Phthalocyanines: From Molecular Structures to Solid-state Arrangements

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Phthalocyanines are highly valued as green and blue pigments, and as photosensitizers in laser printers and photocopiers. In both applications, the physical properties (color, photosensitivity) are dependent on the solid-state molecular arrangement. The single-crystal structures of most phthalocyanine pigments and photosensitizers, together with their corresponding structure-property relationships, have still yet to be established. However, with the support of X-ray powder diffraction and structure calculation therefrom, detailed knowledge of the structures and properties of characterized phthalocyanines can be collated and compared to draw vital conclusions regarding the precise structural details of as yet undetermined phthalocyanines. Moreover, with almost 70 years of phthalocyanine crystal structure research, the need to compile and categorize a comprehensive list of all available structures is paramount. To address this issue, an extensive phthalocyanine structural review, highlighting the common characteristics, was first compiled in 1997 (230 structures),¹ and was later followed by a more broader review in 2003 (580 structures).² Here, we present a summary of this data, and attempt to classify the phthalocyanine single-crystal structures in accordance with their molecular structure and arrangement patterns.

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1) Engel, M. K. Kawamura Rikagaku Kenkyusho Hokoku 1997, 8, 11-54 (English)