

# A Guide to CIF for Authors



International Union of Crystallography

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The Editorial Office of the journals of the International Union of Crystallography (*Acta Crystallographica*, *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation*) is located at 5 Abbey Square, Chester CH1 2HU, England.

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## COMCIFS

The Committee for the Maintenance of the CIF Standard (COMCIFS) has been established by the IUCr to direct and monitor the development of further CIF dictionaries, and to ensure that CIF fulfils its role as a universal data transfer and archive medium within the field of crystallography. Correspondence on any aspect of the CIF standard should be addressed to the Chairman or the Coordinating Secretary. The current membership is:

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The current list of members is always available for inspection through the IUCr WWW server.

## IUCr Policy on the Use of CIF

The Crystallographic Information File (Hall, Allen & Brown, 1991) is, as of January 1992, the recommended method for submitting publications to *Acta Crystallographica*. The International Union of Crystallography holds the Copyright on the CIF, and has applied for Patents\* on the STAR File syntax which is the basis for the CIF format.

It is a principal objective of the IUCr to promote the use of CIF for the exchange and storage of scientific data. The IUCr's sponsorship of the CIF development was motivated by its responsibility to its scientific journals, which set the standards in crystallographic publishing. The IUCr intends that CIFs will be used increasingly for electronic submission of manuscripts to these journals in future. The IUCr recognises that, if the CIF and the STAR File are to be adopted as a means for universal data exchange, the syntax of these files must be strictly and uniformly adhered to. Even small deviations from the syntax would ultimately cause the demise of the universal file concept. Through its Copyrights and Patents the IUCr has taken the steps needed to ensure strict conformance with this syntax.

The IUCr policy on the use of the CIF and STAR File processes is as follows:

1. **CIFs and STAR Files may be generated, stored or transmitted, without permission or charge**, provided their purpose is not specifically for profit or commercial gain, and provided that the published syntax is strictly adhered to.
2. **Computer software may be developed for use with CIFs or STAR files, without permission or charge**, provided it is distributed in the public domain. This condition also applies to software for which a charge is made, provided that its primary function is for use with files that satisfy condition 1 and that it is distributed as a minor component of a larger package of software.
3. **Permission will be granted** for the use of CIFs and STAR Files for specific commercial purposes (such as databases or network exchange processes), and for the distribution of commercial CIF/STAR software, on written application to the IUCr Executive Secretary, 2 Abbey Square, Chester CH1 2HU, England. The nature, terms and duration of the licences granted will be determined by the IUCr Executive and Finance Committees.

In summary, the IUCr wishes to promote the use of the STAR File concepts as a standard universal data file. It will insist on strict compliance with the published syntax for all applications. To assist with this compliance, the IUCr provides public domain software for checking the logical integrity of a CIF, and for validating the data name definitions contained within a CIF. Detailed information on this software, and the associated dictionaries, may be obtained from the IUCr Office at 5 Abbey Square, Chester CH1 2HU, England.

\* The STAR concept is protected by UK Patent No. GB 2 243 467 B.

## A Guide to CIF for Authors

If you are very lucky, you won't have to read this guide at all. Your crystal structure refinement software may generate a CIF that satisfies all the requirements for publishing a data set in *Acta Crystallographica*. It may even supply a template for the extra fields that you need to complete. Your colleague or co-worker may have already submitted CIF papers to *Acta*, and may be able to fill you in on the few extra details you require.

If you aren't so very lucky, you may need to read through some of this guide. But it is intended mostly as a reference manual, to be consulted, rather than a set text to be studied in depth and memorised. And you may find, with the help of the software described in the guide, and the electronic **checkcif** and **printcif** services that the IUCr provides, that effective use of CIF is not so very difficult, after all.

These guidelines are directed primarily at authors of single-crystal structure papers to be published in *Acta Crystallographica Section C*. However, most of the details apply equally to papers reporting powder structure determinations, and to the preparation of CIFs containing structural data that accompany papers submitted to *Section B* of *Acta*. Some comments on these special cases are given later in the *Guide*.

### What is a CIF?

The Crystallographic Information File (CIF) is the standard for crystallographic data exchange prescribed by the International Union of Crystallography. It was described in a paper in *Acta Cryst.* (1991). A47, 655–685 by S. R. Hall, F. H. Allen and I. D. Brown. (Copies of this document may be ordered from the Managing Editor, IUCr, 5 Abbey Square, Chester CH1 2HU, England; or consulted online at the WorldWide Web location <http://www.iucr.ac.uk/welcome.html>).

It is based on a very simple principle: data appear in a simple text file, along with an identifying label. One may retrieve the data by supplying the required labels to an appropriate program. If you want to know the volume of a crystallographic unit cell, you need only ask for `'_cell_volume'`. If you want to know all the fractional atomic coordinates of atoms in a cell, ask for `'_atom_site_label'`, `'_atom_site_fract_x'`, `'_atom_site_fract_y'` and `'_atom_site_fract_z'`.

It is as simple as that; and in due course, that is perhaps all the user of CIFs need know. User-friendly editors will appear, with dialogue boxes prompting for entry of required information, and checking that the user is entering data correctly. For the present, however, the CIF created by a structure refinement program will usually require manual augmentation with a text editor, and so the prospective author will need to know a certain amount of extra detail. It is the intention of this *Guide* to supply that extra knowledge.

### CIF syntax rules

#### 1. Character set

The structure of a CIF is very simple, and the rules for entering or modifying data in such a file can be learned in moments. But the relatively free format of the file means that programs retrieving data must be able to peruse the entire contents of the file in sequence. A corollary of this is that a syntax error early in the file may confuse file-reading software. Certainly, many of the files we receive in Chester do suffer from 'small' syntax errors (a missing quote mark or semicolon) that cause problems that are sometimes difficult to trace, and so it is worth spending a little while on recapitulating the principles of the file structure.

First, the file must contain only 'printable' ASCII characters (these are defined as characters from the ASCII set with decimal integer values from 32 to 126, as well as horizontal and vertical tabs, line feed, form feed and carriage return characters). This includes the standard alphanumeric and punctuation characters on a US computer keyboard, but it excludes any accented letters or characters that may be available on International keyboards.

The reason for this is that the ASCII character set uses only 7 bits to identify the character. Accented characters require the use of an additional bit. However, not all electronic data transmission protocols reliably handle 8-bit characters (many old e-mail systems still do not). Since one requirement for a standard data interchange file was that it could be transmitted by e-mail, it is not feasible to use 8-bit character sets.

Besides, different 8-bit encodings exist. It is not in general possible to guarantee that an acute accent (like é) generated by a particular word processor under MS-DOS can be printed as such by some other printing utility on a Unix workstation.

So, for now at least, please use only ASCII characters in the CIF. Special codes to indicate accented and other special characters are listed in a later section. You may of course use a word processor to edit CIFs, but you must ensure that you save your work as an ASCII file – most word processors permit this.

#### 2. Line length

Lines in a CIF must be no longer than 80 characters. Again, this is in the interest of ensuring transportability through older e-mail systems. (It also facilitates programming software that needs to read CIFs.) Because some software can get confused over what constitutes the length of a line (is the 'newline' character or set of characters counted, or not?) it is good practice to keep all lines well within the 80-character restriction.

It is not necessary to pad lines out to a width of 80 characters with trailing spaces – that simply wastes file space.

It is also advisable to avoid the use of tab characters, which are sometimes transformed by e-mail into groups of up to eight space characters – something that can cause the line-length limits to be exceeded.

#### 3. Data blocks

A CIF may contain one or more sets of data. Each data set is preceded by a code beginning with the characters `data_`. Further characters must follow this sequence, but you are entirely at liberty to choose what these may be – there is no significance to the code chosen other than the requirement that it be unique within a file. Authors typically use this as a device for indexing their own collection of structures: `data_THPO`, `data_THPO-C1`, `data_950523(1)`, `data_james` are all legitimate codes, each conveying more or less information to the originator of the CIF, but otherwise serving only to separate data sets within a file (or collection of files).

Note that this means that the first statement in a CIF (apart perhaps from comment lines) must be a `data_` block code statement. And, remember, the code used must be used only once within a given file.

#### 4. Data names

The labels identifying the nature of associated data begin with an underscore character '\_'. They may occur in two contexts.

##### (a) Associated single data values

Where there is a single value associated with a data item, that value immediately follows the data name. For example

```
_cell_length_a    5.959(1)
```

##### (b) Associated multiple data values

In the case of a table of data, where there are many values of a single item (for instance a set of atomic fractional coordinates), the relevant data names are collected together in a group, prefaced by the reserved word 'loop\_'. The associated values follow in strict rotation. For instance

```
loop_
  _atom_site_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
O1      .4254(4)   .5699(1)   .3026(1)
C2      .5630(5)   .5087(2)   .3246(1)
```

Any label beginning with an underscore may play the role of a data name, and is permitted in the CIF. However, a set of data names has been defined as having precise meanings. This set is the CIF Dictionary, which will be described later.

You may add to a CIF any data names (and associated values) that you wish, provided that you ensure they do not conflict with any standard data names as defined in the existing CIF Dictionary (or Dictionaries). One way to achieve this is to use a prefix which will be issued on request by COMCIFS (the CIF standards body, details of which are given later). For instance, the *Xtal* program system uses a number of local data names beginning `_xtal_` which have meaning to the *Xtal* system only.

#### 5. Data values

Each data name is associated with one or several values (several if it is declared in a loop header). The value may be numeric, it may be a short character string, or it may be a section of text. Normally the CIF Dictionary will indicate what type of data is expected to be associated with any standard data name.

The important thing to remember is that a data value can only include spaces if it is surrounded by matching quote marks ('), double-quote marks ("), or by semicolons at the beginning of the first and trailing lines. For instance,

```
_diffrn_radiation_source    'X-ray tube'
```

or

```
_diffrn_radiation_source    "X-ray tube"
```

or even

```
_diffrn_radiation_source
; X-ray tube
;
```

(though this last example is an awkward way of handling a short phrase). It is also possible to employ underscores instead of spaces, so one could also put

```
_diffrn_radiation_source    X-ray_tube
```

Quote marks may surround any character string, even if it does not have embedded spaces, but it is generally considered poor style to use such delimiters where they are not required.

By the way, don't be misled by the fact that *Acta Cryst.* prints numerical values with a space between the value and its standard uncertainty, for example 0.2227 (1). The value must be given in the CIF without such a space, as 0.2227(1).

Character strings delimited by quote marks must fit on one line; it is not permitted to break the string across a line. Hence, this example is wrong:

```
_refine_ls_extinction_expression    'Crystallographic
Computing [1970, equation (22), p. 292]'
```

but by changing the layout, we obtain the following acceptable alternative:

```
_refine_ls_extinction_expression
'Crystallographic Computing [1970, equation (22), p. 292]'
```

If you need to write a block of text that stretches over more than one line, you must surround it with semicolons as the first character on the first line and trailing line. Here is an example:

```
;
  This is the first of many lines of text.
  This is the second...
;
```

It must be emphasised that the semicolon has to be the *very first* character on the lines on which it occurs (not simply the first non-blank character). Incidentally, it usually does not matter whether the introductory semicolon is on a line by itself, or has text following. The above example could equally well have begun

```
; This is the first...
```

though the *usual* style is to have the text on the same line as the opening semicolon.

Probably the greatest number of syntax problems we see arise because a final semicolon has been omitted from a text field. It's not easy to trap this error, because in principle any text may occur in a text field, so simple parsing software cannot tell that you intended to finish a block of continuous text. Please take especial care that your text fields are properly delimited.

The program *vcif*, available from the IUCr office (details at the end of this *Guide*) may be used to check a CIF against all the syntax rules listed above.

### How to create your CIF

Most of the standard crystallographic refinement packages now have an option allowing them to output their results in CIF format. Usually, the output is a file containing only the results of the refinement. The prospective author will need to augment this by adding details of the experiment, and the text of the commentary if the CIF is to form a submission to *Acta*. In some cases, the output CIF contains the necessary data names, and requires only editing. In other cases, the additional information may be imported from another file. In yet other cases, the author may need to input by hand all the required data names.

As an illustrative example, the program *SHELXL93* (Sheldrick, 1993) will generate a CIF (and a structure-factor listing file, also in CIF format) if the instruction **ACTA** is included in the **.ins** instruction file. The *SHELXL93* distribution also includes an ancillary program, *CIFTAB*, which can resolve unknown data values in the CIF by cross-referencing another file in CIF format – hence the diffractometer operating parameters, for instance, which are not stored in the *SHELXL* program, can be inserted from a master template file containing these parameters.

The *Xtal* program package includes a powerful utility, *CIFIO* (Hall, 1993a), which can input and output data in CIF format. The output file includes a number of data items tagged (with comment lines) as items required in a submission to *Acta*. The *Xtal* program system supplies values for these data items where it is able to do so from the calculations it has performed; the other fields may be edited by hand.

Other large crystallographic software packages have similar facilities.

Some other programs exist that will create CIF output files. For example, *PARSTCIF* (Nardelli, 1995) will take the output from the structural analysis program *PARST* (Nardelli, 1983)

and convert it to CIF form. *PLATON* (Spek, 1990) is another structural analysis program that will produce CIF output.

If all else fails, a standard template can be obtained from the IUCr offices, and manually edited. Provided this is done carefully, the resultant CIF will be entirely suitable for submission of a paper; however, the author choosing this approach must take especial care to check the consistency and integrity of the file contents.

### What should be in a CIF?

A CIF intended for publication in *Acta Cryst.* should meet the guidelines laid down by the IUCr Commission on Journals. These are described in detail in the Notes for Authors, as published *e.g.* in *Acta Cryst.* (1995), C51, 159–174 (and also available online). The most recent copy of the Notes should always be studied before submitting your paper.

Because these requirements try to ensure that the maximum relevant information is recorded, they amount to a formidable list that may daunt the faint-hearted. But here is an example of how CIF can make life easier. If you make a list of the data names given in Appendix 2 of the Notes for Authors, and feed this list to a data extraction program such as *QUASAR*, the program will extract these items from a file that you intend to submit for publication. You can then easily check that they are all present and have reasonable values in the CIF. This is a simple application of the ‘ask and you shall be given’ principle of CIF data transfer.

It’s not even necessary to type up this list: download the file <ftp://ftp.iucr.ac.uk/pub/actac.req> and use this as the request list for *QUASAR*. Here’s an example of how this might work. Suppose you have a file **test.cif** that you propose to submit to *Acta*, and that you have the Commission on Journals request list in a file **actac.req**. Add the following three lines to the top of **actac.req**:

```
star_arc_test.cif
star_out_test.out
data_testblock
```

where ‘*testblock*’ should be replaced by the actual name of the data block containing the information in the CIF. Then run *QUASAR* on this. How you do it is dependent on your operating system, but on a Unix system, you typically type

```
quasar < actac.req
```

The output will appear in the file **test.out**. Provided all the data names in that file take reasonable values, the Commission requirements may be considered as having been met. You may exercise some sensible judgement here: there is no need for **\_exptl\_crystal\_size\_rad** (the crystal radius) to take a value if there are already values for **\_exptl\_crystal\_size\_max**, **\_mid** and **\_min** fields.

These comments refer to the experimental information required in the paper. A complete submission also includes the text of the paper and tables of atomic positions and geometry. Again, the most recent copy of Notes for Authors should be consulted for the exact set of data names required, but at present they are as follows.

Details of the contact author and requested journal:

```
_publ_contact_author
_publ_contact_author_email
_publ_contact_author_fax
_publ_contact_author_phone
_publ_contact_letter
_publ_requested_coeditor_name
_publ_requested_journal
```

The manuscript text information is entered as the data items:

```
_publ_author_name
_publ_author_address
_publ_section_title
_publ_section_abstract
_publ_section_comment
_publ_section_experimental
_publ_section_exptl_prep
_publ_section_exptl_refinement
_publ_section_acknowledgements
_publ_section_references
_publ_section_figure_captions
_publ_section_table_legends
```

Atomic site information is entered as a list of data items. The following items must be supplied:

```
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
```

Additional items can be included where appropriate, *e.g.* site occupancies as **\_atom\_site\_occupancy** or disorder flags as **\_atom\_site\_disorder\_group**.

Structural geometry data (distances and angles) are entered as separate lists, in the data item categories:

```
_geom_bond_*
_geom_contact_*
_geom_angle_*
_geom_torsion_*
```

Each distance or angle value must be tagged with a **\*\_publ\_flag** value of **yes** if it is to be published in a table.

An example of a complete CIF submission is given in Appendix 1; careful study of this example, and comparison with the paper generated from the file and reproduced as Appendix 2, will show how the various components listed above are fitted together.

The complete collection of data names routinely requested by the *Acta* typesetting software is available as the file **request.lst** from the IUCr ftp site.

### Checking if you’ve got it right

This probably still seems like a lot of detail, and indeed it is. However, your CIF generating program will probably attend to most of the details, and once you’ve mastered the trick of creating and completing the CIF once or twice, it should seem quite simple. In order to make it easier still, we’ve established a couple of services that prospective authors are encouraged to use to check the completeness of their paper before submitting it, and to produce a preprint of how the paper will look after the CIF has been processed by the Chester typesetting system. (Indeed, you are free to use these to check and display the contents of any CIF – there is no obligation to publish with *Acta*.) Both these services are accessed by e-mail: you send your CIF to a designated e-mail address, where it is handled entirely automatically, and the results are returned to you. It’s important to realise that this system is completely automatic, so you must send only the CIF in your message – anything else, like an accompanying letter, or even a signature line, will confuse the software. Signature lines are especially tricky, because some mailers automatically append them to your message – you need to figure out how to stop this on your own system.

First send your CIF to the address

**checkcif@iucr.ac.uk**

You should receive back a report describing any syntax errors that were found in the file, and a list of data names found in the file that didn’t match any in the CIF Core Dictionary. Any syntax errors are described fully on their first occurrence, and suggestions are made as to how they might have arisen. You

need to be aware that this check uses only simple syntax rules, and makes no attempt to interpret the data. Consequently, a mistake at one point in the file (especially if it involves missing out a semicolon delimiting a block of text) may only throw up problems in an apparently unconnected part of the file.

The list of data names not found in the Core Dictionary is purely advisory – it is quite legitimate to include your own data names in a CIF. However, this provides a useful check on any ‘official’ data names you intended to include, but mis-spelled.

If the CIF shows no syntax errors, further checks are then carried out to determine whether any Commission requirements need to be fulfilled, and then some numerical checks are performed to ensure the self-consistency of the included data. At this stage, too, the invaluable *MISSYM* program (Le Page, 1988) is run to search for possible higher symmetry in the space-group assignment.

If the **checkcif** report indicates any problem, you should endeavour to fix it, and then you may resend the file to **checkcif** as often as necessary to get it right. When you are happy with the outcome, you might also wish to send the file to the e-mail address

**printcif@iucr.ac.uk**

to obtain a PostScript file representing the paper that *Acta* will publish from your CIF data set. The paper that is returned to you may have portions highlighted: these represent queries that the editorial staff might pose when the paper is submitted; so now is a good time to attend to these potential problems.

If you don’t wish to see these annotations (for instance, if you require a ‘clean’ copy of the paper to obtain approval for publication from your funding authority), place the word ‘**PROOF**’ in the Subject: line of your e-mail message.

At the present time, we can supply **printcif** output only as a PostScript file.

## Using special symbols

It must be remembered that the CIF is primarily a data file, and we have already explained in some detail why it is not appropriate to use the clever facilities of modern word processors to impose a formatting style on the CIF. Nonetheless, it is important to be able to indicate special characters (such as Greek letters, sub- and superscripts, and a few others) for typesetting purposes. We have therefore established a small set of special codes to achieve this. The set has deliberately been kept small to discourage authors from trying to impose any particular style – there are no codes to indicate italic or boldface type, for instance. However, it is intended to be adequate for most purposes. A complete set of current codes will always appear in Notes for Authors. At present, the recognised codes are as follows.

### 1. Greek letters

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

$\alpha$	A	<code>\a</code>	<code>\A</code>	alpha
$\beta$	B	<code>\b</code>	<code>\B</code>	beta
$\chi$	X	<code>\c</code>	<code>\C</code>	chi
$\delta$	$\Delta$	<code>\d</code>	<code>\D</code>	delta
$\epsilon$	E	<code>\e</code>	<code>\E</code>	epsilon
$\varphi$	$\Phi$	<code>\f</code>	<code>\F</code>	phi
$\gamma$	$\Gamma$	<code>\g</code>	<code>\G</code>	gamma
$\eta$	H	<code>\h</code>	<code>\H</code>	eta
$\iota$	I	<code>\i</code>	<code>\I</code>	iota
$\kappa$	K	<code>\k</code>	<code>\K</code>	kappa

$\lambda$	$\Lambda$	<code>\l</code>	<code>\L</code>	lambda
$\mu$	M	<code>\m</code>	<code>\M</code>	mu
$\nu$	N	<code>\n</code>	<code>\N</code>	nu
$o$	O	<code>\o</code>	<code>\O</code>	omicron
$\pi$	$\Pi$	<code>\p</code>	<code>\P</code>	pi
$\theta$	$\Theta$	<code>\q</code>	<code>\Q</code>	theta
$\rho$	R	<code>\r</code>	<code>\R</code>	rho
$\sigma$	$\Sigma$	<code>\s</code>	<code>\S</code>	sigma
$\tau$	T	<code>\t</code>	<code>\T</code>	tau
$\upsilon$	$\Upsilon$	<code>\u</code>	<code>\U</code>	upsilon
$\omega$	$\Omega$	<code>\w</code>	<code>\W</code>	omega
$\xi$	$\Xi$	<code>\x</code>	<code>\X</code>	xi
$\psi$	$\Psi$	<code>\y</code>	<code>\Y</code>	psi
$\zeta$	Z	<code>\z</code>	<code>\Z</code>	zeta

### 2. 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):

<code>\'</code>	acute (é)	<code>\"</code>	umlaut (ü)	<code>\=</code>	overbar (ō)
<code>\`</code>	grave (à)	<code>\~</code>	tilde (ñ)	<code>\.</code>	overdot (ô)
<code>\^</code>	circumflex (â)	<code>\;</code>	ogonek (ś)	<code>\&lt;</code>	hacek (č)
<code>\,</code>	cedilla (ç)	<code>\&gt;</code>	Hungarian umlaut (ő)	<code>\(</code>	breve (ö)

### 3. Other characters

Other special alphabetic characters should be indicated as follows:

<code>\%a</code>	a-ring (â)	<code>\?i</code>	dotless i (i)	<code>\&amp;s</code>	German "ss" (ß)
<code>\/o</code>	o-slash (ø)	<code>\/l</code>	Polish l (ł)	<code>\/d</code>	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	<code>Csp<sup>3</sup></code>	for	<code>Csp<sup>3</sup></code>
subscripts	<code>U<sub>eq</sub></code>	for	<code>U<sub>eq</sub></code>

It’s important to remember the closing symbol, otherwise the rest of your paper may be set as a subscript!

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

<code>\%</code>	degree (°)	<code>\\times</code>	×
<code>--</code>	dash ( <i>e.g.</i> 4–7)	<code>\\neq</code>	≠
<code>---</code>	bond symbol	<code>\\square</code>	□
<code>+-</code>	±	<code>\\rangle</code>	⟩
<code>-+</code>	∓	<code>\\langle</code>	⟨
<code>\\sim</code>	~	<code>\\rightarrow</code>	→
( <i>N.B.</i> ~ is the code for subscript)		<code>\\leftarrow</code>	←
<code>\\simeq</code>	≈	<code>\\infty</code>	∞

### 4. For experts only

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.* `Ueq` would have to be denoted by `U$_{\rm eq}`.

## Adding extra information to your paper

Your paper in *Acta* is built from the request list of CIF data items referred to above (as the file **request.lst**). Usually, if you wish to

add more detail to the paper, you may do this by adding commentary to the free-text fields (such as `_publ_section_comment`). However, if the additional information already exists as a CIF data item, you may direct the typesetting software to add this item to the request list, and thereby incorporate the extra information in the paper. The way to do this is to list the additional data name or names that you want treated this way as values of `'_publ_manuscript_incl_extra_item'`. The example below shows how you may request that the atom site multiplicities and Wyckoff symbols be added to the table of atomic positions. These are data names defined in the Core Dictionary, which may be indicated by supplying `'yes'` as the value of `_publ_manuscript_incl_extra_defn`. Suppose you also wish to include in the paper the value of the magnetic permeability of the crystal, which does not have a standard dictionary definition, but which you always record in your CIFs under a local data name, say `_Smith_crystal_magnetic_perm`. Note that for this item, `_publ_manuscript_incl_extra_defn` takes the value `'no'`. Normally the Chester typesetting software will not be able to handle this, but it may be possible by prior arrangement for us to extract and format this additional data item in future submissions, so long as you continue to list it under `_publ_manuscript_incl_extra_item`.

```
loop_
  _publ_manuscript_incl_extra_item
  _publ_manuscript_incl_extra_defn
  'atom_site_symmetry_multiplicity'  yes
  'atom_site_Wyckoff_symbol'         yes
  '_Smith_crystal_magnetic_perm'      no
```

There are three points to watch when employing this device.

(1) The extra items requested must be surrounded by quote marks, otherwise CIF software will try to interpret them as active data names.

(2) The list is cumulative – if several such loops appear in the file (one per datablock) the request list that is generated will include all the extra items that appear in all of these loops, and that request list will be applied in full to all the datablocks in the file. So it is not possible to ask for an extra item from one datablock but not another.

(3) Not all possible dictionary terms are yet recognised and handled sensibly by our software. Please check what the typesetting system will do with your extra requested items before submitting the paper by using the **printcif** service, described above. If you don't get the desired result, please contact us to explain what needs to be done.

A specific example of the usefulness of this approach is the requirement to print tables of hydrogen bonds. These are not routinely generated, because hydrogen bonding is often unremarkable, but it is convenient to have a mechanism for printing them when they are of interest. In this instance, the author has added comment lines to make the file more readable, though they have no other function. First, the extra items for extraction are identified. (Notice, by the way, that any other extra items that you wish to be printed would be added to this *same* list.)

```
#####
# EXTRA DATA H-BOND INFORMATION
#####
loop_
  _publ_manuscript_incl_extra_item
  _publ_manuscript_incl_extra_info
  _publ_manuscript_incl_extra_defn
#
# New Data Names to Describe Hydrogen Bonding Geometry
# =====
# Name                explanation      standard?
# ----                -
'_geom_bond_atom_site_label_D'  'H-bond donor'      no
'_geom_bond_atom_site_label_H'  'H-bond hydrogen'   no
```

```
'_geom_contact_atom_site_label_A'  'H-bond acceptor'   no
'_geom_bond_distance_DH'           'H-bond D-H'        no
'_geom_contact_distance_HA'        'H-bond H...A'      no
'_geom_contact_distance_DA'        'H-bond D...A'      no
'_geom_angle_DHA'                  'H-bond D-H...A'    no
'_geom_contact_site_symmetry_A'    'symmetry operation' no
```

At some other point in the file, the actual hydrogen-bond data appear, again with a cosmetic set of table headings.

```
loop_
  _geom_bond_atom_site_label_D
  _geom_bond_atom_site_label_H
  _geom_contact_atom_site_label_A
  _geom_bond_distance_DH
  _geom_contact_distance_HA
  _geom_contact_distance_DA
  _geom_angle_DHA
  _geom_contact_site_symmetry_A
#
# Hydrogen bonding scheme
# =====
#
# D      H      A      D-H      H...A      D...A      D-H...A      symm
# -      -      -      -      -      -      -      -
N10     H10    O6      0.95     1.99     2.816(5)    145     3_745
C3      H3      O31     0.95     2.23     2.640(7)    105     .
C4A     H4A     O51     0.95     2.26     2.735(5)    110     .
C7      H7A     O8       0.95     2.19     2.647(7)    109     .
```

*Caution:* the data names in this example, and used for some time in *Acta*, are local names that may be replaced in the future by an alternative set approved by COMCIFS. Consult the most recent version of the Core Dictionary for any approved terms describing hydrogen-bond geometry.

The Chester office is also developing special mechanisms for extra geometry tables, but these are currently discussed with authors on an individual basis. Please contact us for assistance if you wish to experiment with this.

## How to handle multiple structures

Many papers submitted to *Acta C* report the structures of more than one compound. To create a CIF that may be used as the basis for such a paper, we recommend that you concatenate data blocks, each containing all the data for an individual structure, together with an additional data block which contains the material appropriate for the entire paper (mostly the `_publ_items`). Fig. 1 is a skeleton example of how this might be done. The form template distributed from the IUCr office as <ftp://ftp.iucr.ac.uk/pub/form.cif> gives a more complete example.

## Structure-factor listings

*Acta Crystallographica* requires structure-factor listings to be deposited. These may now be supplied as machine-readable files, and the preferred format is, of course, CIF. Because of the large size of reflection data sets, it is best to transfer these as separate files to the IUCr office by ftp (details of the procedure are given in Notes for Authors). Each set of data should be given in a data block using the same code as used in the accompanying CIF (*i.e.* if you have submitted a structure in the CIF data block `data_structure(1)`, store the reflection data in a data block called `data_structure(1)` in the accompanying structure-factors file).

Fig. 2 is a short extract from a *SHELXL93* `.fcf` file, which is ideal for this purpose.

## Submitting a powder paper

At the time of writing, the full mechanism for handling papers in *Acta C* describing the result of a structure determination

```
# ----- Material relevant to the entire paper -----

data_paper
  _publ_section_title
  ; Two dimeric nickel(II) carboxylates
  ;
  loop_
    _publ_author_name
    _publ_author_address
    'Morooka, Mitsuo'
  ; Department of Chemistry
  ...
  ;
  'Ohba, Shigeru'
  ; Department of Chemistry
  ...
  ;
  _publ_section_abstract
  ; The structures of two dimeric NiII carboxylates
  and one dimeric NiII silanecarboxylate have been
  determined. ...
  ;

# ----- Material relevant to the first compound ----

data_(1)
  _chemical_formula_sum          'C34 H54 N2 Ni2 O8'
  _chemical_formula_moiety      'C34 H54 N2 Ni2 O8'
  _chemical_formula_weight      736.2
  _symmetry_cell_setting        monoclinic
  loop_
    _symmetry_equiv_pos_as_xyz
  +x,+y,+z          -x,+y,1/2-z
  -x,-y,-z          +x,-y,1/2+z
  1/2+x,1/2+y,+z    1/2-x,1/2+y,1/2-z
  1/2-x,1/2-y,-z    1/2+x,1/2-y,1/2+z
  _symmetry_space_group_name_H-M 'C 1 2/c 1'
  _cell_length_a      20.520(2)
  _cell_length_b      10.647(1)
  _cell_length_c      18.260(2)
  _cell_angle_alpha   90.00000
  _cell_angle_beta    91.015(8)
  _cell_angle_gamma   90.00000

# --- Material relevant to the second compound ----

data_(2)
  _chemical_formula_sum          'C80 H68 Cl6 N2 Ni2 O8'
  _chemical_formula_moiety
  'C78 H66 N2 Ni2 O8,2(C H Cl3)'
  _chemical_formula_weight      1515.5
  _symmetry_cell_setting        triclinic
  loop_
    _symmetry_equiv_pos_as_xyz
  +x,+y,+z          -x,-y,-z
  _symmetry_space_group_name_H-M 'P -1'
  _cell_length_a      13.231(1)
  _cell_length_b      13.857(1)
  _cell_length_c      11.425(1)
  _cell_angle_alpha   99.48(1)
  _cell_angle_beta    104.63(1)
  _cell_angle_gamma   109.68(1)
```

Fig. 1. Structure of a CIF describing several compounds.

from powder diffraction had not been completely worked out. However, the principles are identical to submission of a single-crystal paper, and the only thing you need to be aware of is the additional set of data items from the powder CIF dictionary that will be specified in the appropriate request list. A file listing these data items will be made available through the IUCr WorldWide Web server, and complete details will be given in Notes for Authors in due course. If you wish to submit a powder paper in the mean time, please contact us for advice.

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared)
# and status flag
#
data_clpl
  _shelx_title 'C8H9CLO'
  _shelx_refl_list_code 4
  _shelx_F_calc_maximum 124.92
  _exptl_crystal_F_000 656.00
  _shelx_F_squared_multiplier 1.000
  loop_
    _refln_index_h
    _refln_index_k
    _refln_index_l
    _refln_F_squared_calc
    _refln_F_squared_meas
    _refln_F_squared_sigma
    _refln_observed_status
  2 0 0 355.77 330.30 34.69 o
  4 0 0 506.58 521.69 20.30 o
  6 0 0 245.80 220.49 18.17 o
```

Fig. 2. Example of structure-factor listing submitted in CIF format.

## Submitting a paper to *Acta B*

Many papers published in *Section B* of *Acta Crystallographica* include crystal structure data, and such data should be supplied in CIF format, following the details in this *Guide*. Normally these CIFs will complement the manuscript, rather than replacing it as in *Section C*, because the more expanded discussion encouraged in *Section B* papers is not well suited to the constraints of a data interchange file. In consequence, the submitted CIFs will contain only the structural data generated directly by the computer program package used, and will require minimal hand editing (though you do need to ensure that they fulfil the complete set of Journals Commission requirements). Notes for Authors of *Section B* provides an up-to-date summary of any special considerations in preparing CIFs for that journal.

## How to read the CIF Dictionary

The standard data names to be understood by all applications are defined in the CIF Dictionary. The original Dictionary was published in the CIF specification paper of Hall, Allen & Brown (1991). An augmented version of these core definitions became available in 1995, and extension dictionaries for powder and macromolecular applications have also become available during 1995. It is a general principle of CIF definitions that they may be added to, but never deleted, so that the original Core Dictionary may continue to be used. However, later versions have been issued in a somewhat different format, so a few words are in order on the formalism of the dictionary. The description applies to the 1995 version.

The dictionaries are available in two formats (obtainable from the IUCr ftp and e-mail server): as a PostScript file and an ASCII file. The PostScript file, when printed, provides a typeset rendering of the information in the dictionary, in a format designed to allow comfortable reading. The ASCII file is itself in a CIF-like form: it is designed to allow a computer program to extract information about the items defined, and hence allow the construction of automatic data validators. It can also be read by humans, but is possibly less convenient. However, the two versions are identical in substance, since the PostScript version is generated automatically from the ASCII file using the same software employed for typesetting CIFs in *Acta Cryst.*

Here are a few examples of definitions from the Core Dictionary, in both formats.

### 1. A simple definition of a well-defined quantity

```
_symmetry_Int_Tables_number (numb)
Space-group number from International Tables for Crystallography,
Vol. A (1987).
[symmetry]
```

Here the data name appears as the headword of the dictionary entry; its *type* (number) is given in parentheses, followed by a textual definition; and its *category* (symmetry) is appended to the entry in square brackets. The category classifies the families of data names described in the dictionary, and defines how data names should be clustered in the CIF.

The formal entry in the master dictionary file looks like this:

```
data_symmetry_Int_Tables_number
  _name      '_symmetry_Int_Tables_number'
  _category  symmetry
  _type      numb
  _definition
; Space-group number from International Tables
  for Crystallography, Vol. A (1987).
;
```

Each data name is described within its own data block. The terms defining and describing the properties of the data name constitute the 'Dictionary Definition Language' or DDL. A full formal description of the DDL can be obtained from the IUCr WWW server. The `_name`, `_category`, `_type` and `_definition` terms fulfil the functions outlined above for the typeset entry.

### 2. A data name that may take a restricted set of values

In this example, a finite set of allowed values (here, character codes) is permitted. The cell setting must be described using one of these codes (this means that, even if the CIF represents a paper written in French or German, the cell setting must be described as 'monoclinic', 'tetragonal' etc.).

```
_symmetry_cell_setting (char)
The cell settings for this space-group symmetry.
triclinic
monoclinic
orthorhombic
tetragonal
rhombohedral
trigonal
hexagonal
cubic
[symmetry]
```

In the DDL representation, the set of permitted values is looped under the data name `_enumeration`:

```
data_symmetry_cell_setting
  _name      '_symmetry_cell_setting'
  _category  symmetry
  _type      char
  loop _enumeration
    triclinic
    monoclinic
    orthorhombic
    tetragonal
    rhombohedral
    trigonal
    hexagonal
    cubic
  _definition
; The cell settings for this space-group symmetry.
;
```

### 3. Looped data

Many data items appear in a looped list. For example, the properties of the atomic sites located within a crystal structure are tabulated under a set of data names beginning `_atom_site_`. Here is an example of one such data item, where the definition also contains information about the range of possible values associated with it.

```
_atom_site_attached_hydrogens (numb)
The number of hydrogen atoms attached to the atom at this site excluding any H atoms for which coordinates (measured or calculated) are given.
Appears in list containing _atom_site_label. Where no value is given, the assumed value is '0'. The permitted range is 0 → 4.
Example(s): '2' (water oxygen), '1' (hydroxyl oxygen), '4' (ammonium nitrogen).
[atom_site]
```

Note how the identification of the list to which this data name belongs is made using the DDL terms `_list` and `_list_reference`. The permitted range of values and the assumed value if none is given are expressed using `_enumeration_range` and `_enumeration_default`.

This definition also contains explanatory examples.

```
data_atom_site_attached_hydrogens
  _name      '_atom_site_attached_hydrogens'
  _category  atom_site
  _type      numb
  _list      yes
  _list_reference '_atom_site_label'
  _enumeration_range  0:4
  _enumeration_default  0
  loop _example
    _example_detail  2  'water oxygen'
                    1  'hydroxyl oxygen'
                    4  'ammonium nitrogen'
  _definition
; The number of hydrogen atoms attached to the atom
  at this site excluding any H atoms for which
  coordinates (measured or calculated) are given.
;
```

### 4. Relationships between loops

The dictionary also contains much essential information on the relationships between data items defined in different entries in the file. Consider the table of bond distances. Each entry in that table requires the labels of the two atoms participating in the bond. These labels are defined in the following way:

```
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2 (char)
The labels of two atom sites that form a bond. These must match labels specified as _atom_site_label in the atom list.
Appears in list as essential element of loop structure. Must match data name _atom_site_label.
[geom_bond]
```

Although the textual definition describes the relationship of these labels to the atom labels used in the table of atomic positions, it is useful for software to be able to check on this relationship, and so the DDL representation of this entry in the dictionary uses `_list_mandatory` to indicate that these items must be present ('appears in list as essential element . . .') if the list is to make any sense; and `_list_link_parent` to

indicate the matching component of the related list. This means, in practice, that a value of `_geom_bond_atom_site_label_1`, for instance, must be identically equal to some value in the `_atom_site_label` list. If an atomic position is described in the atom site list as C2, the atom occupying that position must be labelled in the bond list as C2, and not as C(2), C\_2, Cb or anything else.

```

data_geom_bond_atom_site_label_
loop_ name      '_geom_bond_atom_site_label_1'
      '_geom_bond_atom_site_label_2'
  _category      geom_bond
  _type          char
  _list          yes
  _list_mandatory yes
  _list_link_parent '_atom_site_label'
  _definition
; The labels of two atom sites that form a bond.
  These must match labels specified as
  _atom_site_label in the atom list.
;

```

### Doing it yourself

An earlier section described how the 'printcif' e-mail utility can be used to retrieve a PostScript preprint of the paper you have submitted to *Acta*. Because it is intended to serve this specific function, it is relatively inflexible. We offer two other utilities for formatting CIFs in a preprint-like style.

For systems equipped with a Fortran compiler, a C compiler and the public-domain typesetting system  $\text{\TeX}$ , the IUCr *ciftex* package is available by ftp as <ftp://ftp.iucr.ac.uk/pub/ciftex.tar.Z>. This includes the basic software used in typesetting *Acta*, but without all the additional checking and formatting elements that are available (and updated on a daily basis) through **printcif**. However, it can be used by knowledgeable  $\text{\TeX}$  users to format the paper (or portions thereof) in any style whatsoever. Prospective users are warned, however, that we cannot provide support for modifying the  $\text{\TeX}$  macros supplied.

For users without access to  $\text{\TeX}$ , an earlier utility is available. Again, C and Fortran compilers are needed, but the output is simple ASCII (and only crudely formatted). This may be obtained by ftp as <ftp://ftp.iucr.ac.uk/pub/cifms.shar>. Note that the request lists supplied with this package do not fully match the current ones in use. This package is no longer formally supported by us, but may be of some limited use to some users, and is offered on that basis.

### Additional software for CIFs

We have mentioned already a few of the software packages that create CIFs. The number of programs that can read CIFs is still rather small, despite the potential that the format offers for universal data interchange. Below are the programs that we know about. Software developers are asked to advise us of new CIF-entry programs when they become available.

#### 1. Structure checking and visualization

The *Xtal\_GX* package (Hall, 1995) is a public-domain version of the CIF input/output, graphics, symmetry checking and geometry calculation modules of the *Xtal* system, available in precompiled binary format for a variety of Unix workstations and for IBM-type PC's. The program also checks file syntax and validates data against CIF dictionaries

*PLATON* (Spek, 1990) is a program for Unix workstations that generates a complete listing of the geometry of a crystal structure, creates thermal-ellipsoid plots, checks space-group symmetry and searches for voids in a crystal lattice.

*BUILDER* (Davies, 1995) is a professional program that will check the geometry calculated from the atomic coordinates in a CIF against the geometrical details listed in the file. It allows a complete investigation of the structural geometry, and interconverts between CIF and the internal file format of the Cambridge Structural Database. It is a Unix program. All inquiries regarding this software should be addressed to the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England.

#### 2. Graphics

Most programs that display a graphical representation of a structure described in a CIF also allow some analysis of the structure, but the following programs are primarily for graphical rendering.

*PLUTON* (Spek, 1990) allows stick, ball-and-stick, ball-and-straw or space-filling visualizations of single molecules or cell contents.

*CRYSTINFO* (Bergmann, 1995) is a crystallographic visualizer for the MS-Windows environment.

#### 3. File manipulation utilities

There are a number of utilities for manipulating CIFs, which may be primarily of interest to the programmer.

The *CIFtbx* (Hall, 1993b) library of Fortran subroutines offers a toolbox for Fortran programmers needing to write a CIF input/output interface to existing applications.

*Stargrep* (Kunstleve, 1995) is a small utility for extracting a requested string from a file in STAR format.

*Zinc* (Stampf, 1994) is a facility for converting a CIF into and back from an intermediate format better suited for handling with Unix shell tools such as *grep* or *sed*.

*Star\_Base* (Spadaccini & Hall, 1994) is a powerful program for extracting data from any STAR file, and so is not restricted to CIF applications. It employs a versatile query language to return data in STAR format.

### References

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## APPENDIX 1

### Example of a CIF submission

There is, of course, no such thing as a perfect paper, and so it would be pointless to try to place before you an example of the perfect CIF submission. Nevertheless, it is useful to study a complete CIF as it might be submitted to *Acta Cryst.*, and to compare the file, shown here, with the typeset paper generated from it (and shown in Appendix 2).

Both the CIF and the paper (which is that chosen for illustrative purposes in the *Acta C* Notes for Authors) are annotated to indicate points meriting special attention.

<pre> 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 ; Dr Ulrich Fl"orke   Anorganische und Analytische Chemie   Universit"at-GH Paderborn   Warburgerstr. 100   D-4790 Paderborn   Germany ; _publ_contact_author_email      floe@mvoxac.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 C' # TITLE AND AUTHOR LIST _publ_section_title ; The First Dinuclear Cobalt--Rhenium Cluster Compound:   Hexacarbonylbis(\m-dicyclohexylphosphanido)cobaltrhenium ; loop_   _publ_author_name   _publ_author_address   'Fl"orke, Ulrich' ; Anorganische und Analytische Chemie   Universit"at-GH Paderborn   Warburgerstrasse 100   D-4790 Paderborn   Germany ;   'Haupt, Hans-J"urgen' ; Anorganische und Analytische Chemie   Universit"at-GH Paderborn   Warburgerstrasse 100   D-4790 Paderborn   Germany ; # TEXT _publ_section_abstract ; The title compound [hexacarbonyl-1\k^4C, 2\k^2C-bis(\m-   dicyclohexylphosphido-1:2\k^2P)-cobaltrhenium(Co---Re)] 0.5-   methanol solvate], [CoRe(C^12^H^22^P)^2(CO)^6].0.5CH^3OH,   belongs to a type of edge-linked tetrahedron--octahedron   coordination complex. The molecule has local C^2v symmetry   with eclipsed conformation of the carbonyl ligands at both   metal centres, and a Co---Re single-bond length of 2.786(1) \AA. ; _publ_section_comment ; In the course of our work on phosphanido-bridged homo- and   heteronuclear metal-atom cluster compounds (Haupt, Balsa &amp;   Fl"orke, 1988; Haupt, Heinekamp &amp; Fl"orke, 1989; Fl"orke &amp;   Haupt, 1993), we isolated the title compound (I) in which a </pre>	<p>All CIFs must start with a <code>data_blockcode</code> line. The block code should be no more than 32 characters long.</p> <p>It is valuable to record the origin of the file. Most software CIF generators supply this field automatically.</p> <p><code>_journal_</code> 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.</p> <p>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'.</p> <p>The email address of the contact author is used to acknowledge receipt of the paper.</p> <p>All correspondence relating to the submission should be embedded within the CIF. Supply here any special requirements relating to the presentation of your paper.</p> <p>Give authors' names as 'Surname, Forenames'. Note that names should be given in mixed upper and lower case, not all in capitals.</p> <p>If the paper has several authors, the names and addresses should be looped, as here. If there is only one author, the layout can be</p> <pre>   _publ_author_name      'Fl"orke, Ulrich'   _publ_author_address   ; Anorganische und ...   ; </pre> <p>(i.e. <code>loop_</code> is not required, and entries follow each data name). Sometimes there are additional address details to be published (such as current address). Include these in the <code>_publ_author_address</code> field, separated by a blank line from the normal address, e.g.</p> <pre>   _publ_author_address   ; Anorganische und ...   Germany    Current address: Department of Chemistry ...   ; </pre> <p>Keep line lengths less than 80 characters.</p> <p>The headings in the paper (Abstract, Comment etc.) are automatically generated by the typesetting software. Don't include these headings in your text fields.</p>
---	--

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

```
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 CoReP2-
ring is nearly planar; the maximum deviation from the best
plane is 0.02 Å 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) Å] as well as for Re [2.541(1) and
2.544(1) Å]. 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) Å. 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
[Co2+Re(m3--CC6-H4-Me-4)(CO)10-] (Jeffery, Lewis, Lewis
& Stone, 1985), with Co---Re bond lengths of 2.686(1) and
2.720(1) Å. 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

```
;
```

```
Florke, U. & Haupt, H.-J. (1993). Acta Cryst. C49, 374--376.
```

```
Haupt, H.-J., Balsaa, P. & Florke, U. (1988).
Inorg. Chem. 27, 280--286.
```

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Haupt, H.-J., Heinekamp, C. & Florke, 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.
```

```
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 Re2+(CO)10-,
Co2+(CO)8- and HP(C6-H11)2- (molar ratio 1:1:2) in xylene
solution for 10 h at 423 K in a glass tube. Recrystallization
was from MeOH.
```

#### \_publ\_section\_exptl\_refinement

```
; The enclosed CH3OH solvent molecule had a site occupation
factor of 0.5. Cyclohexyl H atoms were fixed at ideal positions
with common isotropic displacement parameters (Uiso = 0.08
Å2). Structure solution and refinement used SHELXTL-Plus
(Sheldrick, 1990). Other programs include PARST
(Nardelli, 1983).
```

```
#####
```

#### data\_ (I)

```
# CHEMICAL DATA
```

```
_chemical_name_systematic
; [Hexacarbonyl-1-k4C, 2-k2C-bis(m-dicyclohexylphosphido-
1:2-k2P)-cobalt-rhenium(Co---Re)] 0.5-methanol solvate]
;
```

Separate paragraphs in lengthy text fields with a blank line.

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

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.

Use the new 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. The older \_publ\_section\_experimental field may be used if the experimental discussion cannot be categorised in this way.

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_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   '[CoRe(C 12 H 22 P)2(CO)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'

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_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  ?
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_exptl_crystal_F_000      826
_exptl_absorpt_coefficient_mu 4.07
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_exptl_absorpt_correction_T_min 0.690
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# EXPERIMENTAL DATA

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_diffn_measurement_device 'Siemens R3m/V'
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_diffn_reflns_limit_k_max 15
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_diffn_reflns_limit_l_max 21
_diffn_standards_number  4
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_diffn_standards_interval_time ?
_diffn_standards_decay_% 0

# REFINEMENT DATA

_refine_special_details   ?

_reflns_number_total      8161
_reflns_number_observed  6813
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_refine_ls_structure_factor_coef F
_refine_ls_R_factor_obs   0.038
_refine_ls_wR_factor_obs  0.034
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_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_atom_type_scatter_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 items (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_scatter_source` is taken to refer to all atoms. But a preferable layout lists data for each atom species, e.g.

```

loop_
  _atom_type_symbol
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  _atom_type_scatter_dispersion_imag
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C .017 .009
; International Tables for X-ray Crystallography (1974,
  Vol. IV, Table 2.3.1)
;
N .029 .018
; International Tables for X-ray Crystallography (1974,
  Vol. IV, Table 2.3.1)
;

```

```
# ATOMIC COORDINATES AND THERMAL PARAMETERS

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  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_thermal_displace_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
C4 0.1264(7) -0.1761(6) 0.1055(4) 0.062(4) Uani C
O4 0.0725(5) -0.2773(4) 0.0804(3) 0.082(4) Uani O
C5 0.1174(8) 0.2127(6) 0.3180(5) 0.074(5) Uani C
O5 0.0439(7) 0.2631(6) 0.3357(5) 0.132(5) Uani O
C6 0.3598(7) 0.1483(7) 0.3744(4) 0.067(4) Uani C
O6 0.4420(6) 0.1602(6) 0.4263(4) 0.113(5) Uani O
C11 0.5479(6) 0.2618(6) 0.2073(4) 0.056(4) Uani C
C12 0.6243(6) 0.2560(7) 0.1253(4) 0.069(4) Uani C
C13 0.7736(7) 0.2760(8) 0.1443(5) 0.087(6) Uani C
C14 0.8445(8) 0.3902(9) 0.2000(6) 0.095(7) Uani C
C15 0.7702(7) 0.3955(8) 0.2803(5) 0.080(5) Uani C
... ..

loop_
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  _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

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  _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
Co P1 . 2.111(1) yes
Co P2 . 2.116(1) yes
Co C5 . 1.750(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
Re Co P2 60.6(1) yes
P1 Co P2 121.3(1) yes
Re P1 Co 72.9(1) yes
Re P2 Co 72.8(1) yes
... ..

#####
```

Ensure that there are no spaces between values and their e.s.d.'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 form part of the supplementary material accompanying the paper.

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—Coi 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 form part of the supplementary material.

## APPENDIX 2

## Annotated example of a Section C paper

## The First Dinuclear Cobalt–Rhenium Cluster Compound: Hexacarbonylbis( $\mu$ -dicyclohexylphosphanido)cobaltrhenium

ULRICH FLÖRKE AND HANS-JÜRGEN HAUPT

*Anorganische und Analytische Chemie, Universität-GH Paderborn, Warburgerstrasse 100, D-4790 Paderborn, Germany*

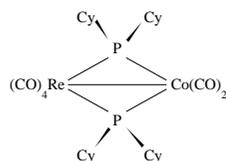
(Received 12 March 1993; accepted 18 May 1993)

### Abstract

The title compound [hexacarbonyl-1 $\kappa^4$ C,2 $\kappa^2$ C-bis( $\mu$ -dicyclohexylphosphido-1:2 $\kappa^2$ P)cobaltrhenium(Co—Re) 0.5-methanol solvate], [CoRe(C<sub>12</sub>H<sub>22</sub>P)<sub>2</sub>(CO)<sub>6</sub>].0.5CH<sub>3</sub>OH, belongs to a type of edge-linked tetrahedron–octahedron coordination complex. The molecule has local C<sub>2v</sub> symmetry with eclipsed conformation of the carbonyl ligands at both metal centres, and a Co—Re single-bond length of 2.786 (1) Å.

### Comment

In the course of our work on phosphanido-bridged homo- and heteronuclear metal-atom cluster compounds (Haupt, Balsaa & Flörke, 1988; Haupt, Heinekamp & Flörke, 1989; Flörke & Haupt, 1993), we isolated the title compound (I) in which a Co—Re bond is symmetrically bridged by two dicyclohexylphosphanido groups.



(I)

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<sub>2</sub> ring is nearly planar; the maximum deviation from the best plane is 0.02 Å 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) Å] as well as for Re [2.541 (1) and 2.544 (1) Å]. 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 title should be concise yet descriptive. It must include the chemical name or the formula. Because all papers in Acta C describe structures, phrases such as 'Structure of' may be omitted.

The authors' names should include the full first name.

The Abstract should contain the full IUPAC chemical name and formula (if it is not present in the title), and basic data which identify the type of chemistry and structure studied. Any special geometry should be highlighted.

The Comment section should start with background information on the chemical, mineralogical and/or crystallographic origins of the material reported. The reasons why the structure was studied should be explained carefully. References to related studies should be included.

A chemical diagram is mandatory for molecular structure studies. This diagram will also be used for the Contents section of the journal (a synopsis will appear in the Contents listings for non-molecular structures).

Only the novel aspects of the structural geometry should be emphasized. These should be related to studies of similar structures and to studies of the compound using other techniques (NMR, IR, etc.). Any unusual geometry should be compared with the standard data listed in §9 of International Tables for Crystallography, Volume C.

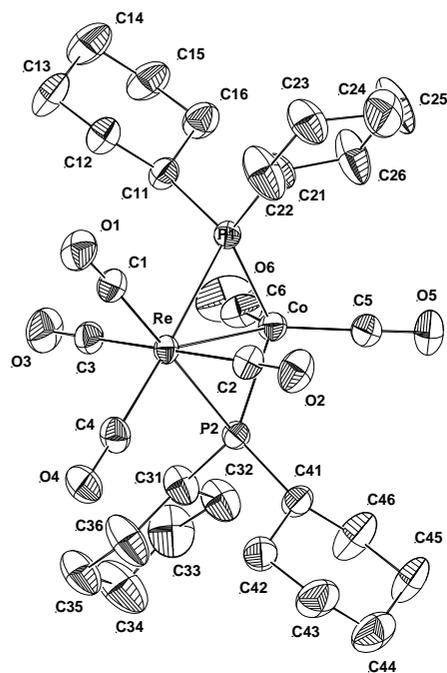


Fig. 1. Molecular structure showing 50% probability displacement ellipsoids. H atoms are omitted for clarity.

A good molecular diagram is essential for a structural paper and it must be oriented to show the most important geometry. The atom labels must be readable when the diagram is reduced to one-column width (80 mm). Labels should clearly identify the atom sites and must match those listed in the table of atom coordinates and  $U$  values. Ellipsoid plots are preferred to line, ball-and-stick or CPK plots because they aid visualization of the atomic displacements and hence provide disorder and thermal-motion information. Unrefined H-atom sites may be omitted, or shown as balls. Distance and angle values should not be placed on the diagram.

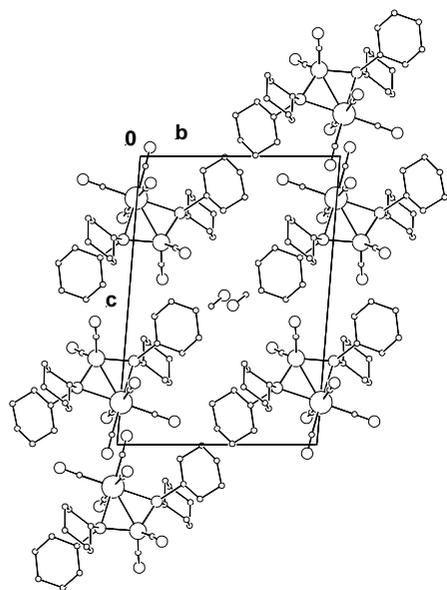


Fig. 2. Packing diagram viewed down the  $a$  axis. Note the solvent molecule in the centre of the cell.

A cell plot is useful if hydrogen bonding, solvent molecules or close van der Waals contacts need to be shown. This diagram can be stylized to emphasize packing information. The orientation of the cell must be displayed with respect to a set of right-handed axes. Hydrogen bonds are normally shown as dashed lines with the donor and acceptor sites suitably labelled.

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) Å. 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<sub>2</sub>Re(μ<sub>3</sub>-CC<sub>6</sub>H<sub>4</sub>Me-4)(CO)<sub>10</sub>] (Jeffery, Lewis, Lewis & Stone, 1985), with Co—Re bond lengths of 2.686 (1) and 2.720 (1) Å. 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 . . .

### Experimental

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

#### Crystal data

[CoRe(C<sub>12</sub>H<sub>22</sub>P)<sub>2</sub>(CO)<sub>6</sub>].-  
0.5CH<sub>3</sub>OH

*M<sub>r</sub>* = 823.7

Triclinic

*P* $\bar{1}$

*a* = 10.452 (3) Å

*b* = 11.664 (4) Å

*c* = 15.641 (4) Å

$\alpha$  = 94.37 (2)°

$\beta$  = 89.75 (2)°

$\gamma$  = 111.87 (2)°

*V* = 1763.8 (8) Å<sup>3</sup>

*Z* = 2

*D<sub>x</sub>* = 1.551 Mg m<sup>-3</sup>

*D<sub>m</sub>* not measured

#### Data collection

Siemens R3m/V diffractometer

$\omega$ -2 $\theta$  scans

Absorption correction:

empirical via  $\psi$  scans

*T<sub>min</sub>* = 0.690, *T<sub>max</sub>* =

0.894

15 189 measured reflections

8161 independent reflections

6813 observed reflections

[*F* > 4σ(*F*)]

#### Refinement

Refinement on *F*

*R* = 0.038

*wR* = 0.034

*S* = 1.583

6813 reflections

379 parameters

H-atom parameters not

refined

Mo K $\alpha$  radiation

$\lambda$  = 0.71073 Å

Cell parameters from 40 reflections

$\theta$  = 7–16°

$\mu$  = 4.07 mm<sup>-1</sup>

*T* = 293 K

Prism

0.50 × 0.34 × 0.28 mm

Red

*R<sub>int</sub>* = 0.022

$\theta_{\max}$  = 27.5°

*h* = -13 → 13

*k* = -15 → 15

*l* = -21 → 21

4 standard reflections

monitored every 400

reflections

intensity decay: none

*w* = 1/[σ<sup>2</sup>(*F*) + 0.0001*F*<sup>2</sup>]

( $\Delta/\sigma$ )<sub>max</sub> = 0.001

$\Delta\rho_{\max}$  = 0.95 e Å<sup>-3</sup>

$\Delta\rho_{\min}$  = -0.80 e Å<sup>-3</sup>

Extinction correction: none

Atomic scattering factors

from *SHELXTL-Plus*

(Sheldrick, 1990)

If there is more than one structure, each experimental data set should be identified with a sequence code [e.g. (1), (2), ... or (I), (II), ...].

A brief summary of the chemical and crystal preparation should be given in sufficient detail to reproduce these aspects of the experiment.

The wavelength  $\lambda$  refers to the radiation used to measure intensities (i.e. mean K $\alpha$  rather than K $\alpha_1$ ).

The absorption coefficient  $\mu$  is in mm<sup>-1</sup> not cm<sup>-1</sup>.

The calculated density, *D<sub>x</sub>*, must be supplied; *D<sub>m</sub>* should be measured if at all possible and details of the method given.

$\theta_{\max}$  refers to the diffraction angle  $\theta$  not 2 $\theta$ .

The absorption transmission factors *T* should range from 0.0 to 1.0. *T<sub>min</sub>* must be ≤ *T<sub>max</sub>*. Co-editors will query *T<sub>max</sub>* values that exceed 1.1, or *T<sub>max</sub>*/*T<sub>min</sub>* ratios that are inappropriate for the crystal under study.

The observed reflection threshold should be as low as possible so as not to bias the structure refinement. Use thresholds of 2σ(*I*) [or 4σ(*F*)], or lower, to ensure that the number of reflections used in the least-squares refinement is as large as possible.

The *R* value is always calculated on *F*, whereas *wR* is calculated with the coefficient used in the least-squares refinement (*F*, *F*<sup>2</sup> or *I*).

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

$$U_{\text{eq}} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i\cdot\mathbf{a}_j.$$

	x	y	z	$U_{\text{eq}}$
Re	0.2227 (1)	-0.0032 (1)	0.1460 (1)	0.042 (1)
Co	0.2347 (1)	0.1392 (1)	0.2992 (1)	0.046 (1)
P1	0.3589 (1)	0.2221 (1)	0.1970 (1)	0.044 (1)
P2	0.1068 (2)	-0.0511 (1)	0.2891 (1)	0.046 (1)
C1	0.3087 (6)	0.0299 (6)	0.0346 (4)	0.057 (4)
O1	0.3569 (5)	0.0449 (5)	-0.0308 (3)	0.079 (3)
C2	0.0662 (6)	0.0396 (6)	0.1118 (4)	0.056 (4)
O2	-0.0268 (5)	0.0626 (5)	0.0927 (3)	0.087 (4)
C3	0.3789 (7)	-0.0423 (6)	0.1896 (4)	0.063 (4)
O3	0.4690 (5)	-0.0639 (5)	0.2137 (4)	0.109 (4)
C4	0.1264 (7)	-0.1761 (6)	0.1055 (4)	0.062 (4)
O4	0.0725 (5)	-0.2773 (4)	0.0804 (3)	0.082 (4)
C5	0.1174 (8)	0.2127 (6)	0.3180 (5)	0.074 (5)
O5	0.0439 (7)	0.2631 (6)	0.3357 (5)	0.132 (5)
C6	0.3598 (7)	0.1483 (7)	0.3744 (4)	0.067 (4)
O6	0.4420 (6)	0.1602 (6)	0.4263 (4)	0.113 (5)
C11	0.5479 (6)	0.2618 (6)	0.2073 (4)	0.056 (4)
C12	0.6243 (6)	0.2560 (7)	0.1253 (4)	0.069 (4)
C13	0.7736 (7)	0.2760 (8)	0.1443 (5)	0.087 (6)
C14	0.8445 (8)	0.3902 (9)	0.2000 (6)	0.095 (7)
C15	0.7702 (7)	0.3955 (8)	0.2803 (5)	0.080 (5)
C16	0.6220 (7)	0.3776 (7)	0.2601 (5)	0.072 (5)
C21	0.3424 (7)	0.3479 (6)	0.1367 (4)	0.066 (4)
C22	0.2909 (12)	0.3202 (8)	0.0493 (5)	0.115 (8)
C23	0.2763 (10)	0.4240 (7)	0.0032 (5)	0.101 (6)
C24	0.2284 (11)	0.5054 (9)	0.0555 (6)	0.136 (8)
C25	0.2913 (13)	0.5398 (8)	0.1420 (6)	0.127 (8)
...	...	...	...	...

Equivalent isotropic displacement parameters are calculated as follows:

From  $U_{ij}$

$$U_{\text{eq}} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i\cdot\mathbf{a}_j.$$

$$B_{\text{eq}} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i\cdot\mathbf{a}_j.$$

From  $B_{ij}$

$$U_{\text{eq}} = (1/24\pi^2)\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i\cdot\mathbf{a}_j.$$

$$B_{\text{eq}} = (1/3)\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i\cdot\mathbf{a}_j.$$

From  $\beta_{ij}$

$$U_{\text{eq}} = (1/6\pi^2)\sum_i\sum_j \beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j.$$

$$B_{\text{eq}} = (4/3)\sum_i\sum_j \beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j.$$

Note that hydrogen-atom data should only be included in the table of coordinates if they have been refined. They will be published at the Co-editor's discretion.

Table 2. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Re—Co	2.786 (1)	Co—P1	2.111 (1)
Re—P1	2.544 (1)	Co—P2	2.116 (1)
Re—P2	2.541 (1)		
Co—Re—P1	46.4 (1)	Re—Co—P2	60.6 (1)
Co—Re—P2	46.5 (1)	P1—Co—P2	121.3 (1)
P1—Re—P2	92.9 (1)	Re—P1—Co	72.9 (1)
Re—Co—P1	60.8 (1)	Re—P2—Co	72.8 (1)

Only geometric data (distances and angles) that need to be drawn to the special attention of the reader should be listed. Torsion angles, intermolecular contact distances and/or deviations from planes that are needed to describe novel features of the structure should be included.

The enclosed  $\text{CH}_3\text{OH}$  solvent molecule had a site occupation factor of 0.5. Cyclohexyl H atoms were fixed at ideal positions with common isotropic displacement parameters ( $U_{\text{iso}} = 0.08 \text{\AA}^2$ ). Structure solution and refinement used *SHELXTL-Plus* (Sheldrick, 1990). Other programs include *PARST* (Nardelli, 1983).

The text of the Experimental section should report specific technical data about the tables and details of the software used in the structure calculation and presentation. These details should be sufficient that, given access to the supplementary data, the presented results could be reproduced.

## References

- Allen, F. H., Ballard, 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.
- Flörke, U. & Haupt, H.-J. (1993). *Acta Cryst.* **C49**, 374–376.
- Haupt, H.-J., Balsaa, P. & Flörke, U. (1988). *Inorg. Chem.* **27**, 280–286.
- Haupt, H.-J., Heinekamp, C. & Flörke, 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.

Reference information must be submitted in the *Acta* style. First and last page numbers are mandatory.

## How to obtain software, documentation and further information

A comprehensive archive of CIF resources is maintained by the IUCr at its Chester office. You can access this most conveniently through a WorldWide Web browser (such as *mosaic* or *Netscape Navigator*), connecting either to the IUCr home page <http://www.iucr.ac.uk/welcome.html>, or to the main CIF information page <http://www.iucr.ac.uk/cif/home.html>.

Most of the software is also available by anonymous ftp to the address [ftp.iucr.ac.uk](ftp://ftp.iucr.ac.uk) (search in the directories `pub` and `cifdics`), or by an e-mail based resource server (for details, send an e-mail containing the word **HELP** to the address [sendcif@iucr.ac.uk](mailto:sendcif@iucr.ac.uk)).

Here is a list (with URLs) of some of the CIF material that is available from our Web server. Connect to <http://www.iucr.ac.uk/cif/home.html> for the most current information.

### General

- Official statement of policy on the use of CIF (as reproduced inside the front cover of this *Guide*) (<http://www.iucr.ac.uk/ipr.html>)
- COMCIFS: list of current members (<http://www.iucr.ac.uk/cif/comcifs/members>)

### Current CIF Dictionaries

- Original CIF Core Dictionary (<ftp://ftp.iucr.ac.uk/pub/cifdic.c91>)
- DDL (Dictionary Definition Language) Dictionary. This is a description of the terms used in the other dictionaries. Version 1.4 (used in the Core and powder dictionaries) (<ftp://ftp.iucr.ac.uk/pub/ddldic.c95>)
- Version 2.0.16 (used in the macromolecular dictionary) (<ftp://ftp.iucr.ac.uk/pub/ddl2.c95>)
- Revised and extended CIF Core (1995 version) (<ftp://ftp.iucr.ac.uk/pub/cifdic.c95>)
- Macromolecular dictionary (<ftp://ftp.iucr.ac.uk/pub/cifdic.m95>)
- Powder dictionary (<ftp://ftp.iucr.ac.uk/pub/cifdic.p95>)

*How to interpret URLs.* The location of the files described above is specified by the WWW Universal Resource Locator string. If you supply this to a WWW browser, you can fetch the file directly. Alternatively, for URLs beginning with **ftp:**, you may connect by anonymous ftp to the machine indicated (normally [ftp.iucr.ac.uk](ftp://ftp.iucr.ac.uk)). Supply the username *anonymous* to log in, and enter your e-mail address when asked for a password. The remainder of the URL specifies the directory (usually **pub**) and file name you require.

### Software tools

- *vcif* syntax checker (compressed tar archive for Unix) (<ftp://ftp.iucr.ac.uk/pub/vcif.tar.Z>)
- *vcif* syntax checker (executable version for MS-DOS) (<ftp://ftp.iucr.ac.uk/pub/vcif.exe>)
- *QUASAR*, a CIF syntax checking and file manipulation tool (<ftp://ftp.iucr.ac.uk/pub/quasar>)
- *CYCLOPS*, a CIF dataname checker (against `cifdic.C91`) (<ftp://ftp.iucr.ac.uk/pub/cyclops>)
- *CIFtbx*, a toolbox of Fortran routines for handling CIF data (<ftp://ftp.iucr.ac.uk/pub/ciftbx>)
- *CIFtex*, the IUCr typesetting tool (compressed tar archive for Unix) [this requires *QUASAR* and  $\text{T}_{\text{E}}\text{X}$ ] (<ftp://ftp.iucr.ac.uk/pub/ciftex.tar.Z>)

### Documentation on CIF

- The original paper describing the CIF standard (<http://www.iucr.ac.uk/cif/standard/cifstd1.html>)
- Description of how *Acta Cryst.* is typeset from CIFs (<http://www.iucr.ac.uk/cif/cifpub.html>)
- Description of the Dictionary Definition Language (DDL) used in CIF dictionaries ([http://www.iucr.ac.uk/cif/ddl\\_brussels.html](http://www.iucr.ac.uk/cif/ddl_brussels.html))

### Publication services

- Notes for Authors of *Acta Crystallographica Section C* ([http://www.iucr.ac.uk/journals/acta/actac\\_notes.html](http://www.iucr.ac.uk/journals/acta/actac_notes.html))
- Notes for Authors of *Acta Crystallographica Section B* ([http://www.iucr.ac.uk/journals/acta/actab\\_notes.html](http://www.iucr.ac.uk/journals/acta/actab_notes.html))
- List of data names forming the Journals Commission requirements for *Acta Crystallographica Section C* (<ftp://ftp.iucr.ac.uk/pub/actac.req>)
- Complete request list of data names extracted in typesetting *Acta Crystallographica Section C* (<ftp://ftp.iucr.ac.uk/pub/request.lst>)

## Checklist for CIF Submission to *Acta*

Based on the most common problems we see.

### Syntax

#### Do's

- Check that the file begins with a `data_` block code.
- Keep all lines shorter than 80 characters.
- Ensure that block codes and data names are no longer than 32 characters.
- Check that character strings with embedded spaces are delimited by correctly balanced quote marks.
- Ensure that text fields have initial and final semicolons as the first character on a line.
- Ensure that superscript (^) or subscript (~) codes occur in pairs.
- Preface each loop header with a `loop_` keyword.
- Ensure that the number of data values in a loop is an exact multiple of the number of data names declared in the header.
- Carefully check spelling of data names used that appear in the CIF Dictionary.
- Use the ASCII character set, with the codes listed in this *Guide* for special symbols.

#### Don'ts

- Don't append signature lines to CIFs submitted by e-mail.
- Don't include *any* additional text before or after a CIF submitted to *Acta* by e-mail.
- Don't duplicate a data name within a data block.
- Don't enter a data name without a value – if you have no information, delete the data name or insert the value ?.
- Don't use unnecessary quote marks around character data.
- Don't break a character string (surrounded by quote marks) over a line.
- Don't put spaces before standard uncertainty values (e.s.d.'s) in numerical data.
- Don't try to indicate bold or italic typeface.
- Don't use ~ to indicate approximately (it's the code for subscript) – use `\\sim`.
- Don't enter accented or other special characters from a word processor.

### Content

#### Do's

- Ensure (as far as possible) that all Commission on Journals requirements are met.
- Give the name *and* address of the contact author in the `_publ_contact_author` field.
- Supply an e-mail address for correspondence in the `_publ_contact_author_email` field.
- Separate each component of the Hermann-Mauguin space-group symbol with a space.
- Format chemical formulae in the `_chemical_formula` fields according to the CIF Dictionary rules.
- Indicate additional fields for publication by use of `_publ_manuscript_incl_extra_item`.
- Separate paragraphs with blank lines.
- Use **yes** or **no** in the `_geom*_publ_flag` fields to indicate which values to print.
- Use the `_publ_section_table_legends` field to list captions for tables *other* than the standard coordinate and geometry tables.
- Enter all references in *Acta* style, separated by blank lines, in the `_publ_section_references` field.
- List all figure captions, separated by blank lines, in the `_publ_section_figure_captions` field. Preface each caption with its number – 'Fig. 1', *etc.*

#### Don'ts

- Don't put several names in a single `_publ_author_name` field, even where they share an address.
- Don't indicate subscripts or superscripts in `_chemical_formula` and `_symmetry_space_group_name` fields.
- Don't forget to state explicitly whether or not the density was measured in the `_exptl_crystal_density_meas` field, and whether or not an extinction correction was made in the `_refine_ls_extinction_method` field.
- Don't add text to indicate the units of quantities – these are defined in the CIF Dictionary.
- Don't put arbitrary text in fields which permit only a fixed set of code words (like `_symmetry_cell_setting`).
- Don't indicate symmetry codes of transformed atoms in the geometry tables by superscripts or 'x,y,z' notation – use the *n\_mmm* convention illustrated in the *Guide*.
- Don't put bond symbols (---) into the geometry loops.
- Don't put headings such as *Abstract*, *Comment*, *etc.* in your text fields; these are generated automatically by the typesetting software.
- Don't use only capital letters in text (especially authors' names) – use normal upper and lower case.