

Versiliaite and apuanite: derivative structures related to schafarzikite

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Abstract

Schafarzikite, FeSb_2O_4 , is tetragonal, space group $P4_2/mbc$, with $a = 8.59$, $c = 5.91\text{\AA}$. The crystal structure is characterized by the presence of edge-sharing iron octahedra connected with corner-sharing antimony ψ -tetrahedra (Fischer and Pertlik, 1975).

Versiliaite is orthorhombic, space group $Pbam$, $a = 8.492$, $b = 8.326$, $c = 11.938\text{\AA}$. Its crystal structure is related to that of schafarzikite in the following manner: every fourth Sb^{3+} ion in the ψ -tetrahedral chains is substituted by a Fe^{3+} ion and a sulphide anion is added between two Fe^{3+} cations in adjacent chains. The corner-sharing Fe^{3+} tetrahedra connect the chains to build double-chain ribbons. The charge balance, altered by the insertion of sulphide anions, is restored by the substitution of Fe^{2+} cations in the octahedral chains by Fe^{3+} cations.

Apuanite is tetragonal, space group $P4_2/mbc$, $a = 8.372$, $c = 17.974\text{\AA}$. Its crystal structure can be derived from that of schafarzikite by substituting every third Sb^{3+} ion in the ψ -tetrahedral chains with an Fe^{3+} cation and adding sulphide anions which connect adjacent chains to build infinite layers. As in versiliaite the charge balance is restored by substitution of Fe^{2+} cations in octahedral chains with Fe^{3+} cations.

The crystal chemistry of these minerals is clarified and the vacancies in sulphide sites as well as the incompleteness in cationic substitutions are explained. The lines for a systematic derivation of possible, yet unknown, related structures are developed.

Introduction

Versiliaite and apuanite were described by Mellini *et al.* (1979); they showed the close chemical, physical, and crystallographic relationships of the two minerals with schafarzikite, FeSb_2O_4 , from which versiliaite and apuanite can be derived by a concerted mechanism of insertion, substitution, and oxidation.

The aim of this paper is to describe and discuss the main features of their crystal structures and to develop a comprehensive crystal chemistry for the schafarzikite group of minerals.

Structure determination

The experimental parameters characterizing the intensity data collection step are summarized in Table 1. Two equivalent sets were collected for both crystals; the diffraction intensities were corrected for the usual geometrical factors, as well as for absorption by the semiempirical method of North *et al.* (1968); symmetry-related reflections were thereafter checked for equivalence and averaged to pro-

duce the unique sets. In the subsequent structure-factor calculations, all the scattering factors for neutral atoms and anomalous dispersion corrections were taken from the International Tables for X-ray Crystallography, or calculated from them when a hybrid curve was used.

Versiliaite

The structure determination was undertaken in the centrosymmetric space group $Pbam$, indicated by the statistical averages and distribution of E_{hkl} values; the choice appeared correct in the subsequent refinement stage. A trial model was built, starting from the parameters given by Fischer and Pertlik (1975) for schafarzikite and taking account of the doubled c parameter. The use of the scattering factors of antimony for atoms at $z = 0.0$ and $z = 0.25$ and of arsenic for an atom at $z = 0.5$ led to the doubling of the c translation. Moreover we used the full reflections set, including the weakest ones corresponding to $l = 2n + 1$. The refinement was led by Fourier syntheses and least-squares cycles for all the three-coordinated and

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3 4079-4582 4 3572 3665 H,0,1 5 34 -38 9 0 4 7 8 207 165

4 1073-1028 5 311 -294 2 0 6 7 166 175 H,8,1 9 97 -110 H,6,2

5 513 455 6 203 -135 4 309 -318 8 105 -90

6 185 154 7 304 327 6 310 320 9 0 33 8 0 011 292 -256 27 6 869 -864

7 687 -688 8 2064 2066 8 108 7810 130 -8

8 616 654 9 195 -21910 238 -26411 234 -273 H,0,2 H,3,2 7 73 127

9 2707-266210 1291 1254 0 897 -772 3 1012 -91410 8 538 605

10 343 -28411 206 191 H,1,1 H,4,1 2 1099 925 4 86 -119 9 21 -29

11 236 205 H,5,0 2 1295-1147 5 1436-1431 4 1425 1390 5 481 409 H,7,2 625 582

H,2,0

5 419 385 4 1148 1019 7 676 687 8 522 526 7 1189 116917 65 -49

3 1433 1389 6 0 -16 5 87 55 8 117 -11810 1052 1056 8 68 87 8 29 -66

4 3663 3773 7 451 -457 5 324 347 9 464 421

5 54 -8 8 325 -354 7 158 -17710 28 125

6 1402-1332 9 2187-2202 8 1243-124611 1096-1070 H,1,2 10 79 3 623 644

7 922 -922910 59 -50 9 45 -25

8 3283 3284 10 748 805 H,5,1 1 63 -85 11 347 419 H,8,2

9 453 461 H,6,0 11 191 191

10 1335 1336 H,2,1 6 28 50 4 0 -14 4 53 -98 H,0,3

11 0 23 7 421 483 8 960 990 6 0 -62 6 1065 1057 2 462 399

H,3,0

8 1372-1406 3 556 -566 9 864 -908 8 208 145 8 204 -189 4 243 -250

9 78 -47 4 82 8110 864 -908 9 692 671 9 56 38

3 3760 377010 7 476 -491 H,0,4 H,3,4 9 71 38 5 834 803 H,6,5

4 0 57 H,1,4 H,7,4 H,8,4

6 215 -218 9 216 202 0 1793-1656 3 1401-1319 H,7,4 7 6 688 -695 7 303 246

8 131 13510 4 11 304 2 1270 1106 4 51 -38 8 90 131 8 89 -134

10 142 -9611 274 318 4 1772 1734 5 840 763 8 0 -114 9 88 -24 9 372 -339

H,1,3

8 609 573 7 1251 1262 H,8,4 11 613 640 H,7,5

2 5220 6011 5 3694 3730 10 1194 1179 8 78 111 11 613 640 H,7,5

3 165 -140 6 388 411 H,1,4 10 10 47 8 157 77 H,3,5 8 815 -832

4 5506-5921 7 3605-3647 H,0,5 5 286 300 9 122 92

5 104 -89 8 198 -174 1 124 -118 11 579 639 H,0,6 5 217 223 H,0,6

| | | | | | | | | | | | | | | | | | | |
|---|--------|-------|---|--------|-------|---|--------|------|------|---|--------|-------|------|--------|-------|--------|--------|------|
| 0 | 3192 | 3220 | 3 | 4927 | 5063 | 7 | 26 | 148 | 55 | 5 | 286 | 225 | 0 | 1502 | -1594 | 2 | 43 | 52 |
| 2 | 3068 | -3063 | 4 | 88 | 43 | 4 | 88 | 133 | 119 | 2 | H,0,21 | 2 | 747 | 813 | 4 | 30 | -108 | |
| 4 | 2583 | -2530 | 5 | 1370 | -1384 | 4 | H,2,19 | 254 | 274 | 3 | H,0,21 | 4 | 1007 | 1052 | 4 | H,1,23 | | |
| 6 | 1962 | 1989 | 6 | 210 | 172 | 6 | 210 | 147 | -206 | 2 | 107 | 149 | 4 | 194 | -193 | 2 | 254 | 194 |
| 8 | 2329 | -2259 | 7 | 158 | 39 | 3 | 71 | 273 | 224 | 4 | 194 | -193 | 4 | H,1,22 | | 2 | 87 | -11 |
| | H,1,18 | | | H,4,18 | | | H,4,18 | 63 | 19 | 1 | H,1,21 | 1 | 303 | -319 | 3 | 338 | -253 | |
| 1 | 2129 | 2105 | 4 | 135 | 42 | 7 | 1053 | 346 | 341 | 2 | 2534 | 2515 | 3 | 955 | 978 | 4 | H,2,23 | |
| 2 | 505 | -486 | 5 | 279 | 269 | 4 | H,3,19 | 173 | 164 | 5 | 324 | -304 | 3 | 70 | -87 | 3 | 166 | -142 |
| 3 | 565 | -576 | 6 | 1744 | -1688 | 5 | H,5,18 | 14 | 31 | 6 | 494 | 439 | 2 | 143 | -210 | 4 | H,0,24 | |
| 4 | 259 | 246 | 7 | 210 | -238 | 4 | H,4,19 | 173 | -81 | 3 | H,2,21 | 2 | 143 | -210 | 4 | H,0,24 | | |
| 5 | 2471 | 2448 | 4 | 205 | 183 | 4 | H,3,20 | 154 | 44 | 4 | 291 | -273 | 4 | 397 | -379 | 0 | 4345 | 4411 |
| 6 | 57 | -84 | 5 | 37 | 50 | 5 | H,3,20 | 69 | 34 | 6 | 199 | 182 | 5 | 134 | 102 | 2 | 821 | -848 |
| 7 | 1328 | 1323 | 6 | 36 | -72 | 6 | H,2,21 | 199 | 182 | 5 | 134 | 102 | 2 | 821 | -848 | | | |
| 8 | 89 | 137 | 5 | 2176 | 2131 | 7 | H,3,21 | 132 | -120 | 3 | 1524 | -1593 | 1 | 318 | -281 | | | |
| | H,2,18 | | | H,0,19 | | | H,3,21 | 132 | -120 | 3 | 1524 | -1593 | 1 | 318 | -281 | | | |
| 2 | 171 | 175 | 3 | 574 | 578 | 3 | H,4,20 | 292 | 296 | 4 | H,4,22 | | | H,2,24 | | | | |
| 3 | 379 | 379 | 2 | 247 | -88 | 6 | H,4,20 | 64 | 69 | 5 | 0 | 15 | | H,2,24 | | | | |
| 4 | 454 | -329 | 4 | 13 | 10 | 5 | H,3,21 | 59 | -67 | 2 | 1863 | -1790 | | | | | | |
| 5 | 363 | -381 | 6 | 165 | 182 | 6 | H,4,21 | 363 | -380 | 2 | 1970 | 1853 | | | | | | |
| 6 | 2331 | -2317 | | H,0,20 | | | H,4,21 | 363 | -380 | 2 | 1970 | 1853 | | | | | | |
| 7 | 52 | -119 | | H,1,19 | | | H,4,21 | 363 | -380 | 2 | 1970 | 1853 | | | | | | |
| 8 | 478 | 375 | | H,5,20 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,0,19 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,4,19 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,0,20 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,4,20 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,0,21 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,4,21 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,0,22 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,4,22 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,0,23 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,4,23 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,0,24 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,4,24 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,0,25 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |
| | | | | H,4,25 | | | H,5,20 | 1864 | 1886 | 5 | 1864 | 1886 | | | | | | |