Anexa 2a

Titlu proiect: ***Polioxometalati imobilizati: sinteza, caracterizare si aplicatii in fotocataliza***
Categoria de proiect: Cercetare
Contractul de finanţare: ORDINUL IUCN nr. 96 din 15.02.2016

Manager proiect: Prof. univ. dr. Doina Humelnicu

Lista rezultate

Nr. crt.	NUME AUTORI	TITLUL ARTICOLULUI/ CĂRŢII / COMUNICĂRII ŞTIINŢIFICE	REVISTA / VOLUMUL/EDITURA IN CARE A APARUT / CONFERINTA LA CARE S-A COMUNICAT	ANUL PUBLICARII/ COMUNICARII
ARTICOLE ISI				
1				
n				
	ARTICOLE ALTE BAZE DE DATE			
1				
n				
CARTI				
1				
n				
COMUNICARI STIINTIFICE NATIONALE				
1	D. Humelnicu, M.L. Craus, I. Humelnicu, M. Ignat	Lanthanide Isopolyoxometalates: synthesis, structure and photocatalytic activity	Conferinţa Facultăţii de Chimie, 27-28 Octombrie, 2016, Iaşi	2016
COMUNICARI STIINTIFICE INTERNATIONALE				
1				
n				
ATLASE, DICTIONARE DE SPECIALITATE				
1				
n				
CERERI BREVET DE INVENTII/BREVET OBTINUT				
ALTE rezultate				
1				
n				

Raport tehnico-stiintific privind grantul:

Tema din Planul tematic al IUCN:

Denumire: ***Investigation of Condensed Matter by Modern Neutron Scattering Methods"***.

Numar: *04-4-1121-2015/2017*

Conducator: Dr. D.P. Kozlenko

Responsabil din Romania:

Nume, prenume: conf. Dr. Doina Humelnicu, **Facultatea de Chimie a Universitatii "Al. I. Cuza" Iasi (UAIC);**

General objectives

The aims of this projects were: 1) The exploration of the possible synthetic routes to adjust the composition of different type of POMs. 2) The investigation of crystalline structures of the obtained clusters. 3) The evaluation of photocatalytic activity of support, POM and supported POM materials.

We obtained a compound of polyoxometalate of type Sm^{3+} - $[W_5O_{18}]^{9-}$ and we tested it from photocatalytic activity point of view.

Polyoxomolybdate was obtained hydrothermally from the reaction of $Na_2WO_4 \cdot 2H_2O$, $Sm(NO_3)_3$ in an aqueous solution at a pH value of 7.4-7.55 adjusted by acetic acid solution. The characterization of the systems Sm^{3+}- POM was accomplished by means of FTIR, UV-Vis spectroscopy and thermal analysis. A Bruker Alpha spectrophotometer was used for Fourier transform infrared (FT-IR) spectroscopy. Spectra were recorded onto a KBr thin disk with a spectral resolution better than 2 cm^{-1} and a wave number accuracy of 0.01 cm^{-1}.

The structure of Sm^{3+} - $[W_5O_{18}]^{9-}$ is formed by two anionic $[W_5O_{18}]^{9-}$ moieties sandwiching the central ion of samarium. The anionic clusters are surrounded by sodium cations that are octahedrally coordinated by oxygen atoms. These hydrated sodium cations interact with the highly charged $[Sm(W_5O_{18})_2]^{9-}$ anions for the electroneutrality.

The preliminary results of our work, "*Sm(III) polyoxometalates: structure and photocatalytic activity for dye degradation*" – D. Humelnicu, O.M. Apostu, M.L. Craus, M. Ignat, I. Humelnicu will be presented to Faculty of Chemistry Conference, 27-29 October, 2016, Iasi.

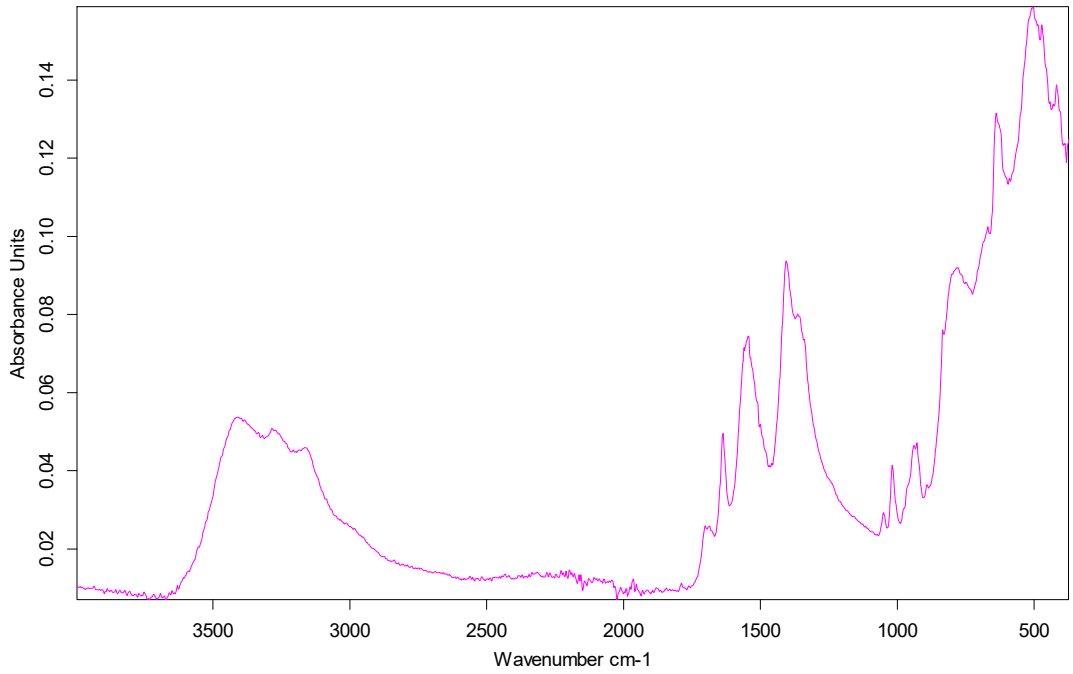

Fig. 1. FT-IR spectrum of obtained compound.

Photocatalysis is an attractive property for POMs because of potential applications in decomposition of water contaminants. Methyl Blue, Methylene Blue and Rhodamine 6G, which are typically difficult to decompose in waste water were employed to study the photocatalytic activities of synthesized POM. For the evaluation of catalytic activity, the catalyst was suspended in an aqueous solution of dyes in a Pyrex reactor. Photodegradation reactions of colorants upon 6W lamp irradiation employing POM as the photocatalyst have been examined by UV-Vis spectroscopy. The efficiency of catalyst was calculated by the following formula:

$$\text{Efficiency}(\%) = \frac{(A_0 - A)}{A_0} \cdot 100$$

where A_0 and A referred to the absorbance of the colorant before and after reaction, respectively.

Results obtained in photocatalytic degradation of organic dyes are presented below.

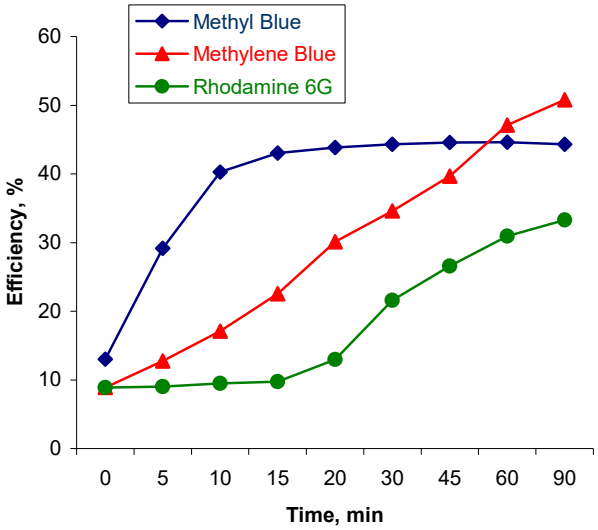

Fig.2. Photocatalytic efficiency of Sm^{3+} - $[W_5O_{18}]^{6-}$.

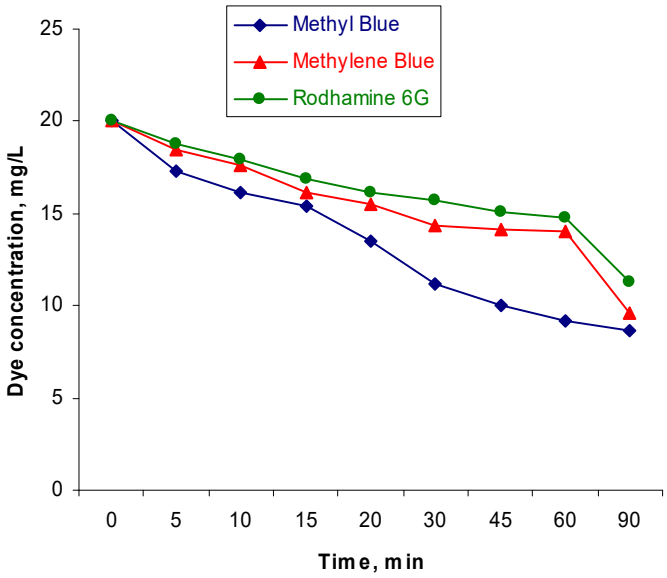

Fig. 3 Variation of dye concentration in photocatalytic degradation.

Theoretical investigations on the electronic properties of the studied compound were performed using Gaussian 09 suite of program and Density Functional Theory (DFT). The PBE0 hybrid density functional (PBE1PBE - the generalized-gradient-approximation exchange-correlation functional of Perdew, Burke, Ernzerhof - in Gaussian) was used as a general method of investigation. For describing the Sm and W atoms, the ECP52MWB 4 52 and ECP60MDF 5 60 Stuttgart-Dresden relativistic effective core potentials and the corresponding basic set have been used. Some results was depicted in figures 4 and 5.