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Charge Density and Optical Properties of Multicomponent Crystals Containing APIs

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Technological progress forces improved material performance therefore controlling synthesis of new crystal phases requires moving from the trial-and-error method to comprehensive solutions. Active Pharmaceutical Ingredients (API) are of particular interest in crystal engineering [1]. Molecular flexibility reflected in many polymorphic forms and appropriate spatial distribution of hydrogen bond donors and acceptors make many known drugs useful for designing optically active materials [2]. The effective correlation between properties and structural features of a given material is possible through quantitative crystal engineering combined with in silico crystal engineering. Quantitative crystal engineering utilizes modern charge density analysis and properties calculations, whereas in silico crystal engineering assesses synthon formation capability probing weak interactions existing within the crystal phases. Optical properties of a crystal strongly depend upon spatial distribution of molecules in the crystal structure, as well as on the electronic properties of molecular building blocks (dipole moments, polarizabilities, hyperpolarizabilities)[3]. Recently we have investigated materials based on pharmaceutically active ingredients: barbiturates, antiarrhythmic drugs, alkaloids, combined with organic molecules and/or transition metal salts. Partial results of our research have already been published [2]. Factors that contribute to molecular recognition in the selected polar/chiral crystal phases (derived through charge densityand Hirshfeld Surfaces Analysis) have been determined. The predicted values of refractive indices were confirmed experimentally using the immersion oil method. Second Harmonic Generation efficiency was assessed using a modified Kurtz-Perry technique [2].

[1] *Brittain, Cryst. Growth Des., 2012, 12 (11), 5823–5832.,* ***[2]*** *M. Gryl, M. Kozieł M, K. Stadnicka et al., CrystEngComm, 2013, 15, 3275; M. Gryl, T. Seidler, K. Stadnicka, et al., CrystEngComm, 2014, DOI: 10.1039/C4CE00178H.,* ***[3]*** *J. M. Cole. Royal Soc. Phil. Trans. A 361 (2003) 2751-2770.*

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