

Supplementary Information

Nazarovite, Ni_{12}P_5 , a new terrestrial and meteoritic mineral structurally related to nickelporphide, Ni_3P

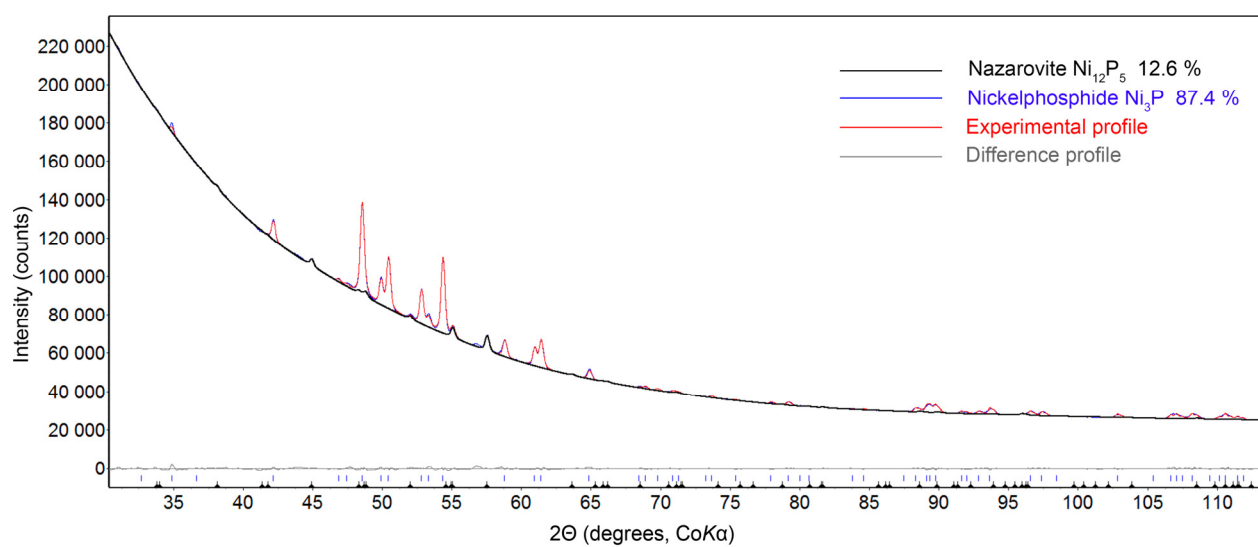


Figure S1. Rietveld refinement plot of acid-resistant precipitate from the Marjalahti pallasite.

Table S1. Rietveld refinement details for nazarovite from the Marjalahti pallasite

Radiation	CoK α_1 / CoK α_2
μ (mm ⁻¹)	60.76
Exposure time (s)	3600
$2\Theta_{\min}$ – $2\Theta_{\max}$ (°)	30–115
R_p, R_{wp}, R_B (%), GoF	0.32, 0.45, 0.216, 1.07

Table S2. Fractional atomic coordinates and isotropic displacement parameters for nazarovite from the Marjalahti pallasite

Site	x	y	z	B_{iso} (Å ²)
Ni1	0.1152(6)	0.1830(6)	0.251(2)	0.47(10)
Ni2	0.3644(9)	0.0610(11)	0	0.47(10)
P1	0.1854(19)	0.4295(17)	0	0.47(10)
P2	0	0	0	0.47(10)

Table S3. Crystal parameters, data collection and single-crystal structure refinement details for nazarovite from the Hatrurim basin (the holotype specimen)

Crystal data	
Chemical formula	Ni ₁₂ P ₅
Crystal system, space group	Tetragonal, <i>I4/m</i>
<i>a</i> (Å)	8.640(1)
<i>c</i> (Å)	5.071(3)
<i>V</i> (Å ³)	378.5(2)
<i>Z</i>	2
<i>D_x</i> (g cm ⁻³)	7.539
Crystal size (mm)	0.01 × 0.005 × 0.002
Data collection and refinement	
Diffractometer	Bruker Kappa Apex DUO CCD
Radiation	MoKα
Temperature (K)	296
μ (mm ⁻¹)	30.06
<i>F</i> (000)	822
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	988, 278, 214
<i>R</i> _{int} , <i>R</i> _σ	0.046, 0.029
<i>h</i> , <i>k</i> , <i>l</i> min→max	−7→11, −11→11, −6→6
2Θ _{max} (°)	52
No. of parameters	24
<i>R</i> ₁ , <i>wR</i> ₂ , <i>S</i>	0.052, 0.124, 1.149
Data completeness	0.996
Δρ _{min} , Δρ _{max} (e Å ⁻³)	−1.44, 1.40