Energy ranking results for 15 organic molecules are presented, including ethane, ethylene, acetylene, methanol, urea, acetic acid, cyclohexane-1,4-dione, paracetamol, CCDC blind test molecules I-VI and a pharmaceutical compound for which crystal structures have been predicted in a blind test fashion. In 14 out of 15 cases, the experimental crystal structure is found among the two most stable predicted crystal structures. The planned implementation of a free energy correction is expected to improve the success rate even further.
All calculations have been carried out with the development version of a novel software package, GRACE (Generation, Ranking And Characterization Engine), which uses VASP as an external component.

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MS14 O4

Stationary state equilibrium conditions for the electron density distribution Julian Henn, *Department of Inorganic Chemistry, University of Göttingen, 37077 Göttingen, Germany* **.** E-mail: julianhenn@web.de

Keywords: mem, multipole refinement, accuracy

Stationary state equilibrium conditions describing the electron density distribution in equilibrium (not necessarily the ground state) as derived from Levy and Perdew [1] *via* the Hellmann-Feynman theorem [2] may be employed to put the experimental electron density reconstruction process on a self-consistency scheme. This should increase the accuracy in present day multipole refinements [3] and maximum entropy methods [4].

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MS14 O5

Refinement of a one electron density matrix from Compton and Bragg pseudo data : the diatomic molecule case J.-M. Gillet, *Ecole Centrale Paris, laboratoire SPMS UMR8580, Grande Voie des Vignes, 92295 Chatenay-Malabry,France.*
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High resolution x-ray diffraction, convergent beam electron diffraction, deep inelastic x-ray scattering (Compton scattering), e-2e and γ-e-γ spectroscopies are all directly related to the One-electron Reduced Density Matrix (1-RDM [1] On the other hand, it is well known [2][3] that the 1-RDM contains all the information about the electronic structure available at the one-electron level. Unfortunately, and to our best knowledge, few attempts for refining 1-RDM models have been carried out [3]-[6]. With the exceptions of Schmider [7][8] for atomic systems, and Schulke and co-workers [9]} only x-ray diffraction data were employed as experimental references.
The purpose of this talk is to discuss to what extent the successfull decomposition of the electron density into aspherical pseudo-atomic contributions [10] can be adapted to the 1-RDM case. Furthermore, we intend to show that, with such a model, the complementarities between very different experiments can be better exploited through a joint refinement.
Emphasis will be put on the difficulties which are specific to a joint refinement of 1-matrices from different experimental data as opposed to usual "mono-experimental" refinements..

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