

Knowledge resources for the crystallographers of tomorrow

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Crystallography for the next generation: the legacy of IUCr

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Outline of talk

- Historical context
- Scientific Publications of the IUCr
- Web and social media services on IUCr servers
- Educational resources

Historical context

Knowledge resources for the crystallographers of tomorrow

knowledge = *scientia* (Latin)

 ***science***

The Translation Movement

- Some exposure to Hellenic ideas during Arab expansion under Umayyads
- Aristotle appears to Caliph Al-Mamun in dream (8th century CE)
- 8th-10th century: Abbasid Caliphs promote the flowering of Arabic philosophy, mathematics and Persian literature
- Western Europe receives Greek ideas via Arabian tradition
- Al-Kindi, Avicenna (Ibn Sina), Averroes (Ibn Rushd)



Al-Kindi (801-873 CE)



Avicenna (980-1037 CE)



Averroes (1126-1198 CE)

Out of the Dark Ages I

– the survival of ideas

- ‘Publication’
- Translation
- Communication

*‘If I have seen further it is by standing on
the shoulders of giants.’*



Isaac Newton (1643-1727 CE)

Out of the Dark Ages II

2. The situation by 1939

The scientific foundations of modern crystallography were laid in 1912 by Laue's discovery of X-ray diffraction followed immediately by the invention of crystal structure analysis by the two Braggs - son and father.

Three committees were set up to investigate a coordinated abstracting scheme, the preparation of standardized space-group tables and the standardization of crystallographic nomenclature.

The Tables Committee consolidated its plans at a 12 day meeting organized by Ewald and Bernal and held at Paul Niggli's institute in Zurich in 1930. The eventual outcome was the publication in 1935 of the splendid two volumes of the *Internationale Tabellen zur Bestimmung von Kristallstrukturen (International Tables for the Determination of Crystal Structures)*.

The *Strukturbericht*, edited at first by Ewald and Hermann and then by Hermann alone, provided critical summaries of structure papers covering the years 1913 to 1939.

The internationally recognized but commercially owned journal *Zeitschrift für Kristallographie*, which had been founded by Paul Groth in 1877, had Paul Niggli as its Editor-in-Chief.

Acta Cryst. (1998). **A54**, 687-696

Aspects of the history of the International Union of Crystallography

D. W. J. Cruickshank

Chemistry Department, UMIST, Manchester M60 1QD, England
(Received 14 August 1998; accepted 1 September 1998)



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WWII 1939-1945

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Out of the Dark Ages II

3. 1941-1946

World War II put a stop to many crystallographic activities, but not completely.

In March 1944, Ewald ... ended with a strong plea for the formation of an international society or union which would represent the new crystallography.

The union he envisaged would be responsible for **publishing an international journal of crystallography as well as archives, abstracts, space-group tables and structure reports.**

At about the same time, ideas for a crystallographic journal were being developed in the USA.

Publications Sub-Committee under Sir Lawrence Bragg ... looked seriously at the possibilities.

views ... communicated both to the Americans and to Russian crystallographers.

The Russians were keen for an international journal of crystallography to be founded to replace the then defunct *Zeitschrift für Kristallographie*.

Once the war was over, there was a **widening circle of correspondence** with leading crystallographers in several countries.

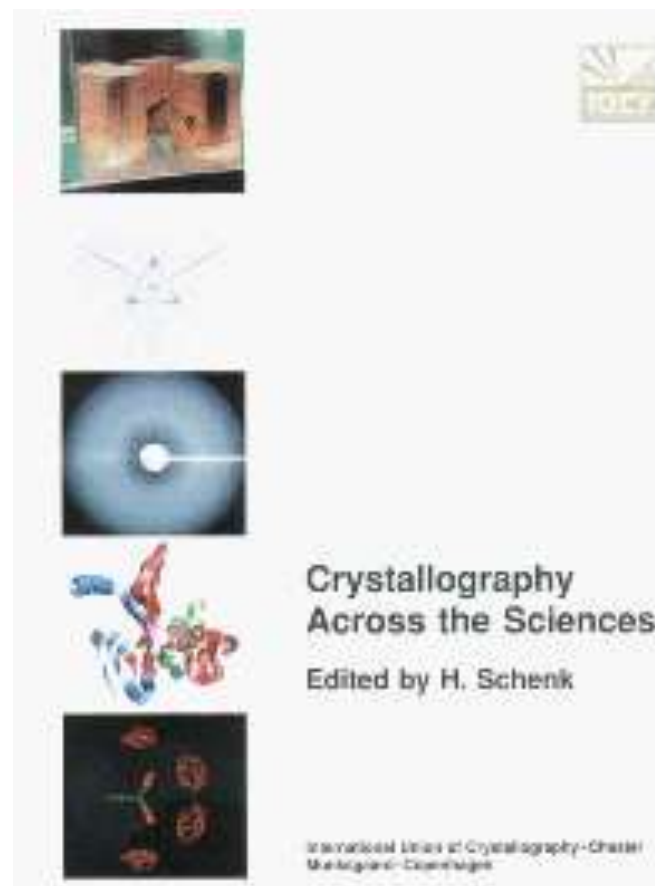
The upshot was an international conference held in London ... explore the starting of a journal and the formation of an International Union.

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Aspects of the history of the International Union of Crystallography

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Birth of an International Scientific Union

- **7 April 1947** IUCr admitted to ICSU
- **1 March 1948** First issue of *Acta Crystallographica*
- **28 July–3 August 1948** First Congress and General Assembly, Harvard University, USA



J. D. Bernal, C. V. Raman, C. Palache, P. P. Ewald, A. L. Patterson. (From the collection of C. Frondel. AIP Niels Bohr Library.)

An International Scientific Union

= an International Union of ***Scientists***

- Freedom of movement and expression (ICSU Statute No. 5; Principle of Universality in Science)
- Representation on bodies with aims that overlap with the aims and activities of the Union (ICTNS, ICSTI, CODATA, ICSU, COSPAR)
- Capacity building (Initiative in Africa; IYCr2014)
- Support travel and meeting attendance (Calendar Subcommittee; Visiting Professorships)
- Ewald Prize
- *Voice of crystallographers*
 - Ethics in science
 - Unacceptability of plagiarism/data falsification
 - Inappropriateness of bibliometrics as sole proxy for evaluation

An International Scientific Union

= an International Union of ***Science***

Objectives (<http://www.iucr.org>)

- to promote international cooperation in crystallography
- to contribute to all aspects of crystallography
- to promote international publication of crystallographic research
- to facilitate standardization of methods, units, nomenclatures and symbols
- to form a focus for the relations of crystallography to other sciences.

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For all mankind – collaborations with UNESCO

The IUCr enjoyed financial support from UNESCO (among others) for

- *Acta Crystallographica*

It has been agreed to fix the subscription at £2. 10s. 0d. or \$10 per volume, and to ask for subsidies in order to keep the price at this level. It is hoped that this moderate price will ensure a large number of subscribers. Subsidies have been obtained from U.N.E.S.C.O., from British and American firms, Research Associations, and other scientific bodies.

and their editors, feel that the discovery of neutron or electron diffraction in a crystal is undoubtedly better placed in a journal devoted to pure physics; the application of these diffraction effects to the study of the scattering by individual crystalline substances, however, would appropriately come within the domain of *Acta*.

The best scheme for the publication of scientific investigations is a problem of outstanding importance for the sound development of science, and is particularly acute in those fields which touch on many different branches of study. On the one hand the results of crystal investigations should be presented to physicists, chemists, mineralogists, metallurgists and biologists in a form which enables them to grasp readily the implications for their sciences; they are not interested in the details of the methods by which the results have been achieved, and if such details are published in the existing journals, the majority of the readers may not be prepared to follow the argument. On the other hand, it is essential that the methods by which the results have been gained, and the data on which they are founded, should be fully published so that they may be subjected to the expert criticism necessary to assess their reliability. *Acta*, in trying to reassemble the crystallographic work now scattered through a great variety of

all expression, should fulfil an the general mechanism of is frankly intended to be the in crystallography the world all important new lines of ted in it, and that *Acta* will sion of problems of crystallo-

on, *Acta Crystallographica* is y belonging to the crystallo- the property of an Inter-. The INTERNATIONAL UNION as established in 1947 after t the meeting of crystallo- s of the world held in London tation of the X-ray Analysis Physics under the Chairman-

ship of Sir Lawrence Bragg. At this meeting a Provisional International Crystallographic Committee was formed consisting of some thirty of those present, and this in turn charged one of its Sub-Committees to take the necessary steps for the formation of a journal, the editors of which were nominated at the meeting.

As a result of this, Statutes of the Union were prepared and approved by the Provisional Committee with their acceptance by the International Council of Scientific Unions on 7 April 1947 the Union of Crystallography came into being. Pending the first General Assembly of the new Union, the Provisional International Committee represents the Union, and the Sub-Committee formed at the London meeting serves as its provisional Executive Committee.

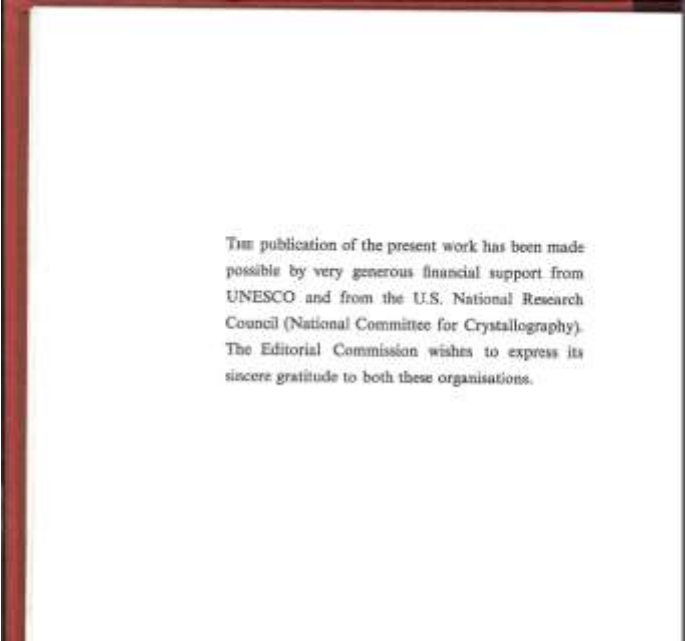
The question of arrangements for a centre of publication of *Acta* was very carefully considered; specifications for the printing were drawn up and tenders invited from firms in various European countries and in the U.S.A. The final decision to entrust the printing to the Cambridge University Press was governed largely by considerations of convenience of editing and publication. The Cambridge University Press is charged with the printing and distribution of *Acta* in accordance with the wishes of the Union. Much to the satisfaction of the Provisional Committee, the international character of the arrangements for *Acta* has been enhanced by the offer of the American Institute of Physics to collect subscriptions in the United States of America, its territories and possessions, in Canada and in Mexico.

It has been agreed to fix the subscription at £2. 10s. 0d. or \$10 per volume, and to ask for subsidies in order to keep the price at this level. It is hoped that this moderate price will ensure a large number of subscribers. Subsidies have been obtained from U.N.E.S.C.O., from British and American firms, Research Associations, and other scientific bodies. This is not the place to list these contributions, but we most gratefully express the sincere thanks of the promoters, the editors, and the readers of *Acta* to those whose moral and material help has made possible the production of this journal.

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- *Acta Crystallographica*
- *International Tables for X-ray Crystallography*



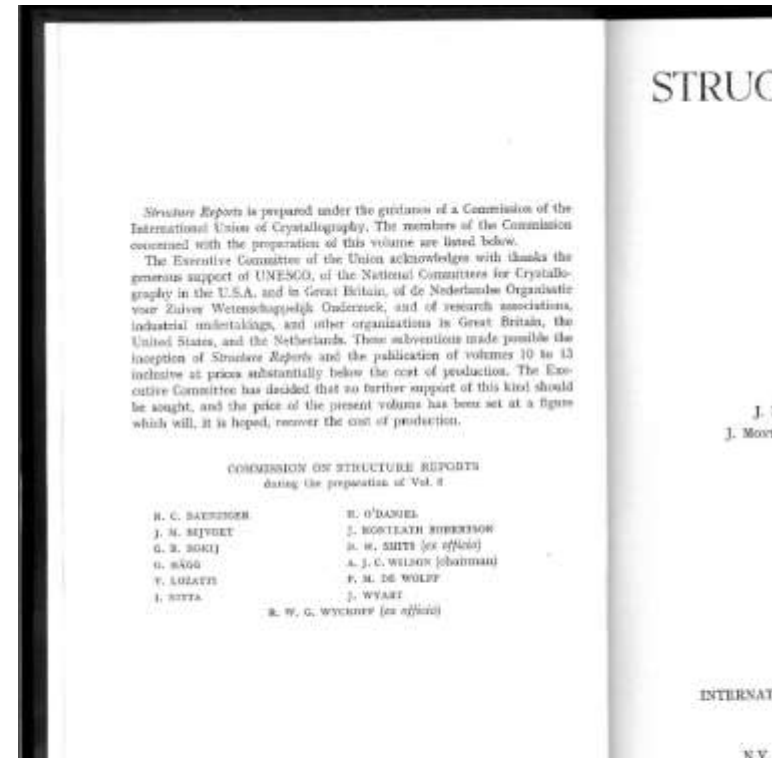
The publication of the present work has been made possible by very generous financial support from UNESCO and from the U.S. National Research Council (National Committee for Crystallography). The Editorial Commission wishes to express its sincere gratitude to both these organisations.

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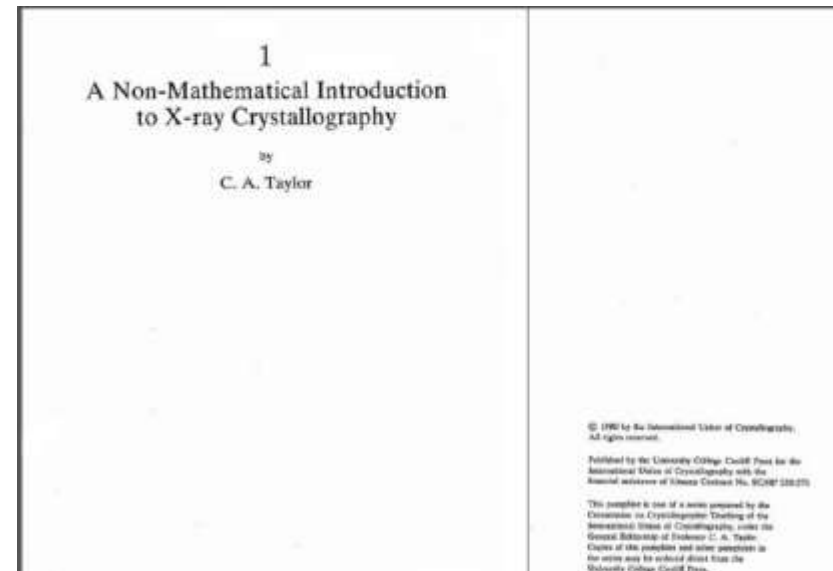


The Executive Committee of the Union acknowledges with thanks the generous support of UNESCO, of the National Committees for Crystallography in the U.S.A. and in Great Britain, of de Nederlandse Organisatie voor Zuiver Wetenschappelijk Onderzoek, and of research associations, industrial undertakings, and other organizations in Great Britain, the United States, and the Netherlands.

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- Teaching Pamphlets



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- IUCr-UNESCO Project on the Teaching of Crystallography

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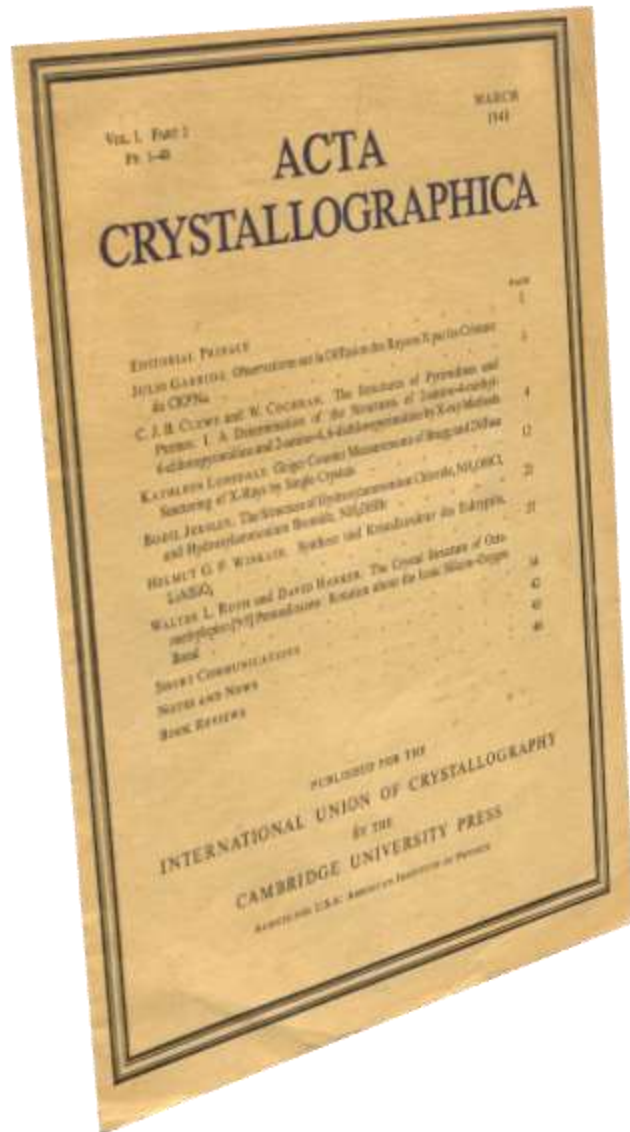
Under this project jointly sponsored by the International Union of Crystallography and UNESCO, funds were provided by the latter organization to assist in the development of some new learning materials in the field of crystallography [see *Acta Crystallographica* (1969), **A25**, 724].

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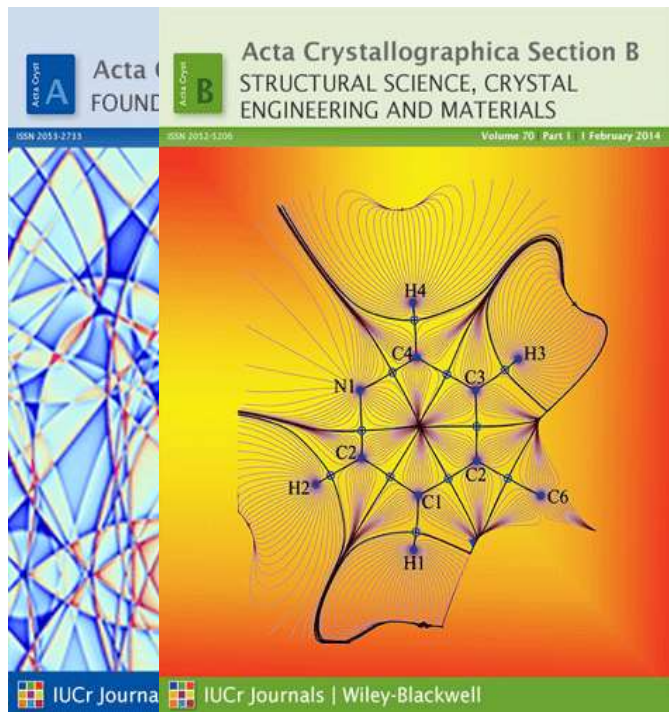
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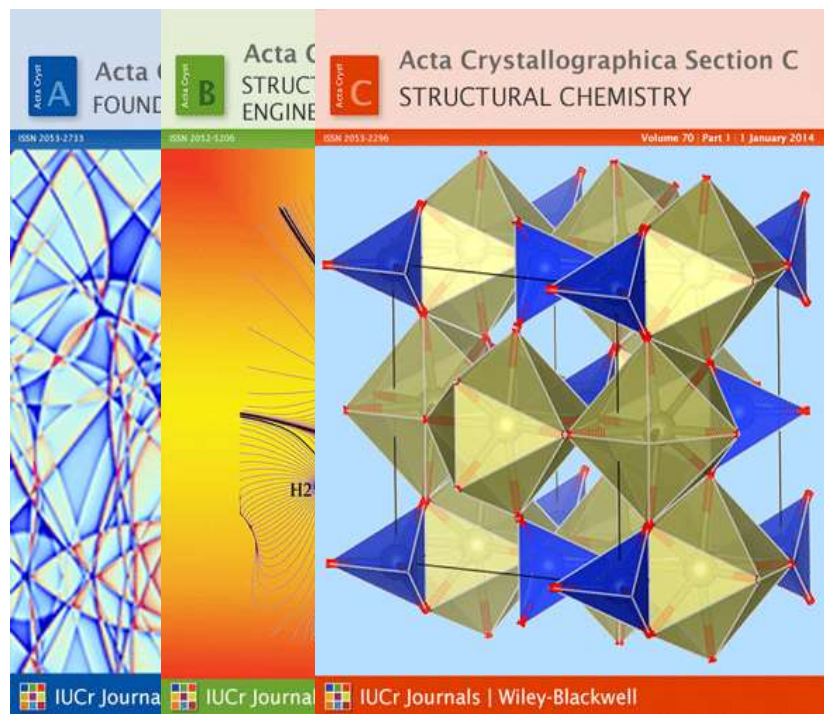
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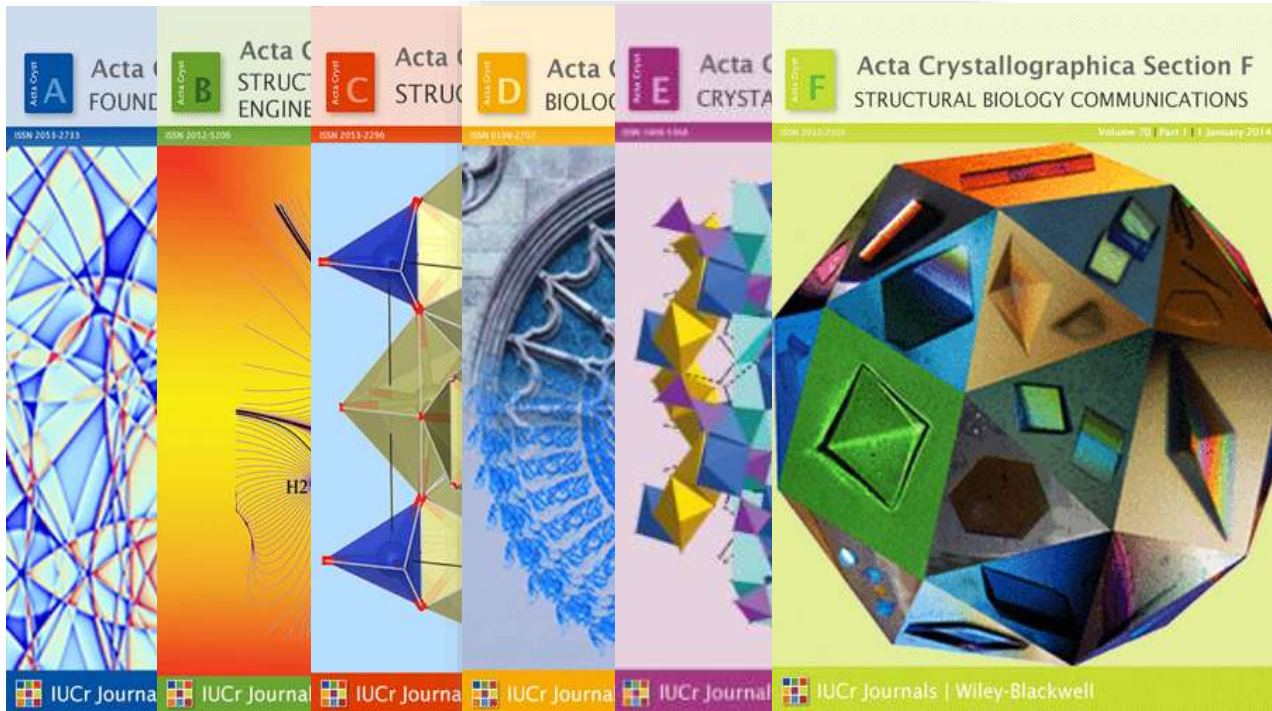
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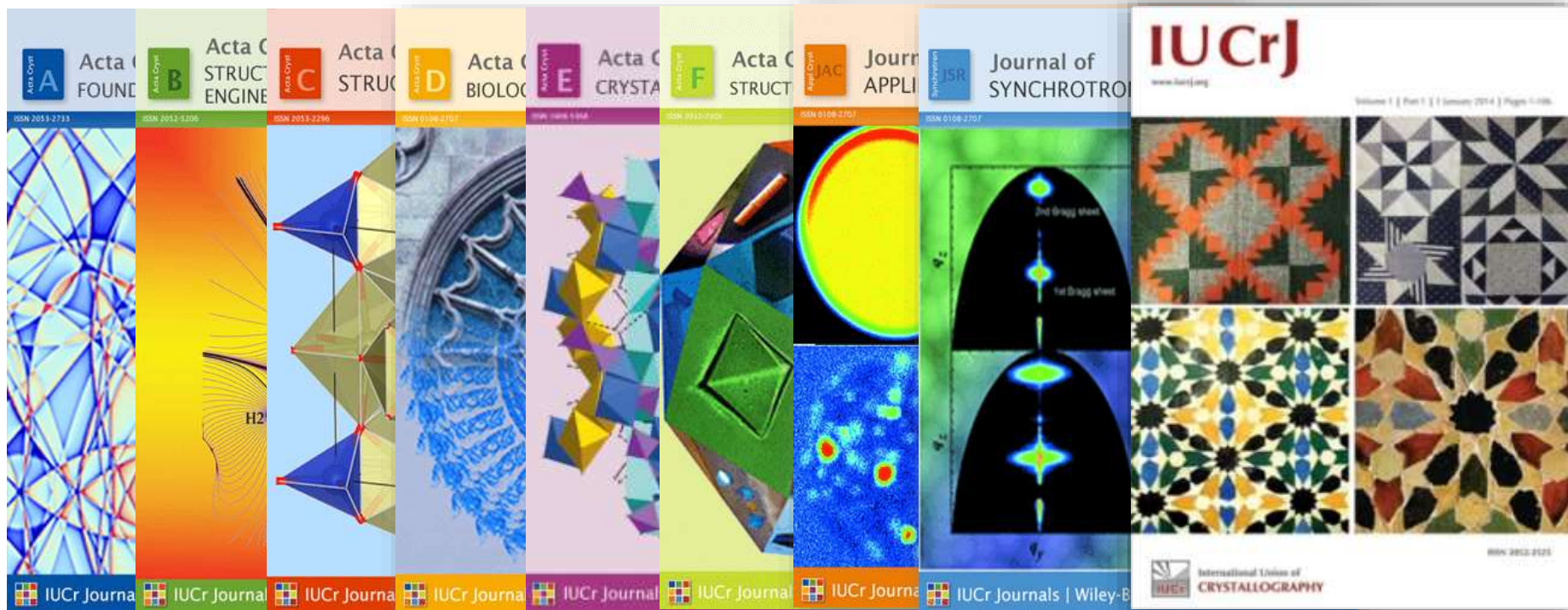
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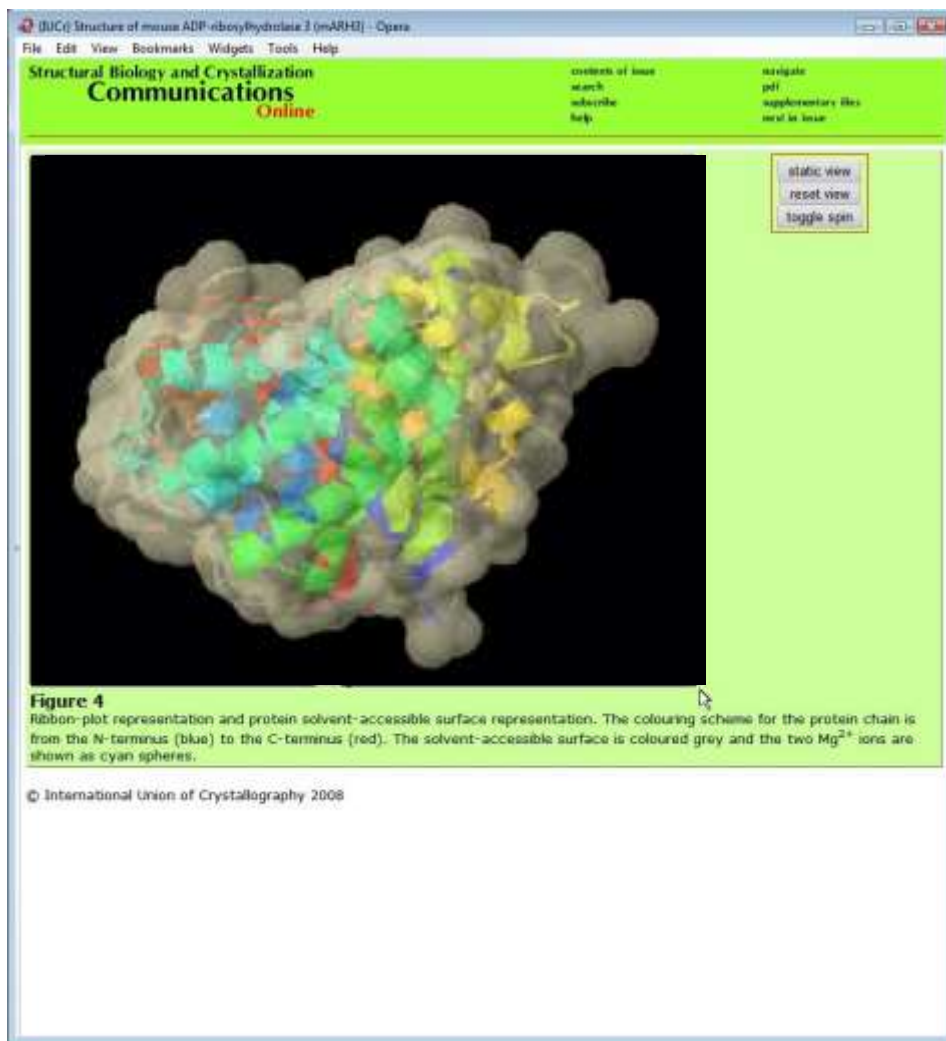
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- 1948 Structure factors (data deposition) required
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An enhanced figure created by the author for an article in *Acta Crystallographica Section F*

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Karle & Karle	The symbolic addition procedure for phase determination for centrosymmetric and noncentrosymmetric crystals	Acta Cryst. (1966), 21, 849–859
Karle & Karle	An application of a new phase determination procedure to the structure of <i>cyclo</i> (hexaglycyl) hemihydrate	Acta Cryst. (1963), 16, 969–975
Ibers & Hamilton	Dispersion corrections and crystal structure refinements	Acta Cryst. (1964), 17, 781–782
Schomaker & Trueblood	On the rigid-body motion of molecules in crystals	Acta Cryst. (1968), B24, 63–76
Doyle & Turner	Relativistic Hartree–Fock X-ray and electron scattering factors	Acta Cryst. (1968), A24, 390–397
Shannon & Prewitt	Effective ionic radii in oxides and fluorides	Acta Cryst. (1969), B25, 925–946
McWeeny	X-ray scattering by aggregates of bonded atoms. I. Analytical approximations in single-atom scattering	Acta Cryst. (1951), 4, 513–519
Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal	New calculations of atomic scattering factors	Acta Cryst. (1955), 8, 478–483
Blow & Crick	The treatment of errors in the isomorphous replacement method	Acta Cryst. (1959), 12, 794–802
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Virtual hyperglossary

The image shows a virtual hyperglossary interface. On the left, there is a sidebar with navigation buttons (up, down, search, etc.) and a list of items, including a link to a 'point group' entry. The main content area is a browser window displaying the 'Point group' entry from the Online Dictionary of Crystallography. The entry includes a title, a list of views (Page, Discussion, View source, History), personal tools (Log in / create account), and a toolbox (What links here, Related changes, Special pages, Printable version, Permanent link). The definition section explains that a point group is a group of symmetry operations that leave at least one point unmoved. The occurrence section states that crystallographic point groups occur in vector space and point space. The 'See also' section is empty.

Point group - Online Dictionary of Crystallography - Google Chrome
reference.iucr.org/dictionary/Point_group

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Point group

Groupe ponctuel (Fr); Punktgruppe (Ge); Gruppo punto (It); 点群 (Ja).

Definition

A **point group** is a group of symmetry operations all of which leave at least one point unmoved. A *crystallographic* point group is a point group that maps a point lattice onto itself: in three dimensions rotations and rotoinversions are restricted to 1, 2, 3, 4, 6 and $\bar{1}$, $\bar{2}$ (= m), $\bar{3}$, $\bar{4}$, $\bar{6}$ respectively.

Occurrence

Crystallographic point groups occur:

- in vector space, as symmetries of the external shapes of crystals (morphological symmetry), as well as symmetry of the physical properties of the crystal ("vector-point group");
- in point space, as site-symmetry groups of points in lattices or in crystal structures, and as symmetries of atomic groups and coordination polyhedra ("point-point group").

See also

Views

- Page
- Discussion
- View source
- History

Personal tools

- Log in / create account

Toolbox

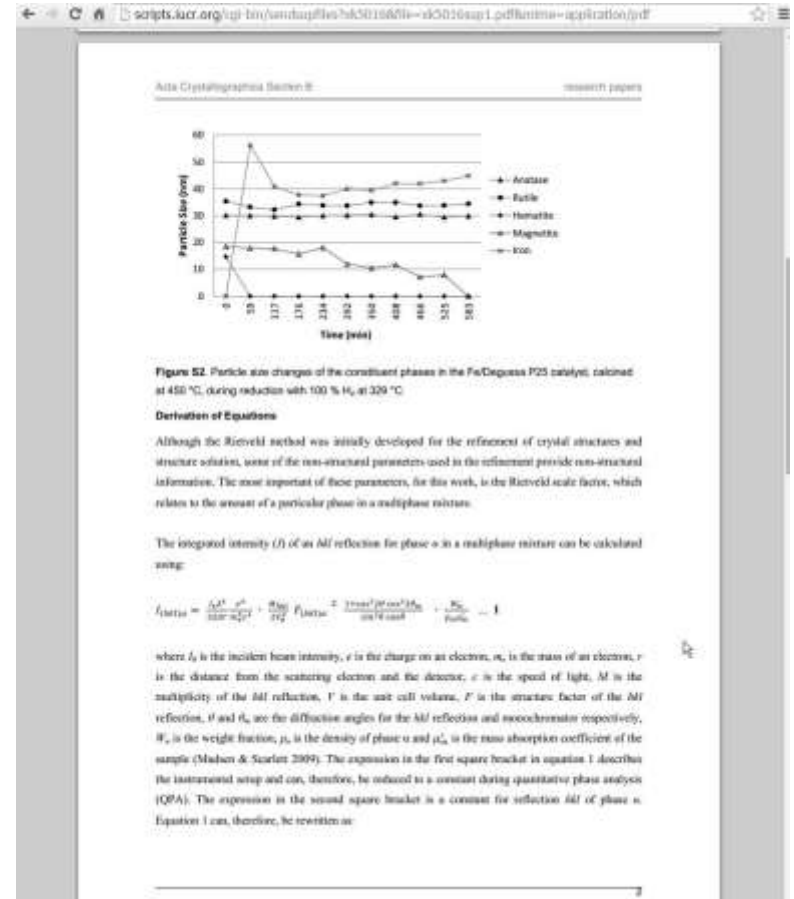
- What links here
- Related changes
- Special pages
- Printable version
- Permanent link

CCDC reference: 1006924

IUCr Journals are *useful!*

- More full-text (HTML) downloads than most other scholarly publishers
- Virtual hyperglossary for technical terms
- Immediate access to supplementary information

Supporting information is freely available



IUCr Journals are *useful!*

- More full-text (HTML) downloads than most other scholarly publishers
- Virtual hyperglossary for technical terms
- Immediate access to supplementary information
- Access to structural and experimental **data**

But what you *really* want is the data!

The screenshot shows a web browser window displaying the CIF database interface. The URL is publids.iucr.org/cifmoldb/gul/dj/mol.php?cifid=wm5025sup1. The page title is "3D view" and it includes journal information: "Volume 70 | Part 7 | July 2014 | Page 138" and "doi:10.1107/S1600536814013087". The main content area displays the title "Tripotassium iron(III) bis(orthamolybdate) dimolybdate" and its chemical formula $K_3Fe(MoO_4)_2Mo_2O_7$. Crystallographic data is provided: $M_r = 796.91$, Monoclinic, $C2/m$, $a = 32.873(2) \text{ \AA}$, $b = 5.7137(7) \text{ \AA}$, $c = 7.9177(6) \text{ \AA}$, $\beta = 91.143(3)^\circ$, $V = 1406.9(3) \text{ \AA}^3$, and $Z = 4$. A 3D ball-and-stick model of the structure is shown, with axes labeled a, b, and c. To the right of the model are controls for "molecule", "unit cell", and "polyhedra". At the bottom of the main content area, there are icons for "GIF", "3D", and "Jmol" and a "change 3D viewer" link. The footer includes "Acta Cryst. E" information, social media links for "Follow Acta Cryst. E", "E-alerts", "Twitter", "Facebook", and "RSS", and a search bar with fields for "search term", "author", "all journals", "volume", and "page", along with a "GO" button and "advanced search" link. The copyright notice at the bottom reads "Copyright © International Union of Crystallography".

For **every** small crystal structure in IUCr journals

But what you *really* want is the data!

publcf.iucr.org/cifmoldb/gui/cifjmol.php?cifid=wm5025sup1

3D view

Volume 70 | Part 7 | July 2014 | Page 138
doi:10.1107/S1600536814013087
OPEN ACCESS

STRUCTURE REPORTS
ISSN: 1600-5368

Tripotassium iron(III) bis(orthomolybdate) dimolybdate

$K_3Fe(MoO_4)_2Mo_2O_7$
 $M_r = 796.91$
Monoclinic, $C2/m$
 $a = 32.873(2) \text{ \AA}$
 $b = 5.7137(7) \text{ \AA}$
 $c = 7.5177(9) \text{ \AA}$
 $\beta = 91.143(8)^\circ$
 $V = 1486.5(3) \text{ \AA}^3$
 $Z = 4$

molecule unit cell
polyhedra

change 3D viewer

Acta Cryst. E
ISSN: 1600-5368
STRUCTURE REPORTS

Volume 70 | Part 7 | July 2014 | Page 138
doi:10.1107/S1600536814013087
OPEN ACCESS

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search term: doi | GO | advanced search

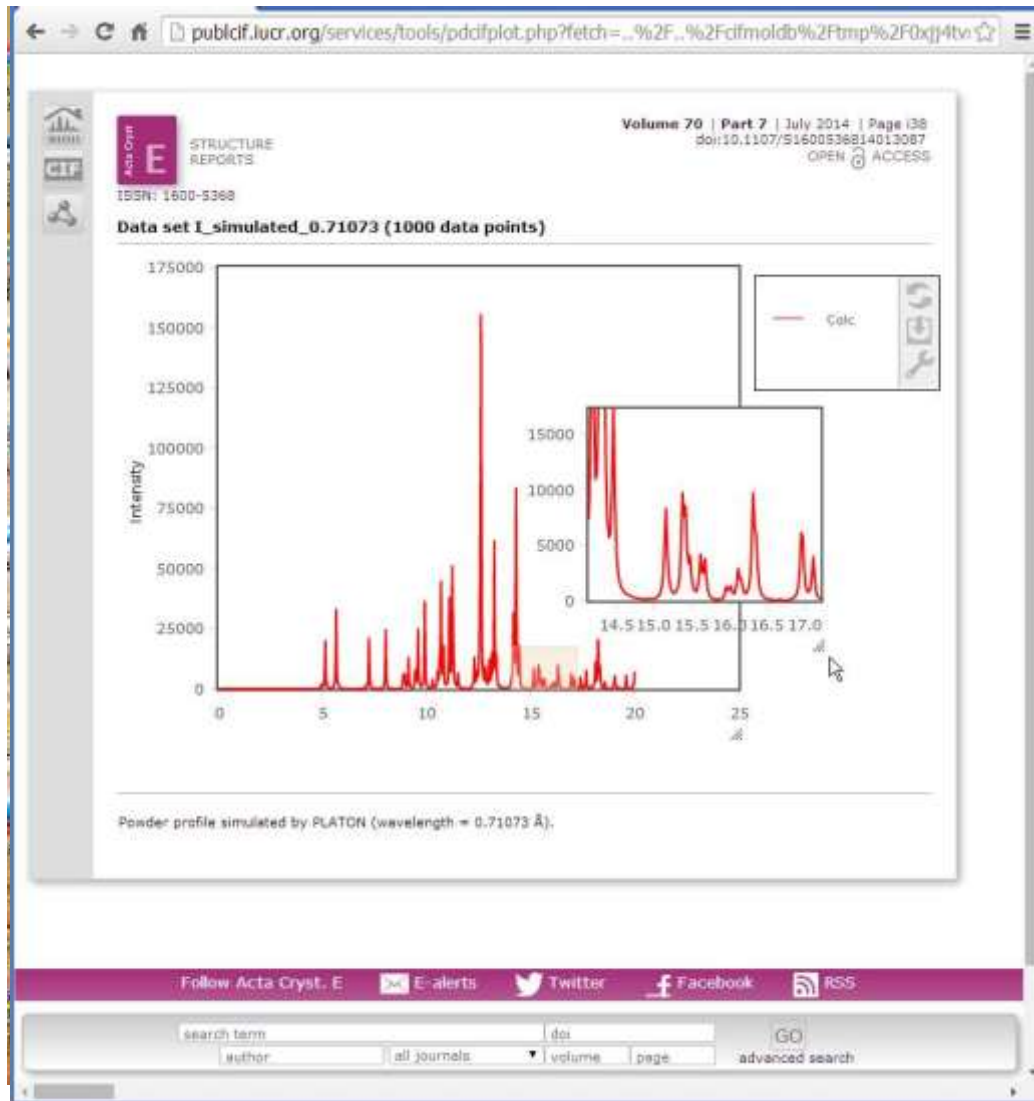
author | all journals | volume | page

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For **every** small crystal structure in IUCr journals

- Interactive visualization (*Jmol*)

But what you *really* want is the data!



For **every** small crystal structure in IUCr journals

- Interactive visualization (*Jmol*)
- Powder pattern visualization/prediction

But what you *really* want is the data!

Acta Cryst. E
ISSN: 1600-5368
STRUCTURE REPORTS

7-Chloro-4-oxo-4H-chromene-3-carbaldehyde
C10H7ClO3
Mr = 209.60
Triclinic, P1
a = 3.823 (2) Å
b = 5.973 (3) Å
c = 18.386 (8) Å
α = 85.99 (4)°
β = 87.74 (4)°
γ = 86.58 (4)°
V = 417.8 (4) Å³
Z = 2

Acta Cryst. E
ISSN: 1600-5368
STRUCTURE REPORTS

Follow Acta Cryst. E | E-alerts | Twitter

search term: | doi: |
author: | all journals | volume: | page: |

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3-acetyl-6-chloro-2H-chromen-2-one
C11H7ClO3

3-Methyl-4H-chromen-4-one
C10H8O2

For **every** small crystal structure in IUCr journals

- Interactive visualization (*Jmol*)
- Powder pattern visualization/prediction
- Search for similar structures

But what you *really* want is the data!

```
pubcif.iucr.org/cifmoldb/tmp/0xj4tvrmp.cif
*****
* This CIF contains the data in a paper accepted for publication in
* Acta Crystallographica Section E. It conforms to the requirements of
* Notes for Authors for Acta Crystallographica Section E, and has been
* peer reviewed under the auspices of the IUCr Commission on Journals.
*
* Full details of the Crystallographic Information File format
* are given in the paper "The Crystallographic Information File (CIF):
* a New Standard Archive File for Crystallography" by S. R. Hall, F. H.
* Allen and I. D. Brown [Acta Cryst. (1991), A47, 655-685].
*
* The current version of the core CIF dictionary is obtainable from:
* ftp://ftp.iucr.org/pub/cif_core.dic.
*
* software is freely available for graphical display of the structure(s)
* in this CIF. For information consult the CIF software page
* http://www.iucr.org/resources/cif/software.
*
* This file may be used for bona fide research purposes within the
* scientific community so long as proper attribution is given to the journal
* article from which it was obtained.
*****
data_1
_audit_creation_method SHELXL-3
_journal_date_recd_electronic 2014-05-09
_journal_date_accepted 2014-06-05
_journal_name_full 'Acta Crystallographica, Section E'
_journal_year 2014
_journal_volume 70
_journal_issue 7
_journal_page_first 138
_journal_page_last 138
_journal_paper_category QE
_journal_paper_doi 10.1107/S160036814012087
_journal_coeditor_code W5025
_publ_contact_author_name 'Dr. A. Souliem'
_publ_contact_author_address
|
| Laboratoire de Mat'eriaux et Cristallographie
| Facult'e des Sciences de Tunis
| universit'e de Tunis ElManar
| 2092 Manar II Tunis
| Tunisia
|
|_publ_contact_author_email 'souliem_ah@yahoo.fr'
|_publ_contact_author_fax '+216 71 58 34 24'
|_publ_contact_author_phone '+216 71 57 26 00'
|_publ_section_title
|
| 5-K-3-Fs(M60-4)-2-Mo-2-O-7-
|_loop
|_publ_author_name
|_publ_author_address
| 'Souliem, Amra'
|
| Laboratoire de Mat'eriaux et Cristallographie
| Facult'e des Sciences de Tunis
| universit'e de Tunis ElManar
| 2092 Manar II Tunis
| Tunisia
|
| 'Zid, Mohamed Faouzi'
|
| Laboratoire de Mat'eriaux et Cristallographie
| Facult'e des Sciences de Tunis
| universit'e de Tunis ElManar
| 2092 Manar II Tunis
| Tunisia
|
| 'Driss, Ahmed'
|
| Laboratoire de Mat'eriaux et Cristallographie
| Facult'e des Sciences de Tunis
| universit'e de Tunis ElManar
| 2092 Manar II Tunis
| Tunisia
```

For **every** small crystal structure in IUCr journals

- Interactive visualization (*Jmol*)
- Powder pattern visualization/prediction
- Search for similar structures
- Download processed data

But what you *really* want is the data!

No syntax errors found. Please wait while processing CIF dictionary Interpreting this report.

Datablock: I

Bond precision: Fe-O = 0.0053 Å Wavelength=0.71073
Cell: a=32.873(2) b=5.7137(7) c=7.9177(9)
alpha=90 beta=91.143(8) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	1486.9(3)	1486.9(3)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Noticity formula	Fe Mo4 O15, 3(K)	Fe K3 Mo4 O15
Sum formula	Fe K3 Mo4 O15	Fe K3 Mo4 O15
M _r	796.91	796.91
D _x , g cm ⁻³	3.560	3.560
Z	4	4
Nu (mm ⁻¹)	5.146	5.146
F ₀₀₀	1484.0	1484.0
F ₀₀₀ ^l	1460.82	
h, k, l _{max}	41, 7, 10	41, 7, 10
N _{ref}	1791	1789
T _{min} , T _{max}	0.267, 0.396	0.285, 0.488
T _{min} ^l	0.151	

Correction method= PSI-SCAN Theta(max)= 26.970
Data completeness= 0.999
R(reflections)= 0.0291(1636) wR2(reflections)= 0.0764(1789)
S = 1.063 Npar= 138

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level C

PLAT213_ALERT_2_C Atom O4 has ADP max/min Ratio 3.3 nrorat

PLAT215_ALERT_2_C
PLAT242_ALERT_2_C
And 2 other PLAT242:
Less ...

PLAT242_ALERT_2_C L
PLAT242_ALERT_2_C L
PLAT250_ALERT_2_C L

Alert level G

PLAT004_ALERT_5_G P
PLAT042_ALERT_1_G C
PLAT082_ALERT_2_G S
PLAT232_ALERT_2_G H
PLAT301_ALERT_3_G N
PLAT794_ALERT_5_G T

0 ALERT level A =
0 ALERT level B =
6 ALERT level C =
6 ALERT level G =

1 ALERT type 1 CIF
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement methodology, query or suggestion

PLAT213 - Google Chrome
journals.iucr.org/services/cif/checking/PLAT213.html

PLAT213

PLAT213 Type_2 Test ratio adp max/min in main residue(s)

The maximum and minimum main axis ADP ratio (Angstrom Units) is tested for the main residue. Large values may indicate unresolved disorder.

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IUCr Webmaster

For *every* small crystal structure in IUCr journals

- Interactive visualization (*Jmol*)
- Powder pattern visualization/prediction
- Search for similar structures
- Download processed data
- Validate the model

But what you *really* want is the data!

```
journals.test.iucr.org/e/issues/2014/07/00/wm5025/wm5025sup2.hkl

# h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag
data_1
_sheX_title ' ntris in C 2/n1'
_sheX_refln_list_code 4
_sheX_F_calc_maximum 728.15
_expt1_crystal_F_000 1484.00
_reflns_d_resolution_high 0.7895

loop
_symmetry_equiv_pos_as_xyz
'X, Y, Z'
'-X, Y, -Z'
'x+1/2, y+1/2, z'
'-x+1/2, y+1/2, -z'
'-X, -Y, Z'
'X, -Y, -Z'
'-x+1/2, -y+1/2, -z'
'x+1/2, -y+1/2, z'

_cell_length_a 32.8733
_cell_length_b 5.7137
_cell_length_c 7.9177
_cell_angle_alpha 90.000
_cell_angle_beta 91.143
_cell_angle_gamma 90.000

_sheX_F_squared_multiplier 1.000

loop
_refln_index_h
_refln_index_k
_refln_index_l
_refln_F_squared_calc
_refln_F_squared_meas
_refln_F_squared_sigma
_refln_observed_status
4 0 0 1472.79 1061.78 50.30 0
6 0 0 56.28 32.73 52.85 0
8 0 0 125040.30 131712.69 1119.63 0
10 0 0 23290.92 23744.94 227.82 0
12 0 0 2.54 151.15 110.40 0
14 0 0 4673.19 1409.51 107.08 0
16 0 0 17033.45 18199.24 249.83 0
18 0 0 49137.25 51012.02 450.44 0
20 0 0 896.15 835.89 51.76 0
22 0 0 44.45 122.84 39.52 0
24 0 0 92551.67 96671.88 727.10 0
26 0 0 2294.50 2076.75 138.66 0
28 0 0 21244.30 22246.91 369.29 0
30 0 0 34599.45 31135.31 460.27 0
32 0 0 12466.38 12332.90 307.30 0
34 0 0 142.11 61.26 177.77 0
36 0 0 7648.71 8326.24 502.07 0
38 0 0 178.27 152.85 102.01 0
40 0 0 517.28 447.84 175.75 0
1 1 0 18858.07 17145.08 238.21 0
3 1 0 27620.63 25552.25 262.49 0
5 1 0 11088.90 10046.63 93.83 0
7 1 0 103920.29 96894.84 1131.61 0
9 1 0 188411.81 175545.48 2251.08 0
11 1 0 27281.74 25958.99 172.16 0
13 1 0 40775.63 41683.90 352.37 0
15 1 0 50326.66 51241.23 420.94 0
17 1 0 134619.52 135042.50 1165.61 0
19 1 0 42793.82 44017.50 429.79 0
21 1 0 636.46 642.40 31.59 0
23 1 0 3373.97 3340.77 94.38 0
25 1 0 728.89 716.71 28.66 0
27 1 0 13987.39 13179.50 340.02 0
29 1 0 8921.98 9101.47 173.77 0
31 1 0 7016.59 7462.72 188.41 0
33 1 0 2776.20 2682.89 95.53 0
35 1 0 964.07 935.17 39.75 0
37 1 0 154.87 106.11 50.92 0
39 1 0 1009.10 1069.90 111.71 0
41 1 0 4754.72 4233.25 174.60 0
0 2 0 530196.31 444304.58 6291.25 0
```

For **every** small crystal structure in IUCr journals

- Interactive visualization (*Jmol*)
- Powder pattern visualization/prediction
- Search for similar structures
- Download processed data
- Validate the model
- Download experimental data (and do your own refinement!)

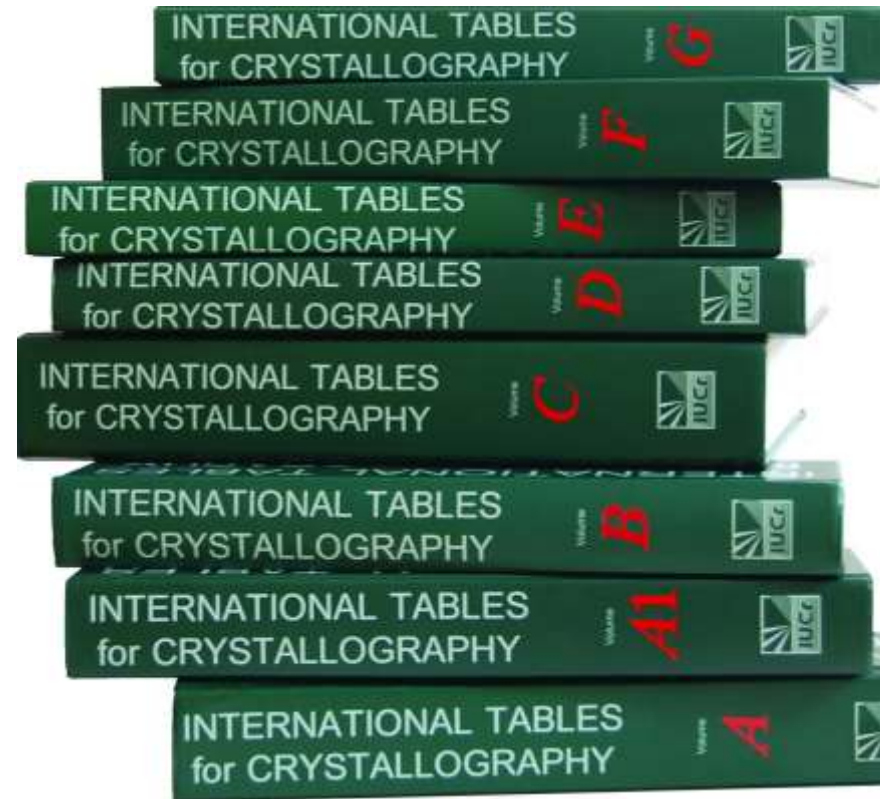
International Tables for Crystallography

- 1935-1944 *International Tables for the Determination of Crystal Structures* (2 volumes)
- 1952-1989 *International Tables for X-ray Crystallography* (4 volumes)



International Tables for Crystallography

- 1935-1944 *International Tables for the Determination of Crystal Structures* (2 volumes)
- 1952-1989 *International Tables for X-ray Crystallography* (4 volumes)
- 1983- *International Tables for Crystallography* (8 volumes)



International Tables for Crystallography

- 1935-1944 *International Tables for the Determination of Crystal Structures* (2 volumes)
- 1952-1989 *International Tables for X-ray Crystallography* (4 volumes)
- 1983- *International Tables for Crystallography* (8 volumes)
- 2006- *International Tables Online*

INTERNATIONAL TABLES Space-group symmetry

Go to: space group No. 1 (P 3) Go

Home > Volume A > Contents > Space group 143

P3 C_3^1 3

No. 143 P3 Trigonal

Pattern symmetry P-3

Positions

Multiplicity, Wyckoff letter, site symmetry	Coordinates	Reflection conditions
3 d 1	(1) x, y, z (2) $-y, x - y, z$ (3) $-x + y, -z$	General: no conditions
1 e 3 ₂	$2/3, 1/3, z$	Special: as above, plus no extra conditions
1 b 3 ₂	$1/3, 2/3, z$	no extra conditions
1 a 3 ₂	$0, 0, z$	no extra conditions

Symmetry of special projections

Along [001] $P3$ $a' = a$ $b' = b$ $c' = c$
 Origin at $0, 0, z$

Along [100] $P1$ $a' = 1/2(a + 3b)$ $b' = c$
 Origin at $x, 0, 0$

Along [210] $P1$ $a' = 1/3b$ $b' = c$
 Origin at $x, 1/2x, 0$

Maximal non-isomorphic subgroups

I	[3] $P1$ (1)	I
IIa	none	
IIb	[3] $P3_2$ ($c' = 3c$) (145), [3] $P3$ ($c' = 3c$) (144), [3] $P3$ ($a' = a, b' = a + 3b, c' = 3c$) (146), [3] $P3$ ($a' = 2a + b, b' = -a + b, c' = 3c$) (146)	

Maximal isomorphic subgroups of lowest index

IIc	[2] $P3$ ($c' = 2c$) (145), [2] $P3$ ($a' = 3a, b' = 3b$) (P3, 143)
-----	---

Minimal non-isomorphic supergroups

I	[7] $P-3$ (147), [2] $P312$ (148), [3] $P321$ (150), [7] $P3m1$ (150), [7] $P31m$ (152), [7] $P3c1$ (152), [4] $P31c$ (152), [7] $P6$ (168), [7] $P6c$ (173), [12] D_6 (174)
---	--

International Tables for Crystallography

Enhanced use on the Web

International Tables for Crystallography

The screenshot shows the website interface for the International Tables for Crystallography. The main content area displays the space group $P3$ (No. 147) with its symbol C_3^1 and a diagram of the unit cell. A search bar at the top allows users to search for space groups. A navigation menu includes options like 'Home', 'Resources', 'Purchase', and 'Contact us'. A sidebar on the left contains links for 'Home', 'Resources', 'Purchase', and 'Contact us'. The main content area is divided into sections for 'Space group', 'Subgroups', and 'Supergroups'. A search bar is also present in the top right corner. The main content area displays the space group $P3$ (No. 147) with its symbol C_3^1 and a diagram of the unit cell. A search bar at the top allows users to search for space groups. A navigation menu includes options like 'Home', 'Resources', 'Purchase', and 'Contact us'. A sidebar on the left contains links for 'Home', 'Resources', 'Purchase', and 'Contact us'. The main content area is divided into sections for 'Space group', 'Subgroups', and 'Supergroups'. A search bar is also present in the top right corner.

Download a pdf

Interactive help

Links to subgroups and supergroups

Hyperlinking to related information

International Tables for Crystallography

Interactive
space-group
help

http://it.iucr.org - (International Tables) Space-group help - Mozilla Firefox

INTERNATIONAL TABLES Space-group help
Move your mouse over or click on the [links](#) to get information about each item. Detailed information on the space-group tables is given in [Chapter 2.2](#).

Cmm2 C_{2v}^{11} *mmm* Crystal class (point group) [close] Orthorhombic
See Section 10.1.1 and Chapter 12.1

No. 35 *Cmm2* Patterson symmetry *Cmmm*

Origin on *mmm* 2
Asymmetric unit $0 \leq x < 1/4; 0 \leq y < 1/2; 0 \leq z < 1$

International Tables for Crystallography

Browsable
crystallographic
ontologies (CIF
dictionaries)

INTERNATIONAL TABLES Definition and exchange of crystallographic data

Contents > Part 4 > Chapter 4.5 > Resources

Macromolecular dictionary (mmCIF)

Definitions are arranged alphabetically by category and within category.

- Revision history
- Category groups
- Extended data types
- Unit codes
- atom_site
 - [atom_site.B_equiv_geom_mean](#)
 - [atom_site.B_equiv_geom_mean_esd](#)
 - [atom_site.B_iso_or_equiv](#)
 - [atom_site.B_iso_or_equiv_esd](#)
 - [atom_site.Cartm_x](#)
 - [atom_site.Cartm_x_esd](#)
 - [atom_site.Cartm_y](#)
 - [atom_site.Cartm_y_esd](#)
 - [atom_site.Cartm_z](#)
 - [atom_site.Cartm_z_esd](#)
 - [atom_site.U_equiv_geom_mean](#)
 - [atom_site.U_equiv_geom_mean_esd](#)
 - [atom_site.U_iso_or_equiv](#)
 - [atom_site.U_iso_or_equiv_esd](#)
 - [atom_site.Wyckoff_symbol](#)
 - [atom_site.adp_type](#)
 - [atom_site.aniso_B\[1\]\[1\]](#)
 - [atom_site.aniso_B\[1\]\[1\]_esd](#)
 - [atom_site.aniso_B\[1\]\[2\]](#)
 - [atom_site.aniso_B\[1\]\[2\]_esd](#)
 - [atom_site.aniso_B\[1\]\[3\]](#)
 - [atom_site.aniso_B\[1\]\[3\]_esd](#)
 - [atom_site.aniso_B\[2\]\[2\]](#)
 - [atom_site.aniso_B\[2\]\[2\]_esd](#)
 - [atom_site.aniso_B\[2\]\[3\]](#)
 - [atom_site.aniso_B\[2\]\[3\]_esd](#)
 - [atom_site.aniso_B\[3\]\[3\]](#)

INTERNATIONAL TABLES Definition and exchange of crystallographic data

Contents > Part 4 > Chapter 4.5 > Resources

_atom_site.aniso_B[1][1]

Name:
'_atom_site.aniso_B[1][1]'

Definition:

The [1][1] element of the anisotropic atomic displacement matrix B , which appears in the structure-factor term as:

$$T = \exp(-1/8 \sin^2 \theta [(h-a)^2 / a^2 + (k-b)^2 / b^2 + (l-c)^2 / c^2])$$

h = the Miller indices
 a^* = the reciprocal space cell lengths

These matrix elements may appear with atomic coordinates in the [ATOM_SITE](#) category, or they may appear in the separate [ATOM_SITE_ANISOTROPIC](#) category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either B's or U's, but not as both.

The unique elements of the real symmetric matrix are entered by row.

The IUCr Commission on Nomenclature recommends against the use of B for reporting atomic displacement parameters. U , being directly proportional to B , is preferred.

Type: float

Type conditions: esd

Mandatory items: no

Related items: [_atom_site.aniso_B\[1\]\[1\]_esd \(associated_esd\)](#)
[_atom_site.aniso_U\[1\]\[1\] \(conversion_constant\)](#)
[_atom_site.anisotrop_B\[1\]\[1\] \(conversion_constant\)](#)
[_atom_site.aniso_U\[1\]\[1\] \(alternate_exclusive\)](#)
[_atom_site.anisotrop_B\[1\]\[1\] \(alternate_exclusive\)](#)
[_atom_site.anisotrop_U\[1\]\[1\] \(alternate_exclusive\)](#)

Category: atom_site

Date:

International Tables for Crystallography

Symmetry
database

The screenshot shows a web browser window titled "Symmetry database: Group I 41 - Mozilla Firefox". The page is for the space group $I4_1$ (No. 80). It features a navigation menu with links for home, resources, purchase, contact us, help, and related sites (IUCr, IUCr Journals). The main content area includes a "General position" section with a "Transform" button and input fields for "Transformaton: a, b, 2c" and "Origin shift: 0, 0, 0". Below this, several symmetry operations are listed as coordinate transformations:

$$x, y, z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
$$-x + 1/2, -y + 1/2, z + 1/2 = \begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$$
$$-y, x + 1/2, z + 1/4 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 1/2 \\ 0 & 0 & 1 & 1/4 \end{pmatrix}$$
$$y + 1/2, -x, z + 3/4 = \begin{pmatrix} 0 & 1 & 0 & 1/2 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 3/4 \end{pmatrix}$$
$$x + 1/2, y + 1/2, z + 1/2 = \begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$$
$$(-1 \ 0 \ 0 \ 0)$$

International Tables for Crystallography

Superspace Group Finder

Superspace Group Finder - Mozilla Firefox

Superspace Group Finder

home | resources | purchase | contact us | help | RELATED SITES: IUCr | IUCr Journals

INTERNATIONAL TABLES - Superspace Group Finder

| A | A1 | B | C | D | E | F | G |

Home > Resources > Superspace Group Finder

Superspace Group Finder
3D derivatives of (3+1)D space groups in analytical form.

- Displays real-space sections of superspace groups
- Finds parental (3+1)D superspace group for a set of 3D groups
- Of special use for phase transitions and modular structures

Browse (3+1)D groups...

First, select the crystal system, then browse the categories from left to right:

Systems	Classes	3D groups	(3+1)D groups
triclinic	6	191, P6/mmm	192.1 P6/mcc(00g)
monoclinic	-6	192, P6/mcc	192.2 P6/mcc(00g)s00s
orthorhombic	6/m	193, P63/mcm	
tetragonal	622	194, P63/mmc	
trigonal	6mm		
hexagonal	-6m2		
	-62m		
	6/mmm		

(3+1)D special reflection condition
00lm: m=2n, 0klm: l=2n, hklm: l+m=2n

Reference / comments

3+1D to 3D group transformation for commensurate modulation
Modulation vector $q=(D1/N1, D2/N2, D3/N3)$, or DN if there is only one non-zero component.
3D derivatives admit base of parental (3+1)D group.
To obtain specific group notations and symbols a base transformation might be necessary.

Constraints of t level. Variable n stands for any integer.

	General	n/N	$1/4n+n/N$	$1/2n+n/N$	$3/4n+n/N$
0 0 2n+1/2n+1	P31c	P-31c	P-62c	P-31c	P-62c
0 0 2n/2n+1	P3c1	P-3c1	P-6c2	P-3c1	P-6c2
0 0 2n+1/2n	P63	P63/m	P6322	P63/m	P6322

...or search for 3D group set

Type desired 3D space groups separated by space.

P-31c, P3c1, P63 Search

Search results
Click a record below to see 3+1D to 3D transformation

Complete match:

- P6/mcc(00g)s00s
- P63/mcm(00g)00ss
- P63/mcc(00g)00ss

Incomplete match (2 of 3):

- P6cc(00g)s0s
- P63cm(00g)0ss
- P63mc(00g)0ss

Incomplete match (1 of 3):

- P3m1(00g)0s0
- P3c1(00g)
- R3m(00g)0s
- R3c(00g)
- P-31m(00g)00s
- P-31c(00g)
- P-3m1(00g)
- P-3m1(00g)0s0

International Tables for Crystallography

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printed
tabulations
replaced ...

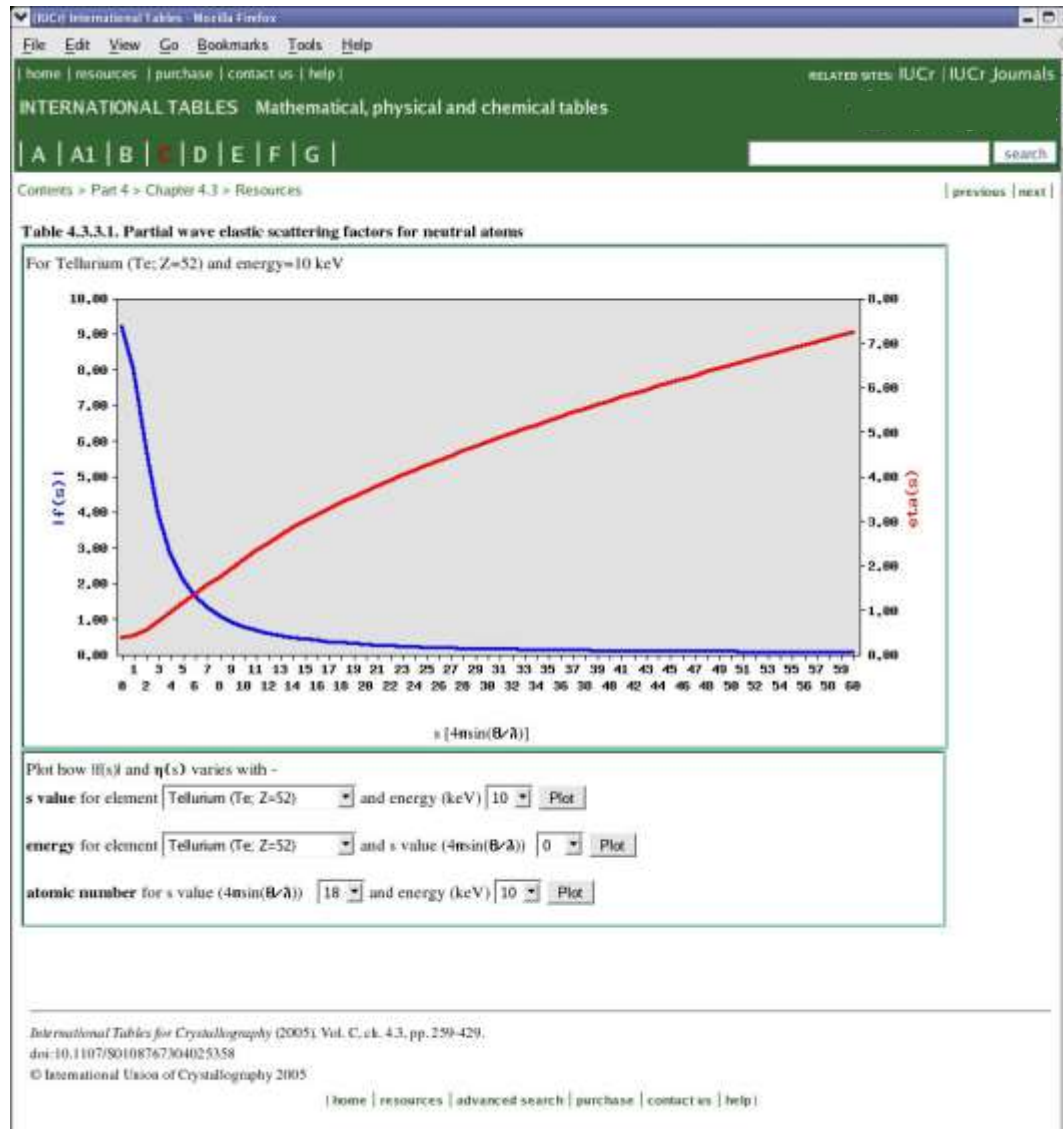
4. PRODUCTION AND PROPERTIES OF RADIATIONS

Table 4.3.3.1. Partial wave elastic scattering factors for neutral atoms
H, Z = 1

s	10 keV		40 keV		60 keV		90 keV	
	f(s)	g(s)	f(s)	g(s)	f(s)	g(s)	f(s)	g(s)
0	5.3956E-01	2.1835E-02	5.7106E-01	1.1403E-02	5.8301E-01	9.6111E-03	6.0222E-01	8.2636E-03
1	4.8779E-01	2.3657E-02	5.1682E-01	1.2341E-02	5.3150E-01	1.0365E-02	5.5125E-01	8.8468E-03
2	3.7546E-01	2.8959E-02	3.9784E-01	1.5102E-02	4.1121E-01	1.2624E-02	4.3188E-01	1.0053E-02
3	2.6708E-01	3.7159E-02	2.8276E-01	1.9391E-02	2.9248E-01	1.6207E-02	3.0790E-01	1.3658E-02
4	1.8733E-01	4.7200E-02	1.9824E-01	2.4676E-02	2.0522E-01	2.0617E-02	2.1554E-01	1.7432E-02
5	1.3383E-01	5.8258E-02	1.4159E-01	3.0404E-02	1.4658E-01	2.5411E-02	1.5436E-01	2.1443E-02
6	9.8468E-02	6.9249E-02	1.0417E-01	3.6154E-02	1.0784E-01	3.0211E-02	1.1349E-01	2.5524E-02
7	7.4696E-02	7.9743E-02	7.9010E-02	4.1905E-02	8.1814E-02	3.4784E-02	8.5989E-02	2.9037E-02
8	5.8260E-02	8.9502E-02	6.1621E-02	4.6690E-02	6.3789E-02	3.9055E-02	6.7184E-02	3.1990E-02
9	4.6554E-02	9.8462E-02	4.9235E-02	5.1360E-02	5.0981E-02	4.2952E-02	5.3638E-02	3.6328E-02
10	3.7970E-02	1.0665E-01	4.0156E-02	5.5626E-02	4.1569E-02	4.6555E-02	4.3702E-02	3.9995E-02
11	3.1489E-02	1.1414E-01	3.3300E-02	5.9529E-02	3.4468E-02	4.9806E-02	3.6249E-02	4.2156E-02
12	2.6551E-02	1.2100E-01	2.8077E-02	6.3104E-02	2.9065E-02	5.2796E-02	3.0577E-02	4.4678E-02
13	2.2685E-02	1.2732E-01	2.3987E-02	6.6395E-02	2.4832E-02	5.5549E-02	2.6126E-02	4.7004E-02
14	1.9591E-02	1.3316E-01	2.0715E-02	6.9437E-02	2.1445E-02	5.8097E-02	2.2568E-02	4.9144E-02
15	1.7086E-02	1.3858E-01	1.8065E-02	7.2263E-02	1.8702E-02	6.0463E-02	1.9680E-02	5.1163E-02
16	1.5030E-02	1.4364E-01	1.5891E-02	7.4898E-02	1.6451E-02	6.2669E-02	1.7307E-02	5.3039E-02
17	1.3322E-02	1.4838E-01	1.4085E-02	7.7366E-02	1.4581E-02	6.4736E-02	1.5344E-02	5.4773E-02
18	1.1889E-02	1.5283E-01	1.2569E-02	7.9685E-02	1.3012E-02	6.6678E-02	1.3692E-02	5.6427E-02
19	1.0674E-02	1.5703E-01	1.1285E-02	8.1873E-02	1.1682E-02	6.8509E-02	1.2290E-02	5.7987E-02
20	9.6165E-03	1.6100E-01	1.0188E-02	8.3943E-02	1.0546E-02	7.0243E-02	1.1097E-02	5.9439E-02
21	8.7427E-03	1.6477E-01	9.2423E-03	8.5908E-02	9.5673E-03	7.1887E-02	1.0067E-02	6.0840E-02
22	7.9675E-03	1.6836E-01	8.4206E-03	8.7776E-02	8.7186E-03	7.3452E-02	9.1718E-03	6.2174E-02
23	7.2908E-03	1.7178E-01	7.7070E-03	8.9558E-02	7.9778E-03	7.4943E-02	8.3943E-03	6.3421E-02
24	6.6968E-03	1.7505E-01	7.0789E-03	9.1261E-02	7.3275E-03	7.6369E-02	7.7096E-03	6.4635E-02
25	6.1724E-03	1.7818E-01	6.5244E-03	9.2892E-02	6.7534E-03	7.7754E-02	7.1041E-03	6.5801E-02
26	5.7072E-03	1.8118E-01	6.0325E-03	9.4456E-02	6.2442E-03	7.9043E-02	6.5697E-03	6.6894E-02
27	5.2927E-03	1.8407E-01	5.5942E-03	9.5959E-02	5.7904E-03	8.0301E-02	6.0920E-03	6.7965E-02
28	4.9217E-03	1.8685E-01	5.2019E-03	9.7406E-02	5.3842E-03	8.1512E-02	5.6635E-03	6.9001E-02
29	4.5884E-03	1.8952E-01	4.8494E-03	9.8800E-02	5.0193E-03	8.2679E-02	5.2805E-03	6.9973E-02
30	4.2878E-03	1.9211E-01	4.5116E-03	1.0014E-01	4.6903E-03	8.3805E-02	4.9342E-03	7.0931E-02
31	4.0157E-03	1.9460E-01	4.2440E-03	1.0145E-01	4.3925E-03	8.4893E-02	4.6200E-03	7.1865E-02
32	3.7688E-03	1.9702E-01	3.9829E-03	1.0270E-01	4.1222E-03	8.5946E-02	4.3363E-03	7.2741E-02
33	3.5440E-03	1.9936E-01	3.7451E-03	1.0392E-01	3.8760E-03	8.6966E-02	4.0773E-03	7.3607E-02
34	3.3387E-03	2.0162E-01	3.5280E-03	1.0510E-01	3.6513E-03	8.7954E-02	3.8401E-03	7.4456E-02
35	3.1507E-03	2.0382E-01	3.3293E-03	1.0625E-01	3.4455E-03	8.8913E-02	3.6241E-03	7.5254E-02
36	2.9781E-03	2.0598E-01	3.1468E-03	1.0736E-01	3.2566E-03	8.9845E-02	3.4254E-03	7.6044E-02
37	2.8194E-03	2.0804E-01	2.9790E-03	1.0844E-01	3.0828E-03	9.0751E-02	3.2419E-03	7.6823E-02
38	2.6736E-03	2.1006E-01	2.8242E-03	1.0949E-01	2.9236E-03	9.1631E-02	3.0738E-03	7.7585E-02
39	2.5377E-03	2.1202E-01	2.6812E-03	1.1052E-01	2.7745E-03	9.2485E-02	2.9180E-03	7.8328E-02
40	2.4124E-03	2.1394E-01	2.5487E-03	1.1152E-01	2.6374E-03	9.3344E-02	2.7732E-03	7.9002E-02
41	2.2962E-03	2.1581E-01	2.4258E-03	1.1249E-01	2.5101E-03	9.4138E-02	2.6397E-03	7.9679E-02
42	2.1882E-03	2.1763E-01	2.3116E-03	1.1344E-01	2.3919E-03	9.4934E-02	2.5153E-03	8.0351E-02
43	2.0876E-03	2.1941E-01	2.2053E-03	1.1437E-01	2.2818E-03	9.5709E-02	2.3991E-03	8.1021E-02
44	1.9939E-03	2.2115E-01	2.1061E-03	1.1527E-01	2.1791E-03	9.6466E-02	2.2913E-03	8.1649E-02
45	1.9062E-03	2.2284E-01	2.0134E-03	1.1616E-01	2.0832E-03	9.7207E-02	2.1905E-03	8.2275E-02
46	1.8243E-03	2.2451E-01	1.9268E-03	1.1702E-01	1.9935E-03	9.7931E-02	2.0957E-03	8.2901E-02
47	1.7475E-03	2.2613E-01	1.8456E-03	1.1787E-01	1.9095E-03	9.8638E-02	2.0075E-03	8.3489E-02
48	1.6755E-03	2.2771E-01	1.7694E-03	1.1870E-01	1.8306E-03	9.9331E-02	1.9246E-03	8.4073E-02
49	1.6078E-03	2.2927E-01	1.6979E-03	1.1951E-01	1.7565E-03	1.0001E-01	1.8463E-03	8.4662E-02
50	1.5441E-03	2.3080E-01	1.6306E-03	1.2030E-01	1.6868E-03	1.0068E-01	1.7732E-03	8.5214E-02
51	1.4842E-03	2.3229E-01	1.5672E-03	1.2108E-01	1.6212E-03	1.0133E-01	1.7042E-03	8.5761E-02
52	1.4277E-03	2.3376E-01	1.5074E-03	1.2184E-01	1.5593E-03	1.0197E-01	1.6388E-03	8.6315E-02
53	1.3743E-03	2.3519E-01	1.4510E-03	1.2259E-01	1.5009E-03	1.0259E-01	1.5775E-03	8.6837E-02
54	1.3239E-03	2.3660E-01	1.3977E-03	1.2333E-01	1.4457E-03	1.0321E-01	1.5195E-03	8.7353E-02
55	1.2762E-03	2.3798E-01	1.3473E-03	1.2405E-01	1.3935E-03	1.0381E-01	1.4644E-03	8.7876E-02
56	1.2311E-03	2.3934E-01	1.2995E-03	1.2476E-01	1.3441E-03	1.0440E-01	1.4125E-03	8.8368E-02
57	1.1882E-03	2.4068E-01	1.2543E-03	1.2545E-01	1.2972E-03	1.0499E-01	1.3633E-03	8.8858E-02
58	1.1476E-03	2.4199E-01	1.2113E-03	1.2614E-01	1.2528E-03	1.0556E-01	1.3162E-03	8.9357E-02
59	1.1091E-03	2.4327E-01	1.1706E-03	1.2681E-01	1.2105E-03	1.0612E-01	1.2719E-03	8.9826E-02
60	1.0724E-03	2.4454E-01	1.1319E-03	1.2746E-01	1.1705E-03	1.0667E-01	1.2301E-03	9.0263E-02

International Tables for Crystallography

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Structure Reports

- Pre-electronic abstracting and indexing
- Now defunct (electronic search engines)
- Precursor to structural databases (CSD, PDB, COD, ICSD etc.)

- *Structure Reports for 1940-1950, Volumes 8-13: Metals, Inorganic and Organic Sections* by A. J. Pearson
- *Structure Reports for 1951-1960, Volumes 15-24 Cumulative Index for 1951-1960, Volume 25: Metals* by A. J. Pearson
- *Structure Reports for 1961, Volume 26: Metals, Inorganic and Organic Sections* by W. B. Pearson
- *Structure Reports for 1962, Volume 27: Metals, Inorganic and Organic Sections* by W. B. Pearson
- *Structure Reports for 1963, Volume 28: Metals, Inorganic and Organic Sections* by W. B. Pearson
- *Structure Reports for 1964, Volume 29: Metals, Inorganic and Organic Sections* by W. B. Pearson
- *Structure Reports for 1965, Volume 30A: Metals and Inorganic Sections* by W. B. Pearson, H. W. Pearson
- *Structure Reports for 1965, Volume 30B: Organic Section* by W. B. Pearson and A. W. Hanson
- *Structure Reports for 1966, Volume 31A: Metals and Inorganic Sections* by W. B. Pearson and J. Trotter
- *Structure Reports for 1966, Volume 31B: Organic Section* by W. B. Pearson and J. Trotter
- *Structure Reports for 1967, Volume 32A: Metals and Inorganic Sections* by W. B. Pearson, C. B. Pearson
- *Structure Reports for 1967, Volume 32B: Organic Section* by W. B. Pearson and G. Ferguson
- *Structure Reports for 1968, Volume 33A: Metals and Inorganic Sections* by W. B. Pearson, C. B. Pearson
- *Structure Reports for 1968, Volume 33B: Organic Section* by W. B. Pearson and J. Trotter
- *Structure Reports for 1969, Volume 34A: Metals and Inorganic Sections* by W. B. Pearson, C. B. Pearson
- *Structure Reports for 1969, Volume 34B: Organic Section* by W. B. Pearson and J. Trotter
- *Structure Reports for 1970, Volume 35A: Metals and Inorganic Sections* by W. B. Pearson, L. D. Searles
- *Structure Reports for 1970, Volume 35B: Organic Section* by W. B. Pearson and J. Trotter
- *Structure Reports, Volume 36: Cumulative Index for 1961-1970* by W. B. Pearson, N. E. Sennema

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However and correction for this increases the bond length to 1.46 Å crystal molecules are linked into dimers about centres of symmetry. Hydrogen bonds (2.85 Å).

1. Structure Reports, 30B, 115.

10aα-CFAM0-1a,4αp-ODMETHYL-7-ETHOXY-2a-METHOXY-1,2,3,4,6a,9,10,10a-OCTAHYDRO-1a-PHENANTHRENE

$C_{22}H_{22}NO_3$

R. H. STANFORD and T. C. McELENIE, 1974. Acta Cryst., B30, 421

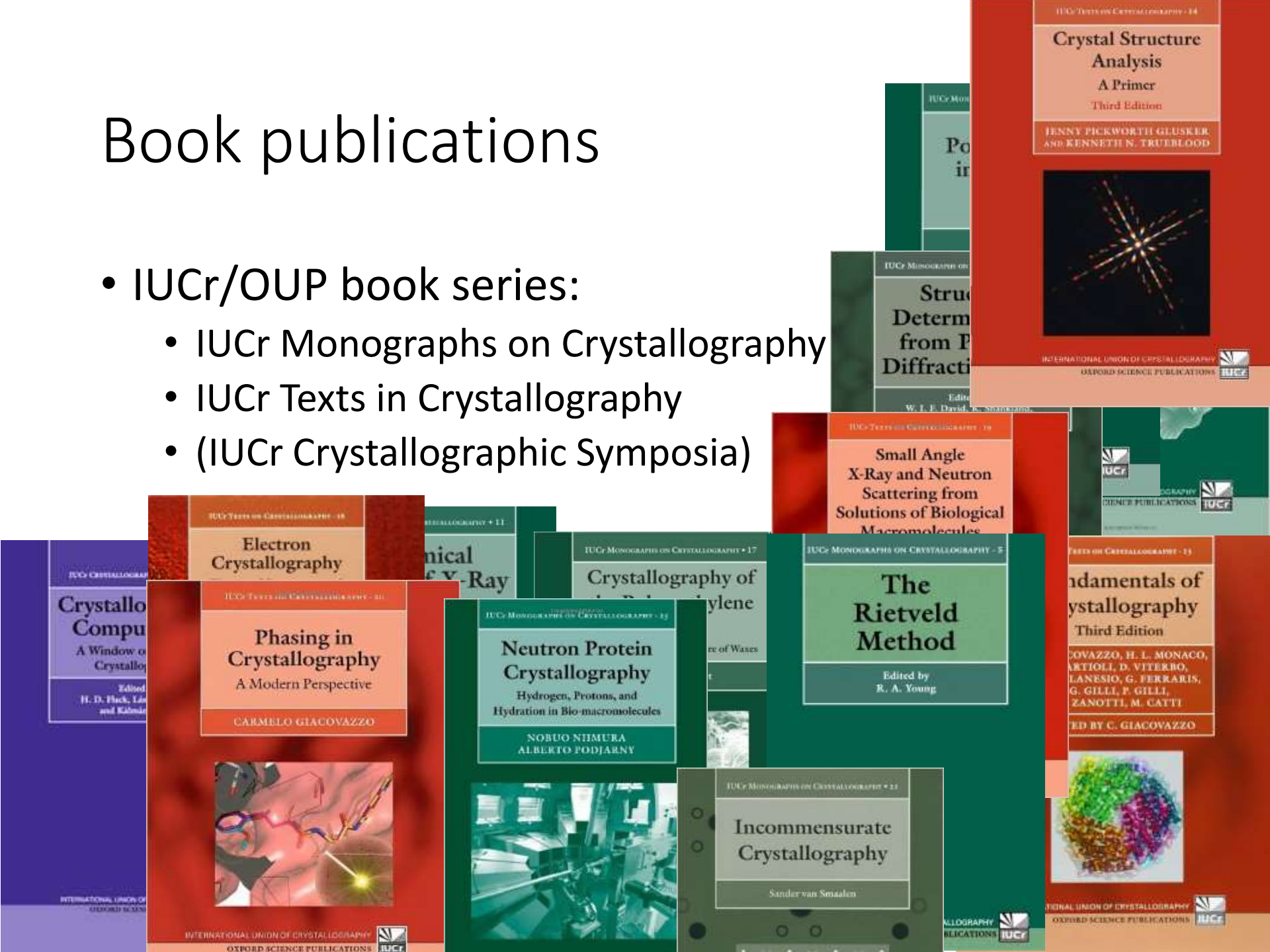
Monoclinic, $P2_1/a$, $a = 15.188$, $b = 7.144$, $c = 27.884$, $\beta = 107.11^\circ$, D_4 . Cu radiation, $\lambda = 0.801$ for 2829 reflections.

The molecule has a chair conformation with the hydroxyl group O (Fig. 1); the torsion angle O(21)-C(1)-C(12)-H is -174° . There is an interaction between O(21) and a hydrogen atom attached to C(17) and this C(17) to twist away from the angular methyl group. The ring containing group is further distorted because of an intramolecular hydrogen bond and D(21). The six atoms of the aromatic ring are planar but the three nitro atoms are displaced from this plane, especially C(16) (deviation

Fig. 1. The conformation of $C_{22}H_{22}NO_3$.

Book publications

- IUCr/OUP book series:
 - IUCr Monographs on Crystallography
 - IUCr Texts in Crystallography
 - (IUCr Crystallographic Symposia)



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- Acta Cryst. A**: FOUNDATIONS ADVANCES
- Acta Cryst. B**: STRUCTURAL SCIENCE, CRYSTAL ENGINEERING, MATERIALS
- Acta Cryst. C**: STRUCTURAL CHEMISTRY
- Acta Cryst. D**: BIOLOGICAL CRYSTALLOGRAPHY
- Acta Cryst. E**: CRYSTALLOGRAPHIC COMMUNICATIONS
- Acta Cryst. F**: STRUCTURAL BIOLOGY COMMUNICATIONS
- Appl. Cryst.**: JOURNAL OF APPLIED CRYSTALLOGRAPHY
- Synchrotron**: JOURNAL OF SYNCHROTRON RADIATION
- IUCrJ**: IUCr

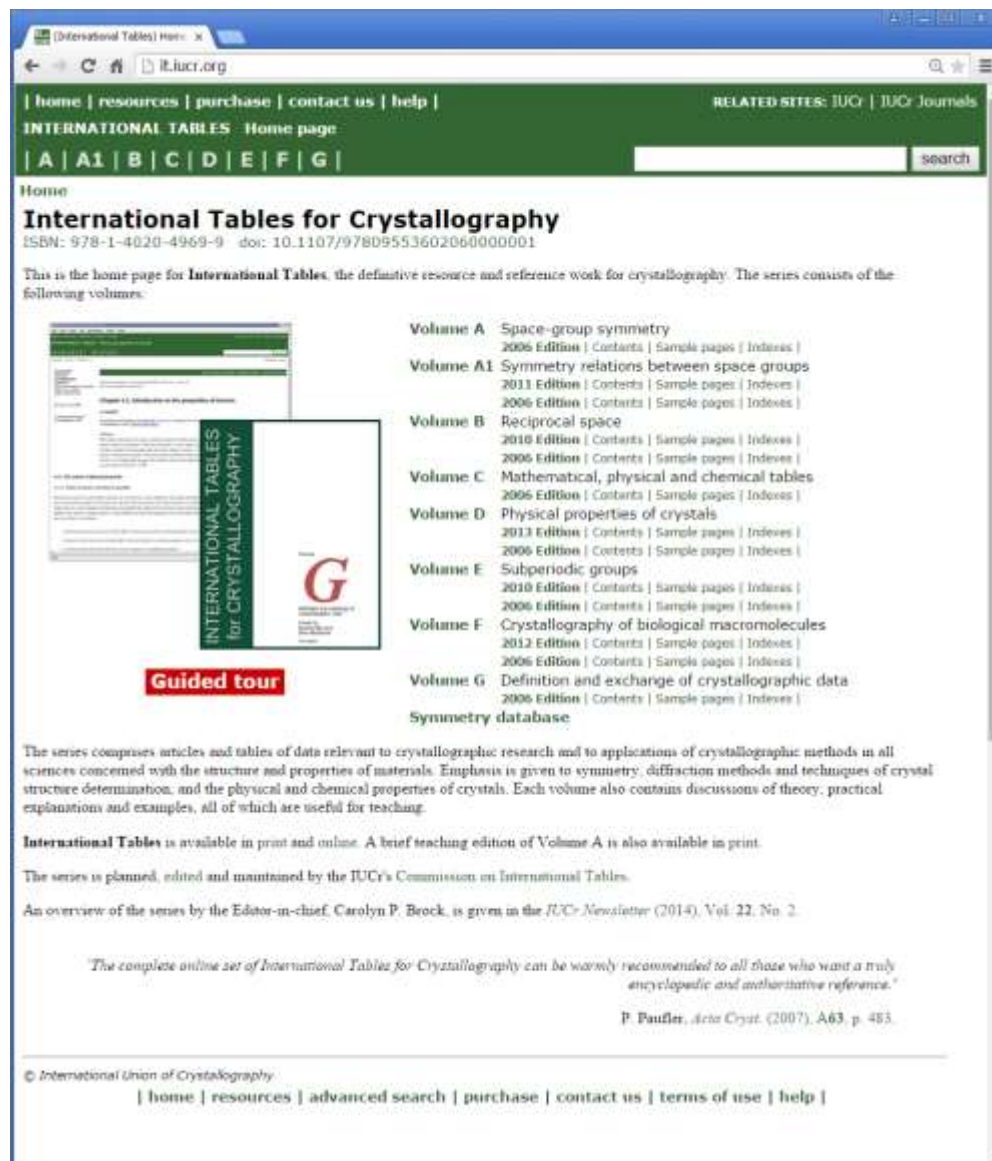
Below the grid, a featured research paper is highlighted with a green 'RESEARCH PAPERS' icon. The title is 'Structure, hydrogen bonding and thermal expansion'. The abstract text reads: 'Single-crystal neutron diffraction, ab initio calculations and Raman spectroscopy are applied to understand the structure and hydrogen bonding of ammonium carbonate monohydrate, a till now poorly characterised substance, particularly in relation to other ammonium-bearing compounds.' To the left of the text is a 2D map showing the distribution of hydrogen atoms in the structure, with a color scale from blue (low density) to red (high density). A 'Read more' link is provided below the figure.

At the bottom, another 'RESEARCH PAPERS' section is visible, with the title 'Human norovirus polymerase'.

On the right side of the page, there is a red banner for the '2014 International year of crystallography' and a section titled 'Editorial Boards of IUCr Journals' listing various sections and their respective editors. Below that, a 'News and jobs' section lists several opportunities, including a Postdoctoral Position at CHESS, a Post-Doctoral Fellow position, a PhD Thesis Student position, and a Beamline Scientist position.

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The screenshot shows the homepage of the International Tables for Crystallography website. The browser address bar displays it.iucr.org. The navigation menu includes links for home, resources, purchase, contact us, and help. The main heading is "INTERNATIONAL TABLES Home page" with a search bar and a search button. Below the heading, there are links for volumes A through G. The "Home" section features the title "International Tables for Crystallography" with ISBN and DOI information. A paragraph describes the series as the definitive resource and reference work for crystallography. A "Guided tour" button is visible. A list of volumes (A through G) is provided, each with links to editions, contents, sample pages, and indexes. A quote from P. Paufler is included at the bottom, along with the copyright notice for the International Union of Crystallography.

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INTERNATIONAL TABLES Home page

| A | A1 | B | C | D | E | F | G | search

Home

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ISBN: 978-1-4020-4969-9 doi: 10.1107/97809553602060000001

This is the home page for **International Tables**, the definitive resource and reference work for crystallography. The series consists of the following volumes:



Volume A Space-group symmetry
2006 Edition | Contents | Sample pages | Indexes |

Volume A1 Symmetry relations between space groups
2011 Edition | Contents | Sample pages | Indexes |
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Volume B Reciprocal space
2010 Edition | Contents | Sample pages | Indexes |
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Volume D Physical properties of crystals
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International Tables is available in print and online. A brief teaching edition of Volume A is also available in print.

The series is planned, edited and maintained by the IUCr's Commission on International Tables.

An overview of the series by the Editor-in-chief, Carolyn P. Beckett, is given in the *IUCr Newsletter* (2014), Vol. 22, No. 2.

The complete online set of International Tables for Crystallography can be warmly recommended to all those who want a truly encyclopaedic and authoritative reference.

P. Paufler, *Acta Cryst.* (2007), A63, p. 483.

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The screenshot shows the IUCr website homepage. At the top, there is a navigation bar with links for journals, books, news, education, people, resources, and iucr2014. Below this is a header section with the IUCr logo and the text "International Union of CRYSTALLOGRAPHY". A search bar is located on the right side of the header.

The main content area is divided into several sections:

- Research news:** A section titled "Combined effort for structural determination" with a sub-heading "Making carbonylase friends". It includes a "SHARE" button and a small image of a protein structure.
- Regional Associate meetings:** A banner for the ACA (Asian Crystallographic Association) meeting in Hyderabad, India, from 3-8 December 2013.
- Legacy Conference:** A banner for the "IUCr Legacy Conference: Crystallography for the Next Generation" in Rabat, Morocco, from 22-24 April 2015.
- 2014 International Year of Crystallography:** A red banner celebrating the 100th anniversary of the IUCr, with the text "Crystallography for the next generation: the legacy of IUCr" and "22-24 April 2015, Rabat II Academy of Science and Technology, Rabat, Morocco".
- Log in to your entry in the World Directory:** A login form with fields for "IUCr ID" (2895) and "Password", and a "Log in" button.
- Latest notices:** A section with two notices: "DIALS DEALS workshop - Diffraction Integration for Advanced Light Sources: Roring, Creative 23rd Aug 2015" and "DAWN: Automating and Simplifying Reduction of 3D powder diffraction data with DAWN, ECM28 satellite: Roring, Creative 23rd Aug 2013".
- Pedagogical Position at CHESS: Complex Electronic Materials:** A notice from Bhatia NY dated 23rd Aug 2013.
- Post-Doctoral Fellow for the high resolution powder diffraction:** A notice from Gumbale dated 23rd Aug 2013.

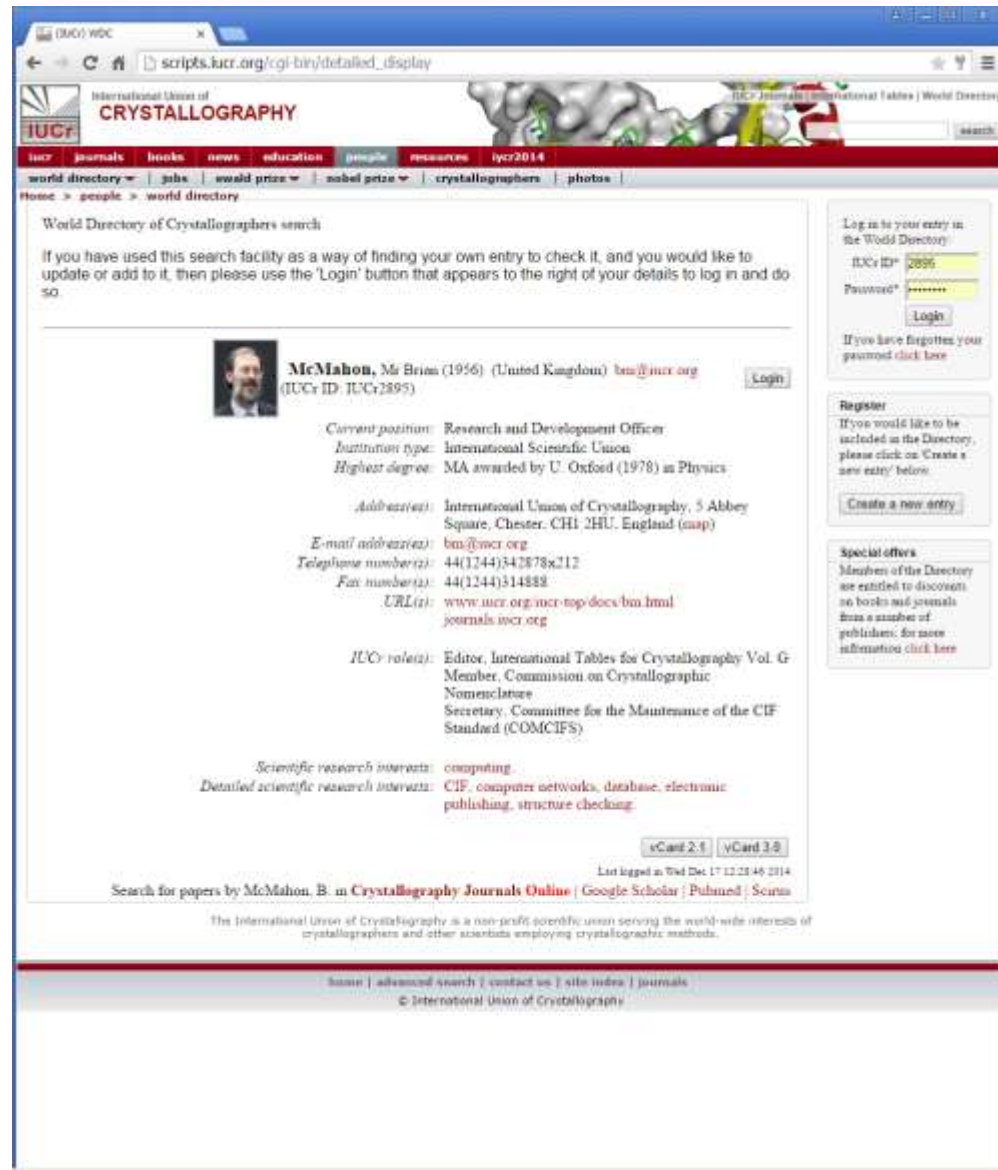
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- International Year of Crystallography
 - <http://www.iycr2014.org>

The screenshot shows the homepage of the International Year of Crystallography 2014 website. The browser address bar displays 'www.iycr2014.org'. The main navigation menu includes 'home', 'about', 'events', 'opportunities', 'activities', 'sponsors', 'participate', and 'learn'. A prominent red banner at the top reads 'Crystallography matters ... more!' and 'events and outcomes from the international year of crystallography 2014'. Below the banner, the page is organized into several columns. On the left, there is a section for 'IUCr Supporters' divided into 'Commercial' and 'Organisations', with logos for various institutions like ICSU, IMAAS, and IAP. The middle column features a 'Plans for 2015 and beyond ...' section with a 'click here to explore future initiatives' link, followed by a 'Latest news' section. The news section includes a headline 'UNESCO Associated Schools Network: Laureates of the crystal growing competition announced' and a sub-headline 'Under the High Patronage of the King Mohamed VI'. The right column contains 'Coming events' with details for 'Crystallography for the next generation: the legacy of IUCr' in Rabat, Morocco, and 'Bruker OpenLab' events in Algeria and Tunisia. At the bottom right, there is a section for 'IUCr awarded ICSU grant'.

IUCr web sites

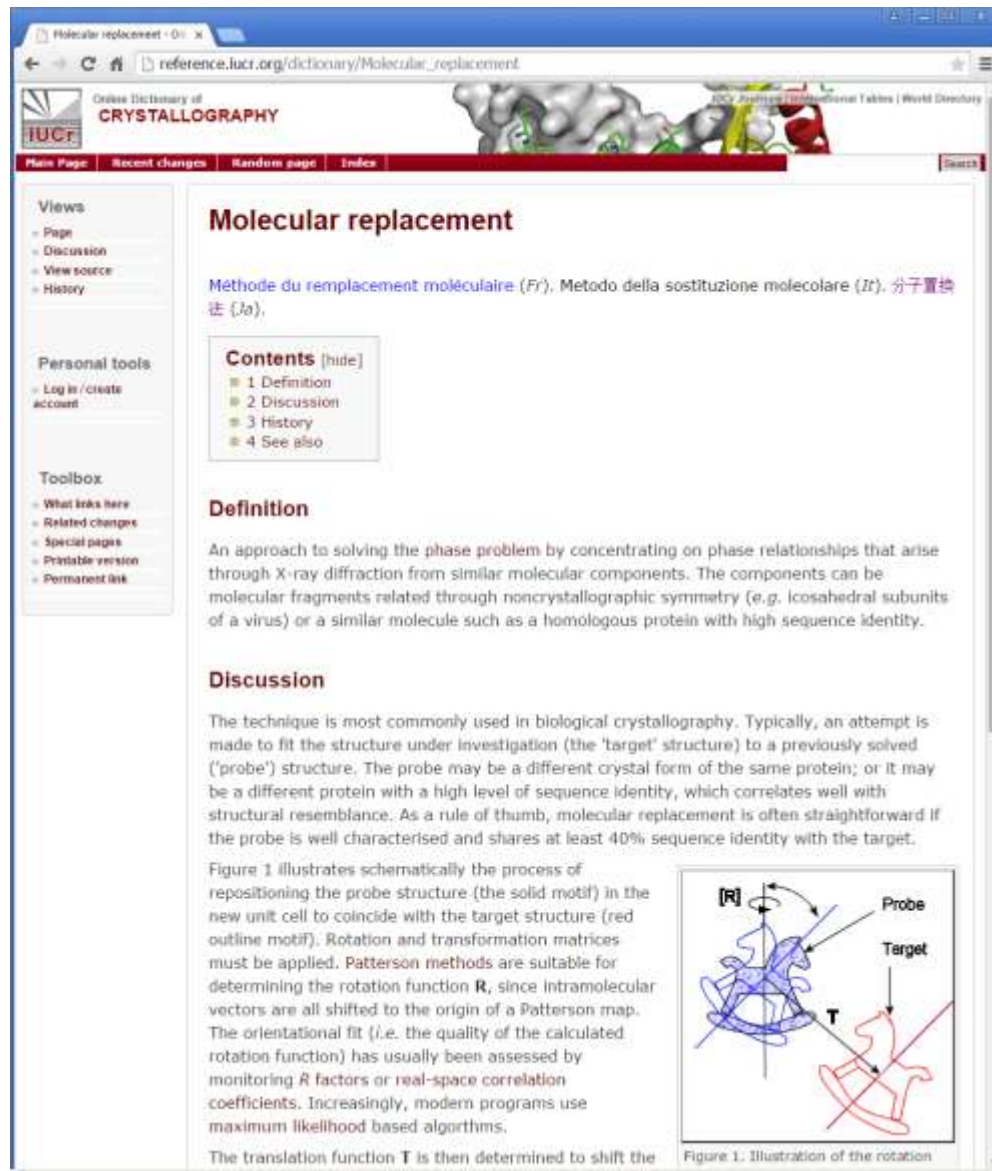
- Crystallography Journals Online
- International Tables Online
- International Union of Crystallography
- International Year of Crystallography
- World Directory of Crystallographers
 - <http://wdc.iucr.org>



The screenshot shows the IUCr World Directory of Crystallographers search results page for Brian McMahon. The page is titled "World Directory of Crystallographers search" and includes a search bar and a "Login" button. The profile information for Brian McMahon is displayed, including his name, birth year (1956), location (United Kingdom), and IUCr ID (IUCr ID: IUCr2895). His current position is Research and Development Officer at the International Scientific Union. His highest degree is a MA awarded by U. Oxford (1978) in Physics. His address is International Union of Crystallography, 5 Abbey Square, Chester, CH1 2HU, England. His email address is bm@iucr.org, and his telephone and fax numbers are 44(1244)542878x212 and 44(1244)514888, respectively. His URL is www.iucr.org/iucr-top/docs/bm.html. His IUCr role is Editor, International Tables for Crystallography Vol. G Member, Commission on Crystallographic Nomenclature Secretary, Committee for the Maintenance of the CIF Standard (COMCIFS). His scientific research interests are computing, and his detailed scientific research interests are CIF, computers networks, database, electronic publishing, structure checking. The page also includes a "Register" section and a "Special offers" section. The footer of the page contains the IUCr logo and contact information.

IUCr web sites

- Crystallography Journals Online
- International Tables Online
- International Union of Crystallography
- International Year of Crystallography
- World Directory of Crystallographers
- Online Dictionary of Crystallography
 - <http://reference.iucr.org>



The screenshot shows a web browser window displaying the IUCr Online Dictionary of Crystallography page for "Molecular replacement". The page title is "Molecular replacement" and the URL is "reference.iucr.org/dictionary/Molecular_replacement". The page content includes a navigation menu, a sidebar with "Views", "Personal tools", and "Toolbox", and the main article text. The article is titled "Molecular replacement" and includes a definition, a discussion, and a schematic diagram (Figure 1) illustrating the process of repositioning a probe structure to coincide with a target structure.

Molecular replacement

Méthode du remplacement moléculaire (*Fr*), Metodo della sostituzione molecolare (*It*), 分子置換法 (*Ja*).

Contents [hide]

- 1 Definition
- 2 Discussion
- 3 History
- 4 See also

Definition

An approach to solving the phase problem by concentrating on phase relationships that arise through X-ray diffraction from similar molecular components. The components can be molecular fragments related through noncrystallographic symmetry (e.g. icosahedral subunits of a virus) or a similar molecule such as a homologous protein with high sequence identity.

Discussion

The technique is most commonly used in biological crystallography. Typically, an attempt is made to fit the structure under investigation (the 'target' structure) to a previously solved ('probe') structure. The probe may be a different crystal form of the same protein; or it may be a different protein with a high level of sequence identity, which correlates well with structural resemblance. As a rule of thumb, molecular replacement is often straightforward if the probe is well characterised and shares at least 40% sequence identity with the target.

Figure 1 illustrates schematically the process of repositioning the probe structure (the solid motif) in the new unit cell to coincide with the target structure (red outline motif). Rotation and transformation matrices must be applied. Patterson methods are suitable for determining the rotation function R , since intramolecular vectors are all shifted to the origin of a Patterson map. The orientational fit (i.e. the quality of the calculated rotation function) has usually been assessed by monitoring R factors or real-space correlation coefficients. Increasingly, modern programs use maximum likelihood based algorithms.

The translation function T is then determined to shift the

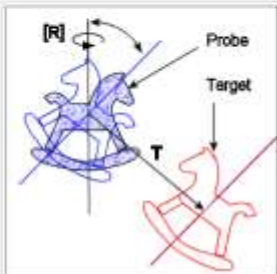
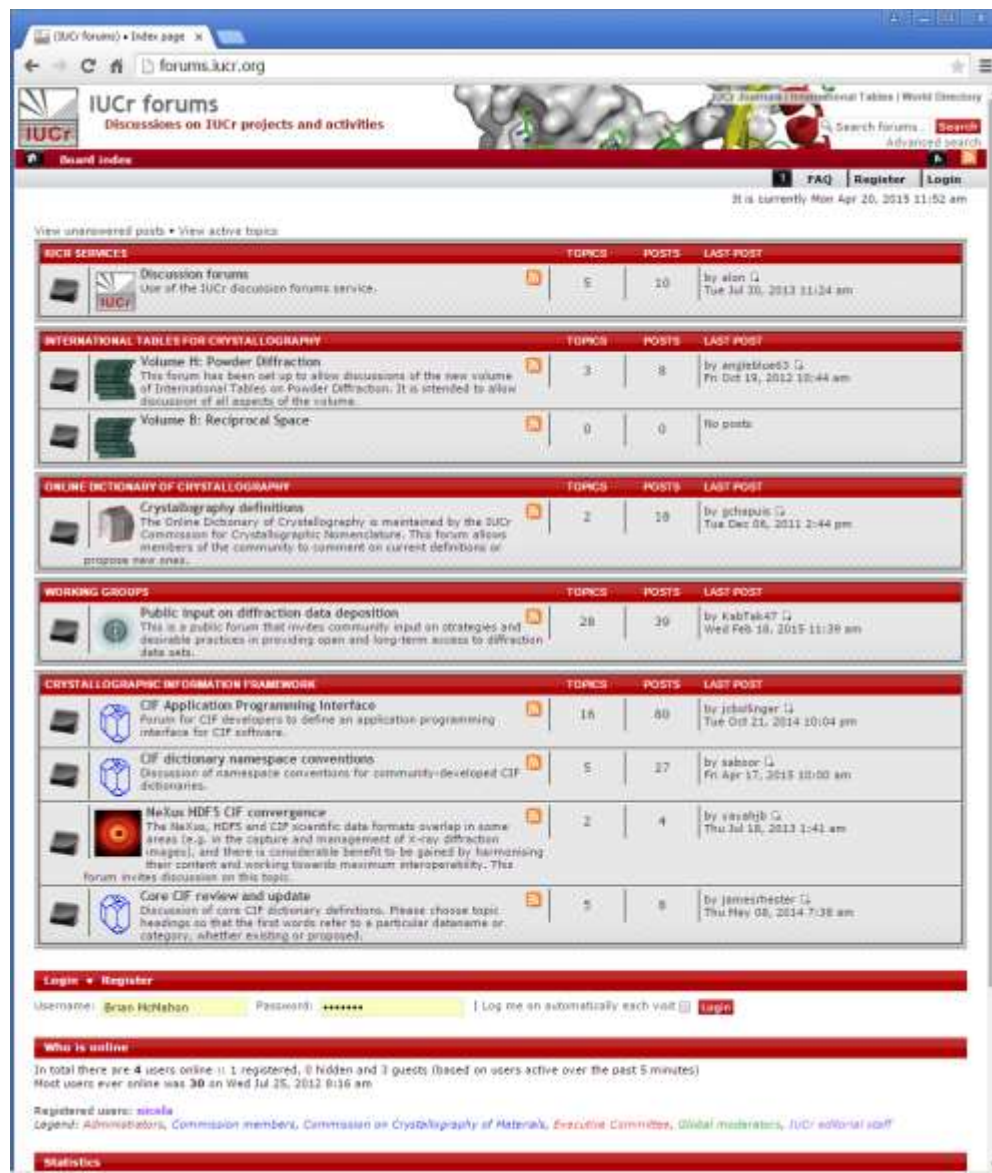


Figure 1. Illustration of the rotation

IUCr web sites

- Crystallography Journals Online
- International Tables Online
- International Union of Crystallography
- International Year of Crystallography
- World Directory of Crystallographers
- Online Dictionary of Crystallography
- Discussion forums
 - <http://forums.iucr.org>



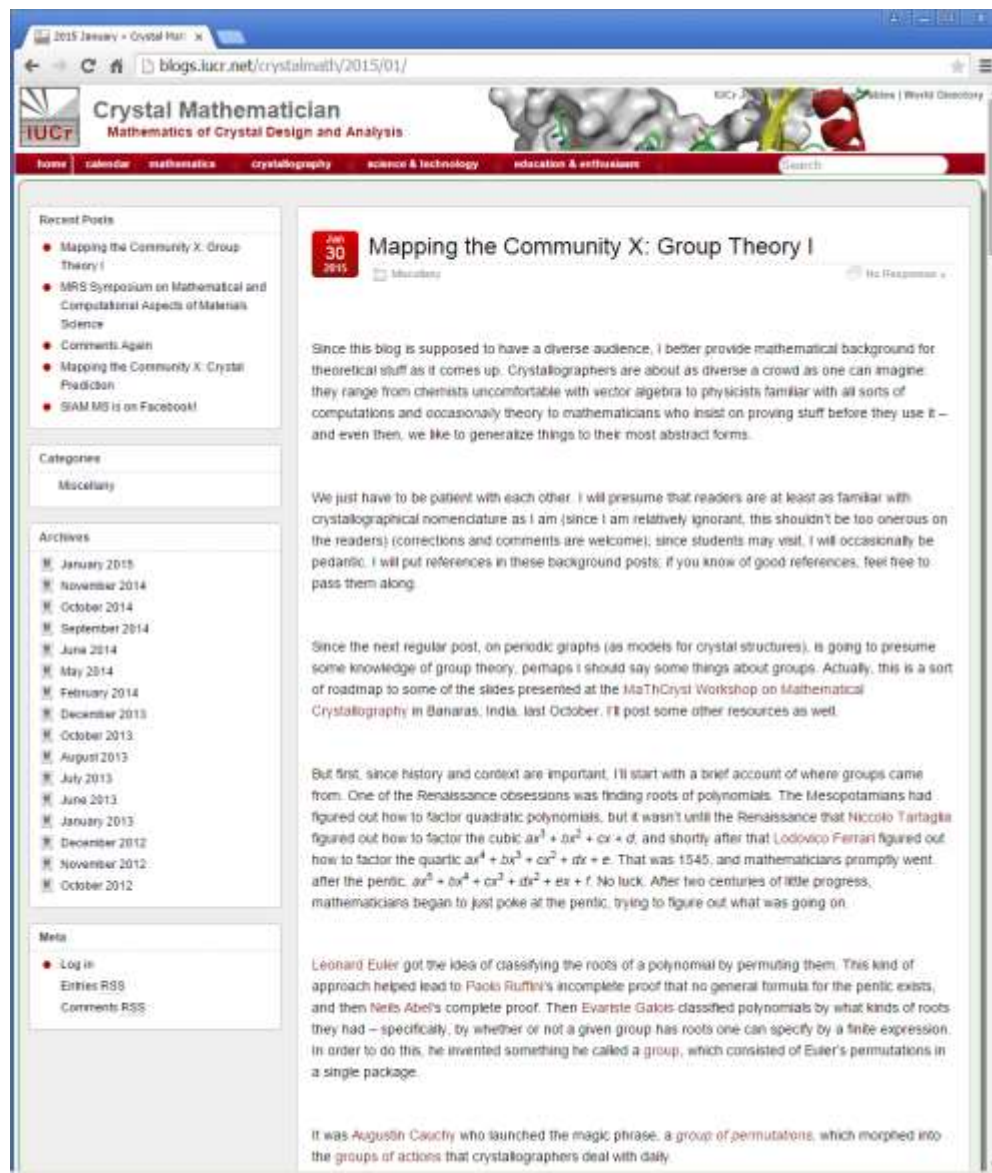
The screenshot shows the IUCr forums website interface. The header includes the IUCr logo, the text "IUCr forums Discussions on IUCr projects and activities", and a search bar. Below the header, there are navigation links for "Board index", "FAQ", "Register", and "Login". The main content area displays a list of forum topics, each with a category icon, a title, a description, and statistics for topics, posts, and last post.

Category	Topic	Topics	Posts	Last Post
RICR SERVICES	Discussion forums Use of the IUCr discussion forums service.	5	10	by alan 1 Tue Jul 30, 2013 11:24 am
INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY	Volume H: Powder Diffraction This forum has been set up to allow discussions of the new volume of International Tables on Powder Diffraction. It is intended to allow discussion of all aspects of the volume.	3	8	by angblued3 1 Fri Oct 19, 2012 10:44 am
	Volume B: Reciprocal Space	0	0	No posts
ONLINE DICTIONARY OF CRYSTALLOGRAPHY	Crystallography definitions The Online Dictionary of Crystallography is maintained by the IUCr Commission for Crystallographic Nomenclature. This forum allows members of the community to comment on current definitions or propose new ones.	2	10	by jchrisp 1 Tue Dec 05, 2011 2:44 pm
WORKING GROUPS	Public input on diffraction data deposition This is a public forum that invites community input on strategies and desirable practices in providing open and long-term access to diffraction data sets.	28	29	by kabFeb47 1 Wed Feb 10, 2015 11:39 am
CRYSTALLOGRAPHIC INFORMATION FRAMEWORK	CIF Application Programming Interface Forum for CIF developers to define an application programming interface for CIF software.	16	80	by jrbfing 1 Tue Oct 21, 2014 10:04 pm
	CIF dictionary namespace conventions Discussion of namespace conventions for community-developed CIF dictionaries.	5	27	by sabhor 1 Fri Apr 17, 2015 10:00 am
	NeXus HDF5 CIF convergence The NeXus, HDF5 and CIF scientific data formats overlap in some areas (e.g. in the capture and management of X-ray diffraction images), and there is considerable benefit to be gained by harmonising their content and working towards maximum interoperability. This forum invites discussion on this topic.	2	4	by vashjib 1 Thu Jul 18, 2013 1:41 am
	Core CIF review and update Discussion of core CIF dictionary definitions. Please choose topic headings so that the first words refer to a particular dataname or category, whether existing or proposed.	5	8	by jameshester 1 Thu May 08, 2014 7:38 am

At the bottom of the page, there is a login section with fields for "Username" (Brian Hefeban) and "Password" (masked with asterisks), a "Log me in automatically each visit" checkbox, and a "Login" button. Below the login section, there is a "Who is online" section stating "In total there are 4 users online (1 registered, 0 hidden and 3 guests (based on users active over the past 5 minutes). Most users ever online was 30 on Wed Jul 25, 2012 9:16 am." and a "Registered users" section listing "nicola". A legend at the bottom identifies user roles: Administrators, Commission members, Commission on Crystallography of Materials, Executive Committee, Global moderators, IUCr editorial staff, and Statistics.

IUCr web sites

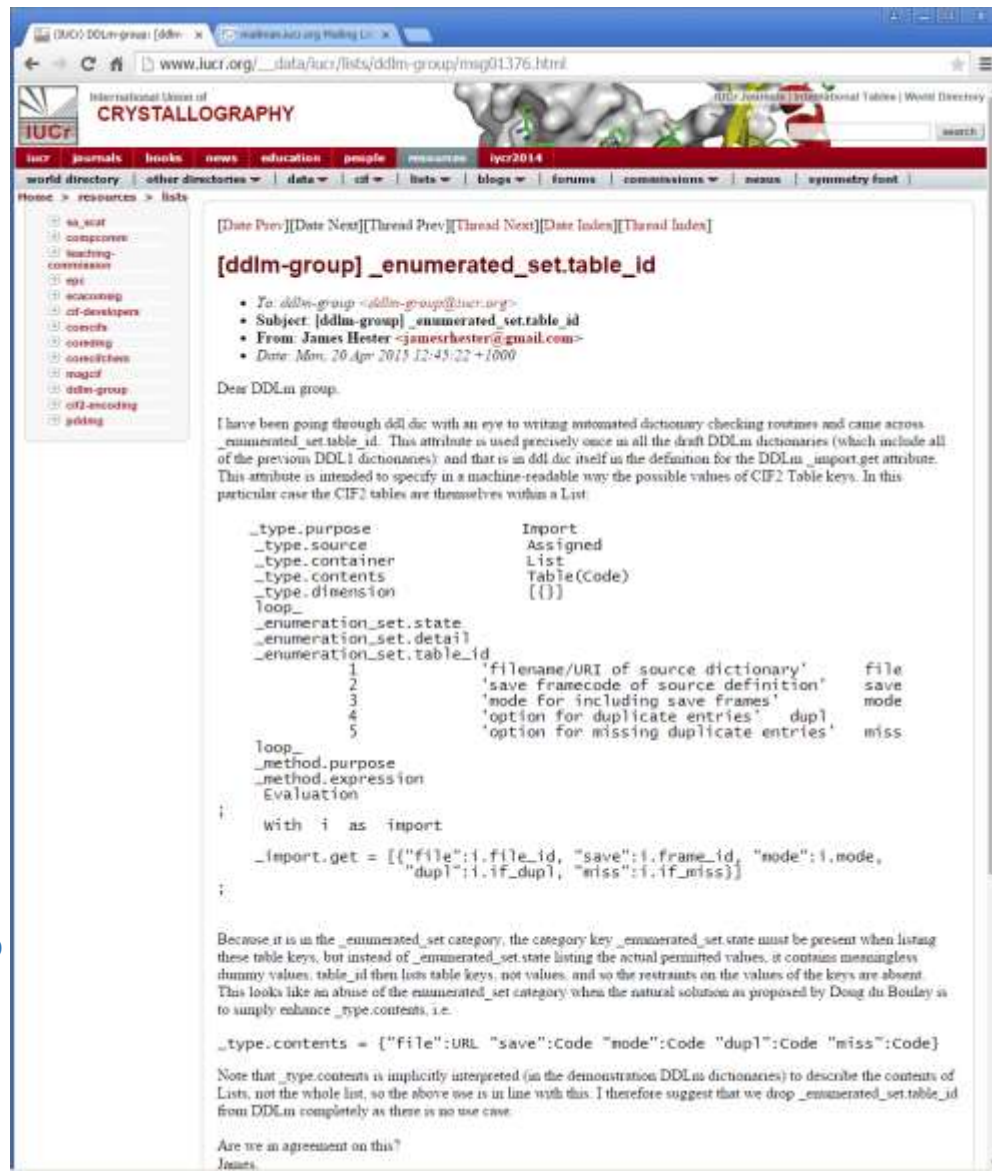
- Crystallography Journals Online
- International Tables Online
- International Union of Crystallography
- International Year of Crystallography
- World Directory of Crystallographers
- Online Dictionary of Crystallography
- Discussion forums
- Blogs
 - <http://blogs.iucr.net>
 - <http://blogs.iucr.org>



The screenshot shows a web browser window displaying a blog post on the 'Crystal Mathematician' website. The browser's address bar shows the URL blogs.iucr.net/crystalmath/2015/01/. The page header includes the IUCr logo and the title 'Crystal Mathematician: Mathematics of Crystal Design and Analysis'. A navigation menu at the top lists 'home', 'calendar', 'mathematics', 'crystallography', 'science & technology', 'education & activities', and a search bar. The main content area features a post titled 'Mapping the Community X: Group Theory I' dated January 30, 2015. The post text discusses the blog's audience, the historical context of group theory, and the author's plans for future posts. The sidebar on the left contains sections for 'Recent Posts', 'Categories' (listing 'Miscellany'), 'Archives' (listing months from January 2015 to October 2012), and 'Meta' (with links for 'Log in', 'Entries RSS', and 'Comments RSS').

IUCr web sites

- Crystallography Journals Online
- International Tables Online
- International Union of Crystallography
- International Year of Crystallography
- World Directory of Crystallographers
- Online Dictionary of Crystallography
- Discussion forums
- Blogs
- Email discussion lists
 - <http://mailman.iucr.org/mailman/listinfo>



The screenshot shows a web browser window displaying an email from the IUCr mailing list. The page header includes the IUCr logo and navigation links. The email subject is "[ddlm-group]_enumerated_set.table_id" and is dated Monday, 20 April 2010. The body of the email discusses the use of the `_enumerated_set.table_id` attribute in DDLm dictionaries and includes a table of its attributes and their import values.

Attribute	Import
<code>_type.purpose</code>	Assigned
<code>_type.source</code>	List
<code>_type.container</code>	Table(Code)
<code>_type.contents</code>	{}
<code>_type.dimension</code>	
<code>Loop_</code>	
<code>_enumeration_set.state</code>	
<code>_enumeration_set.detail</code>	
<code>_enumeration_set.table_id</code>	
1	'filename/URI of source dictionary' file
2	'save framecode of source definition' save
3	'mode for including save frames' mode
4	'option for duplicate entries' dupl
5	'option for missing duplicate entries' miss
<code>Loop_</code>	
<code>_method.purpose</code>	
<code>_method.expression</code>	
Evaluation	

```
with i as import
_import.get = [{"file":i.file_id, "save":i.frame_id, "mode":i.mode,
               "dupl":i.if_dupl, "miss":i.if_miss}]
```

Because it is in the `_enumerated_set` category, the category key `_enumerated_set.state` must be present when listing these table keys, but instead of `_enumerated_set.state` listing the actual permitted values, it contains meaningless dummy values, `table_id` then lists table keys, not values, and so the restraints on the values of the keys are absent. This looks like an abuse of the `_enumerated_set` category when the natural solution as proposed by Doug du Boulay is to simply enhance `_type.contents`, i.e.

```
_type.contents = [{"file":URL "save":Code "mode":Code "dupl":Code "miss":Code}
```

Note that `_type.contents` is implicitly interpreted (in the demonstration DDLm dictionaries) to describe the contents of Lists, not the whole list, so the above use is in line with this. I therefore suggest that we drop `_enumerated_set.table_id` from DDLm completely as there is no use case.

Are we in agreement on this?
James

More IUCr web sites

- Regional associates
 - <http://asca.iucr.org>

AsCA: About us

asca.iucr.org/aboutus

Home About us History Media Meetings Contact us

As
C
A

Asian
Crystallographic
Association

About us

AsCA was founded in 1987 at the Perth IUCr Congress following almost a decade of discussions among crystallographers in the region.

The current membership is as follows

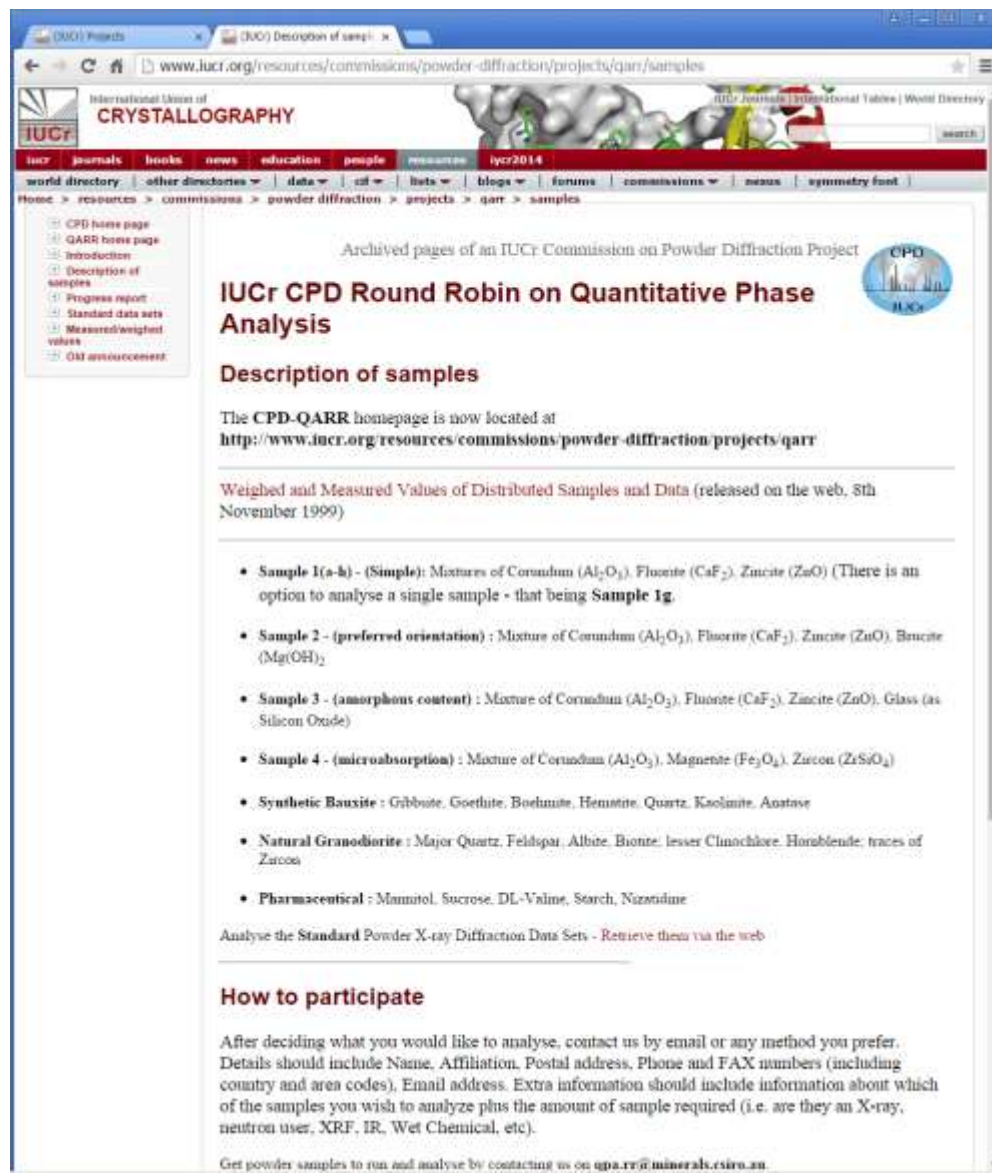
- Australia (category D) - Society of Crystallographers in Australia and New Zealand
- Bangladesh (category B) - Bangladesh Crystallographic Association
- China, People's Republic of (category D) - Chinese Crystallographic Society
- China, Taipei (category C) - The Academy of Sciences Located in Taipei
- India (category E) - Indian Crystallographic Association
- Indonesia (category B)
- Japan (category D) - Crystallographic Society of Japan
- Korea, Republic of (category C) - Korean Crystallographic Association
- Malaysia (category B)
- Mongolia (category B)
- New Zealand (category C) - Royal Society of New Zealand
- Pakistan (category B) - Pakistan Crystallographic Association
- Philippines (category B)
- Singapore (category B)
- Sri Lanka (category B)
- Thailand (category B)
- Vietnam (category B)

All enquiries about membership should be directed to the secretary.

Membership map

More IUCr web sites

- Regional associates
- Commission web sites
 - e.g. <http://cpd.iucr.org>



The screenshot shows a web browser window displaying the IUCr website. The page title is "IUCr CPD Round Robin on Quantitative Phase Analysis". The main content area is titled "Description of samples" and lists several sample types for analysis, including mixtures of Corundum, Fluorite, Zincite, and various synthetic and natural minerals. The page also includes a section for "How to participate" and contact information for the CPD Round Robin.

Archived pages of an IUCr Commission on Powder Diffraction Project

IUCr CPD Round Robin on Quantitative Phase Analysis

Description of samples

The CPD-QARR homepage is now located at <http://www.iucr.org/resources/commissions/powder-diffraction/projects/qarr>

Weighted and Measured Values of Distributed Samples and Data (released on the web, 8th November 1999)

- **Sample 1(a-b) - (Simple)**: Mixtures of Corundum (Al_2O_3), Fluorite (CaF_2), Zincite (ZnO) (There is an option to analyse a single sample - that being **Sample 1g**.)
- **Sample 2 - (preferred orientation)**: Mixture of Corundum (Al_2O_3), Fluorite (CaF_2), Zincite (ZnO), Brucite ($Mg(OH)_2$)
- **Sample 3 - (amorphous content)**: Mixture of Corundum (Al_2O_3), Fluorite (CaF_2), Zincite (ZnO), Glass (as Silicon Oxide)
- **Sample 4 - (microabsorption)**: Mixture of Corundum (Al_2O_3), Magnetite (Fe_3O_4), Zircon ($ZrSiO_4$)
- **Synthetic Bauxite**: Gibbsite, Goethite, Boehmite, Hematite, Quartz, Kaolinite, Anatase
- **Natural Granodiorite**: Major Quartz, Feldspar, Albite, Biotite, lesser Clinoclase, Hornblende, traces of Zircon
- **Pharmaceutical**: Mannitol, Sucrose, DL-Valine, Starch, Nizatidine

Analyse the Standard Powder X-ray Diffraction Data Sets - Retrieve them via the web

How to participate

After deciding what you would like to analyse, contact us by email or any method you prefer. Details should include Name, Affiliation, Postal address, Phone and FAX numbers (including country and area codes), Email address. Extra information should include information about which of the samples you wish to analyze plus the amount of sample required (i.e. are they an X-ray, neutron user, XRF, IR, Wet Chemical, etc).

Get powder samples to run and analyse by contacting us on cpd.rro@minerals.csiro.au

More IUCr web sites

- Regional associates
- Commission web sites
 - e.g. <http://cpd.iucr.org>
 - <http://crysac.iucr.org>



The screenshot shows the website for the Commission on Crystallography in Art and Cultural Heritage. The page features a navigation menu with links to 'iucr', 'journals', 'books', 'news', 'education', 'people', 'resources', and 'iucr2014'. Below the navigation, there is a header for the 'International Union of Crystallography Commission on Crystallography in Art and Cultural Heritage'. A large image of a classical column is displayed on the left. The main content area is titled 'Commission on Crystallography in Art and Cultural Heritage' and includes a paragraph about its formation in 2008. A list of bullet points describes the commission's goals, such as promoting crystallography in art, offering analytical tools, and fostering interdisciplinary collaboration. The right sidebar contains 'CrysAC News' with a 'IYCr2014' banner, a photo of an opening ceremony, and 'Next Events' including the 31st Meeting X-ray and other techniques in Krakow, Poland, and the 23rd IUCr Congress in Montreal, Canada.

More IUCr web sites

- Regional associates
- Commission web sites
- checkCIF
 - <http://checkcif.iucr.org>



The screenshot shows the checkCIF website interface in a browser window. The browser address bar displays "checkcif.iucr.org". The main content area includes the following sections:

- checkCIF**: A service of the International Union of Crystallography.
- checkCIF reports on the consistency and integrity of crystal structure determinations reported in CIF format.**
- Please upload your CIF using the form below.**
- File name:** Choose File | No file chosen
- Select form of checkCIF report:** HTML PDF
- Select validation type:** Full validation of CIF and structure factors. Validation of CIF only (no structure factors)
- Output Validation Response Form:** Level A alerts only Level A and B alerts Level A, B and C alerts None
- Send CIF for checking** button
- Information about this version of checkCIF ...**
- Useful links**
 - Prepublication check for submissions to IUCr journals
 - Details of checkCIF/PLATON tests
 - CIF dictionary
 - Download CIF editor (pubCIF) from the IUCr
 - Download CIF editor (enCIFer) from the CCDC

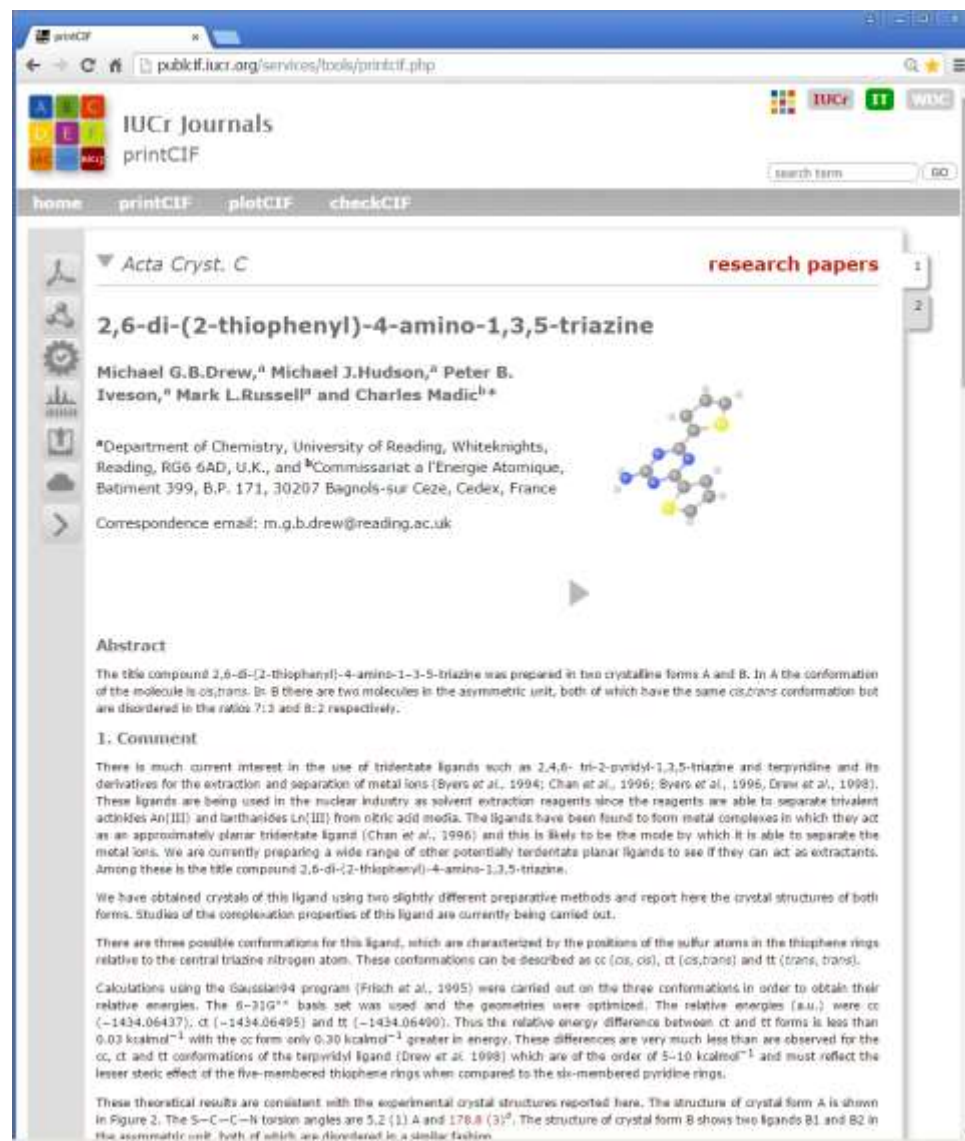
On the right side of the page, there is a vertical column of logos and text:

- checkCIF is sponsored by
- Crystallography Journals Online
- Four colored circles (red, orange, yellow, green)
- A logo with the letters A, B, C and a triangle
- ELSEVIER logo
- WILEY logo
- ROYAL SOCIETY OF CHEMISTRY logo
- THE CHEMICAL SOCIETY OF JAPAN logo

At the bottom right, there is a link: "Become a sponsor."

More IUCr web sites

- Regional associates
- Commission web sites
- checkCIF
- Publication tools
 - e.g. <http://publCIF.iucr.org>



The screenshot shows a web browser window displaying the publCIF website. The page title is "IUCr Journals printCIF". The main content area shows a research paper entry for "2,6-di-(2-thiophenyl)-4-amino-1,3,5-triazine" in the journal "Acta Cryst. C". The authors listed are Michael G.B. Drew, Michael J. Hudson, Peter B. Iveson, Mark L. Russell, and Charles Madic. A ball-and-stick model of the molecule is shown to the right. The abstract describes the preparation of two crystalline forms, A and B, and discusses the conformation of the molecule. The comment section provides a detailed discussion of the ligand's properties and the authors' work on its conformational isomers.

publCIF

publCIF.iucr.org/services/tools/printcif.php

IUCr Journals
printCIF

home printCIF plotCIF checkCIF

Acta Cryst. C research papers

2,6-di-(2-thiophenyl)-4-amino-1,3,5-triazine

Michael G.B. Drew,^a Michael J. Hudson,^a Peter B. Iveson,^a Mark L. Russell^a and Charles Madic^{b*}

^aDepartment of Chemistry, University of Reading, Whiteknights, Reading, RG6 6AD, U.K., and ^bCommissariat à l'Énergie Atomique, Batiment 399, B.P. 171, 30207 Bagnols-sur Ceze, Cedex, France

Correspondence email: m.g.b.drew@reading.ac.uk

Abstract

The title compound 2,6-di-(2-thiophenyl)-4-amino-1,3,5-triazine was prepared in two crystalline forms A and B. In A the conformation of the molecule is *cis,trans*. In B there are two molecules in the asymmetric unit, both of which have the same *cis,trans* conformation but are disordered in the ratios 7:1 and 8:2 respectively.

1. Comment

There is much current interest in the use of tridentate ligands such as 2,4,6-tri-2-pyridyl-1,3,5-triazine and terpyridine and its derivatives for the extraction and separation of metal ions (Byers *et al.*, 1994; Chan *et al.*, 1996; Byers *et al.*, 1996; Drew *et al.*, 1998). These ligands are being used in the nuclear industry as solvent extraction reagents since the reagents are able to separate trivalent actinides An(III) and lanthanides Ln(III) from nitric acid media. The ligands have been found to form metal complexes in which they act as an approximately planar tridentate ligand (Chan *et al.*, 1996) and this is likely to be the mode by which it is able to separate the metal ions. We are currently preparing a wide range of other potentially tridentate planar ligands to see if they can act as extractants. Among these is the title compound 2,6-di-(2-thiophenyl)-4-amino-1,3,5-triazine.

We have obtained crystals of this ligand using two slightly different preparative methods and report here the crystal structures of both forms. Studies of the complexation properties of this ligand are currently being carried out.

There are three possible conformations for this ligand, which are characterized by the positions of the sulfur atoms in the thiophene rings relative to the central triazine nitrogen atom. These conformations can be described as *cc* (*cis, cis*), *ct* (*cis, trans*) and *tt* (*trans, trans*).

Calculations using the Gaussian94 program (Frisch *et al.*, 1995) were carried out on the three conformations in order to obtain their relative energies. The 6-31G** basis set was used and the geometries were optimized. The relative energies (a.u.) were *cc* (-1434.06437), *ct* (-1434.06495) and *tt* (-1434.06400). Thus the relative energy difference between *ct* and *tt* forms is less than 0.03 kcalmol⁻¹ with the *cc* form only 0.30 kcalmol⁻¹ greater in energy. These differences are very much less than are observed for the *cc*, *ct* and *tt* conformations of the terpyridyl ligand (Drew *et al.*, 1998) which are of the order of 5-10 kcalmol⁻¹ and must reflect the lesser steric effect of the five-membered thiophene rings when compared to the six-membered pyridine rings.

These theoretical results are consistent with the experimental crystal structures reported here. The structure of crystal form A is shown in Figure 2. The S-C-C-N torsion angles are 5.2 (1) Å and 176.8 (3)°. The structure of crystal form B shows two ligands B1 and B2 in the asymmetric unit, both of which are disordered in a similar fashion.

More IUCr web sites

- Regional associates
- Commission web sites
- checkCIF
- Publication tools
- Facebook (IUCr)
 - <https://facebook.com/iucr.org>



The screenshot shows the Facebook page for the International Union of Crystallography (IUCr). The page header includes the Facebook logo and the text "International Union of Crystallography (IUCr) Community Page about Crystallography". Below the header is a cover photo of a group of people, with the IUCr logo overlaid. The page has 1,215 likes and 9 visits. The "ABOUT" section describes the IUCr as a non-profit scientific union serving the world-wide interests of crystallographers and other scientists. The "PHOTOS" section shows a grid of images, including a map of Africa with highlighted regions. A post from April 27, 2015, announces a grant for "Building Science Capacity in Africa via Crystallography" under the ICSU Grants Programme 2015. The post includes a link to the grant information and a map of Africa with highlighted regions. The post is liked by Sanjosh Parghar, Sarva Nair, Sam Goffman, and 5 others.

More IUCr web sites

- Regional associates
- Commission web sites
- checkCIF
- Publication tools
- Facebook (IUCr)
- Facebook (IYCr2014)
 - <https://fb.com/iycr2014.org>



The image shows a screenshot of a Facebook page for the International Year of Crystallography 2014. The page features a blue header with the Facebook logo and a search bar. Below the header is a red banner with the text "2014 International year of crystallography" and "CONFERENCE Crystallography for the next generation: the legacy of IYCr". The banner also mentions the location "Hassan II Academy of Science and Technology, Rabat (Morocco)" and the dates "22-24 April 2015". The page includes a "PEOPLE" section with 4,032 likes, an "ABOUT" section with a description of the event, and a "PHOTOS" section with a grid of images. A post from the page is visible, titled "IYCr2014 - Launch conference", with a photo of a building and text inviting people to attend the conference.

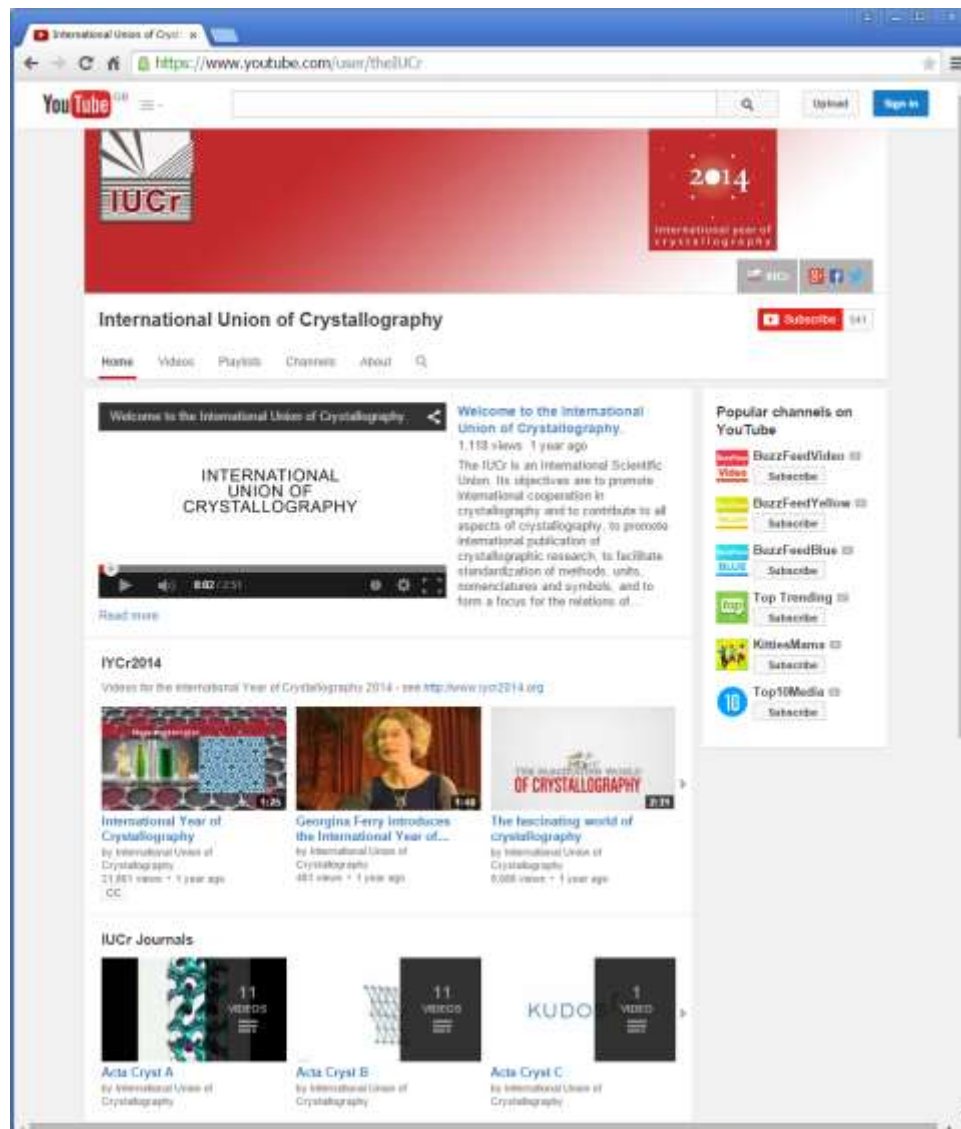
More IUCr web sites

- Regional associates
- Commission web sites
- checkCIF
- Publication tools
- Facebook (IUCr)
- Facebook (IYCr2014)
- Twitter
 - <https://twitter.com/IUCr>



More IUCr web sites

- Regional associates
- Commission web sites
- checkCIF
- Publication tools
- Facebook (IUCr)
- Facebook (IYCr2014)
- Twitter
- YouTube
 - <https://youtube.com/theIUCr>

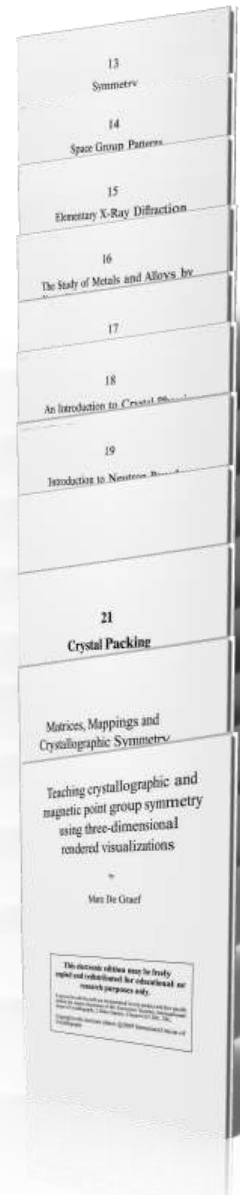
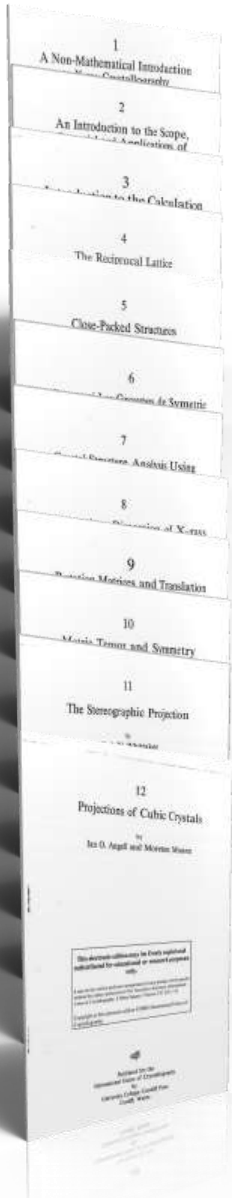


The image shows a screenshot of the IUCr YouTube channel page. The browser address bar displays the URL <https://www.youtube.com/user/theIUCr>. The channel banner features the IUCr logo on the left and a red box on the right that says "2014 International year of Crystallography". Below the banner, the channel name "International Union of Crystallography" is displayed with a "Subscribe" button showing 141 subscribers. The main content area includes a video player with a video titled "Welcome to the International Union of Crystallography" (1:18 views, 1 year ago). Below the video player, there is a section for "IYCr2014" with three video thumbnails: "International Year of Crystallography" (21,861 views), "Georgina Ferry introduces the International Year of..." (481 views), and "The fascinating world of crystallography" (8,006 views). At the bottom, there are three "IUCr Journals" sections: "Acta Cryst A" (11 videos), "Acta Cryst B" (11 videos), and "Acta Cryst C" (1 video).

Educational resources

Teaching pamphlets

- Prepared mostly in 1980s
- IUCr Commission on Crystallographic Teaching
- Financial support from UNESCO
- Distinguished authors
- **Still** widely used
- Now all available as PDF and HTML
- Free to download and distribute
- Accompanied by teaching materials
- Mostly undergraduate level
- Some school level
- Model for future (online-intensive) projects




Crystallography 365

Crystallography matters ... more!

events and outcomes from the international year of crystallography 2014






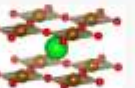

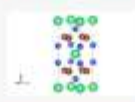

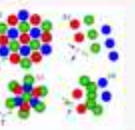


Crystallography365

Shipping a crystal structure a day in 2014



Select month: | January | February | March | April | May | June | July | August | September | October | November | December |

A perpetual calendar of crystallography - May

<p>1</p>  <p>Magnetic monopoles in the pyrochlore lattice</p>	<p>2</p>  <p>From crystallography, to naming the country</p>	<p>3</p>  <p>FeCo magnets - May the 3rd be with you</p>	<p>4</p>  <p>It's a bird, it's a plane... it's a SuperHyd!</p>	<p>5</p>  <p>Elements Under Pressure: Boron</p>	<p>6</p>  <p>Square planar boron: creating up or with only atomic precursors</p>
<p>7</p>  <p>Milestone: 'The Miracle Ice'</p>	<p>8</p>  <p>ThO₂(111), giving it the old 1-0-2</p>	<p>9</p>  <p>J. D. Bertini and the structure of water</p>	<p>10</p>  <p>Water ice under pressure - the structure of IceXVI-A</p>	<p>11</p>  <p>Dorothy Crowfoot Hodgkin and the structure of Vitamin B₁₂</p>	<p>12</p>  <p>Sulfuric acid out of the box</p>

Timelines of crystallography

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2014 international year of crystallography

Timelines of Crystallography

1. Click on the buttons to show or hide timelines (up to 5 can be shown side by side)

2. Drag the timeline or select a date: 1500 | 1600 | 1700 | 1750 | 1800 | 1850 | 1900 | 1950 | 1975 | 2000 | 2010 | 2014

3. Show ("filter") or highlight entries containing a given word

Filter: Highlight: Clear All

2009

Membrane proteins
Fleck parameter
Quasicrystals
enbrane proteins

Transcription of genetic information
Structure of the ribosome
Kepler's Conjecture proved
Understanding life from crystal structures

Neutron diffraction developed and won the Nobel Prize
Crystallography characterises a photosynthesis site

Fermi surface of copper
Thermoelectric effect in terms of Fermi surface
Electron microscopic studies of Lamer-Cottrell locks
Ferroelectricity and soft phonon modes
Ferroelectricity and soft phonon modes
Ferroelectricity and soft phonon modes
Development of studies on one-dimensional d

Effective ionic radii
Classification of complex intermetallic structures based on coordination
Packing description of complex ions
Importance of carbon distribution o

USA: Snowflake
Korea: Crystallography characterises a photosynthesis site

UK: Dorothy Hodgkin
Guinea Bissau: W.L. Bragg
Guinea Bissau: W.L. Bragg
Germany: Wilhelm Conrad Röntgen

Argentina: Quartz
Australia: W.L. Bragg
Austria: Felix P
Israel: Quasi-Pe
Moldova: Perio
Poland: Crysta

Crystallography and Philately

a sheet of perforated postage stamps is a typical example of a plane lattice (Fig. 1), the type of symmetry (in two dimensions) that is matched by the three-dimensional structure of a crystal lattice. Perhaps this is one reason why there are many crystallographers who appreciate philately - the study of postage stamps and their history. Commemorative stamps from countries all over the world illustrate historical events, often in miniature works of art of great beauty. Very stamp-collectors have isolated crystallographic specimens, scientific results of individual scientists. The picture highlights some of the most noteworthy and beautiful examples.

Source: original illustrations by: Daniel Alesbrovich, U. North Carolina at Charlotte, USA; Santiago Garcia-Chando and A. Florjanczyk, U. Oviedo, Spain; and Japannath Watt, Bangalore, India. Image implemented by Dany Hanny, Alun School, Maid, Wales, UK.

Dr. Dorothy Hodgkin

25 February 2010 Dorothy Hodgkin was credited with the development of protein crystallography. She was awarded the Nobel Prize in Chemistry in 1964. This stamp was issued on the 150th anniversary of the Royal Society.

Web teaching/learning resources

The image displays a collage of web browser windows showcasing various resources for teaching and learning crystallography. At the top, a red banner features the text "2014 international year of crystallography" and logos for the International Union of Crystallography (IUCr) and the Royal Canadian Mounted Police (RCMP). Below this, several browser windows are visible:

- A window titled "Learn about crystallography" with a URL of materials.cmu.edu/degraeef/pq/pq_bar-43m.gif, showing a 3D molecular model of a crystal structure with blue and red atoms and a central red triangle.
- A window titled "Symmetry" from symmetry.otterbein.edu/gallery/, displaying a point group selection interface. The "Point Group Type" is set to "All", and the "Select Molecule" list includes options like 1,1-dichloroethylene, 1,2-dichloroethylene (cis), 1,2-dichloroethylene (trans), 10-crown-6, C_{60} -(C_{60})²⁺, Sn_2 , BF_3 , C_{3v} , S_6 , and $(\text{Co}_2/\text{Co}_2)$ cluster. A 3D ball-and-stick model of a molecule is shown next to the interface.
- A window titled "CSIC Cristalografía" from www.xtal.igih.csic.es/Cristalografia/, featuring a list of resources and a 3D lattice diagram with a red dot at the origin.
- A window titled "Symmetry" from www.crystallography.net/, showing a 3D lattice diagram with a red dot at the origin.

Crystal growing competitions for schools


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2015 crystal-growing competition for schoolchildren

Following the great success of the IYC/2014 competition, we announce the 2015 edition of a worldwide competition, open to all schoolchildren, to introduce students to the exciting, challenging and sometimes frustrating world of growing crystals. The winners will be those who most successfully convey their experiences to the panel of judges in a video report.



Download high-definition version of the video (195 MB, MP4 format)

Winners of the 2014 edition

[Click here to watch the videos](#)

How to participate?

The aim of the competition is to grow your own crystals (whether involved in a regional/national competition or not) and to convey your experiences through a video. The following guidelines are applicable:

- maximal duration of three minutes, format mpag, avi or mov, or hosted on a public video platform (e.g. YouTube, Vimeo)

Each contribution should clearly show or mention the experimental work carried out by the participants during the growing of their single crystals (compounds and methods used are free of choice). Furthermore the contribution should reflect in a creative way on the experimental work and theoretical background and/or applications.

Rules

- The closing date for submissions is **22 November 2015**.
- The competition is open to students of primary or secondary schools; maximum age 18.
- Language: mother language of participant or English.
- A maximum of one entry may be submitted by any individual or team.
- The judging panel will be nominated by the International Union of Crystallography. The decisions of the judging panel are final.

[Click here to submit your entry.](#)

Prizes

The winning contributors in each category will receive 'Young crystal growers' certificates and exciting prizes to stimulate further interest in science.

Criteria for evaluation

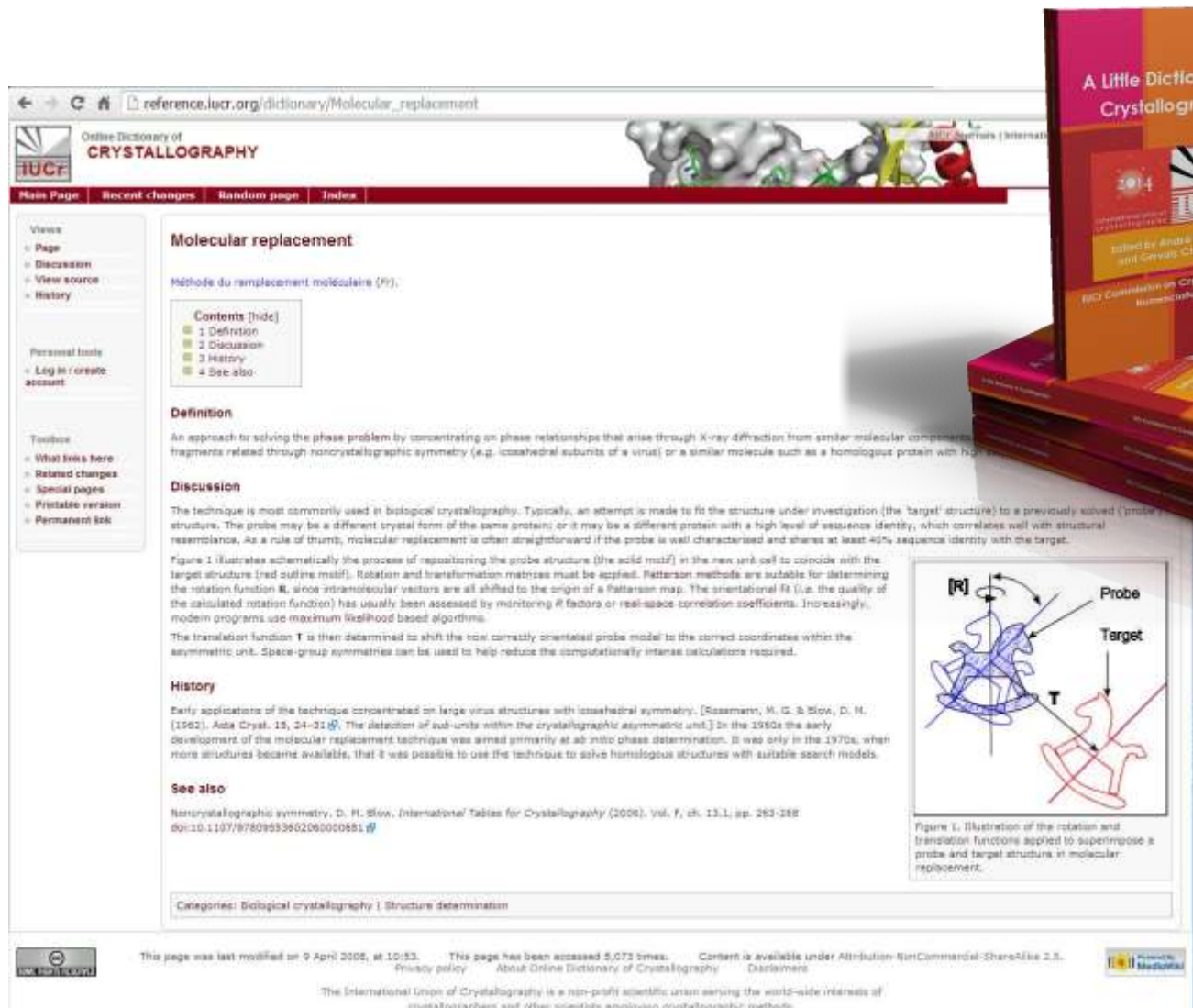
A panel of judges will evaluate the entries. The following criteria will be used: creativity, aesthetic value, description of working plan and experimental work, clarity of explanations and scientific background.

Contact: iyc2014@iucr.org facebook [Site map](#) © IUCr

Local coordinators

Teachers and pupils may have a lot of questions during the competition. To prevent the mailbox of the coordinator from being overloaded, it is very practical to work with local coordinators who are the contacts for a certain region. Together all local coordinators can act as help!

Online dictionary of crystallography



reference.iucr.org/dictionary/Molecular_replacement

Online Dictionary of
CRYSTALLOGRAPHY

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Discussion
View source
History

Personal tools
Log in / create account

Tools
What links here
Related changes
Special pages
Printable version
Permanent link

Molecular replacement

Méthode du remplacement moléculaire (FR)

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- 2 Discussion
- 3 History
- 4 See also

Definition

An approach to solving the phase problem by concentrating on phase relationships that arise through X-ray diffraction from similar molecular components or fragments related through noncrystallographic symmetry (e.g. isosubunits of a virus) or a similar molecule such as a homologous protein with high sequence identity.

Discussion

The technique is most commonly used in biological crystallography. Typically, an attempt is made to fit the structure under investigation (the 'target' structure) to a previously solved ('probe' structure). The probe may be a different crystal form of the same protein; or it may be a different protein with a high level of sequence identity, which correlates well with structural resemblance. As a rule of thumb, molecular replacement is often straightforward if the probe is well characterized and shares at least 40% sequence identity with the target.

Figure 1 illustrates schematically the process of repositioning the probe structure (the solid motif) in the new unit cell to coincide with the target structure (red outline motif). Rotation and transformation matrices must be applied. Patterson methods are suitable for determining the rotation function R , since intramolecular vectors are all shifted to the origin of a Patterson map. The orientational fit (i.e. the quality of the calculated rotation function) has usually been assessed by monitoring R factors or real-space correlation coefficients. Increasingly, modern programs use maximum likelihood based algorithms.

The translation function T is then determined to shift the now correctly orientated probe model to the correct coordinates within the asymmetric unit. Space-group symmetries can be used to help reduce the computationally intense calculations required.

History

Early applications of the technique concentrated on large virus structures with icosahedral symmetry. [Rossmann, M. G. & Blow, D. H. (1962). *Acta Cryst.* **15**, 24–31.] The detection of sub-units within the crystallographic asymmetric unit, in the 1960s the early development of the molecular replacement technique was aimed primarily at ab initio phase determination. It was only in the 1970s, when more structures became available, that it was possible to use the technique to solve homologous structures with suitable search models.

See also

Noncrystallographic symmetry, D. H. Blow, *International Tables for Crystallography* (2006), Vol. F, ch. 13.1, pp. 263–288
doi:10.1107/9780955362060000681

Categories: Biological crystallography | Structure determination

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The International Union of Crystallography is a non-profit scientific union serving the world-wide interests of crystallographers and other scientists employing crystallographic methods.

A Little Dictionary of Crystallography
Edited by André Authier and Lorenzo Ciampelli
IUCr Commission on Crystallographic Nomenclature

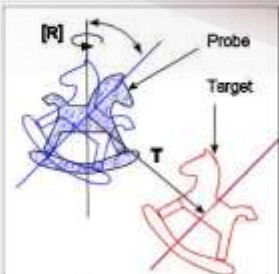


Figure 1. Illustration of the rotation and translation functions applied to superimpose a probe and target structures in molecular replacement.

Concluding remarks

- Outreach activities during IYCr2014 have opened new avenues for communication and education
- New member countries of IUCr bringing younger scientific communities together worldwide
- As the scientific world expands, IUCr remains committed to preservation and sharing of knowledge
- ... and to passing it on to future generations

Thank you!

Brian McMahon

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