.2897 (3)	0.0188 (8)	

O3	0.6941 (4)	0.9870 (6)	0.2974 (3)	0.0162 (8)	
O4	0.4411 (6)	0.7500	0.4247 (3)	0.0155 (11)	
O5	0.4506 (7)	0.2500	0.4132 (3)	0.0163 (11)	
O6	0.4188 (6)	0.2500	0.2599 (3)	0.0139 (10)	
O7	−0.0182 (6)	0.2500	0.3997 (4)	0.0173 (12)	
O8	−0.0426 (8)	0.7500	0.3124 (5)	0.0336 (16)	
O9	0.8728 (7)	0.7500	0.4391 (4)	0.0265 (14)	
O10	0.5571 (6)	0.2500	0.1626 (3)	0.0126 (10)	
O11	0.4043 (6)	0.7500	0.2490 (3)	0.0131 (10)	
O12	0.5392 (6)	0.7500	0.1478 (3)	0.0125 (10)	
O13	0.2698 (5)	0.4894 (6)	0.1113 (3)	0.0163 (8)	
O14	0.7944 (5)	−0.0248 (7)	0.1322 (3)	0.0200 (9)	
O15	0.5537 (9)	0.6795 (13)	0.0037 (5)	0.022 (2)	0.50
O16	0.0593 (10)	0.2500	−0.0231 (4)	0.047 (2)	
O17	0.0244 (7)	0.2500	0.1174 (4)	0.0314 (15)	
H1	0.479 (13)	0.7500	0.338 (7)	0.05 (3)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0277 (8)	0.0207 (9)	0.0174 (7)	0.000	0.0102 (6)	0.000
A1CE	0.0277 (8)	0.0207 (9)	0.0174 (7)	0.000	0.0102 (6)	0.000
A2CE	0.0131 (2)	0.0222 (3)	0.0119 (2)	0.000	0.00335 (16)	0.000
A2CA	0.0131 (2)	0.0222 (3)	0.0119 (2)	0.000	0.00335 (16)	0.000
A3CE	0.0213 (3)	0.0596 (5)	0.0092 (2)	0.000	0.00362 (19)	0.000
A3CA	0.0213 (3)	0.0596 (5)	0.0092 (2)	0.000	0.00362 (19)	0.000
A4CE	0.0120 (2)	0.0221 (3)	0.0113 (2)	0.000	0.00343 (16)	0.000
A4CA	0.0120 (2)	0.0221 (3)	0.0113 (2)	0.000	0.00343 (16)	0.000
M1AL	0.0100 (10)	0.0132 (12)	0.0121 (11)	−0.0003 (8)	0.0044 (8)	−0.0006 (9)
M1FE	0.0100 (10)	0.0132 (12)	0.0121 (11)	−0.0003 (8)	0.0044 (8)	−0.0006 (9)
M2AL	0.0092 (7)	0.0116 (8)	0.0132 (8)	−0.0006 (5)	0.0043 (6)	−0.0009 (6)
M2FE	0.0092 (7)	0.0116 (8)	0.0132 (8)	−0.0006 (5)	0.0043 (6)	−0.0009 (6)
M3FE	0.0177 (7)	0.0168 (8)	0.0237 (8)	0.000	0.0107 (6)	0.000
M3AL	0.0177 (7)	0.0168 (8)	0.0237 (8)	0.000	0.0107 (6)	0.000
Si1	0.0122 (9)	0.0139 (10)	0.0109 (9)	0.000	0.0035 (7)	0.000
Si2	0.0099 (9)	0.0115 (10)	0.0136 (9)	0.000	0.0057 (8)	0.000
Si3	0.0076 (8)	0.0133 (10)	0.0099 (9)	0.000	0.0048 (7)	0.000
Si4	0.0101 (8)	0.0158 (10)	0.0120 (9)	0.000	0.0062 (7)	0.000
Si5	0.0072 (8)	0.0109 (10)	0.0106 (9)	0.000	0.0024 (7)	0.000
O1	0.0157 (17)	0.0168 (19)	0.030 (2)	−0.0022 (15)	0.0124 (17)	−0.0075 (18)
O2	0.0172 (18)	0.024 (2)	0.0177 (19)	0.0043 (16)	0.0103 (15)	−0.0006 (17)
O3	0.0123 (17)	0.0097 (18)	0.0203 (19)	−0.0009 (14)	0.0014 (15)	−0.0011 (16)

O4	0.015 (2)	0.016 (3)	0.012 (2)	0.000	0.003 (2)	0.000
O5	0.020 (3)	0.019 (3)	0.012 (2)	0.000	0.009 (2)	0.000
O6	0.012 (2)	0.016 (3)	0.017 (3)	0.000	0.009 (2)	0.000
O7	0.006 (2)	0.004 (2)	0.022 (3)	0.000	−0.012 (2)	0.000
O8	0.031 (4)	0.034 (4)	0.049 (4)	0.000	0.030 (3)	0.000
O9	0.026 (3)	0.044 (4)	0.009 (3)	0.000	0.007 (2)	0.000
O10	0.014 (2)	0.007 (2)	0.015 (2)	0.000	0.005 (2)	0.000
O11	0.013 (2)	0.011 (3)	0.014 (2)	0.000	0.004 (2)	0.000
O12	0.011 (2)	0.013 (3)	0.015 (2)	0.000	0.007 (2)	0.000
O13	0.0122 (16)	0.0085 (17)	0.022 (2)	−0.0028 (14)	0.0024 (15)	0.0000 (15)
O14	0.022 (2)	0.014 (2)	0.031 (2)	−0.0025 (16)	0.0185 (18)	−0.0013 (17)
O15	0.020 (4)	0.033 (6)	0.010 (3)	−0.004 (3)	0.005 (3)	−0.004 (3)
O16	0.059 (5)	0.056 (5)	0.008 (3)	0.000	0.000 (3)	0.000
O17	0.019 (3)	0.053 (4)	0.027 (3)	0.000	0.015 (3)	0.000

HU_01

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.7329 (2)	0.2500	0.41004 (10)	0.0180 (6)	0.964 (3)
A1CE	0.7329 (2)	0.2500	0.41004 (10)	0.0180 (6)	0.036 (3)
A2CE	0.89190 (7)	0.2500	0.24953 (3)	0.01674 (19)	0.974 (5)
A2CA	0.89190 (7)	0.2500	0.24953 (3)	0.01674 (19)	0.026 (5)
A3CE	0.74007 (8)	0.2500	0.00964 (3)	0.0322 (3)	0.952 (5)
A3CA	0.74007 (8)	0.2500	0.00964 (3)	0.0322 (3)	0.048 (5)
A4CE	0.07839 (7)	0.7500	0.16573 (3)	0.01624 (18)	0.946 (5)
A4CA	0.07839 (7)	0.7500	0.16573 (3)	0.01624 (18)	0.054 (5)
M1AL	0.5000	0.5000	0.5000	0.0140 (8)	0.952 (8)
M1FE	0.5000	0.5000	0.5000	0.0140 (8)	0.048 (8)
M2AL	0.4812 (2)	−0.0005 (3)	0.20501 (10)	0.0116 (5)	0.970 (6)
M2FE	0.4812 (2)	−0.0005 (3)	0.20501 (10)	0.0116 (5)	0.030 (6)
M3FE	0.19448 (18)	0.7500	0.37652 (9)	0.0162 (5)	0.742 (9)
M3AL	0.19448 (18)	0.7500	0.37652 (9)	0.0162 (5)	0.258 (9)
Si1	0.1620 (3)	0.2500	0.47756 (14)	0.0118 (5)	
Si2	0.8051 (3)	0.7500	0.33553 (14)	0.0112 (5)	
Si3	0.3051 (3)	0.2500	0.31258 (14)	0.0097 (5)	
Si4	0.6702 (3)	0.7500	0.10310 (14)	0.0124 (5)	
Si5	0.1549 (3)	0.2500	0.07757 (14)	0.0109 (5)	

O1	0.2673 (5)	0.4902 (7)	0.4823 (2)	0.0168 (10)	
O2	0.1801 (5)	0.4756 (8)	0.2893 (2)	0.0156 (10)	
O3	0.6941 (5)	−0.0125 (7)	0.2983 (2)	0.0161 (10)	
O4	0.4408 (7)	0.7500	0.4253 (3)	0.0137 (13)	
O5	0.4487 (7)	0.2500	0.4126 (3)	0.0116 (13)	
O6	0.4181 (6)	0.2500	0.2591 (3)	0.0091 (12)	
O7	−0.0150 (7)	0.2500	0.3976 (3)	0.0157 (14)	
O8	−0.0422 (9)	0.7500	0.3117 (4)	0.0321 (18)	
O9	0.8726 (8)	0.7500	0.4384 (4)	0.0258 (16)	
O10	0.5572 (7)	0.2500	0.1626 (3)	0.0108 (13)	
O11	0.4035 (7)	0.7500	0.2499 (3)	0.0122 (13)	
O12	0.5414 (7)	0.7500	0.1485 (3)	0.0138 (13)	
O13	0.2678 (5)	0.4896 (7)	0.1102 (2)	0.0156 (10)	
O14	0.7934 (5)	0.5254 (8)	0.1316 (3)	0.0211 (11)	
O15	0.5499 (9)	0.8190 (16)	0.0043 (5)	0.025 (3)	0.50
O16	0.0641 (9)	0.2500	−0.0223 (4)	0.041 (2)	
O17	0.0219 (8)	0.2500	0.1169 (4)	0.0343 (19)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0245 (11)	0.0144 (11)	0.0186 (9)	0.000	0.0127 (7)	0.000
A1CE	0.0245 (11)	0.0144 (11)	0.0186 (9)	0.000	0.0127 (7)	0.000
A2CE	0.0137 (3)	0.0213 (4)	0.0134 (3)	0.000	0.00431 (19)	0.000
A2CA	0.0137 (3)	0.0213 (4)	0.0134 (3)	0.000	0.00431 (19)	0.000
A3CE	0.0234 (4)	0.0573 (6)	0.0120 (3)	0.000	0.0044 (2)	0.000
A3CA	0.0234 (4)	0.0573 (6)	0.0120 (3)	0.000	0.0044 (2)	0.000
A4CE	0.0133 (3)	0.0209 (4)	0.0129 (3)	0.000	0.0044 (2)	0.000
A4CA	0.0133 (3)	0.0209 (4)	0.0129 (3)	0.000	0.0044 (2)	0.000
M1AL	0.0145 (15)	0.0122 (16)	0.0170 (13)	0.0037 (11)	0.0084 (10)	0.0007 (9)
M1FE	0.0145 (15)	0.0122 (16)	0.0170 (13)	0.0037 (11)	0.0084 (10)	0.0007 (9)
M2AL	0.0095 (9)	0.0096 (10)	0.0149 (9)	0.0002 (7)	0.0045 (6)	−0.0001 (6)
M2FE	0.0095 (9)	0.0096 (10)	0.0149 (9)	0.0002 (7)	0.0045 (6)	−0.0001 (6)
M3FE	0.0147 (9)	0.0141 (9)	0.0170 (7)	0.000	0.0045 (6)	0.000
M3AL	0.0147 (9)	0.0141 (9)	0.0170 (7)	0.000	0.0045 (6)	0.000
Si1	0.0108 (12)	0.0116 (14)	0.0129 (11)	0.000	0.0051 (9)	0.000
Si2	0.0107 (13)	0.0090 (14)	0.0156 (11)	0.000	0.0074 (9)	0.000
Si3	0.0068 (12)	0.0098 (14)	0.0140 (11)	0.000	0.0059 (8)	0.000
Si4	0.0101 (12)	0.0155 (15)	0.0131 (11)	0.000	0.0064 (9)	0.000
Si5	0.0100 (12)	0.0080 (13)	0.0118 (10)	0.000	0.0023 (8)	0.000
O1	0.016 (2)	0.011 (3)	0.026 (2)	0.0007 (19)	0.0115 (18)	−0.0013 (18)
O2	0.018 (2)	0.016 (3)	0.017 (2)	0.0067 (19)	0.0106 (17)	0.0035 (17)

O3	0.016 (2)	0.009 (2)	0.021 (2)	0.0004 (18)	0.0056 (17)	0.0004 (17)
O4	0.007 (3)	0.014 (4)	0.019 (3)	0.000	0.004 (2)	0.000
O5	0.011 (3)	0.009 (3)	0.015 (3)	0.000	0.006 (2)	0.000
O6	0.008 (3)	0.002 (3)	0.022 (3)	0.000	0.011 (2)	0.000
O7	0.010 (3)	0.011 (4)	0.018 (3)	0.000	−0.001 (2)	0.000
O8	0.035 (5)	0.031 (5)	0.042 (4)	0.000	0.027 (3)	0.000
O9	0.027 (4)	0.034 (5)	0.018 (3)	0.000	0.011 (3)	0.000
O10	0.010 (3)	0.007 (3)	0.014 (3)	0.000	0.003 (2)	0.000
O11	0.005 (3)	0.009 (3)	0.019 (3)	0.000	0.002 (2)	0.000
O12	0.011 (3)	0.014 (4)	0.019 (3)	0.000	0.008 (2)	0.000
O13	0.011 (2)	0.006 (2)	0.025 (2)	0.0004 (17)	0.0033 (17)	0.0011 (17)
O14	0.020 (3)	0.014 (3)	0.034 (3)	0.004 (2)	0.017 (2)	0.001 (2)
O15	0.013 (4)	0.037 (10)	0.020 (4)	0.004 (4)	0.005 (3)	0.005 (4)
O16	0.054 (5)	0.044 (6)	0.015 (3)	0.000	0.006 (3)	0.000
O17	0.017 (4)	0.059 (6)	0.039 (4)	0.000	0.024 (3)	0.000

ST2_02 (room temperature)

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73253 (13)	0.2500	0.41004 (7)	0.0167 (3)	0.971 (2)
A1CE	0.73253 (13)	0.2500	0.41004 (7)	0.0167 (3)	0.029 (2)
A2CE	0.89172 (4)	0.2500	0.249439 (19)	0.01466 (10)	0.973 (4)
A2CA	0.89172 (4)	0.2500	0.249439 (19)	0.01466 (10)	0.027 (4)
A3CE	0.73964 (4)	0.2500	0.00971 (2)	0.02963 (14)	0.950 (4)
A3CA	0.73964 (4)	0.2500	0.00971 (2)	0.02963 (14)	0.050 (4)
A4CE	0.07827 (4)	0.7500	0.16571 (2)	0.01393 (10)	0.943 (4)
A4CA	0.07827 (4)	0.7500	0.16571 (2)	0.01393 (10)	0.057 (4)
M1AL	0.5000	0.5000	0.5000	0.0101 (5)	0.993 (7)
M1FE	0.5000	0.5000	0.5000	0.0101 (5)	0.007 (7)
M2AL	0.48138 (11)	0.00031 (18)	0.20506 (7)	0.0103 (3)	0.973 (6)
M2FE	0.48138 (11)	0.00031 (18)	0.20506 (7)	0.0103 (3)	0.027 (6)
M3FE	0.19564 (10)	0.7500	0.37645 (6)	0.0140 (3)	0.687 (8)
M3AL	0.19564 (10)	0.7500	0.37645 (6)	0.0140 (3)	0.313 (8)
Si1	0.16227 (16)	0.2500	0.47723 (9)	0.0103 (3)	
Si2	0.80569 (16)	0.7500	0.33580 (9)	0.0094 (3)	
Si3	0.30475 (15)	0.2500	0.31276 (9)	0.0090 (3)	
Si4	0.67013 (16)	0.7500	0.10315 (9)	0.0113 (3)	

Si5	0.15495 (15)	0.2500	0.07761 (9)	0.0089 (3)	
O1	0.2675 (3)	0.4898 (4)	0.48169 (18)	0.0158 (6)	
O2	0.1807 (3)	0.4757 (5)	0.28945 (17)	0.0164 (6)	
O3	0.6949 (3)	0.9867 (4)	0.29765 (17)	0.0139 (5)	
O4	0.4424 (4)	0.7500	0.4252 (2)	0.0118 (7)	
O5	0.4507 (4)	0.2500	0.4130 (2)	0.0110 (7)	
O6	0.4200 (4)	0.2500	0.2595 (2)	0.0104 (7)	
O7	−0.0159 (4)	0.2500	0.3972 (2)	0.0150 (8)	
O8	−0.0425 (5)	0.7500	0.3114 (3)	0.0290 (10)	
O9	0.8723 (5)	0.7500	0.4383 (2)	0.0221 (9)	
O10	0.5578 (4)	0.2500	0.1620 (2)	0.0100 (7)	
O11	0.4039 (4)	0.7500	0.2486 (2)	0.0119 (7)	
O12	0.5381 (4)	0.7500	0.1478 (2)	0.0095 (7)	
O13	0.2690 (3)	0.4903 (4)	0.11070 (17)	0.0150 (6)	
O14	0.7942 (3)	−0.0242 (5)	0.13243 (19)	0.0195 (6)	
O15	0.5513 (6)	0.6812 (8)	0.0034 (3)	0.0215 (14)	0.50
O16	0.0619 (6)	0.2500	−0.0232 (3)	0.0430 (13)	
O17	0.0226 (5)	0.2500	0.1170 (3)	0.0293 (10)	
H1	0.440 (7)	0.7500	0.322 (4)	0.020 (16)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0195 (5)	0.0169 (6)	0.0151 (6)	0.000	0.0089 (4)	0.000
A1CE	0.0195 (5)	0.0169 (6)	0.0151 (6)	0.000	0.0089 (4)	0.000
A2CE	0.01140 (14)	0.01948 (18)	0.01022 (16)	0.000	0.00220 (11)	0.000
A2CA	0.01140 (14)	0.01948 (18)	0.01022 (16)	0.000	0.00220 (11)	0.000
A3CE	0.01906 (18)	0.0565 (3)	0.00847 (17)	0.000	0.00172 (13)	0.000
A3CA	0.01906 (18)	0.0565 (3)	0.00847 (17)	0.000	0.00172 (13)	0.000
A4CE	0.01024 (14)	0.01890 (18)	0.01011 (16)	0.000	0.00219 (11)	0.000
A4CA	0.01024 (14)	0.01890 (18)	0.01011 (16)	0.000	0.00219 (11)	0.000
M1AL	0.0081 (7)	0.0108 (8)	0.0108 (8)	0.0009 (5)	0.0036 (6)	−0.0001 (6)
M1FE	0.0081 (7)	0.0108 (8)	0.0108 (8)	0.0009 (5)	0.0036 (6)	−0.0001 (6)
M2AL	0.0070 (5)	0.0097 (5)	0.0120 (6)	0.0004 (3)	0.0024 (4)	−0.0002 (4)
M2FE	0.0070 (5)	0.0097 (5)	0.0120 (6)	0.0004 (3)	0.0024 (4)	−0.0002 (4)
M3FE	0.0116 (4)	0.0137 (5)	0.0136 (5)	0.000	0.0029 (3)	0.000
M3AL	0.0116 (4)	0.0137 (5)	0.0136 (5)	0.000	0.0029 (3)	0.000
Si1	0.0080 (6)	0.0109 (6)	0.0101 (7)	0.000	0.0024 (5)	0.000
Si2	0.0089 (6)	0.0095 (6)	0.0095 (7)	0.000	0.0038 (5)	0.000
Si3	0.0057 (5)	0.0122 (6)	0.0087 (6)	0.000	0.0028 (5)	0.000
Si4	0.0080 (6)	0.0145 (7)	0.0109 (7)	0.000	0.0039 (5)	0.000
Si5	0.0066 (5)	0.0086 (6)	0.0094 (6)	0.000	0.0016 (5)	0.000

O1	0.0106 (11)	0.0133 (12)	0.0240 (15)	−0.0022 (9)	0.0080 (11)	−0.0044 (11)
O2	0.0151 (12)	0.0191 (13)	0.0162 (14)	0.0079 (10)	0.0082 (10)	0.0043 (11)
O3	0.0109 (11)	0.0108 (12)	0.0147 (13)	0.0001 (9)	0.0008 (10)	−0.0024 (10)
O4	0.0072 (14)	0.0129 (17)	0.0121 (18)	0.000	0.0013 (13)	0.000
O5	0.0139 (16)	0.0094 (16)	0.0092 (17)	0.000	0.0045 (13)	0.000
O6	0.0082 (14)	0.0097 (16)	0.0137 (18)	0.000	0.0051 (13)	0.000
O7	0.0088 (15)	0.0132 (17)	0.0159 (19)	0.000	−0.0011 (14)	0.000
O8	0.027 (2)	0.034 (2)	0.037 (3)	0.000	0.024 (2)	0.000
O9	0.0229 (19)	0.031 (2)	0.012 (2)	0.000	0.0078 (16)	0.000
O10	0.0092 (14)	0.0081 (16)	0.0123 (17)	0.000	0.0045 (13)	0.000
O11	0.0092 (15)	0.0088 (16)	0.0163 (19)	0.000	0.0044 (14)	0.000
O12	0.0081 (14)	0.0094 (16)	0.0133 (18)	0.000	0.0068 (13)	0.000
O13	0.0094 (10)	0.0106 (12)	0.0196 (14)	−0.0025 (9)	0.0016 (10)	−0.0005 (10)
O14	0.0211 (13)	0.0123 (13)	0.0328 (17)	−0.0015 (10)	0.0191 (13)	−0.0028 (12)
O15	0.029 (3)	0.023 (4)	0.013 (2)	−0.006 (2)	0.009 (2)	−0.003 (2)
O16	0.050 (3)	0.056 (3)	0.009 (2)	0.000	0.000 (2)	0.000
O17	0.0150 (18)	0.046 (3)	0.033 (3)	0.000	0.0165 (19)	0.000

ST2_02 (*T* = 350 °C)

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.73097 (14)	0.2500	0.40952 (7)	0.0167 (3)	0.969 (3)
A1CE	0.73097 (14)	0.2500	0.40952 (7)	0.0167 (3)	0.031 (3)
A2CE	0.89003 (4)	0.2500	0.24934 (2)	0.01453 (10)	0.967 (5)
A2CA	0.89003 (4)	0.2500	0.24934 (2)	0.01453 (10)	0.033 (5)
A3CE	0.73897 (5)	0.2500	0.01002 (2)	0.02951 (14)	0.949 (5)
A3CA	0.73897 (5)	0.2500	0.01002 (2)	0.02951 (14)	0.051 (5)
A4CE	0.08032 (4)	0.7500	0.16496 (2)	0.01478 (10)	0.938 (5)
A4CA	0.08032 (4)	0.7500	0.16496 (2)	0.01478 (10)	0.062 (5)
M1AL	0.5000	0.5000	0.5000	0.0103 (5)	0.983 (8)
M1FE	0.5000	0.5000	0.5000	0.0103 (5)	0.017 (8)
M2AL	0.48102 (13)	−0.00068 (19)	0.20474 (7)	0.0099 (4)	0.983 (7)
M2FE	0.48102 (13)	−0.00068 (19)	0.20474 (7)	0.0099 (4)	0.017 (7)
M3FE	0.19811 (12)	0.7500	0.37572 (6)	0.0136 (3)	0.676 (9)
M3AL	0.19811 (12)	0.7500	0.37572 (6)	0.0136 (3)	0.324 (9)
Si1	0.16199 (18)	0.2500	0.47648 (9)	0.0099 (3)	
Si2	0.80607 (17)	0.7500	0.33617 (9)	0.0092 (3)	

Si3	0.30586 (17)	0.2500	0.31298 (9)	0.0090 (3)	
Si4	0.67081 (18)	0.7500	0.10328 (10)	0.0114 (3)	
Si5	0.15510 (17)	0.2500	0.07744 (9)	0.0092 (3)	
O1	0.2663 (3)	0.4910 (5)	0.48012 (19)	0.0156 (6)	
O2	0.1817 (4)	0.4776 (5)	0.29112 (18)	0.0151 (6)	
O3	0.6949 (3)	0.9875 (5)	0.29716 (18)	0.0137 (5)	
O4	0.4428 (5)	0.7500	0.4252 (2)	0.0119 (7)	
O5	0.4517 (5)	0.2500	0.4134 (2)	0.0113 (7)	
O6	0.4181 (5)	0.2500	0.2596 (2)	0.0110 (7)	
O7	−0.0177 (5)	0.2500	0.3970 (3)	0.0148 (8)	
O8	−0.0392 (6)	0.7500	0.3138 (3)	0.0275 (11)	
O9	0.8678 (6)	0.7500	0.4385 (3)	0.0253 (10)	
O10	0.5574 (5)	0.2500	0.1626 (2)	0.0108 (7)	
O11	0.4038 (5)	0.7500	0.2477 (3)	0.0126 (7)	
O12	0.5402 (4)	0.7500	0.1472 (2)	0.0105 (7)	
O13	0.2692 (3)	0.4911 (5)	0.11027 (19)	0.0150 (6)	
O14	0.7954 (4)	−0.0246 (5)	0.1328 (2)	0.0188 (6)	
O15	0.5535 (7)	0.6789 (9)	0.0044 (3)	0.0197 (13)	0.50
O16	0.0615 (8)	0.2500	−0.0232 (3)	0.0481 (16)	
O17	0.0246 (6)	0.2500	0.1175 (3)	0.0293 (11)	
H1	0.414 (16)	0.7500	0.313 (8)	0.10 (4)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0175 (5)	0.0177 (6)	0.0162 (5)	0.000	0.0088 (4)	0.000
A1CE	0.0175 (5)	0.0177 (6)	0.0162 (5)	0.000	0.0088 (4)	0.000
A2CE	0.00975 (15)	0.01958 (18)	0.01051 (15)	0.000	0.00112 (11)	0.000
A2CA	0.00975 (15)	0.01958 (18)	0.01051 (15)	0.000	0.00112 (11)	0.000
A3CE	0.01816 (19)	0.0559 (3)	0.00866 (17)	0.000	0.00077 (13)	0.000
A3CA	0.01816 (19)	0.0559 (3)	0.00866 (17)	0.000	0.00077 (13)	0.000
A4CE	0.01058 (15)	0.01930 (18)	0.01034 (15)	0.000	0.00093 (11)	0.000
A4CA	0.01058 (15)	0.01930 (18)	0.01034 (15)	0.000	0.00093 (11)	0.000
M1AL	0.0076 (7)	0.0105 (8)	0.0109 (8)	0.0003 (5)	0.0023 (6)	0.0006 (5)
M1FE	0.0076 (7)	0.0105 (8)	0.0109 (8)	0.0003 (5)	0.0023 (6)	0.0006 (5)
M2AL	0.0060 (5)	0.0090 (6)	0.0119 (6)	0.0004 (4)	0.0014 (4)	−0.0005 (4)
M2FE	0.0060 (5)	0.0090 (6)	0.0119 (6)	0.0004 (4)	0.0014 (4)	−0.0005 (4)
M3FE	0.0094 (4)	0.0140 (5)	0.0131 (5)	0.000	0.0011 (4)	0.000
M3AL	0.0094 (4)	0.0140 (5)	0.0131 (5)	0.000	0.0011 (4)	0.000
Si1	0.0069 (6)	0.0104 (6)	0.0094 (6)	0.000	0.0010 (5)	0.000
Si2	0.0067 (6)	0.0095 (6)	0.0100 (6)	0.000	0.0023 (5)	0.000
Si3	0.0054 (6)	0.0120 (6)	0.0081 (6)	0.000	0.0016 (5)	0.000

Si4	0.0086 (6)	0.0140 (7)	0.0111 (7)	0.000	0.0039 (5)	0.000
Si5	0.0049 (6)	0.0100 (6)	0.0092 (6)	0.000	0.0000 (5)	0.000
O1	0.0080 (11)	0.0138 (13)	0.0237 (15)	−0.0016 (10)	0.0058 (11)	−0.0050 (11)
O2	0.0110 (12)	0.0189 (14)	0.0150 (13)	0.0077 (10)	0.0054 (10)	0.0026 (10)
O3	0.0072 (11)	0.0106 (12)	0.0156 (13)	0.0002 (9)	−0.0020 (10)	−0.0012 (10)
O4	0.0064 (15)	0.0134 (17)	0.0132 (17)	0.000	0.0019 (14)	0.000
O5	0.0108 (16)	0.0122 (17)	0.0085 (16)	0.000	0.0020 (14)	0.000
O6	0.0088 (16)	0.0107 (17)	0.0159 (18)	0.000	0.0078 (15)	0.000
O7	0.0063 (16)	0.0166 (19)	0.0124 (18)	0.000	−0.0040 (14)	0.000
O8	0.021 (2)	0.031 (3)	0.042 (3)	0.000	0.024 (2)	0.000
O9	0.028 (2)	0.034 (3)	0.0118 (19)	0.000	0.0068 (18)	0.000
O10	0.0082 (15)	0.0106 (16)	0.0113 (17)	0.000	0.0023 (14)	0.000
O11	0.0088 (16)	0.0095 (17)	0.0185 (19)	0.000	0.0052 (15)	0.000
O12	0.0060 (15)	0.0108 (16)	0.0133 (17)	0.000	0.0031 (13)	0.000
O13	0.0067 (11)	0.0104 (12)	0.0211 (14)	−0.0013 (10)	0.0000 (10)	−0.0016 (10)
O14	0.0202 (14)	0.0117 (13)	0.0318 (17)	−0.0045 (11)	0.0181 (14)	−0.0021 (11)
O15	0.020 (3)	0.028 (4)	0.007 (2)	−0.005 (2)	0.002 (2)	−0.0013 (19)
O16	0.055 (4)	0.063 (4)	0.007 (2)	0.000	−0.004 (2)	0.000
O17	0.013 (2)	0.048 (3)	0.031 (3)	0.000	0.014 (2)	0.000

ST2_02 (*T* = 450 °C)

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.72680 (13)	0.2500	0.40752 (7)	0.0166 (3)	0.965 (3)
A1CE	0.72680 (13)	0.2500	0.40752 (7)	0.0166 (3)	0.035 (3)
A2CE	0.88481 (4)	0.2500	0.24952 (2)	0.01379 (10)	0.971 (4)
A2CA	0.88481 (4)	0.2500	0.24952 (2)	0.01379 (10)	0.029 (4)
A3CE	0.73652 (5)	0.2500	0.01121 (2)	0.02915 (14)	0.952 (4)
A3CA	0.73652 (5)	0.2500	0.01121 (2)	0.02915 (14)	0.048 (4)
A4CE	0.09081 (4)	0.7500	0.16334 (2)	0.01527 (11)	0.944 (4)
A4CA	0.09081 (4)	0.7500	0.16334 (2)	0.01527 (11)	0.056 (4)
M1AL	0.5000	0.5000	0.5000	0.0098 (5)	0.968 (7)
M1FE	0.5000	0.5000	0.5000	0.0098 (5)	0.032 (7)
M2AL	0.47938 (13)	−0.00399 (17)	0.20399 (7)	0.0103 (3)	0.963 (6)
M2FE	0.47938 (13)	−0.00399 (17)	0.20399 (7)	0.0103 (3)	0.037 (6)
M3FE	0.20443 (11)	0.7500	0.37397 (6)	0.0111 (3)	0.665 (8)
M3AL	0.20443 (11)	0.7500	0.37397 (6)	0.0111 (3)	0.335 (8)

Si1	0.16127 (17)	0.2500	0.47477 (9)	0.0082 (3)	
Si2	0.80490 (17)	0.7500	0.33735 (9)	0.0087 (3)	
Si3	0.30815 (17)	0.2500	0.31380 (9)	0.0080 (3)	
Si4	0.67490 (17)	0.7500	0.10428 (10)	0.0107 (3)	
Si5	0.15468 (17)	0.2500	0.07526 (9)	0.0090 (3)	
O1	0.2645 (3)	0.4944 (4)	0.47594 (18)	0.0123 (5)	
O2	0.1839 (3)	0.4805 (4)	0.29463 (17)	0.0120 (5)	
O3	0.6961 (3)	0.9893 (4)	0.29638 (18)	0.0120 (5)	
O4	0.4436 (4)	0.7500	0.4267 (2)	0.0102 (7)	
O5	0.4546 (4)	0.2500	0.4138 (2)	0.0095 (7)	
O6	0.4159 (4)	0.2500	0.2592 (2)	0.0095 (7)	
O7	−0.0206 (4)	0.2500	0.3979 (3)	0.0139 (8)	
O8	−0.0307 (5)	0.7500	0.3229 (3)	0.0197 (9)	
O9	0.8570 (5)	0.7500	0.4377 (3)	0.0223 (9)	
O10	0.5569 (4)	0.2500	0.1626 (2)	0.0090 (7)	
O11	0.4001 (4)	0.7500	0.2435 (2)	0.0114 (7)	
O12	0.5420 (4)	0.7500	0.1464 (2)	0.0108 (7)	
O13	0.2695 (3)	0.4910 (4)	0.10708 (19)	0.0155 (6)	
O14	0.7990 (4)	−0.0222 (5)	0.1345 (2)	0.0206 (7)	
O15	0.5597 (7)	0.6749 (8)	0.0057 (3)	0.0180 (12)	0.50
O16	0.0590 (7)	0.2500	−0.0244 (3)	0.0497 (16)	
O17	0.0277 (6)	0.2500	0.1166 (3)	0.0327 (11)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0176 (5)	0.0197 (6)	0.0141 (6)	0.000	0.0084 (4)	0.000
A1CE	0.0176 (5)	0.0197 (6)	0.0141 (6)	0.000	0.0084 (4)	0.000
A2CE	0.01134 (15)	0.01718 (16)	0.00978 (16)	0.000	0.00201 (11)	0.000
A2CA	0.01134 (15)	0.01718 (16)	0.00978 (16)	0.000	0.00201 (11)	0.000
A3CE	0.0213 (2)	0.0535 (3)	0.00813 (18)	0.000	0.00254 (14)	0.000
A3CA	0.0213 (2)	0.0535 (3)	0.00813 (18)	0.000	0.00254 (14)	0.000
A4CE	0.01433 (16)	0.02044 (18)	0.00869 (16)	0.000	0.00310 (12)	0.000
A4CA	0.01433 (16)	0.02044 (18)	0.00869 (16)	0.000	0.00310 (12)	0.000
M1AL	0.0079 (7)	0.0089 (7)	0.0108 (8)	0.0004 (5)	0.0027 (6)	0.0010 (5)
M1FE	0.0079 (7)	0.0089 (7)	0.0108 (8)	0.0004 (5)	0.0027 (6)	0.0010 (5)
M2AL	0.0091 (5)	0.0093 (5)	0.0111 (6)	0.0006 (3)	0.0034 (4)	−0.0001 (4)
M2FE	0.0091 (5)	0.0093 (5)	0.0111 (6)	0.0006 (3)	0.0034 (4)	−0.0001 (4)
M3FE	0.0090 (4)	0.0113 (4)	0.0109 (5)	0.000	0.0025 (3)	0.000
M3AL	0.0090 (4)	0.0113 (4)	0.0109 (5)	0.000	0.0025 (3)	0.000
Si1	0.0067 (6)	0.0082 (6)	0.0074 (7)	0.000	0.0011 (5)	0.000
Si2	0.0085 (6)	0.0080 (6)	0.0093 (7)	0.000	0.0036 (5)	0.000

Si3	0.0064 (6)	0.0096 (6)	0.0071 (6)	0.000	0.0022 (5)	0.000
Si4	0.0093 (6)	0.0129 (6)	0.0101 (7)	0.000	0.0045 (5)	0.000
Si5	0.0063 (6)	0.0092 (6)	0.0090 (7)	0.000	0.0011 (5)	0.000
O1	0.0089 (12)	0.0103 (11)	0.0168 (14)	−0.0012 (9)	0.0050 (10)	−0.0012 (10)
O2	0.0122 (12)	0.0113 (11)	0.0112 (13)	0.0013 (9)	0.0039 (10)	−0.0010 (10)
O3	0.0092 (11)	0.0077 (11)	0.0145 (14)	−0.0010 (8)	0.0014 (10)	0.0002 (9)
O4	0.0106 (16)	0.0092 (15)	0.0106 (18)	0.000	0.0047 (14)	0.000
O5	0.0071 (16)	0.0099 (15)	0.0092 (18)	0.000	0.0018 (13)	0.000
O6	0.0119 (17)	0.0060 (14)	0.0120 (18)	0.000	0.0067 (14)	0.000
O7	0.0072 (16)	0.0159 (17)	0.0127 (19)	0.000	−0.0008 (14)	0.000
O8	0.015 (2)	0.025 (2)	0.020 (2)	0.000	0.0094 (17)	0.000
O9	0.026 (2)	0.031 (2)	0.012 (2)	0.000	0.0109 (18)	0.000
O10	0.0104 (16)	0.0094 (15)	0.0069 (17)	0.000	0.0035 (13)	0.000
O11	0.0096 (16)	0.0113 (16)	0.0123 (19)	0.000	0.0040 (14)	0.000
O12	0.0074 (16)	0.0093 (15)	0.0150 (19)	0.000	0.0042 (14)	0.000
O13	0.0074 (11)	0.0081 (11)	0.0225 (15)	0.0003 (9)	−0.0007 (10)	0.0003 (10)
O14	0.0239 (15)	0.0125 (12)	0.0346 (19)	−0.0028 (10)	0.0212 (14)	−0.0013 (12)
O15	0.019 (3)	0.022 (3)	0.011 (3)	−0.0023 (19)	0.005 (2)	−0.002 (2)
O16	0.051 (4)	0.067 (4)	0.012 (3)	0.000	−0.003 (2)	0.000
O17	0.020 (2)	0.049 (3)	0.036 (3)	0.000	0.019 (2)	0.000

ST2_02 (*T* = 550 °C)

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.7256 (3)	0.2500	0.40768 (12)	0.0201 (7)	0.959 (4)
A1CE	0.7256 (3)	0.2500	0.40768 (12)	0.0201 (7)	0.041 (4)
A2CE	0.88349 (8)	0.2500	0.24984 (4)	0.0163 (2)	0.939 (7)
A2CA	0.88349 (8)	0.2500	0.24984 (4)	0.0163 (2)	0.061 (7)
A3CE	0.73516 (9)	0.2500	0.01143 (4)	0.0310 (3)	0.923 (7)
A3CA	0.73516 (9)	0.2500	0.01143 (4)	0.0310 (3)	0.077 (7)
A4CE	0.09167 (8)	0.7500	0.16323 (4)	0.0176 (2)	0.921 (7)
A4CA	0.09167 (8)	0.7500	0.16323 (4)	0.0176 (2)	0.079 (7)
M1AL	0.5000	0.5000	0.5000	0.0140 (9)	0.945 (11)
M1FE	0.5000	0.5000	0.5000	0.0140 (9)	0.055 (11)
M2AL	0.4792 (2)	−0.0034 (4)	0.20405 (12)	0.0106 (7)	0.987 (9)
M2FE	0.4792 (2)	−0.0034 (4)	0.20405 (12)	0.0106 (7)	0.013 (9)
M3FE	0.2050 (2)	0.7500	0.37438 (11)	0.0161 (6)	0.709 (12)

M3AL	0.2050 (2)	0.7500	0.37438 (11)	0.0161 (6)	0.291 (12)
Si1	0.1603 (3)	0.2500	0.47448 (17)	0.0116 (6)	
Si2	0.8049 (3)	0.7500	0.33787 (16)	0.0117 (6)	
Si3	0.3081 (3)	0.2500	0.31345 (16)	0.0100 (6)	
Si4	0.6756 (3)	0.7500	0.10481 (17)	0.0121 (6)	
Si5	0.1547 (3)	0.2500	0.07432 (16)	0.0104 (6)	
O1	0.2642 (6)	0.4933 (8)	0.4751 (3)	0.0179 (12)	
O2	0.1829 (6)	0.4810 (9)	0.2940 (3)	0.0151 (11)	
O3	0.6952 (6)	0.9893 (8)	0.2958 (3)	0.0172 (11)	
O4	0.4439 (8)	0.7500	0.4270 (4)	0.0147 (15)	
O5	0.4526 (8)	0.2500	0.4133 (4)	0.0135 (15)	
O6	0.4170 (8)	0.2500	0.2589 (4)	0.0136 (15)	
O7	−0.0234 (8)	0.2500	0.3998 (4)	0.0167 (15)*	
O8	−0.0296 (9)	0.7500	0.3249 (5)	0.0223 (17)	
O9	0.8559 (9)	0.7500	0.4388 (4)	0.029 (2)	
O10	0.5567 (8)	0.2500	0.1634 (4)	0.0109 (14)	
O11	0.3996 (8)	0.7500	0.2428 (4)	0.0155 (16)	
O12	0.5424 (8)	0.7500	0.1470 (4)	0.0146 (15)	
O13	0.2702 (6)	0.4901 (8)	0.1065 (3)	0.0198 (12)	
O14	0.7995 (6)	−0.0214 (9)	0.1358 (3)	0.0217 (12)	
O15	0.5605 (12)	0.6725 (16)	0.0064 (6)	0.025 (3)	0.50
O16	0.0597 (13)	0.2500	−0.0247 (6)	0.067 (4)	
O17	0.0275 (10)	0.2500	0.1146 (5)	0.036 (2)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0217 (12)	0.0216 (13)	0.0171 (11)	0.000	0.0088 (8)	0.000
A1CE	0.0217 (12)	0.0216 (13)	0.0171 (11)	0.000	0.0088 (8)	0.000
A2CE	0.0142 (4)	0.0212 (4)	0.0111 (3)	0.000	0.0037 (2)	0.000
A2CA	0.0142 (4)	0.0212 (4)	0.0111 (3)	0.000	0.0037 (2)	0.000
A3CE	0.0244 (4)	0.0554 (6)	0.0097 (3)	0.000	0.0046 (3)	0.000
A3CA	0.0244 (4)	0.0554 (6)	0.0097 (3)	0.000	0.0046 (3)	0.000
A4CE	0.0165 (4)	0.0255 (4)	0.0101 (3)	0.000	0.0054 (2)	0.000
A4CA	0.0165 (4)	0.0255 (4)	0.0101 (3)	0.000	0.0054 (2)	0.000
M1AL	0.0113 (15)	0.0164 (17)	0.0137 (14)	0.0025 (11)	0.0052 (11)	0.0003 (11)
M1FE	0.0113 (15)	0.0164 (17)	0.0137 (14)	0.0025 (11)	0.0052 (11)	0.0003 (11)
M2AL	0.0103 (11)	0.0110 (11)	0.0096 (10)	0.0009 (8)	0.0038 (8)	−0.0005 (7)
M2FE	0.0103 (11)	0.0110 (11)	0.0096 (10)	0.0009 (8)	0.0038 (8)	−0.0005 (7)
M3FE	0.0123 (10)	0.0149 (10)	0.0220 (10)	0.000	0.0085 (7)	0.000
M3AL	0.0123 (10)	0.0149 (10)	0.0220 (10)	0.000	0.0085 (7)	0.000
Si1	0.0103 (13)	0.0125 (14)	0.0110 (12)	0.000	0.0040 (10)	0.000

Si2	0.0128 (14)	0.0116 (14)	0.0127 (13)	0.000	0.0076 (11)	0.000
Si3	0.0098 (13)	0.0128 (14)	0.0095 (12)	0.000	0.0064 (10)	0.000
Si4	0.0105 (13)	0.0164 (15)	0.0116 (12)	0.000	0.0070 (10)	0.000
Si5	0.0099 (13)	0.0084 (14)	0.0107 (12)	0.000	0.0027 (10)	0.000
O1	0.010 (3)	0.015 (3)	0.028 (3)	−0.002 (2)	0.007 (2)	−0.004 (2)
O2	0.018 (3)	0.019 (3)	0.016 (2)	0.002 (2)	0.013 (2)	−0.001 (2)
O3	0.019 (3)	0.013 (3)	0.016 (2)	−0.001 (2)	0.004 (2)	0.000 (2)
O4	0.018 (4)	0.017 (4)	0.012 (3)	0.000	0.009 (3)	0.000
O5	0.014 (4)	0.013 (4)	0.013 (3)	0.000	0.007 (3)	0.000
O6	0.019 (4)	0.009 (3)	0.018 (4)	0.000	0.013 (3)	0.000
O8	0.022 (4)	0.029 (4)	0.025 (4)	0.000	0.020 (3)	0.000
O9	0.032 (5)	0.047 (5)	0.011 (4)	0.000	0.013 (3)	0.000
O10	0.012 (3)	0.009 (3)	0.011 (3)	0.000	0.004 (3)	0.000
O11	0.013 (4)	0.016 (4)	0.017 (4)	0.000	0.006 (3)	0.000
O12	0.011 (3)	0.012 (4)	0.019 (4)	0.000	0.004 (3)	0.000
O13	0.017 (3)	0.014 (3)	0.025 (3)	0.002 (2)	0.006 (2)	−0.001 (2)
O14	0.023 (3)	0.018 (3)	0.037 (3)	−0.007 (2)	0.025 (3)	−0.004 (2)
O15	0.027 (6)	0.038 (8)	0.011 (4)	0.007 (5)	0.009 (4)	−0.002 (4)
O16	0.067 (7)	0.072 (8)	0.021 (5)	0.000	−0.017 (5)	0.000
O17	0.022 (5)	0.048 (5)	0.040 (5)	0.000	0.016 (4)	0.000

ST2_02 (*T* = 650 °C)

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.72593 (13)	0.2500	0.40731 (7)	0.0154 (3)	0.969 (2)
A1CE	0.72593 (13)	0.2500	0.40731 (7)	0.0154 (3)	0.031 (2)
A2CE	0.88360 (4)	0.2500	0.249966 (19)	0.01345 (10)	0.965 (4)
A2CA	0.88360 (4)	0.2500	0.249966 (19)	0.01345 (10)	0.035 (4)
A3CE	0.73457 (5)	0.2500	0.01157 (2)	0.02828 (14)	0.959 (4)
A3CA	0.73457 (5)	0.2500	0.01157 (2)	0.02828 (14)	0.041 (4)
A4CE	0.09327 (4)	0.7500	0.16328 (2)	0.01517 (10)	0.947 (4)
A4CA	0.09327 (4)	0.7500	0.16328 (2)	0.01517 (10)	0.053 (4)
M1AL	0.5000	0.5000	0.5000	0.0084 (4)	0.957 (7)
M1FE	0.5000	0.5000	0.5000	0.0084 (4)	0.043 (7)
M2AL	0.47861 (12)	−0.00454 (19)	0.20368 (6)	0.0085 (3)	0.977 (5)
M2FE	0.47861 (12)	−0.00454 (19)	0.20368 (6)	0.0085 (3)	0.023 (5)
M3FE	0.20510 (11)	0.7500	0.37351 (6)	0.0099 (3)	0.677 (7)

M3AL	0.20510 (11)	0.7500	0.37351 (6)	0.0099 (3)	0.323 (7)
Si1	0.16117 (17)	0.2500	0.47445 (9)	0.0076 (3)	
Si2	0.80488 (16)	0.7500	0.33795 (9)	0.0081 (3)	
Si3	0.30771 (16)	0.2500	0.31347 (8)	0.0067 (3)	
Si4	0.67627 (17)	0.7500	0.10507 (9)	0.0101 (3)	
Si5	0.15405 (17)	0.2500	0.07393 (9)	0.0083 (3)	
O1	0.2637 (3)	0.4947 (5)	0.47528 (17)	0.0107 (5)	
O2	0.1825 (3)	0.4809 (5)	0.29410 (17)	0.0112 (5)	
O3	0.6956 (3)	0.9884 (5)	0.29618 (17)	0.0117 (5)	
O4	0.4442 (4)	0.7500	0.4272 (2)	0.0079 (6)	
O5	0.4544 (4)	0.2500	0.4132 (2)	0.0089 (7)	
O6	0.4146 (4)	0.2500	0.2587 (2)	0.0089 (7)	
O7	−0.0222 (4)	0.2500	0.3970 (2)	0.0129 (7)	
O8	−0.0305 (5)	0.7500	0.3235 (3)	0.0166 (8)	
O9	0.8553 (5)	0.7500	0.4377 (3)	0.0210 (9)	
O10	0.5577 (4)	0.2500	0.1631 (2)	0.0088 (7)	
O11	0.3975 (4)	0.7500	0.2418 (2)	0.0120 (7)	
O12	0.5433 (4)	0.7500	0.1464 (2)	0.0087 (7)	
O13	0.2684 (3)	0.4907 (5)	0.10568 (18)	0.0144 (5)	
O14	0.7997 (4)	−0.0221 (5)	0.1355 (2)	0.0195 (6)	
O15	0.5610 (6)	0.6712 (9)	0.0070 (3)	0.0164 (12)	0.50
O16	0.0598 (7)	0.2500	−0.0254 (3)	0.0477 (15)	
O17	0.0277 (6)	0.2500	0.1153 (3)	0.0336 (12)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0156 (5)	0.0187 (6)	0.0120 (5)	0.000	0.0062 (4)	0.000
A1CE	0.0156 (5)	0.0187 (6)	0.0120 (5)	0.000	0.0062 (4)	0.000
A2CE	0.01136 (15)	0.01746 (18)	0.00745 (14)	0.000	0.00064 (11)	0.000
A2CA	0.01136 (15)	0.01746 (18)	0.00745 (14)	0.000	0.00064 (11)	0.000
A3CE	0.01963 (19)	0.0536 (3)	0.00613 (15)	0.000	0.00097 (13)	0.000
A3CA	0.01963 (19)	0.0536 (3)	0.00613 (15)	0.000	0.00097 (13)	0.000
A4CE	0.01291 (16)	0.0229 (2)	0.00630 (14)	0.000	0.00133 (11)	0.000
A4CA	0.01291 (16)	0.0229 (2)	0.00630 (14)	0.000	0.00133 (11)	0.000
M1AL	0.0068 (7)	0.0092 (7)	0.0070 (7)	−0.0002 (5)	0.0012 (5)	0.0005 (5)
M1FE	0.0068 (7)	0.0092 (7)	0.0070 (7)	−0.0002 (5)	0.0012 (5)	0.0005 (5)
M2AL	0.0064 (5)	0.0082 (5)	0.0083 (5)	0.0002 (4)	0.0012 (4)	−0.0006 (4)
M2FE	0.0064 (5)	0.0082 (5)	0.0083 (5)	0.0002 (4)	0.0012 (4)	−0.0006 (4)
M3FE	0.0080 (4)	0.0102 (5)	0.0096 (4)	0.000	0.0022 (3)	0.000
M3AL	0.0080 (4)	0.0102 (5)	0.0096 (4)	0.000	0.0022 (3)	0.000
Si1	0.0055 (5)	0.0089 (6)	0.0060 (6)	0.000	0.0005 (5)	0.000

Si2	0.0070 (6)	0.0086 (6)	0.0070 (6)	0.000	0.0018 (5)	0.000
Si3	0.0052 (5)	0.0078 (6)	0.0050 (6)	0.000	0.0005 (4)	0.000
Si4	0.0077 (6)	0.0142 (7)	0.0074 (6)	0.000	0.0026 (5)	0.000
Si5	0.0061 (6)	0.0076 (6)	0.0083 (6)	0.000	0.0006 (5)	0.000
O1	0.0071 (11)	0.0096 (12)	0.0146 (13)	−0.0006 (9)	0.0043 (9)	−0.0004 (10)
O2	0.0106 (11)	0.0120 (12)	0.0087 (11)	0.0024 (10)	0.0024 (9)	−0.0008 (10)
O3	0.0081 (11)	0.0099 (12)	0.0118 (12)	−0.0001 (9)	−0.0002 (9)	−0.0017 (10)
O4	0.0056 (14)	0.0111 (17)	0.0056 (15)	0.000	0.0014 (12)	0.000
O5	0.0084 (15)	0.0084 (17)	0.0070 (16)	0.000	0.0010 (12)	0.000
O6	0.0086 (15)	0.0091 (17)	0.0104 (16)	0.000	0.0056 (13)	0.000
O7	0.0061 (15)	0.0166 (19)	0.0082 (16)	0.000	−0.0037 (13)	0.000
O8	0.0111 (17)	0.022 (2)	0.017 (2)	0.000	0.0067 (15)	0.000
O9	0.025 (2)	0.030 (2)	0.0111 (19)	0.000	0.0105 (17)	0.000
O10	0.0059 (15)	0.0117 (17)	0.0073 (15)	0.000	0.0016 (13)	0.000
O11	0.0123 (16)	0.0106 (18)	0.0157 (18)	0.000	0.0085 (15)	0.000
O12	0.0082 (15)	0.0071 (17)	0.0101 (16)	0.000	0.0035 (13)	0.000
O13	0.0073 (11)	0.0076 (12)	0.0204 (14)	−0.0007 (10)	−0.0007 (10)	0.0002 (11)
O14	0.0228 (14)	0.0096 (13)	0.0348 (18)	−0.0032 (11)	0.0207 (14)	−0.0023 (12)
O15	0.019 (3)	0.020 (3)	0.008 (2)	−0.0034 (19)	0.004 (2)	−0.0034 (19)
O16	0.050 (3)	0.063 (4)	0.010 (2)	0.000	−0.004 (2)	0.000
O17	0.018 (2)	0.056 (3)	0.030 (3)	0.000	0.014 (2)	0.000

ST2_02 (*T* = 750 °C)

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

	x/a	*y/b*	*z/c*	U_{eq} (U_{iso}*)	occupancy
A1CA	0.72579 (13)	0.2500	0.40754 (7)	0.0131 (3)	0.983 (2)
A1CE	0.72579 (13)	0.2500	0.40754 (7)	0.0131 (3)	0.017 (2)
A2CE	0.88310 (4)	0.2500	0.250255 (19)	0.01253 (10)	0.967 (4)
A2CA	0.88310 (4)	0.2500	0.250255 (19)	0.01253 (10)	0.033 (4)
A3CE	0.73345 (5)	0.2500	0.01178 (2)	0.02701 (13)	0.971 (4)
A3CA	0.73345 (5)	0.2500	0.01178 (2)	0.02701 (13)	0.029 (4)
A4CE	0.09424 (4)	0.7500	0.16332 (2)	0.01457 (10)	0.954 (4)
A4CA	0.09424 (4)	0.7500	0.16332 (2)	0.01457 (10)	0.046 (4)
M1AL	0.5000	0.5000	0.5000	0.0076 (4)	0.947 (7)
M1FE	0.5000	0.5000	0.5000	0.0076 (4)	0.053 (7)
M2AL	0.47817 (12)	−0.00480 (17)	0.20360 (6)	0.0078 (3)	0.963 (5)
M2FE	0.47817 (12)	−0.00480 (17)	0.20360 (6)	0.0078 (3)	0.037 (5)

M3FE	0.20512 (11)	0.7500	0.37322 (6)	0.0083 (3)	0.641 (7)
M3AL	0.20512 (11)	0.7500	0.37322 (6)	0.0083 (3)	0.359 (7)
Si1	0.16111 (17)	0.2500	0.47426 (9)	0.0066 (3)	
Si2	0.80462 (17)	0.7500	0.33805 (9)	0.0070 (3)	
Si3	0.30750 (17)	0.2500	0.31344 (8)	0.0061 (2)	
Si4	0.67717 (18)	0.7500	0.10549 (9)	0.0097 (3)	
Si5	0.15369 (17)	0.2500	0.07333 (9)	0.0076 (3)	
O1	0.2634 (3)	0.4939 (4)	0.47511 (16)	0.0092 (5)	
O2	0.1823 (3)	0.4811 (4)	0.29390 (16)	0.0091 (5)	
O3	0.6957 (3)	0.9889 (4)	0.29645 (16)	0.0102 (5)	
O4	0.4438 (4)	0.7500	0.4272 (2)	0.0070 (6)	
O5	0.4539 (4)	0.2500	0.4134 (2)	0.0068 (6)	
O6	0.4135 (5)	0.2500	0.2581 (2)	0.0091 (7)	
O7	−0.0218 (4)	0.2500	0.3974 (2)	0.0109 (7)	
O8	−0.0304 (5)	0.7500	0.3238 (3)	0.0154 (8)	
O9	0.8555 (5)	0.7500	0.4381 (2)	0.0184 (8)	
O10	0.5580 (4)	0.2500	0.1633 (2)	0.0079 (6)	
O11	0.3967 (4)	0.7500	0.2413 (2)	0.0096 (7)	
O12	0.5432 (4)	0.7500	0.1465 (2)	0.0087 (7)	
O13	0.2688 (3)	0.4906 (4)	0.10508 (18)	0.0146 (5)	
O14	0.8013 (4)	−0.0227 (5)	0.13623 (19)	0.0181 (6)	
O15	0.5618 (7)	0.6710 (9)	0.0072 (3)	0.0159 (11)	0.50
O16	0.0607 (8)	0.2500	−0.0265 (3)	0.0469 (15)	
O17	0.0273 (6)	0.2500	0.1145 (3)	0.0366 (13)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
A1CA	0.0120 (5)	0.0168 (5)	0.0108 (5)	0.000	0.0055 (4)	0.000
A1CE	0.0120 (5)	0.0168 (5)	0.0108 (5)	0.000	0.0055 (4)	0.000
A2CE	0.01032 (15)	0.01646 (16)	0.00724 (14)	0.000	0.00085 (11)	0.000
A2CA	0.01032 (15)	0.01646 (16)	0.00724 (14)	0.000	0.00085 (11)	0.000
A3CE	0.01774 (19)	0.0518 (3)	0.00637 (16)	0.000	0.00101 (13)	0.000
A3CA	0.01774 (19)	0.0518 (3)	0.00637 (16)	0.000	0.00101 (13)	0.000
A4CE	0.01098 (16)	0.02324 (17)	0.00655 (14)	0.000	0.00140 (11)	0.000
A4CA	0.01098 (16)	0.02324 (17)	0.00655 (14)	0.000	0.00140 (11)	0.000
M1AL	0.0049 (7)	0.0081 (6)	0.0066 (7)	−0.0002 (5)	−0.0002 (5)	0.0002 (5)
M1FE	0.0049 (7)	0.0081 (6)	0.0066 (7)	−0.0002 (5)	−0.0002 (5)	0.0002 (5)
M2AL	0.0056 (5)	0.0076 (5)	0.0080 (5)	0.0004 (3)	0.0012 (4)	−0.0003 (3)
M2FE	0.0056 (5)	0.0076 (5)	0.0080 (5)	0.0004 (3)	0.0012 (4)	−0.0003 (3)
M3FE	0.0056 (4)	0.0087 (4)	0.0092 (4)	0.000	0.0021 (3)	0.000
M3AL	0.0056 (4)	0.0087 (4)	0.0092 (4)	0.000	0.0021 (3)	0.000

Si1	0.0051 (6)	0.0068 (5)	0.0058 (6)	0.000	0.0007 (5)	0.000
Si2	0.0063 (6)	0.0072 (5)	0.0068 (6)	0.000	0.0024 (5)	0.000
Si3	0.0037 (6)	0.0086 (5)	0.0052 (6)	0.000	0.0013 (5)	0.000
Si4	0.0068 (6)	0.0129 (6)	0.0095 (6)	0.000	0.0037 (5)	0.000
Si5	0.0043 (6)	0.0071 (5)	0.0084 (6)	0.000	0.0003 (5)	0.000
O1	0.0047 (11)	0.0084 (10)	0.0136 (12)	−0.0010 (9)	0.0034 (10)	−0.0008 (9)
O2	0.0087 (11)	0.0082 (10)	0.0099 (11)	0.0024 (9)	0.0038 (9)	0.0016 (9)
O3	0.0090 (11)	0.0062 (10)	0.0121 (12)	0.0021 (9)	0.0018 (10)	−0.0002 (9)
O4	0.0033 (14)	0.0085 (14)	0.0070 (15)	0.000	0.0004 (13)	0.000
O5	0.0051 (15)	0.0056 (14)	0.0058 (15)	0.000	−0.0010 (13)	0.000
O6	0.0106 (16)	0.0076 (14)	0.0101 (16)	0.000	0.0056 (14)	0.000
O7	0.0059 (16)	0.0110 (15)	0.0119 (17)	0.000	0.0005 (14)	0.000
O8	0.0108 (18)	0.0226 (19)	0.0158 (19)	0.000	0.0086 (16)	0.000
O9	0.020 (2)	0.027 (2)	0.0092 (18)	0.000	0.0081 (16)	0.000
O10	0.0082 (16)	0.0072 (14)	0.0093 (16)	0.000	0.0047 (14)	0.000
O11	0.0074 (16)	0.0073 (14)	0.0132 (17)	0.000	0.0038 (14)	0.000
O12	0.0071 (15)	0.0068 (14)	0.0120 (17)	0.000	0.0042 (14)	0.000
O13	0.0066 (11)	0.0082 (11)	0.0219 (14)	−0.0008 (9)	0.0001 (10)	0.0005 (10)
O14	0.0211 (15)	0.0099 (11)	0.0320 (17)	−0.0028 (11)	0.0196 (14)	−0.0026 (11)
O15	0.017 (3)	0.017 (2)	0.011 (2)	−0.001 (2)	0.004 (2)	−0.0026 (19)
O16	0.048 (4)	0.070 (4)	0.009 (2)	0.000	0.001 (2)	0.000
O17	0.016 (2)	0.066 (3)	0.034 (3)	0.000	0.017 (2)	0.000