

Template for Preparation of Papers for International seminar of Hydrogeology and Environment

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Abstract—The treatment of water polluted by metals and solvents, as well as reducing emissions of polluting gases by implementing alternative energy are major environmental issues. Porous materials characterized by low density network meet these industrial applications.

This article focuses on the synthesis by soft chemistry of hybrid materials using new technical, to applications such as molecular sieves, receivers and enantioselective catalysts are described. In addition, the storage capacity of porous solids prepared will be evaluated based on reasoned changes to their molecular architecture, pore size and chemical reactivity.

Key-Words— single-crystal X-ray study, pore,

I. INTRODUCTION

In the course of a study on mixed squarate of amines and metals, the role of the amine group has been investigated in the topology of the organic-inorganic framework. The synthesis led to a new mixed squarate of yttrium and ethylenediamine.

The design of these new materials based on transition metals and amines (organic ligands) has taken an increasing interest in recent years. The objective in this area is the design of new solids with new physical properties prospects of new applications, such as storage molecules [1] [2].

This technique is based on the capacity that have some solid materials to retain liquid compounds.

To get a good return abatement of water, we need the catalyst the most efficient as possible. The idea is to produce porous catalytic materials that are fixed and then let a very easy to use. To prepare a porous material we chose the method by soft chemistry.

II. EXPERIMENTAL

The title compound, $Y(C_4O_4)_3(C_2H_{10}N_2)1.54H_2O$ was prepared from an aqueous solution of dissolved yttrium nitrate, ethylenediamine and 3,4-dihydroxy-3-cyclobutene-1,2-dione, also named squaric acid.

The slow evaporation at room temperature leads after some hours to the formation of the title compound together with two polymorphs of $(HC_4O_4)_2(C_2H_{10}N_2)(H_2O)$ [3].

III. REFINEMENT

All H atoms were found from Fourier difference maps. H atoms attached to C were fixed geometrically and treated as riding with C—H = 0.97 Å with $U_{iso}(H) = 1.2U_{eq}$. As H atoms attached to N and O are not geometrically tightened, they were refined using restraints of N—H = 0.89 (1) Å and O—H = 0.97 (1) Å with $U_{iso}(H) = 1.2U_{eq}(N)$ and $U_{iso}(H) = 1.5U_{eq}(O)$, respectively. In the last cycles of refinement, they were treated as riding on their parent atoms.

IV. DESCRIPTION OF STRUCTURE

Yttrium is eightfold coordinated in the shape of a square antiprism. YO_8 polyhedra are connected along the b axis

through bis(monodentate) squarates in the form zigzag chains. Amine groups from are located between the chains and are connected to them through hydrogen bonds involving oxygen atoms from squarate groups. Other hydrogen bonds between squarate [4].

The asymmetric unit contains one yttrium cation in an antiprismatic environment, three squarate groups, one and a half protonated ethylenediamine molecules and four water molecules. YO_8 polyhedra are connected through bis(monodentate) squarates, leading to infinite zigzag chains, in between which are located ammonium groups. A framework of hydrogen bonds between protonated amine N atoms, water molecules and squarate anions ensures the cohesion of the structure.

Yttrium is environment by 8 oxygen atoms. So a square base YO_8 antiprism (a cube which is the upper face turned 45° relative to the base) is formed.

These antiprisms formed by the contribution of the four oxygen atoms of the four ligands squarates and the four oxygen atoms of four water molecules formed a straight chain Y - squarate - Y (zigzag) along the b axis. Amines located between the channels involved by their powerful N-H ... O hydrogen bonds to interconnect these chains forming layers in the (ab) as shown in figure 1

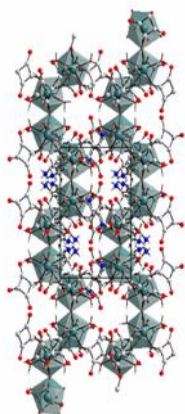


Figure 1. Projection of the structure of Y (C4O4)₃ (C2H10N2)_{1.5}.4H2O along the c axis

These layers are developed in parallel planes (bc) are stacked along the c axis. They are located approximately 18A ° to one another. The layer arrangement leaves appear channels which develops parallel to the c axis.

The chemical structure of this compound is bound via hydrogen bonds involving the protonated amine as shown in figure 2.

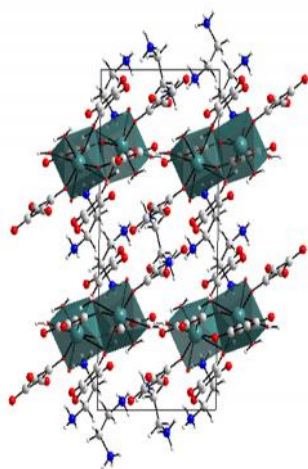


Figure 2. Projection of the structure of Y (C4O4)₃ (C2H10N2)_{1.5}.4H2O along the b axis.

The final atomic coordinates and isotropic atomic displacement parameters, as well as the positions of the hydrogen atoms have been study.

APPLICATIONS

The absorption of porous solid is mainly used to treat water polluted by oil or hydrocarbons. This is why materials that will be both oleophilic and hydrophobic be used[5] [6].

V. CONCLUSION

A new hybrid material was prepared. Characterization was carried out by X-ray diffraction by the crystal. This compound has a two-dimensional structure held by hydrogen bonds.

The idea is to make a kind of porous catalytic materials that would be fixed and then let a very easy to use. To a porous material we chose the method by soft chemistry. We are successfully manufacturing cluster. This cluster is then bridged by entities to form a network containing pores.

For now we are trying to control the bridging process with minimal molecular defect and we control the pore size and we'll get one the greatest possible surface area.

Following this study tests will show if the performance is better and especially will highlight the ease of use of this material.

APPENDIX

Appendixes, if needed, appear before the acknowledgment.

Données cristallographique	
Formula	(HC ₄ O ₄) ₂ (C ₂ H ₁₀ N ₂) ₂ .H ₂ O
Masse moléculaire (g.mol ⁻¹)	330.66
Système cristallin	Monoclinique
Groupe d'espace	P 2/a
a (Å)	10.941(1)
b (Å)	9.022(1)
c (Å)	14.191(1)
(°)	90.000
(°)	111.789(1)
(°)	90.000
V (Å ³)	1300.7(2)
Z	4
F(000)	670
(Mo K) Å	0.71073
u (mm ⁻¹)	2.328
ρ	1.689
R1	0.0586
wR2	0.1688
Goof	1.032

Refinement

R[F² > 2 (F²)] = 0.044 190 parameters
wR(F²) = 0.116 H-atom parameters constrained
S = 1.06 max = 0.28 e Å⁻³
2957 reflections min = -0.24 e Å⁻³

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