Acta Cryst. (1998). **C54**, 153–168

International Union of Crystallography

Acta Crystallographica Section C

Notes for Authors

Acta Crystallographica Section C: Crystal Structure Communications publishes crystal structures determined by diffraction methods. It specialises in the rapid dissemination and archiving (for Internet access) of high-quality studies of interesting and novel chemical structures, compounds and materials. The journal's unique checking, editing and publishing facilities are directed specifically at these objectives.

These Notes for Authors provide the submission and publication requirements of *Acta Crystallographica Section C: Crystal Structure Communications* as stipulated by the policies of the IUCr Commission on Journals for the rapid publication of crystal structure studies.

The Notes are divided into the following sections:

§1. Submission requirements
§2. Publication requirements
§3. Data standards
§4. Diagram requirements
§5. Nomenclature
§6. References

Appendix 1. Guidelines for editing CIF text
Appendix 2. Transferring large electronic files
Appendix 3. Required CIF data items
Appendix 4. Standard codes for data items
Appendix 5. Example of a CIF submission
Appendix 6. Transfer of Copyright Agreement form

1. Submission requirements

1.1. *Author checking of manuscripts*

All papers must be submitted in Crystallographic Information File (CIF) ASCII format (MIME or other encoded formats should be avoided if possible). To avoid delays in editorial handling, authors are asked to pre-check their submission by e-mailing the CIF to **checkcif@iucr.org**. This will be mandatory after 30 June 1998. A check report will be returned automatically to the sender's e-mail address. The text and tables of a paper, as distributed to the Co-editors and referees, may be previewed by sending the CIF (after completing the pre-check) to **printcif@iucr.org**. A PostScript file of the paper will be returned for local printing. Note that use of these automatic facilities does not constitute a submission to *Section C*.

1.2. *Categories of submission*

Section C publishes three categories of papers. The requested category must be specified in the submitted CIF as `_publ_requested_category`, using one of the codes listed below.

(*a*) Full papers describe one or more structure determinations. These submissions are validated (see §3) and peer reviewed. The accepted paper is printed in the journal and the CIF is accessible from the *Section C* web address `http://www.iucr.org/actac.html`. The category codes used to identify these papers are `FI` for inorganic, `FM` for metal–organic, and `FO` for organic structures.

(*b*) CIF-access papers describe one or more structure determinations. The submitted CIF is validated identically to (*a*) but the text is not peer reviewed. The title, authors, synopsis and scheme of the paper will appear in the Table of Contents of the journal and the CIF is accessible from the address `http://www.iucr.org/actac.html`. The category codes used to identify these papers are `CI` for inorganic, `CM` for metal–organic, and `CO` for organic structures.

(*c*) *Addenda and Errata* are short printed papers describing additions to, comments on, or errata to existing *Section C* publications and are *not* intended for interim reports of work in progress. The text should not exceed 1000 words. Addenda and Errata are peer reviewed. The category code for these papers is `AD`.

1.3. *Method of submission*

CIFs for full papers should be sent to the e-mail address **cifpub@iucr.org**, whereas cif-access submissions should be sent to **cifaccess@iucr.org**.

Authors are requested not to send the additional material required for submission until the CIF validation checks summarized in §3 have been carried out and they have received formal acknowledgement of the submission. At that time the Transfer of Copyright Agreement form (*Appendix* 6) should be posted to

The Managing Editor
International Union of Crystallography
5 Abbey Square
Chester CH1 2HU
England

Telephone: 44 1244 342878
Fax: 44 1244 314888

Large diagram files (if required for full submissions), and structure-factor lists in CIF format (necessary for all submissions), should be sent by ftp (*Appendix* 2). Note that structure factors should always be supplied in a separate file.

1.4. *Languages of submission*

The languages of publication are English, French, German and Russian.

1.5. *Author's warranty*

The submission of a paper is taken as an implicit guarantee that the work is original, that it is the author(s) own work, that all authors concur with and are aware of the submission, that all workers involved in the study are listed as authors or given proper credit in the acknowledgements, that the results have not already been published (in any language or medium) or deposited in a public access database, and that the paper is not being considered and will not be offered elsewhere while under consideration for an IUCr journal. For these reasons, the submission must be made over the signature of at least one author.

1.6. *Copyright*

Except as required otherwise by national laws, the author must sign and submit a copy of the Transfer of Copyright Agreement form (*Appendix* 6) for each manuscript before it can be accepted.

1.7. *Handling of manuscripts*

Each submitted CIF is checked in Chester for completeness and data integrity. If incomplete or inadequate it will be returned to the author for correction. The data-validation criteria applied in these checks are summarized in §3, and more detailed information is available from the web site `http://www.iucr.org/actac.html`. Papers failing to meet these criteria may still be accepted if sufficient explanation or justification is given. Papers accepted for publication will be assigned an IUCr data-validation number (*e.g.* IUC9800856). This will be published in the journal to allow retrieval of the CIF from the IUCr archives.

For CIF-access papers the title, authors, synopsis and scheme for molecular compounds will normally appear in the journal within two months of data validation. Full papers will be forwarded, together with the *Check Report*, to a Co-editor, who is responsible for the review steps and future communications with the authors up to the acceptance stage. Failure to respond to a communication from either a Co-editor or the Chester editorial staff *within three months* will result in the automatic withdrawal of the paper. If major revisions are made to the submission the journal reserves the right to reset the date of receipt of the paper to the date of re-submission. Any amendments to a paper during its review **must be indicated on the printed manuscript provided**, as this document is used by the editorial staff to update and revise the archived CIF.

Once a paper is accepted, it is the responsibility of the Managing Editor to prepare the paper for printing and to correspond with the authors and/or the Co-editor to resolve publication ambiguities or inadequacies. The date of acceptance that will appear on the published paper will be the date on which the Managing Editor receives the last item needed.

1.8. *Status of a submission*

Authors may obtain information about the current status of a paper either from the web site `http://www.iucr.org/journals/status.html` or by sending an e-mail, containing the reference code of the paper and the author's name as the subject line (*e.g.* JA1325 Smith), to the address **status@iucr.org**.

1.9. *Reprints*

Twenty-five reprints of each printed article will be provided to the contact author free of charge.

1.10. *Author grievance procedure*

An author who believes that a paper has been unjustifiably treated by the Co-editor may appeal initially to the Section Editor, and then to the Editor-in-Chief if still aggrieved by the decision.

2. Publication requirements

The publication requirements for the text, tabular and graphical material are described in this section. The standards for numerical and codified data are summarized in §3, and a list of all items required for submission is given in *Appendix* 3. Each item described in this section is required for a full paper submission. Only the items described in §§2.1, 2.2, 2.4, 2.5, 2.6, 2.7, 2.9, 2.11 and 2.13 are required for a CIF-access submission. Crystal diagrams should not be supplied for a CIF-access submission.

2.1. *Title and authors*

The *Title* should be short and informative. Avoid complicated IUPAC names and redundant phrases such as '*Crystal Structure of ...*'. The full first name of each author is preferred. The e-mail address of the contact author should be included in the CIF using the data item `_publ_contact_author_email`. Note that data items `_publ_section_title_footnote` and `_publ_author_footnote` are for inserting footnotes to the title and to individual authors.

2.2. *Abstract*

The *Abstract* must be written in English and should summarize *only the most important aspects of the study*. It should not contain the crystal data. The systematic IUPAC name and the chemical formula should be given here, if they are not included in the *Title*.

2.3. *Comment*

The *Comment* is the descriptive section of the study. It should be as concise as possible and cover the following aspects of the study:

(*a*) Why the structure determination was undertaken.

(*b*) The origin of the material studied. General chemical background material and references should be included. Details of the chemical extraction, synthesis and crystallization processes should be given in the *Experimental* section (see §2.4).

(*c*) Novel or unusual aspects of the coordination, geometry, conformation, crystal packing, *etc*. A discussion of geometry values that agree with established values (see *International Tables for Crystallography*, Volume C, §§9.4–9.6) is not warranted.

2.4. *Experimental data*

Experimental data (see *Appendix* 3) are tabulated under the sub-headings *Crystal data, Data collection* and *Refinement*. The descriptive text item `_publ_section_exptl_prep` should give sufficient information on the chemical and crystal preparation, and identification (*e.g.* on melting points and densities), to reproduce the experiment. Additional measurements (*e.g.* NMR spectra) supporting the crystallographic study may also be included. The item `_publ_section_exptl_refinement` details special aspects of the data collection, space-group identification, data processing, structure determination, refinement and hydrogen-atom treatment.

2.5. *Acknowledgements*

Acknowledgement should be given for any assistance provided to the study (see §1.5).

2.6. *References*

References to published work must be cited in the format detailed in §6. If reference is made to unpublished work, prior consent must be first obtained from the authors of that work.

2.7. *Atomic sites*

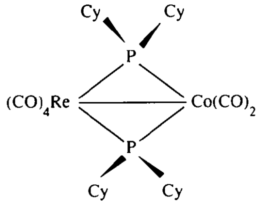
Except for structures involving special site symmetries, atom coordinate and displacement parameters *will not be printed*. These will be available to readers from the archived CIF. The `_atom_site_` coordinate and displacement parameters must be supplied with standard uncertainty values (see §5.1). The parameter constraints and restraints applied to the refinement process, and the anisotropic atomic displacement parameters (as U^{ij}), must also be supplied. If atomic displacement parameters other than U or U^{ij} are used, the exact form of the displacement-factor expression should be indicated in `_publ_section_exptl_refinement`.

2.8. *Selected geometrical data*

Interatomic bond lengths, intermolecular non-bonded contact distances, bond angles and torsion angles should be supplied, but only values that are *novel* should be flagged for printing by setting the `_geom_..._flag` value to `yes`. The data to be printed will be reviewed by the Co-editor. All submitted geometry data will be accessible from the archived CIF.

2.9. *Chemical scheme*

A chemical structural diagram (see below) must be included for molecular compounds.



2.10. *Crystallographic diagram*

Only one crystallographic diagram is usually permitted for each structure presented in the paper. Diagram requirements are given in §4. A displacement ellipsoid diagram is required either for publication or to be used in the review process.

2.11. *Contents requirements*

The Table of Contents of the journal will list the title and author(s) of all papers. For full papers, each entry will be accompanied by either a chemical structural diagram (see §2.9) for molecular compounds or a written synopsis for compounds that cannot be shown as a chemical structural diagram. For CIF-access papers, all Table of Contents entries will include a written synopsis; for molecular compounds this will be accompanied by a chemical structural diagram. The synopsis should be one or two sentences (less than 40 words) in length and should be given in `_publ_section_synopsis`.

2.12. *Powder diffraction data*

A CIF powder template and list of data items for inclusion in a powder diffraction paper are available by ftp (files `/pub/rietform.cif` and `/pub/rietreq.lst`, respectively). The numerical intensity of each measured point on the profile (as a function of scattering angle) will be deposited with the IUCr and, in the case of X-ray diffraction data, sent by the Co-editor to the International Centre for Diffraction Data (ICDD), 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. These data will be checked and assigned an ICDD reference number which will, where possible, be published in the paper. Papers reporting Rietveld refinements should include a figure showing the diffraction profile and the difference between the measured and calculated profiles.

2.13. *Structure factors*

The reflection data h, k, l, $Y_{\rm meas}$, $\sigma Y_{\rm meas}$, $Y_{\rm calc}$ (where Y is I, F^2, or F), should be supplied as an electronic file in CIF format. Authors should indicate if the Y values are corrected for absorption and extinction effects in this file and in the `_publ_section_exptl_refinement` section of the paper.

3. Data standards

A list of all data required for submission is given in *Appendix* 3. If the submitted data are incomplete, inadequate or incorrect the author will be informed promptly. Authors are required to pre-check each CIF (see §1.1) prior to submission. A more complete description of the data-validation checks applied to submitted CIFs is available from the web site `http://www.iucr.org/actac.html`.

The most important data requirements are summarized below.

`_chemical_formula_moiety`
`_chemical_formula_sum`

The chemical formula must be consistent with the atomic content specified by the `_atom_site_` information, and match the `_chemical_formula_weight` (see *Appendix* 3).

`_symmetry_space_group_name_H-M`

The space group must encompass the highest symmetry permitted by the diffraction intensities, and be consistent with the `_cell_length_` and `_cell_angle_` values (see *Appendix* 3).

`_cell_formula_units_Z`

The number of formula units in the unit cell must comply with that expected from the chemical formula, the space group and the `_atom_site_` data.

`_exptl_crystal_colour`

The crystal colour should comply with the codes listed in *Appendix* 4.

`_exptl_absorpt_correction_type`

Permitted absorption-type codes are listed in *Appendix* 4. A type code must be accompanied by a reference to the method or the software used; this should be given in the field `_exptl_absorpt_process_details`. The need for absorption corrections, and the appropriate type of correction, is dependent on the μ value `_exptl_absorpt_coefficient_mu` and the crystal size values `_exptl_crystal_size_min`, `_mid` and `_max`. If x is the medial size `_mid`, the product μx provides a gauge to the type of correction needed. Analytical or numerical corrections are strongly recommended if μx exceeds 1.0 and mandatory if μx is above 3.0. If μx is below 0.1 corrections are usually unnecessary, otherwise ψ-scan or empirical methods are acceptable. Refined absorption methods are discouraged except in special circumstances. The transmission-factor limits `_exptl_absorpt_correction_T_min` and `_max` should agree with those expected for the crystal shape and size, and μ.

`_reflns_number_total`

The number of symmetry-independent reflections excludes the systematically extinct intensities. Authors are encouraged to use all of these reflections in the refinement of the structure parameters.

`_reflns_threshold_expression`

This is identical to the item `_reflns_observed_criterion`. This threshold, which is based on multiples of σI, σF^2 or σF, serves to identify the significantly intense reflections, the number of which is given by `_reflns_number_gt`. These reflections are used in the calculation of `_refine_ls_R_factor_gt`. The multiplier in the threshold expression should be as small as possible.

`_diffrn_reflns_theta_max`

The $\theta_{\max}$ of measured reflections should be such that $\sin\theta_{\max}/\lambda$ exceeds $0.6\,\text{Å}^{-1}$ (*i.e.* $\theta_{\max} > 25°$ for Mo $K\alpha$; $\theta_{\max} > 67°$ for Cu $K\alpha$). This provides the minimum number of reflections recommended for an average structural study.

`_diffrn_measured_fraction_theta_max`

This is intended for area-detector data, but is also useful as a general measure of data completeness. It is the fraction of unique (symmetry-independent) reflections measured out to `_diffrn_reflns_theta_max`. Ideally, this should be as close to 1.0 as possible.

`_diffrn_reflns_theta_full`

This is intended for area-detector data. θ_{full} is the diffractometer angle at which the measured reflection count is close to complete. The fraction of unique reflections measured out to this angle is given by `_diffrn_measured_fraction_theta_full`. Alternatively, a breakdown of data completeness and merging statistics as a function of θ may be requested if deemed necessary.

`_diffrn_reflns_av_R_equivalents`

Sufficient symmetry-equivalent reflections must be measured to provide a good estimate of the intensity repeatability. This is particularly important when absorption corrections are applied (this value is calculated *after* the corrections are applied to the intensities).

`_refine_ls_R_factor_gt`

This is identical to the item `_refine_ls_R_factor_obs` and is calculated for the number of reflections `_reflns_number_gt`. Note that this value is not intended as a reliable gauge of structure precision; this is better determined from the standard uncertainties of the parameters (which depend on the number and the reliability of the measured structure factors used in the refinement process).

`_refine_ls_number_reflns`

The number of reflections used in the refinement should be as large as possible, and is expected to be an order of magnitude greater than the number of refined parameters `_refine_ls_number_parameters`. If the number of refinement reflections is set equal to `_reflns_number_gt`, then the σ multiplier in `_reflns_threshold_expression` should be kept as small as possible.

`_refine_ls_number_parameters`

This is the number of coordinate, atomic displacement, scale, occupancy, constraint and restraint parameters refined independently in the least-squares process. It is possible, and sometimes desirable, to reduce that number by the appropriate application of geometric constraints.

`_refine_ls_hydrogen_treatment`

The codes which identify the treatment of H-atom parameters are listed in *Appendix* 4. Detailed text about the refinement of H-atom sites should be placed in `_publ_section_exptl_refinement`. Authors should note that the method by which the H-atom parameters are determined dictates how the hydrogen-bond geometry may be considered in the paper.

`_refine_ls_weighting_scheme`

Refinements based on unit weights are not acceptable.

`_refine_ls_shift/su_max`

This is identical to the item `_refine_ls_shift/esd_max`. It is the largest ratio of the refinement shift to standard uncertainty and typically is within ±0.01. A value outside ±0.1 is considered unusual and values beyond this are a signal of incomplete refinement, unaccounted-for disorder or high correlation between parameters that should be constrained. Authors should explain the reasons for a high value in `_publ_section_exptl_refinement`.

`_refine_diff_density_min`
`_refine_diff_density_max`

These values are expected to be small, especially for light-atom structures. If their magnitudes exceed $1\,\text{e}\,\text{Å}^{-3}$, the label and the distance of the closest atom site should be reported in `_publ_section_exptl_refinement`.

`_geom_`

All geometry values must originate from the submitted `_atom_site_fract_` values. Only novel geometry values of significance to the structure will be printed. These must be identified with a `_geom_..._flag` value of `yes` in the submitted CIF; all other geometry values must be flagged with a `no`.

`_atom_site_`

Atomic coordinates for molecular structures should be supplied as connected sets. `atom_site_occupancy` values should be 1.0 except for disordered or non-stoichiometric atom sites. Atom sites constrained to model disorder must be indicated by `_atom_site_disorder_group`. The overall packing in the structure will be checked for significant vacant regions (*i.e.* voids) indicating omitted solvent molecules.

`_atom_site_aniso_U_`

Checks will be made for non-positive-definite anisotropic atomic displacement parameters. The ratio of maximum to minimum eigenvalues should not, except in special circumstances (*e.g.* disorder), exceed 5.

`_refine_ls_abs_structure_details`

This item should describe the method applied, and the number of Friedel-related reflections used, in the measurement of the absolute structure parameter (*e.g.* `_refine_ls_abs_structure_Flack`). If the structure is non-centrosymmetric, and atoms heavier than Si are present, an absolute structure parameter is expected. The reliability of this parameter increases with the number of Friedel-related intensities, and a complete set of Friedel pairs is strongly recommended.

4. Diagram requirements

4.1. *Publication*

Diagrams are only required for full papers. Normally only one diagram will be published per structure. For papers reporting molecular structures this should be a molecular diagram; otherwise it should be a packing or polyhedron diagram. Unique atom sites should be identified with labels consistent with those for the supplied atom coordinates. Distances and angles should not be shown in the crystallographic diagram. A chemical structural diagram must be supplied for molecular compounds (see §2.9 for a typical example).

4.2. *Submission*

Authors should not send diagrams with the CIF submission. They will be contacted when the diagram material is required. Electronic submission as PostScript or HPGL files is preferred (see *Appendix* 2 for details) but high-quality prints may be sent by post or courier (see §1.3).

4.3. *Quality*

It is essential that diagrams be of *publication* quality. A clear, well presented crystallographic diagram encapsulates the stereochemistry, the geometry, and, if it is a displacement ellipsoid plot, the structural disorder and thermal motion.

4.4. *Size*

Each diagram should be provided separately without reduction. Diagrams will be reduced by the printer to fit an 80 mm column. The orientation and labelling of the diagram should take this into account.

4.5. *Lettering and symbols*

Fine-scale details and lettering must be large enough to be clearly legible (not less than 1.2 mm in height) when the diagram is one column (80 mm) in width. Atom site labels in crystallographic diagrams should match labels used in the atom site lists and text. The labels should not overlap ellipsoids or bonds. Descriptive matter should be placed in the legend. Packing diagrams must show the cell-axis directions (labelled *a*, *b*, *c*) and the cell origin (labelled *0*), but should normally exclude H-atom sites.

4.6. *Numbering and legends*

Diagrams and photographs are to be numbered as figures in a single series, normally in the order in which they are referred to in the text. A list of the legends ('figure captions') should be included in `_publ_section_figure_captions`. Legends of ellipsoid plots must state the probability limit used.

5. Nomenclature

5.1. *Crystallographic nomenclature*

Atom sites not related by space-group symmetry should be identified by unique labels composed of a number appended to the IUPAC chemical symbol (*e.g.* C5, C7 *etc.*). Label numbers *should not* be placed in parentheses. Chemical and crystallographic numbering should be in agreement wherever possible. Crystallographically equivalent atoms in *different* asymmetric units should be identified in diagrams and text with lower-case roman numeral superscripts appended to the original atom labels (*e.g.* $C5^{i}$ and $C7^{iv}$).

Space groups should be designated by the Hermann–Mauguin symbols. Standard cell settings, as listed in Volume A of *International Tables for Crystallography*, should be used unless objective reasons to the contrary are stated. A list of equivalent positions should also be supplied. Hermann–Mauguin symbols should be used for designating point groups and molecular symmetry. If there is a choice of origin, this should be stated in `_publ_section_exptl_refinement`. The choice of axes should normally follow the recommendations of the Commission on Crystallographic Data [Kennard *et al.* (1967). *Acta Cryst.* **22**, 445–449].

Authors are encouraged to follow the recommendation of the International Organization for Standardization (ISO) and use the term standard uncertainty, abbreviated s.u., in place of the traditional term estimated standard deviation [see Schwarzenbach *et al.* (1995). *Acta Cryst.* A**51**, 565–569]. The standard uncertainty should be expressed as a number in parentheses following the numerical result and should be on the scale of the least significant digits of the result. The s.u. value should be in the range 2–19.

Anisotropic displacement parameters should be reported as U values with the indices ij given as superscripts [see Trueblood *et al.* (1996). *Acta Cryst.* A**52**, 770–781].

5.2. *Nomenclature of chemical compounds*

Names of chemical compounds and minerals should conform to the nomenclature rules of the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry and Molecular Biology (IUBMB), the International Mineralogical Association and other appropriate bodies. Any accepted trivial or non-systematic name may be retained, but the corresponding systematic (IUPAC) name should also be given. If help on assigning systematic names is sought from advisory sources, authors are requested to indicate the source consulted.

5.3. *Units*

The International System of Units (SI) is used except that the ångström (symbol Å, defined as 10^{-10} m) is generally preferred to the nanometre (nm) or picometre (pm) as the appropriate unit of length. Recommended prefixes of decimal multiples should be used rather than '$\times 10^{n}$'.

6. References

References to published work must be indicated by giving the authors' names followed immediately by the year of publication, *e.g.* Neder & Schulz (1998) or (Neder & Schulz, 1998). Where there are three or more authors the reference in the text should be indicated in the form Smith *et al.* (1989) or (Smith *et al.*, 1989) *etc.*

In the reference list, entries for journals [abbreviated in the style of *Chemical Abstracts* (the abbreviations *Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.* are exceptions)], books, multi-author books, computer programs, personal communications and undated documents should be arranged alphabetically and conform with the following style:

Bürgi, H.-B. (1989). Acta Cryst. B45, 383–390.

Ferguson, G., Schwan, A. L., Kalin, M. L. & Snelgrove, J. L. (1997). Acta Cryst. C53, IUC9700009.

Hervieu, M. & Raveau, B. (1983a). Chem. Scr. 22, 117–122.

Hervieu, M. & Raveau, B. (1983b). Chem. Scr. 22, 123–128.

Hummel, W., Hauser, J. & Bürgi, H.-B. (1998). In preparation.

International Union of Crystallography (1998). (IUCr) Acta Crystallographica Section C, http://www.iucr.org/actac.html.

Jones, P. T. (1987). Personal communication.

McCrone, W. C. (1965). Physics and Chemistry of the Organic Solid State, Vol. 2, edited by D. Fox, M. M. Labes & A. Weissberger, pp. 725–767. New York: Interscience.

Perkins, P. (undated). PhD thesis, University of London, England.

Sheldrick, G. M. (1993). SHELXL93. Program for the Refinement of Crystal Structures. University of Göttingen, Germany.

Smith, J. V. (1988). Chem. Rev. 88, 149–182.

Smith, J. V. & Bennett, J. M. (1981). Am. Mineral. 66, 777–788.

Stanlow, D. J. (1998). Acta Cryst. B54. In the press.

Vogel, A. (1978). Textbook of Practical Organic Chemistry, 4th ed. London: Longman.

Note that **inclusive** page numbers *must* be given.

APPENDIX 1
Guidelines for editing CIF text

A limited number of special characters (such as Greek letters, sub- and superscripts, and a few others) may be indicated in CIF text for typesetting purposes, using the special codes listed below. Authors are discouraged from trying to impose any particular style on the submitted text, and codes for italic and boldface characters have been omitted intentionally.

Greek letters

In general, the corresponding letter of the Latin alphabet, prefixed by a backslash character. The complete set is:

α	A	`\a`	`\A`	alpha
β	B	`\b`	`\B`	beta
χ	X	`\c`	`\C`	chi
δ	Δ	`\d`	`\D`	delta
ε	E	`\e`	`\E`	epsilon
φ	Φ	`\f`	`\F`	phi
γ	Γ	`\g`	`\G`	gamma
η	H	`\h`	`\H`	eta
ι	I	`\i`	`\I`	iota
κ	K	`\k`	`\K`	kappa
λ	Λ	`\l`	`\L`	lambda
μ	M	`\m`	`\M`	mu
ν	N	`\n`	`\N`	nu
ο	O	`\o`	`\O`	omicron
π	Π	`\p`	`\P`	pi
θ	Θ	`\q`	`\Q`	theta
ρ	R	`\r`	`\R`	rho
σ	Σ	`\s`	`\S`	sigma
τ	T	`\t`	`\T`	tau
υ	Υ	`\u`	`\U`	upsilon
ω	Ω	`\w`	`\W`	omega
ξ	Ξ	`\x`	`\X`	xi
ψ	Ψ	`\y`	`\Y`	psi
ζ	Z	`\z`	`\Z`	zeta

Accented letters

Accents should be indicated by using the following codes before the letter to be modified (*i.e.* use `\'e` for an acute e):

`\'`	acute (é)	`\"`	umlaut (ü)	`\=`	overbar (ō)
`\'`	grave (à)	`\~`	tilde (ñ)	`\.`	overdot (ȯ)
`\^`	circumflex (â)	`\;`	ogonek (ş)	`\<`	hacek (č)
`\,`	cedilla (ç)	`\>`	Hungarian umlaut (ő)	`\(`	breve (ŏ)

Other characters

Other special alphabetic characters should be indicated as follows:

`\%a`	a-ring (å)	`\?i`	dotless i (ı)	`\&s`	German "ss" (ß)
`\/o`	o-slash (ø)	`\/l`	Polish l (ł)	`\/d`	barred d (đ)

Capital letters may also be used in these codes, so an ångström symbol (Å) may be given as `\%A`.

Superscripts and subscripts should be indicated by bracketing relevant characters with circumflex or tilde characters, thus:

superscripts	`Csp^3^`	for	Csp^3
subscripts	`U~eq~`	for	U$_{eq}$

The closing symbol is essential to return to normal text.

Other codes are also recognized by the IUCr software. These are:

`\%`	degree (°)	`\\times`	×
`--`	dash (*e.g.* 4–7)	`+-`	±
`---`	single bond (*e.g.* C—C)	`-+`	∓
`\\db`	double bond (*e.g.* C═C)	`\\square`	□
`\\tb`	triple bond (*e.g.* C≡C)	`\\neq`	≠
`\\ddb`	delocalized double bond (*e.g.* C⋯C)	`\\rangle`	⟩
`\\sim`	∼	`\\langle`	⟨
(*N.B.* ~ is the code for subscript)		`\\rightarrow`	→
`\\simeq`	≃	`\\leftarrow`	←
		`\\infty`	∞

Note that `\\db`, `\\tb` and `\\ddb` should always be followed by a space, e.g. C≡C is denoted by `C\\tb C`.

Complete text using TEX

One further mechanism exists to allow the use of a wider range of special symbols. If, in a text field (one surrounded by semicolons), the first two non-blank characters are '`%T`', the *entire contents of that field* will be passed unchanged to the TEX formatting program. Hence, any symbols known to the powerful TEX system may be used, and indeed arbitrarily complex text may be typeset. Any macros defined by the author are valid only through the field in which they are defined, however. It should be stressed that the usual CIF special symbols are not valid in such a field, *e.g.* U$_{eq}$ would have to be denoted by `U$_{\rm eq}$`.

APPENDIX 2
Transferring large electronic files

File transfer protocol (ftp) should be used to transfer large electronic files exceeding 100K bytes to the Editorial Office in Chester. Files need to be deposited in a directory called 'incoming/c' with a filename constructed from the *reference code* supplied by Chester.

Files containing reflection data in CIF format should be identified by the filename extension `.hkl`. Where more than one structure is reported in the CIF, the names of the files containing the reflection data should be in the form *`ref.id`*`.hkl` where *`id`* is the `data_` block code for the corresponding structure in the CIF. Files containing diagrams in HPGL, PostScript or encapsulated PostScript format should be given the extensions `.hpg`, `.ps` or `.eps`, respectively. Multiple files for the same submission should be identified by filenames constructed as *`ref.id.ext`* where *`id`* indicates the contents, *e.g.* `xz1087.fig1.ps` and `xz1087.fig2.ps`.

The procedure for transferring files is shown below.

(i) On your workstation enter:	`ftp ftp.iucr.org`
(ii) Wait for `Login`: prompt and enter:	`anonymous`
(iii) Wait for `Password`: prompt and enter:	*your e-mail address*
(iv) Wait for `ftp>` prompt and enter:	`cd incoming/c`
(v) Transfer a file from your account (*e.g.* b28.cif) as an identifiable name (*e.g.* zb1032.hkl):	`put b28.cif zb1032.hkl`
(vi) Wait for `ftp>` prompt before sending another file	
(vii) Finish off the ftp session by entering:	`bye`
(viii) Send an e-mail to Chester (`checkin@iucr.org`) with a list of the files transferred by ftp	

APPENDIX 3
Required CIF data items

The detailed description of most required data items is provided in the published *CIF Core Dictionary* [Hall *et al.* (1991). *Acta Cryst.* A**47**, 655–685] and subsequent revisions available from `http://www.iucr.org/CIF/`. The dictionary is available free of charge from the IUCr Editorial Office in Chester (see §1.3 for address).

New names listed below are flagged with (*new*) and in some cases are followed by old names [in regular type and flagged with (*old*)] which are accepted but will be discontinued in the future. Authors may also include other data items in the CIF (see the two `_publ_manuscript_incl_extra_` entries towards the end of the list) provided their data names are also listed in the `_publ_contact_letter` text.

Text items

`_publ_contact_author_name`	Contact author's name
`_publ_contact_author_address`	Contact author's address
`_publ_contact_author`	Contact author's name and address (*old*)
`_publ_contact_author_email`	E-mail address to be published
`_publ_contact_author_fax`	For editorial communications
`_publ_contact_author_phone`	For editorial communications
`_publ_contact_letter`	Letter of submission, with date
`_publ_requested_journal`	`'Acta Crystallographica Section C'`
`_publ_requested_category`	Publication choice (`FI FM FO CI CM CO AD`)
`_publ_section_title`	Title of paper (see §2.1)
`_publ_section_title_footnote`	Footnote to title of paper
`_publ_author_name`	List of author(s) name(s)
`_publ_author_footnote`	Footnote(s) to author(s) name(s)
`_publ_author_address`	Author(s) address(es) (see §2.1)
`_publ_section_synopsis`	Synopsis for compounds that cannot be shown as a chemical diagram and for all CIF-access papers (see §2.11)
`_publ_section_abstract`	Abstract of paper in English (see §2.2)
`_publ_section_comment`	Discussion of study (see §2.3)
`_publ_section_acknowledgements`	Acknowledgements (see §2.5)
`_publ_section_references`	References (see §2.6)
`_publ_section_figure_captions`	Legends to figures (see §4)

Experimental data (*machine and author generated*)

`_publ_section_exptl_prep`	Compound preparation details (see §2.4)

_chemical_formula_sum	Chemical formula as sum of elements
_chemical_formula_moiety	Chemical formula in moieties
_chemical_formula_weight	Chemical formula mass (Da)
_chemical_melting_point	Melting point (K) (*new*)
_symmetry_cell_setting	Code for cell setting (see *Appendix* 4)
_symmetry_space_group_name_H-M	Space-group symbol, including unique axis
_symmetry_equiv_pos_as_xyz	Equivalent positions in order used by `_geom_`
_cell_length_a **_cell_length_b** **_cell_length_c**	Unit-cell lengths (Å)
_cell_angle_alpha **_cell_angle_beta** **_cell_angle_gamma**	Unit-cell angles (°)
_cell_volume	Unit-cell volume (Å^3)
_cell_formula_units_Z	Number of formulae per unit cell
_exptl_crystal_density_diffrn	Density calculated from unit cell and contents (Mg m^{-3})
_exptl_crystal_density_meas	Density measured experimentally (Mg m^{-3})
_exptl_crystal_density_method	Method used to measure density experimentally
_diffrn_radiation_type	Radiation type (*e.g.* neutron or Mo $K\alpha$)
_diffrn_radiation_wavelength	Radiation wavelength (Å)
_cell_measurement_reflns_used	Number of reflections used to measure unit cell
_cell_measurement_theta_min	Minimum θ of reflections used to measure unit cell (°)
_cell_measurement_theta_max	Maximum θ of reflections used to measure unit cell (°)
_cell_measurement_temperature	Measurement temperature (K)
_exptl_absorpt_coefficient_mu	Linear absorption coefficient (mm^{-1})
_exptl_crystal_description	Crystal habit description
_exptl_crystal_size_max	Maximum dimension of crystal (mm)
_exptl_crystal_size_mid	Medial dimension of crystal (mm)
_exptl_crystal_size_min	Minimum dimension of crystal (mm)
_exptl_crystal_size_rad	Radius of spherical or cylindrical crystal (mm)
_exptl_crystal_colour	Crystal colour (see *Appendix* 4)
_diffrn_measurement_device_type	Diffractometer make and type
_diffrn_measurement_device	Diffractometer make and type (*old*)
_diffrn_measurement_method	Mode of intensity measurement and scan
_diffrn_detector_area_resol_mean	Resolution of area detector (pixels mm^{-1})
_exptl_absorpt_correction_type	Code for absorption correction (see *Appendix* 4)
_exptl_absorpt_process_details	Literature reference for absorption correction [*e.g.* `'(North et al., 1968)'`]
_exptl_absorpt_correction_T_min	Minimum transmission factor from corrections
_exptl_absorpt_correction_T_max	Maximum transmission factor from corrections
_diffrn_reflns_number	Total number of reflections measured
_reflns_number_total	Number of symmetry-independent reflections
_reflns_number_gt	Number of reflections > σ threshold
_reflns_number_observed	Number of 'observed' reflections (*old*)
_reflns_threshold_expression	σ expression for F, F^2 or I threshold
_reflns_observed_criterion	σ expression for 'observed' F, F^2 or I threshold (*old*)
_diffrn_reflns_theta_max	Maximum θ of measured reflections (°)
_diffrn_reflns_theta_full	θ to which available reflections are 'complete' (°)
_diffrn_measured_fraction_theta_max	Fraction of unique reflections measured to $\theta_{\max}$
_diffrn_measured_fraction_theta_full	Fraction of unique reflections measured to θ_{full}
_diffrn_reflns_av_R_equivalents	R factor for symmetry-equivalent intensities
_diffrn_reflns_limit_h_min **_diffrn_reflns_limit_h_max**	Minimum/maximum h index of measured data
_diffrn_reflns_limit_k_min **_diffrn_reflns_limit_k_max**	Minimum/maximum k index of measured data
_diffrn_reflns_limit_l_min **_diffrn_reflns_limit_l_max**	Minimum/maximum l index of measured data
_diffrn_standards_number	Number of standards used in measurement

_diffrn_standards_interval_count	(*alternate*)	Number of measurements between standards
_diffrn_standards_interval_time		Time (min) between standards
_diffrn_standards_decay_%		Percentage decrease in standards intensity
_refine_ls_structure_factor_coef		Code for F, F^2 or I used in least-squares refinement (see *Appendix* 4)
_refine_ls_R_factor_gt		R factor of F for reflections > threshold
_refine_ls_R_factor_obs		R factor of F for 'observed' reflections (*old*)
_refine_ls_wR_factor_ref		R factor of coefficient for refinement reflections
_refine_ls_wR_factor_obs		R factor of coefficient for 'observed' reflections (*old*)
_refine_ls_goodness_of_fit_ref		Goodness of fit S for refinement reflections
_refine_ls_goodness_of_fit_obs		Goodness of fit S for 'observed' reflections (*old*)
_refine_ls_number_reflns		Number of reflections used in refinement
_refine_ls_number_parameters		Number of parameters refined
_refine_ls_weighting_scheme		Code for weight type (see *Appendix* 4)
_refine_ls_weighting_details		Weighting expression
_refine_ls_hydrogen_treatment		Code for H-atom treatment (see *Appendix* 4)
_refine_ls_shift/su_max		Maximum shift/s.u. ratio after final refinement cycle
_refine_ls_shift/esd_max		Maximum shift/e.s.d. ratio after final refinement cycle (*old*)
_refine_diff_density_max **_refine_diff_density_min**		Maximum/minimum values of final difference map (e Å^{-3})
_refine_ls_extinction_method		Description of extinction methods applied
_refine_ls_extinction_coef		Extinction coefficient applied in corrections
_refine_ls_abs_structure_details		Absolute structure method and Friedel-pair number
_refine_ls_abs_structure_Flack	(*alternate*)	Measure of absolute structure
_refine_ls_abs_structure_Rogers		Measure of absolute structure
_publ_section_exptl_refinement		Special details of the refinement (see §2.4)
_computing_data_collection		Reference to data-collection software
_computing_cell_refinement		Reference to cell-refinement software
_computing_data_reduction		Reference to data-reduction software
_computing_structure_solution		Reference to structure-solution software
_computing_structure_refinement		Reference to structure-refinement software
_computing_molecular_graphics		Reference to visualization software
_computing_publication_material		Reference to publication preparation software
loop_		
_atom_type_symbol		Atom type symbol (usually element symbol)
_atom_type_description		Description of atom type
_atom_type_scat_source		Reference to scattering factors applied
_atom_type_scat_dispersion_real		Real anomalous-dispersion value applied
_atom_type_scat_dispersion_imag		Imaginary anomalous-dispersion value applied
loop_		
_atom_site_label		Unique label identifying the atom site
_atom_site_fract_x **_atom_site_fract_y** **_atom_site_fract_z**		Fractional coordinates of atom site
_atom_site_U_iso_or_equiv		Isotropic atomic displacement parameter, or equivalent from anisotropic atomic displacement parameters
_atom_site_occupancy		Occupancy fraction for site (default is 1.0)
_atom_site_disorder_assembly		Code that identifies functional group suffering disorder
_atom_site_disorder_group		Code that identifies disorder group
_atom_site_adp_type		Atomic displacement parameter type
_atom_site_thermal_displace_type		Atomic displacement parameter type (*old*)

`loop_`	
`_atom_site_aniso_label`	Unique label identifying the atom site

`_atom_site_aniso_U_11`
`_atom_site_aniso_U_22`
`_atom_site_aniso_U_33`
`_atom_site_aniso_U_12`
`_atom_site_aniso_U_13`
`_atom_site_aniso_U_23`
	Elements of anisotropic atomic displacement parameter tensor

`loop_`	
`_geom_bond_atom_site_label_1` `_geom_bond_atom_site_label_2`	Labels identifying the atom sites 1 and 2
`_geom_bond_site_symmetry_1` `_geom_bond_site_symmetry_2`	Symmetry codes (*e.g.* `2_554`) for atom sites 1 and 2
`_geom_bond_distance`	Distance between atom sites 1 and 2 (Å)
`_geom_bond_publ_flag`	Flag for print request (`yes` or `no`)
`loop_`	

`_geom_angle_atom_site_label_1`
`_geom_angle_atom_site_label_2`
`_geom_angle_atom_site_label_3`
	Labels identifying the atom sites 1, 2 and 3

`_geom_angle_site_symmetry_1`
`_geom_angle_site_symmetry_2`
`_geom_angle_site_symmetry_3`
	Symmetry codes for atom sites 1, 2 and 3

`_geom_angle`	Angle between atom sites 1, 2 and 3 (°)
`_geom_angle_publ_flag`	Flag for print request (`yes` or `no`)
`loop_`	

`_geom_torsion_atom_site_label_1`
`_geom_torsion_atom_site_label_2`
`_geom_torsion_atom_site_label_3`
`_geom_torsion_atom_site_label_4`
	Labels identifying the atom sites 1, 2, 3 and 4

`_geom_torsion_site_symmetry_1`
`_geom_torsion_site_symmetry_2`
`_geom_torsion_site_symmetry_3`
`_geom_torsion_site_symmetry_4`
	Symmetry codes for atom sites 1, 2, 3 and 4

`_geom_torsion`	Torsion angle between atom sites 1, 2, 3 and 4 (°)
`_geom_torsion_publ_flag`	Flag for print request (`yes` or `no`)
`loop_`	
`_geom_hbond_atom_site_label_D`	Donor-atom label in hydrogen bond
`_geom_hbond_atom_site_label_H`	H-atom label in hydrogen bond
`_geom_hbond_atom_site_label_A`	Acceptor-atom label in hydrogen bond
`_geom_hbond_site_symmetry_D`	Symmetry code for donor site
`_geom_hbond_site_symmetry_H`	Symmetry code for H-atom site
`_geom_hbond_site_symmetry_A`	Symmetry code for acceptor site
`_geom_hbond_distance_DH`	Donor atom-to-H-atom distance (Å)
`_geom_hbond_distance_HA`	H-atom-to-acceptor atom distance (Å)
`_geom_hbond_distance_DA`	Donor atom-to-acceptor atom distance (Å)
`_geom_hbond_angle_DHA`	Donor—H· · ·acceptor angle (°)
`_geom_hbond_publ_flag`	Flag for print request (`yes` or `no`)

Author requested items

`loop_`	
`_publ_manuscript_incl_extra_item`	Additional CIF item submitted for publication
`_publ_manuscript_incl_extra_defn`	Is item defined in Core dictionary? (`yes` or `no`)

Structure-factor lists should be submitted as separate files

loop_

_refln_index_h **_refln_index_k** **_refln_index_l**		Miller indices *h*, *k* and *l*
_refln_F_meas	*(alternate)*	Measured *F*
_refln_F_squared_meas		Measured F^2
_refln_F_sigma	*(alternate)*	Standard uncertainty of *F*
_refln_F_squared_sigma		Standard uncertainty of F^2
_refln_F_calc	*(alternate)*	Calculated *F*
_refln_F_squared_calc		Calculated F^2

APPENDIX 4
Standard codes for data items

Cell-setting codes

The following codes should be used with _symmetry_cell_setting.

triclinic
monoclinic
orthorhombic
tetragonal
rhombohedral
trigonal
hexagonal
cubic

Colour codes

The following colour codes should be used with _exptl_crystal_colour. The code may be constructed from three attributes *appearance*, *intensity* and *base colour*, in that order, of which only the base-colour string is mandatory. The colour code may be enclosed in quotes (*e.g.* 'light blue'), or the attribute strings may be joined by underscore characters (*e.g.* metallic_gold). Colour codes constructed from two base colours are also allowed (*e.g.* red-brown).

Appearance	Intensity	Base colour
metallic	dark	black
lustrous	light	blue
translucent	intense	bronze
fluorescent	pale	brown
clear		colourless
		gold
		green
		grey
		orange
		pink
		purple
		red
		silver
		violet
		white
		yellow

Absorption-type codes

The following codes should be used with _exptl_absorpt_correction_type. Note that this data item should contain only the type code. A reference to the computer program used to apply the absorption corrections should be given in _exptl_absorpt_process_details.

none	No absorption corrections applied (*default*)
analytical	Analytical corrections applied using crystal faces (*e.g.* Tompa method)
integration numerical gaussian	Numerical integration corrections applied using crystal faces
empirical	Corrections using intensity measurements
psi-scan	Corrections using ψ-scan measurements
multi-scan	Corrections using symmetry-related measurements
refdelf	Corrections as part of the refinement model
cylinder	Corrections for a cylinder mounted on the φ axis
sphere	Corrections for a sphere

Structure-factor codes

The following codes should be used with _refine_ls_structure_factor_coef.

F	Structure-factor magnitude
Fsqd	Structure factor squared
Inet	Net intensity

H-atom treatment codes

The following codes should be used with _refine_ls_hydrogen_treatment. Note that this data item should only contain the type code. Any detailed text about the determination and refinement of H-atom parameters should be placed in _publ_section_exptl_refinement.

none	No H atoms present (*default*)
undef	H-atom parameters are not defined
noref	No refinement of H-atom parameters
refall	H-atom parameters are refined independently
refxyz	H-atom coordinate parameters are refined only
refU	H-atom displacement parameters are refined only
constr	H-atom parameters are constrained to parent site (*e.g.* riding model)
mixed	H atoms treated by a mixture of independent and constrained refinement

Weighting-scheme codes

The following codes should be used with _refine_ls_weighting_scheme. Note that this data item should contain only the type code. The weighting expression should be given in _refine_ls_weighting_details.

sigma	Based on measured s.u.'s (*default*)
calc	Calculated weights applied

APPENDIX 5
Example of a CIF submission

```
data_global

_audit_creation_method        'manual editing of form.cif'

# PROCESSING SUMMARY (IUCr Office Use Only)

_journal_date_recd_electronic     93-03-12
_journal_date_from_coeditor       93-05-18
_journal_date_accepted            93-05-18
_journal_coeditor_code            SE1031

# SUBMISSION DETAILS

_publ_contact_author_name     'Dr Ulrich Fl\"orke'
_publ_contact_author_address
; Anorganische und Analytische Chemie
  Universit\"at-GH Paderborn
  Warburgerstr. 100
  D-4790 Paderborn
  Germany
;
_publ_contact_author_email    floe@mvaxac.uni-paderborn.de
_publ_contact_author_fax          '49(5251)603423'
_publ_contact_author_phone        '49(5251)602496'

_publ_contact_letter
; Please consider this CIF submission for publication in
  Acta Cryst. C. This file is a resubmission of a revised
  version of the paper SE1031, as requested by the Coeditor.
;
_publ_requested_journal     'Acta Crystallographica Section C'
_publ_requested_category          FM


# TITLE AND AUTHOR LIST

_publ_section_title
; The First Dinuclear Cobalt--Rhenium Cluster Compound:
  Hexacarbonylbis(\m-dicyclohexylphosphanido)cobaltrhenium
;
_publ_section_title_footnote
; Contribution No. ...
;


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
 'Fl\"orke, Ulrich'  .
; Anorganische und Analytische Chemie
  Universit\"at-GH Paderborn
  Warburgerstrasse 100
  D-4790 Paderborn
  Germany
;
 'Haupt, Hans-J\"urgen'
; Current address: Department of Chemistry ...
;
; Anorganische und Analytische Chemie
  Universit\"at-GH Paderborn
  Warburgerstrasse 100
  D-4790 Paderborn
  Germany
;


# TEXT

_publ_section_abstract
; The title compound [hexacarbonyl-1\k^4^C, 2\k^2^C-bis(\m-
dicyclohexylphosphido-1:2\k^2^P)-cobaltrhenium(Co---Re)] 0.5-
methanol solvate], [CoRe(C~12~H~22~P)~2~(CO)~6~].0.5CH~3~OH,
belongs to a type of edge-linked tetrahedron--octahedron
coordination complex. The molecule has local C~2v~ symmetry
with ecliptic conformation of the carbonyl ligands at both
metal centres, and a Co---Re single-bond length of 2.786(1) \%A.
;


_publ_section_comment
; In the course of our work on phosphanido-bridged homo- and
heteronuclear metal-atom cluster compounds (Haupt, Balsaa &
Fl\"orke, 1988; Haupt, Heinekamp & Fl\"orke, 1989; Fl\"orke &
Haupt, 1993), we isolated the title compound (I) in which a
```

All CIFs must start with a `data_blockcode` *line. The block code should be no more than 32 characters long.*

It is valuable to record the origin of the file. Most software CIF generators supply this field automatically.

`_journal_` *entries are added by Chester software and should not be modified by authors. They contain information about received and accepted dates, production codes, and other book-keeping information.*

The name and address of the contact author should be in a format that allows the automatic printing of address labels for sending proofs. Give the name as '(Title) Forenames Surname'.

The email address of the contact author is used to acknowledge receipt of the paper.

All correspondence relating to the submission should be embedded within the CIF. Supply here any special requirements relating to the presentation of your paper.

The requested paper category (see §1.5) should be given within the CIF.

Use the new field `_publ_section_title_footnote` *to insert footnotes to the title*

Give authors' names as 'Surname, Forenames'. Note that names should be given in mixed upper and lower case, not all in capitals.

Sometimes there are additional author details to be published (such as current address). Include these in the new `_publ_author_footnote` *field. Use a single full point if no footnote is relevant to the current author in a loop.*

Keep line lengths less than 80 characters.

*The headings in the paper (*Abstract, Comment *etc.) are automatically generated by the typesetting software. Don't include these headings in your text fields.*

```
Co---Re bond is symmetrically bridged by two
dicyclohexylphosphanido groups.
```

Separate paragraphs in lengthy text fields with a blank line.

```
The Co atom has distorted tetrahedral coordination from two
carbonyl ligands and the bridging P atoms. These bridging atoms
and four of the carbonyl groups give rise to distorted
octahedral coordination at the Re atom. The central CoReP~2~
ring is nearly planar; the maximum deviation from the best
plane is 0.02 \%A with a dihedral angle of 2.2\%. With respect
to the different metal atomic radii, the ring may be regarded
as regular. It shows two equal M---P bond lengths for Co
[2.111(1)and 2.116(1) \%A] as well as for Re [2.541(1) and
2.544(1) \%A]. The enclosed ring angles at both P atoms are
acute [72.8(1) and 72.9(1)\%], and the P---M---P angles reflect
the distorted coordination polyhedron of each metal atom
[121.3(1) and 92.9(1)\% for Co and Re, respectively]. The
most interesting structural feature is the Co---Re single bond
which meets the requirement of 18 valence electrons for each
metal atom and has a length of 2.786(1) \%A. We have
established, by use of the Cambridge Structural Database
(Allen et al., 1979), that the only other cobalt--rhenium
cluster reported so far is
[Co~2~Re(\m~3~-CC~6~H~4~Me-4)(CO)~10~] (Jeffery, Lewis, Lewis
& Stone, 1985), with Co---Re bond lengths of 2.686(1) and
2.720(1) \%A. This triangular cluster has distinctly different
bonding and bridging patterns, so direct comparison of the
heteronuclear bond lengths of both compounds is not possible.
However, . . .
;
_publ_section_acknowledgements                 ?

_publ_section_references
; Allen, F. H., Bellard, S., Brice, M. D., Cartwright, B. A.,
Doubleday, A., Higgs, H., Hummelink, T., Hummelink-Peters,
B. G., Kennard, O., Motherwell, W. D. S., Rodgers, J. R. &
Watson, D. G. (1979). Acta Cryst. B35, 2331--2339.

Fl\"orke, U. & Haupt, H.-J. (1993). Acta Cryst. C49, 374--376.
```

Separate each reference, as with paragraphs, with a blank line.

```
Haupt, H.-J., Balsaa, P. & Fl\"orke, U. (1988).
Inorg. Chem. 27, 280--286.

Haupt, H.-J., Heinekamp, C. & Fl\"orke, U. (1989).
Inorg. Chem. 29, 2955--2963.

Jeffery, J. C., Lewis, D. B., Lewis, G. E. & Stone,
F. G. A. (1985). J. Chem. Soc. Dalton Trans. pp. 2001--2007.

Nardelli, M. (1983). Comput. Chem. 7, 95--98.

Sheldrick, G. M. (1990). SHELXTL-Plus. Structure Determination
Software Programs. Siemens Analytical X-ray Instruments Inc.,
Madison, Wisconsin, USA.
;

_publ_section_figure_captions
; Fig. 1. Molecular structure showing 50% probability
displacement ellipsoids. H atoms are omitted for clarity.
```

The list of figure captions should be in the single text field `_publ_section_figure_captions`. Separate each with a blank line. Give complete text of figure captions, including initial 'Fig. 1' etc.

```
Fig. 2. Packing diagram viewed down the a axis. Note the
solvent molecule in the centre of the cell.
;

_publ_section_exptl_prep
; Synthesis was carried out by reaction of Re~2~(CO)~10~,
Co~2~(CO)~8~ and HP(C~6~H~11~)~2~ (molar ratio 1:1:2) in xylene
solution for 10 h at 423 K in a glass tube. Recrystallization
was from MeOH.
;
```

Use the fields `_publ_section_exptl_prep` for details of the chemical and crystal preparation, and `_publ_section_exptl_refinement` for special aspects of the structure determination and refinement.

```
_publ_section_exptl_refinement
; The enclosed CH~3~OH solvent molecule had a site occupation
factor of 0.5. Cyclohexyl H atoms were fixed at ideal positions
with common isotropic displacement parameters (U~iso~ = 0.08
\%A^2^). Structure solution and refinement used SHELXTL-Plus
(Sheldrick, 1990). Other programs include PARST
(Nardelli, 1983).
;

############################################################

data_(I)
```

Here another `data_` block header introduces the structural data for the compound reported. This is optional for a single-compound paper, but should be used to separate structures in a multi-compound paper.

```
# CHEMICAL DATA

_chemical_name_systematic
; [Hexacarbonyl-1\k^4^C, 2\k^2^C-bis(\m-dicyclohexylphosphido-
  1:2\k^2^P)-cobaltrhenium(Co---Re)] 0.5-methanol solvate]
;
```

```
_chemical_formula_moiety  'C30 H44 Co O6 P2 Re,0.5(C H4 O)'
_chemical_formula_sum               'C30.5 H46 Co1 O6.5 P2 Re1'
_chemical_formula_iupac
          '[Co Re (C12 H22 P)2 (C O)6].0.5C H3 O H'
_chemical_formula_weight            823.7

# CRYSTAL DATA
_symmetry_cell_setting              triclinic
_symmetry_space_group_name_H-M      'P -1'

loop_
    _symmetry_equiv_pos_as_xyz
'x,y,z'
'-x,-y,-z'

_cell_length_a                       10.452(3)
_cell_length_b                       11.664(4)
_cell_length_c                       15.641(4)
_cell_angle_alpha                     94.37(2)
_cell_angle_beta                      89.75(2)
_cell_angle_gamma                    111.87(2)
_cell_volume                        1763.8(8)
_cell_formula_units_Z               2
_cell_measurement_reflns_used       40
_cell_measurement_theta_min         7
_cell_measurement_theta_max         16
_cell_measurement_temperature       293

_exptl_crystal_description          prism
_exptl_crystal_colour               red
_exptl_crystal_size_max             0.50
_exptl_crystal_size_mid             0.34
_exptl_crystal_size_min             0.28
_exptl_crystal_size_rad             ?
_exptl_crystal_density_diffrn       1.551
_exptl_crystal_density_meas         ?
_exptl_crystal_density_method       'not measured'
_exptl_crystal_F_000                826
_exptl_absorpt_coefficient_mu       4.07
_exptl_absorpt_correction_type      psi-scan
_exptl_absorpt_process_details
          '(North, Phillips & Mathews, 1968)'
_exptl_absorpt_correction_T_min     0.131
_exptl_absorpt_correction_T_max     0.320

# EXPERIMENTAL DATA
_diffrn_radiation_type              'Mo K\a'
_diffrn_radiation_wavelength        0.71073
_diffrn_measurement_device_type     'Siemens R3m/V'
_diffrn_measurement_method          \w--2\q
_diffrn_reflns_number               15189
_diffrn_reflns_av_R_equivalents     0.022
_diffrn_reflns_theta_max            27.5
_diffrn_reflns_limit_h_min          -13
_diffrn_reflns_limit_h_max          13
_diffrn_reflns_limit_k_min          -15
_diffrn_reflns_limit_k_max          15
_diffrn_reflns_limit_l_min          -21
_diffrn_reflns_limit_l_max          21
_diffrn_standards_number            4
_diffrn_standards_interval_count    400
_diffrn_standards_interval_time     ?
_diffrn_standards_decay_%           0

# REFINEMENT DATA

_refine_special_details             ?

_reflns_number_total                8161
_reflns_number_gt                   6813
_reflns_threshold_expression        F>4\s(F)

_refine_ls_structure_factor_coef    F
_refine_ls_R_factor_gt              0.038
_refine_ls_wR_factor_ref            0.034
_refine_ls_hydrogen_treatment       noref
_refine_ls_number_reflns            6813
_refine_ls_number_parameters        379
_refine_ls_goodness_of_fit_ref      1.583
_refine_ls_weighting_scheme         calc
_refine_ls_weighting_details  'w - 1/[\s^2^(F) + 0.0001F^2^]'

_refine_ls_shift/su_max             0.001
_refine_diff_density_max            0.95
_refine_diff_density_min            -0.80
_refine_ls_extinction_method        none
_refine_ls_extinction_coef          ?
_atom_type_scat_source        'SHELXTL-Plus (Sheldrick, 1990)'
```

The sum and moiety formulae should be present, and entered according to the rules of the CIF Dictionary. Do not *indicate sub- or superscripts.*

`_chemical_formula_iupac` *is used to express chemical formulae according to IUPAC rules.*

The full *Hermann-Mauguin space-group symbol should be used, with a space between each separate component of the symbol.*

Loop all *symmetry equivalent positions for the space group, including any for lattice centring and a centre of symmetry.*

Do not *include the units of physical quantities – these are included in the definitions for each data name.*

Authors are encouraged to measure the crystal density. However, if the crystal density was not measured, this should be explicitly stated.

Comment lines in the CIF are never parsed by software, but can be used to improve the visual layout of the file.

All data names (if present at all in the file) must have a corresponding value – use ? (without surrounding quotes) if there is no information on the value.

Fields denoted '`*_special_details`*' are not normally printed in the published paper, but may contain information (often generated by the refinement program) important for critical review purposes.*

We accept the convention that a single occurrence of `_atom_type_scat_source` *is taken to refer to all atoms. But a preferable layout lists data for each atom species, e.g.*

```
loop_
     _atom_type_symbol
     _atom_type_scat_dispersion_real
     _atom_type_scat_dispersion_imag
     _atom_type_scat_source
 C  .017  .009
; International Tables for X-ray Crystallography
  (Vol. IV)
;
 N  .029  .018
; International Tables for X-ray Crystallography
  (Vol. IV)
;
```

```
# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
     _atom_site_label
     _atom_site_fract_x
     _atom_site_fract_y
     _atom_site_fract_z
     _atom_site_U_iso_or_equiv
     _atom_site_adp_type
     _atom_site_type_symbol
Re   0.2227(1)  -0.0032(1)   0.1460(1)    0.042(1)   Uani   Re
Co   0.2347(1)   0.1392(1)   0.2992(1)    0.046(1)   Uani   Co
P1   0.3589(1)   0.2221(1)   0.1970(1)    0.044(1)   Uani   P
P2   0.1068(2)  -0.0511(1)   0.2891(1)    0.046(1)   Uani   P
C1   0.3087(6)   0.0299(6)   0.0346(4)    0.057(4)   Uani   C
O1   0.3569(5)   0.0449(5)  -0.0308(3)    0.079(3)   Uani   O
C2   0.0662(6)   0.0396(6)   0.1118(4)    0.056(4)   Uani   C
O2  -0.0268(5)   0.0626(5)   0.0927(3)    0.087(4)   Uani   O
C3   0.3789(7)  -0.0423(6)   0.1896(4)    0.063(4)   Uani   C
O3   0.4690(5)  -0.0639(5)   0.2137(4)    0.109(4)   Uani   O
...     ...        ...         ...          ...       ...    ...


loop_
     _atom_site_aniso_label
     _atom_site_aniso_U_11
     _atom_site_aniso_U_22
     _atom_site_aniso_U_33
     _atom_site_aniso_U_23
     _atom_site_aniso_U_13
     _atom_site_aniso_U_12
     _atom_site_aniso_type_symbol
Re    .045(1)  .045(1)  .036(1)  .001(1)  .002(1)  .021(1)  Re
Co    .050(1)  .048(1)  .042(1) -.001(1)  .006(1)  .015(1)  Co
P1    .044(1)  .045(1)  .044(1)  .004(1)  .002(1)  .018(1)   P
P2    .049(1)  .046(1)  .042(1)  .004(1)  .004(1)  .018(1)   P
...     ...      ...      ...      ...      ...      ...    ...


# MOLECULAR GEOMETRY

loop_
     _geom_bond_atom_site_label_1
     _geom_bond_atom_site_label_2
     _geom_bond_site_symmetry_1
     _geom_bond_site_symmetry_2
     _geom_bond_distance
     _geom_bond_publ_flag
Re Co   .   .  2.786(1)   yes
Re P1   .   .  2.544(1)   yes
Re P2   .   .  2.541(1)   yes
Re C1   .   .  1.955(6)   no
Re C2   .   .  1.967(4)   no
Re C3   .   .  1.987(5)   no
... ...  ...  ...    ...    ...


loop_
     _geom_angle_atom_site_label_1
     _geom_angle_atom_site_label_2
     _geom_angle_atom_site_label_3
     _geom_angle
     _geom_angle_publ_flag
Co Re P1             46.4(1)   yes
Co Re P2             46.5(1)   yes
Co Re C1            134.8(2)   no
P1 Re P2             92.9(1)   yes
P1 Re C1             88.4(2)   no
Re Co P1             60.8(1)   yes
... ... ...            ...      ...


loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
O6  H6  O3 0.98(3) 1.69(3)  2.664(3)  172(3)  2_675
O6  H6  O4 0.98(3) 1.71(2)  2.661(3)  166(3)  .
... ... ... ...      ...       ...       ...     ...

##########################################################
```

Ensure that there are no spaces between values and their s.u.'s.

Authors are required to provide the U^{ij} values for checking purposes.

It is essential to check (especially if the U^{ij} values are manually entered, or imported from another file) that the order of data names in the loop header corresponds to the order of values tabulated.

This table is not usually published, but will be available over the Internet.

The geometry tables are generated from CIF data loops. Bond symbols must not be entered in these loops.

In this example, the symmetry code for each atom site has the default value denoted by '.' (in such circumstances, these values need not appear at all, as in the following table). Suppose the first set of entries in this list included a symmetry code as below:

`Re  Co   .   1_565    2.786(1)    yes`

The specific atom site undergoing a symmetry transformation (here the Co site) is labelled with a symbol 1_565, where the number preceding the underscore is the sequence number of the symmetry operation in the `_symmetry_equiv_pos_as_xyz` *loop (in this example, that would be 'x,y,z'), and the digits following the underscore refer to unit translations along the x, y and z axes respectively, where the base cell is located at 555. So the example cited would refer to the symmetry operator 'x,1+y, z', and the resultant table entry would be printed as*

Re—Co^{i} 2.786 (1)

with a footnote to the table:

Symmetry code: (i) x, $1+y$, z.

Only bonds, angles and torsion angles flagged with '`yes`*' will be published. Others will be available over the Internet.*

Hydrogen-bond details should be included using the new `_geom_hbond_` *data items.*

APPENDIX 6

International Union of Crystallography
Transfer of Copyright Agreement

Title of Article (*Please type or use capital letters*)

. . . .

. . . .

Authors (*Please type or use capital letters*)

. . . .

. . . .

Copyright to the above article is hereby transferred (except as otherwise required by national laws*) to the International Union of Crystallography, effective if and when the article is accepted for publication in *Acta Crystallographica*, *Journal of Applied Crystallography* or *Journal of Synchrotron Radiation*. In addition to reproduction in conventional printed form your article will be stored electronically. Your assignment of Copyright signifies your agreement to the journal making arrangements to include your paper in document delivery services, CD-ROMs and electronic databases, *etc.*, worldwide. This transfer of copyright also applies to data submitted in machine-readable form. However, the authors reserve the following:

(1) All proprietary rights other than copyright, such as patent rights.
(2) The right to use all or part of this article in future works prepared by or on the behalf of the author.
(3) In the case of 'work for hire', the right of the employer to incorporate all or part of this article in future works.
(4) The royalty-free right of the employer to make copies of this article, without further permission, for his or her own use but not for resale. Any identification or notice appearing on the pages to be reproduced must not be deleted.

Signature	Signature . . . .
Name and position, if not author	Name and position, if not author
. . . .	. . . .
. . . .	. . . .
Date	Date . . . .

This Transfer of Copyright Agreement must be signed by at least one of the authors (who agrees to inform the others, if any) or, in the case of a 'work made for hire', by the employer.

By signing this form you certify that your contribution is your original work, has not been published before (in any language or medium) and is not being considered for publication elsewhere; that you have obtained permission for and acknowledged the source of any excerpts from other copyright works; and that to the best of your knowledge your paper contains no statements which are libellous, unlawful or in any way actionable.

The signed statement must be received before the article can be accepted for publication. Requests for further information should be sent to the Executive Secretary of the Union.

---

* In this case please give further details overleaf.

For use of the International Union of Crystallography only.

M. E. Ref.	Co-editor Ref.	Issue	Journal

This form may be photocopied.