American Mineralogist, Volume 92, pages 1262–1269, 2007

Crystal-chemical and carbon-isotopic characteristics of karpatite ($C_{24}H_{12}$) from the Picacho Peak Area, San Benito County, California: Evidences for the hydrothermal formation

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Abstract

Karpatite from the Picacho Peak Area, San Benito County, California, has been characterized as an exceptionally pure crystal of coronene ($C_{24}H_{12}$) by infrared absorption analysis, Raman scattering analysis, and differential thermal analysis. Furthermore, the crystal structure of karpatite was determined using a single-crystal X-ray diffraction method for the first time. The mineral crystallizes in the monoclinic system, space group $P2_1/a$, with unit-cell dimensions of a = 16.094(9), b = 4.690(3), c = 10.049(8) Å, β = 110.79(2)°, V = 709.9(8) Å^3, and Z = 2. The structure was solved and finally refined to R_1 = 3.44% and wR_2 = 2.65%, respectively. The coronene molecules in the crystal structure of karpatite are all isolated and the intermolecular distances correspond to van der Waals interactions. The coronene molecules have the high degree of aromaticity and no overcrowded hydrogen atoms, both of which avoid a mixing of other polycyclic aromatic hydrocarbons (PAHs) in karpatite. The corrugated arrangement of coronene molecules constituting karpatite prevents intercalation reactions, accounting for the exceptional purity of this mineral.

The isotopic composition of carbon was measured, using an elemental analyzer-isotopic ratio mass spectrometer (EA/IRMS). The present karpatite yielded a $\delta^{13}C$ value of –22.39 ± 0.18‰ (vs. VPDB), which is similar to carbon isotopic compositions of sedimentary organic matter in the far-reaching tectonic regions. This organic matter might be converted to coronene molecules by hydrothermal fluids leading to formation of karpatite. Textural relationships indicate that after the strong concentration of coronene molecules in hydrothermal fluids, karpatite growth postdates both hydrothermal quartz precipitation, and subsequent cinnabar formation.

Keywords: Crystal structure, karpatite, stable isotopes, coronene, IR spectroscopy, Raman spectroscopy, DTA, polycyclic aromatic hydrocarbons