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Hartite from Bílina

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ABSTRACT

In the Bílina Mine (Czech Republic), a very chemically pure material corresponding to hartite was found as a product of distillation into the pelosiderite nodule during coalification of a lignite seam in the Miocene or later. The amount of the material available allowed characterizing this natural mineral equivalent of the hydrocarbon (+)-phyllocladane [16α(H)-phyllocladane] thoroughly.

Elementary analysis of hartite from Bílina gave C = 87.45 wt% and H = 12.55 wt%, which corresponds to the formula $C_{20}H_{34}$. The IR spectrum demonstrated the presence of gem-dimethyl groups (doublet $\delta_s CH_3$ at 1369 and 1383 cm^{-1}). Other bands indicated the presence of methyl and methylene groups. NMR studies showed that the hydrocarbon (hartite) molecule contains four CH_3 groups, nine CH_2 groups, four CH groups, and three quaternary carbon atoms. The sample exhibits a well-defined melting point between 71 and 71.5 °C. Measurements of optical rotation gave $[\alpha]_D = +24.2°$ ($CHCl_3$, $c = 0.7$). Lattice parameters from single-crystal study measured at 293(2) K were $a = 11.407$ (1), $b = 20.952$ (2), $c = 7.4060$ (8) Å, $\alpha = 93.941$ (9)°, $\beta = 100.750$ (8)°, and $\gamma = 80.499$ (9)°. The crystal system is triclinic with space group *P*l, $Z = 4$, $V = 1713.8$ (3) $Å^3$. Densities are $D_m = 1.04$ g/cm^3 and $D_x = 1.064$ g/cm^3, respectively. Isotopic composition of C in hartite from Bílina gave $\delta^{13}C_{(PDB)} = -24.4(1)$ ‰, a common value for coal and organic sedimentary material derived from higher plants.