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Magnetically Oriented Powder Crystal to Indexing and Structure Determination

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In pharmaceutical sciences, the crystal structure is of primary importance because it influences drug efficacy. Due to difficulties of growing a large single crystal suitable for the single crystal X-ray diffraction analysis, powder diffraction method is widely used. In powder method, two-dimensional diffraction information is projected onto one dimension, which impairs the accuracy of the resulting crystal structure. To overcome this problem, we recently proposed a novel method of fabricating a magnetically oriented microcrystal array (MOMA), a composite in which microcrystals are aligned three-dimensionally in a polymer matrix. The X-ray diffraction of the MOMA is equivalent to that of the corresponding large single crystal, enabling the determination of the crystal lattice parameters and crystal structure of the embedded microcrytals.[1-3] Because we make use of the diamagnetic anisotropy of crystal, those crystals that exhibit small magnetic anisotropy do not take sufficient three-dimensional alignment. However, even for these crystals that only align uniaxially, the determination of the crystal lattice parameters can be easily made compared with the determination by powder diffraction pattern. Once these parameters are determined, crystal structure can be determined by X-ray powder diffraction method. In this paper, we demonstrate possibility of the MOMA method to assist the structure analysis through X-ray powder and single crystal diffraction methods. We applied the MOMA method to various microcrystalline powders including L-alanine, 1,3,5-triphenyl benzene, and cellobiose. The obtained MOMAs exhibited well-resolved diffraction spots, and we succeeded in determination of the crystal lattice parameters and crystal structure analysis.

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