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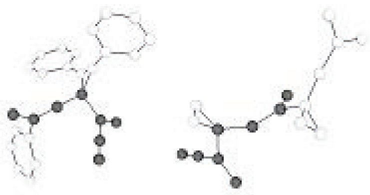
A Further Improved Structure Matching Algorithm. N. David Brown[a], James Haestier[a], Mustapha Sadki[a], Amber L. Thompson[a], David J. Watkin[a]. [a]*Chemical Crystallography, Inorganic Chemistry Department, University of Oxford.*
E-mail: dave.brown@chem.ox.ac.uk

Since publication of the classic Ullmann algorithm for subgraph isomorphism [1], a variety of works have successfully augmented the algorithm's behaviour for graph matching, such as that presented by Cordella *et al*. [2]. Their paper describes a generic implementation of Ullmann with emphasis on an efficient implementation utilising linear data arrays rather than the matrices Ullmann originally specified.

As part of "Age Concern", a joint project between the crystallography laboratories in Durham and Oxford, funded by the EPSRC (grant EP/C536282/1), Oxford team members have developed an improved version of the Cordella algorithm, to be used for chemical structure matching. We explore the problem by considering graph and chemical theory in parallel, and allowing tailoring of the algorithm's behaviour to perform structure matching bespoke to any context via parameters specified prior to execution.



The state tree for any chemical structure matching algorithm is a search space of all possible atom-to-atom mappings between two input structures. Through parameterisation of our algorithm, we are able to winnow choices at every stage of our state search and maximise pruning of the state tree, as much as is possible for any given chemical context, according to the knowledge of the user. Pre-specified similarity conditions for both individual atoms as well as atom environments can be considered during matching, allowing 'chemically similar' fragments and molecules to be rapidly identified, as well as those which are 'structurally similar'. We provide distinct definitions of 'graph isomorphism' and 'chemical isomorphism' to clarify our proposal.

Additionally, by leveraging the arbitrary mapping of certain single-degree atoms within any input chemical structure, we are able to further improve the efficiency of the original graph matching algorithm [2]. A working demonstration of the algorithm will be available at the poster presentation.

[1]J.R. Ullmann, **1976**. *Journal of the Association for Computing Machinery*, 23, 31-42 . [2] L.P. Cordella, P. Foggia, C. Sansone, M. Vento, **2004**. *IEEE Trans. On Patt. Anal. & Mach. Intell.*, 26, 10, 1367-1372.

Keywords: crystallographic analysis; computing methods in crystallography; structural similarity

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OLEX2 News. Oleg V. Dolomanov[a], Luc J. Bourhis[a], Richard J. Gildea[a], Judith A. K. Howard[a], Horst Puschmann[a]. [a]*Department of Chemistry, Durham University, Durham, DH1 3LE, UK.*
E-mail: oleg.dolomanov@durham.ac.uk

OLEX2 is a portable open-source program for structure analysis and visualisation which provides a workflow driven user interface to manipulate crystal structures [1]. The workflow seamlessly links all aspects of the structure solution, refinement and publication process. Numerous built in functions, such as space group determination, void calculation, hydrogen atoms placement, electron density maps and structure alignment help the user with the structure solution, refinement and analysis. Our current work on the small molecule toolbox smtbx [2] and its integration with OLEX2 provides new potential for the development of small molecule refinement software. This poster presents new developments on the interface and structure analysis sides which have taken place since previous presentations at IUCr conferences.

[1] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard and H. Puschmann **2009**. *J. Appl. Cryst.*, 42, 339-341. [2] L.J. Bourhis, R.W. Grosse-Kuntsleve, P.D. Adams **2007**. *IUCr Commission on Crystallographic Computing Newsletter*,8, 74-80.

Keywords: structure analysis; structure visualisation; open-source

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Harnessing the Power of the CCTBX with OLEX2. Richard Gildea[a], Luc Bourhis[a], Oleg Dolomanov[a], Judith Howard[a], Horst Puschmann[a]. [a]*Department of Chemistry, Durham University, UK.*
E-mail: r.j.gildea@durham.ac.uk

The Computational Crystallography Toolbox (cctbx) [1] is an open-source portable library of reusable crystallographic algorithms. Whilst much of the current development of the cctbx is driven towards macromolecular crystallography, the core of the cctbx is completely general to all aspects of crystallography.

As a part of the cctbx, we are developing the small molecule toolbox (smtbx) module [2], which contains algorithms specifically for small molecule work. The algorithms developed within the smtbx will be made accessible through the OLEX2 software [3]. Currently available are a charge-flipping structure solution routine [4], and a refinement routine using an LBFGS minimiser [5].

Recent development involves the implementation of restraints and constraints specific to small-molecule work in the refinement module, and final structure report generation. Currently we use OLEX2 as the main interface to formulate the restraints and constraints and all other aspects of the refinement model, however, the library is designed to be easily reused in building or extending other crystallographic software.