[1] Kolb, U., Gorelik, T., Kübel, C., Otten, M.T. and Hubert, D. *Ultramicroscopy* **2007**, 107, 507. [2] Kolb, U., Gorelik, T. and Otten, M.T. *Ultramicroscopy* **2008**, 108, 763. [3] Mugnaioli, E., Gorelik, T. and Kolb, U. *Ultramicroscopy* **2009**, 109, 758. [4] Nikishova, L.V., Lazebnik, K.A. and Lazebnik, Yu.D. In *Crystalchemistry and Structure of Minerals*. Leningrad Ed. Nauka, **1975**, p. 100-105. [5] Rozhdestvenskaya, I.V., Kogure, T. and Drits, V.A. Abstracts of Meeting "Crystal chemistry and X-ray diffraction of Minerals", Miass **2007**, p. 48-49.

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***"Ab initio"* Structure Solution of Organic Materials from Electron Diffraction to Mography Data.**

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Electron diffraction has been always an attractive method to solve crystal structures, firstly because of its fine lateral resolution (the method can easily probe volumes down to several tenth of nanometers, thus making nano phases as well as agglomerated materials assessable), secondly electrons have different scattering factors than X-rays, which allow to "see" relatively light elements in the presence of heavy atoms.
One of the major complications in the electron diffraction data processing is the presence of dynamical effects, which severely modify the data, and hamper structure determination. These difficulties are not so strong for organic materials, which typically diffract in "quasi-kinematical" manner.
Although use of electron diffraction data for structure solution of organic materials promises obvious benefits, it has been rarely used in the past [1, 2]. Recently a new method of collecting and processing of electron diffraction data was developed (ADT) [3, 4]. Practically the method allows sampling of up to 2/3 of reciprocal space from a single nano crystal. This data is powerful enough to give a solution of the structure directly from the raw data. Several organic structures of difference classes of compounds were solved from the ADT data "ab initio" using SIR08 [5].

[1] Kolb, U., and G.N. Matveeva, Z. Krist. spezial issue: *Electron crystallography,* 218 (4), 259-268, **2003**. [2] Dorset, D. L., McCourt, M. P., Li Gao, Voigt-Martin I. G., J. Appl. Cryst., 31 (4), 544-553, **1998**. [3] Kolb, U.., Gorelik, T., Kübel, C., Otten, M.T. and Hubert, D., *Ultramicroscopy,* **2007**, 107, 507. [4] Kolb, U., Gorelik, T. and Otten, M.T., *Ultramicroscopy,* **2008**, 108, 763. [5] Burla, M.C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G.L., De Caro, L. Giacovazzo, C., Polidorim, G. and Spagna, R. *J. Appl. Cryst.,* **2005**, 38, 381.