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). A**39**, 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). C**41**, 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 ($Å^3$)
  - 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
  - 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 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 $R_{\rm int}$ ($\sum|F-\langle F\rangle|/\sum F$ 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, $(\Delta/\sigma)_{\rm max}$
Justification of $(\Delta/\sigma)_{\rm max}$ value if it exceeds 1.0
Maximum positive and maximum negative electron density in final difference Fourier synthesis, $(\Delta\rho)_{\rm max}$, $(\Delta\rho)_{\rm min}$
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 $8\frac{1}{2}\times$ 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 $1\frac{1}{4}$ 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^{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
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). 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
ACS Symp. Ser.	ACSMC8
Acta Chem. Scand. Ser. A	ACAPCT
Acta Chem. Scand. Ser. B	ACBOCV
Acta Cryst.	ACCRA9
Acta Cryst. A	ACACEQ
Acta Cryst. B	ASBSDK
Acta Cryst. C	ACSCEE
Acta Metall.	AMETAR
Adv. Chem. Ser. (ACS)	ADCSAJ
Adv. Inorg. Chem. Radiochem.	AICRAH
Adv. Struct. Res. Diffr. Methods	ASDMA9
Am. Mineral.	AMMIAY
Angew. Chem.	ANCEAD
Angew. Chem. Int. Ed. Engl.	ACIEAY
Ann. Chim. (Paris)	ANCPAC
Ann. Chim. (Rome)	ANCRAI
Ann. N.Y. Acad. Sci.	ANYAA9
Ann. Phys. (Leipzig)	ANPYA2
Annu. Rev. Phys. Chem.	ARPLAP
Ark. Kemi	ARKEAD
Arzneim.-Forsch.	ARZNAD
Atti Accad. Naz. Lincei. Cl. Sci. Fis. Mat. Nat. Rend.	AANLAW
Aust. J. Chem.	AJCHAS
Ber. Bunsenges. Phys. Chem.	BBPCAX
Ber. Dtsch. Chem. Ges.	BDCGAS
Ber. Dtsch. Chem. Ges. A	BDCAAA
Ber. Dtsch. Chem. Ges. B	BDCBAD
Biochem. Biophys. Res. Commun.	BBRCA9
Biochim. Biophys. Acta	BBACAQ
Bioinorg. Chem.	BICHBX
Bioorg. Khim.	BIKHD7
Biopolymers	BIPMAA
Bull. Acad. Pol. Sci. Ser. Sci. Chim.	BAPCAQ
Bull. Chem. Soc. Jpn.	BCSJA8
Bull. Soc. Chim. Belg.	BSCBAG
Bull. Soc. Chim. Fr.	BSCFAS
Bull. Soc. Fr. Minéral. Cristallogr.	BUFCAE
Can. J. Chem.	CJCHAG
Can. J. Phys.	CJPHAD
Can. Mineral.	CAMIA6
Carbohydr. Res.	CRBRAT
Carbon	CRBNAH
Carnegie Inst. Washington Yearb.	CIWYAO
Chem. Ber.	CHBEAM
Chem. Commun.	CCOMA8
Chem. Commun. Univ. Stockholm	CCUSBN
Chem. Erde	CERDAA
Chem. Ind. (London)	CHINAG
Chem. Lett.	CMLTAG
Chem. Pharm. Bull. (Jpn)	CPBTAL
Chem. Phys. Lett.	CHPLBC
Chem. Scr.	CSRPB9
Chem. Zvesti	CHZVAN
Chimia	CHIMAD
Coll. Czech. Chem. Commun.	CCCCAK
Coord. Chem. Rev.	CCHRAM
C.R. Séances Acad. Sci. Sér. C	CHDCAQ
C.R. Séances Acad. Sci. Sér. 2	CRSUDO
Croat. Chem. Acta	CCACAA
Cryst. Lattice Defects	CLADA8
Cryst. Res. Technol.	CRTEDF
Cryst. Struct. Commun.	CSCMCS
Curr. Sci. (India)	CUSCAM
Discuss. Faraday Soc.	DFSOAW
Dokl. Akad. Nauk SSSR	DANKAS
Dokl. Akad. Nauk SSSR Ser. Khim.	DASKAJ
Dopov. Akad. Nauk Ukr. RSR, Ser. B	DANND6
Eur. J. Biochem.	EJBCAI
Experientia	EXPEAM
FEBS Lett.	FEBLAL
Ferroelectrics	FEROA8
Finn. Chem. Lett.	FCMLAS
Fiz. Tverd. Tela (Leningrad)	FTVTAC
Fortschr. Mineral.	FMRLAL
Gazz. Chim. Ital.	GCITA9
Gold Bull.	GLDBBS
Helv. Chim. Acta	HCACAV
Heterocycles	HTCYAM
Indian Chem. J.	ICLJAG
Indian J. Chem.	IJOCAP
Indian J. Phys.	IJPYAS
Indian J. Phys. Part A	INJADP
Indian J. Phys. Part B	IJPBDU
Inorg. Chem.	INOCAJ
Inorg. Chim. Acta	ICHAA3
Inorg. Nucl. Chem. Lett.	INUCAF
Int. J. Pept. Protein Res.	IJPPC3
Isr. J. Chem.	ISJCAT
Izv. Akad. Nauk SSSR Neorg. Mater.	IVNMAW
J. Am. Chem. Soc.	JACSAT
J. Appl. Cryst.	JACGAR
J. Biol. Chem.	JBCHA3
J. Chem. Phys.	JCPSA6
J. Chem. Res. Synop.	JRPSDC
J. Chem. Soc. A	JCSIAP
J. Chem. Soc. B	JCSPAC
J. Chem. Soc. Chem. Commun.	JCCCAT
J. Chem. Soc. Dalton Trans.	JCDTBI
J. Chem. Soc. Perkin Trans. 1	JCPRB4
J. Chem. Soc. Perkin Trans. 2	JCPKBH
J. Chim. Phys. Phys. Chim. Biol.	JCPBAN
J. Coord. Chem.	JCCMBQ
J. Cryst. Growth	JCRGAE
J. Cryst. Mol. Struct.	JCMLB5
J. Crystallogr. Spectrosc. Res.	JCREDB
J. Electrochem. Soc.	JESOAN
J. Electron Mater.	JECMA5
J. Fluorine Chem.	JFLCAR
J. Heterocycl. Chem.	JHTCAD
J. Inclusion Phenom.	JOIPDF
J. Inorg. Biochem.	JIBIDJ
J. Inorg. Nucl. Chem.	JINCAO
J. Less Common Met.	JCOMAH
J. Magn. Reson.	JOMRA4
J. Mater. Sci.	JMTSAS
J. Mol. Biol.	JMOBAK
J. Mol. Spectrosc.	JMOSA3
J. Mol. Struct.	JMOSB4
J. Nat. Prod.	JNPRDF
J. Nucl. Mater.	JNUMAM
J. Org. Chem.	JOCEAH
J. Organomet. Chem.	JORCAI
J. Pharmacol. Exp. Ther.	JPETAB
J. Phys. C	JPSOAW
J. Phys. F	JPFMAT
J. Phys. Chem.	JPCHAX
J. Phys. Chem. Solids	JPCSAW
J. Phys. Lett.	JPSLBO
J. Phys. Soc. Jpn	JUPSAU
J. Polym. Sci.	JPSCAU
J. Polym. Sci. Polym. Chem. Ed.	JPLCAT
J. Prakt. Chem.	JPCEAO
J. Raman Spectrosc.	JRSPAF
J. Solid State Chem.	JSSCBI
J. Struct. Chem. (Engl. Trans.)	JSTCAM
Jpn. J. Appl. Phys.	JJAPA5
Jpn. J. Appl. Phys. Part 1	JAPNDE
Jpn. J. Appl. Phys. Part 2	JAPLD8
Justus Liebigs Ann. Chem.	JLACBF
Khim. Prir. Soedin.	KPSUAR
Koord. Khim.	KOKHDC
Kristallografiya	KRISAJ
Krist. Tech.	KRTEAW
Life Sci.	LIFSAK
Makromol. Chem.	MACEAK
Mater. Res. Bull.	MRBUAC
Mater. Sci.	MSCJDS
Mater. Sci. Eng.	MSCEAA
Mineral. J.	MJTOAS
Mineral. Mag.	MNLMBB
Mol. Cryst. Liq. Cryst.	MCLCA5
Monatsh. Chem.	MOCMB7
Natl. Bur. Stand. US Circ.	NBSCAA
Natl. Bur. Stand. US Monogr.	NBSMA6
Natl. Bur. Stand. US Spec. Publ.	XNBSAV
Natl. Bur. Stand. US Tech. Note	NBTNAE
Nature (London)	NATUAS
Naturwissenschaften	NATWAY
Neues Jahrb. Mineral. Abh.	NJMIAK
Neues Jahrb. Mineral. Monatsh.	NJMMAW
Nouv. J. Chim.	NJCHD4
Organometallics	ORGND7
Philos. Mag.	PHMAA4
Physica A (Amsterdam)	PHYADX
Physica B & C (Amsterdam)	PHBCDQ
Physica (Utrecht)	PHYSAG
Phys. Kondens. Mater.	PKOMA3
Phys. Rev. B: Condens. Matter	PRBMDO
Phys. Rev. B: Solid State	PLRBAQ
Phys. Status Solidi	PHSSAK

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

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).