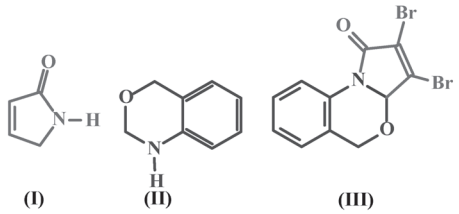
MS43-P15 **2,3-Dibromo-3a*H*,5*H*-4-oxa-9b-aza-cyclopenta[*a*]naphthalene-1-one** Mustafa Odabasoglu[a] & Orhan Büyükgüngör[b] [a]*Pamukkale University, Department of Chemical Technology, 20020, Denizli-Turkey,* [b]*Ondokuz Mayis University, Department of Physics, 55139, Samsun-Turkey*
E-mail: mustafaodabasoglu@gmail.com

1*H*-pyrrol-2(5*H*)-one (I) and 2,4-dihydro-1*H*-benzo[*d*][1,3] oxazine (II) units are commonly present in synthetic and natural products as simple structures or as a part of complex systems. A search of the literature revealed that some 1*H*-pyrrol-2(5*H*)-one derivatives have important effective the central nervous system (CNS), therefore 8a-phenyl-tetrahydro-2*H*-pyrrolo[2,1-*b*][1,3]oxazin-6(7*H*)-one to be used such as anti-depressants over the past 30 [1]. Some 1,3-benzoxazine derivatives have anti-HIV [2], anti-viral [3], anti-bacterial [4],, anti-malarial [5] activities and some of them uses as dopamin and seratonin receptor [6]. It was assumed that compounds having both 1*H*-pyrrol-2(5*H*)-one and 1,3-benzoxazine residues in the same molecule may possess some interesting biological activities. With this in mind, the synthesis and structure determination of the title compounds (III) were undertaken.



(I) (II) (III)

The crystal structure of the (III) exhibit C-H…O, C-H…Br and C-Br…O interactions generating an edge-fused $R_6^6(31)$ ring motif [7]. There are two symmetry-independent molecules in the asymmetric unit. The dihedral angle between the pyrrol-2-one and aromatic rings in (III) are 26.5(2)° and 22.1(2)°.

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[5] Ren, H., *et al.,* (2001). *Bioorg. Med. Chem. Lett.* 2001, 11, 1851–1854.
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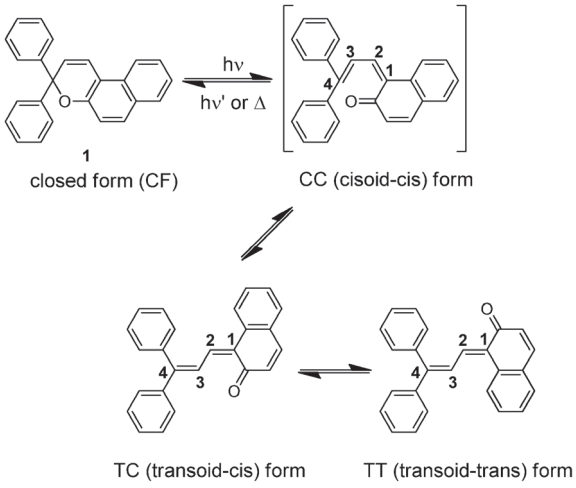
[7] Etter, M. C. (1990). *Acc. Chem. Res.* 23, 120–126.

Keywords: Pyrrol-2-one, and 1,3-benzoxazine, X-Ray Analysis.

MS43-P16 **Solid-State Photochromism of Chromenes.** Keiichiro Ogawa, KeigoUeki, Jun Harada[a] *The University of Tokyo, Japan.* [a]*Hokkaido University, Japan.*
E-mail: Keiichiro.Ogawa@post.c.u-tokyo.ac.jp

Solid-state photochromism of benzopyrans and naphthopyrans, which are often generically referred to as chromenes, has been studied extensively. The mechanism of the photochromism has been investigated almost exclusively for the reactions in solution and proposed to proceed through the following mechanism (Scheme I): Upon UV irradiation of colorless closed form (CF), cleavage of the C(sp^3)-O bond of the pyran ring takes place to yield a metastable ring-opened species referred to as CC form. The CC form undergoes rotation about the C2-C3 bond to give stable photoproducts, TC and TT forms. Solid-state photochromism of chromenes, however, has been reported only in a few papers and the mechanism of the reactionsremains unexplored.



Scheme 1

We have investigated solid-state photochromism of chromenes in the temperature range between 300 and 80 K [1]. Variable-temperature diffuse reflectance spectroscopy of microcrystalline powders showed that the extent of photocoloration was greatly enhanced at low temperatures. All the chromenes examined exhibited solid-state photochromism at low temperature, even when they showed little or no photocoloration at room temperature. The solid-state photochromic properties of the chromenes were quite similar to those reported for analogous photochromic compounds of spiropyrans and spirooxazines [2], which indicates that these classes of compounds are generally photochromic even in the solid state. In addition to two stable planar merocyanine forms, which are usually observed in the photochromic reactions in solution, photoreactions at low temperatures allowed us to observe unstable colored species, which were tentatively assigned as nonplanar CC forms, and were stabilized in the solid state at low temperatures.

[1] Harada, J., Ueki, K.,Anada, M., Kawazoe, Y., Ogawa, K.(2011) . *Chem. Eur. J.*,**17**, 14111-14119.[2] Harada, J., Kawazoe, Y., Ogawa, K. (2010). *Chem. Commun.,***46**, 2593-2595.

Keywords: photochromism; solid-state reactions;solid-state spectroscopy