

Supplementary Data

to the article

Negevite, the pyrite-type NiP_2 , a new terrestrial phosphide

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Table S1. Reflectance values for negevite

<i>R</i> (%)	λ (nm)	<i>R</i> (%)	λ (nm)
53.4	400	55.1	560
53.9	420	55.2	580
54.3	440	55.3	589 ^{<i>a</i>}
54.5	460	55.3	600
54.6	470 ^{<i>a</i>}	55.4	620
54.6	480	55.5	640
54.8	500	55.6	650 ^{<i>a</i>}
54.9	520	55.6	660
55.0	540	55.7	680
55.0	546 ^{<i>a</i>}	55.8	700

^{*a*} Reflectance values for four wavelengths recommended by the Commission on Ore Mineralogy, I.M.A.

Table S2. Crystal parameters, data collection and structure refinement details for negevite

Crystal data	
Chemical formula	NiP ₂
Crystal size (mm)	0.01 x 0.01 x 0.01
Crystal system, space group	Cubic, $Pa\bar{3}$
a (Å), V (Å ³), Z	5.4816 (5), 164.71(3), 4
D_x (g/cm ³)	4.865
Data collection and refinement	
Instrument	Bruker APEX DUO (CCD detector)
X-ray source and optics	MoK α , microfocus tube, 50 kV, 0.6 mA
2 Θ range (°)	13.0–54.0
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1920, 62, 52
h, k, l range	–7→6, –6→7, –7→7
$R_{\text{int}}, R_{\sigma}$	0.067, 0.018
R_1 ($ F_o \geq 4\sigma_F$), wR_2 , $S=GoF$	0.017, 0.037, 1.115

Table S3. Calculated X-ray powder diffraction pattern for negevite

I_{calc}	d_{calc} (Å)	hkl
54	3.1648	111
95	2.7408	200
42	2.4514	210
35	2.2379	211
54	1.9380	220
100	1.6528	311
17	1.5824	222
13	1.5203	320
17	1.4650	321
12	1.2576	331
14	1.2257	420