

*Acta Cryst.* (1985). B41, 1-4

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

Papers are considered for publication in Section B if they contribute to an advance in structural science. The following three criteria should be met:

1. The paper must contain a major structural element. This component may be an original determination of one or more structures (a single structure should generally have been studied under more than one condition of temperature or pressure), a theoretical structural investigation including new methodology, a study of structural relationships based on a search of the literature, or similar study.

2. The paper should also present an experimental and/or theoretical contribution to one of the natural sciences that is novel, original and of high quality.

3. The paper should combine these two types of contribution to provide new structural insight for that science or for crystallography.

In future, Lead Articles will be published on an occasional basis in Section B. Although Lead Articles may contain a review element, their primary emphasis will be with the direction in which an area of structural science is moving, indicating major problems, with suggestions for future development of the subject. Lead Articles will normally be invited but authors wishing to contribute such papers are asked to discuss their proposal with the Editor in advance. Such articles will be subject to normal review.

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* [*Acta Cryst.* (1983). A39, 174-196], 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. See also Hamor, Steinfink & Willis [*Acta Cryst.* (1985). C41, 301-303] for a summary of recommended techniques used in crystal structure determinations.

The checklist below is provided for the convenience of authors submitting papers for publication in Section B. Fuller information is given in *Notes for Authors*. Checklists for authors of papers submitted to Sections A and C 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 B, 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 10 000 words for full articles  
Maximum of 1000 words for Short Communications  
(For typography see *Notes for Authors*, § 9)
- (c) *Title*  
Short but informative, emphasizing the structural science reported  
Not to include long compound names
- (d) *Abstract*  
About 200 words  
Suitable for reproduction by abstracting services without change of wording  
Any references to be given in full  
Sufficiently informative to obviate need for *Conclusion* section  
Structure determination component 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  
Principal results stated as specifically and quantitatively as possible
- (e) *Experimental section*  
Structure determination component 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 value (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
- As small as possible consistent with legibility
- High information density
- Lettering not less than 4 mm high on International A4 sized paper (210 × 297 mm) or 8½ × 11 in (and *pro rata*)
- Figure captions in separate list
- Chemical and structural formulae preferably in camera-ready form
- Stereofigures:
- One 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
- 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
- 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<sup>i</sup>) *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
- Table 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
- Figures that duplicate information given elsewhere

## 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>	ACHRE4	<i>Chimia</i>	CHIMAD	<i>J. Inorg. Biochem.</i>	JIBIDJ
<i>ACS Symp. Ser.</i>	ACSMC8	<i>Coll. Czech. Chem. Commun.</i>	CCCCAK	<i>J. Inorg. Nucl. Chem.</i>	JINCAO
<i>Acta Chem. Scand. Ser. A</i>	ACAPCT	<i>Coord. Chem. Rev.</i>	CCHRAM	<i>J. Less Common Met.</i>	JCOMAH
<i>Acta Chem. Scand. Ser. B</i>	ACBOCV	<i>C.R. Séances Acad. Sci. Sér. C</i>	CHDCAQ	<i>J. Magn. Reson.</i>	JOMRA4
<i>Acta Cryst.</i>	ACCRA9	<i>C.R. Séances Acad. Sci. Sér. 2</i>	CRSUDO	<i>J. Mater. Sci.</i>	JMTSAS
<i>Acta Cryst. A</i>	ACACEQ	<i>Croat. Chem. Acta</i>	CCACAA	<i>J. Mol. Biol.</i>	JMOBAK
<i>Acta Cryst. B</i>	ASBSDK	<i>Cryst. Lattice Defects</i>	CLADA8	<i>J. Mol. Spectrosc.</i>	JMOSA3
<i>Acta Cryst. C</i>	ACSCEE	<i>Cryst. Res. Technol.</i>	CRTEDF	<i>J. Mol. Struct.</i>	JMOSB4
<i>Acta Metall.</i>	AMETAR	<i>Cryst. Struct. Commun.</i>	CSCMCS	<i>J. Nat. Prod.</i>	JNPRDF
<i>Adv. Chem. Ser. (ACS)</i>	ADCSAJ	<i>Curr. Sci. (India)</i>	CUSCAM	<i>J. Nucl. Mater.</i>	JNUMAM
<i>Adv. Inorg. Chem. Radiochem.</i>	AICRAH	<i>Discuss. Faraday Soc.</i>	DFSOAW	<i>J. Org. Chem.</i>	JOCEAH
<i>Adv. Struct. Res. Diffr. Methods</i>	ASDMA9	<i>Dokl. Akad. Nauk SSSR</i>	DANKAS	<i>J. Organomet. Chem.</i>	JORCAI
<i>Am. Mineral.</i>	AMMIAY	<i>Dokl. Akad. Nauk SSSR Ser. Khim.</i>	DASKAJ	<i>J. Pharmacol. Exp. Ther.</i>	JPETAB
<i>Angew. Chem.</i>	ANCEAD	<i>Dopov. Akad. Nauk Ukr. RSR, Ser. B</i>	DANND6	<i>J. Phys. C</i>	JPSOAW
<i>Angew. Chem. Int. Ed. Engl.</i>	ACIEAY	<i>Eur. J. Biochem.</i>		<i>J. Phys. F</i>	JPFMAT
<i>Ann. Chim. (Paris)</i>	ANCPAC	<i>Experientia</i>	EJBCAI	<i>J. Phys. Chem.</i>	JPCHAX
<i>Ann. Chim. (Rome)</i>	ANCRAI	<i>FEBS Lett.</i>	EXPEAM	<i>J. Phys. Chem. Solids</i>	JPCSAW
<i>Ann. N.Y. Acad. Sci.</i>	ANYAA9	<i>Ferroelectrics</i>	FEBLAL	<i>J. Phys. Lett.</i>	JPSLBO
<i>Ann. Phys. (Leipzig)</i>	ANPYA2	<i>Finn. Chem. Lett.</i>	FEROA8	<i>J. Phys. Soc. Jpn</i>	JUPS AU
<i>Annu. Rev. Phys. Chem.</i>	ARPLAP	<i>Fiz. Tverd. Tela (Leningrad)</i>	FCMLAS	<i>J. Polym. Sci.</i>	JPSCAU
<i>Ark. Kemi</i>	ARKEAD	<i>Fortschr. Mineral.</i>	FTVTAC	<i>J. Polym. Sci. Polym. Chem. Ed.</i>	JPLCAT
<i>Arzneim.-Forsch.</i>	ARZNA D	<i>Gazz. Chim. Ital.</i>	FMR LAL	<i>J. Prakt. Chem.</i>	JPEAO
<i>Atti Accad. Naz. Lincei. Cl. Sci. Fis. Mat. Nat. Rend.</i>	AANLAW	<i>Gold Bull.</i>	GCITA9	<i>J. Raman Spectrosc.</i>	JRSPAF
<i>Aust. J. Chem.</i>	AJCHAS	<i>Helv. Chim. Acta</i>	GLDBBS	<i>J. Solid State Chem.</i>	JSSCBI
<i>Ber. Bunsenges. Phys. Chem.</i>	BBPCAX	<i>Heterocycles</i>	HCACAV	<i>J. Struct. Chem. (Engl. Trans.)</i>	JSTCAM
<i>Ber. Dtsch. Chem. Ges.</i>	BDCGAS	<i>Indian Chem. J.</i>	HTCYAM	<i>Jpn. J. Appl. Phys.</i>	JJAPA5
<i>Ber. Dtsch. Chem. Ges. A</i>	BDCAAA	<i>Indian J. Chem.</i>	ICLJAG	<i>Jpn. J. Appl. Phys. Part 1</i>	JAPNDE
<i>Ber. Dtsch. Chem. Ges. B</i>	BDCBAD	<i>Indian J. Phys.</i>	IJOCAP	<i>Jpn. J. Appl. Phys. Part 2</i>	JAPLD8
<i>Biochem. Biophys. Res. Commun.</i>	BBRCA9	<i>Indian J. Phys. Part A</i>	IJPYAS	<i>Justus Liebig's Ann. Chem.</i>	JLACBF
<i>Biochim. Biophys. Acta</i>	BBACAQ	<i>Indian J. Phys. Part B</i>	INJADP	<i>Khim. Prir. Soedin.</i>	KPSUAR
<i>Biinorg. Chem.</i>	BICHBX	<i>Inorg. Chem.</i>	IJPBDU	<i>Koord. Khim.</i>	KOKHDC
<i>Bioorg. Khim.</i>	BIKHD7	<i>Inorg. Chim. Acta</i>	INOC AJ	<i>Kristallografiya</i>	KRISAJ
<i>Biopolymers</i>	BIPMAA	<i>Inorg. Nucl. Chem. Lett.</i>	ICHAA3	<i>Krist. Tech.</i>	KRTEAJ
<i>Bull. Acad. Pol. Sci. Ser. Sci. Chim.</i>	BAPCAQ	<i>Int. J. Pept. Protein Res.</i>	INUCA F	<i>Life Sci.</i>	LIFSAK
<i>Bull. Chem. Soc. Jpn.</i>	BCSJA8	<i>Isr. J. Chem.</i>	IJPPC3	<i>Makromol. Chem.</i>	MACEAC
<i>Bull. Soc. Chim. Belg.</i>	BSCBAG	<i>Izv. Akad. Nauk SSSR Neorg. Mater.</i>	ISJCAT	<i>Mater. Res. Bull.</i>	MRBUAC
<i>Bull. Soc. Chim. Fr.</i>	BSCFAS	<i>J. Am. Chem. Soc.</i>	IVNMAW	<i>Mater. Sci.</i>	MSCJDS
<i>Bull. Soc. Fr. Minéral. Cristallogr.</i>	BUFCAE	<i>J. Appl. Cryst.</i>	JACSAT	<i>Mater. Sci. Eng.</i>	MSC EAA
<i>Can. J. Chem.</i>	CJCHAG	<i>J. Biol. Chem.</i>	JACGAR	<i>Mineral. J.</i>	MJTOAS
<i>Can. J. Phys.</i>	CJPHAD	<i>J. Chem. Phys.</i>	JBCHA3	<i>Mineral. Mag.</i>	MNLMBB
<i>Can. Mineral.</i>	CAMIA6	<i>J. Chem. Res. Synop.</i>	JCPSA6	<i>Mol. Cryst. Liq. Cryst.</i>	MCLCA5
<i>Carbohydr. Res.</i>	CRBRAT	<i>J. Chem. Soc. A</i>	JRPSDC	<i>Monatsh. Chem.</i>	MOCMB7
<i>Carbon</i>	CRBNAH	<i>J. Chem. Soc. B</i>	JCSIA P	<i>Natl. Bur. Stand. US Circ.</i>	NBSCAA
<i>Carnegie Inst. Washington Yearb.</i>	CIWYAO	<i>J. Chem. Soc. Chem. Commun.</i>	JCSPAC	<i>Natl. Bur. Stand. US Monogr.</i>	NBSMA6
<i>Chem. Ber.</i>	CHBEAM	<i>J. Chem. Soc. Dalton Trans.</i>	JCCCAT	<i>Natl. Bur. Stand. US Spec. Publ.</i>	XNBSAV
<i>Chem. Commun.</i>	CCOMA8	<i>J. Chem. Soc. Perkin Trans. 1</i>	JCDTBI	<i>Natl. Bur. Stand. US Tech. Note</i>	NBTNAE
<i>Chem. Commun. Uniu. Stockholm</i>	CCUSB N	<i>J. Chem. Soc. Perkin Trans. 2</i>	JCPRB4	<i>Nature (London)</i>	NATUAS
<i>Chem. Erde</i>	CERDAA	<i>J. Chim. Phys. Phys. Chim. Biol.</i>	JCPKBH	<i>Naturwissenschaften</i>	NATWAY
<i>Chem. Ind. (London)</i>	CHINAG	<i>J. Coord. Chem.</i>	JCPBAN	<i>Neues Jahrb. Mineral. Abh.</i>	NJMIAK
<i>Chem. Lett.</i>	CMLTAG	<i>J. Cryst. Growth</i>	JCCMBQ	<i>Neues Jahrb. Mineral. Monatsh.</i>	NJMMAW
<i>Chem. Pharm. Bull. (Jpn)</i>	CPBTAL	<i>J. Cryst. Mol. Struct.</i>	JCRGAE	<i>Nouv. J. Chim.</i>	NJCHD4
<i>Chem. Phys. Lett.</i>	CHPLBC	<i>J. Crystallogr. Spectrosc. Res.</i>	JCMLB5	<i>Organometallics</i>	ORGND7
<i>Chem. Scr.</i>	CSRPB9	<i>J. Electrochem. Soc.</i>	JCREDB	<i>Philos. Mag.</i>	PHMAA4
<i>Chem. Zvesti</i>	CHZVAN	<i>J. Electron Mater.</i>	JESOAN	<i>Physica A (Amsterdam)</i>	PHYADX
		<i>J. Fluorine Chem.</i>	JECMA5	<i>Physica B &amp; C (Amsterdam)</i>	PHBCDQ
		<i>J. Heterocycl. Chem.</i>	JFLCAR	<i>Physica (Utrecht)</i>	PHYSAG
		<i>J. Inclusion Phenom.</i>	JHTCAD	<i>Phys. Kondens. Mater.</i>	PKOMA3
			JOIPDF	<i>Phys. Rev. B: Condens. Matter</i>	PRBMDO
				<i>Phys. Rev. B: Solid State</i>	PLRBAQ
				<i>Phys. Status Solidi</i>	PHSSAK

## CHECKLIST FOR AUTHORS

<i>Phys. Status Solidi A</i>	PSSABA	<i>S. Afr. J. Chem.</i>	SAJCDG	<i>Trans. Metall. Soc. AIME</i>	TMSAAB
<i>Phys. Status Solidi B</i>	PSSBBD	<i>Schweiz. Mineral. Petrogr. Mitt.</i>	SMPTA8	<i>Transition Met. Chem. (N.Y.)</i>	TRMCAM
<i>Pol. J. Chem.</i>	PJCHDQ	<i>Science</i>	SCIEAS	<i>Transition Met. Chem. (Weinheim)</i>	TMCHDN
<i>Polyhedron</i>	PLYHDE	<i>Solid State Commun.</i>	SSCOA4	<i>Tschermaks Mineral. Petrogr. Mitt.</i>	MPMTAG
<i>Pramana</i>	PRAMCI	<i>Sov. Phys.-Crystallogr. (Engl. Trans.)</i>	SPHCA6	<i>Z. Anorg. Allg. Chem.</i>	ZAACAB
<i>Proc. Natl. Acad. Sci. USA</i>	PNASA6	<i>Sov. Phys.-Solid State (Engl. Trans.)</i>	SPSSA7	<i>Z. Anorg. Chem.</i>	ZACMAH
<i>Proc. R. Soc. London Ser. A</i>	PRLAAZ	<i>Spectrochim Acta</i>	SPACA5	<i>Z. Elektrochem.</i>	ZEELAI
<i>Proc. R. Soc. London Ser. B</i>	PRLBA4	<i>Spectrochim Acta Part A</i>	SAMCAS	<i>Z. Kristallogr.</i>	ZEKRDZ
<i>Prog. Inorg. Chem.</i>	PIOCAR	<i>Struct. Bonding (Berlin)</i>	STBGAG	<i>Z. Metallkd.</i>	ZEMTAE
<i>Prog. Med. Chem.</i>	PMDCAY	<i>Suom. Kemistil.B</i>	SUKBAJ	<i>Z. Naturforsch Teil A</i>	ZTAKDZ
<i>Q. Rev. Chem. Soc.</i>	QUREA7	<i>Tetrahedron</i>	TETRAB	<i>Z. Naturforsch. Teil B</i>	ZNBAD2
<i>Recl. J. R. Neth. Chem. Soc.</i>	RJRSDK	<i>Tetrahedron Lett.</i>	TELEAY	<i>Z. Phys. Chem. (Frankfurt am Main)</i>	ZPCFAX
<i>Recl. Trav. Chim. Pays-Bas</i>	RTCPA3	<i>Theor. Chim. Acta</i>	TCHAAM	<i>Z. Phys. Chem. (Leipzig)</i>	ZPCLAH
<i>Rev. Chim. Minér.</i>	RVCMA8	<i>TMPM Tschermaks Mineral. Petrogr. Mitt.</i>	TTMMDZ	<i>Zh. Neorg. Khim.</i>	ZNOKAQ
<i>Rev. Sci. Instrum.</i>	RSINAK	<i>Trans. Am. Crystallogr. Assoc.</i>	TACAAH	<i>Zh. Obshch. Khim.</i>	ZOKHA4
<i>Ric. Sci.</i>	RISCAZ	<i>Trans. Faraday Soc.</i>	TFSOA4	<i>Zh. Strukt. Khim.</i>	ZSTKAI
<i>Rocz. Chem</i>	ROCHAC				
<i>Russ. J. Inorg. Chem. (Engl. Trans.)</i>	RJICAQ				

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*).