Structural evidence of the formation of ZnPc-DBU complex during recrystallisation of commercially available ZnPc dye.

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Streszczenie

Recrystallisation of commercially available ZnPc dye in a liquid 2-cyanopyridine or 4-cyanopyridine leads to formation of well developed parallelepipedal violet single crystals with the same composition in both cases. A combination of X-ray single crystal analysis and NMR spectroscopy together with an elemental analysis enable to identify the composition and the structure of the obtained ZnPc-DBU crystals (where DBU is 1,8-diazabicyclo[4.5.0]undec-7-ene). The commercially available ZnPc dye contains DBU as impurity, since DBU is usually used as a strong base in the synthesis of phthalocyanines, and therefore recrystallisation in 2- or 4-cyanopyridine as weaker bases leads to formation of ZnPc-DBU crystals. The ZnPc-DBU crystallizes in the centrosymmetric space group of the monoclinic system with four molecules per unit cell. The Zn center is equatorially coordinated by four isoindole N atom of phthalocyaninato macrocycle and by the N atom of DBU ligand in an axial position. Thus the ZnPc unit of the ZnPc-DBU molecule adopts a saucer shape form. The ZnPc-DBU compound exhibits better solubility than the parent ZnPc compound due to the steric hindrance of the axial DBU ligand that lowers the aggregation in solution. The electronic spectra in DBU and cyclohexane solutions exhibit the B and Q bands typical of the phthalocyaninate(2-) macrocycle. The bands are blue shifted in cyclohexane solution in relation to DBU solution.

Słowa kluczowe

ZnPc-diazabicycloundecene complex, NMR, UV-vis, crystal structure, Phthalocyanine

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