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Titlul proiectului Materiale luminescente cu proprietati de cristale lichide pe baza de compusi organoplatinati(II)

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Cristale lichide - metalomezogeni

Compusi cu proprietati de cristale lichide bazate pe complexi metalici, denumiti in continuare *metalomezogeni*, sunt cunoscuti inca de la începutul secolului al XX-lea, fiind priviti la vremea respectiva mai mult ca pe o curiozitate. Date cu privire la existenta acestora au fost publicate mai mult sporadic pâna în anii '80. Renasterea acestui subiect este atribuita lui Giroud si Mueller-Westerhoff, odata cu publicarea rezultatelor lor in 1977 [1], despre sinteza si proprietatile de cristale lichide ale unor compusi ai Ni(II) cu liganzi de tip ditiolene.

De atunci, acest domeniu s-a dezvoltat uluitor, facand subiectul mai multor carti de specialitate si culminand cu includerea unui capitol special dedicat combinatiilor complexe cu proprietati de cristale lichide in ultima editie *Comprehensive Coordination Chemistry* din 2003 [2] si, de asemenea in editia din 2006 *Comprehensive Organometallic Chemistry* [3].

[1]. A.-M. Giroud, U.T. Mueller-Westerhoff, *Mol. Cryst., Liq. Cryst.*, **1977**, 41, 11.

[2]. B. Donnio, D. Guillon, R. Deschenaux, D.W. Bruce, in *Comprehensive Coordination Chemistry II*; Eds. J.A. McCleverty and T.J. Meyer, Elsevier, Oxford, UK, **2003**, Vol. 7, chapter 7.9, pp. 357-627.

[3]. B. Donnio, D. Guillon, R. Deschenaux, D. W. Bruce in *Comprehensive Organometallic Chemistry III*; Eds. R. H. Crabtree and D. M. P. Mingos, Elsevier, Vol. 12, chapter 12.3, **2006**.

Avantajele includerii ionilor metalici in sistemele cu proprietati de cristale lichide

Atunci cand se introduce un ion metalic intr-un sistem cu proprietati de cristale lichide trebuie avut in vedere o serie de factori ce pot influenta proprietatile sistemului rezultat si

anume: mobilitatea densitatii electronice pe centru metalic, existenta electronilor impari si, desigur, culoarea.

Culoarea – Aceasta este cea mai evidenta dintre proprietatile conferite de complexii metalici. Pentru constructia monitoarelor TV color inca se utilizeaza materiale cristale lichide incolore si filtre pentru obtinerea culorilor dorite.

Polarizabilitate – Este bine cunoscut faptul ca ionii metalici poseda o densitate de electroni polarizabila, iar birefringenta si constantele dielectrice depind de polarizabilitate si chiar a fost demonstrat faptul ca stabilitatea termica a fazelor cristalelor lichide depinde intr-o oarecare masura de polarizabilitate.

Magnetism – Sunt studiate intens sistemele feromagnetice, dar exista putine perspective in utilizarea acestor sisteme pentru a influenta timpul de switching, in mare masura datorita faptului ca spinul poate fi privit ca fiind izotrop in intr-un astfel de sistem.

Rol structural – introducerea ionilor metalici in sistemele organice produce structuri noi prin abilitatea acestora de a adopta geometrii de coordinatie diferite, conducând la obtinerea de proprietati noi ce un sunt caracteristice doar sistemelor simple pur organice

Obiectivele proiectului :

- 1. Prepararea de noi materiale cu proprietati de cristale lichide***
- 2. Caracterizarea structurala a noilor sisteme metalomesogenice***
- 3. Corelarea structurii complexilor metalici cu comportamentul mesomorfic si a proprietatilor luminescente***

Membrii echipei de cercetare:

- 1. Viorel Cîrcu – Director proiect***
- 2. Claudia Maria Simonescu – Lector dr.***
- 3. Monica Victoria Ilis – Asist. Dr.***
- 4. Simona Pasculescu – Doctorand***
- 5. Ionela Neagoe – Asistent cercetare***
- 6. Ana Sorina Mocanu – Asistent cercetare***

Director proiect : Dr. Viorel Cîrcu

Principalele articole publicate :

1. Reactivity of a Rhodium(I) Complex towards oxygen enhanced by a cyano ligand. Structure of $[\text{Rh}(\text{CN})(\text{O}_2)(\text{PPh}_3)_2(\text{XNC})]$ (XNC = xylyl isocyanide) - V. Cîrcu, M. Fernandes, L. Carlton, *Polyhedron*, **2002**, 21, p. 1775.

2. Reaction of bis(phosphine)hydrotris(3,5-dimethylpyrazolyl)borate rhodium(I) complexes with phenylacetylene, p-nitrobenzaldehyde and triphenyltin hydride. Structures of $[\text{Rh}(\text{Tp}^*)(\text{PPh}_3)_2]$, $[\text{Rh}(\text{Tp}^*)(\text{H})(\text{C}_2\text{Ph})\{\text{P}(\text{C}_6\text{H}_4\text{F})_3\}]$, $[\text{Rh}(\text{Tp}^*)(\text{H})(\text{CO}-\text{C}_6\text{H}_4-\text{NO}_2)(\text{PPh}_3)]$ and $[\text{Rh}(\text{Tp}^*)(\text{H})(\text{SnPh}_3)(\text{PPh}_3)]$ - V. Cîrcu, M.A. Fernandes, L. Carlton, *Inorg. Chem.*, **2002**, 41, p. 3859.

3. Reactions of $[\text{Rh}(\text{Tp}^*)(\text{PPh}_3)_2]$ ($\text{Tp}^* = \text{hydrotris}(3,5\text{-dimethylpyrazolyl})\text{borate}$) involving fragmentation or loss of Tp^* . Structures of $[\text{Rh}(\text{H})(\text{Cl})_2(\text{PPh}_3)(\text{pz}^*)]$, $[\text{Rh}_2(\mu\text{-SC}_6\text{F}_5)_2(\text{SC}_6\text{F}_5)(\text{H})(\text{PPh}_3)(\text{pz}^*)]$ and $[\text{Rh}_2(\mu\text{-Hg})(\text{Cl})_4(\text{PPh}_3)_4]$ - V. Cîrcu, M.A. Fernandes, L. Carlton, *Polyhedron*, **2003**, 22, p. 3293.
4. Possible Rod-Disc Transition in *Ortho*-metallated Imine Complexes of Palladium(II). Crystal and Molecular Structure of Three Palladium Complexes, L. Omnès, V. Cîrcu, P. T. Hutchins, S. J. Coles, M. B. Hursthouse and D. W. Bruce, *Liq. Cryst.* **2005**, 32, 1439-49.
5. Orthometallated palladium(II) imine complexes as candidate materials for the biaxial nematic phase. Crystal and molecular structure of three palladium imine complexes, V. Cîrcu, T. J. K. Gibbs, L. Omnes, P. N. Horton, M. B. Hursthouse, D. W. Bruce, *J. Mater. Chem.*, **2006**, 16, 4316.

Conferinte:

1. Liquid crystal properties of ortho-metallated imine complexes of the β -diketonatoplatinum(II) fragment, V. Cîrcu, P.N. Horton, M.B. Hursthouse, D.W. Bruce, ICCS 37, August 13 – 18, 2006, Cape Town, South Africa.
2. Liquid crystalline materials based on N,N'-disubstituted thiurea derivatives (poster), A. Deleanu, M. Ilis, T. Rosu, V. Cîrcu, International Conference of Physical Chemistry – ROMPHYSICHEM – 12, September 6-8 2006, Bucharest, Romania.
3. Ortho-metallated Pd(II) complexes (poster), A. Deleanu, M. Ilis, T. Rosu, V. Cîrcu, ICOSECS 5, International Conference of the Chemical Societies of the South-East European Countries, 10 – 14 Spetember 2006, Ohrid, Macedonia.
4. Orthometallated palladium(II) imine complexes as candidate materials for the biaxial nematic phase, V. Cîrcu, T.J.K. Gibbs, L. Omnes, P.N. Horton, S.J. Coles, M.B. Hursthouse, D.W. Bruce, 10th International Symposium on Metallomesogens, 30 May – 2 June, Cetraro, Italy.
5. Synthesis and liquid crystal properties of ortho-metallated Pd(II) complexes containing N-benzoyl thiourea derivatives, V. Cîrcu, M. Ilis, T. Rosu, P.N. Horton, M.B. Hursthouse, D.W. Bruce, 9th European Conference on Liquid Crystals, July 2-6 2007, Lisbon, Portugal.