

# IUCr meeting changing needs: the future of scholarly communications

Crystallography for the next generation 22-24 April 2015, Rabat, Morocco

Dr Jonathan Agbenyega, business development manager

[ja@iucr.org](mailto:ja@iucr.org)

## My role

- Discover new opportunities for the IUCr
- Improve on existing activities, such as journals, books, teaching material and other services
- Meet scientists to keep aware of field and attract top research
- Encourage best practise in how to get published in high impact journals
- Developing other business critical opportunities which fit the IUCr strategic business plan

# The Chester office



# Continuity and change

**Funding bodies** are looking more closely at impact factors, journal metrics and usage

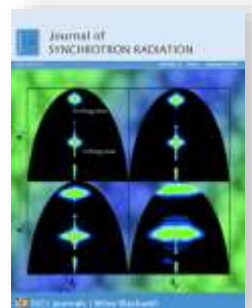
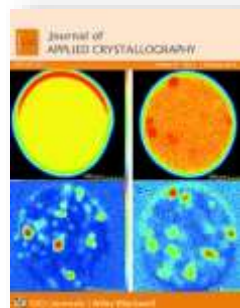
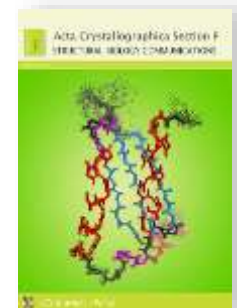
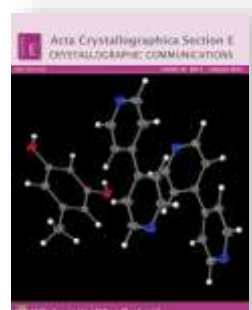
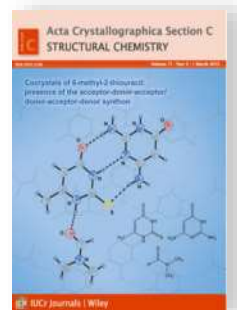
**Research is becoming more digital** – In both the way it is carried out and consumed

**Emerging regions** – Research is truly global

**Research is becoming more interdisciplinary** – Chemists, biologists and physicists are joining forces to answer global research problems

# IUCr Journals

- Acta Cryst A
- Acta Cryst B
- Acta Cryst C
- Acta Cryst D
- Acta Cryst E
- Acta Cryst F
- IUCrJ
- Appl Cryst JAC
- Synchrotron JSR



- New covers
- New article design
- New web pages



# New design Download statistics

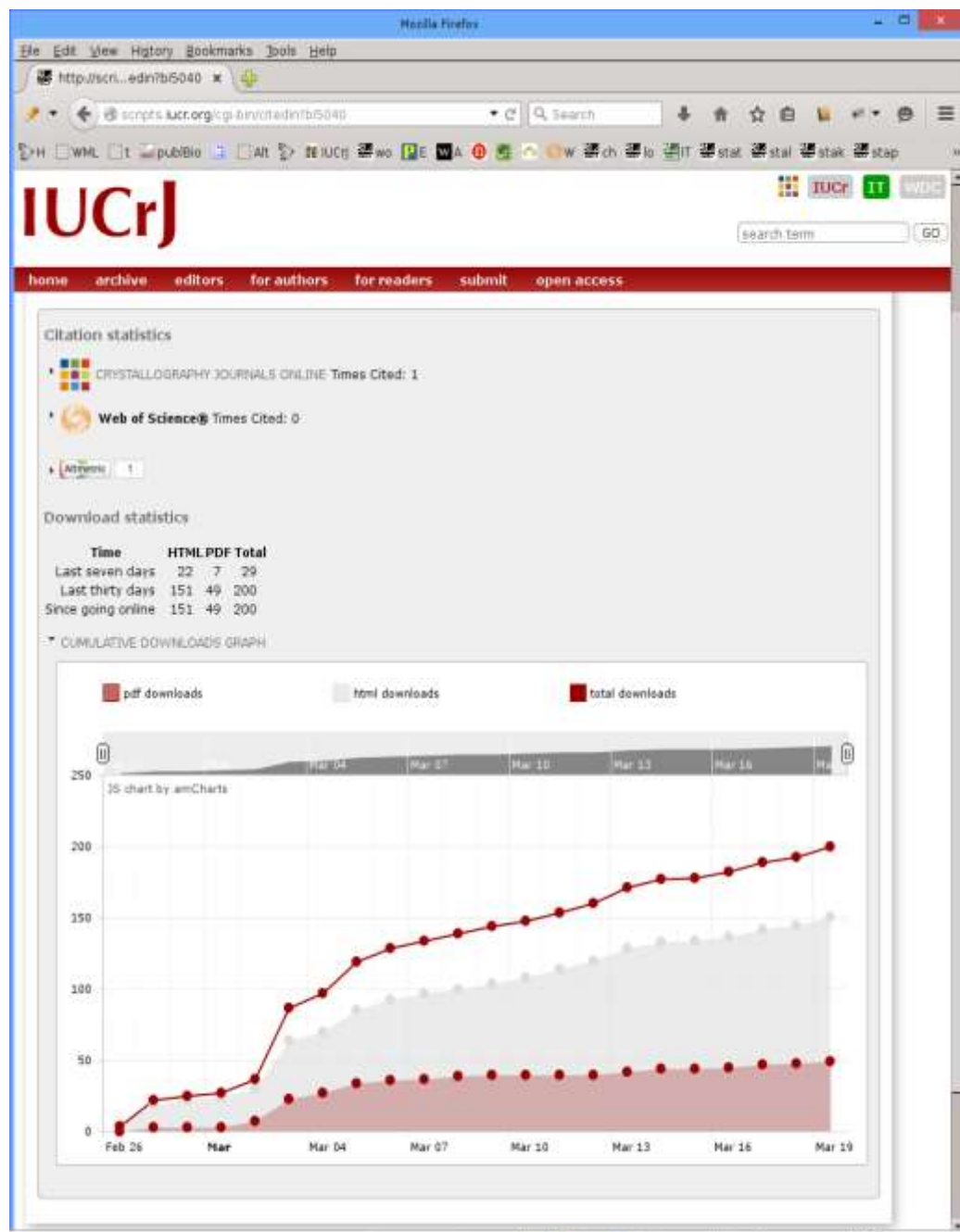
The screenshot shows the IUCr journal website interface. At the top, there is a navigation bar with links for 'home', 'archive', 'editors', 'for authors', 'for readers', 'submit', and 'open access'. The main content area displays the article title 'Solvent-vapour-assisted pathways and the role of pre-organization in solid-state transformations of coordination polymers' by James S. Wright, Inigo J. Vitorica-Yrezabal, Harry Adams, Stephen P. Thompson, Adrian H. Hillig, and Lee Brammer. Below the title, there is a table showing page views over time:

Time	HTML	PDF	Total
Last seven days	22	7	29
Last thirty days	151	49	200
Since going online	151	49	200

Below the table, there is a link to 'more article statistics ...'. The article abstract is partially visible, discussing the formation of ether polymorphs and the templating effect of toluene and *p*-xylene over *o*-xylene or *m*-xylene in the formation of arene-containing architecture 1. The abstract also mentions the conversion of coordination polymers 1 to 2a and 2b.

# New design

## Detailed statistics



# New design Journal home

(IUCr) - Mozilla Firefox

File Edit View History Bookmarks Tools Help

cif.publcryst.co.uk/journalstart.htm

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CURRENT ISSUE | SUBMIT

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Appl. Cryst. JAC JOURNAL OF APPLIED CRYSTALLOGRAPHY  
CURRENT ISSUE | SUBMIT

Synchrotron JSR JOURNAL OF SYNCHROTRON RADIATION  
CURRENT ISSUE | SUBMIT

IUCrJ IUCrJ  
CURRENT ISSUE | SUBMIT

International year of crystallography 2014

Forthcoming special issues

- A Special issue on mathematical crystallography
- B Special issue on non-ambient crystallography
- C Special issue on nanostructures
- D Special issue on scorpionates
- E Special issue on the interplay of crystallography, spectroscopy and theoretical methods for solving chemical problems
- F Special issue on computational materials discovery
- G Special issue on pharmaceuticals, drug discovery and natural products
- H CCP4 Study Weekend 2014 Complementary Techniques, Nottingham, January 2014
- I Diffraction Data Deposition Working Group meeting (DDD WG)
- J IYCr Crystallization Series
- K Special issue on diffraction imaging techniques
- L 15th Small-Angle Scattering Meeting (SAS2012)
- M 11th Biennial Conference on High Resolution X-ray Diffraction and Imaging (XTOP2012)
- N Diffraction-limited storage rings

latest articles | most read | most cited | highlighted articles

*Reflections on the magnetic pair distribution function.* W. Ratcliff II (2014), *Acta Cryst.* **A70**, 1-2.

*Spin-coupling in dimers of 2,3-dicyano-5,6-dichlorosemiquinone radical anions in the crystalline state.* K. Molcanov, D. Babic, B. Kojic-Prodic, J. Stera, N. Malter-Strmedki & L. Andros (2014), *Acta Cryst.* **B70**, doi:10.1107/S2052520613027170.

*$\pi$ -stacking and C-H...D ( $X = H, NO_2$ ;  $D = O, \pi$ ) interactions in the crystal network of both C-H...N and  $\pi$ -stacked dimers of 1,2-bis(4-bromophenyl)-1H-benzimidazole and 2-(4-bromophenyl)-1-(4-nitrophenyl)-1H-benzimidazole.* J. E. González-Padilla, M. C. Rosales-Hernández, I. J. Padilla-Martínez, E. V. García-Báez, S. Rojas-Lima & W. Salazar-Pereda (2014), *Acta Cryst.* **C70**, doi:10.1107/S2053220613033329.

*X-ray crystallographic studies of family 14 xylanase Michaelis and product complexes: implications for the catalytic mechanism.* Q. Wang, Q. Zhang, S. Hamilton-Brehm, K. Weiss, M. Muslyayimov, L. Coates, P. Langen, D. Graham & A. Kovalevsky (2014), *Acta Cryst.* **D70**, doi:10.1107/S1399004713023626.

*(E)-3-Amino-4-(2-phenylhydrazinylidene)-1H-pyrazol-5(4H)-one. Corrigendum.* G. H. Elgarni, S. H. Sayed & P. G. Jones (2014), *Acta Cryst.* **E70**, e1.

*Crystallization and structure determination of a symmetrical "football" complex of the mammalian mitochondrial Hsp60. Hsp10 chaperonins.* S. Naimblatt, A. Parnas, O. Yaniv, A. Azem & F. Frolow (2014), *Acta Cryst.* **F70**, doi:10.1107/S2053230X1303389X.

*A quantitative approach to tune metal oxide network morphology based on grazing-incidence small-angle X-ray scattering investigations.* K. Sarkar, M. Rawolle, M. A. Niedermeier, W. Wang, C. M. Herzig, V. Korstgens, A. Buffet, S. V. Roth & P. Müller-Buschbaum (2014), *J. Appl. Cryst.* **47**, doi:10.1107/S1600576713027775.

*X-ray absorption near-edge structure anomalous behaviour in structures with buried layers containing silicon nano-crystals.* V. A. Terkhov, D. J. Tetelbaum, O. E. Spirin, K. N. Pankov, A. N. Mikhailov, A. I. Belov, A. V. Ershov & S. Yu. Turishchev (2014), *J. Synchrotron Rad.* **21**, 209-214.

IUCr JOURNALS ONLINE

A B C  
D E F  
JAC JSR IUCrJ



# New design journal homepage

**IUCrJ**

home archive editors for authors for readers submit open access

IUCrJ is a new fully open-access peer-reviewed journal from the International Union of Crystallography (IUCr).

The journal will publish high-profile articles on all aspects of the sciences and technologies supported by the IUCr via its commissions, including emerging fields where structural results underpin the science reported in the article. Our aim is to make IUCrJ the natural home for high-quality structural science results. Chemists, biologists, physicists and material scientists will be actively encouraged to report their structural studies in IUCrJ.

IUCrJ covers five broad areas:

- biology and medicine
- chemistry and crystal engineering
- materials and computation
- medicine and synchrotron science and technology
- physics and free electron laser science and technology

The journal has been launched to commemorate the International Year of Crystallography.

**Editorial board**  
ISSN: 2052-2523

[Current issue](#) | [Previous issues](#)


The value of exploring Mars to Marskind

Curiosity's Landing

**Why choose IUCrJ?**

- High profile, high impact
- Fast publication, excellent technical editing
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**KUDOS**   
IUCr Journals

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# World directory of crystallographers

- First formal meeting of the IUCr at Harvard University in July 1948
- WDC would have started as an organisational tool
- Used to facilitate international contacts and keep track of growing number of crystallographers
- In 1957, 2255 crystallographers coming from 52 countries made up the first edition of the world directory
- Strong feeling of a single family
- Today: Over 12,000 searchable entries in the world directory





# INTRODUCTION

Why we undertook this project

Wiley undertook a piece of research to understand what individuals value from societies and associations

Research will help IUCr develop strategies for information and education products and services

# About the respondents

5%

Lower than a  
Bachelor's Degree

14%

Bachelor's Degree

31%

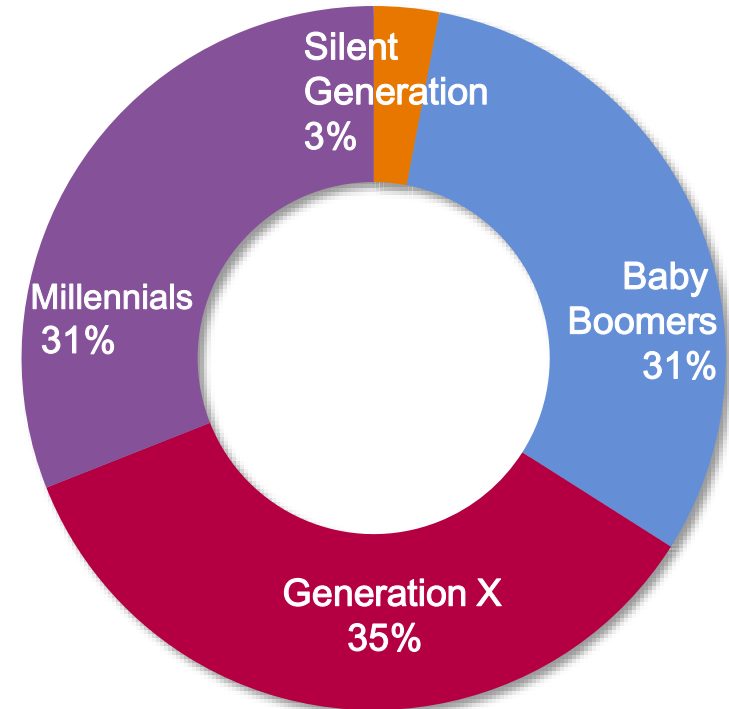
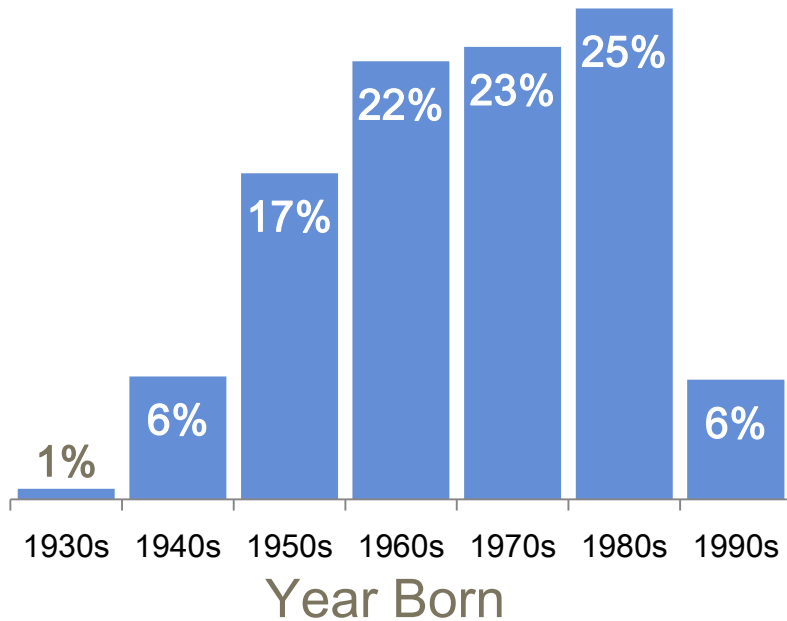
Master's Degree

13%

Professional Degree

37%

Doctorate Degree





# KEY FINDINGS

1

## VALUED BENEFITS

Both members and nonmembers highly value the peer-reviewed journal and opportunities for continuing education.

2

## REASONS FOR JOINING

The quality of a society's content is the top reason people initially join. They renew because they feel connected to the community.

3

## REASONS FOR NOT JOINING

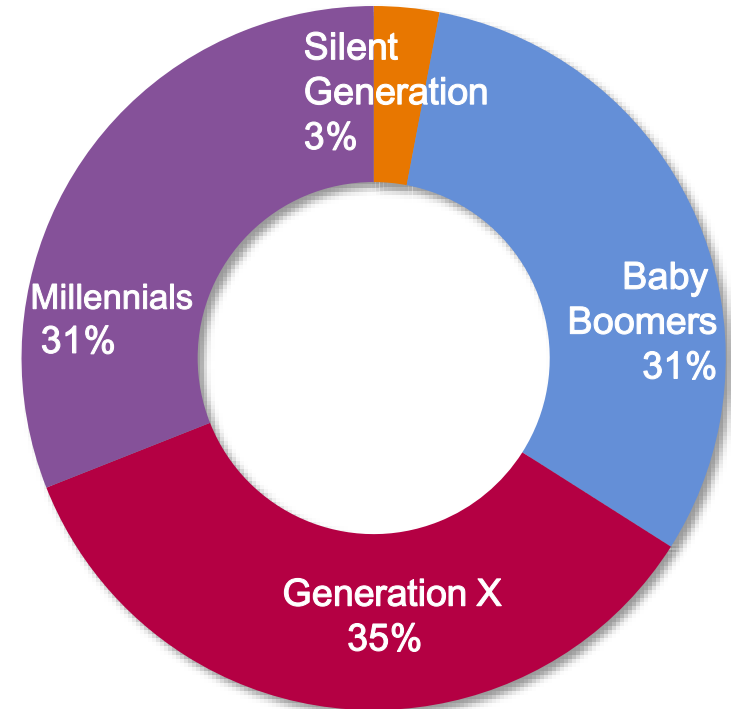
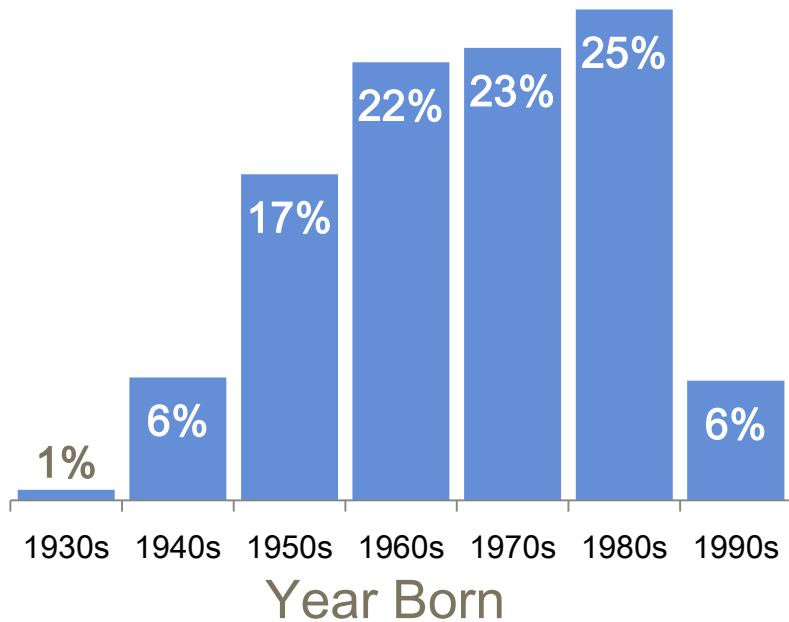
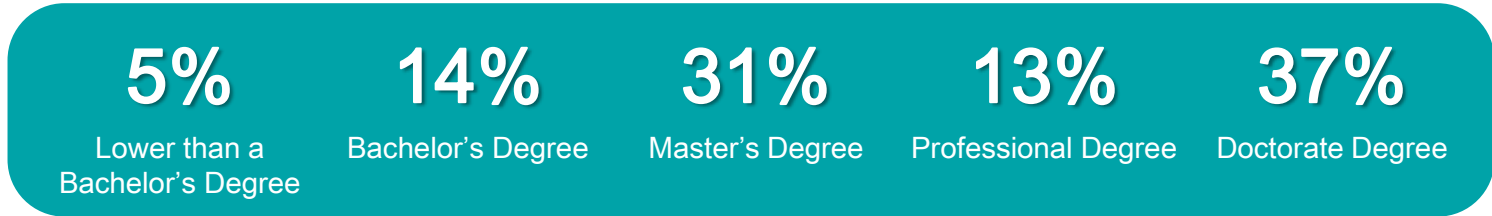
Often, nonmembers don't join societies because the cost is too high, and a surprising percentage haven't joined because they were never invited.

4

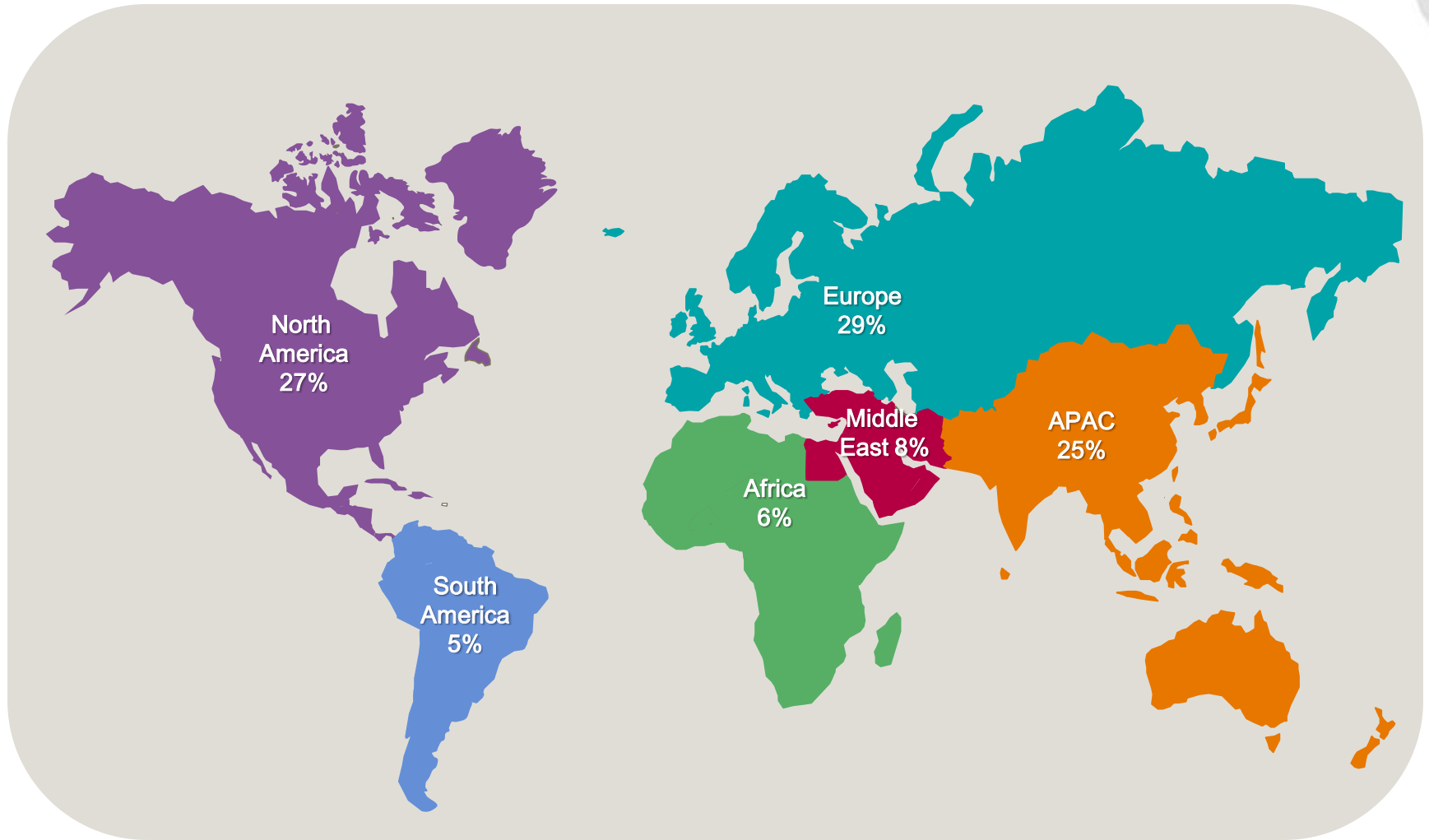
## SATISFACTION AND ENGAGEMENT

Members are satisfied with their society more often than not and almost three-fourths of members say they actively read the association's publications.

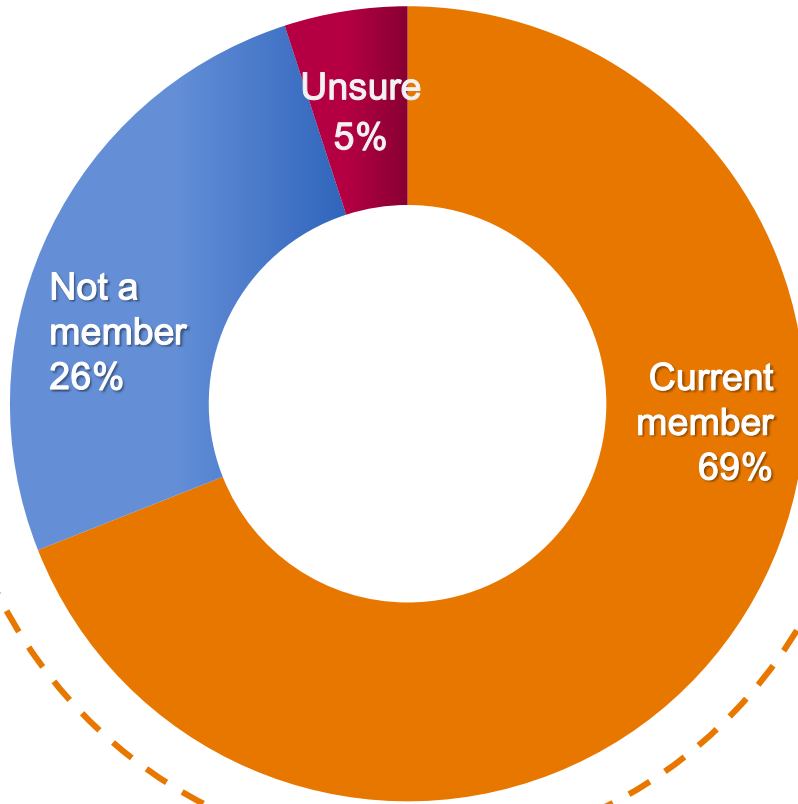
# About the respondents



# Country of Residence



# Branching Question: Membership Status





# Reasons for Joining

	Importance Ranking ("1" is best)
Quality of research-based content	1.94
Prestige of organization	2.28
Required to attend meeting	2.33
Required certification for career	2.35
Networking opportunities	2.4
Value of membership benefits to me	2.5
Recommendation from a colleague/ mentor	2.61
Great Reputation	2.64
Required for publication	2.86
Representation within my region	2.93
Number of membership benefits	3.06

## Reasons for Renewing



*"I feel connected to the community"*



*"I receive good value"*

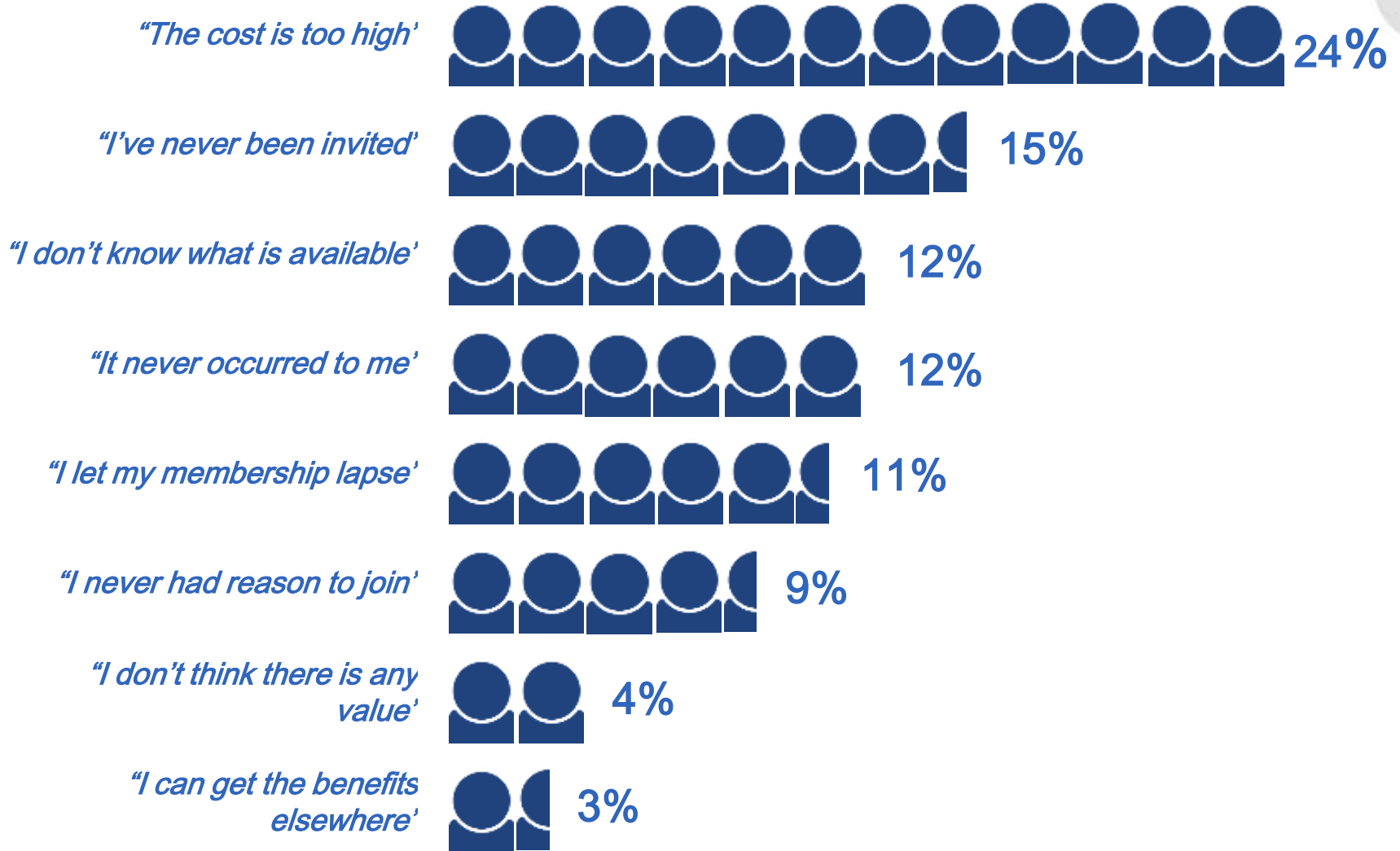
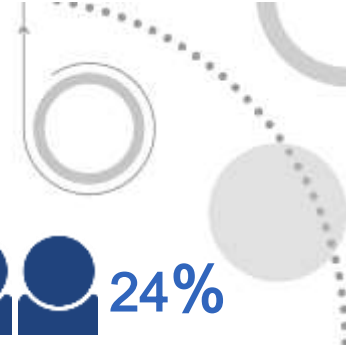


*"I am in a leadership position"*



*"I have never thought about it"*

# Reasons for Not Joining



# Most Valued Benefits (1 through 5)

MEMBERS

## Journal

Peer-reviewed journal that publishes academic/scholarly research

## Continuing Education

Opportunities for continuing education and training

## Magazine

Publication (typically magazine) with latest techniques, trends in your field

## Standards

Standards, guidelines and reference guides for your field

## Conference

Capability to attend an in-person event(s) (i.e. annual meeting)

## Continuing Education

Opportunities for continuing education and training

## Journal

Peer-reviewed journal that publishes academic/scholarly research

## Magazine

Publication (typically magazine) with latest techniques, trends in your field

## Expert Advice

Expert advice from professionals in your field

## Leadership Experience

Opportunities to gain leadership experience

NONMEMBERS

# Somewhat Valued Benefits (6 through 11)

MEMBERS

## Expert Advice

Expert Advice from professionals in your field

## Leadership Experience

Opportunities to gain leadership experience

## Career Resources

Career Resources (job board, networking events, interviewing advice, etc.)

## Community Outreach

Outreach program to improve your professions' standing in the community

## Government Advocacy

Government advocacy program that represents your field

## Online Presentations

Online presentations on topics related to your work

## Standards

Standards, guidelines and reference guides for you field

## Career Resources

Career resources (job board, networking events, interviewing advice, etc.)

## Conference

Capability to attend an in-person event(s) (i.e. annual meeting)

## Online Presentations

Online presentation on topics related to your work

## Community Outreach

Outreach program to improve your professions' standing in the community

## Government Advocacy

Government advocacy program that represents your field

NONMEMBERS



# Least Valued Benefits (12 through 16)

MEMBERS

## Newsletter

Newsletter with news from your field

## Peer Mentoring

Ability to participate in peer mentoring program(s)

## Local Chapters

Local chapters allowing you to connect to near-by members

## Salary Benchmarking

Salary benchmark data and information

## Discounts

Member discounts to products not included in membership

## Peer Mentoring

Ability to participate in peer mentoring program(s)

## Newsletter

Newsletter with news from your field

## Salary Benchmarking

Salary benchmark data and information

## Local Chapters

Local chapters allowing you to connect to near-by members

## Discounts

Member discounts to products not included in membership

NONMEMBERS

# Communicating science

## Five W's and an H

- Where?
- Why?
- Who?
- What?
- When?
- How?

# Where is our audience?



## Why?

- To engage our audience and



extend our reach

2013 in a typical month

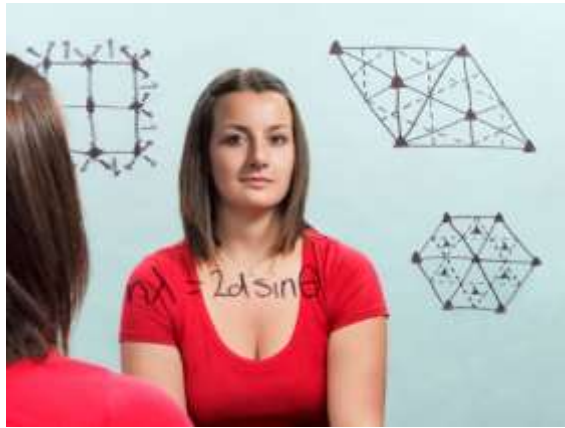
**45,000 unique visitors**

2015 in a typical month

**71,000 unique visitors**



# Who?




# What?

 **Jenny Martin** @JennyMartin\_UQ · 1h

How to set up crystallography in Africa. The @iucr initiative



View more photos and videos

 **AMG** @MikeGlazer1 Following

Thats nice. Our paper on disorder in PZT [bit.ly/1yrM85T](http://bit.ly/1yrM85T) has been given Spriggs Award by American Ceramic Society. #crystallography

RETWEETS 3 FAVORITES 6

5:00 PM - 15 Apr 2015

## When?

- Experiment!
- Often
- Repeatedly
- Use the tools available

How?

We are all marketers



# Kudos homepage on IUCr

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## IUCr Journals and Kudos

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During 2013 kudos ran a pilot scheme with a number of other publishers where it saw an average of 19% higher daily downloads of articles shared in this way.

*'I have found kudos really useful', says Philip Gale, Professor of Supramolecular Chemistry and Head of the School of Chemistry at the University of Southampton. 'It not only helps me improve the visibility of my papers, by highlighting them to my social network, but also provides a way of widening the audience for the work by linking a lay summary of the work to the paper.'*

After publication of an article within an IUCr Journal, authors will receive a personalized email from the IUCr in-house editorial team, sent by kudos, requesting them to log on to the kudos platform. On the platform, authors will be led through various steps that prompt them to explain their article; add content via links to other content such as images and data; and share their article via social networks and email.

The kudos platform will enable authors to see the effect of their actions on altmetrics and usage data.

The service is free for users; IUCr Journals pay a small fee for authors to receive a premium level of service, including customized guidance on how to make best use of the service, and the addition of usage data to help authors evaluate the impact of their efforts.

To find out more about kudos and our plans, please contact Dr Jonathan Agbenyega, Business Development Manager, IUCr ([ja@iucr.org](mailto:ja@iucr.org)).

#### Examples of articles with lay summaries

- [Acta Cryst. A](#)
- [A new theory for X-ray diffraction](#)
- [Acta Cryst. B](#)
- [Crystal structure of beta-Pigment Red 170](#)
- [Modulated structure of adamantan-1-iumonium 4-fluorobenzoate at low temperature](#)
- [Acta Cryst. D](#)
- [Fingerprinting crystal structures with Raman spectroscopy](#)
- [pH measurement with a spectrophotometer](#)
- [J. Appl. Cryst.](#)
- [How does the Nb-content change the martensite crystallography in Ti-Nb alloys?](#)
- [J. Synchrotron Rad.](#)
- [Achieve sub-10 pm spatial resolution using EXAFS](#)

<http://www.iucr.org/resources/article/101107/20132731401133>

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EN 26/01/2013



# Kudos widget

The screenshot displays the Acta Crystallographica Section A website. At the top, the journal title and navigation menu are visible. The main content area features a research paper titled "Viruses and fullerenes - symmetry as a common thread?" by P.-P. Dechant, J. Wardman, T. Keef, and R. Twarock. The paper's abstract and keywords are provided. Below the abstract, a Kudos widget is present, which includes a summary of the paper and a list of resources. The Kudos logo is also visible in the bottom right corner of the page.

Acta Cryst. (2014), A70, 162-167  
doi:10.1107/S2053273313034220

## Viruses and fullerenes - symmetry as a common thread?

P.-P. Dechant, J. Wardman, T. Keef and R. Twarock

The principle of affine symmetry is applied here to the nested fullerene cages (carbon onions) that arise in the context of carbon chemistry. Previous work on affine extensions of the icosahedral group has revealed a new organizational principle in virus structure and assembly. This group-theoretic framework is adapted here to the physical requirements dictated by carbon chemistry, and it is shown that mathematical models for carbon onions can be derived within this affine symmetry approach. This suggests the applicability of affine symmetry in a wider context in nature, as well as offering a novel perspective on the geometric principles underpinning carbon chemistry.

Keywords: **symmetry**; **viruses**; **fullerenes**; **carbon onions**; **Coxeter groups**; **affine extensions**; **quasicrystals**.

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The following simple language summary of this publication has been provided by the author(s):

### Virus structure inspires novel understanding of onion-like carbon nanoparticles

**What is it about?**

Symmetry is ubiquitous in the natural world. It occurs in gemstones and snowflakes and even in biology, an area typically associated with complexity and diversity. There are striking examples: the shapes of virus particles, such as those causing the common cold, are highly symmetrical and look like tiny footballs. We have developed new mathematical tools to better understand the implications of this high degree of symmetry to virus structure, assembly and dynamics.

**Why is this important?**

In this paper we show that these generalised symmetries apply more widely in the natural world and also account for the structures of Russian-doll-like arrangements of carbon cages known as carbon onions. It was known previously that individual shells could be modeled using symmetry techniques, but the fact that the entire structure is collectively constrained by a single symmetry principle is a surprising new result with implications for assembly and potential applications to nanotechnology.

[Read more on Kudos \(?\)](#)

### Virus structure inspires novel understanding of onion-like carbon nanoparticles

**Resources**

- [International Union of Crystallography Press Release](#)  
A press release explaining the context and content of the article in laypeople's terms.
- [Nature Physics Research Highlight](#)  
Nature selected our article as a Physics Research Highlight.
- [Durham Mathematical Sciences Department Press Release](#)  
A press release from the Durham Mathematics Department concerning the article and the media attention it got.


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RESEARCH PAPERS  
Acta Cryst. (2014), D70, 1289–1296  
doi:10.1107/S1399004714004039




## Fingerprinting redox and ligand states in haemprotein crystal structures using resonance Raman spectroscopy

D. Kokkili, F. S. N. Dworkowski, G. Pompidor, M. R. Fuchs, C. R. Andrew, S. Antonyuk, R. W. Strange, J. R. Eady, S. S. Hasnain and M. A. Hough

It is crucial to assign the correct redox and ligand states to crystal structures of proteins with an active redox centre to gain valid functional information and prevent the misinterpretation of structures. Single-crystal spectroscopies, particularly when applied *in situ* at macromolecular crystallography beamlines, allow spectroscopic investigations of redox and ligand states and the identification of reaction intermediates in protein crystals during the collection of structural data. Single-crystal resonance Raman spectroscopy was carried out in combination with macromolecular crystallography on Swiss Light Source beamline X10SA using cytochrome *c* from *Alcaligenes xylosoxidans*. This allowed the fingerprinting and validation of different redox and ligand states, identification of vibrational modes and identification of intermediates together with monitoring of radiation-induced changes. This combined approach provides a powerful tool to obtain complementary data and correctly assign the true oxidation and ligand state(s) in redox-protein crystals.

**Keywords:** resonance Raman spectroscopy; haemproteins; cytochrome *c*; redox states; ligand states.

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Supporting Information.

PDB references: 4cYUcp, 4cda, 4cdy, 4cdv, 4cdp, 4cdg, 4cde

The following simple language summary of the publication has been provided by the author(s):

### Fingerprinting crystal structures with Raman spectroscopy

**What is it about?**  
X-ray crystallography is a vital means of understanding protein structure. It is important to ensure that the structures generated by this method represent the true state of the protein in the organism and also that the X-rays have not changed or damaged the protein. In this paper we used a spectroscopic method to obtain 'fingerprints' for different states of the protein. This approach allows us to identify the starting state of the protein as well as to monitor any changes due to X-ray exposure.

**Why is this important?**  
This work, carried out in collaboration with Swiss Light Source scientists shows the use of Raman spectroscopy as an efficient fingerprinting tool. It has the potential to be applied at other synchrotrons for structure validation and to maximise the information content of combined spectroscopic-crystallographic experiments.

[Read more on PubMed \(7\)](#)

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The kudos platform will enable authors to see the effect of their actions on altmetrics and usage data.

The service is free for users; IUCr Journals pay a small fee for authors to receive a premium level of service, including customized guidance on how to make best use of the service, and the addition of usage data to help authors evaluate the impact of their efforts.

To find out more about kudos and our plans, please contact Dr Jonathan Agbenyega, Business Development Manager, IUCr (ja@iucr.org).

#### Examples of articles with lay summaries

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EN 26/01/2014

# Kudos widget

The screenshot displays the Acta Crystallographica Section A website. At the top, the journal title "Acta Crystallographica Section A" and the subtitle "FOUNDATIONS AND ADVANCES" are visible. A navigation bar includes links for "home", "archive", "editors", "for authors", "for readers", "submit", and "subscribe". A search bar is located in the top right corner. The main content area features a research paper titled "Viruses and fullerenes - symmetry as a common thread?" by P.-P. Dechant, J. Wardman, T. Keef, and R. Twarock. The paper's abstract discusses the application of affine symmetry to carbon onions and virus structures. A "Kudos" widget is embedded on the page, providing a summary of the paper and highlighting its significance. The widget includes a "What is it about?" section, a "Why is this important?" section, and a "Resources" section with links to press releases and research highlights.

Acta Cryst. (2014), A70, 162-167  
doi:10.1107/S2053273313034220

## Viruses and fullerenes - symmetry as a common thread?

P.-P. Dechant, J. Wardman, T. Keef and R. Twarock

The principle of affine symmetry is applied here to the nested fullerene cages (carbon onions) that arise in the context of carbon chemistry. Previous work on affine extensions of the icosahedral group has revealed a new organizational principle in virus structure and assembly. This group-theoretic framework is adapted here to the physical requirements dictated by carbon chemistry, and it is shown that mathematical models for carbon onions can be derived within this affine symmetry approach. This suggests the applicability of affine symmetry in a wider context in nature, as well as offering a novel perspective on the geometric principles underpinning carbon chemistry.

Keywords: **symmetry**; **viruses**; **fullerenes**; **carbon onions**; **Coxeter groups**; **affine extensions**; **quasicrystals**.

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The following simple language summary of this publication has been provided by the author(s):

### Virus structure inspires novel understanding of onion-like carbon nanoparticles

**What is it about?**

Symmetry is ubiquitous in the natural world. It occurs in gemstones and snowflakes and even in biology, an area typically associated with complexity and diversity. There are striking examples: the shapes of virus particles, such as those causing the common cold, are highly symmetrical and look like tiny footballs. We have developed new mathematical tools to better understand the implications of this high degree of symmetry to virus structure, assembly and dynamics.

**Why is this important?**

In this paper we show that these generalised symmetries apply more widely in the natural world and also account for the structures of Russian-doll-like arrangements of carbon cages known as carbon onions. It was known previously that individual shells could be modeled using symmetry techniques, but the fact that the entire structure is collectively constrained by a single symmetry principle is a surprising new result with implications for assembly and potential applications to nanotechnology.

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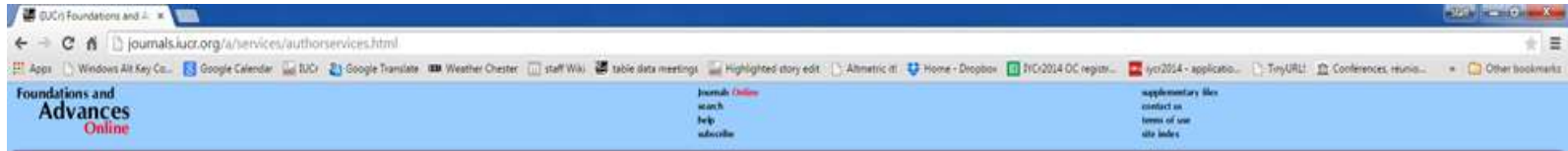
### Virus structure inspires novel understanding of onion-like carbon nanoparticles

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A press release explaining the context and content of the article in laypeople's terms.
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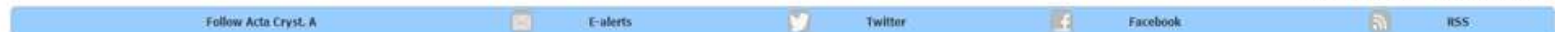
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Paul P. Ewald, Acta Crystallographica (1948), 1, 2.



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