

Crystal structure of karpatite (C₂₄H₁₂: coronene): application of Huckel rule to the paragenesis of PAH minerals.

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http://www.geo.tsukuba.ac.jp/Mineralogy_Web/Kimata_Labo/index.html

The crystal structure of karpatite, C₂₄H₁₂, from Picacho Peak Area, San Benito County, California, monoclinic, P2₁/c, a = 10.06(1) Å, b = 4.694(5) Å, c = 16.08(3) Å, beta = 69.19(5) deg., V = 980.9(4) cubic Å, Z = 2, was solved by direct methods and refined with full-matrix least squares techniques to R = 0.050 and Rw = 0.078 for 1921 observed reflections [I_o is larger than 5 sigma (I_o)] collected using MoK-alfa radiation.