

LETTER

Icosahedral coordination of phosphorus in the crystal structure of melliniite, a new phosphide mineral from the Northwest Africa 1054 acapulcoite

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ABSTRACT

Melliniite, ideally (Ni,Fe)₄P, is a new mineral from the Northwest Africa 1054 acapulcoite. It occurs as anhedral to subhedral grains up to 100 μm, associated with kamacite and nickelporphide. Melliniite is opaque with a metallic luster and possesses a gray streak. It is brittle with an uneven fracture; the Vickers microhardness (VHN₅₀₀) is 447 kg/mm² (range 440–454) (calculated Mohs hardness of 8–8½). The calculated density is 7.88 g/cm³ (on the basis of the empirical formula). In plane-polarized reflected light, melliniite is cream-yellowish. Between crossed polars it is isotropic, with no internal reflections. Reflectance percentages (*R*) for the four standard COM wavelengths are 60.5 (471.1 nm), 50.4 (548.3 nm), 52.5 (586.6 nm), and 55.9 (652.3 nm), respectively. Electron-microprobe analyses give the chemical formula (Ni_{2.30}Fe_{1.64}Co_{0.01})_{Σ=3.95}P_{1.05} on the basis of total atoms = 5.

Melliniite is cubic, space group *P*2₁3, with *a* = 6.025(1) Å, *V* = 218.71(6) Å³, and *Z* = 4. The crystal structure has been solved and refined to *R* = 2.72% using single-crystal X-ray diffraction data. It shows the AlAu₄-type structure, which is an ordered form of the β-Mn structure. The metal atoms occupying the 12*b* site (M1) are effectively 14 coordinated whereas the metals at the 4*a* site (M2) are 12 coordinated by three P atoms and nine metals. The phosphorus atoms (4*a* site) coordinate 12 metal atoms in a somewhat distorted icosahedral arrangement. This new phosphide is the first phase with such a high coordination-number for phosphorus.

The new mineral is named after Marcello Mellini, Professor of Mineralogy, who strongly developed the study of meteorites in Italy. The new mineral and mineral name have been approved by the IMA Commission on New Minerals and Mineral Names (2005-027).

Keywords: Melliniite, chemical composition, meteorites, X-ray data, new mineral