

非対称ベンズイミダゾール[3]アレンからなる多孔性金属錯体 Metal-Benzimidazole[3]arene Framework-1 (MBAF-1)の分子吸着 特性と構造変化

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Molecular adsorption properties and structural transformation of metal-benzimidazole[3]arene framework-1 (MBAF-1) composed of unsymmetric benzimidazole[3]arene (¹*Graduate School of Science, The University of Tokyo*) ○Yoshiki Okajima,¹ Shohei Tashiro,¹ Mitsuhiro Shionoya¹

Metal-organic frameworks (MOFs) have received a great deal of attention as a porous material with high surface areas and chemical modularity. Therefore, porous crystals with undulations, asymmetric nature, and flexibility that are characteristics of the surface of biomolecules have the potential to exhibit excellent molecular adsorption capacity and molecular recognition characteristics not found in typical porous crystals with flat and pores. We have previously reported the synthesis and molecular adsorption structures of MBAF-1, a porous crystal with an asymmetric and undulating pore surface consisting of the C_1 -symmetric macrocyclic ligand, benzimidazole[3]arene. As a result of detailed examination of the adsorption structure of solvent molecules, it was found that MBAF-1 shows a change in the shape of the adsorption site depending on the type of the immersion solvent, and expands and contracts isotropically or anisotropically.

Keywords : Silver; Porous crystal; Single-crystal X-ray diffraction; Porous coordination polymer; Macrocycle

高い比表面積や化学修飾性を備えた多孔性材料として、金属有機構造体(MOF)が注目されている。生体分子の表面に特徴的な起伏、非対称性、柔軟性を備えた多孔性結晶は、平坦かつ剛直な細孔をもつ典型的な多孔性結晶にはない優れた分子吸着能や分子認識特性を発現する可能性がある。先に我々は、 C_1 対称の大環状配位子ベンズイミダゾール[3]アレン¹からなる非対称で起伏に富んだ細孔表面をもつ多孔性結晶 MBAF-1 の合成と分子吸着構造を報告した。今回、溶媒の吸着構造を詳細に調べた結果、MBAF-1 は浸漬溶媒の種類によって吸着部位の形状が変化し、等方的または異方的に膨張および収縮することを見出した。

1) S. Tashiro, T. Umeki, R. Kubota and M. Shionoya, *Chem. Sci.* **2018**, 9, 7614–7619.

