

## ONLINE MATERIALS

### Discovery of an Earthborn quasicrystal approximant

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Table 1. Reflectance of proxitwelvefoldite compared to Bi bearing melonite (Criddle and Stanley 1993)

| Proxitwelvefoldite |            |            | Melonite       |       |       |
|--------------------|------------|------------|----------------|-------|-------|
| $\lambda$ (nm)     | $R_{\max}$ | $R_{\min}$ | $\lambda$ (nm) | $R_o$ | $R_e$ |
| 471.1              | 49.8       | 48.7       | 470            | 55.8  | 54.3  |
| 548.3              | 51.0       | 49.8       | 546            | 61.9  | 57.2  |
| 586.6              | 53.6       | 52.4       | 589            | 65.5  | 60.9  |
| 652.3              | 56.5       | 54.4       | 650            | 68.9  | 64.2  |

Reflectance was measured in air using a Zeiss MPM-200 microphotometer equipped with an MSP-20 system processor on a Zeiss Axioplan ore microscope. The filament temperature was approximately 3350 K. Readings were taken for specimen and standard (SiC) maintained under the same focus conditions. The diameter of the circular measuring area was 0.01 mm.

Table 2. Crystal and experimental data for proxitwelvefoldite.

| Crystal data                          |                                    |
|---------------------------------------|------------------------------------|
| Crystal size (mm <sup>3</sup> )       | 0.025 × 0.023 × 0.017              |
| Cell setting, space group             | Tetragonal, $P4_2/mnm$             |
| $a$ (Å)                               | 10.2641(11)                        |
| $c$ (Å)                               | 5.4015(7)                          |
| $V$ (Å <sup>3</sup> )                 | 569.06(14)                         |
| $Z$                                   | 2                                  |
| Data collection and refinement        |                                    |
| Radiation, wavelength (Å)             | MoK $\alpha$ , $\lambda = 0.71073$ |
| Temperature (K)                       | 293                                |
| $2\theta_{\max}$ (°)                  | 69.94                              |
| Measured reflections                  | 6895                               |
| Unique reflections                    | 721                                |
| Reflections with $F_o > 4\sigma(F_o)$ | 428                                |
| $R_{\text{int}}$                      | 0.0356                             |
| Range of $h, k, l$                    | $0 \leq h \leq 11,$                |
| $R [F_o > 4\sigma(F_o)]$              | 0.0216                             |
| $R$ (all data)                        | 0.0234                             |
| $wR$ (on $F^2$ )                      | 0.0473                             |
| GooF                                  | 0.806                              |
| Number of least-squares parameters    | 26                                 |
| Maximum and                           | 0.75 (at 0.03 Å from Te2)          |

Table 3. Wyckoff positions, atom coordinates, and equivalent isotropic displacement parameters (Å<sup>2</sup>) for proxitwelvefoldite.

| atom | Wyckoff | $x/a$      | $y/b$      | $z/c$         | $U_{\text{iso}}$ |
|------|---------|------------|------------|---------------|------------------|
| Pd1  | 2b      | 0          | 0          | $\frac{1}{2}$ | 0.03997(16)      |
| Pd2  | 4f      | 0.10125(3) | 0.10125(3) | 0             | 0.03765(11)      |
| Ni   | 8i      | 0.36882(8) | 0.03664(8) | 0             | 0.05354(17)      |
| Te1  | 8i      | 0.56594(4) | 0.23940(5) | 0             | 0.06161(12)      |
| Te2  | 8j      | 0.31719(2) | 0.31719(2) | 0.25210(8)    | 0.05684(10)      |

Table 4. Selected bond distances (Å) for proxitwelvefoldite.

|      |     |            |      |
|------|-----|------------|------|
| Pd1- | Pd2 | 3.0747(4)  | (×4) |
|      | Te1 | 2.7591(6)  | (×4) |
|      | Te2 | 2.9826(4)  | (×4) |
| Pd2- | Pd1 | 3.0747(3)  | (×2) |
|      | Pd2 | 2.9394(10) |      |
|      | Ni  | 2.8253(8)  | (×2) |
|      | Te1 | 3.1781(4)  | (×4) |
|      | Te2 | 3.3158(6)  | (×4) |
|      | Te2 | 3.4175(5)  | (×2) |
| Ni-  | Ni  | 2.7960(16) |      |
|      | Te1 | 2.9025(10) |      |
|      | Te1 | 2.9114(9)  |      |
|      | Te1 | 2.9357(4)  | (×2) |
|      | Pd2 | 2.8253(8)  |      |
|      | Ni  | 3.3471(7)  | (×4) |
|      | Te2 | 3.2291(4)  | (×2) |
|      | Te2 | 3.2422(4)  | (×2) |
| Te1- | Te1 | 2.8257(9)  |      |
|      | Te2 | 2.9633(6)  | (×2) |
|      | Te2 | 3.0018(8)  | (×2) |
| Te2- | Te2 | 2.6781(10) |      |
|      | Te2 | 2.7234(10) |      |
|      | Te1 | 2.9633(6)  | (×2) |
|      | Te1 | 3.0018(8)  | (×2) |