National University, Canberra, ACT, Australia.
E-mail: echanj@rsc.anu.edu.au

The drug benzocaine (ethyl-4-aminobenzoate), commonly used as a local anesthetic, is a bimorphic solid at room temperature. Form(I) is monoclinic $P2_1/c$ [1]. The metastable form(II) is orthorhombic $P2_12_12_1$ [2]. We describe the study and comparison of the thermal diffuse scattering (TDS) observed in both room temperature forms. Three dimensional diffuse X-ray scattering data was collected on the 11-ID-B beamline at the Advanced Photon Source (APS). In both forms broad diffuse streaks are observed in the 0kl section which indicate a strong correlation between molecules in the [0 3 1] direction. Streaks extending between Bragg peaks in the hk0 section normal to [1 0 0] correspond to correlated motions between in-plane linked N-H...O=C hydrogen bonded ribbon pairs. Subsequent interrogation and comparison of models developed using Monte Carlo simulations for both forms provide details of the local structure and relative magnitudes of intermolecular interactions between the ribbon pair layers. The work is part of preliminary results which demonstrate how X-ray diffuse scattering studies of polymorphic compounds contain information about dynamic structure-related phenomena e.g. temperature controlled phase transitions.

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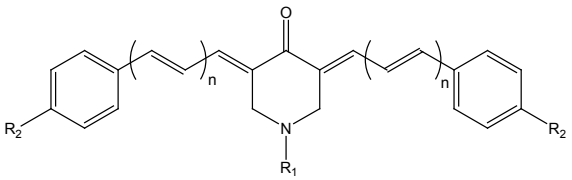
Structure and Spectroscopy of Potential Drugs for Photodynamic Therapy. Tatiana V. Timofeeva[a], Tiffany L. Kinnibrugh[a], Kurt W. Short[a], Michael V. Makarov[b], Irina L. Odinets[b], Mikhail Yu. Antipin[a,b]. *[a]New Mexico Highlands University, Las Vegas, NM, USA. [b]Institute of Organoelement compounds, Moscow, Russia.*
E-mail: tvtimofeeva@nmhu.edu

Photodynamic therapy (PDT) is a treatment that uses specific drugs, called photosensitizers, which with exposure to a specific wavelength of light produce a form of oxygen that kills harmful cells. At present, in clinical applications several drugs that are porphyrin derivatives are used. Their mechanism of action is related to a one-photon excitation process, in which relaxation of an exited state in the presence of molecular oxygen produces singlet oxygen ($^1O_2$) or superoxide (O_2^-) that induces cell damage. Recent approachs to PDT include so-called two-photon photosensitizers, that have the same mechanism of action but are excited with lower energy light (less harmful for healthy tissues). These non-absorbed longer wavelengths penetrate under the skin to a depth of up to 5-7 cm in the tumor location. We are



presenting structural and spectroscopic characteristics of about twenty new arylidenepiperidones with the structural formula Donor – π-Bridge – Acceptor – π-Bridge – Donor, that is standard for two-photon absorbing materials. Variation of substituents at the N atom (R_1) was used to improve water-solubility of the photosensitizers, and as donors (R_2) we used NMe_2 and NEt_2 groups. Increased length of the pi-conjugated bridge results in higher two-photon cross sections, that correspond to predictions from quantum-chemical computations [1]. Also, there is a better ratio between dark and phototoxicity. Consequantly, materials with a longer chain of conjugation are more valuable candidates for future bioassay. Intrinsic fluorescence of the presented materials makes them even more attractive for further testing, since their imaging can be done without additional modifications of their structure.

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