COORDINATIVE ALIGNMENT OF MOLECULES IN CHIRAL METAL ORGANIC FRAMEWORKS

Tech ID: 26003 / UC Case 2017-006-0

PATENT STATUS

Country	Type	Number	Dated	Case
Germany	Issued Patent	60 2017 093 647.2	01/21/2026	2017-006
European Patent Office	Issued Patent	EP3496838	01/21/2026	2017-006
France	Issued Patent	EP3496838	01/21/2026	2017-006
United Kingdom	Issued Patent	EP3496838	01/21/2026	2017-006
Japan	Issued Patent	7049318	03/29/2022	2017-006
United States Of America	Issued Patent	10,766,911	09/08/2020	2017-006
United States Of America	Issued Patent	11,370,805	06/28/2000	2017-006

BRIEF DESCRIPTION

Single-crystal x-ray diffraction is a powerful technique for the definitive identification of chemical structures. Although most molecules and molecular complexes can be crystallized, often enthalpic and entropic factors introduce orientational disorder that prevent determination of a high-resolution structure. Several strategies based on the inclusion of guests in a host framework that helps maintain molecular orientation have been used to overcome this challenge. However, most of these methods rely primarily on weak interactions to induce crystalline order of the included molecules.

Researchers at UC Berkeley have developed a strategy for crystallization of molecules within the pores of chiral metal-organic frameworks (MOFs) using coordinative bonding, which includes covalent and ionic bonds, and/or using chirality.

SUGGESTED USES

The invention can be used to determine the precise crystal structure of pharmaceutical molecules, natural products, and protein structures by diffraction techniques, such as, x-ray, neutron, and electron diffractions.

ADVANTAGES

Advantages of this strategy include: (i) the molecules make covalent bonds to well-defined metal sites of the MOF; these bonds anchor them and lower their motional degrees of freedom, thereby promoting their alignment into an ordered pattern across the interior of the crystalline framework; and (ii) the absolute structure of the chiral MOF framework serves as a reference for the direct determination of the absolute configuration of bound chiral molecules. Indeed, this latter feature forgoes the reported pseudo-symmetry problems that have obscured the absolute structures that specify the enantiomorph in achiral host framework systems.

RELATED MATERIALS

ADDITIONAL TECHNOLOGIES BY THESE INVENTORS

- Exceptional Zeolitic Imidazolate Frameworks And A General Strategy To Make More
- Hydroxamate-Based Metal-Organic Frameworks
- Mof Heterolites: Mesoscopic Heterogeneity Within Order With Porous Nanocrystals
- PFAS Removal from Water Through Fluorinated Cationic Reticular Materials
- Sorption-Based Atmospheric Water Harvesting Device

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OTHER INFORMATION

KEYWORDS

crystallization coordinative bonding

CATEGORIZED AS

» **Imaging**

» Molecular

» **Materials & Chemicals**

» Chemicals

RELATED CASES

2017-006-0

- Molecular Weaving Additives To Enhance The Mechanical Properties Of Materials
- Hydrochromic Reticular Materials
- Thiazole-Based Covalent Organic Frameworks For Low-Humidity Water Adsorption

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