

## Checklist for Authors of Papers Submitted to *Acta Crystallographica*, Section C

### Short-Format Papers – a New Section

Papers are considered for publication in Section C that report the results of one or more crystal structure determinations and that are primarily concerned only with the crystal and molecular structure results.

Following recent decisions by the Commission on Journals, *Acta Crystallographica*, Section C is to be divided into two parts. The format of papers for publication in the first part will remain essentially identical with that currently used for Section C papers. The second part, to be entitled Short-Format Papers, will include shorter papers that will differ from the current format in having neither *Introduction* nor *Discussion* sections (*i.e.* they shall comprise only *Abstract*, *Experimental*, tables and figures, and *Related literature*). The structural criteria for both parts will be identical. Concise presentation is essential in either format. There are some additional changes affecting the form of the title and the content of the *Abstract* and *Experimental* sections (see below).

Papers submitted for consideration in *Acta Crystallographica*, Section C, subject to the Co-editor's discretion, should conform with the following arrangement:

The *Title* should be both short and informative and not include long compound names. It should relate the structure to the chemical or other interest in the crystal, *e.g.* 'The structure of a morphine derivative . . . . .'.  
 The *Abstract* should consist of the information given in §(d) of the checklist below (in abbreviated telegraphic form and preferably in the order given).

The *Introduction* (not applicable to Short-Format Papers) should briefly state the reason for undertaking the structure determination and its chemical, physical, biological or other interest. If organic, or containing complicated organic ligands, a display of the structural formula of the material studied should be given, in accordance with IUPAC convention.

The *Experimental* section should include the information in §(e) of the checklist below, either in tabular or abbreviated telegraphic form. Any further details, say of refinement, should be treated as normal text, but kept as brief as possible. The *Experimental* will generally include not more than two tables and two figures per structure as described in §2.1 of *Notes for Authors* [*Acta Cryst.* (1983). A39, 174–186]. Additional tables and figures may be deposited. If the table of bond distances and angles is very long, this will be deposited and only values that are unusual and relevant to the discussion will be retained for publication.

The *Discussion* (not applicable to Short-Format Papers) should include comment on any unusual features of coordination, bonding, bond lengths, bond angles, thermal vibrations *etc.*

Attention is drawn to the *Suggested guidelines for the publication of Rietveld analyses and pattern decomposition studies* [*J. Appl. Cryst.* (1982). 15, 357–359] and to *Recommendations of the Ad-hoc Committee on Criteria for Publication of Charge Density Studies* [*J. Appl. Cryst.* (1984). 17, 369]. Determinations based on powder data should be accompanied by copies of the data in the appropriate format (see *Notes for Authors*, Appendix III); these will be deposited both with the JCPDS, Swarthmore, and at the Union's office in Chester. Papers on polytypes will be treated no differently from those on other materials and basic diffraction data relating to these should be made available either for publication or for deposition. Recommended techniques for improving the standard of many crystal structure investigations will be published in *Acta Cryst.* (1985). C41, 301–303.

The checklist below is provided for the convenience of authors submitting papers for publication in Section C. Fuller information is given in *Notes for Authors*. Checklists for authors of papers submitted to Sections A and B of *Acta Crystallographica* and to *Journal of Applied Crystallography* are given in the first issue of those journals for 1985.

**All papers submitted for publication in *Acta Crystallographica*, Section C, should be checked against the following list:**

- (a) Signed *Transfer of Copyright* form with manuscript
- (b) *Typescripts*  
 Submitted in triplicate to any Co-editor  
 Double-spaced with wide margins (*e.g.* 30 mm)  
 Authors' addresses in full  
 Maximum of 4000 words for full articles on a single structure, 2500 words for each additional structure determination  
 Maximum of 2000 words for Short-Format Papers  
 Maximum of 1000 words for Short Communications  
 (For typography see *Notes for Authors*, §9)
- (c) *Title*  
 Short, informative and related to the chemistry or other relevant interest in the compound  
 Not to include long compound names

(d) *Abstract*

Suitable for reproduction by abstracting services without change of wording

Any references to be given in full

To include:

Systematic IUPAC name

Chemical formula

Formula weight

Space group

Unit-cell dimensions

Volume of unit cell ( $\text{\AA}^3$ )

$Z$

Measured and calculated densities  $D_m, D_x$

Radiation and wavelength

Linear absorption coefficient

$F(000)$

Temperature of measurement

Final value of  $R = [\sum(|F_o| - |F_c|)] / \sum |F_o|$  and number of unique reflections

Discussion of principal structural results (in about 50 additional words)

(e) *Experimental section*

To include:

Source of material

Crystal shape and size

Method of measuring  $D_m$

Diffractometer used

Method of measuring intensities

Number and  $\theta$  range of reflections used for measuring lattice parameters

Absorption correction applied (with maximum and minimum values)

Maximum value of  $(\sin\theta)/\lambda$  reached in intensity measurements

Range of  $h, k$  and  $l$

Standard reflections and their intensity variation throughout experiment

Number of reflections measured

Number of unique reflections

Value of  $R_{\text{int}} = [\sum |F - \langle F \rangle|] / \sum F$ , from merging equivalent reflections]

Number of unobserved reflections

Criterion for recognizing unobserved reflections [ $I < n\sigma(I)$ ]

Method used to solve structure

Definition of origin for polar structures

Independent physical measurements made to check polarity or chirality as applicable

Use of  $F$  or  $F^2$  magnitudes in least-squares refinement

Methods of locating and refining H atoms if applicable

Parameters refined

Values of  $R$ ,  $wR = [\sum w(|F_o| - |F_c|)^2 / \sum wF_o^2]^{1/2}$  and  $S = [\sum w(|F_o| - |F_c|)^2 / (m - n)]^{1/2}$  (or the  $F^2$  equivalents)

Method used to calculate  $w$

Ratio of maximum least-squares shift to error in final refinement cycle,  $(\Delta/\sigma)_{\text{max}}$

Justification of  $(\Delta/\sigma)_{\text{max}}$  value if it exceeds 1.0

Maximum positive and maximum negative electron density in final difference Fourier synthesis,  $(\Delta\rho)_{\text{max}}, (\Delta\rho)_{\text{min}}$

Primary- and secondary-extinction values (if used)

Source of atomic scattering factors and  $f', f''$  values

All computer programs used (see also § 10 of *Notes for Authors*)

(f) *Diagrams and photographs*

Drawings in black ink or high-quality glazed prints

Cited in text

Typically two per structure (projection of molecule and stereoview or projection of unit-cell packing)

As small as possible consistent with legibility

High information density

Lettering not less than 4 mm high on International A4 sized (210 × 297 mm) or 8½ × 11 in paper (and *pro rata*)

Figure captions in separate list

Chemical and structural formulae preferably in camera-ready form

Stereofigures:

One of the two figures per structure

Centre-to-centre separation of 55 mm or less

Atom labelling on left and right views that remains legible and higher than 1¼ mm after reduction

(g) *Tables*

Not to repeat information given in text or diagrams

Cited in text

Typically two per structure (coordinates and bonding geometry)

Table number and title to be given for each

To occupy minimum space consistent with clarity

To include e.s.d.'s for all derived quantities (especially all varied parameters)

The following generally to be deposited: structure factors, anisotropic thermal parameters, least-squares planes, unrefined H-atom coordinates

(h) *References*

In form: authors' names followed by year of publication

Alphabetic order in reference list

All references in text to be given in reference list and *vice-versa*

Inclusive page numbers to be given in reference list

- Short-Format Papers should cite essential references under *Related literature* and give full bibliographic details in reference list
- Codens-type notation with volume and initial page number to be used in multi-reference structural papers (see Table)
- (i) *Units and Nomenclature*
- SI units to be used throughout (except for Å)
- Atom labels as C(1) *etc.*
- Space groups in Hermann–Mauguin notation (Schönflies symbols may be used in addition for molecular symmetry)
- Choice of axes as recommended by Kennard, Speakman & Donnay [*Acta Cryst.* (1967). **22**, 445–449]
- Symmetry-equivalent atoms to be denoted as C(1) *etc.*, with symmetry operations defined in terms of equivalent positions
- Reflections, planes, directions and forms to be unambiguously distinguished (see *Notes for Authors*, §8)
- Chemical names and formulae to conform to IUPAC rules, including spelling of element names
- Acronyms to be defined
- Nomenclature of polytypes to conform to Guinier recommendations [*Acta Cryst.* (1984). **A40**, 399–404]
- (j) *Data to be deposited*
- In general:
- Structure factors
- Anisotropic temperature factors
- Least-squares planes and deviations
- Calculated H-atom coordinates
- Normal intermolecular distances
- Tables of non-essential bond lengths and angles
- At the Co-editor's discretion:
- Details of experimental procedures
- Details of mathematical derivations
- Lengthy mathematical appendices
- Lengthy discussion not of general interest
- For macromolecular papers:
- Atomic coordinates, thermal parameters and structure factors in machine-readable form with the Brookhaven Protein Data Bank [see *Acta Cryst.* (1981). **B37**, 1161–1162; *Acta Cryst.* (1982). **B38**, 1050]
- For powder-data papers:
- Powder data (in standard format – see *Notes for Authors*, Appendix III) with the JCPDS *Format of deposited material* (for all papers other than macromolecular):
- Not to exceed A4 size (210 × 297 mm) or 8½ × 11 in
- Minimum character height 1.5 mm
- Three copies, of good photocopyable quality

## Codens for journals frequently referenced in crystallographic papers

<i>Acc. Chem. Res.</i>	ACHREA	<i>Biopolymers</i>	BIPMAA	<i>Discuss. Faraday Soc.</i>	DFSOAW
<i>ACS Symp. Ser.</i>	ACSMC8	<i>Bull. Acad. Pol. Sci. Ser. Sci. Chim.</i>	BAPCAQ	<i>Dokl. Akad. Nauk SSSR</i>	DANKAS
<i>Acta Chem. Scand. Ser. A</i>	ACAPCT			<i>Dokl. Akad. Nauk SSSR Ser. Khim.</i>	DASKAJ
<i>Acta Chem. Scand. Ser. B</i>	ACBOCV	<i>Bull. Chem. Soc. Jpn</i>	BCSJA8	<i>Dopov. Akad. Nauk Ukr. RSR, Ser. B</i>	DANND6
<i>Acta Cryst.</i>	ACCRA9	<i>Bull. Soc. Chim. Belg.</i>	BSCBAG		
<i>Acta Cryst. A</i>	ACACEQ	<i>Bull. Soc. Chim. Fr.</i>	BSCFAS	<i>Eur. J. Biochem.</i>	EJBCAI
<i>Acta Cryst. B</i>	ASBSDK	<i>Bull. Soc. Fr. Minéral. Cristallogr.</i>	BUFCAE	<i>Experientia</i>	EXPEAM
<i>Acta Cryst. C</i>	ACSCEE	<i>Can. J. Chem.</i>	CJCHAG	<i>FEBS Lett.</i>	FEBLAL
<i>Acta Metall.</i>	AMETAR	<i>Can. J. Phys.</i>	CJPHAD	<i>Ferroelectrics</i>	FEROAS
<i>Adv. Chem. Ser. (ACS)</i>	ADCSAJ	<i>Can. Mineral.</i>	CAMIA6	<i>Finn. Chem. Lett.</i>	FCMLAS
<i>Adv. Inorg. Chem. Radiochem.</i>	AICRAH	<i>Carbohydr. Res.</i>	CRBRAT	<i>Fiz. Tverd. Tela (Leningrad)</i>	FTVTAC
<i>Adv. Struct. Res. Diffr. Methods</i>	ASDMA9	<i>Carbon</i>	CRBNAH	<i>Fortschr. Mineral.</i>	FMRLAL
<i>Am. Mineral.</i>	AMMIAY	<i>Carnegie Inst. Washington Yearb. Chem. Ber.</i>	CIWYAO	<i>Gazz. Chim. Ital.</i>	GCITA9
<i>Angew. Chem.</i>	ANCEAD	<i>Chem. Commun.</i>	CHBEAM	<i>Gold Bull.</i>	GLDBBS
<i>Angew. Chem. Int. Ed. Engl.</i>	ACIEAY	<i>Chem. Commun. Univ. Stockholm</i>	CCOMA8	<i>Helv. Chim. Acta Heterocycles</i>	HCACAV
<i>Ann. Chim. (Paris)</i>	ANCPAC	<i>Chem. Erde</i>	CCUSBN	<i>Indian Chem. J.</i>	HTCYAM
<i>Ann. Chim. (Rome)</i>	ANCRAI	<i>Chem. Ind. (London)</i>	CERDAA	<i>Indian J. Chem.</i>	ICLJAG
<i>Ann. N.Y. Acad. Sci.</i>	ANYAA9	<i>Chem. Lett.</i>	CHINAG	<i>Indian J. Phys.</i>	IJOCAP
<i>Ann. Phys. (Leipzig)</i>	ANPYA2	<i>Chem. Pharm. Bull. (Jpn)</i>	CMLTAG	<i>Indian J. Phys. Part A</i>	IJPYAS
<i>Annu. Rev. Phys. Chem.</i>	ARPLAP	<i>Chem. Phys. Lett.</i>	CPBTAL	<i>Indian J. Phys. Part B</i>	INJADP
<i>Ark. Kemi</i>	ARKEAD	<i>Chem. Zvesti</i>	CHPLBC	<i>Inorg. Chem.</i>	IJPBDU
<i>Arzneim.-Forsch.</i>	ARZNAD	<i>Chimia</i>	CSRPB9	<i>Inorg. Chim. Acta</i>	INUCAJ
<i>Atti Accad. Naz. Lincei. Cl. Sci. Fis. Mat. Nat. Rend.</i>	AANLAW	<i>Coll. Czech. Chem. Commun. Coord. Chem. Rev.</i>	CHZVAN	<i>Int. J. Pept. Protein Res.</i>	ICHAA3
<i>Aust. J. Chem.</i>	AJCHAS	<i>C. R. Séances Acad. Sci. Sér. C</i>	CHIMAD	<i>Isr. J. Chem.</i>	INUCAF
<i>Ber. Bunsenges. Phys. Chem.</i>	BBPCAX	<i>C. R. Séances Acad. Sci. Sér. 2</i>	CCCCAK	<i>Izv. Akad. Nauk SSSR Neorg. Mater.</i>	IUPPC3
<i>Ber. Dtsch. Chem. Ges.</i>	BDCGAS	<i>Croat. Chem. Acta</i>	CCHRAM	<i>J. Am. Chem. Soc.</i>	ISICAT
<i>Ber. Dtsch. Chem. Ges. A</i>	BDCAAA	<i>Cryst. Lattice Defects</i>	CHDCAQ	<i>J. Appl. Cryst.</i>	IVNMAW
<i>Ber. Dtsch. Chem. Ges. B</i>	BDCBAD	<i>Cryst. Res. Technol.</i>	CRSUDO	<i>J. Biol. Chem.</i>	
<i>Biochem. Biophys. Res. Commun.</i>	BBRCA9	<i>Cryst. Struct. Commun.</i>	CCACAA	<i>J. Chem. Phys.</i>	JACSAT
<i>Biochim. Biophys. Acta</i>	BBACAQ		CLADA8		JACGAR
<i>Bioinorg. Chem.</i>	BICHBX		CRTEDF		JBCHA3
<i>Bioorg. Khim.</i>	BIKHD7		CSCMCS		JCPSA6

## CHECKLIST FOR AUTHORS

<i>J. Chem. Res. Synop.</i>	JRPSDC	<i>Justus Liebigs Ann. Chem.</i>	JLACBF	<i>Recl Trav. Chim. Pays-Bas</i>	RTCPA3
<i>J. Chem. Soc. A</i>	JCSIAP	<i>Khim. Prir. Soedin.</i>	KPSUAR	<i>Rev. Chim. Minér.</i>	RVCMA8
<i>J. Chem. Soc. B</i>	JCSPAC	<i>Koord. Khim.</i>	KOKHDC	<i>Rev. Sci. Instrum.</i>	RSINAK
<i>J. Chem. Soc. Chem. Commun.</i>	JCCCAT	<i>Kristallografiya</i>	KRISAJ	<i>Ric. Sci.</i>	RISCAZ
<i>J. Chem. Soc. Dalton Trans.</i>	JCDTBI	<i>Krist. Tech.</i>	KRTEAW	<i>Rocz. Chem.</i>	ROCHAC
<i>J. Chem. Soc. Perkin Trans. 1</i>	JCPRB4	<i>Life Sci.</i>	LIFSAK	<i>Russ. J. Inorg. Chem. (Engl. Trans.)</i>	RJICAQ
<i>J. Chem. Soc. Perkin Trans. 2</i>	JCPKBH	<i>Makromol. Chem.</i>	MACEAK	<i>S. Afr. J. Chem.</i>	SAJCDG
<i>J. Chim. Phys. Phys. Chim. Biol.</i>	JCPBAN	<i>Mater. Res. Bull.</i>	MRBUAC	<i>Schweiz. Mineral. Petrogr. Mitt. Science</i>	SMPTA8
<i>J. Coord. Chem.</i>	JCCMBQ	<i>Mater. Sci.</i>	MSCJDS	<i>Solid State Commun.</i>	SCIEAS
<i>J. Cryst. Growth</i>	JCRGAE	<i>Mater. Sci. Eng.</i>	MSCEAA	<i>Sov. Phys.-Crystallogr. (Engl. Trans.)</i>	SSCOA4
<i>J. Cryst. Mol. Struct.</i>	JCMLB5	<i>Mineral. J.</i>	MJTOAS	<i>Sov. Phys.-Solid State (Engl. Trans.)</i>	SPSSA7
<i>J. Crystallogr. Spectrosc. Res.</i>	JCREDB	<i>Mineral. Mag.</i>	MNLMBB	<i>Spectrochim Acta</i>	SPACA5
<i>J. Electrochem. Soc.</i>	JESOAN	<i>Mol. Cryst. Liq. Cryst.</i>	MCLCA5	<i>Spectrochim Acta Part A</i>	SAMCAS
<i>J. Electron Mater.</i>	JECMA5	<i>Monatsh. Chem.</i>	MOCMB7	<i>Struct. Bonding (Berlin)</i>	STBGAG
<i>J. Fluorine Chem.</i>	JFLCAR	<i>Natl Bur. Stand. US Circ.</i>	NBSCAA	<i>Suom. Kemistil. B</i>	SUKBAJ
<i>J. Heterocycl. Chem.</i>	JHTCAD	<i>Natl Bur. Stand. US Monogr.</i>	NBSMA6	<i>Tetrahedron</i>	TETRAB
<i>J. Inclusion Phenom.</i>	JOIPDF	<i>Natl Bur. Stand. US Spec. Publ.</i>	XNBSAV	<i>Tetrahedron Lett.</i>	TELEAY
<i>J. Inorg. Biochem.</i>	JIBIDJ	<i>Natl Bur. Stand. US Tech. Note</i>	NBTNAE	<i>Theor. Chim. Acta</i>	TCHAAM
<i>J. Inorg. Nucl. Chem.</i>	JINCAO	<i>Nature (London)</i>	NATUAS	<i>TMPM Tschermaks Mineral. Petrogr. Mitt.</i>	TTMMDZ
<i>J. Less Common Met.</i>	JCOMAH	<i>Naturwissenschaften</i>	NATWAY	<i>Trans. Am. Crystallogr. Assoc.</i>	TACAAH
<i>J. Magn. Reson.</i>	JOMRA4	<i>Neues Jahrb. Mineral. Abh.</i>	NJMIAK	<i>Trans. Faraday Soc.</i>	TFSOA4
<i>J. Mater. Sci.</i>	JMTSAS	<i>Neues Jahrb. Mineral. Monatsh.</i>	NJMMAW	<i>Trans. Metall. Soc. AIME</i>	TMSAAB
<i>J. Mol. Biol.</i>	JMOBAK	<i>Nouv. J. Chim.</i>	NJCHD4	<i>Transition Met. Chem. (N.Y.)</i>	TRMCAM
<i>J. Mol. Spectrosc.</i>	JMOSA3	<i>Organometallics</i>	ORGND7	<i>Transition Met. Chem. (Weinheim)</i>	TMCHDN
<i>J. Mol. Struct.</i>	JMOSB4	<i>Philos. Mag.</i>	PHMAA4	<i>Tschermaks Mineral. Petrogr. Mitt.</i>	MPMTAG
<i>J. Nat. Prod.</i>	JNPRDF	<i>Physica A (Amsterdam)</i>	PHYADX	<i>Z. Anorg. Allg. Chem.</i>	ZAACAB
<i>J. Nucl. Mater.</i>	JNUMAM	<i>Physica B &amp; C (Amsterdam)</i>	PHBCDQ	<i>Z. Anorg. Chem.</i>	ZACMAH
<i>J. Org. Chem.</i>	JOCEAH	<i>Physica (Utrecht)</i>	PHYSAG	<i>Z. Elektrochem.</i>	ZEELAI
<i>J. Organomet. Chem.</i>	JORCAI	<i>Phys. Kondens. Mater.</i>	PKOMA3	<i>Z. Kristallogr.</i>	ZEKRDZ
<i>J. Pharmacol. Exp. Ther.</i>	JPETAB	<i>Phys. Rev. B: Condens. Matter</i>	PRBMDO	<i>Z. Metallkd.</i>	ZEMTAE
<i>J. Phys. C</i>	JPSOAW	<i>Phys. Rev. B: Solid State</i>	PLRBAQ	<i>Z. Naturforsch. Teil A</i>	ZTAKDZ
<i>J. Phys. F</i>	JPFMAT	<i>Phys. Status Solidi</i>	PHSSAK	<i>Z. Naturforsch. Teil B</i>	ZNBAD2
<i>J. Phys. Chem.</i>	JPCHAX	<i>Phys. Status Solidi A</i>	PSSABA	<i>Z. Phys. Chem. (Frankfurt am Main)</i>	ZPCFAX
<i>J. Phys. Chem. Solids</i>	JPCSAW	<i>Phys. Status Solidi B</i>	PSSBBD	<i>Z. Phys. Chem. (Leipzig)</i>	ZPCLAH
<i>J. Phys. Lett.</i>	JPSLBO	<i>Pol. J. Chem.</i>	PJCHDQ	<i>Zh. Neorg. Khim.</i>	ZNOKAQ
<i>J. Phys. Soc. Jpn</i>	JUPSAU	<i>Polyhedron</i>	PLYHDE	<i>Zh. Obshch. Khim.</i>	ZOKHA4
<i>J. Polym. Sci.</i>	JPSCAU	<i>Pramana</i>	PRAMCI	<i>Zh. Strukt. Khim.</i>	ZSTKAI
<i>J. Polym. Sci. Polym. Chem. Ed.</i>	JPLCAT	<i>Proc. Natl Acad. Sci. USA</i>	PNASA6		
<i>J. Prakt. Chem.</i>	JPCEAO	<i>Proc. R. Soc. London Ser. A</i>	PRLAAZ		
<i>J. Raman Spectrosc.</i>	JRSPAF	<i>Proc. R. Soc. London Ser. B</i>	PRLBA4		
<i>J. Solid State Chem.</i>	JSSCBI	<i>Prog. Inorg. Chem.</i>	PIOCAR		
<i>J. Struct. Chem. (Engl. Trans.)</i>	JSTCAM	<i>Prog. Med. Chem.</i>	PMDCAY		
<i>Jpn. J. Appl. Phys.</i>	JJAPA5	<i>Q. Rev. Chem. Soc.</i>	QUREA7		
<i>Jpn. J. Appl. Phys. Part 1</i>	JAPNDE	<i>Recl. J. R. Neth. Chem. Soc.</i>	RJRSDK		
<i>Jpn. J. Appl. Phys. Part 2</i>	JAPLD8				

The required form of the Codens-type notation for references in multi-reference structural papers is ACSCEE 41 1 (representing page 1 of Volume 41 of the journal *Acta Cryst. Section C*).