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The electron density of isoindole derivatives from synchrotron diffraction data. Lilianna Chęcińska^a, Magdalena Malecka^a, Agnieszka Rybarczyk-Pirek^a, Carsten Paulmann^{b,c}, Simon Grabowsky^d, Peter Luger^d
^aDepartment of Crystallography and Crystal Chemistry University of Łódź, Tamka 12, 91-403 Łódź, Poland, ^bc/o DESY/HASYLAB, Notkestr. 85, D-22603 Hamburg, Germany, ^cMineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany, ^dInstitut für Chemie und Biochemie/ Kristallographie, Freie Universität Berlin, Fabeckstr. 36a, D-14195 Berlin, Germany
 E-mail: lilach@uni.lodz.pl

The isoindolin-1-ones are the important structural units found in natural products, biologically active substances and synthetic intermediates [1], [2]. Here, the electron density of two isoindole derivatives is considered: 3-hydroxy-2-phenyl-2,3-dihydro-isoindol-1-one (I) and 5-hydroxy-6-phenyl-5,6-dihydro-pyrrolo[3,4-*b*]pyridin-7-one (II).

The high-resolution synchrotron-diffraction data sets were collected at beamline F1 at Hasylab/DESY (Hamburg, Germany). The *XDS* [3] was used for an integration of frames and data reduction. Initial spherical refinements were performed with *SHELXL97* [4] providing starting values for subsequent aspherical-atom least-squares refinements with *XDLSM* of *XD2006* program package [5].

Two analyzed molecular structures of I/II consist of isoindol-1-one/aza-isoindol-1-one moiety substituted by phenyl and hydroxyl groups at position 2 and 3, respectively. The geometry of the investigated molecules is similar but not

identical, but their arrangement in the crystal structures is different.

In I, the molecules are linked by intermolecular hydrogen bond O-H...O ($\frac{1}{2}-x, \frac{1}{2}+y, z$) forming an infinite chain along [010] direction. In the aza-isoindole derivative (II) additional nitrogen atom is an accepting centre of hydrogen bonding, instead of oxygen atom, and O-H...N ($x, \frac{1}{2}-y, \frac{1}{2}+z$) is observed. This interaction generates an infinite chain along [001] direction.

The qualitative and quantitative analysis of the electron density distribution within isoindole moieties and hydrogen bonding areas will be presented in the poster.

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Keywords: structure and charge-density analysis, synchrotron X-ray diffraction, isoindole derivatives

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Mismatched interactions in bis(phenolato) metal complexes Thomas S. Dols^{a,b}, Thomas P. Spaniol^a, Jun Okuda^a, Christian W. Lehmann^b, ^aInstitut für anorganische Chemie, RWTH Aachen University, Germany, ^bMPI für Kohlenforschung, Mülheim, Germany
 E-mail: thomas.dols@ac.rwth-aachen.de

Three-dimensional crystal structures have become an indispensable tool in modern catalyst research. To improve the product properties, the structural changes of homogeneous catalysts and their precatalysts are correlated with their impact on polymerization. We are investigating transition metal complexes with bridged bisphenolato ligands that are used in olefin-polymerization. The molecular structure of the ligand has a strong influence on the stereochemistry of the resulting polymer[1,2]. For this reason, the bis(phenolate) ligands have been tuned by different substituents on the aromatic rings as well as by modifying the bridging unit. S atoms as part of the bridge can improve the catalytic activity, obviously as a result of hemilabile interactions between the soft donor S atom and the hard metal center [3].

In several S-C-C-S-bridged bis(phenolato)titanium complexes, the M...S interactions lead to a stereorigid O,S,S,O-tetradentate coordination in solution [4]. Such a system has made it possible to polymerize styrene in homogeneous phase to give isotactic polystyrene for the first time [1]. The results prove the high conformational stability of the metal complexes under the conditions of polymerization.

The focus of our investigations is on metal complexes where, according to the HSAB principle, the hard metal centers are interacting with the sulfur atom of the bisphenolato ligand. It