

Synthesis, crystal structure and magnetic properties of indium(III) diphthalocyanine.

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New form indium(III) phthalocyanine was obtained by the direct reaction of InMg alloy with 1,2-dicyanobenzene at 210 °C. The InPc_2 is isostructural with SnPc_2 ; it crystallizes in the orthorhombic system, space group $P2_12_12_1$, with unit cell parameters $a = 10.569(3) \text{ \AA}$, $b = 50.868(11) \text{ \AA}$, $c = 8.899(2) \text{ \AA}$, $V = 4784.1 \text{ \AA}^3$, and $Z = 4$. The crystal structure was refined to $R = 0.0322$, $R_w = 0.0457$, and $S = 1.11$ for 731 refined parameters and 3898 independent reflections having with $F > 4\sigma(F)$. The crystals of InPc_2 contain sandwich-type molecules in which the indium atom is 8-fold coordinated by the isoindole nitrogens of two phthalocyanine rings. The average value of the In-N bond distance is $2.333 \text{ \AA}$ ($2.327(4)$ - $2.346(4) \text{ \AA}$). The distance between phthalocyanine planes in this sandwich macromolecule is equal to $2.741(7) \text{ \AA}$. The two phthalocyaninato moieties are rotated about $41.2(4)^\circ$ with respect to one another. The magnetic susceptibility measurement shows a typical Curie-Weiss behavior. The effective magnetic moment is $1.67 \mu_B$. The EPR spectrum of InPc_2 exhibits a single strong signal at $g = 2.0025$. © 1995, American Chemical Society. All rights reserved.

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