

Publications in IUCr journals

Acta Cryst. (2014). A70, 309-316 [[doi:10.1107/S2053273314010626](https://doi.org/10.1107/S2053273314010626)]

On the temperature dependence of H- U_{iso} in the riding hydrogen model

[J. Lübben](#), [C. Volkmann](#), [S. Grabowsky](#), [A. Edwards](#), [W. Morgenroth](#), [F. P. A. Fabbiani](#), [G. M. Sheldrick](#) and [B. Dittrich](#)

Synopsis: The temperature dependence of hydrogen U_{iso} and parent U_{eq} in the riding hydrogen model is investigated by neutron diffraction, aspherical-atom refinements and QM/MM and MO/MO cluster calculations. Fixed values of 1.2 or 1.5 appear to be underestimated, especially at temperatures below 100 K.

Online 28 May 2014

J. Appl. Cryst. (2014). 47 [[doi:10.1107/S1600576714010838](https://doi.org/10.1107/S1600576714010838)]

***PolaBer*: a program to calculate and visualize distributed atomic polarizabilities based on electron density partitioning**

[A. Krawczuk](#), [D. Pérez](#) and [P. Macchi](#)

Synopsis: A program is presented for the calculation and visualization of distributed atomic polarizabilities, quantities which are useful for the evaluation of crystal properties such as the optical indicatrix.

Online 14 June 2014

PHYSICS | FELS

IUCrJ (2014) **1**, 194-199

doi: [10.1107/S2052252514007283](https://doi.org/10.1107/S2052252514007283)

First spin-resolved electron distributions in crystals from combined polarized neutron and X-ray diffraction experiments

M. Deutsch, **B. Gillon**, **N. Claiser**, **J.-M. Gillet**, **C. Lecomte** and **M. Souhassou**

A method to map spin-resolved electron distribution from combined polarized neutron and X-ray diffraction is described and applied for the first time to a molecular magnet and it is shown that spin up density is 5% more contracted than spin down density.

Acta Cryst. (2014). A70, 291-299 [[doi:10.1107/S2053273314006305](https://doi.org/10.1107/S2053273314006305)]

On the assessment of time-resolved diffraction results

[B. Fournier](#) and [P. Coppens](#)

Synopsis: Agreement factors based on the ratio of intensities R collected in dynamic structure pump-probe crystallography experiments are shown to be analogous to the R factors widely used in standard crystallographic refinements. Fourier photodifference maps allow the visualization of the externally induced structural changes in the crystal, but also can be used during refinement to monitor its progress. Photodeformation maps are modified to separate the photo-induced structural change from the effect of the temperature increase on laser exposure.

Online 2 May 2014

Acta Cryst. (2014). A70, 248-256 [[doi:10.1107/S2053273314000898](https://doi.org/10.1107/S2053273314000898)]

About systematic errors in charge-density studies

[J. Henn](#) and [K. Meindl](#)

Synopsis: An indicator of systematic errors based on theoretical R values is introduced and applied to charge-density data.

Online 13 March 2014

CHEMISTRY | CRYSTENG

IUCrJ (2014) **1**, 119-128

doi: [10.1107/S2052252514003327](https://doi.org/10.1107/S2052252514003327)

The enrichment ratio of atomic contacts in crystals, an indicator derived from the Hirshfeld surface analysis

[C. Jelsch](#), [K. Ejsmont](#) and [L. Huder](#)

An enrichment ratio is derived from the decomposition of the crystal contact surface between pairs of interacting chemical species. The propensity of different contact types to form is investigated.

Acta Cryst. (2014). A70, 39-48 [[doi:10.1107/S2053273313026600](https://doi.org/10.1107/S2053273313026600)]

Experimental determination of core electron deformation in diamond

[N. Bindzus](#), [T. Straasø](#), [N. Wahlberg](#), [J. Becker](#), [L. Bjerg](#), [N. Lock](#), [A.-C.](#)

Dippel and B. B. Iversen

Synopsis: Based on benchmark synchrotron powder X-ray diffraction data, the subtleties in the electron density of diamond are explored. A contraction of the core density inherently linked to covalent bond formation is experimentally observed.

Online 17 December 2013

Acta Cryst. (2014). **A70**, 72-91 [[doi:10.1107/S2053273313028313](https://doi.org/10.1107/S2053273313028313)]

Statistical analysis of multipole-model-derived structural parameters and charge-density properties from high-resolution X-ray diffraction experiments

R. Kaminski, S. Domagala, K. N. Jarzemska, A. A. Hoser, W. F. Sanjuan-Szklarz, M. J. Gutmann, A. Makal, M. Malinska, J. M. Bak and K. Wozniak

Synopsis: A comprehensive analysis of various properties derived from multiple high-resolution X-ray diffraction experiments is reported. The study indicates the precision and reliability of the analysed quantities and their usefulness in charge-density studies of organic molecules.

Online 20 December 2013

Acta Cryst. (2013). **A69**, 570-582 [[doi:10.1107/S0108767313024458](https://doi.org/10.1107/S0108767313024458)]

Comparative study of X-ray charge-density data on CoSb₃

M. S. Schmøkel, L. Bjerg, F. K. Larsen, J. Overgaard, S. Cenedese, M. Christensen, G. K. H. Madsen, C. Gatti, E. Nishibori, K. Sugimoto, M. Takata and B. B. Iversen

Synopsis: Experimental electron-density studies of inorganic, extended solids containing heavy elements are highly challenging. Such a study on a particularly problematic case, CoSb₃, is presented and discussed.

Online 17 October 2013

J. Appl. Cryst. (2013). **46**, 1513-1517 [[doi:10.1107/S0021889813020098](https://doi.org/10.1107/S0021889813020098)]

***NCImilano*: an electron-density-based code for the study of noncovalent interactions**

G. Saleh, L. Lo Presti, C. Gatti and D. Ceresoli

Synopsis: A code to investigate noncovalent interactions making use only of the electron density distribution (theoretically or experimentally derived) is presented.

Online 11 September 2013

J. Appl. Cryst. (2013). **46**, 1151-1161 [[doi:10.1107/S0021889813013903](https://doi.org/10.1107/S0021889813013903)]

Diffraction studies under *in situ* electric field using a large-area hybrid pixel XPAD detector

P. Fertey, P. Alle, E. Wenger, B. Dinkespiler, O. Cambon, J. Haines, S. Hustache, K. Medjoubi, F. Picca, A. Dawiec, P. Breugnon, P. Delpierre, C. Mazzoli and C. Lecomte

Synopsis: The diffraction response of a single crystal subjected to an *in situ* electric field periodically reversed is recorded with an XPAD large-area hybrid pixel detector. This new approach to the field-switching method offers unprecedented perspectives to analyse the electric field-induced structural deformations.

Online 18 July 2013

Acta Cryst. (2013). **A69**, 427-434 [[doi:10.1107/S0108767313010143](https://doi.org/10.1107/S0108767313010143)]

Digital electron diffraction - seeing the whole picture

R. Beanland, P. J. Thomas, D. I. Woodward, P. A. Thomas and R. A. Roemer

Synopsis: Computer control of beam tilt and image capture allows the collection of electron diffraction patterns over a large angular range, without any overlap in diffraction data and from a region limited only by the size of the electron beam. This results in a significant improvement in data volumes and ease of interpretation.

Online 21 May 2013

J. Appl. Cryst. (2013). **46**, 649-655 [[doi:10.1107/S002188981300592X](https://doi.org/10.1107/S002188981300592X)]

Element-selective charge density visualization of endohedral metallofullerenes using synchrotron X-ray multi-wavelength anomalous powder diffraction data

[S. Maki](#), [E. Nishibori](#), [D. Kawaguchi](#), [M. Sakata](#), [M. Takata](#), [T. Inoue](#) and [H. Shinohara](#)

Synopsis: An algorithm for determining the element-selective charge density is developed using multi-wavelength anomalous synchrotron X-ray powder diffraction data. The method is employed in order to resolve the disordered structure of yttrium in $(Y@C_{82})(C_6H_5CH_3)$.

Online 6 April 2013

Acta Cryst. (2013). **A69**, 309-321 [[doi:10.1107/S0108767313005011](https://doi.org/10.1107/S0108767313005011)]

Anisotropic displacement parameters for molecular crystals from periodic Hartree-Fock and density functional theory calculations

[A. Ø. Madsen](#), [B. Civalleri](#), [M. Ferrabone](#), [F. Pascale](#) and [A. Erba](#)

Synopsis: An approach to calculating anisotropic displacement parameters based on periodic *ab initio* calculations is introduced. Calculations on urea, benzene, urotropine and L-alanine are discussed and validated against available experimental results.

Online 16 April 2013

J. Appl. Cryst. (2012). **45**, 1254-1260
[[doi:10.1107/S0021889812041283](https://doi.org/10.1107/S0021889812041283)]

Special directions in momentum space. II. Hexagonal, tetragonal and trigonal symmetries

[G. Kontrym-Sznajd](#) and [M. Samsel-Czekala](#)

Synopsis: Special directions in the Brillouin zone for hexagonal, tetragonal and trigonal lattices are defined. They optimize a description of various physical quantities having full symmetry of the Brillouin zone, and they define the projections, measured either in Compton scattering or in positron annihilation experiments, that allow reconstruction of electron momentum densities with the highest efficiency.

Online 15 November 2012

Acta Cryst. (2012). **A68**, 675-686 [[doi:10.1107/S0108767312031996](https://doi.org/10.1107/S0108767312031996)]

Experimental determination of spin-dependent electron density by joint

refinement of X-ray and polarized neutron diffraction data

[M. Deutsch](#), [N. Claiser](#), [S. Pillet](#), [Y. Chumakov](#), [P. Becker](#), [J.-M. Gillet](#), [B. Gillon](#), [C. Lecomte](#) and [M. Souhassou](#)

Synopsis: An algorithm for joint multipolar charge and spin refinement against X-ray and polarized neutron diffraction data is described and applied for the first time to molecular magnetic crystals. This algorithm is implemented in the software *MOLLYNX*.

Online 18 September 2012

Acta Cryst. (2012). **A68**, 705-714 [[doi:10.1107/S010876731203317X](https://doi.org/10.1107/S010876731203317X)]

Is it possible to derive quantitative information on polarization of electron density from the multipolar model?

[J. M. Bak](#), [Z. Czyznikowska](#) and [P. M. Dominiak](#)

Synopsis: Tests were carried out to determine whether the Hansen-Coppens multipolar model is accurate enough to study changes of electrostatic properties under the influence of a crystal field. The study revealed that electrostatic properties obtained from the multipolar model are significantly different from those obtained from theoretical cluster or perturbation theory calculations.

Online 25 September 2012

A critical analysis of dipole-moment calculations as obtained from experimental and theoretical structure factors

[A. Poulain-Paul](#), [A. Nassour](#), [C. Jelsch](#), [B. Guillot](#), [M. Kubicki](#) and [C. Lecomte](#)

Synopsis: Three charge-density models were tested against theoretical and experimental X-ray diffraction data and the resulting molecular dipole moments are compared.

Online 5 October 2012

Acta Cryst. (2012). **A68**, 750-762 [[doi:10.1107/S0108767312037269](https://doi.org/10.1107/S0108767312037269)]

Maximum-entropy-method charge densities based on structure-factor extraction with the commonly used Rietveld refinement programs *GSAS*, *FullProf* and *Jana2006*

[N. Bindzus](#) and [B. B. Iversen](#)

Synopsis: Synchrotron powder X-ray diffraction data are analysed with generally available Rietveld refinement software and strategies are suggested for subsequent calculation of

maximum-entropy-method charge densities.

Online 18 October 2012

Acta Cryst. (2012). A68, 568-581 [[doi:10.1107/S0108767312029005](https://doi.org/10.1107/S0108767312029005)]

Experimental dynamic electron densities of multipole models at different temperatures

[S. Mondal](#), [S. J. Prathapa](#) and [S. van Smaalen](#)

Synopsis: The dynamic electron densities of multipole models and independent atom models are computed by inverse Fourier transform of accurately computed structure factors of α -glycine and D,L-serine at different temperatures. A topological analysis of the dynamic electron densities provides a quantitative measure for the effects of zero-point vibrations and temperature on electron densities.

Online 2 August 2012

Acta Cryst. (2012). A68, 589-594 [[doi:10.1107/S0108767312027614](https://doi.org/10.1107/S0108767312027614)]

Radial integrals for the magnetic form factor of the 5*d* electrons of rare earth elements

[K. Kobayashi](#), [T. Nagao](#) and [M. Ito](#)

Synopsis: The radial integrals $\langle j_L \rangle$, where $L = 0, 2, 4$, for several electronic configurations of the 5*d* electrons of rare earth elements are calculated. Gaussian analytical expressions with four exponential terms are fitted to the resultant values and the coefficients of the expressions are tabulated.

Online 26 July 2012

Acta Cryst. (2012). A68, 435-442 [[doi:10.1107/S0108767312013001](https://doi.org/10.1107/S0108767312013001)]

Crystal-field effects in L-homoserine: multipoles *versus* quantum chemistry

[B. Dittrich](#), [E. Sze](#), [J. J. Holstein](#), [C. B. Hübschle](#) and [D. Jayatilaka](#)

Synopsis: Crystal-field effects in the non-standard amino acid L-homoserine were investigated. Benchmark results from periodic B3LYP calculations are well reproduced by point-charge models. Basis-set representations of the electron density show subtle features further away from the nuclei, which cannot be retrieved by the Hansen/Coppens multipole model.

Online 1 May 2012

Acta Cryst. (2012). A68, 452-463 [[doi:10.1107/S0108767312016571](https://doi.org/10.1107/S0108767312016571)]

Charge-density analysis and electrostatic properties of 2-carboxy-4-methylanilinium chloride monohydrate obtained using a multipolar and a spherical-charges model

[N. Dadda](#), [A. Nassour](#), [B. Guillot](#), [N. Benali-Cherif](#) and [C. Jelsch](#)

Synopsis: The multipolar electron distribution of the title compound was compared with a spherical-charge modelling of the atoms, bonding density and lone pairs.

Online 10 May 2012

Acta Cryst. (2012). A68, 464-469 [[doi:10.1107/S0108767312015772](https://doi.org/10.1107/S0108767312015772)]

A practical study of the electron-density-map variance

[C. Giacovazzo](#) and [A. Mazzone](#)

Synopsis: An algorithm for the calculation of the variance of electron-density maps *via* fast Fourier transform is proposed. A study of the related features is described.

Online 15 May 2012

Acta Cryst. (2012). A68, 337-351 [[doi:10.1107/S0108767312008197](https://doi.org/10.1107/S0108767312008197)]

An improved experimental databank of transferable multipolar atom models - ELMAM2. Construction details and applications

[S. Domagala](#), [B. Fournier](#), [D. Liebschner](#), [B. Guillot](#) and [C. Jelsch](#)

Synopsis: The construction and application of the generalized ELMAM2 databank of experimentally derived aspherical atom types are described. With this new database, it is possible to transfer multipolar parameters to proteins and various organic molecules within the limitation of the currently available atom types.

Online 29 March 2012

Acta Cryst. (2012). A68, 244-255 [[doi:10.1107/S0108767311053281](https://doi.org/10.1107/S0108767311053281)]

Covariance and correlation estimation in electron-density maps

[A. Altomare](#), [C. Cuocci](#), [C. Giacovazzo](#), [A. Moliterni](#) and [R. Rizzi](#)

Synopsis: The covariance between two points of an electron-density map has been calculated, no matter the correlation between the model and target structures.

Online 25 January 2012

Acta Cryst. (2012). **A68**, 301-303 [doi:10.1107/S0108767312003066]

On the significance of Bragg reflections

[M. R. V. Jørgensen](#), [H. Svendsen](#), [M. S. Schmøkel](#), [J. Overgaard](#) and [B. B. Iversen](#)

Synopsis: The statistical descriptor, W , recently introduced by Henn & Meindl [*Acta Cryst.* (2010), **A66**, 676-684] is modified to include the scale factors introduced in data processing, and the effects of using empirical error models on the final significance distribution are discussed.

Online 16 February 2012

Acta Cryst. (2012). **A68**, 304 [doi:10.1107/S010876731200325X]

Response to *On the significance of Bragg reflections* by Jørgensen *et al.*

[J. Henn](#) and [K. Meindl](#)

Synopsis: A response is given to the article *On the significance of Bragg reflections* by Jørgensen *et al.* [*Acta Cryst.* (2012). **A68**, 301-303].

Online 16 February 2012

Acta Cryst. (2012). **A68**, 110-116 [doi:10.1107/S0108767311037974]

On QM/MM and MO/MO cluster calculations of all-atom anisotropic displacement parameters for molecules in crystal structures

[B. Dittrich](#), [S. Pfitzenreuter](#) and [C. B. Hübschle](#)

Synopsis: A computationally efficient method to calculate anisotropic displacement parameters (ADPs) by QM/MM or MO/MO cluster calculations is described. Calculated ADPs are used in place of experimentally refined ADPs in three examples and provide a significant improvement over the isotropic description.

Online 11 November 2011

Acta Cryst. (2012). **A68**, 139-147 [doi:10.1107/S0108767311042176]

New version of the theoretical databank of transferable aspherical pseudoatoms, UBDB2011 - towards nucleic acid modelling

[K. N. Jarzemska](#) and [P. M. Dominiak](#)

Synopsis: The extended theoretical databank of aspherical pseudoatoms (UBDB2011) and the related *LSDB* program are presented. The applicability of the databank to electrostatic energy estimation for chemical systems containing nucleic base and amino-acid fragments was extensively tested.

Online 17 November 2011

Acta Cryst. (2011). **A67**, 473-480 [[doi:10.1107/S010876731102633X](https://doi.org/10.1107/S010876731102633X)]

Radial integrals for the magnetic form factor of *5d* transition elements

[K. Kobayashi](#), [T. Nagao](#) and [M. Ito](#)

Synopsis: The radial integrals, $\langle j_L \rangle$, where $L = 0, 2, 4$, for several electronic configurations in the *5d* electrons of transition metal atoms and ions are calculated. The resultant values are fitted to Gaussian analytical expressions with four exponential terms, and the coefficients of the expressions are tabulated.

Online 3 August 2011
