Poster Presentations

[MS10-P01] Structures and Properties of Benzimidazole Derivatives from Invariom Modelling. Akmal Tojiboev[a], Birger Dittrich[b], Nasirkhon Mukhamedov[c], Kudaybergen Abdireymov[c].

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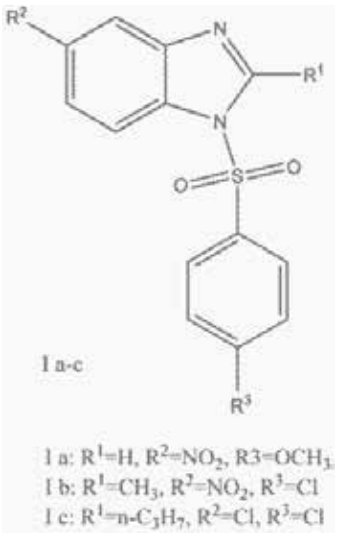
Biological activity of a wide range of derivatives of benzimidazole like e.g. the anti-ulcer drug omeprazole gave rise to lasting interest in this class of compounds. [1-5] Our continuing research on synthesis and reactions of benzimidazole derivatives led to investigations in arylsulfonation of 5 - (chloro, nitro, methyl)-2-alkylbenzimidazoles. To further investigate the nature of chemical bonds and of intermolecular interactions in these derivatives [6] we had carried out single-crystal X-ray structure determinations in the past. We have recently added several new crystal structures determinations of benzimidazole derivatives. A classical charge density study on a whole series of derivatives of benzimidazole is not possible because large single crystals are often hard to grow for these molecules. Furthermore, the presence of disorder in one or several of a series of related compounds prohibits a complete comparative charge density study: often only one out of several compounds is really suitable for a high-resolution experiment. Therefore we have chosen to evaluate a series of single-crystal diffraction experiments carried out on a home source and at the SLS synchrotron to normal resolution (sin θ/λ around 0.6 $Å^{-1}$) by invariom modeling instead [7,8]. Invariom modeling takes into account the asphericity of the electron density distribution in the scattering factor, and it allows obtaining a more accurate structure from the diffraction data than refinements with the independent atom model. Structural properties of molecules can also be derived, even in the presence of disorder. Structural data now also allows us a more complete representation of the most common patterns of their intra- and intermolecular interactions.



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