building blocks. Barbituric acid molecule seems to be a valuable component in designing of new materials possesing prospective properties i.e NLO properties [1,2,3]. Organic materials modified with inorganic components are interesting from the viewpoint of their outstanding properties as NLO materials i.e. high SHG responce, appropriate mechanical and optical resistance. Recently we have discovered the usage of barbituric acid and selected inorganic metal salts to form polar structures such as cadmium barbiturate dihydrate (Iba2) or copper barbiturate trihydrate (Fdd2) [4]. Moreover we have obtained centrosymmetric structure of silver barbiturate hydrate (P2(1)/m), which can be further modified to obtain the polar structure. For those three structures experimental charge density study and its topological properties were analyzed using XD2006 package [5]. The studies revealed different topological features for the three oxygen atoms of the barbituric acid. Molecular recognition and the formation of specific hydrgen patterns in all of the examined structures seems to have origin in the resonance structures of the barbituric acid molecule.

[1] Kondo K., Fukutome N., Ohnishi, N., Aso H., (1991), J. J. Appl. Phys. 30: 3419. [2] Kondo K., Ochiai S., Takemoto K., Irie M., (1990), Appl. Phys. Lett. 56(8): 718. [3] Gryl, M.; Krawczuk, A.; Stadnicka, K.;(2008), Acta Cryst. B64, , 623. [4] Ya Xiong, Chun He, Tai-Cheng An, Chang-Hong Cha, Xi-Hai Zhu, Trans. Metal Chem. 28 (2003) 69. [5] Volkov T., Macchi P., Farrugia L.J., Gatti C., Mallinson P., Richter T., Koritsanszky T. (2006). XD 2006: A Computer Program Package for Multipole Refinement, Topological Analysis of Charge Densities and Evaluation of Intermolecular Energies from Experimental and Theoretical Structure Factors.

Keywords: crystal engineering, experimental charge densities, nonlinear optics

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Anharmonic Nuclear Motion in Charge Density Studies. Regine Herbst-Irmer, Julian Henn, Kathrin Meindl. *Institute of Inorganic Chemistry, University of Göttingen, Germany*
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In some of our recent charge density studies we had severe problems in appropriately refining the model to a flat and featureless residual density. In 9-diphenylthiophosphinoyl-anthracene unreasonable high residual density peaks remained close to the sulfur atoms [1]. These peaks disappeared only when Gram-Charlier anharmonic coefficients were introduced. Data sets at 15 K, 100 K and room temperature were collected. For all temperatures a typical shashlik-like residual density pattern could be found [2]. Although the room temperature data set was not of the quality and resolution sufficient for a multipole refinement, this pattern was also present and could be removed by refining anharmonic Gram-Charlier-coefficients. This was observed with a spherical-atom as well as with an invariom refinement [3, 4]. However, the drop in the R-value was only small.
There are two independent molecules in the asymmetric unit that differ in their amount of vibration but have similar geometrical parameters. Therefore, also the anharmonic motion differs.
Calculations with theoretical data showed that the amount of noise and thus the quality of data seems to be important for the detection and successful refinement of anharmonic motion [2]. The dependence of temperature, resolution, data quality and vibration on the Gram-Charlier coefficients will be presented. The correlation with further parameters of a multipole refinement will be discussed.

[1] Herbst-Irmer R., Henn J., Kratzert D., Stern D., Stalke D., *Acta Crystallogr.* 2009, A65, s109. [2] Meindl K., Herbst-Irmer R., Henn J., *Acta Crystallogr.* 2010, A66, in press. [3] Volkov A., Macchi P., Farrugia L.J., Gatti C., Mallinson P.R., Richter T., Koritsanszky T., *XD2006* (2006). [4] Dittrich B., Koritsanszky T., Luger P., *Angew. Chem. Int. Ed.* 2003, 43, 314.

Keywords: charge density, anharmonic refinement, residual electron density

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Chemical Experimental Charge Density Study of γ–B_{28}. Swastik Mondal[a], Sander van Smaalen[a], Andreas Schönleber[a], Yaroslav Filinchuk[b], Dmitry Chernyshov[b], Evgeniya Yu. Zarechnaya[c], Leonid Dubrovinsky[c], Natalia Dubrovinskaia[d,a] , [a] *Laboratory of Crystallography, University of Bayreuth, Germany,* [b]*Swiss-Norwegian Beam line, ESRF, Grenoble, France,* [c]*Bayerisches Geoinstitut, University of Bayreuth, Germany,* [d]*Mineralphysics, Institute of Earth Sciences, University of Heidelberg, Germany*
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The latest discovery of γ–B_{28}, a superhard, high-pressure form of boron [1,2] has attracted much attention due to unique properties of this material. The present electron density study of γ–B_{28} has been undertaken in order to extract experimental information about peculiarities of chemical bonding in γ–B_{28}. The study has been carried out using low-temperature, high-resolution, single-crystal synchrotron X-ray diffraction data. Electron densities of γ–B_{28} have been obtained by the multipole refinement using the computer program *XD2006* [3], and by the maximum entropy method (MEM) using the computer program *BayMEM* [4]. Experimental charge densities have been analyzed with the aid of Bader's *Atoms in Molecule* (AIM) theory [5]. Quantitative interpretation of the electron density using Bader analysis reveals the polar-ovalent nature of chemical bonding in γ–B_{28}. Detailed analysis of the charge transfer is provided.

[1] Zarechnaya, E. Yu.; Dubrovinsky, L.; Dubrovinskaia, N.; Filinchuk, Y.; Chernyshov, D.; Dmitriev, V.; Miyajima, N.; El Goresy, A.; Braun, H. F.; Van Smaalen, S.; Kantor, I.; Kantor, A.; Prakapenka, V.; Hanfland, M.; Mikhaylushkin, A. S.; Abrikosov, I. A.; Simak, S. I. *Phys. Rev. Lett.* 2009, 102, 185501. [2] Oganov, A. R.; Chen, J. H.; Gatti, C.; Ma, Y. Z.; Ma, Y. M.; Glass, C. W.; Liu, Z. X.; Yu, T.; Kurakevych, O. O.; Solozhenko, V. L. *Nature* 2009, 457, 863; Addendum: *Nature* 2009, 460, 292. [3] Volkov, A.; Macchi, P.; Farrugia, L. J.; Gatti, C.; Mallinson, P. R.; Richter, T.; Koritsanszky, T. *XD2006*, 2006. [4] van Smaalen, S.; Palatinus, L.; Schneider, M. *Acta Crystallogr.* 2003, A59, 459. [5] Bader, R. F. W. *Atoms in Molecules*, Oxford University Press, 1990.

Keywords: boron, charge density, X-ray diffraction

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Direct visualization of disordered polymer chain structure in polyoxymethylene crystal by MEM. Kunihisa Sugimoto[a], Sono Sasaki[b], Kohji Tashiro[c], Yoshie Nakamura[d], Masaki Takata[d,e], [a]*JASRI/SPring-8, Hyougo, 679-5198 Japan,* [b] *Kyoto Institute of*