# Supplementary Materials: New Mineral with Modular Structure Derived from Hatrurite from the Pyrometamorphic Rocks of the Hatrurim Complex: Ariegilatite, $BaCa_{12}(SiO_4)_4(PO_4)_2F_2O$, from Negev Desert, Israel

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**Table S1.** Calculated powder pattern for ariegilatite. Intensities were calculated using the software JANA2006 [30].

| *h* | *k* | *l* | $d_{hkl}$ [Å] | *I* [%] | *h* | *k* | *l* | $d_{hkl}$ [Å] | *I* [%] | *h* | *k* | *l* | $d_{hkl}$ [Å] | *I* [%] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 3 | 13.768 | 3 | 3 | 0 | 9 | 1.884 | 23 | 3 | −2 | 14 | 1.834 | 3 |
| 0 | 0 | 6 | 6.884 | 2 | 4 | −1 | 23 | 1.242 | 4 | 1 | 0 | 22 | 1.797 | 3 |
| 1 | −1 | 2 | 5.935 | 17 | 4 | −4 | 20 | 1.239 | 3 | 4 | −2 | 0 | **1.789** | **92** |
| 1 | 0 | 4 | 5.313 | 13 | 2 | −2 | 31 | 1.224 | 4 | 2 | −2 | 19 | 1.780 | 10 |
| 1 | 0 | 7 | 4.273 | 8 | 5 | 0 | 8 | 1.205 | 2 | 3 | −3 | 12 | 1.771 | 12 |
| 1 | −1 | 8 | 3.967 | 8 | 6 | −3 | 0 | 1.193 | 5 | 1 | −1 | 23 | 1.725 | 4 |
| 2 | −1 | 0 | **3.578** | **51** | 4 | −3 | 25 | 1.191 | 4 | 2 | 0 | 20 | 1.718 | 17 |
| 2 | −1 | 3 | 3.463 | 30 | 6 | −4 | 1 | 1.171 | 8 | 4 | −1 | 8 | 1.631 | 8 |
| 1 | 0 | 10 | **3.437** | **45** | 4 | −2 | 27 | 1.163 | 2 | 1 | 0 | 25 | 1.596 | 8 |
| 1 | −1 | 11 | 3.211 | 8 | 6 | −3 | 9 | 1.154 | 3 | 4 | −1 | 11 | 1.563 | 3 |
| 2 | −1 | 6 | 3.174 | 17 | 6 | −4 | 7 | 1.149 | 6 | 2 | 0 | 23 | 1.554 | 2 |
| 2 | −2 | 1 | **3.090** | **100** | 6 | −2 | 8 | 1.142 | 7 | 2 | −1 | 24 | 1.551 | 15 |
| 2 | −2 | 4 | 2.968 | 6 | 2 | −2 | 34 | 1.131 | 5 | 4 | 0 | 1 | 1.548 | 10 |
| 2 | 0 | 5 | 2.901 | 19 | 6 | −4 | 10 | 1.127 | 2 | 3 | −3 | 18 | 1.535 | 3 |
| 1 | 0 | 13 | 2.827 | 18 | 4 | −3 | 28 | 1.119 | 4 | 4 | −4 | 5 | 1.523 | 3 |
| 2 | −1 | 9 | **2.822** | **82** | 2 | 0 | 35 | 1.103 | 4 | 4 | −2 | 15 | 1.500 | 38 |
| 0 | 0 | 15 | **2.754** | **62** | 4 | −2 | 30 | 1.091 | 6 | 4 | 0 | 7 | 1.498 | 6 |
| 2 | −2 | 7 | **2.743** | **51** | 6 | −2 | 14 | 1.088 | 4 | 4 | −1 | 14 | 1.485 | 2 |
| 1 | −1 | 14 | 2.664 | 2 | 6 | −5 | 8 | 1.088 | 3 | 4 | −4 | 8 | 1.484 | 4 |
| 2 | 0 | 8 | 2.657 | 17 | 5 | −2 | 25 | 1.078 | 4 | 3 | −1 | 22 | 1.465 | 4 |
| 2 | −1 | 12 | 2.480 | 34 | 6 | −4 | 16 | 1.066 | 9 | 2 | −2 | 25 | 1.458 | 2 |
| 2 | 0 | 11 | 2.390 | 3 | 5 | −4 | 24 | 1.063 | 6 | 1 | 0 | 28 | 1.435 | 3 |
| 1 | 0 | 16 | 2.383 | 6 | 6 | 0 | 0 | 1.033 | 8 | 3 | −2 | 23 | 1.425 | 4 |
| 3 | −2 | 2 | 2.327 | 13 | 6 | −4 | 19 | 1.031 | 2 | 0 | 0 | 30 | 1.377 | 2 |
| 0 | 0 | 18 | 2.295 | 2 | 5 | −2 | 28 | 1.024 | 3 | 4 | −4 | 14 | 1.372 | 4 |
| 3 | −1 | 4 | 2.284 | 3 | 6 | −2 | 20 | 1.019 | 3 | 5 | −1 | 0 | 1.352 | 5 |
| 3 | −2 | 5 | 2.253 | 3 | 7 | −5 | 6 | 0.982 | 3 | 3 | −1 | 25 | 1.350 | 5 |
| 2 | −2 | 13 | 2.218 | 3 | 7 | −2 | 9 | 0.970 | 6 | 5 | −2 | 10 | 1.344 | 5 |
| 3 | −1 | 7 | 2.177 | 20 | 6 | 0 | 15 | 0.967 | 4 | 5 | −3 | 11 | 1.330 | 2 |
| 2 | 0 | 14 | 2.137 | 36 | 6 | −6 | 15 | 0.967 | 3 | 4 | 0 | 16 | 1.328 | 7 |
| 3 | −2 | 8 | 2.133 | 35 | 4 | −2 | 36 | 0.966 | 3 | 5 | −1 | 6 | 1.327 | 4 |
| 3 | 0 | 0 | 2.066 | 3 | 4 | 0 | 34 | 0.956 | 3 | 3 | 0 | 24 | 1.322 | 10 |
| 3 | −3 | 3 | 2.043 | 5 | 7 | −5 | 12 | 0.953 | 2 | 5 | −2 | 13 | 1.298 | 4 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | −1 | 10 | 2.037 | 9 | 6 | −5 | 23 | 0.946 | 2 | 5 | −4 | 9 | 1.297 | 10 |
| 2 | −2 | 16 | **1.983** | **47** | 4 | −4 | 35 | 0.939 | 3 | 5 | −1 | 9 | 1.297 | 2 |
| 3 | −3 | 6 | 1.978 | 14 | 7 | −3 | 22 | 0.895 | 2 | 4 | −3 | 22 | 1.268 | 2 |
| 3 | −1 | 13 | 1.885 | 3 | 8 | −4 | 0 | 0.894 | 7 | 4 | 0 | 19 | 1.262 | 2 |
| 3 | −3 | 9 | 1.884 | 4 | 6 | −4 | 31 | 0.880 | 3 | 5 | −4 | 12 | 1.259 | 2 |