MS14 P01

Problem Structures: Attempts to Rationalize their Description and Refinement A. David Rae, *Research School of Chemistry, the Australian National University, Canberra, ACT 0200, Australia.*
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Keywords: Refinement, problem structures, twin-disorder.

The author is completing an update to his program *RAELS* prior to general release. The program's concept includes using multiple components to describe an intensity, the combination of which is determined by modeling and refinement. Each component specifies a selection of cell, atoms, symmetry elements and reflection indices. Component reflections may partially overlap. This allows a most general description of twin-disorder, including stacking faults that combine different orientations and origins of a prototype (ideally ordered) structure. It also allows the coexistence of polymorphic structures that interchange across a commensurate surface. Reflections can be monitored according to user set index conditions $\mathbf{h} = \mathbf{g} + m\mathbf{q}$ where m is associated with particular symmetrized components. Often structures can be described as a modulation of a parent structure of higher symmetry that corresponds to parent reflections **g**, allowing the identification of a twin-disorder mechanisms involving pseudo symmetry at an interface. Symmetrized components of the scattering density may be constructed and correspond to particular combinations of pseudo equivalent reflections. This identifies minor components of the scattering density and possible false minima since each component may be separately scaled and has its own systematic absences, global phase and content. Sensible constraint-restraint procedures should restrict minor components. Solved structures will be presented detailing relevant concepts.

MS14 P02

One electron Reduced Density matrix of a urea under electric field Pierre Boquel, Dario Sangiovani, Jean-Michel Gillet *Ecole Centrale Paris, Laboratoire SPMS UMR CNRS 8580, Grande Voie des Vignes, 92295 Chatenay-Malabry France.* E-mail: jean-michel.gillet@ecp.fr

Keywords: Density Matrix-, polarization, electric field

The one electron reduced density matrix (1-RDM) is a handy quantity that can often be substituted to the N-electron wavefunction when it comes to the computation of one electron properties. Moreover, the 1-RDM is intimately connected to x-rays scattering experiments since its diagonal elements (the charge density) can be recovered from a large set of the structure factors and the off-diagonal elements are linked to the auto-correlation function or the so-called directional Compton profiles (DCP).
The purpose of this poster is to give some preliminary results concerning the changes over the density matrix when a molecule is excited by a static electric field. Rough solid state effects can also be observed since a trimere of urea was also computed.
Charge transfers, atomic polarization as well as changes in the characters of the chemical bonds are displayed with emphasis on the off-diagonal contributions to the 1-RDM. Separations between π and σ electronic behaviors are tentatively made.

MS14 P03

Processing and Scaling Algorithms for Small Molecules, Macromolecules and Twins. Ina Dix[a*], Madhumati Sevvana[b], Regine Herbst-Irmer[a], George M. Sheldrick[a], [a]*Department of Structural Chemistry, University of Göttingen, Tammannstr. 4, 37077 Göttingen, Germany.* [b]*Department of Biotechnique, University of Erlangen-Nürnberg, IZMP, Henkestr. 91, 91052 Erlangen, Germany.* E-mail: inadix@shelx.uni-ac.gwdg.de

Keywords: twinning, scaling, data processing.

Non-merohedral twinning is one of the challenging problems in data collection and data processing characterised by a not exact overlap of the reciprocal lattices of the different domains. Over the last years, processing X-ray data of non-merohedrally twinned small molecule crystals became more or less routine. We have applied theses methods in macro-molecule crystallography in order to solve twinned protein structures using Single Wavelength Anomalous Dispersion (SAD) and then refine them.
After data integration using all orientation matrices simultaneously, resulting in a raw data file containing overlapping and non-overlapping reflections, one key step in data analysis is the scaling of this multi-component raw file [1], [2]. The program TWINABS is able to do the scaling and absorption correction of theses raw files producing two kinds of HKL formats: detwinned HKLF4 format used for structure solution and HKLF5 format distinguishing between overlapping and non-overlapping reflections [3].
A new algorithm is used in TWINABS to create the merged HKLF4 format file of unique reflections. Each measured intensity of single and overlapping reflections is treated as an observational equation, and this over determined system of equations is solved for the unique reflection intensities and twins ratios. For this purpose, but not for scaling, it is essential that the different twin components are consistently indexed.

[1] Bruker, *SAINT*, Bruker AXS Inc. Madison (2001).
[2] A. J. M. Duisenberg, L- M. J. Kroon-Batenburg, A. M. M. Schreurs, *J Appl. Crystallogr.* ,2003, 36, 220-229.
[3] G. M. Sheldrick, *TWINABS*, University of Göttingen (2002).

MS14 P04

The Structure of different phases for solid Uranium Hexafluoride, S .M. El-Sheikh, *Department of Physics, American University in Cairo, Egypt*.
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Keywords: structure transitions, accurate phase determination , molecular dynamics simulations.

The constant temperature constant pressure (T, P, N) molecular dynamics technique is applied to UF_6 to investigate its properties in its condensed phases, using an intermolecular potential model includes dispersion, characteristic, and induction terms. A numerical value of the melting temperature at high pressure as well as pressures at phase transitions was estimated . The structure of these phases was identified.