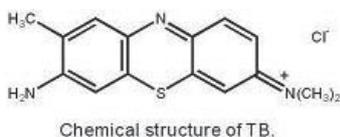


Information Sciences, 79-2, Tokiwadai, Hodogaya-ku, Yokohama, Kanagawa, 240-8501, Japan, ²University of Latvia, Ratsupites 1, LV 1067 Riga, Latvia, ³Rigaku Corporation, 3-9-12, Matsubara-cho, Akishima-shi, Tokyo, 196-0003, Japan, E-mail: d07ta003@ynu.ac.jp

Toluidine blue O (TB), one of popular cationic dyes, has been used in biological and medical fields as a important cytological probe because of its metachromatic effects. Its metachromasy has been considered to be caused by the formation of a certain dye aggregate. It is very important to understand the relationship between the metachromatic spectral change and the aggregates, in order to obtain structural information of biomolecules from metachromatic staining. But regarding TB, structural data of both TB itself and TB - biomolecule complexes have not been reported. We then approached the structure analysis of TB. TB was crystallized as blue needles by means of solvent diffusion method using ion-exchanged water and acetone as good and poor solvents, respectively. However, the thickness of the needles was unsuitable for X-ray structure analysis. On the other hand, thick crystals were obtained after exchanging the chloride ion to hexafluorophosphate ion. Its crystal analysis is now under investigation.



Keywords: crystal structure of organic compounds, dye compounds, molecular biology

V.A., Sivaev I.B., Lobanova I.A., Bregadze V.I., Buravov L.I., Dyachenko O.A., J. Organomet. Chem. 692 (2007) 5033.

Keywords: organic conductors, X-ray analysis, materials properties

P08.14.157

Acta Cryst. (2008). A64, C466

Optical activity of *N*-benzoylglycine crystals

Kentaro Kato, Tomoya Taniguchi, Masanari Otsuka, Hideko Koshima

Ehime University, Department of Material Science and Biotechnology, Graduate School of Science and Engineering, 3, Bunkyo-cho, Matsuyama, Ehime, 790-8577, Japan, E-mail: u843015x@mails.cc.ehime-u.ac.jp

Every chiral organic crystal has inherent optical activity. The sign and the magnitude of the optical activity of an organic crystal should reflect the molecular structure and the packing arrangement because the freedom of molecules is severely restricted in the crystal lattice. We report here the optical rotatory power of chiral crystals self-assembled from achiral *N*-benzoylglycine determined by HAUP (high accuracy universal polarimeter) method. The magnitude of rotatory powers was 10 to 100 times larger than that for ordinary organic crystals. It revealed that the helically arranged aromatic p electrons as well as the helical ionic and hydrogen bond networks in the crystal contributed to the enhancement of the magnitude of these rotations.

Keywords: optical activity, *N*-benzoylglycine, chiral crystal

P08.14.156

Acta Cryst. (2008). A64, C466

Structure of new organic semiconductors with cobalt bis(dicarbollide) bromine anion

Olga Kazheva¹, Grigori Alexandrov², Oleg Dyachenko¹

¹Institute of Problems of Chemical Physics of RAS, 1, Semenov av., Chernogolovka, Moscow Region, 142432, Russia, ²N.S.Kurnakov Institute of General and Inorganic Chemistry of RAS, Moscow, Russia, E-mail: koh@icp.ac.ru

New molecular semiconductors on the base of 8,8'-dibromo cobalt bis(dicarbollide) anion, (BEDT-TTF)₂[8,8'-Br₂-3,3'-Co(1,2-C₂B₉H₁₀)₂] (1), (BEDT-TTF)[8,8'-Br₂-3,3'-Co(1,2-C₂B₉H₁₀)₂] (2) and (BMDT-TTF)₄[8,8'-Br₂-3,3'-Co(1,2-C₂B₉H₁₀)₂] (3) were synthesized and investigated. Recently we have started investigation of the structure-property relationship in a series of fulvalene salts of cobalt bis(dicarbollide) anion and its derivatives [1,2]. These counter anions are particularly interesting owing to their enormous variability. The cobalt bis(dicarbollide) anion [3,3'-Co(1,2-C₂B₉H₁₀)₂]⁻ offers several distinct ways of chemical modification: (1) substitution at carbon atoms; (2) substitution at boron atoms in upper belt of the dicarbollide ligand; and (3) substitution at boron atoms in lower belt of the dicarbollide ligand. As a result, molecules with a wide variety of properties in almost unlimited variations can be prepared. In this contribution, we present synthesis and structure of the first electroconducting salts of the dibromo derivative of cobalt bis(dicarbollide) anion [8,8'-Br₂-3,3'-Co(1,2-C₂B₉H₁₀)₂]⁻. Crystal structure of (BEDT-TTF)₂[8,8'-Br₂-3,3'-Co(1,2-C₂B₉H₁₀)₂] (1) is formed by the BEDT-TTF radical cations in general positions of the unit cell, and the [8,8'-Br₂-3,3'-Co(1,2-C₂B₉H₁₀)₂]⁻ anions in special centrosymmetric positions (Fig.1). Fig. 1. Atomic designations in (BEDT-TTF)₂[8,8'-Br₂-3,3'-Co(1,2-C₂B₉H₁₀)₂] (1)

[1] Kazheva O.N., Chekhlov A.N., Alexandrov G.G., Buravov L.I., Kravchenko A.V., Starodub V.A., Sivaev I.B., Bregadze V.I., Dyachenko O.A., J. Organomet. Chem. 691 (2006) 4225.

[2] Kazheva O.N., Alexandrov G.G., Kravchenko A.V., Starodub

P08.14.158

Acta Cryst. (2008). A64, C466-467

New photoluminescent microporous metal phosphate as a hybrid intrinsic yellow phosphor

Sue-Lein Wang, Yaching Yang

National Tsing Hua University, Chemistry, 101, 2nd Sec. Kuangfu Rd., Hsinchu, Taiwan, 30013, Taiwan, E-mail: slwang@mx.nthu.edu.tw

Photoluminescence is a new property of microporous materials. Recently some extra-large channel zinc and gallium phosphates are found to emit blue light [1-5] or even synchronize dual wavelengths to give out white light under the excitation of UV light [6]. This intriguing optical property has allowed us to discover microporous metal phosphates a new class of inorganic phosphors with distinct emission centers different from conventional understanding. In current lighting technology, yellow light phosphor integrated with blue LED to produce white light is of the most importance. Demands on inorganic yellow-light phosphors are increasing. Yet they are limited in number and kind. Existing inorganic yellow phosphors are all extrinsic illuminants, i.e. a condensed host lattice with doped lighting elements. No inorganic host without doped metal activators could emit yellow light. The extraordinary intrinsic yellow emission of NTHU-4 is speculated to closely correlate with defects resulting from the disorderliness near large pores. In this presentation, we report the synthesis, structure and some property of a new yellow phosphor, NTHU-6 [7], which has a unique MOF-like organic-inorganic hybrid open framework with high PL quantum efficiency (PLQE). It is the first hybrid microporous yellow light phosphor ever discovered.

1. Feng, P. Chem. Comm. 2001, 1668.

2. Liao, Y.C.; Liao, F.L.; Chang, W.K.; Wang, S.L. J. Am. Chem. Soc. 2004, 126, 1320.