Acta Cryst. (1985). C**41**, 1–4

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). A**39**, 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). C**41**, 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 (Å^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 θ 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_{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, $(\Delta/\sigma)_{max}$
- Justification of $(\Delta/\sigma)_{max}$ value if it exceeds 1·0
- Maximum positive and maximum negative electron density in final difference Fourier synthesis, $(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$
- 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 $8\frac{1}{2} \times 11$ 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 $1\frac{1}{4}$ 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^{i}) *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). A**40**, 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). B**37**, 1161–1162; *Acta Cryst.* (1982). B**38**, 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 $8\frac{1}{2} \times 11$ in

Minimum character height 1·5 mm

Three copies, of good photocopiable quality

Codens for journals frequently referenced in crystallographic papers

Acc. Chem. Res.	ACHRE4	*Biopolymers*	BIPMAA	*Discuss. Faraday Soc.*	DFSOAW
ACS Symp. Ser.	ACSMC8	*Bull. Acad. Pol. Sci. Ser. Sci. Chim.*	BAPCAQ	*Dokl. Akad. Nauk SSSR*	DANKAS
Acta Chem. Scand. Ser. A	ACAPCT			*Dokl. Akad. Nauk SSSR Ser. Khim.*	DASKAJ
Acta Chem. Scand. Ser. B	ACBOCV	*Bull. Chem. Soc. Jpn*	BCSJA8		
Acta Cryst.	ACCRA9	*Bull. Soc. Chim. Belg.*	BSCBAG	*Dopov. Akad. Nauk Ukr. RSR, Ser. B*	DANND6
Acta Cryst. A	ACACEQ	*Bull. Soc. Chim. Fr.*	BSCFAS		
Acta Cryst. B	ASBSDK	*Bull. Soc. Fr. Minéral. Cristallogr.*	BUFCAE	*Eur. J. Biochem.*	EJBCAI
Acta Cryst. C	ACSCEE	*Can. J. Chem.*	CJCHAG	*Experientia*	EXPEAM
Acta Metall.	AMETAR	*Can. J. Phys.*	CJPHAD	*FEBS Lett.*	FEBLAL
Adv. Chem. Ser. (ACS)	ADCSAJ	*Can. Mineral.*	CAMIA6	*Ferroelectrics*	FEROA8
Adv. Inorg. Chem. Radiochem.	AICRAH	*Carbohydr. Res.*	CRBRAT	*Finn. Chem. Lett.*	FCMLAS
Adv. Struct. Res. Diffr. Methods	ASDMA9	*Carbon*	CRBNAH	*Fiz. Tverd. Tela (Leningrad)*	FTVTAC
Am. Mineral.	AMMIAY	*Carnegie Inst. Washington Yearb.*	CIWYAO	*Fortschr. Mineral.*	FMRLAL
Angew. Chem.	ANCEAD	*Chem. Ber.*	CHBEAM	*Gazz. Chim. Ital.*	GCITA9
Angew. Chem. Int. Ed. Engl.	ACIEAY	*Chem. Commun.*	CCOMA8	*Gold Bull.*	GLDBBS
Ann. Chim. (Paris)	ANCPAC	*Chem. Commun. Univ. Stockholm*	CCUSBN	*Helv. Chim. Acta*	HCACAV
Ann. Chim. (Rome)	ANCRAI	*Chem. Erde*	CERDAA	*Heterocycles*	HTCYAM
Ann. N.Y. Acad. Sci.	ANYAA9	*Chem. Ind. (London)*	CHINAG	*Indian Chem. J.*	ICLJAG
Ann. Phys. (Leipzig)	ANPYA2	*Chem. Lett.*	CMLTAG	*Indian J. Chem.*	IJOCAP
Annu. Rev. Phys. Chem.	ARPLAP	*Chem. Pharm. Bull. (Jpn)*	CPBTAL	*Indian J. Phys.*	IJPYAS
Ark. Kemi	ARKEAD	*Chem. Phys. Lett.*	CHPLBC	*Indian J. Phys. Part A*	INJADP
Arzneim.-Forsch.	ARZNAD	*Chem. Scr.*	CSRPB9	*Indian J. Phys. Part B*	IJPBDU
Atti Accad. Naz. Lincei. Cl. Sci. Fis. Mat. Nat. Rend.	AANLAW	*Chem. Zvesti*	CHZVAN	*Inorg. Chem.*	INOCAJ
		Chimia	CHIMAD	*Inorg. Chim. Acta*	ICHAA3
Aust. J. Chem.	AJCHAS	*Coll. Czech. Chem. Commun.*	CCCCAK	*Inorg. Nucl. Chem. Lett.*	INUCAF
Ber. Bunsenges. Phys. Chem.	BBPCAX	*Coord. Chem. Rev.*	CCHRAM	*Int. J. Pept. Protein Res.*	IJPPC3
Ber. Dtsch. Chem. Ges.	BDCGAS	*C. R. Séances Acad. Sci. Sér. C*	CHDCAQ	*Isr. J. Chem.*	ISJCAT
Ber. Dtsch. Chem. Ges. A	BDCAAA	*C. R. Séances Acad. Sci. Sér. 2*	CRSUDO	*Izv. Akad. Nauk SSSR Neorg. Mater.*	IVNMAW
Ber. Dtsch. Chem. Ges. B	BDCBAD	*Croat. Chem. Acta*	CCACAA		
Biochem. Biophys. Res. Commun.	BBRCA9	*Cryst. Lattice Defects*	CLADA8	*J. Am. Chem. Soc.*	JACSAT
Biochim. Biophys. Acta	BBACAQ	*Cryst. Res. Technol.*	CRTEDF	*J. Appl. Cryst.*	JACGAR
Bioinorg. Chem.	BICHBX	*Cryst. Struct. Commun.*	CSCMCS	*J. Biol. Chem.*	JBCHA3
Bioorg. Khim.	BIKHD7	*Curr. Sci. (India)*	CUSCAM	*J. Chem. Phys.*	JCPSA6

J. Chem. Res. Synop.	JRPSDC	*Justus Liebigs Ann. Chem.*	JLACBF	*Recl Trav. Chim. Pays-Bas*	RTCPA3
J. Chem. Soc. A	JCSIAP	*Khim. Prir. Soedin.*	KPSUAR	*Rev. Chim. Minér.*	RVCMA8
J. Chem. Soc. B	JCSPAC	*Koord. Khim.*	KOKHDC	*Rev. Sci. Instrum.*	RSINAK
J. Chem. Soc. Chem. Commun.	JCCCAT	*Kristallografiya*	KRISAJ	*Ric. Sci.*	RISCAZ
J. Chem. Soc. Dalton Trans.	JCDTBI	*Krist. Tech.*	KRTEAW	*Rocz. Chem.*	ROCHAC
J. Chem. Soc. Perkin Trans. 1	JCPRB4	*Life Sci.*	LIFSAK	*Russ. J. Inorg. Chem.* (*Engl. Trans.*)	RJICAQ
J. Chem. Soc. Perkin Trans. 2	JCPKBH	*Makromol. Chem.*	MACEAK		
J. Chim. Phys. Phys. Chim. Biol.	JCPBAN	*Mater. Res. Bull.*	MRBUAC	*S. Afr. J. Chem.*	SAJCDG
J. Coord. Chem.	JCCMBQ	*Mater. Sci.*	MSCJDS	*Schweiz. Mineral. Petrogr. Mitt.*	SMPTA8
J. Cryst. Growth	JCRGAE	*Mater. Sci. Eng.*	MSCEAA	*Science*	SCIEAS
J. Cryst. Mol. Struct.	JCMLB5	*Mineral. J.*	MJTOAS	*Solid State Commun.*	SSCOA4
J. Crystallogr. Spectrosc. Res.	JCREDB	*Mineral. Mag.*	MNLMBB	*Sov. Phys.-Crystallogr.* (*Engl. Trans.*)	SPHCA6
J. Electrochem. Soc.	JESOAN	*Mol. Cryst. Liq. Cryst.*	MCLCA5		
J. Electron Mater.	JECMA5	*Monatsh. Chem.*	MOCMB7	*Sov. Phys.-Solid State* (*Engl. Trans.*)	SPSSA7
J. Fluorine Chem.	JFLCAR	*Natl Bur. Stand. US Circ.*	NBSCAA		
J. Heterocycl. Chem.	JHTCAD	*Natl Bur. Stand. US Monogr.*	NBSMA6	*Spectrochim Acta*	SPACA5
J. Inclusion Phenom.	JOIPDF	*Natl Bur. Stand. US Spec. Publ.*	XNBSAV	*Spectrochim Acta Part A*	SAMCAS
J. Inorg. Biochem.	JIBIDJ	*Natl Bur. Stand. US Tech. Note*	NBTNAE	*Struct. Bonding* (*Berlin*)	STBGAG
J. Inorg. Nucl. Chem.	JINCAO	*Nature* (*London*)	NATUAS	*Suom. Kemistil. B*	SUKBAJ
J. Less Common Met.	JCOMAH	*Naturwissenschaften*	NATWAY	*Tetrahedron*	TETRAB
J. Magn. Reson.	JOMRA4	*Neues Jahrb. Mineral. Abh.*	NJMIAK	*Tetrahedron Lett.*	TELEAY
J. Mater. Sci.	JMTSAS	*Neues Jahrb. Mineral. Monatsh.*	NJMMAW	*Theor. Chim. Acta*	TCHAAM
J. Mol. Biol.	JMOBAK	*Nouv. J. Chim.*	NJCHD4	*TMPM Tschermaks Mineral. Petrogr. Mitt.*	TTMMDZ
J. Mol. Spectrosc.	JMOSA3	*Organometallics*	ORGND7		
J. Mol. Struct.	JMOSB4	*Philos. Mag.*	PHMAA4	*Trans. Am. Crystallogr. Assoc.*	TACAAH
J. Nat. Prod.	JNPRDF	*Physica A* (*Amsterdam*)	PHYADX	*Trans. Faraday Soc.*	TFSOA4
J. Nucl. Mater.	JNUMAM	*Physica B & C* (*Amsterdam*)	PHBCDQ	*Trans. Metall. Soc. AIME*	TMSAAB
J. Org. Chem.	JOCEAH	*Physica* (*Utrecht*)	PHYSAG	*Transition Met. Chem.* (*N.Y.*)	TRMCAM
J. Organomet. Chem.	JORCAI	*Phys. Kondens. Mater.*	PKOMA3	*Transition Met. Chem.* (*Weinheim*)	TMCHDN
J. Pharmacol. Exp. Ther.	JPETAB	*Phys. Rev. B: Condens. Matter*	PRBMDO	*Tschermaks Mineral. Petrogr. Mitt.*	MPMTAG
J. Phys. C	JPSOAW	*Phys. Rev. B: Solid State*	PLRBAQ		
J. Phys. F	JPFMAT	*Phys. Status Solidi*	PHSSAK	*Z. Anorg. Allg. Chem.*	ZAACAB
J. Phys. Chem.	JPCHAX	*Phys. Status Solidi A*	PSSABA	*Z. Anorg. Chem.*	ZACMAH
J. Phys. Chem. Solids	JPCSAW	*Phys. Status Solidi B*	PSSBBD	*Z. Elektrochem.*	ZEELAI
J. Phys. Lett.	JPSLBO	*Pol. J. Chem.*	PJCHDQ	*Z. Kristallogr.*	ZEKRDZ
J. Phys. Soc. Jpn	JUPSAU	*Polyhedron*	PLYHDE	*Z. Metallkd.*	ZEMTAE
J. Polym. Sci.	JPSCAU	*Pramana*	PRAMCI	*Z. Naturforsch. Teil A*	ZTAKDZ
J. Polym. Sci. Polym. Chem. Ed.	JPLCAT	*Proc. Natl Acad. Sci. USA*	PNASA6	*Z. Naturforsch. Teil B*	ZNBAD2
J. Prakt. Chem.	JPCEAO	*Proc. R. Soc. London Ser. A*	PRLAAZ	*Z. Phys. Chem.* (*Frankfurt am Main*)	ZPCFAX
J. Raman Spectrosc.	JRSPAF	*Proc. R. Soc. London Ser. B*	PRLBA4		
J. Solid State Chem.	JSSCBI	*Prog. Inorg. Chem.*	PIOCAR	*Z. Phys. Chem.* (*Leipzig*)	ZPCLAH
J. Struct. Chem. (*Engl. Trans.*)	JSTCAM	*Prog. Med. Chem.*	PMDCAY	*Zh. Neorg. Khim.*	ZNOKAQ
Jpn. J. Appl. Phys.	JJAPA5	*Q. Rev. Chem. Soc.*	QUREA7	*Zh. Obshch. Khim.*	ZOKHA4
Jpn. J. Appl. Phys. Part 1	JAPNDE	*Recl: J. R. Neth. Chem. Soc.*	RJRSDK	*Zh. Strukt. Khim.*	ZSTKAI
Jpn. J. Appl. Phys. Part 2	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).