```
##############################################################################
#                                                                            #
#                      Image CIF Dictionary (imgCIF)                         #
#            and Crystallographic Binary File Dictionary (CBF)               #
#           Extending the Macromolecular CIF Dictionary (mmCIF)              #
#                                                                            #
#                              Version 1.5.2                                 #
#                              of 2007-05-07                                 #
#    ##################################################################      #
#    # *** WARNING *** THIS IS A DRAFT FOR DISCUSSSION *** WARNING *** #      #
#    #                  SUBJECT TO CHANGE WITHOUT NOTICE                #      #
#    #     VERSIONS WILL BE POSTED AS cif_img_1.5_DDMMMYY_draft.html    #      #
#    #       SEND COMMENTS TO imgcif-l@iucr.org CITING THE VERSION      #      #
#    ##################################################################      #
#                  This draft edited by H. J. Bernstein                      #
#                                                                            #
#     by Andrew P. Hammersley, Herbert J. Bernstein and John D. Westbrook    #
#                                                                            #
# This dictionary was adapted from format discussed at the imgCIF Workshop,  #
# held at BNL Oct 1997 and the Crystallographic Binary File Format Draft     #
# Proposal by Andrew Hammersley.  The first DDL 2.1 Version was created by   #
# John Westbrook.  This version was drafted by Herbert J. Bernstein and      #
# incorporates comments by I. David Brown, John Westbrook, Brian McMahon,    #
# Bob Sweet, Paul Ellis, Harry Powell, Wilfred Li, Gotzon Madariaga,         #
# Frances C. Bernstein, Chris Nielsen, Nicola Ashcroft and others.           #
##############################################################################

data_cif_img.dic

    _dictionary.title          cif_img.dic
    _dictionary.version        1.5.2
    _dictionary.datablock_id   cif_img.dic

##############################################################################
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#        category  DIFFRN_DETECTOR_AXIS
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#
```

```
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#                  _diffrn_measurement.details
#                  _diffrn_measurement.device
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#                  _diffrn_measurement.id
#                  _diffrn_measurement.method
#                  _diffrn_measurement.number_of_axes
#                  _diffrn_measurement.specimen_support
#
#        category  DIFFRN_MEASUREMENT_AXIS
#
#                  _diffrn_measurement_axis.axis_id
#                  _diffrn_measurement_axis.measurement_device
#                  _diffrn_measurement_axis.measurement_id
#
#        category  DIFFRN_RADIATION
#
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#                  _diffrn_radiation.diffrn_id
#                  _diffrn_radiation.div_x_source
#                  _diffrn_radiation.div_y_source
#                  _diffrn_radiation.div_x_y_source
#                  _diffrn_radiation.filter_edge'
#                  _diffrn_radiation.inhomogeneity
#                  _diffrn_radiation.monochromator
#                  _diffrn_radiation.polarisn_norm
#                  _diffrn_radiation.polarisn_ratio
#                  _diffrn_radiation.polarizn_source_norm
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#
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#
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#                  _diffrn_scan.date_start
#                  _diffrn_scan.integration_time
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#                  _diffrn_scan.frame_id_end
#                  _diffrn_scan.frames
#
#        category  DIFFRN_SCAN_AXIS
#
#                  _diffrn_scan_axis.axis_id
#                  _diffrn_scan_axis.angle_start
#                  _diffrn_scan_axis.angle_range
#                  _diffrn_scan_axis.angle_increment
#                  _diffrn_scan_axis.angle_rstrt_incr
#                  _diffrn_scan_axis.displacement_start
#                  _diffrn_scan_axis.displacement_range
#                  _diffrn_scan_axis.displacement_increment
#                  _diffrn_scan_axis.displacement_rstrt_incr
#                  _diffrn_scan_axis.reference_angle
#                  _diffrn_scan_axis.reference_displacement
#                  _diffrn_scan_axis.scan_id
#
#        category  DIFFRN_SCAN_FRAME
#
#                  _diffrn_scan_frame.date
#                  _diffrn_scan_frame.frame_id
#                  _diffrn_scan_frame.frame_number
#                  _diffrn_scan_frame.integration_time
#                  _diffrn_scan_frame.scan_id
#
#         category  DIFFRN_SCAN_FRAME_AXIS
#
#                  _diffrn_scan_frame_axis.axis_id
#                  _diffrn_scan_frame_axis.angle
#                  _diffrn_scan_frame_axis.angle_increment
#                  _diffrn_scan_frame_axis.angle_rstrt_incr
#                  _diffrn_scan_frame_axis.displacement
#                  _diffrn_scan_frame_axis.displacement_increment
#                  _diffrn_scan_frame_axis.displacement_rstrt_incr
#                  _diffrn_scan_frame_axis.reference_angle
#                  _diffrn_scan_frame_axis.reference_displacement
#                  _diffrn_scan_frame_axis.frame_id
#
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#                  _map.diffrn_id
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#                  _map.id
#
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#                  _map_segment.binary_id
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#                  _map_segment.mask_binary_id
#                  _map_segment.id
#                  _map_segment.map_id
#                  _map_segment.details
#
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#
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#                  _diffrn_measurement_axis.id
#
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#
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#                  _diffrn_frame_data.binary_id
#                  _diffrn_frame_data.detector_element_id
#                  _diffrn_frame_data.id
#                  _diffrn_frame_data.details
#
#
#         ITEM_TYPE_LIST
#         ITEM_UNITS_LIST
#         DICTIONARY_HISTORY
#
##############################################################################


########################
## CATEGORY_GROUP_LIST ##
########################

      loop_
     _category_group_list.id
     _category_group_list.parent_id
     _category_group_list.description
              'inclusive_group'   .
;             Categories that belong to the dictionary extension.
;
             'array_data_group'
             'inclusive_group'
;             Categories that describe array data.
;
             'axis_group'
             'inclusive_group'
;             Categories that describe axes.
;
```

```
            'diffrn_group'
            'inclusive_group'
;           Categories that describe details of the diffraction experiment.
;


##################
## SUB_CATEGORY ##
##################

     loop_
    _sub_category.id
    _sub_category.description
             'matrix'
;             The collection of elements of a matrix.
;
             'vector'
;             The collection of elements of a vector.
;



##############
# ARRAY_DATA #
##############


save_ARRAY_DATA
    _category.description
;    Data items in the ARRAY_DATA category are the containers for
     the array data items described in the category ARRAY_STRUCTURE.
;
    _category.id                   array_data
    _category.mandatory_code       no
     loop_
    _category_key.name             '_array_data.array_id'
                                   '_array_data.binary_id'
    loop_
    _category_group.id             'inclusive_group'
                                   'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;
        Example 1 -

        This example shows two binary data blocks.  The first one
        was compressed by the CBF_CANONICAL compression algorithm and is
        presented as hexadecimal data.  The first character 'H' on the
        data lines means hexadecimal.  It could have been 'O' for octal
        or 'D' for decimal.  The second character on the line shows
        the number of bytes in each word (in this case '4'), which then
        requires eight hexadecimal digits per word.  The third character
        gives the order of octets within a word, in this case '<'
        for the ordering 4321 (i.e. 'big-endian').  Alternatively, the
        character '>' could have been used for the ordering 1234
        (i.e. 'little-endian').  The block has a 'message digest'
        to check the integrity of the data.

        The second block is similar, but uses CBF_PACKED compression
        and BASE64 encoding.  Note that the size and the digest are
        different.
;
;


        loop_
        _array_data.array_id
        _array_data.binary_id
        _array_data.data
        image_1 1
        ;
        --CIF-BINARY-FORMAT-SECTION--
        Content-Type: application/octet-stream;
             conversions="X-CBF_CANONICAL"
        Content-Transfer-Encoding: X-BASE16
        X-Binary-Size: 3927126
        X-Binary-ID: 1
        Content-MD5: u2sTJEovAHkmkDjPi+gWsg==

        # Hexadecimal encoding, byte 0, byte order ...21
        #
        H4< 0050B810 00000000 00000000 00000000 000F423F 00000000 00000000 ...
        ....
        --CIF-BINARY-FORMAT-SECTION----
        ;
        image_2 2
        ;
        --CIF-BINARY-FORMAT-SECTION--
        Content-Type: application/octet-stream;
             conversions="X-CBF-PACKED"
        Content-Transfer-Encoding: BASE64
        X-Binary-Size: 3745758
        X-Binary-ID: 2
        Content-MD5: lzsJjWPfol2GYl2V+QSXrw==

        ELhQAAAAAAAA...
        ...
        --CIF-BINARY-FORMAT-SECTION----
        ;
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
save_


save__array_data.array_id
    _item_description.description
;             This item is a pointer to _array_structure.id in the
              ARRAY_STRUCTURE category.
;
    _item.name                  '_array_data.array_id'
    _item.category_id             array_data
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__array_data.binary_id
    _item_description.description
;             This item is an integer identifier which, along with
              _array_data.array_id, should uniquely identify the
              particular block of array data.

              If _array_data.binary_id is not explicitly given,
              it defaults to 1.

              The value of _array_data.binary_id distinguishes
              among multiple sets of data with the same array
              structure.

              If the MIME header of the data array specifies a
              value for X-Binary-ID, the value of  _array_data.binary_id
              should be equal to the value given for X-Binary-ID.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
             '_array_data.binary_id'            array_data
                                                          implicit
             '_diffrn_data_frame.binary_id'     diffrn_data_frame
                                                        implicit
             '_array_intensities.binary_id'     array_intensities
```

```
                                                        implicit
     loop_
    _item_linked.child_name
    _item_linked.parent_name
             '_diffrn_data_frame.binary_id'     '_array_data.binary_id'
             '_array_intensities.binary_id'     '_array_data.binary_id'

    _item_default.value           1
    _item_type.code               int
     loop_
    _item_range.maximum
    _item_range.minimum
                           1  1
                           .  1
     save_


save__array_data.data
    _item_description.description
;             The value of _array_data.data contains the array data
              encapsulated in a STAR string.

              The representation used is a variant on the
              Multipurpose Internet Mail Extensions (MIME) specified
              in RFC 2045-2049 by N. Freed et al.  The boundary
              delimiter used in writing an imgCIF or CBF is
              '\n--CIF-BINARY-FORMAT-SECTION--' (including the
              required initial '\n--').

              The Content-Type may be any of the discrete types permitted
              in RFC 2045; 'application/octet-stream' is recommended.
              If an octet stream was compressed, the compression should
              be specified by the parameter
                'conversions="X-CBF_PACKED"'
              or the parameter
                'conversions="X-CBF_CANONICAL"'
              or the parameter
                'conversions="X-CBF_BYTE_OFFSET"'

              If the parameter
                'conversions="X-CBF_PACKED"'
              is given it may be further modified with the parameters
                '"uncorrelated_sections"'
              or
                '"flat"'

              If the '"uncorrelated_sections"' parameter is
              given, each section will be compressed without using
              the prior section for averaging.

              If the '"flat"' parameter is given, each the
              image will be treated as one long row.

              The Content-Transfer-Encoding may be 'BASE64',
              'Quoted-Printable', 'X-BASE8', 'X-BASE10',
              'X-BASE16' or 'X-BASE32K', for an imgCIF or 'BINARY'
              for a CBF.  The octal, decimal and hexadecimal transfer
              encodings are provided for convenience in debugging and
              are not recommended for archiving and data interchange.

              In a CIF, one of the parameters 'charset=us-ascii',
              'charset=utf-8' or 'charset=utf-16' may be used on the
              Content-Transfer-Encoding to specify the character set
              used for the external presentation of the encoded data.
              If no charset parameter is given, the character set of
              the enclosing CIF is assumed.  In any case, if a BOM
              flag is detected (FE FF for big-endian UTF-16, FF FE for
              little-endian UTF-16 or EF BB BF for UTF-8) is detected,
              the indicated charset will be assumed until the end of the
              encoded data or the detection of a different BOM.  The
              charset of the Content-Transfer-Encoding is not the character
              set of the encoded data, only the character set of the
              presentation of the encoded data and should be respecified
              for each distinct STAR string.

              In an imgCIF file, the encoded binary data begins after
              the empty line terminating the header.  In an imgCIF file,
              the encoded binary data ends with the terminating boundary
              delimiter '\n--CIF-BINARY-FORMAT-SECTION----'
              in the currently effective charset or with the '\n; '
              that terminates the STAR string.

              In a CBF, the raw binary data begins after an empty line
              terminating the header and after the sequence:

              Octet   Hex   Decimal  Purpose
                0     0C       12    (ctrl-L) Page break
                1     1A       26    (ctrl-Z) Stop listings in MS-DOS
                2     04       04    (Ctrl-D) Stop listings in UNIX
                3     D5      213    Binary section begins

              None of these octets are included in the calculation of
              the message size or in the calculation of the
              message digest.

              The X-Binary-Size header specifies the size of the
              equivalent binary data in octets.  If compression was
              used, this size is the size after compression, including
              any book-keeping fields.  An adjustment is made for
              the deprecated binary formats in which eight bytes of binary
              header are used for the compression type.  In this case,
              the eight bytes used for the compression type are subtracted
              from the size, so that the same size will be reported
              if the compression type is supplied in the MIME header.
              Use of the MIME header is the recommended way to
              supply the compression type.  In general, no portion of
              the  binary header is included in the calculation of the size.

              The X-Binary-Element-Type header specifies the type of
              binary data in the octets, using the same descriptive
              phrases as in _array_structure.encoding_type.  The default
              value is 'unsigned 32-bit integer'.

              An MD5 message digest may, optionally, be used. The 'RSA Data
              Security, Inc. MD5 Message-Digest Algorithm' should be used.
              No portion of the header is included in the calculation of the
              message digest.

              If the Transfer Encoding is 'X-BASE8', 'X-BASE10' or
              'X-BASE16', the data are presented as octal, decimal or
              hexadecimal data organized into lines or words.  Each word
              is created by composing octets of data in fixed groups of
              2, 3, 4, 6 or 8 octets, either in the order ...4321 ('big-
              endian') or 1234... ('little-endian').  If there are fewer
              than the specified number of octets to fill the last word,
              then the missing octets are presented as '==' for each
              missing octet.  Exactly two equal signs are used for each
              missing octet even for octal and decimal encoding.
              The format of lines is:

              rnd xxxxxx xxxxxx xxxxxx

              where r is 'H', 'O' or 'D' for hexadecimal, octal or
              decimal, n is the number of octets per word and d is '<'
              or '>' for the '...4321' and '1234...' octet orderings,
              respectively.  The '==' padding for the last word should
              be on the appropriate side to correspond to the missing
              octets, e.g.

              H4< FFFFFFFF FFFFFFFF 07FFFFFF ====0000

              or

              H3> FF0700 00====
```

```
For these hexadecimal, octal and decimal formats only,
comments beginning with '#' are permitted to improve
readability.

BASE64 encoding follows MIME conventions.  Octets are
in groups of three: c1, c2, c3.  The resulting 24 bits
are broken into four six-bit quantities, starting with
the high-order six bits (c1 >> 2) of the first octet, then
the low-order two bits of the first octet followed by the
high-order four bits of the second octet [(c1 & 3)<<4 | (c2>>4)],
then the bottom four bits of the second octet followed by the
high-order two bits of the last octet [(c2 & 15)<<2 | (c3>>6)],
then the bottom six bits of the last octet (c3 & 63).  Each
of these four quantities is translated into an ASCII character
using the mapping:

          1         2         3         4         5         6
012345678901234567890123456789012345678901234567890123456789012345
|         |         |         |         |         |         |
ABCDEFGHIJKLMNOPQRSTUVWXYZabcdefghijklmnopqrstuvwxyz0123456789+/

With short groups of octets padded on the right with one '='
if c3 is missing, and with '==' if both c2 and c3 are missing.

X-BASE32K encoding is similar to BASE64 encoding, except that
sets of 15 octets are encoded as sets of 8 16-bit unicode
characters, by breaking the 120 bits into 8 15-bit quantities.
256 is added to each 15 bit quantity to bring it into a
printable uncode range.  When encoding, zero padding is used
to fill out the last 15 bit quantity.  If 8 or more bits of
padding are used, a single equals sign (hexadecimal 003D) is
appended.  Embedded whitespace and newlines are introduced
to produce lines of no more than 80 characters each.  On
decoding, all printable ascii characters and ascii whitespace
characters are ignored except for any trailing equals signs.
The number of trailing equals signs indicated the number of
trailing octets to be trimmed from the end of the decoded data.
(see Georgi Darakev, Vassil Litchev, Kostadin Z. Mitev, Herbert
J. Bernstein, 'Efficient Support of Binary Data in the XML
Implementation of the NeXus File Format',absract W0165,
ACA Summer Meeting, Honolulu, HI, July 2006).

QUOTED-PRINTABLE encoding also follows MIME conventions, copying
octets without translation if their ASCII values are 32...38,
42, 48...57, 59, 60, 62, 64...126 and the octet is not a ';'
in column 1.  All other characters are translated to =nn, where
nn is the hexadecimal encoding of the octet.  All lines are
'wrapped' with a terminating '=' (i.e. the MIME conventions
for an implicit line terminator are never used).

The "X-Binary-Element-Byte-Order" can specify either
'"BIG_ENDIAN"' or '"LITTLE_ENDIAN"' byte order of the imaage
data.  Only LITTLE_ENDIAN is recommended.  Processors
may treat BIG_ENDIAN as a warning of data that can
only be processed by special software.

The "X-Binary-Number-of-Elements" specifies the number of
elements (not the number of octets) in the decompressed, decoded
image.

The optional "X-Binary-Size-Fastest-Dimension" specifies the
number of elements (not the number of octets) in one row of the
fastest changing dimension of the binary data array. This
information must be in the MIME header for proper operation of
some of the decompression algorithms.

The optional "X-Binary-Size-Second-Dimension" specifies the
number of elements (not the number of octets) in one column of
the second-fastest changing dimension of the binary data array.
This information must be in the MIME header for proper operation
of some of the decompression algorithms.

            The optional "X-Binary-Size-Third-Dimension" specifies the number
            of sections for the third-fastest changing dimension of the
            binary data array.

            The optional "X-Binary-Size-Padding" specifies the size in
            octets of an optional padding after the binary array data and
            before the closing flags for a binary section.
;
    _item.name                  '_array_data.data'
    _item.category_id             array_data
    _item.mandatory_code          yes
    _item_type.code               binary
save_


#####################
# ARRAY_ELEMENT_SIZE #
#####################


save_ARRAY_ELEMENT_SIZE
    _category.description
;    Data items in the ARRAY_ELEMENT_SIZE category record the physical
     size of array elements along each array dimension.
;
    _category.id                   array_element_size
    _category.mandatory_code       no
     loop_
    _category_key.name             '_array_element_size.array_id'
                                   '_array_element_size.index'
    loop_
    _category_group.id             'inclusive_group'
                                   'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;       Example 1 - A regular 2D array with a uniform element dimension
                    of 1220 nanometres.
;
;
       loop_
      _array_element_size.array_id
      _array_element_size.index
      _array_element_size.size
       image_1   1    1.22e-6
       image_1   2    1.22e-6
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_


save__array_element_size.array_id
    _item_description.description
;             This item is a pointer to _array_structure.id in the
              ARRAY_STRUCTURE category.
;
    _item.name                  '_array_element_size.array_id'
    _item.category_id             array_element_size
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__array_element_size.index
    _item_description.description
;             This item is a pointer to _array_structure_list.index in
              the ARRAY_STRUCTURE_LIST category.
;
    _item.name                  '_array_element_size.index'
    _item.category_id             array_element_size
```

```
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__array_element_size.size
    _item_description.description
;               The size in metres of an image element in this
                dimension. This supposes that the elements are arranged
                on a regular grid.
;
    _item.name               '_array_element_size.size'
    _item.category_id          array_element_size
    _item.mandatory_code       yes
    _item_type.code            float
    _item_units.code           'metres'
     loop_
    _item_range.maximum
    _item_range.minimum
                             .   0.0
     save_


####################
# ARRAY_INTENSITIES #
####################


save_ARRAY_INTENSITIES
    _category.description
;               Data items in the ARRAY_INTENSITIES category record the
                information required to recover the intensity data from
                the set of data values stored in the ARRAY_DATA category.

                The detector may have a complex relationship
                between the raw intensity values and the number of
                incident photons.  In most cases, the number stored
                in the final array will have a simple linear relationship
                to the actual number of incident photons, given by
                _array_intensities.gain.  If raw, uncorrected values
                are presented (e.g. for calibration experiments), the
                value of _array_intensities.linearity will be 'raw'
                and _array_intensities.gain will not be used.

;
    _category.id                   array_intensities
    _category.mandatory_code       no
    loop_
    _category_key.name             '_array_intensities.array_id'
                                   '_array_intensities.binary_id'
    loop_
    _category_group.id             'inclusive_group'
                                   'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;
        Example 1
;
;
        loop_
        _array_intensities.array_id
        _array_intensities.linearity
        _array_intensities.gain
        _array_intensities.overload
        _array_intensities.undefined_value
        _array_intensities.pixel_fast_bin_size
        _array_intensities.pixel_slow_bin_size
        _array_intensities.pixel_binning_method
        image_1   linear  1.2    655535   0   2   2    hardware
;
```

```
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_


save__array_intensities.array_id
    _item_description.description
;               This item is a pointer to _array_structure.id in the
                ARRAY_STRUCTURE category.
;
    _item.name                  '_array_intensities.array_id'
    _item.category_id             array_intensities
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__array_intensities.binary_id
    _item_description.description
;               This item is a pointer to _array_data.binary_id in the
                ARRAY_DATA category.
;
    _item.name                  '_array_intensities.binary_id'
    _item.category_id             array_intensities
    _item.mandatory_code          implicit
    _item_type.code               int
     save_


save__array_intensities.gain
    _item_description.description
;                Detector 'gain'. The factor by which linearized
                 intensity count values should be divided to produce
                 true photon counts.
;
    _item.name               '_array_intensities.gain'
    _item.category_id          array_intensities
    _item.mandatory_code       yes
    _item_type.code            float
     loop_
    _item_range.maximum
    _item_range.minimum
                             .   0.0
    _item_units.code           'counts_per_photon'
     loop_
    _item_related.related_name
    _item_related.function_code  '_array_intensities.gain_esd'
                                 'associated_value'
    save_


save__array_intensities.gain_esd
    _item_description.description
;             The estimated standard deviation in detector 'gain'.
;
    _item.name               '_array_intensities.gain_esd'
    _item.category_id          array_intensities
    _item.mandatory_code       yes
    _item_type.code            float
     loop_
    _item_range.maximum
    _item_range.minimum
                             .   0.0

    _item_units.code           'counts_per_photon'
     loop_
    _item_related.related_name
    _item_related.function_code  '_array_intensities.gain'
                                 'associated_esd'
    save_


save__array_intensities.linearity
```

```
    _item_description.description
;               The intensity linearity scaling method used to convert
                from the raw intensity to the stored element value:

                'linear' is linear.

                'offset'  means that the value defined by
                _array_intensities.offset should be added to each
                 element value.

                'scaling' means that the value defined by
                _array_intensities.scaling should be multiplied with each
                element value.

                'scaling_offset' is the combination of the two previous cases,
                with the scale factor applied before the offset value.

                'sqrt_scaled' means that the square root of raw
                intensities multiplied by _array_intensities.scaling is
                calculated and stored, perhaps rounded to the nearest
                integer. Thus, linearization involves dividing the stored
                values by _array_intensities.scaling and squaring the
                result.

                'logarithmic_scaled' means that the logarithm base 10 of
                raw intensities multiplied by _array_intensities.scaling
                is calculated and stored, perhaps rounded to the nearest
                integer. Thus, linearization involves dividing the stored
                values by _array_intensities.scaling and calculating 10
                to the power of this number.

                'raw' means that the data are a set of raw values straight
                from the detector.
;

    _item.name               '_array_intensities.linearity'
    _item.category_id          array_intensities
    _item.mandatory_code       yes
    _item_type.code            code
     loop_
    _item_enumeration.value
    _item_enumeration.detail
                               'linear' .
                               'offset'
;               The value defined by  _array_intensities.offset should
                be added to each element value.
;
                               'scaling'
;               The value defined by _array_intensities.scaling should be
                multiplied with each element value.
;
                               'scaling_offset'
;               The combination of the scaling and offset
                with the scale factor applied before the offset value.
;
                               'sqrt_scaled'
;               The square root of raw intensities multiplied by
                _array_intensities.scaling is calculated and stored,
                perhaps rounded to the nearest integer. Thus,
                linearization involves dividing the stored
                values by _array_intensities.scaling and squaring the
                result.
;
                               'logarithmic_scaled'
;               The logarithm base 10 of raw intensities multiplied by
                _array_intensities.scaling  is calculated and stored,
                perhaps rounded to the nearest integer. Thus,
                linearization involves dividing the stored values by
                _array_intensities.scaling and calculating 10 to the
                power of this number.
;
                               'raw'
;               The array consists of raw values to which no corrections have
                been applied.  While the handling of the data is similar to
                that given for 'linear' data with no offset, the meaning of
                the data differs in that the number of incident photons is
                not necessarily linearly related to the number of counts
                reported.  This value is intended for use either in
                calibration experiments or to allow for handling more
                complex data-fitting algorithms than are allowed for by
                this data item.
;

    save_


save__array_intensities.offset
    _item_description.description
;               Offset value to add to array element values in the manner
                described by the item _array_intensities.linearity.
;
    _item.name                 '_array_intensities.offset'
    _item.category_id          array_intensities
    _item.mandatory_code       no
    _item_type.code            float
    save_


save__array_intensities.overload
    _item_description.description
;               The saturation intensity level for this data array.
;
    _item.name                 '_array_intensities.overload'
    _item.category_id          array_intensities
    _item.mandatory_code       no
    _item_type.code            float
    _item_units.code          'counts'
    save_


save__array_intensities.pixel_fast_bin_size
    _item_description.description
;               The value of _array_intensities.pixel_fast_bin_size specifies
                the number of pixels that compose one element in the direction
                of the most rapidly varying array dimension.

                Typical values are 1, 2, 4 or 8.  When there is 1 pixel per
                array element in both directions, the value given for
                _array_intensities.pixel_binning_method normally should be
                'none'.

                It is specified as a float to allow for binning algorithms that
                create array elements that are not integer multiples of the
                detector pixel size.
;
    _item.name               '_array_intensities.pixel_fast_bin_size'
    _item.category_id          array_intensities
    _item.mandatory_code       implicit
    _item_type.code            float
    _item_default.value        1.
     loop_
    _item_range.maximum
    _item_range.minimum
                               .   0.0
    _item_units.code           'pixels_per_element'
    save_


save__array_intensities.pixel_slow_bin_size
    _item_description.description
;               The value of _array_intensities.pixel_slow_bin_size specifies
                the number of pixels that compose one element in the direction
                of the second most rapidly varying array dimension.
```

```
                Typical values are 1, 2, 4 or 8.  When there is 1 pixel per
                array element in both directions, the value given for
                _array_intensities.pixel_binning_method normally should be
                'none'.

                It is specified as a float to allow for binning algorithms that
                create array elements that are not integer multiples of the
                detector pixel size.
;
    _item.name              '_array_intensities.pixel_slow_bin_size'
    _item.category_id          array_intensities
    _item.mandatory_code       implicit
    _item_type.code            float
    _item_default.value        1.
     loop_
    _item_range.maximum
    _item_range.minimum
                           .   0.0
    _item_units.code           'pixels_per_element'
    save_


save__array_intensities.pixel_binning_method
    _item_description.description
;               The value of _array_intensities.pixel_binning_method specifies
                the method used to derive array elements from multiple pixels.
;
    _item.name              '_array_intensities.pixel_binning_method'
    _item.category_id          array_intensities
    _item.mandatory_code       implicit
    _item_type.code            code
     loop_
    _item_enumeration.value
    _item_enumeration.detail
                               'hardware'
;               The element intensities were derived from the raw data of one
                or more pixels by used of hardware in the detector, e.g. by use
                of shift registers in a CCD to combine pixels into super-pixels.
;
                               'software'
;               The element intensities were derived from the raw data of more
                than one pixel by use of software.
;
                               'combined'
;               The element intensities were derived from the raw data of more
                than one pixel by use of both hardware and software, as when
                hardware binning is used in one direction and software in the
                other.
;
                               'none'
;               In the both directions, the data has not been binned.  The
                number of pixels is equal to the number of elements.

                When the value of _array_intensities.pixel_binning_method is
                'none' the values of _array_intensities.pixel_fast_bin_size
                and _array_intensities.pixel_slow_bin_size both must be 1.
;
                               'unspecified'
;               The method used to derive element intensities is not specified.
;
    _item_default.value        'unspecified'
    save_

save__array_intensities.scaling
    _item_description.description
;               Multiplicative scaling value to be applied to array data
                in the manner described by item
                _array_intensities.linearity.
;
    _item.name                 '_array_intensities.scaling'
    _item.category_id          array_intensities
    _item.mandatory_code       no
    _item_type.code            float
    save_



save__array_intensities.undefined_value
    _item_description.description
;               A value to be substituted for undefined values in
                the data array.
;
    _item.name                 '_array_intensities.undefined_value'
    _item.category_id          array_intensities
    _item.mandatory_code       no
    _item_type.code            float
    save_


##################
# ARRAY_STRUCTURE #
##################


save_ARRAY_STRUCTURE
    _category.description
;    Data items in the ARRAY_STRUCTURE category record the organization and
     encoding of array data that may be stored in the ARRAY_DATA category.
;
    _category.id                   array_structure
    _category.mandatory_code       no
    _category_key.name             '_array_structure.id'
    loop_
    _category_group.id             'inclusive_group'
                                   'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 -
;
;
     loop_
    _array_structure.id
    _array_structure.encoding_type
    _array_structure.compression_type
    _array_structure.byte_order
     image_1       "unsigned 16-bit integer"  none  little_endian
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_


save__array_structure.byte_order
    _item_description.description
;               The order of bytes for integer values which require more
                than 1 byte.

                (IBM-PC's and compatibles and DEC VAXs use low-byte-first
                ordered integers, whereas Hewlett Packard 700
                series, Sun-4 and Silicon Graphics use high-byte-first
                ordered integers.  DEC Alphas can produce/use either
                depending on a compiler switch.)
;

    _item.name                    '_array_structure.byte_order'
    _item.category_id              array_structure
    _item.mandatory_code           yes
    _item_type.code                ucode
     loop_
    _item_enumeration.value
    _item_enumeration.detail
                                   'big_endian'
;       The first byte in the byte stream of the bytes which make up an
```

```
        integer value is the most significant byte of an integer.
;
                                 'little_endian'
;       The last byte in the byte stream of the bytes which make up an
        integer value is the most significant byte of an integer.
;
     save_


save__array_structure.compression_type
    _item_description.description
;             Type of data-compression method used to compress the array
              data.
;
    _item.name                   '_array_structure.compression_type'
    _item.category_id             array_structure
    _item.mandatory_code          no
    _item_type.code               ucode
    _item_default.value           'none'
     loop_
    _item_enumeration.value
    _item_enumeration.detail
                                 'byte_offset'
;       Using the 'byte_offset' compression scheme as per A. Hammersley
        and the CBFlib manual, section 3.3.3
;
                                 'canonical'
;       Using the 'canonical' compression scheme (International Tables
        for Crystallography Volume G, Section 5.6.3.1) and CBFlib
        manual section 3.3.1
;
                                 'none'
;       Data are stored in normal format as defined by
        _array_structure.encoding_type and
        _array_structure.byte_order.
;
                                 'packed'
;       Using the 'packed' compression scheme, a CCP4-style packing
        as per J. P. Abrahams pack_c.c and CBFlib manual, section 3.3.2.
;
                                 'packed_v2'
;       Using the 'packed' compression scheme, version 2, as per
        J. P. Abrahams pack_c.c and CBFlib manual, section 3.3.2.
;
    save_

save__array_structure.compression_type_flag
    _item_description.description
;             Flags modifying the type of data-compression method used to
              compress the arraydata.
;
    _item.name                   '_array_structure.compression_type_flag'
    _item.category_id             array_structure
    _item.mandatory_code          no
    _item_type.code               ucode
     loop_
    _item_enumeration.value
    _item_enumeration.detail
                                 'uncorrelated_sections'
;       When applying packed or packed_v2 compression on an array with
        uncorrelated sections, do not average in points from the prior
        section.
;
                                 'flat'
;       When applying packed or packed_v2 compression on an array with
        treat the entire image as a single line set the maximum number
        of bits for an offset to 65 bits.

        The flag is included for compatibility with software prior to
        CBFlib_0.7.7, and should not be used for new data sets.

;
```

```
    save_

save__array_structure.encoding_type
    _item_description.description
;               Data encoding of a single element of array data.

                In several cases, the IEEE format is referenced.
                See IEEE Standard 754-1985 (IEEE, 1985).

                Ref: IEEE (1985). IEEE Standard for Binary Floating-Point
                Arithmetic. ANSI/IEEE Std 754-1985. New York: Institute of
                Electrical and Electronics Engineers.
;

    _item.name                 '_array_structure.encoding_type'
    _item.category_id           array_structure
    _item.mandatory_code        yes
    _item_type.code             uline
     loop_
    _item_enumeration.value
                               'unsigned 8-bit integer'
                               'signed 8-bit integer'
                               'unsigned 16-bit integer'
                               'signed 16-bit integer'
                               'unsigned 32-bit integer'
                               'signed 32-bit integer'
                               'signed 32-bit real IEEE'
                               'signed 64-bit real IEEE'
                               'signed 32-bit complex IEEE'
     save_


save__array_structure.id
    _item_description.description
;             The value of _array_structure.id must uniquely identify
              each item of array data.
;
    loop_
    _item.name
    _item.category_id
    _item.mandatory_code
             '_array_structure.id'              array_structure      yes
             '_array_data.array_id'             array_data           yes
             '_array_structure_list.array_id'   array_structure_list yes
             '_array_intensities.array_id'      array_intensities    yes
             '_diffrn_data_frame.array_id'      diffrn_data_frame    yes


    _item_type.code              code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
             '_array_data.array_id'             '_array_structure.id'
             '_array_structure_list.array_id'   '_array_structure.id'
             '_array_intensities.array_id'      '_array_structure.id'
             '_diffrn_data_frame.array_id'      '_array_structure.id'

     save_


########################
# ARRAY_STRUCTURE_LIST #
########################


save_ARRAY_STRUCTURE_LIST
    _category.description
;    Data items in the ARRAY_STRUCTURE_LIST category record the size
     and organization of each array dimension.

     The relationship to physical axes may be given.
```

```
;
    _category.id                    array_structure_list
    _category.mandatory_code        no
     loop_
    _category_key.name              '_array_structure_list.array_id'
                                    '_array_structure_list.index'
    loop_
    _category_group.id              'inclusive_group'
                                    'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;       Example 1 - An image array of 1300 x 1200 elements.  The raster
                    order of the image is left to right (increasing) in the
                    first dimension and bottom to top (decreasing) in
                    the second dimension.
;
;
       loop_
       _array_structure_list.array_id
       _array_structure_list.index
       _array_structure_list.dimension
       _array_structure_list.precedence
       _array_structure_list.direction
       _array_structure_list.axis_set_id
        image_1   1    1300    1     increasing  ELEMENT_X
        image_1   2    1200    2     decreasing  ELEMENY_Y
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_


save__array_structure_list.array_id
    _item_description.description
;             This item is a pointer to _array_structure.id in the
              ARRAY_STRUCTURE category.
;
    _item.name                  '_array_structure_list.array_id'
    _item.category_id             array_structure_list
    _item.mandatory_code          yes
    _item_type.code               code
save_


save__array_structure_list.axis_set_id
    _item_description.description
;               This is a descriptor for the physical axis or set of axes
                corresponding to an array index.

                This data item is related to the axes of the detector
                itself given in DIFFRN_DETECTOR_AXIS, but usually differs
                in that the axes in this category are the axes of the
                coordinate system of reported data points, while the axes in
                DIFFRN_DETECTOR_AXIS are the physical axes
                of the detector describing the 'poise' of the detector as an
                overall physical object.

                If there is only one axis in the set, the identifier of
                that axis should be used as the identifier of the set.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
           '_array_structure_list.axis_set_id'
                                array_structure_list            yes
           '_array_structure_list_axis.axis_set_id'
                                array_structure_list_axis       implicit
    _item_type.code               code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
          '_array_structure_list_axis.axis_set_id'
                                '_array_structure_list.axis_set_id'


     save_


save__array_structure_list.dimension
    _item_description.description
;               The number of elements stored in the array structure in this
                dimension.
;
    _item.name                '_array_structure_list.dimension'
    _item.category_id          array_structure_list
    _item.mandatory_code       yes
    _item_type.code            int
     loop_
    _item_range.maximum
    _item_range.minimum
                               1  1
                               .  1
     save_


save__array_structure_list.direction
    _item_description.description
;              Identifies the direction in which this array index changes.
;
    _item.name                '_array_structure_list.direction'
    _item.category_id          array_structure_list
    _item.mandatory_code       yes
    _item_type.code            code
     loop_
    _item_enumeration.value
    _item_enumeration.detail

                               'increasing'
;         Indicates the index changes from 1 to the maximum dimension.
;
                               'decreasing'
;         Indicates the index changes from the maximum dimension to 1.
;
     save_


save__array_structure_list.index
    _item_description.description
;               Identifies the one-based index of the row or column in the
                array structure.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
           '_array_structure_list.index'        array_structure_list   yes
           '_array_structure_list.precedence'   array_structure_list   yes
           '_array_element_size.index'          array_element_size     yes

    _item_type.code            int

     loop_
    _item_linked.child_name
    _item_linked.parent_name
          '_array_element_size.index'         '_array_structure_list.index'
     loop_
    _item_range.maximum
    _item_range.minimum
                               1  1
                               .  1
     save_
```

```
save__array_structure_list.precedence
    _item_description.description
;               Identifies the rank order in which this array index changes
                with respect to other array indices.  The precedence of 1
                indicates the index which changes fastest.
;
    _item.name                 '_array_structure_list.precedence'
    _item.category_id           array_structure_list
    _item.mandatory_code        yes
    _item_type.code             int
     loop_
    _item_range.maximum
    _item_range.minimum
                             1  1
                             .  1
     save_


############################
# ARRAY_STRUCTURE_LIST_AXIS #
############################

save_ARRAY_STRUCTURE_LIST_AXIS
    _category.description
;    Data items in the ARRAY_STRUCTURE_LIST_AXIS category describe
     the physical settings of sets of axes for the centres of pixels that
     correspond to data points described in the
     ARRAY_STRUCTURE_LIST category.

     In the simplest cases, the physical increments of a single axis correspond
     to the increments of a single array index.  More complex organizations,
     e.g. spiral scans, may require coupled motions along multiple axes.

     Note that a spiral scan uses two coupled axes: one for the angular
     direction and one for the radial direction.  This differs from a
     cylindrical scan for which the two axes are not coupled into one set.
;
    _category.id                    array_structure_list_axis
    _category.mandatory_code        no
     loop_
    _category_key.name
                                   '_array_structure_list_axis.axis_set_id'
                                   '_array_structure_list_axis.axis_id'
     loop_
    _category_group.id             'inclusive_group'
                                   'array_data_group'
     save_


save__array_structure_list_axis.axis_id
    _item_description.description
;               The value of this data item is the identifier of one of
                the axes in the set of axes for which settings are being
                specified.

                Multiple axes may be specified for the same value of
                _array_structure_list_axis.axis_set_id.

                This item is a pointer to _axis.id in the
                AXIS category.
;
    _item.name                 '_array_structure_list_axis.axis_id'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       yes
    _item_type.code            code
     save_


save__array_structure_list_axis.axis_set_id
    _item_description.description
;               The value of this data item is the identifier of the
                set of axes for which axis settings are being specified.

                Multiple axes may be specified for the same value of
                _array_structure_list_axis.axis_set_id.

                This item is a pointer to
                _array_structure_list.axis_set_id
                in the ARRAY_STRUCTURE_LIST category.

                If this item is not specified, it defaults to the corresponding
                axis identifier.
;
    _item.name                 '_array_structure_list_axis.axis_set_id'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       implicit
    _item_type.code            code
     save_


save__array_structure_list_axis.angle
    _item_description.description
;               The setting of the specified axis in degrees for the first
                data point of the array index with the corresponding value
                of _array_structure_list.axis_set_id.  If the index is
                specified as 'increasing', this will be the centre of the
                pixel with index value 1.  If the index is specified as
                'decreasing', this will be the centre of the pixel with
                maximum index value.
;
    _item.name                 '_array_structure_list_axis.angle'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'degrees'
     save_


save__array_structure_list_axis.angle_increment
    _item_description.description
;               The pixel-centre-to-pixel-centre increment in the angular
                setting of the specified axis in degrees.  This is not
                meaningful in the case of 'constant velocity' spiral scans
                and should not be specified for this case.

                See _array_structure_list_axis.angular_pitch.

;
    _item.name                 '_array_structure_list_axis.angle_increment'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'degrees'
     save_


save__array_structure_list_axis.displacement
    _item_description.description
;               The setting of the specified axis in millimetres for the first
                data point of the array index with the corresponding value
                of _array_structure_list.axis_set_id.  If the index is
                specified as 'increasing', this will be the centre of the
                pixel with index value 1.  If the index is specified as
                'decreasing', this will be the centre of the pixel with
                maximum index value.
;
    _item.name                '_array_structure_list_axis.displacement'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
```

```
    _item_units.code           'millimetres'
     save_

save__array_structure_list_axis.fract_displacement
    _item_description.description
;               The setting of the specified axis as a decimal fraction of
                the axis unit vector for the first data point of the array
                index with the corresponding value of
                _array_structure_list.axis_set_id.
                If the index is specified as 'increasing', this will be the
                centre of the pixel with index value 1.  If the index is
                specified as 'decreasing', this will be the centre of the
                pixel with maximum index value.
;
    _item.name               '_array_structure_list_axis.fract_displacement'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
     save_

save__array_structure_list_axis.displacement_increment
    _item_description.description
;               The pixel-centre-to-pixel-centre increment for the displacement
                setting of the specified axis in millimetres.
;
    _item.name
        '_array_structure_list_axis.displacement_increment'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'millimetres'
     save_

save__array_structure_list_axis.fract_displacement_increment
    _item_description.description
;               The pixel-centre-to-pixel-centre increment for the displacement
                setting of the specified axis as a decimal fraction of the
                axis unit vector.
;
    _item.name
        '_array_structure_list_axis.fract_displacement_increment'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'millimetres'
     save_


save__array_structure_list_axis.angular_pitch
    _item_description.description
;               The pixel-centre-to-pixel-centre distance for a one-step
                change in the setting of the specified axis in millimetres.

                This is meaningful only for 'constant velocity' spiral scans
                or for uncoupled angular scans at a constant radius
                (cylindrical scans) and should not be specified for cases
                in which the angle between pixels (rather than the distance
                between pixels) is uniform.

                See _array_structure_list_axis.angle_increment.
;
    _item.name               '_array_structure_list_axis.angular_pitch'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'millimetres'
     save_
```

```
save__array_structure_list_axis.radial_pitch
    _item_description.description
;               The radial distance from one 'cylinder' of pixels to the
                next in millimetres.  If the scan is a 'constant velocity'
                scan with differing angular displacements between pixels,
                the value of this item may differ significantly from the
                value of _array_structure_list_axis.displacement_increment.
;
    _item.name               '_array_structure_list_axis.radial_pitch'
    _item.category_id          array_structure_list_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'millimetres'
     save_


save__array_structure_list_axis.reference_angle
     _item_description.description
;               The value of _array_structure_list_axis.reference_angle
                specifies the setting of the angle of this axis used for
                determining a reference beam center and a reference detector
                distance.  It is normally expected to be identical to the
                value of _array_structure_list.angle.

;
     _item.name '_array_structure_list_axis.reference_angle'
     _item.category_id          array_structure_list_axis
     _item.mandatory_code       implicit
     _item_type.code            float
     _item_units.code           'degrees'
      save_


save__array_structure_list_axis.reference_displacement
     _item_description.description
;               The value of _array_structure_list_axis.reference_displacement
                specifies the setting of the displacement of this axis used
                for determining a reference beam center and a reference detector
                distance.  It is normally expected to be identical to the value
                of _array_structure_list.displacement.

;
     _item.name '_array_structure_list_axis.reference_displacement'
     _item.category_id          array_structure_list_axis
     _item.mandatory_code       implicit
     _item_type.code            float
     _item_units.code           'millimetres'
      save_



########
# AXIS #
########

save_AXIS
    _category.description
;    Data items in the AXIS category record the information required
     to describe the various goniometer, detector, source and other
     axes needed to specify a data collection or the axes defining the
     coordinate system of an image.

     The location of each axis is specified by two vectors: the axis
     itself, given by a  unit vector in the direction of the axis, and
     an offset to the base of the unit vector.

     The vectors defining an axis are referenced to an appropriate
     coordinate system.  The axis vector, itself, is a dimensionless
     unit vector.  Where meaningful, the offset vector is given in
```

millimetres. In coordinate systems not measured in metres,
the offset is not specified and is taken as zero.

The available coordinate systems are:

    The imgCIF standard laboratory coordinate system
    The direct lattice (fractional atomic coordinates)
    The orthogonal Cartesian coordinate system (real space)
    The reciprocal lattice
    An abstract orthogonal Cartesian coordinate frame

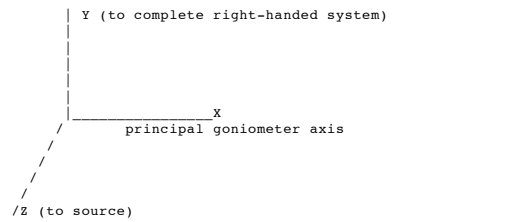
For consistency in this discussion, we call the three coordinate
system axes X, Y and Z. This is appropriate for the imgCIF
standard laboratory coordinate system, and last two Cartesian
coordinate systems, but for the direct lattice, X corresponds
to a, Y to b and Z to c, while for the reciprocal lattice,
X corresponds to a*, Y to b* and Z to c*.

For purposes of visualization, all the coordinate systems are
taken as right-handed, i.e., using the convention that the extended
thumb of a right hand could point along the first (X) axis, the
straightened pointer finger could point along the second (Y) axis
and the middle finger folded inward could point along the third (Z)
axis.

THE IMGCIF STANDARD LABORATORY COORDINATE SYSTEM

The imgCIF satandard laboratory coordinate system is a right-handed
othogonal coordinate similar to the MOSFLM coordinate system,
but puts Z along the X-ray beam, rather than X.

All vectors for the imgCIF standard laboratory coordinate system
is a right-handed Cartesian coordinate system with its origin
in the sample or specimen. The origin of the axis system should,
if possible, be defined in terms of mechanically stable axes to be
in the sample and in the beam. If the sample goniometer or other
sample positioner has two axes the intersection which defines a
unique point at which the sample should be mounted to be bathed
by the beam, that will be the origin of the axis system. If no such
point is defined, then the midpoint of the line of intersection
between the sample and the center of the beam will define the origin.
For this definition the sample positioning system will be set at
its initial reference position for the experiment.



Axis 1 (X): The X-axis is aligned to the mechanical axis pointing from
the sample or specimen along the principal axis of the goniometer or
sample positioning system if the sample positioning system has an axis that
intersects the origin and which form an angle of more than 22.5 degrees
with the beam axis.

Axis 2 (Y): The Y-axis completes an orthogonal right-handed system
defined by the X-axis and the Z-axis (see below).

Axis 3 (Z): The Z-axis is derived from the source axis which goes from
the sample to the source. The Z-axis is the component of the source axis
in the direction of the source orthogonal to the X-axis in the plane
defined by the X-axis and the source axis.

If the conditions for the X-axis can be met, the coordinate system
will be based on the goniometer or other sample positioning system
and the beam and not on the orientation of the detector, gravity etc.
The vectors necessary to specify all other axes are given by sets of
three components in the order (X, Y, Z).
If the axis involved is a rotation axis, it is right-handed, i.e. as
one views the object to be rotated from the origin (the tail) of the
unit vector, the rotation is clockwise. If a translation axis is
specified, the direction of the unit vector specifies the sense of
positive translation.

Note: This choice of coordinate system is similar to but significantly
different from the choice in MOSFLM (Leslie & Powell, 2004). In MOSFLM,
X is along the X-ray beam (the CBF/imgCIF Z axis) and Z is along the
rotation axis.

In some experimental techniques, there is no goniometer or the principal
axis of the goniometer is at a small acute angle with respect to
the source axis. In such cases, other reference axes are needed
to define a useful coordinate system. The order of priority in
defining directions in such cases is to use the detector, then
gravity, then north.

If the X-axis cannot be defined as above, then the
direction (not the origin) of the X-axis should be parallel to the axis
of the primary detector element corresponding to the most rapidly
varying dimension of that detector element's data array, with its
positive sense corresponding to increasing values of the index for
that dimension. If the detector is such that such a direction cannot
be defined (as with a point detector) or that direction forms an
angle of less than 22.5 degrees with respect to the source axis, then
the X-axis should be chosen so that if the Y-axis is chosen
in the direction of gravity, and the Z-axis is chosen to be along
the source axis, a right-handed orthogonal coordinate system is chosen.
In the case of a vertical source axis, as a last resort, the
X-axis should be chosen to point North.

All rotations are given in degrees and all translations are given in mm.

Axes may be dependent on one another. The X-axis is the only goniometer
axis the direction of which is strictly connected to the hardware. All
other axes are specified by the positions they would assume when the
axes upon which they depend are at their zero points.

When specifying detector axes, the axis is given to the beam centre.
The location of the beam centre on the detector should be given in the
DIFFRN_DETECTOR category in distortion-corrected millimetres from
the (0,0) corner of the detector.

It should be noted that many different origins arise in the definition
of an experiment. In particular, as noted above, it is necessary to
specify the location of the beam centre on the detector in terms
of the origin of the detector, which is, of course, not coincident
with the centre of the sample.

The unit cell, reciprocal cell and crystallographic orthogonal
Cartesian coordinate system are defined by the CELL and the matrices
in the ATOM_SITES category.

THE DIRECT LATTICE (FRACTIONAL COORDINATES)

The direct lattice coordinate system is a system of fractional
coordinates aligned to the crystal, rather than to the laboratory.
This is a natural coordinate system for maps and atomic coordinates.
It is the simplest coordinate system in which to apply symmetry.
The axes are determined by the cell edges, and are not necessarily
othogonal. This coordinate system is not uniquely defined and

depends on the cell parameters in the CELL category and the
settings chosen to index the crystal.

Molecules in a crystal studied by X-ray diffracraction are organized
into a repeating regular array of unit cells. Each unit cell is defined
by three vectors, a, b and c. To quote from Drenth,

"The choice of the unit cell is not unique and therefore, guidelines
have been established for selecting the standard basis vectors and
the origin. They are based on symmetry and metric considerations:

 "(1) The axial system should be right handed.
  (2) The basis vectors should coincide as much as possible with
  directions of highest symmetry."
  (3) The cell taken should be the smallest one that satisfies
  condition (2)
  (4) Of all the lattice vectors, none is shorter than a.
  (5) Of those not directed along a, none is shorter than b.
  (6) Of those not lying in the ab plane, none is shorter than c.
  (7) The three angles between the basis vectors a, b and c are
  either all acute (<90 degrees) or all obtuse (>=90 degrees)."

These rules do not produce a unique result that is stable under
the assumption of experimental errors, and the the resulting cell
may not be primitive.

In this coordinate system, the vector (.5, .5, .5) is in the middle
of the given unit cell.

Grid coordinates are an important variation on fractional coordinates
used when working with maps. In imgCIF, the conversion from
fractional to grid coordinates is implicit in the array indexing
specified by _array_structure_list.dimension. Note that this
implicit grid-coordinate scheme is 1-based, not zero-based, i.e.
the origin of the cell for axes along the cell edges with no
specified _array_structure_list_axis.displacement will have
grid coordinates of (1,1,1), i.e. array indices of (1,1,1).

THE ORTHOGONAL CARTESIAN COORDINATE SYSTEM (REAL SPACE)

The orthogonal Cartesian coordinate system is a transformation of
the direct lattice to the actual physical coordinates of atoms in
space. It is similar to the laboratory coordinate system, but
is anchored to and moves with the crystal, rather than being
schored to the laboratory. The transformation from fractional
to orthogonal cartesian coordinates is given by the
        _atom_sites.Cartn_transf_matrix[i][j] and
        _atom_sites.Cartn_transf_vector[i]
tags. A common choice for the matrix of the transformation is
given in the 1992 PDB format document

        | a   b cos(g)   c cos(b) |
        | 0   b sin(g)   c (cos(a) - cos(b)cos(g))/sin(g) |
        | 0   0   V/(a b sin(g)) |

This is a convenient coordinate system in which to do fitting
of models to maps and in which to understand the chemistry of
a molecule.

THE RECIPROCAL LATTICE

The reciprocal lattice coordinate system is used for diffraction
intensitities. It is based on the reciprocal cell, the dual of the cell,
in which reciprocal cell edges are derived from direct cell faces:

   a* = bc sin(a)/V b* = ac sin(b)/V c* = ab sin(g)/V
   cos(a*) = (cos(b) cos(g) - cos(a))/(sin(b) sin(g))
   cos(b*) = (cos(g) cos(g) - cos(b))/(sin(a) sin(g))
   cos(g*) = (cos(a) cos(b) - cos(g))/(sin(a) sin(b))
   V = abc SQRT (1 - cos(a)2 - cos(b)2 - cos(g)2
                    + 2 cos(a) cos(b) cos(g))

      In this form the dimensions of the reciprocal lattice are in reciprocal
      \%Angstroms (\%A^-1). A dimensionless form can be obtained by
      multiplying by the wavelength. Reflections are commonly indexed against
      this coordinate system as (h, k, l) triples.

      References:

      Drenth, J., "Introduction to basic crystallography." chapter
      2.1 in Rossmann, M. G. and Arnold, E. "Crystallography of
      biological macromolecules", Volume F of the IUCr's "International
      tables for crystallography", Kluwer, Dordrecht 2001, pp 44 -- 63

      Leslie, A. G. W. and Powell, H. (2004). MOSFLM v6.11.
      MRC Laboratory of Molecular Biology, Hills Road, Cambridge, England.
      http://www.CCP4.ac.uk/dist/X-windows/Mosflm/.

      Stout, G. H. and Jensen, L. H., "X-ray structure determination",
      2nd ed., Wiley, New York, 1989, 453 pp.

      __, "PROTEIN DATA BANK ATOMIC COORDINATE AND BIBLIOGRAPHIC ENTRY
      FORMAT DESCRIPTION," Brookhaven National Laboratory, February 1992.
;
    _category.id   axis
    _category.mandatory_code   no
     loop_
    _category_key.name   '_axis.id'
                                '_axis.equipment'
     loop_
    _category_group.id   'inclusive_group'
                                 'axis_group'
                                 'diffrn_group'
    loop_
    _category_examples.detail
    _category_examples.case
-
;   Example 1 -

        This example shows the axis specification of the axes of a kappa-
        geometry goniometer [see Stout, G. H. & Jensen, L. H. (1989). X-ray
        structure determination. A practical
        guide, 2nd ed. p. 134. New York: Wiley Interscience].

        There are three axes specified, and no offsets. The outermost axis,
        omega, is pointed along the X axis. The next innermost axis, kappa,
        is at a 50 degree angle to the X axis, pointed away from the source.
        The innermost axis, phi, aligns with the X axis when omega and
        phi are at their zero points. If T-omega, T-kappa and T-phi
        are the transformation matrices derived from the axis settings,
        the complete transformation would be:
            X' = (T-omega) (T-kappa) (T-phi) X
;
;
         loop_
        _axis.id
        _axis.type
        _axis.equipment
        _axis.depends_on
        _axis.vector[1] _axis.vector[2] _axis.vector[3]
        omega rotation goniometer   .   1   0   0
        kappa rotation goniometer omega   -.64279 0   -.76604
        phi   rotation goniometer kappa   1   0   0
;
-
;   Example 2 -

        This example shows the axis specification of the axes of a
        detector, source and gravity. The order has been changed as a
        reminder that the ordering of presentation of tokens is not
        significant. The centre of rotation of the detector has been taken
        to be 68 millimetres in the direction away from the source.

```
;
;
        loop_
        _axis.id
        _axis.type
        _axis.equipment
        _axis.depends_on
        _axis.vector[1] _axis.vector[2] _axis.vector[3]
        _axis.offset[1] _axis.offset[2] _axis.offset[3]
        source        .        source     .       0     0     1   . . .
        gravity       .        gravity    .       0    -1     0   . . .
        tranz     translation detector rotz      0     0     1   0 0 -68
        twotheta  rotation    detector   .       1     0     0   . . .
        roty      rotation    detector twotheta  0     1     0   0 0 -68
        rotz      rotation    detector roty      0     0     1   0 0 -68
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;       Example 3 -

        This example show the axis specification of the axes for a map,
        using fractional coordinates.  Each cell edge has been divided
        into a grid of 50 divisions in the ARRAY_STRUCTURE_LIST_AXIS
        category.  The map is using only the first octant of the grid
        in the ARRAY_STRUCTURE_LIST category.

        The fastest changing axis is the gris along A, then along B,
        and the slowest is along C.

        The map sampling is being done in the middle of each grid
        division

;
;
        loop_
        _axis.id
        _axis.system
        _axis.vector[1] _axis.vector[2] _axis.vector[3]
        CELL_A_AXIS    fractional       1 0 0
        CELL_B_AXIS    fractional       0 1 0
        CELL_C_AXIS    fractional       0 0 1

        loop_
        _array_structure_list.array_id
        _array_structure_list.index
        _array_structure_list.dimension
        _array_structure_list.precedence
        _array_structure_list.direction
        _array_structure_list.axis_id
        MAP 1 25 1 increasing CELL_A_AXIS
        MAP 1 25 2 increasing CELL_B_AXIS
        MAP 1 25 3 increasing CELL_C_AXIS

        loop_
        _array_structure_list_axis.axis_id
        _array_structure_list_axis.fract_displacement
        _array_structure_list_axis.fract_displacement_increment
        CELL_A_AXIS 0.01 0.02
        CELL_B_AXIS 0.01 0.02
        CELL_C_AXIS 0.01 0.02



;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;       Example 4 -

        This example show the axis specification of the axes for a map,
        this time as orthogonal Angstroms, using the same coordinate system
        as for the atomic coordinates.  The map is sampling every 1.5
        Angstroms (1.5e-7 millimeters) in a map segment 37.5 Angstroms on
        a side.
```

```
;
;
        loop_
        _axis.id
        _axis.system
        _axis.vector[1] _axis.vector[2] _axis.vector[3]
        X    orthogonal       1 0 0
        Y    orthogonal       0 1 0
        Z    orthogonal       0 0 1

                loop_
        _array_structure_list.array_id
        _array_structure_list.index
        _array_structure_list.dimension
        _array_structure_list.precedence
        _array_structure_list.direction
        _array_structure_list.axis_id
        MAP 1 25 1 increasing X
        MAP 2 25 2 increasing Y
        MAP 3 25 3 increasing Z

        loop_
        _array_structure_list_axis.axis_id
        _array_structure_list_axis.displacement
        _array_structure_list_axis.displacement_increment
        X 7.5e-8 1.5e-7
        Y 7.5e-8 1.5e-7
        Z 7.5e-8 1.5e-7


;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_


save__axis.depends_on
    _item_description.description
;             The value of _axis.depends_on specifies the next outermost
              axis upon which this axis depends.

              This item is a pointer to _axis.id in the same category.
;
    _item.name                      '_axis.depends_on'
    _item.category_id                 axis
    _item.mandatory_code              no

     save_


save__axis.equipment
    _item_description.description
;             The value of  _axis.equipment specifies the type of
              equipment using the axis:  'goniometer', 'detector',
              'gravity', 'source' or 'general'.
;
    _item.name                      '_axis.equipment'
    _item.category_id                 axis
    _item.mandatory_code              no
    _item_type.code                   ucode
    _item_default.value               general
     loop_
    _item_enumeration.value
    _item_enumeration.detail   goniometer
                              'equipment used to orient or position samples'
                               detector
                              'equipment used to detect reflections'
                               general
                              'equipment used for general purposes'
                               gravity
                              'axis specifying the downward direction'
                               source
                              'axis specifying the direction sample to source'
```

```
     save_


save__axis.offset[1]
    _item_description.description
;              The [1] element of the three-element vector used to specify
               the offset to the base of a rotation or translation axis.

               The vector is specified in millimetres.
;
    _item.name                  '_axis.offset[1]'
    _item.category_id             axis
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
    _item_type.code               float
    _item_units.code              millimetres
     save_


save__axis.offset[2]
    _item_description.description
;              The [2] element of the three-element vector used to specify
               the offset to the base of a rotation or translation axis.

               The vector is specified in millimetres.
;
    _item.name                  '_axis.offset[2]'
    _item.category_id             axis
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
    _item_type.code               float
    _item_units.code              millimetres
     save_


save__axis.offset[3]
    _item_description.description
;              The [3] element of the three-element vector used to specify
               the offset to the base of a rotation or translation axis.

               The vector is specified in millimetres.
;
    _item.name                  '_axis.offset[3]'
    _item.category_id             axis
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
    _item_type.code               float
    _item_units.code              millimetres
     save_


save__axis.id
    _item_description.description
;             The value of _axis.id must uniquely identify
              each axis relevant to the experiment.  Note that multiple
              pieces of equipment may share the same axis (e.g. a twotheta
              arm), so the category key for AXIS also includes the
              equipment.
;
    loop_
    _item.name
    _item.category_id
    _item.mandatory_code
         '_axis.id'                         axis                    yes
         '_array_structure_list_axis.axis_id'
                                            array_structure_list_axis
                                                                    yes
         '_diffrn_detector_axis.axis_id'    diffrn_detector_axis    yes
         '_diffrn_measurement_axis.axis_id' diffrn_measurement_axis yes
         '_diffrn_scan_axis.axis_id'        diffrn_scan_axis        yes
         '_diffrn_scan_frame_axis.axis_id'  diffrn_scan_frame_axis  yes

    _item_type.code              code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
         '_axis.depends_on'                    '_axis.id'
         '_array_structure_list_axis.axis_id' '_axis.id'
         '_diffrn_detector_axis.axis_id'       '_axis.id'
         '_diffrn_measurement_axis.axis_id'    '_axis.id'
         '_diffrn_scan_axis.axis_id'           '_axis.id'
         '_diffrn_scan_frame_axis.axis_id'     '_axis.id'


     save_

save__axis.system
    _item_description.description
;             The value of  _axis.system specifies the coordinate
              system used to define the axis: 'laboratory', 'direct', 'orthogonal',
              'reciprocal' or 'abstract'.
;
    _item.name                    '_axis.system'
    _item.category_id               axis
    _item.mandatory_code            no
    _item_type.code                 ucode
    _item_default.value             laboratory
     loop_
    _item_enumeration.value
    _item_enumeration.detail

laboratory
;  the axis is referenced to the imgCIF standard laboratory Cartesian
   coordinate system
;

direct
;  the axis is referenced to the direct lattice
;

orthogonal
;  the axis is referenced to the cell Cartesian orthogonal coordinates
;

reciprocal
;  the axis is referenced to the reciprocal lattice
;

abstract
;  the axis is referenced to abstract Cartesian cooridinate system
;

     save_


save__axis.type
    _item_description.description
;             The value of _axis.type specifies the type of
              axis:  'rotation' or 'translation' (or 'general' when
              the type is not relevant, as for gravity).
;
    _item.name                    '_axis.type'
    _item.category_id               axis
    _item.mandatory_code            no
    _item_type.code                 ucode
    _item_default.value             general
     loop_
    _item_enumeration.value
    _item_enumeration.detail      rotation
                                 'right-handed axis of rotation'
                                  translation
```

```
                                'translation in the direction of the axis'
                                 general
                                'axis for which the type is not relevant'

     save_


save__axis.vector[1]
    _item_description.description
;               The [1] element of the three-element vector used to specify
                the direction of a rotation or translation axis.
                The vector should be normalized to be a unit vector and
                is dimensionless.
;
    _item.name                  '_axis.vector[1]'
    _item.category_id             axis
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
    _item_type.code               float
     save_

save__axis.vector[2]
    _item_description.description
;               The [2] element of the three-element vector used to specify
                the direction of a rotation or translation axis.
                The vector should be normalized to be a unit vector and
                is dimensionless.
;
    _item.name                  '_axis.vector[2]'
    _item.category_id             axis
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
    _item_type.code               float
     save_

save__axis.vector[3]
    _item_description.description
;               The [3] element of the three-element vector used to specify
                the direction of a rotation or translation axis.
                The vector should be normalized to be a unit vector and
                is dimensionless.
;
    _item.name                  '_axis.vector[3]'
    _item.category_id             axis
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
    _item_type.code               float
     save_



####################
# DIFFRN_DATA_FRAME #
####################


save_DIFFRN_DATA_FRAME
    _category.description
;             Data items in the DIFFRN_DATA_FRAME category record
              the details about each frame of data.

              The items in this category were previously in a
              DIFFRN_FRAME_DATA category, which is now deprecated.
              The items from the old category are provided
              as aliases but should not be used for new work.
;
    _category.id                  diffrn_data_frame
    _category.mandatory_code      no
     loop_
```

```
    _category_key.name            '_diffrn_data_frame.id'
                                  '_diffrn_data_frame.detector_element_id'
    loop_
    _category_group.id            'inclusive_group'
                                  'array_data_group'

    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - A frame containing data from 4 frame elements.
                Each frame element has a common array configuration
                'array_1' described in ARRAY_STRUCTURE and related
                categories.  The data for each detector element are
                stored in four groups of binary data in the
                ARRAY_DATA category, linked by the array_id and
                binary_id.
;
;
       loop_
       _diffrn_data_frame.id
       _diffrn_data_frame.detector_element_id
       _diffrn_data_frame.array_id
       _diffrn_data_frame.binary_id
       frame_1   d1_ccd_1  array_1  1
       frame_1   d1_ccd_2  array_1  2
       frame_1   d1_ccd_3  array_1  3
       frame_1   d1_ccd_4  array_1  4
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
    save_


save__diffrn_data_frame.array_id
    _item_description.description
;             This item is a pointer to _array_structure.id in the
              ARRAY_STRUCTURE category.
;
    _item.name                  '_diffrn_data_frame.array_id'
    _item.category_id             diffrn_data_frame
    _item.mandatory_code          yes
    _item_aliases.alias_name    '_diffrn_frame_data.array_id'
    _item_aliases.dictionary      cif_img.dic
    _item_aliases.version         1.0
    _item_type.code               code
     save_


save__diffrn_data_frame.binary_id
    _item_description.description
;             This item is a pointer to _array_data.binary_id in the
              ARRAY_DATA category.
;
    _item.name                  '_diffrn_data_frame.binary_id'
    _item.category_id             diffrn_data_frame
    _item.mandatory_code          implicit
    _item_aliases.alias_name    '_diffrn_frame_data.binary_id'
    _item_aliases.dictionary      cif_img.dic
    _item_aliases.version         1.0
    _item_type.code               int
     save_


save__diffrn_data_frame.detector_element_id
    _item_description.description
;               This item is a pointer to _diffrn_detector_element.id
                in the DIFFRN_DETECTOR_ELEMENT category.
;
    _item.name                  '_diffrn_data_frame.detector_element_id'
    _item.category_id             diffrn_data_frame
    _item.mandatory_code          yes
    _item_aliases.alias_name    '_diffrn_frame_data.detector_element_id'
    _item_aliases.dictionary      cif_img.dic
```

```
    _item_aliases.version         1.0
    _item_type.code               code
     save_


save__diffrn_data_frame.id
    _item_description.description
;             The value of _diffrn_data_frame.id must uniquely identify
              each complete frame of data.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
          '_diffrn_data_frame.id'        diffrn_data_frame  yes
          '_diffrn_refln.frame_id'       diffrn_refln       yes
          '_diffrn_scan.frame_id_start'  diffrn_scan        yes
          '_diffrn_scan.frame_id_end'    diffrn_scan        yes
          '_diffrn_scan_frame.frame_id'  diffrn_scan_frame  yes
          '_diffrn_scan_frame_axis.frame_id'
                                         diffrn_scan_frame_axis
                                                            yes
    _item_aliases.alias_name    '_diffrn_frame_data.id'
    _item_aliases.dictionary      cif_img.dic
    _item_aliases.version         1.0
    _item_type.code               code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
          '_diffrn_refln.frame_id'        '_diffrn_data_frame.id'
          '_diffrn_scan.frame_id_start'   '_diffrn_data_frame.id'
          '_diffrn_scan.frame_id_end'     '_diffrn_data_frame.id'
          '_diffrn_scan_frame.frame_id'   '_diffrn_data_frame.id'
          '_diffrn_scan_frame_axis.frame_id'
                                          '_diffrn_data_frame.id'
     save_


save__diffrn_data_frame.details
     _item_description.description
;              The value of _diffrn_data_frame.details should give a
               description of special aspects of each frame of data.

               This is an appropriate location in which to record
               information from vendor headers as presented in those
               headers, but it should never be used as a substitute
               for providing the fully parsed information within
               the appropriate imgCIF/CBF categories.
;
    _item.name                  '_diffrn_data_frame.details'
    _item.category_id             diffrn_data_frame
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_frame_data.details'
    _item_aliases.dictionary      cif_img.dic
    _item_aliases.version         1.4
    _item_type.code               text
     loop_
    _item_examples.case
    _item_examples.detail
;
 HEADER_BYTES = 512;
 DIM = 2;
 BYTE_ORDER = big_endian;
 TYPE = unsigned_short;
 SIZE1 = 3072;
 SIZE2 = 3072;
 PIXEL_SIZE = 0.102588;
 BIN = 2x2;
 DETECTOR_SN = 901;
 TIME = 29.945155;
 DISTANCE = 200.000000;
 PHI = 85.000000;
 OSC_START = 85.000000;
 OSC_RANGE = 1.000000;
 WAVELENGTH = 0.979381;
 BEAM_CENTER_X = 157.500000;
 BEAM_CENTER_Y = 157.500000;
 PIXEL SIZE = 0.102588;
 OSCILLATION RANGE = 1;
 EXPOSURE TIME = 29.9452;
 TWO THETA = 0;
 BEAM CENTRE = 157.5 157.5;
;
;               Example of header information extracted from an ADSC Quantum
                315 detector header by CBFlib_0.7.6.  Image provided by Chris
                Nielsen of ADSC from a data collection at SSRL beamline 1-5.
;
      save_



#####################################################################
#  The following is a restatement of the mmCIF DIFFRN_DETECTOR,          #
#  DIFFRN_MEASUREMENT and DIFFRN_RADIATION categories, modified for      #
#  the CBF/imgCIF extensions                                            #
#####################################################################

###################
# DIFFRN_DETECTOR #
###################


save_DIFFRN_DETECTOR
    _category.description
;               Data items in the DIFFRN_DETECTOR category describe the
                detector used to measure the scattered radiation, including
                any analyser and post-sample collimation.
;
    _category.id                  diffrn_detector
    _category.mandatory_code      no
     loop_
    _category_key.name          '_diffrn_detector.diffrn_id'
                                '_diffrn_detector.id'
     loop_
    _category_group.id           'inclusive_group'
                                 'diffrn_group'
     loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - based on PDB entry 5HVP and laboratory records for the
                structure corresponding to PDB entry 5HVP.
;
;
    _diffrn_detector.diffrn_id             'd1'
    _diffrn_detector.detector              'multiwire'
    _diffrn_detector.type                  'Siemens'
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_


save__diffrn_detector.details
    _item_description.description
;               A description of special aspects of the radiation detector.
;
    _item.name                  '_diffrn_detector.details'
    _item.category_id             diffrn_detector
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_detector_details'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code                   text
    _item_examples.case         'slow mode'
```

```
     save_


save__diffrn_detector.detector
    _item_description.description
;               The general class of the radiation detector.
;
    _item.name                   '_diffrn_detector.detector'
    _item.category_id             diffrn_detector
    _item.mandatory_code          no
     loop_
    _item_aliases.alias_name
    _item_aliases.dictionary
    _item_aliases.version        '_diffrn_radiation_detector'
                                  cifdic.c91
                                  1.0
                                 '_diffrn_detector'
                                  cif_core.dic
                                  2.0
    _item_type.code               text
     loop_
    _item_examples.case           'photographic film'
                                  'scintillation counter'
                                  'CCD plate'
                                  'BF~3~ counter'
     save_


save__diffrn_detector.diffrn_id
    _item_description.description
;               This data item is a pointer to _diffrn.id in the DIFFRN
                category.

                The value of _diffrn.id uniquely defines a set of
                diffraction data.
;
    _item.name                   '_diffrn_detector.diffrn_id'
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__diffrn_detector.dtime
    _item_description.description
;               The deadtime in microseconds of the detector(s) used to
                measure the diffraction intensities.
;
    _item.name                   '_diffrn_detector.dtime'
    _item.category_id             diffrn_detector
    _item.mandatory_code          no
     loop_
    _item_aliases.alias_name
    _item_aliases.dictionary
    _item_aliases.version        '_diffrn_radiation_detector_dtime'
                                  cifdic.c91
                                  1.0
                                 '_diffrn_detector_dtime'
                                  cif_core.dic
                                  2.0
     loop_
    _item_range.maximum
    _item_range.minimum            .    0.0
                                  0.0   0.0
    _item_type.code               float
    _item_units.code              microseconds
     save_


save__diffrn_detector.id
    _item_description.description
;               The value of _diffrn_detector.id must uniquely identify
                each detector used to collect each diffraction data set.
                If the value of _diffrn_detector.id is not given, it is
                implicitly equal to the value of
                _diffrn_detector.diffrn_id.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
            '_diffrn_detector.id'         diffrn_detector       implicit
           '_diffrn_detector_axis.detector_id'
                                          diffrn_detector_axis       yes
     loop_
    _item_linked.child_name
    _item_linked.parent_name
            '_diffrn_detector_axis.detector_id'
                                        '_diffrn_detector.id'

    _item_type.code               code
     save_


save__diffrn_detector.number_of_axes
    _item_description.description
;               The value of _diffrn_detector.number_of_axes gives the
                number of axes of the positioner for the detector identified
                by _diffrn_detector.id.

                The word 'positioner' is a general term used in
                instrumentation design for devices that are used to change
                the positions of portions of apparatus by linear
                translation, rotation or combinations of such motions.

                Axes which are used to provide a coordinate system for the
                face of an area detetctor should not be counted for this
                data item.

                The description of each axis should be provided by entries
                in DIFFRN_DETECTOR_AXIS.
;
    _item.name                   '_diffrn_detector.number_of_axes'
    _item.category_id             diffrn_detector
    _item.mandatory_code          no
     loop_
    _item_range.maximum
    _item_range.minimum           .   1
                                  1   1
    _item_type.code               int
     save_


save__diffrn_detector.type
    _item_description.description
;               The make, model or name of the detector device used.
;
    _item.name                   '_diffrn_detector.type'
    _item.category_id             diffrn_detector
    _item.mandatory_code          no
    _item_aliases.alias_name     '_diffrn_detector_type'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
     save_


#########################
# DIFFRN_DETECTOR_AXIS #
#########################


save_DIFFRN_DETECTOR_AXIS
    _category.description
```

```
;    Data items in the DIFFRN_DETECTOR_AXIS category associate
     axes with detectors.
;
    _category.id                    diffrn_detector_axis
    _category.mandatory_code        no
     loop_
    _category_key.name          '_diffrn_detector_axis.detector_id'
                                '_diffrn_detector_axis.axis_id'
     loop_
    _category_group.id           'inclusive_group'
                                 'diffrn_group'
     save_


save__diffrn_detector_axis.axis_id
    _item_description.description
;               This data item is a pointer to _axis.id in
                the AXIS category.
;
    _item.name                  '_diffrn_detector_axis.axis_id'
    _item.category_id            diffrn_detector_axis
    _item.mandatory_code         yes
    _item_type.code              code
     save_


save__diffrn_detector_axis.detector_id
    _item_description.description
;               This data item is a pointer to _diffrn_detector.id in
                the DIFFRN_DETECTOR category.

                This item was previously named _diffrn_detector_axis.id
                which is now a deprecated name.  The old name is
                provided as an alias but should not be used for new work.
;
    _item.name                  '_diffrn_detector_axis.detector_id'
    _item.category_id            diffrn_detector_axis
    _item.mandatory_code         yes
    _item_aliases.alias_name    '_diffrn_detector_axis.id'
    _item_aliases.dictionary     cif_img.dic
    _item_aliases.version        1.0
    _item_type.code              code
     save_


##########################
# DIFFRN_DETECTOR_ELEMENT #
##########################


save_DIFFRN_DETECTOR_ELEMENT
    _category.description
;             Data items in the DIFFRN_DETECTOR_ELEMENT category record
              the details about spatial layout and other characteristics
              of each element of a detector which may have multiple elements.

              In most cases, giving more detailed information
              in ARRAY_STRUCTURE_LIST and ARRAY_STRUCTURE_LIST_AXIS
              is preferable to simply providing the centre of the
              detector element.
;
    _category.id                    diffrn_detector_element
    _category.mandatory_code        no
     loop_
    _category_key.name              '_diffrn_detector_element.id'
                                    '_diffrn_detector_element.detector_id'
    loop_
    _category_group.id              'inclusive_group'
                                    'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
```

```
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;       Example 1 - Detector d1 is composed of four CCD detector elements,
        each 200 mm by 200 mm, arranged in a square, in the pattern

                    1     2
                       *
                    3     4

        Note that the beam centre is slightly displaced from each of the
        detector elements, just beyond the lower right corner of 1,
        the lower left corner of 2, the upper right corner of 3 and
        the upper left corner of 4.
;
;
        loop_
        _diffrn_detector_element.detector_id
        _diffrn_detector_element.id
        _diffrn_detector_element.center[1]
        _diffrn_detector_element.center[2]
        d1     d1_ccd_1  201.5 -1.5
        d1     d1_ccd_2  -1.8  -1.5
        d1     d1_ccd_3  201.6 201.4
        d1     d1_ccd_4  -1.7  201.5
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
    save_


save__diffrn_detector_element.center[1]
    _item_description.description
;               The value of _diffrn_detector_element.center[1] is the X
                component of the distortion-corrected beam centre in
                millimetres from the (0, 0) (lower-left) corner of the
                detector element viewed from the sample side.

                The X and Y axes are the laboratory coordinate system
                coordinates defined in the AXIS category measured
                when all positioning axes for the detector are at their zero
                settings.  If the resulting X or Y axis is then orthogonal to the
                detector, the Z axis is used instead of the orthogonal axis.

;
    _item.name                  '_diffrn_detector_element.center[1]'
    _item.category_id             diffrn_detector_element
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
    _item_type.code               float
    _item_units.code              millimetres

    save_


save__diffrn_detector_element.center[2]
    _item_description.description
;               The value of _diffrn_detector_element.center[2] is the Y
                component of the distortion-corrected beam centre in
                millimetres from the (0, 0) (lower-left) corner of the
                detector element viewed from the sample side.

                The X and Y axes are the laboratory coordinate system
                coordinates defined in the AXIS category measured
                when all positioning axes for the detector are at their zero
                settings.  If the resulting X or Y axis is then orthogonal to the
                detector, the Z axis is used instead of the orthogonal axis.

;
    _item.name                  '_diffrn_detector_element.center[2]'
    _item.category_id             diffrn_detector_element
    _item.mandatory_code          no
    _item_default.value           0.0
    _item_sub_category.id         vector
```

```
    _item_type.code              float
    _item_units.code             millimetres

    save_


save__diffrn_detector_element.id
    _item_description.description
;             The value of _diffrn_detector_element.id must uniquely
              identify each element of a detector.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
           '_diffrn_detector_element.id'
           diffrn_detector_element
           yes
    _item_type.code              code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
           '_diffrn_data_frame.detector_element_id'
           '_diffrn_detector_element.id'

     save_


save__diffrn_detector_element.detector_id
    _item_description.description
;              This item is a pointer to _diffrn_detector.id
               in the DIFFRN_DETECTOR category.
;
    _item.name                  '_diffrn_detector_element.detector_id'
    _item.category_id            diffrn_detector_element
    _item.mandatory_code         yes
    _item_type.code              code
     save_

save__diffrn_detector_element.reference_center_fast
     _item_description.description
;             The value of _diffrn_detector_element.reference_center_fast is
              the fast index axis beam center position relative to the detector
              element face in millimetres along that from the first pixel to
              the point at which the Z-axis (which should be colinear with the
              beam) intersects the face of the detector, if in fact is does.
              At the time of the measurement all settings of the detector
              positioner should be at their reference settings.  If more than
              one reference setting has been used the value given whould be
              representive of the beam center as determined from the ensemble
              of settings.

              It is important to note that the sense of the axis is used,
              rather than the sign of the pixel-to-pixel increments.

;
     _item.name '_diffrn_detector_element.reference_center_fast'
     _item.category_id            diffrn_detector_element
     _item.mandatory_code         no
     _item_type.code              float
     _item_units.code             millimetres

     save_


save__diffrn_detector_element.reference_center_slow
     _item_description.description
;             The value of _diffrn_detector_element.reference_center_slow is
              the slow index axis beam center position relative to the detector
              element face in millimetres along that from the first pixel to
              the point at which the Z-axis (which should be colinear with the
              beam) intersects the face of the detector, if in fact is does.
              At the time of the measurement all settings of the detector
              positioner should be at their reference settings.  If more than
              one reference setting has been used the value givien whould be
              representive of the beam center as determined from the ensemble
              of settings.

              It is important to note that the sense of the axis is used,
              rather than the sign of the pixel-to-pixel increments.

;
     _item.name '_diffrn_detector_element.reference_center_slow'
     _item.category_id            diffrn_detector_element
     _item.mandatory_code         no
     _item_type.code              float
     _item_units.code             millimetres

     save_



########################
## DIFFRN_MEASUREMENT ##
########################


save_DIFFRN_MEASUREMENT
    _category.description
;              Data items in the DIFFRN_MEASUREMENT category record details
               about the device used to orient and/or position the crystal
               during data measurement and the manner in which the
               diffraction data were measured.
;
    _category.id                  diffrn_measurement
    _category.mandatory_code      no
     loop_
    _category_key.name          '_diffrn_measurement.device'
                                '_diffrn_measurement.diffrn_id'
                                '_diffrn_measurement.id'
     loop_
    _category_group.id           'inclusive_group'
                                 'diffrn_group'
     loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;    Example 1 - based on PDB entry 5HVP and laboratory records for the
                 structure corresponding to PDB entry 5HVP
;
;
    _diffrn_measurement.diffrn_id          'd1'
    _diffrn_measurement.device             '3-circle camera'
    _diffrn_measurement.device_type        'Supper model X'
    _diffrn_measurement.device_details     'none'
    _diffrn_measurement.method             'omega scan'
    _diffrn_measurement.details
    ; 440 frames, 0.20 degrees, 150 sec, detector distance 12 cm, detector
      angle 22.5 degrees
    ;
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;     Example 2 - based on data set TOZ of Willis, Beckwith & Tozer
                  [Acta Cryst. (1991), C47, 2276-2277].
;
;
    _diffrn_measurement.diffrn_id       's1'
    _diffrn_measurement.device_type     'Philips PW1100/20 diffractometer'
    _diffrn_measurement.method          'theta/2theta (\q/2\q)'
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_
```

```
save__diffrn_measurement.device
    _item_description.description
;               The general class of goniometer or device used to support
                and orient the specimen.

                If the value of _diffrn_measurement.device is not given,
                it is implicitly equal to the value of
                _diffrn_measurement.diffrn_id.

                Either _diffrn_measurement.device or
                _diffrn_measurement.id may be used to link to other
                categories.  If the experimental setup admits multiple
                devices, then _diffrn_measurement.id is used to provide
                a unique link.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
             '_diffrn_measurement.device'  diffrn_measurement      implicit
             '_diffrn_measurement_axis.measurement_device'
                                           diffrn_measurement_axis implicit
     loop_
    _item_linked.child_name
    _item_linked.parent_name
             '_diffrn_measurement_axis.measurement_device'
                                          '_diffrn_measurement.device'
    _item_aliases.alias_name    '_diffrn_measurement_device'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
     loop_
    _item_examples.case          '3-circle camera'
                                 '4-circle camera'
                                 'kappa-geometry camera'
                                 'oscillation camera'
                                 'precession camera'
     save_


save__diffrn_measurement.device_details
    _item_description.description
;               A description of special aspects of the device used to
                measure the diffraction intensities.
;
    _item.name                  '_diffrn_measurement.device_details'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_measurement_device_details'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
    _item_examples.case
;                                 commercial goniometer modified locally to
                                  allow for 90\% \t arc
;
     save_


save__diffrn_measurement.device_type
    _item_description.description
;               The make, model or name of the measurement device
                (goniometer) used.
;
    _item.name                  '_diffrn_measurement.device_type'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_measurement_device_type'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
     loop_
    _item_examples.case          'Supper model q'
                                 'Huber model r'
                                 'Enraf-Nonius model s'
                                 'home-made'
     save_


save__diffrn_measurement.diffrn_id
    _item_description.description
;               This data item is a pointer to _diffrn.id in the DIFFRN
                category.
;
    _item.name                  '_diffrn_measurement.diffrn_id'
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__diffrn_measurement.details
    _item_description.description
;               A description of special aspects of the intensity
                measurement.
;
    _item.name                  '_diffrn_measurement.details'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_measurement_details'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
    _item_examples.case
;                                 440 frames, 0.20 degrees, 150 sec, detector
                                  distance 12 cm, detector angle 22.5 degrees
;
     save_


save__diffrn_measurement.id
    _item_description.description
;               The value of _diffrn_measurement.id must uniquely identify
                the set of mechanical characteristics of the device used to
                orient and/or position the sample used during the collection
                of each diffraction data set.

                If the value of _diffrn_measurement.id is not given, it is
                implicitly equal to the value of
                _diffrn_measurement.diffrn_id.

                Either _diffrn_measurement.device or
                _diffrn_measurement.id may be used to link to other
                categories.  If the experimental setup admits multiple
                devices, then _diffrn_measurement.id is used to provide
                a unique link.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
             '_diffrn_measurement.id'     diffrn_measurement      implicit
             '_diffrn_measurement_axis.measurement_id'
                                          diffrn_measurement_axis implicit
     loop_
    _item_linked.child_name
    _item_linked.parent_name
             '_diffrn_measurement_axis.measurement_id'
                                         '_diffrn_measurement.id'

    _item_type.code               code
     save_
```

```
save__diffrn_measurement.method
    _item_description.description
;               Method used to measure intensities.
;
    _item.name                  '_diffrn_measurement.method'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_measurement_method'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
    _item_examples.case
      'profile data from theta/2theta (\q/2\q) scans'
     save_


save__diffrn_measurement.number_of_axes
    _item_description.description
;               The value of _diffrn_measurement.number_of_axes gives the
                number of axes of the positioner for the goniometer or
                other sample orientation or positioning device identified
                by _diffrn_measurement.id.

                The description of the axes should be provided by entries in
                DIFFRN_MEASUREMENT_AXIS.
;
    _item.name                  '_diffrn_measurement.number_of_axes'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
     loop_
    _item_range.maximum
    _item_range.minimum           .   1
                                  1   1
    _item_type.code               int
     save_


save__diffrn_measurement.specimen_support
    _item_description.description
;               The physical device used to support the crystal during data
                collection.
;
    _item.name                  '_diffrn_measurement.specimen_support'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_measurement_specimen_support'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
     loop_
    _item_examples.case          'glass capillary'
                                 'quartz capillary'
                                 'fiber'
                                 'metal loop'
     save_


##########################
# DIFFRN_MEASUREMENT_AXIS #
##########################


save_DIFFRN_MEASUREMENT_AXIS
    _category.description
;     Data items in the DIFFRN_MEASUREMENT_AXIS category associate
      axes with goniometers.
;
    _category.id                  diffrn_measurement_axis
    _category.mandatory_code      no
     loop_
    _category_key.name
                            '_diffrn_measurement_axis.measurement_device'
                            '_diffrn_measurement_axis.measurement_id'
                            '_diffrn_measurement_axis.axis_id'
     loop_
    _category_group.id           'inclusive_group'
                                 'diffrn_group'
     save_


save__diffrn_measurement_axis.axis_id
    _item_description.description
;               This data item is a pointer to _axis.id in
                the AXIS category.
;
    _item.name                  '_diffrn_measurement_axis.axis_id'
    _item.category_id             diffrn_measurement_axis
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__diffrn_measurement_axis.measurement_device
    _item_description.description
;               This data item is a pointer to _diffrn_measurement.device
                in the DIFFRN_MEASUREMENT category.
;
    _item.name
      '_diffrn_measurement_axis.measurement_device'
    _item.category_id             diffrn_measurement_axis
    _item.mandatory_code          implicit
    _item_type.code               text
     save_


save__diffrn_measurement_axis.measurement_id
    _item_description.description
;               This data item is a pointer to _diffrn_measurement.id in
                the DIFFRN_MEASUREMENT category.

                This item was previously named _diffrn_measurement_axis.id,
                which is now a deprecated name.  The old name is
                provided as an alias but should not be used for new work.
;
    _item.name                  '_diffrn_measurement_axis.measurement_id'
    _item.category_id             diffrn_measurement_axis
    _item.mandatory_code          implicit
    _item_aliases.alias_name    '_diffrn_measurement_axis.id'
    _item_aliases.dictionary      cif_img.dic
    _item_aliases.version         1.0
    _item_type.code               code
     save_


####################
# DIFFRN_RADIATION #
####################


save_DIFFRN_RADIATION
    _category.description
;               Data items in the DIFFRN_RADIATION category describe
                the radiation used for measuring diffraction intensities,
                its collimation and monochromatization before the sample.

                Post-sample treatment of the beam is described by data
                items in the DIFFRN_DETECTOR category.
;
    _category.id                  diffrn_radiation
    _category.mandatory_code      no
    _category_key.name          '_diffrn_radiation.diffrn_id'
     loop_
    _category_group.id           'inclusive_group'
                                 'diffrn_group'
```

```
     loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - based on PDB entry 5HVP and laboratory records for the
                structure corresponding to PDB entry 5HVP
;
;
    _diffrn_radiation.diffrn_id            'set1'

    _diffrn_radiation.collimation          '0.3 mm double pinhole'
    _diffrn_radiation.monochromator        'graphite'
    _diffrn_radiation.type                 'Cu K\a'
    _diffrn_radiation.wavelength_id         1
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;    Example 2 - based on data set TOZ of Willis, Beckwith & Tozer
               [Acta Cryst. (1991), C47, 2276-2277].
;
;
    _diffrn_radiation.wavelength_id    1
    _diffrn_radiation.type             'Cu K\a'
    _diffrn_radiation.monochromator    'graphite'
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
     save_

save__diffrn_radiation.collimation
    _item_description.description
;              The collimation or focusing applied to the radiation.
;
    _item.name                   '_diffrn_radiation.collimation'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name     '_diffrn_radiation_collimation'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
     loop_
    _item_examples.case          '0.3 mm double-pinhole'
                                 '0.5 mm'
                                 'focusing mirrors'
     save_


save__diffrn_radiation.diffrn_id
    _item_description.description
;              This data item is a pointer to _diffrn.id in the DIFFRN
               category.
;
    _item.name                   '_diffrn_radiation.diffrn_id'
    _item.mandatory_code          yes
    _item_type.code               code
     save_



save__diffrn_radiation.div_x_source
    _item_description.description
;              Beam crossfire in degrees parallel to the laboratory X axis
               (see AXIS category).

               This is a characteristic of the X-ray beam as it illuminates
               the sample (or specimen) after all monochromation and
               collimation.

               This is the standard uncertainty (e.s.d.)  of the directions of
               photons in the XZ plane around the mean source beam
               direction.

               Note that for some synchrotrons this value is specified
               in milliradians, in which case a conversion is needed.
               To convert a value in milliradians to a value in degrees,
               multiply by 0.180 and divide by \p.
;
    _item.name                   '_diffrn_radiation.div_x_source'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_type.code               float
    _item_units.code              degrees
     save_


save__diffrn_radiation.div_y_source
    _item_description.description
;              Beam crossfire in degrees parallel to the laboratory Y axis
               (see AXIS category).

               This is a characteristic of the X-ray beam as it illuminates
               the sample (or specimen) after all monochromation and
               collimation.

               This is the standard uncertainty (e.s.d.) of the directions
               of photons in the YZ plane around the mean source beam
               direction.

               Note that for some synchrotrons this value is specified
               in milliradians, in which case a conversion is needed.
               To convert a value in milliradians to a value in degrees,
               multiply by 0.180 and divide by \p.
;
    _item.name                   '_diffrn_radiation.div_y_source'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_type.code               float
    _item_units.code              degrees
    _item_default.value           0.0
     save_


save__diffrn_radiation.div_x_y_source
    _item_description.description
;              Beam crossfire correlation degrees^2^ between the
               crossfire laboratory X-axis component and the crossfire
               laboratory Y-axis component (see AXIS category).

               This is a characteristic of the X-ray beam as it illuminates
               the sample (or specimen) after all monochromation and
               collimation.

               This is the mean of the products of the deviations of the
               direction of each photon in XZ plane times the deviations
               of the direction of the same photon in the YZ plane
               around the mean source beam direction.  This will be zero
               for uncorrelated crossfire.

               Note that some synchrotrons, this value is specified in
               milliradians^2^, in which case a conversion would be needed.
               To go from a value in milliradians^2^ to a value in
               degrees^2^, multiply by 0.180^2^ and divide by \p^2^.

;
    _item.name                   '_diffrn_radiation.div_x_y_source'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_type.code               float
    _item_units.code              degrees_squared
    _item_default.value           0.0
     save_

save__diffrn_radiation.filter_edge
    _item_description.description
;              Absorption edge in \%Angstroms of the radiation filter used.
;
```

```
    _item.name                  '_diffrn_radiation.filter_edge'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_filter_edge'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
     loop_
    _item_range.maximum
    _item_range.minimum            .    0.0
                                  0.0   0.0
    _item_type.code               float
    _item_units.code              angstroms
     save_

save__diffrn_radiation.inhomogeneity
    _item_description.description
;              Half-width in millimetres of the incident beam in the
               direction perpendicular to the diffraction plane.
;
    _item.name                  '_diffrn_radiation.inhomogeneity'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_inhomogeneity'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
     loop_
    _item_range.maximum
    _item_range.minimum            .    0.0
                                  0.0   0.0
    _item_type.code               float
    _item_units.code              millimetres
     save_

save__diffrn_radiation.monochromator
    _item_description.description
;              The method used to obtain monochromatic radiation. If a
               monochromator crystal is used, the material and the
               indices of the Bragg reflection are specified.
;
    _item.name                  '_diffrn_radiation.monochromator'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_monochromator'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               text
     loop_
    _item_examples.case           'Zr filter'
                                  'Ge 220'
                                  'none'
                                  'equatorial mounted graphite'
     save_

save__diffrn_radiation.polarisn_norm
    _item_description.description
;              The angle in degrees, as viewed from the specimen, between the
               perpendicular component of the polarization and the diffraction
               plane. See _diffrn_radiation_polarisn_ratio.
;
    _item.name                  '_diffrn_radiation.polarisn_norm'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_polarisn_norm'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
     loop_
    _item_range.maximum
    _item_range.minimum           90.0  90.0
                                  90.0 -90.0
                                 -90.0 -90.0
    _item_type.code               float
    _item_units.code              degrees
     save_

save__diffrn_radiation.polarisn_ratio
    _item_description.description
;              Polarization ratio of the diffraction beam incident on the
               crystal. This is the ratio of the perpendicularly polarized to
               the parallel polarized component of the radiation. The
               perpendicular component forms an angle of
               _diffrn_radiation.polarisn_norm to the normal to the
               diffraction plane of the sample (i.e. the plane containing
               the incident and reflected beams).
;
    _item.name                  '_diffrn_radiation.polarisn_ratio'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_polarisn_ratio'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
     loop_
    _item_range.maximum
    _item_range.minimum            .    0.0
                                  0.0   0.0
    _item_type.code               float
     save_


save__diffrn_radiation.polarizn_source_norm
    _item_description.description
;              The angle in degrees, as viewed from the specimen, between
               the normal to the polarization plane and the laboratory Y
               axis as defined in the AXIS category.

               Note that this is the angle of polarization of the source
               photons, either directly from a synchrotron beamline or
               from a monochromater.

               This differs from the value of
               _diffrn_radiation.polarisn_norm
               in that _diffrn_radiation.polarisn_norm refers to
               polarization relative to the diffraction plane rather than
               to the laboratory axis system.

               In the case of an unpolarized beam, or a beam with true
               circular polarization, in which no single plane of
               polarization can be determined, the plane should be taken
               as the XZ plane and the angle as 0.

               See _diffrn_radiation.polarizn_source_ratio.
;
    _item.name                  '_diffrn_radiation.polarizn_source_norm'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
     loop_
    _item_range.maximum
    _item_range.minimum           90.0   90.0
                                  90.0  -90.0
                                 -90.0  -90.0
    _item_type.code               float
    _item_units.code              degrees
    _item_default.value           0.0
     save_


save__diffrn_radiation.polarizn_source_ratio
    _item_description.description
;              (Ip-In)/(Ip+In), where Ip is the intensity
               (amplitude squared) of the electric vector in the plane of
               polarization and In is the intensity (amplitude squared)
               of the electric vector in the plane of the normal to the
               plane of polarization.
```

```
                In the case of an unpolarized beam, or a beam with true
                circular polarization, in which no single plane of
                polarization can be determined, the plane is to be taken
                as the XZ plane and the normal is parallel to the Y axis.

                Thus, if there was complete polarization in the plane of
                polarization, the value of
                _diffrn_radiation.polarizn_source_ratio would be 1, and
                for an unpolarized beam
                _diffrn_radiation.polarizn_source_ratio would have a
                value of 0.

                If the X axis has been chosen to lie in the plane of
                polarization, this definition will agree with the definition
                of 'MONOCHROMATOR' in the Denzo glossary, and values of near
                1 should be expected for a bending-magnet source.  However,
                if the X axis were perpendicular to the polarization plane
                (not a common choice), then the Denzo value would be the
                negative of _diffrn_radiation.polarizn_source_ratio.

                See http://www.hkl-xray.com for information on Denzo and
                Otwinowski & Minor (1997).

                This differs both in the choice of ratio and choice of
                orientation from _diffrn_radiation.polarisn_ratio, which,
                unlike _diffrn_radiation.polarizn_source_ratio, is
                unbounded.

                Reference: Otwinowski, Z. & Minor, W. (1997). 'Processing of
                X-ray diffraction data collected in oscillation mode.' Methods
                Enzymol. 276, 307-326.
;
    _item.name                  '_diffrn_radiation.polarizn_source_ratio'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
     loop_
    _item_range.maximum
    _item_range.minimum           1.0    1.0
                                  1.0   -1.0
                                 -1.0   -1.0
    _item_type.code               float
     save_


save__diffrn_radiation.probe
    _item_description.description
;               Name of the type of radiation used. It is strongly
                recommended that this be given so that the
                probe radiation is clearly specified.
;
    _item.name                  '_diffrn_radiation.probe'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_probe'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               line
     loop_
    _item_enumeration.value      'X-ray'
                                 'neutron'
                                 'electron'
                                 'gamma'
     save_

save__diffrn_radiation.type
    _item_description.description
;               The nature of the radiation. This is typically a description
                of the X-ray wavelength in Siegbahn notation.
;
    _item.name                  '_diffrn_radiation.type'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_type'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               line
     loop_
    _item_examples.case          'CuK\a'
                                 'Cu K\a~1~'
                                 'Cu K-L~2,3~'
                                 'white-beam'

     save_

save__diffrn_radiation.xray_symbol
    _item_description.description
;               The IUPAC symbol for the X-ray wavelength for the probe
                radiation.
;
    _item.name                  '_diffrn_radiation.xray_symbol'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          no
    _item_aliases.alias_name    '_diffrn_radiation_xray_symbol'
    _item_aliases.dictionary      cif_core.dic
    _item_aliases.version         2.0.1
    _item_type.code               line
     loop_
    _item_enumeration.value
    _item_enumeration.detail     'K-L~3~'
                                 'K\a~1~ in older Siegbahn notation'
                                 'K-L~2~'
                                 'K\a~2~ in older Siegbahn notation'
                                 'K-M~3~'
                                 'K\b~1~ in older Siegbahn notation'
                                 'K-L~2,3~'
                                 'use where K-L~3~ and K-L~2~ are not resolved'
     save_

save__diffrn_radiation.wavelength_id
    _item_description.description
;               This data item is a pointer to
                _diffrn_radiation_wavelength.id in the
                DIFFRN_RADIATION_WAVELENGTH category.
;
    _item.name                  '_diffrn_radiation.wavelength_id'
    _item.category_id             diffrn_radiation
    _item.mandatory_code          yes
    _item_type.code               code
     save_



################
# DIFFRN_REFLN #
################


save_DIFFRN_REFLN
    _category.description
;    This category redefinition has been added to extend the key of
     the standard DIFFRN_REFLN category.
;
    _category.id                  diffrn_refln
    _category.mandatory_code      no
    _category_key.name            '_diffrn_refln.frame_id'
     loop_
    _category_group.id            'inclusive_group'
                                  'diffrn_group'
     save_


save__diffrn_refln.frame_id
    _item_description.description
;               This item is a pointer to _diffrn_data_frame.id
```

```
               in the DIFFRN_DATA_FRAME category.
;
     _item.name                  '_diffrn_refln.frame_id'
     _item.category_id            diffrn_refln
     _item.mandatory_code         yes
     _item_type.code              code
      save_


###############
# DIFFRN_SCAN #
###############

save_DIFFRN_SCAN
     _category.description
;     Data items in the DIFFRN_SCAN category describe the parameters of one
      or more scans, relating axis positions to frames.

;
     _category.id                  diffrn_scan
     _category.mandatory_code      no
     _category_key.name           '_diffrn_scan.id'
      loop_
     _category_group.id           'inclusive_group'
                                  'diffrn_group'
      loop_
     _category_examples.detail
     _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;    Example 1 - derived from a suggestion by R. M. Sweet.

    The vector of each axis is not given here, because it is provided in
    the AXIS category.  By making _diffrn_scan_axis.scan_id and
    _diffrn_scan_axis.axis_id keys of the DIFFRN_SCAN_AXIS category,
    an arbitrary number of scanning and fixed axes can be specified for a
    scan.  In this example, three rotation axes and one translation axis
    at nonzero values are specified, with one axis stepping.  There is no
    reason why more axes could not have been specified to step. Range
    information has been specified, but note that it can be calculated from
    the  number of frames and the increment, so the data item
    _diffrn_scan_axis.angle_range could be dropped.

    Both the sweep data and the data for a single frame are specified.

    Note that the information on how the axes are stepped is given twice,
    once in terms of the overall averages in the value of
    _diffrn_scan.integration_time and the values for DIFFRN_SCAN_AXIS,
    and precisely for the given frame in the value for
    _diffrn_scan_frame.integration_time and the values for
    DIFFRN_SCAN_FRAME_AXIS.  If dose-related adjustments are made to
    scan times and nonlinear stepping is done, these values may differ.
    Therefore, in interpreting the data for a particular frame it is
    important to use the frame-specific data.
;
;
       _diffrn_scan.id                   1
       _diffrn_scan.date_start          '2001-11-18T03:26:42'
       _diffrn_scan.date_end            '2001-11-18T03:36:45'
       _diffrn_scan.integration_time     3.0
       _diffrn_scan.frame_id_start       mad_L2_000
       _diffrn_scan.frame_id_end         mad_L2_200
       _diffrn_scan.frames               201

        loop_
       _diffrn_scan_axis.scan_id
       _diffrn_scan_axis.axis_id
       _diffrn_scan_axis.angle_start
       _diffrn_scan_axis.angle_range
       _diffrn_scan_axis.angle_increment
       _diffrn_scan_axis.displacement_start
       _diffrn_scan_axis.displacement_range
       _diffrn_scan_axis.displacement_increment
        1 omega 200.0 20.0 0.1 . . .
        1 kappa -40.0  0.0 0.0 . . .
        1 phi   127.5  0.0 0.0 . . .
        1 tranz  . . .   2.3 0.0 0.0

       _diffrn_scan_frame.scan_id                    1
       _diffrn_scan_frame.date                '2001-11-18T03:27:33'
       _diffrn_scan_frame.integration_time     3.0
       _diffrn_scan_frame.frame_id             mad_L2_018
       _diffrn_scan_frame.frame_number         18

       loop_
       _diffrn_scan_frame_axis.frame_id
       _diffrn_scan_frame_axis.axis_id
       _diffrn_scan_frame_axis.angle
       _diffrn_scan_frame_axis.angle_increment
       _diffrn_scan_frame_axis.displacement
       _diffrn_scan_frame_axis.displacement_increment

        mad_L2_018 omega 201.8  0.1 . .
        mad_L2_018 kappa -40.0  0.0 . .
        mad_L2_018 phi   127.5  0.0 . .
        mad_L2_018 tranz  .     .  2.3 0.0
;

;  Example 2 - a more extensive example (R. M. Sweet, P. J. Ellis &
   H. J. Bernstein).

   A detector is placed 240 mm along the Z axis from the goniometer.
   This leads to a choice:  either the axes of
   the detector are defined at the origin, and then a Z setting of -240
   is entered, or the axes are defined with the necessary Z offset.
   In this case, the setting is used and the offset is left as zero.
   This axis is called DETECTOR_Z.

   The axis for positioning the detector in the Y direction depends
   on the detector Z axis.  This axis is called DETECTOR_Y.

   The axis for positioning the detector in the X direction depends
   on the detector Y axis (and therefore on the detector Z axis).
   This axis is called DETECTOR_X.

   This detector may be rotated around the Y axis.  This rotation axis
   depends on the three translation axes.  It is called DETECTOR_PITCH.

   A coordinate system is defined on the face of the detector in terms of
   2300 0.150 mm pixels in each direction.  The ELEMENT_X axis is used to
   index the first array index of the data array and the ELEMENT_Y
   axis is used to index the second array index.  Because the pixels
   are 0.150mm X 0.150mm, the centre of the first pixel is at (0.075,
   0.075) in this coordinate system.
;

;    ###CBF: VERSION 1.1

     data_image_1

     # category DIFFRN
     _diffrn.id P6MB
     _diffrn.crystal_id P6MB_CRYSTAL7

     # category DIFFRN_SOURCE
     loop_
     _diffrn_source.diffrn_id
     _diffrn_source.source
     _diffrn_source.type
      P6MB synchrotron 'SSRL beamline 9-1'

     # category DIFFRN_RADIATION
     loop_
     _diffrn_radiation.diffrn_id
```

```
_diffrn_radiation.wavelength_id
_diffrn_radiation.monochromator
_diffrn_radiation.polarizn_source_ratio
_diffrn_radiation.polarizn_source_norm
_diffrn_radiation.div_x_source
_diffrn_radiation.div_y_source
_diffrn_radiation.div_x_y_source
 P6MB WAVELENGTH1 'Si 111' 0.8 0.0 0.08
0.01 0.00

# category DIFFRN_RADIATION_WAVELENGTH
loop_
_diffrn_radiation_wavelength.id
_diffrn_radiation_wavelength.wavelength
_diffrn_radiation_wavelength.wt
 WAVELENGTH1 0.98 1.0

# category DIFFRN_DETECTOR
loop_
_diffrn_detector.diffrn_id
_diffrn_detector.id
_diffrn_detector.type
_diffrn_detector.number_of_axes
 P6MB MAR345-SN26 'MAR 345' 4

# category DIFFRN_DETECTOR_AXIS
loop_
_diffrn_detector_axis.detector_id
_diffrn_detector_axis.axis_id
 MAR345-SN26 DETECTOR_X
 MAR345-SN26 DETECTOR_Y
 MAR345-SN26 DETECTOR_Z
 MAR345-SN26 DETECTOR_PITCH

# category DIFFRN_DETECTOR_ELEMENT
loop_
_diffrn_detector_element.id
_diffrn_detector_element.detector_id
 ELEMENT1 MAR345-SN26

# category DIFFRN_DATA_FRAME
loop_
_diffrn_data_frame.id
_diffrn_data_frame.detector_element_id
_diffrn_data_frame.array_id
_diffrn_data_frame.binary_id
 FRAME1 ELEMENT1 ARRAY1 1

# category DIFFRN_MEASUREMENT
loop_
_diffrn_measurement.diffrn_id
_diffrn_measurement.id
_diffrn_measurement.number_of_axes
_diffrn_measurement.method
 P6MB GONIOMETER 3 rotation

# category DIFFRN_MEASUREMENT_AXIS
loop_
_diffrn_measurement_axis.measurement_id
_diffrn_measurement_axis.axis_id
 GONIOMETER GONIOMETER_PHI
 GONIOMETER GONIOMETER_KAPPA
 GONIOMETER GONIOMETER_OMEGA

# category DIFFRN_SCAN
loop_
_diffrn_scan.id
_diffrn_scan.frame_id_start
_diffrn_scan.frame_id_end
_diffrn_scan.frames
 SCAN1 FRAME1 FRAME1 1
```

```
# category DIFFRN_SCAN_AXIS
loop_
_diffrn_scan_axis.scan_id
_diffrn_scan_axis.axis_id
_diffrn_scan_axis.angle_start
_diffrn_scan_axis.angle_range
_diffrn_scan_axis.angle_increment
_diffrn_scan_axis.displacement_start
_diffrn_scan_axis.displacement_range
_diffrn_scan_axis.displacement_increment
 SCAN1 GONIOMETER_OMEGA 12.0 1.0 1.0 0.0 0.0 0.0
 SCAN1 GONIOMETER_KAPPA 23.3 0.0 0.0 0.0 0.0 0.0
 SCAN1 GONIOMETER_PHI -165.8 0.0 0.0 0.0 0.0 0.0
 SCAN1 DETECTOR_Z 0.0 0.0 0.0 -240.0 0.0 0.0
 SCAN1 DETECTOR_Y 0.0 0.0 0.0 0.6 0.0 0.0
 SCAN1 DETECTOR_X 0.0 0.0 0.0 -0.5 0.0 0.0
 SCAN1 DETECTOR_PITCH 0.0 0.0 0.0 0.0 0.0 0.0

# category DIFFRN_SCAN_FRAME
loop_
_diffrn_scan_frame.frame_id
_diffrn_scan_frame.frame_number
_diffrn_scan_frame.integration_time
_diffrn_scan_frame.scan_id
_diffrn_scan_frame.date
 FRAME1 1 20.0 SCAN1 1997-12-04T10:23:48

# category DIFFRN_SCAN_FRAME_AXIS
loop_
_diffrn_scan_frame_axis.frame_id
_diffrn_scan_frame_axis.axis_id
_diffrn_scan_frame_axis.angle
_diffrn_scan_frame_axis.displacement
 FRAME1 GONIOMETER_OMEGA 12.0 0.0
 FRAME1 GONIOMETER_KAPPA 23.3 0.0
 FRAME1 GONIOMETER_PHI -165.8 0.0
 FRAME1 DETECTOR_Z 0.0 -240.0
 FRAME1 DETECTOR_Y 0.0 0.6
 FRAME1 DETECTOR_X 0.0 -0.5
 FRAME1 DETECTOR_PITCH 0.0 0.0

# category AXIS
loop_
_axis.id
_axis.type
_axis.equipment
_axis.depends_on
_axis.vector[1] _axis.vector[2] _axis.vector[3]
_axis.offset[1] _axis.offset[2] _axis.offset[3]
 GONIOMETER_OMEGA rotation goniometer . 1 0 0 . . .
 GONIOMETER_KAPPA rotation goniometer GONIOMETER_OMEGA 0.64279
 0 0.76604 . . .
 GONIOMETER_PHI   rotation goniometer GONIOMETER_KAPPA 1 0 0
. . .
 SOURCE           general source . 0 0 1 . . .
 GRAVITY          general gravity . 0 -1 0 . . .
 DETECTOR_Z       translation detector . 0 0 1 0 0 0
 DETECTOR_Y       translation detector DETECTOR_Z 0 1 0 0 0 0
 DETECTOR_X       translation detector DETECTOR_Y 1 0 0 0 0 0
 DETECTOR_PITCH   rotation    detector DETECTOR_X 0 1 0 0 0 0
 ELEMENT_X        translation detector DETECTOR_PITCH
1 0 0 172.43 -172.43 0
 ELEMENT_Y        translation detector ELEMENT_X
0 1 0 0 0 0

# category ARRAY_STRUCTURE_LIST
loop_
_array_structure_list.array_id
_array_structure_list.index
_array_structure_list.dimension
_array_structure_list.precedence
_array_structure_list.direction
```

```
      _array_structure_list.axis_set_id
       ARRAY1 1 2300 1 increasing ELEMENT_X
       ARRAY1 2 2300 2 increasing ELEMENT_Y

      # category ARRAY_STRUCTURE_LIST_AXIS
      loop_
      _array_structure_list_axis.axis_set_id
      _array_structure_list_axis.axis_id
      _array_structure_list_axis.displacement
      _array_structure_list_axis.displacement_increment
       ELEMENT_X ELEMENT_X 0.075 0.150
       ELEMENT_Y ELEMENT_Y 0.075 0.150

      # category ARRAY_ELEMENT_SIZE
      loop_
      _array_element_size.array_id
      _array_element_size.index
      _array_element_size.size
       ARRAY1 1 150e-6
       ARRAY1 2 150e-6

      # category ARRAY_INTENSITIES
      loop_
      _array_intensities.array_id
      _array_intensities.binary_id
      _array_intensities.linearity
      _array_intensities.gain
      _array_intensities.gain_esd
      _array_intensities.overload
      _array_intensities.undefined_value
       ARRAY1 1 linear 1.15 0.2 240000 0

       # category ARRAY_STRUCTURE
       loop_
       _array_structure.id
       _array_structure.encoding_type
       _array_structure.compression_type
       _array_structure.byte_order
       ARRAY1 "signed 32-bit integer" packed little_endian

      # category ARRAY_DATA
      loop_
      _array_data.array_id
      _array_data.binary_id
      _array_data.data
       ARRAY1 1
      ;
      --CIF-BINARY-FORMAT-SECTION--
      Content-Type: application/octet-stream;
          conversions="X-CBF_PACKED"
      Content-Transfer-Encoding: BASE64
      X-Binary-Size: 3801324
      X-Binary-ID: 1
      X-Binary-Element-Type: "signed 32-bit integer"
      Content-MD5: 07lZFvF+aOcW85IN7usl8A==

      AABRAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAZBQSr1sKNBOeOe9HITdMdDUnbq7bg
      ...
      8REo6TtBrxJ1vKqAvx9YDMD6J18Qg83OMr/tgssjMIJMXATDsZobL90AEXc4KigE

      --CIF-BINARY-FORMAT-SECTION----
      ;
;

;   Example 3 - Example 2 revised for a spiral scan (R. M. Sweet,
    P. J. Ellis & H. J. Bernstein).

   A detector is placed 240 mm along the Z axis from the
   goniometer, as in Example 2 above, but in this example the
   image plate is scanned in a spiral pattern from the outside edge in.

   The axis for positioning the detector in the Y direction depends
   on the detector Z axis.  This axis is called DETECTOR_Y.

   The axis for positioning the detector in the X direction depends
   on the detector Y axis (and therefore on the detector Z axis).
   This axis is called DETECTOR_X.

   This detector may be rotated around the Y axis.  This rotation axis
   depends on the three translation axes.  It is called DETECTOR_PITCH.

   A coordinate system is defined on the face of the detector in
   terms of a coupled rotation axis and radial scan axis to form
   a spiral scan.  The rotation axis is called  ELEMENT_ROT  and the
   radial axis is called ELEMENT_RAD.  A 150 micrometre radial pitch
   and a 75 micrometre 'constant velocity' angular pitch are assumed.

   Indexing is carried out first on the rotation axis and the radial axis
   is made to be dependent on it.

   The two axes are coupled to form an axis set ELEMENT_SPIRAL.
;
;    ###CBF: VERSION 1.1

      data_image_1

      # category DIFFRN
      _diffrn.id P6MB
      _diffrn.crystal_id P6MB_CRYSTAL7

      # category DIFFRN_SOURCE
      loop_
      _diffrn_source.diffrn_id
      _diffrn_source.source
      _diffrn_source.type
       P6MB synchrotron 'SSRL beamline 9-1'

      # category DIFFRN_RADIATION
           loop_
      _diffrn_radiation.diffrn_id
      _diffrn_radiation.wavelength_id
      _diffrn_radiation.monochromator
      _diffrn_radiation.polarizn_source_ratio
      _diffrn_radiation.polarizn_source_norm
      _diffrn_radiation.div_x_source
      _diffrn_radiation.div_y_source
      _diffrn_radiation.div_x_y_source
       P6MB WAVELENGTH1 'Si 111' 0.8 0.0 0.08
      0.01 0.00

      # category DIFFRN_RADIATION_WAVELENGTH
      loop_
      _diffrn_radiation_wavelength.id
      _diffrn_radiation_wavelength.wavelength
      _diffrn_radiation_wavelength.wt
       WAVELENGTH1 0.98 1.0

      # category DIFFRN_DETECTOR
      loop_
      _diffrn_detector.diffrn_id
      _diffrn_detector.id
      _diffrn_detector.type
      _diffrn_detector.number_of_axes
       P6MB MAR345-SN26 'MAR 345' 4

      # category DIFFRN_DETECTOR_AXIS
      loop_
      _diffrn_detector_axis.detector_id
      _diffrn_detector_axis.axis_id
       MAR345-SN26 DETECTOR_X
       MAR345-SN26 DETECTOR_Y
       MAR345-SN26 DETECTOR_Z
       MAR345-SN26 DETECTOR_PITCH
```

```
# category DIFFRN_DETECTOR_ELEMENT
loop_
_diffrn_detector_element.id
_diffrn_detector_element.detector_id
 ELEMENT1 MAR345-SN26

# category DIFFRN_DATA_FRAME
loop_
_diffrn_data_frame.id
_diffrn_data_frame.detector_element_id
_diffrn_data_frame.array_id
_diffrn_data_frame.binary_id
 FRAME1 ELEMENT1 ARRAY1 1

# category DIFFRN_MEASUREMENT
loop_
_diffrn_measurement.diffrn_id
_diffrn_measurement.id
_diffrn_measurement.number_of_axes
_diffrn_measurement.method
 P6MB GONIOMETER 3 rotation

# category DIFFRN_MEASUREMENT_AXIS
loop_
_diffrn_measurement_axis.measurement_id
_diffrn_measurement_axis.axis_id
 GONIOMETER GONIOMETER_PHI
 GONIOMETER GONIOMETER_KAPPA
 GONIOMETER GONIOMETER_OMEGA

# category DIFFRN_SCAN
loop_
_diffrn_scan.id
_diffrn_scan.frame_id_start
_diffrn_scan.frame_id_end
_diffrn_scan.frames
 SCAN1 FRAME1 FRAME1 1

# category DIFFRN_SCAN_AXIS
loop_
_diffrn_scan_axis.scan_id
_diffrn_scan_axis.axis_id
_diffrn_scan_axis.angle_start
_diffrn_scan_axis.angle_range
_diffrn_scan_axis.angle_increment
_diffrn_scan_axis.displacement_start
_diffrn_scan_axis.displacement_range
_diffrn_scan_axis.displacement_increment
 SCAN1 GONIOMETER_OMEGA 12.0 1.0 1.0 0.0 0.0 0.0
 SCAN1 GONIOMETER_KAPPA 23.3 0.0 0.0 0.0 0.0 0.0
 SCAN1 GONIOMETER_PHI -165.8 0.0 0.0 0.0 0.0 0.0
 SCAN1 DETECTOR_Z 0.0 0.0 0.0 -240.0 0.0 0.0
 SCAN1 DETECTOR_Y 0.0 0.0 0.0 0.6 0.0 0.0
 SCAN1 DETECTOR_X 0.0 0.0 0.0 -0.5 0.0 0.0
 SCAN1 DETECTOR_PITCH 0.0 0.0 0.0 0.0 0.0 0.0

# category DIFFRN_SCAN_FRAME
loop_
_diffrn_scan_frame.frame_id
_diffrn_scan_frame.frame_number
_diffrn_scan_frame.integration_time
_diffrn_scan_frame.scan_id
_diffrn_scan_frame.date
 FRAME1 1 20.0 SCAN1 1997-12-04T10:23:48

# category DIFFRN_SCAN_FRAME_AXIS
loop_
_diffrn_scan_frame_axis.frame_id
_diffrn_scan_frame_axis.axis_id
_diffrn_scan_frame_axis.angle
_diffrn_scan_frame_axis.displacement
 FRAME1 GONIOMETER_OMEGA 12.0 0.0
 FRAME1 GONIOMETER_KAPPA 23.3 0.0
 FRAME1 GONIOMETER_PHI -165.8 0.0
 FRAME1 DETECTOR_Z 0.0 -240.0
 FRAME1 DETECTOR_Y 0.0 0.6
 FRAME1 DETECTOR_X 0.0 -0.5
 FRAME1 DETECTOR_PITCH 0.0 0.0

# category AXIS
loop_
_axis.id
_axis.type
_axis.equipment
_axis.depends_on
_axis.vector[1] _axis.vector[2] _axis.vector[3]
_axis.offset[1] _axis.offset[2] _axis.offset[3]
 GONIOMETER_OMEGA rotation goniometer . 1 0 0 . . .
 GONIOMETER_KAPPA rotation goniometer GONIOMETER_OMEGA 0.64279
 0 0.76604 . . .
 GONIOMETER_PHI   rotation goniometer GONIOMETER_KAPPA 1 0 0
. . .
 SOURCE           general source . 0 0 1 . . .
 GRAVITY          general gravity . 0 -1 0 . . .
 DETECTOR_Z       translation detector . 0 0 1 0 0 0
 DETECTOR_Y       translation detector DETECTOR_Z 0 1 0 0 0 0
 DETECTOR_X       translation detector DETECTOR_Y 1 0 0 0 0 0
 DETECTOR_PITCH   rotation    detector DETECTOR_X 0 1 0 0 0 0
 ELEMENT_ROT      translation detector DETECTOR_PITCH 0 0 1 0 0 0
 ELEMENT_RAD      translation detector ELEMENT_ROT 0 1 0 0 0 0

# category ARRAY_STRUCTURE_LIST
loop_
_array_structure_list.array_id
_array_structure_list.index
_array_structure_list.dimension
_array_structure_list.precedence
_array_structure_list.direction
_array_structure_list.axis_set_id
 ARRAY1 1 8309900 1 increasing ELEMENT_SPIRAL

# category ARRAY_STRUCTURE_LIST_AXIS
loop_
_array_structure_list_axis.axis_set_id
_array_structure_list_axis.axis_id
_array_structure_list_axis.angle
_array_structure_list_axis.displacement
_array_structure_list_axis.angular_pitch
_array_structure_list_axis.radial_pitch
 ELEMENT_SPIRAL ELEMENT_ROT 0    .  0.075   .
 ELEMENT_SPIRAL ELEMENT_RAD . 172.5  .    -0.150

# category ARRAY_ELEMENT_SIZE
# the actual pixels are 0.075 by 0.150 mm
# We give the coarser dimension here.
loop_
_array_element_size.array_id
_array_element_size.index
_array_element_size.size
 ARRAY1 1 150e-6

# category ARRAY_INTENSITIES
loop_
_array_intensities.array_id
_array_intensities.binary_id
_array_intensities.linearity
_array_intensities.gain
_array_intensities.gain_esd
_array_intensities.overload
_array_intensities.undefined_value
 ARRAY1 1 linear 1.15 0.2 240000 0

 # category ARRAY_STRUCTURE
 loop_
```

```
       _array_structure.id
       _array_structure.encoding_type
       _array_structure.compression_type
       _array_structure.byte_order
       ARRAY1 "signed 32-bit integer" packed little_endian

      # category ARRAY_DATA
      loop_
      _array_data.array_id
      _array_data.binary_id
      _array_data.data
       ARRAY1 1
      ;
      --CIF-BINARY-FORMAT-SECTION--
      Content-Type: application/octet-stream;
          conversions="X-CBF_PACKED"
      Content-Transfer-Encoding: BASE64
      X-Binary-Size: 3801324
      X-Binary-ID: 1
      X-Binary-Element-Type: "signed 32-bit integer"
      Content-MD5: 07lZFvF+aOcW85IN7usl8A==

      AABRAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAZBQSr1sKNBOeOe9HITdMdDUnbq7bg
      ...
      8REo6TtBrxJ1vKqAvx9YDMD6J18Qg83OMr/tgssjMIJMXATDsZobL90AEXc4KigE

      --CIF-BINARY-FORMAT-SECTION----
      ;
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
       save_


save__diffrn_scan.id
    _item_description.description
;             The value of _diffrn_scan.id uniquely identifies each
              scan.  The identifier is used to tie together all the
              information about the scan.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
       '_diffrn_scan.id'                 diffrn_scan             yes
       '_diffrn_scan_axis.scan_id'       diffrn_scan_axis        yes
       '_diffrn_scan_frame.scan_id'      diffrn_scan_frame       yes
    _item_type.code              code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
       '_diffrn_scan_axis.scan_id'          '_diffrn_scan.id'
       '_diffrn_scan_frame.scan_id'         '_diffrn_scan.id'
     save_


save__diffrn_scan.date_end
    _item_description.description
;             The date and time of the end of the scan.  Note that this
              may be an estimate generated during the scan, before the
              precise time of the end of the scan is known.
;
    _item.name                '_diffrn_scan.date_end'
    _item.category_id         diffrn_scan
    _item.mandatory_code      no
    _item_type.code           yyyy-mm-dd
     save_


save__diffrn_scan.date_start
    _item_description.description
;             The date and time of the start of the scan.
;
    _item.name                '_diffrn_scan.date_start'
    _item.category_id         diffrn_scan
    _item.mandatory_code      no
    _item_type.code           yyyy-mm-dd
     save_


save__diffrn_scan.integration_time
    _item_description.description
;             Approximate average time in seconds to integrate each
              step of the scan.  The precise time for integration
              of each particular step must be provided in
              _diffrn_scan_frame.integration_time, even
              if all steps have the same integration time.
;
    _item.name                '_diffrn_scan.integration_time'
    _item.category_id         diffrn_scan
    _item.mandatory_code      no
    _item_type.code           float
    _item_units.code          'seconds'
     loop_
    _item_range.maximum
    _item_range.minimum
                           .   0.0
     save_


save__diffrn_scan.frame_id_start
    _item_description.description
;             The value of this data item is the identifier of the
              first frame in the scan.

              This item is a pointer to _diffrn_data_frame.id in the
              DIFFRN_DATA_FRAME category.
;
    _item.name                '_diffrn_scan.frame_id_start'
    _item.category_id         diffrn_scan
    _item.mandatory_code      yes
    _item_type.code           code
     save_


save__diffrn_scan.frame_id_end
    _item_description.description
;             The value of this data item is the identifier of the
              last frame in the scan.

              This item is a pointer to _diffrn_data_frame.id in the
              DIFFRN_DATA_FRAME category.
;
    _item.name                '_diffrn_scan.frame_id_end'
    _item.category_id         diffrn_scan
    _item.mandatory_code      yes
    _item_type.code           code
     save_


save__diffrn_scan.frames
    _item_description.description
;             The value of this data item is the number of frames in
              the scan.
;
    _item.name                '_diffrn_scan.frames'
    _item.category_id         diffrn_scan
    _item.mandatory_code      no
    _item_type.code           int
     loop_
    _item_range.maximum
    _item_range.minimum
                           .   1
                           1   1
     save_
```

```
####################
# DIFFRN_SCAN_AXIS #
####################

save_DIFFRN_SCAN_AXIS
    _category.description
;     Data items in the DIFFRN_SCAN_AXIS category describe the settings of
      axes for particular scans.  Unspecified axes are assumed to be at
      their zero points.
;
    _category.id                  diffrn_scan_axis
    _category.mandatory_code      no
     loop_
    _category_key.name
                                 '_diffrn_scan_axis.scan_id'
                                 '_diffrn_scan_axis.axis_id'
     loop_
    _category_group.id           'inclusive_group'
                                 'diffrn_group'
     save_


save__diffrn_scan_axis.scan_id
    _item_description.description
;               The value of this data item is the identifier of the
                scan for which axis settings are being specified.

                Multiple axes may be specified for the same value of
                _diffrn_scan.id.

                This item is a pointer to _diffrn_scan.id in the
                DIFFRN_SCAN category.
;
    _item.name                '_diffrn_scan_axis.scan_id'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      yes
    _item_type.code           code
     save_


save__diffrn_scan_axis.axis_id
    _item_description.description
;               The value of this data item is the identifier of one of
                the axes for the scan for which settings are being specified.

                Multiple axes may be specified for the same value of
                _diffrn_scan.id.

                This item is a pointer to _axis.id in the
                AXIS category.
;
    _item.name                '_diffrn_scan_axis.axis_id'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      yes
    _item_type.code           code
     save_


save__diffrn_scan_axis.angle_start
    _item_description.description
;               The starting position for the specified axis in degrees.
;
    _item.name                '_diffrn_scan_axis.angle_start'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'degrees'
     save_


save__diffrn_scan_axis.angle_range
    _item_description.description
;               The range from the starting position for the specified axis
                in degrees.
;
    _item.name                '_diffrn_scan_axis.angle_range'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'degrees'
     save_


save__diffrn_scan_axis.angle_increment
    _item_description.description
;               The increment for each step for the specified axis
                in degrees.  In general, this will agree with
                _diffrn_scan_frame_axis.angle_increment. The
                sum of the values of _diffrn_scan_frame_axis.angle and
                _diffrn_scan_frame_axis.angle_increment is the
                angular setting of the axis at the end of the integration
                time for a given frame.  If the individual frame values
                vary, then the value of
                _diffrn_scan_axis.angle_increment will be
                representative
                of the ensemble of values of
                _diffrn_scan_frame_axis.angle_increment (e.g.
                the mean).
;
    _item.name                '_diffrn_scan_axis.angle_increment'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'degrees'
     save_


save__diffrn_scan_axis.angle_rstrt_incr
    _item_description.description
;               The increment after each step for the specified axis
                in degrees.  In general, this will agree with
                _diffrn_scan_frame_axis.angle_rstrt_incr.  The
                sum of the values of _diffrn_scan_frame_axis.angle,
                _diffrn_scan_frame_axis.angle_increment
                and  _diffrn_scan_frame_axis.angle_rstrt_incr is the
                angular setting of the axis at the start of the integration
                time for the next frame relative to a given frame and
                should equal _diffrn_scan_frame_axis.angle for this
                next frame.   If the individual frame values
                vary, then the value of
                _diffrn_scan_axis.angle_rstrt_incr will be
                representative
                of the ensemble of values of
                _diffrn_scan_frame_axis.angle_rstrt_incr (e.g.
                the mean).
;
    _item.name                '_diffrn_scan_axis.angle_rstrt_incr'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'degrees'
     save_


save__diffrn_scan_axis.displacement_start
    _item_description.description
;               The starting position for the specified axis in millimetres.
;
```

```
    _item.name                '_diffrn_scan_axis.displacement_start'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'millimetres'
     save_


save__diffrn_scan_axis.displacement_range
    _item_description.description
;              The range from the starting position for the specified axis
               in millimetres.
;
    _item.name                '_diffrn_scan_axis.displacement_range'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'millimetres'
     save_


save__diffrn_scan_axis.displacement_increment
    _item_description.description
;              The increment for each step for the specified axis
               in millimetres.  In general, this will agree with
               _diffrn_scan_frame_axis.displacement_increment.
               The sum of the values of
               _diffrn_scan_frame_axis.displacement and
               _diffrn_scan_frame_axis.displacement_increment is the
               angular setting of the axis at the end of the integration
               time for a given frame.  If the individual frame values
               vary, then the value of
               _diffrn_scan_axis.displacement_increment will be
               representative
               of the ensemble of values of
               _diffrn_scan_frame_axis.displacement_increment (e.g.
               the mean).
;
    _item.name                '_diffrn_scan_axis.displacement_increment'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'millimetres'
     save_


save__diffrn_scan_axis.displacement_rstrt_incr
    _item_description.description
;              The increment for each step for the specified axis
               in millimetres.  In general, this will agree with
               _diffrn_scan_frame_axis.displacement_rstrt_incr.
               The sum of the values of
               _diffrn_scan_frame_axis.displacement,
               _diffrn_scan_frame_axis.displacement_increment and
               _diffrn_scan_frame_axis.displacement_rstrt_incr is the
               angular setting of the axis at the start of the integration
               time for the next frame relative to a given frame and
               should equal _diffrn_scan_frame_axis.displacement
               for this next frame.  If the individual frame values
               vary, then the value of
               _diffrn_scan_axis.displacement_rstrt_incr will be
               representative
               of the ensemble of values of
               _diffrn_scan_frame_axis.displacement_rstrt_incr (e.g.
               the mean).
;
    _item.name                '_diffrn_scan_axis.displacement_rstrt_incr'
    _item.category_id         diffrn_scan_axis
    _item.mandatory_code      no
    _item_default.value       0.0
    _item_type.code           float
    _item_units.code          'millimetres'
     save_


save__diffrn_scan_axis.reference_angle
     _item_description.description
;              The setting of the specified axis in degrees
               against which measurements of the reference beam center
               and reference detector distance should be made.

               In general, this will agree with
               _diffrn_scan_frame_axis.reference_angle.

               If the individual frame values vary, then the value of
               _diffrn_scan_axis.reference_angle will be
               representative of the ensemble of values of
               _diffrn_scan_frame_axis.reference_angle (e.g.
               the mean).

               If not specified, the value defaults to zero.
;
     _item.name                '_diffrn_scan_axis.reference_angle'
     _item.category_id         diffrn_scan_axis
     _item.mandatory_code      implicit
     _item_default.value       0.0
     _item_type.code           float
     _item_units.code          'degrees'
      save_


save__diffrn_scan_axis.reference_displacement
     _item_description.description
;              The setting of the specified axis in millimetres
               against which measurements of the reference beam center
               and reference detector distance should be made.

               In general, this will agree with
               _diffrn_scan_frame_axis.reference_displacement.

               If the individual frame values vary, then the value of
               _diffrn_scan_axis.reference_displacement will be
               representative of the ensemble of values of
               _diffrn_scan_frame_axis.reference_displacement (e.g.
               the mean).

               If not specified, the value defaults to to the value of
               _diffrn_scan_axis.displacement.
;
     _item.name                '_diffrn_scan_axis.reference_displacement'
     _item.category_id         diffrn_scan_axis
     _item.mandatory_code      implicit
     _item_type.code           float
     _item_units.code          'millimetres'
      save_



####################
# DIFFRN_SCAN_FRAME #
####################

save_DIFFRN_SCAN_FRAME
    _category.description
;           Data items in the DIFFRN_SCAN_FRAME category describe
            the relationships of particular frames to scans.
;
    _category.id                 diffrn_scan_frame
    _category.mandatory_code     no
     loop_
    _category_key.name
                                '_diffrn_scan_frame.scan_id'
```

```
                                '_diffrn_scan_frame.frame_id'
     loop_
    _category_group.id           'inclusive_group'
                                 'diffrn_group'
     save_


save__diffrn_scan_frame.date
    _item_description.description
;               The date and time of the start of the frame being scanned.
;
    _item.name                  '_diffrn_scan_frame.date'
    _item.category_id           diffrn_scan_frame
    _item.mandatory_code        no
    _item_type.code             yyyy-mm-dd
     save_


save__diffrn_scan_frame.frame_id
    _item_description.description
;               The value of this data item is the identifier of the
                frame being examined.

                This item is a pointer to _diffrn_data_frame.id in the
                DIFFRN_DATA_FRAME category.
;
    _item.name                  '_diffrn_scan_frame.frame_id'
    _item.category_id           diffrn_scan_frame
    _item.mandatory_code        yes
    _item_type.code             code
     save_


save__diffrn_scan_frame.frame_number
    _item_description.description
;               The value of this data item is the number of the frame
                within the scan, starting with 1.  It is not necessarily
                the same as the value of _diffrn_scan_frame.frame_id,
                but it may be.

;
    _item.name                  '_diffrn_scan_frame.frame_number'
    _item.category_id           diffrn_scan_frame
    _item.mandatory_code        no
    _item_type.code             int
     loop_
    _item_range.maximum
    _item_range.minimum
                            .   0
                            0   0
     save_


save__diffrn_scan_frame.integration_time
    _item_description.description
;               The time in seconds to integrate this step of the scan.
                This should be the precise time of integration of each
                particular frame.  The value of this data item should
                be given explicitly for each frame and not inferred
                from the value of _diffrn_scan.integration_time.
;
    _item.name                  '_diffrn_scan_frame.integration_time'
    _item.category_id           diffrn_scan_frame
    _item.mandatory_code        yes
    _item_type.code             float
    _item_units.code            'seconds'
     loop_
    _item_range.maximum
    _item_range.minimum
                            .   0.0
     save_
```

```
save__diffrn_scan_frame.scan_id
    _item_description.description
;               The value of _diffrn_scan_frame.scan_id identifies the scan
                containing this frame.

                This item is a pointer to _diffrn_scan.id in the
                DIFFRN_SCAN category.
;
    _item.name              '_diffrn_scan_frame.scan_id'
    _item.category_id         diffrn_scan_frame
    _item.mandatory_code      yes
    _item_type.code           code
     save_


#########################
# DIFFRN_SCAN_FRAME_AXIS #
#########################

save_DIFFRN_SCAN_FRAME_AXIS
    _category.description
;     Data items in the DIFFRN_SCAN_FRAME_AXIS category describe the
      settings of axes for particular frames.  Unspecified axes are
      assumed to be at their zero points.  If, for any given frame,
      nonzero values apply for any of the data items in this category,
      those values should be given explicitly in this category and not
      simply inferred from values in DIFFRN_SCAN_AXIS.
;
    _category.id                    diffrn_scan_frame_axis
    _category.mandatory_code        no
     loop_
    _category_key.name
                                   '_diffrn_scan_frame_axis.frame_id'
                                   '_diffrn_scan_frame_axis.axis_id'
     loop_
    _category_group.id             'inclusive_group'
                                   'diffrn_group'
     save_


save__diffrn_scan_frame_axis.axis_id
    _item_description.description
;               The value of this data item is the identifier of one of
                the axes for the frame for which settings are being specified.

                Multiple axes may be specified for the same value of
                _diffrn_scan_frame.frame_id.

                This item is a pointer to _axis.id in the
                AXIS category.
;
    _item.name                  '_diffrn_scan_frame_axis.axis_id'
    _item.category_id           diffrn_scan_frame_axis
    _item.mandatory_code        yes
    _item_type.code             code
     save_


save__diffrn_scan_frame_axis.angle
    _item_description.description
;               The setting of the specified axis in degrees for this frame.
                This is the setting at the start of the integration time.
;
    _item.name                  '_diffrn_scan_frame_axis.angle'
    _item.category_id           diffrn_scan_frame_axis
    _item.mandatory_code        no
    _item_default.value         0.0
    _item_type.code             float
    _item_units.code            'degrees'
     save_
```

```
save__diffrn_scan_frame_axis.angle_increment
    _item_description.description
;               The increment for this frame for the angular setting of
                the specified axis in degrees.  The sum of the values
                of _diffrn_scan_frame_axis.angle and
                _diffrn_scan_frame_axis.angle_increment is the
                angular setting of the axis at the end of the integration
                time for this frame.
;
    _item.name                '_diffrn_scan_frame_axis.angle_increment'
    _item.category_id          diffrn_scan_frame_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'degrees'
     save_


save__diffrn_scan_frame_axis.angle_rstrt_incr
    _item_description.description
;               The increment after this frame for the angular setting of
                the specified axis in degrees.  The sum of the values
                of _diffrn_scan_frame_axis.angle,
                _diffrn_scan_frame_axis.angle_increment and
                _diffrn_scan_frame_axis.angle_rstrt_incr is the
                angular setting of the axis at the start of the integration
                time for the next frame and should equal
                _diffrn_scan_frame_axis.angle for this next frame.
;
    _item.name               '_diffrn_scan_frame_axis.angle_rstrt_incr'
    _item.category_id          diffrn_scan_frame_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'degrees'
     save_


save__diffrn_scan_frame_axis.displacement
    _item_description.description
;               The setting of the specified axis in millimetres for this
                frame.  This is the setting at the start of the integration
                time.
;
    _item.name               '_diffrn_scan_frame_axis.displacement'
    _item.category_id          diffrn_scan_frame_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'millimetres'
     save_


save__diffrn_scan_frame_axis.displacement_increment
    _item_description.description
;               The increment for this frame for the displacement setting of
                the specified axis in millimetres.  The sum of the values
                of _diffrn_scan_frame_axis.displacement and
                _diffrn_scan_frame_axis.displacement_increment is the
                angular setting of the axis at the end of the integration
                time for this frame.
;
    _item.name               '_diffrn_scan_frame_axis.displacement_increment'
    _item.category_id          diffrn_scan_frame_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'millimetres'
     save_
```

```
save__diffrn_scan_frame_axis.displacement_rstrt_incr
    _item_description.description
;               The increment for this frame for the displacement setting of
                the specified axis in millimetres.  The sum of the values
                of _diffrn_scan_frame_axis.displacement,
                _diffrn_scan_frame_axis.displacement_increment and
                _diffrn_scan_frame_axis.displacement_rstrt_incr is the
                angular setting of the axis at the start of the integration
                time for the next frame and should equal
                _diffrn_scan_frame_axis.displacement for this next frame.
;
    _item.name               '_diffrn_scan_frame_axis.displacement_rstrt_incr'
    _item.category_id          diffrn_scan_frame_axis
    _item.mandatory_code       no
    _item_default.value        0.0
    _item_type.code            float
    _item_units.code           'millimetres'
     save_

save__diffrn_scan_frame_axis.frame_id
    _item_description.description
;               The value of this data item is the identifier of the
                frame for which axis settings are being specified.

                Multiple axes may be specified for the same value of
                _diffrn_scan_frame.frame_id.

                This item is a pointer to _diffrn_data_frame.id in the
                DIFFRN_DATA_FRAME category.
;
    _item.name               '_diffrn_scan_frame_axis.frame_id'
    _item.category_id          diffrn_scan_frame_axis
    _item.mandatory_code       yes
    _item_type.code            code
     save_

save__diffrn_scan_frame_axis.reference_angle
     _item_description.description
;               The setting of the specified axis in degrees
                against which measurements of the reference beam center
                and reference detector distance should be made.

                This is normally the same for all frames, but the
                option is provided here of making changes when
                needed.

                If not provided, it is assumed to be zero.
;
     _item.name               '_diffrn_scan_frame_axis.reference_angle'
     _item.category_id          diffrn_scan_frame_axis
     _item.mandatory_code       implicit
     _item_default.value        0.0
     _item_type.code            float
     _item_units.code           'degrees'
      save_


save__diffrn_scan_frame_axis.reference_displacement
     _item_description.description
;               The setting of the specified axis in millimetres for this
                frame against which measurements of the reference beam center
                and reference detector distance should be made.

                This is normally the same for all frames, but the
                option is provided here of making changes when
                needed.

                If not provided, it is assumed to be equal to
                _diffrn_scan_frame_axis.displacement.
;
     _item.name               '_diffrn_scan_frame_axis.reference_displacement'
     _item.category_id          diffrn_scan_frame_axis
```

```
     _item.mandatory_code       implicit
     _item_type.code            float
     _item_units.code           'millimetres'
      save_



#######
# MAP #
#######

save_MAP
    _category.description
;             Data items in the MAP category record
              the details of a maps. Maps record values of parameters,
              such as density, that are functions of position within
              a cell or are functions of orthogonal coordinates in
              three space.

              A map may is composed of one or more map segments
              specified in the MAP_SEGMENT category.

              Examples are given in the MAP_SEGMENT category.
;
    _category.id                  map
    _category.mandatory_code      no
     loop_
    _category_key.name            '_map.id'
                                  '_map.diffrn_id'
                                  '_map.entry_id'
    loop_
    _category_group.id            'inclusive_group'
                                  'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - Identifying an observed density map
                and a calculated density map
;
;

        loop_
        _map.id
        _map.details

        rho_calc
   ;
        density calculated from F_calc derived from the ATOM_SITE list
   ;
        rho_obs
   ;
        density combining the observed structure factors with the
        calculated phases
   ;
;

# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
    save_


save__map.details
     _item_description.description
;              The value of _map.details should give a
               description of special aspects of each map.

;
    _item.name                  '_map.details'
    _item.category_id             map
    _item.mandatory_code          no
    _item_type.code               text
     loop_
```

```
    _item_examples.case
    _item_examples.detail
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - Identifying an observed density map
                and a calculated density map
;
;

        loop_
        _map.id
        _map.details

        rho_calc
    ;
        density calculated from F_calc derived from the ATOM_SITE list
    ;
        rho_obs
    ;
        density combining the observed structure factors with the
        calculated phases
    ;
;

# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      save_

save__map.diffrn_id
    _item_description.description
;             This item is a pointer to _diffrn.id in the
              DIFFRN category.
;
    _item.name                  '_map.diffrn_id'
    _item.category_id             map
    _item.mandatory_code          implicit
    _item_type.code               code
     save_

save__map.entry_id
    _item_description.description
;             This item is a pointer to _entry.id in the
              ENTRY category.
;
    _item.name                  '_map.entry_id'
    _item.category_id             map
    _item.mandatory_code          implicit
    _item_type.code               code
     save_


save__map.id
    _item_description.description
;             The value of _map.id must uniquely identify
              each map for the given diffrn.id or entry.id.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
           '_map.id'                map          yes
          '_map_segment.id'         map_segment  yes
    _item_type.code               code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
          '_map_segment.id'         '_map.id'
     save_



##########################
# MAP_SEGMENT #
```

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


save_MAP_SEGMENT
    _category.description
;             Data items in the MAP_SEGMENT category record
              the details about each segment (section or brick) of a map.
;
    _category.id                   map_segment
    _category.mandatory_code       no
     loop_
    _category_key.name             '_map_segment.id'
                                   '_map_segment.map_id'
    loop_
    _category_group.id             'inclusive_group'
                                   'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - Identifying an observed density map
                and a calculated density map, each consisting of one
                segment, both using the same array structure
                and mask.
;
;

        loop_
        _map.id
        _map.details

        rho_calc
     ;
        density calculated from F_calc derived from the ATOM_SITE list
     ;
        rho_obs
     ;
        density combining the observed structure factors with the
        calculated phases
     ;

        loop_
        _map_segment.map_id
        _map_segment.id
        _map_segment.array_id
        _map_segment.binary_id
        _map_segment.mask_array_id
        _map_segment.mask_binary_id
        rho_calc rho_calc map_structure 1 mask_structure 1
        rho_obs  rho_obs  map_structure 2 mask_structure 1
;

# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
    save_


save__map_segment.array_id
    _item_description.description
;             The value of _map_segment.array_id identifies the array structure
              into which the map is organized.

              This item is a pointer to _array_structure.id in the
              ARRAY_STRUCTURE category.
;
    _item.name                  '_map_segment.array_id'
    _item.category_id             map_segment
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__map_segment.binary_id
    _item_description.description
;             The value of _map_segment.binary_id distinguishes the particular
              set of data organized according to _map_segment.array_id in
              which the data values of the map are stored.

              This item is a pointer to _array_data.binary_id in the
              ARRAY_DATA category.
;
    _item.name                  '_map_segment.binary_id'
    _item.category_id             map_segment
    _item.mandatory_code          implicit
    _item_type.code               int
     save_

save__map_segment.mask_array_id
    _item_description.description
;             The value of _map_segment.mask_array_id, if given, the array
              structure into which the mask for the map is organized.  If no
              value is given, then all elements of the map are valid.  If a
              value is given, then only elements of the map for which the
              corresponding element of the mask is non-zero are valid.  The
              value of _map_segment.mask_array_id differs from the value of
              _map_segment.array_id in order to permit the mask to be given
              as, say, unsigned 8-bit integers, while the map is given as
              a data type with more range.  However, the two array structures
              must be aligned, using the same axes in the same order with the
              same displacements and increments

              This item is a pointer to _array_structure.id in the
              ARRAY_STRUCTURE category.
;
    _item.name                  '_map_segment.mask_array_id'
    _item.category_id             map_segment
    _item.mandatory_code          no
    _item_type.code               code
     save_


save__map_segment.mask_binary_id
    _item_description.description
;             The value of _map_segment.mask_binary_id identifies the
              particular set of data organized according to
              _map_segment.mask_array_id specifying the mask for the map.

              This item is a pointer to _array_data.mask_binary_id in the
              ARRAY_DATA category.
;
    _item.name                  '_map_segment.mask_binary_id'
    _item.category_id             map_segment
    _item.mandatory_code          implicit
    _item_type.code               int
     save_


save__map_segment.id
    _item_description.description
;             The value of _map_segment.id must uniquely
              identify each segment of a map.
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
           '_map_segment.id'
           map_segment
           yes
    _item_type.code               code
     loop_
    _item_linked.child_name
    _item_linked.parent_name
           '_map_data_frame.map_segment_id'
           '_map_segment.id'
```

```
     save_


save__map_segment.map_id
    _item_description.description
;               This item is a pointer to _map.id
                in the MAP category.
;
    _item.name                  '_map_segment.map_id'
    _item.category_id             map_segment
    _item.mandatory_code          yes
    _item_type.code               code
     save_

save__map_segment.details
     _item_description.description
;               The value of _map_segment.details should give a
                description of special aspects of each segment of a map.

;
    _item.name                  '_map_segment.details'
    _item.category_id             map_segment
    _item.mandatory_code          no
    _item_type.code               text
     loop_
    _item_examples.case
    _item_examples.detail
;                Example to be provided
;
;

;
      save_


#########################   DEPRECATED DATA ITEMS ########################

save__diffrn_detector_axis.id
    _item_description.description
;               This data item is a pointer to _diffrn_detector.id in
                the DIFFRN_DETECTOR category.

                DEPRECATED -- DO NOT USE
;
    _item.name                  '_diffrn_detector_axis.id'
    _item.category_id             diffrn_detector_axis
    _item.mandatory_code          yes
    _item_type.code               code
     save_

save__diffrn_measurement_axis.id
    _item_description.description
;               This data item is a pointer to _diffrn_measurement.id in
                the DIFFRN_MEASUREMENT category.

                DEPRECATED -- DO NOT USE
;
    _item.name                  '_diffrn_measurement_axis.id'
    _item.category_id             diffrn_measurement_axis
    _item.mandatory_code          yes
    _item_type.code               code
     save_

#########################   DEPRECATED CATEGORY ##########################
####################
# DIFFRN_FRAME_DATA #
####################


save_DIFFRN_FRAME_DATA
    _category.description
;             Data items in the DIFFRN_FRAME_DATA category record
              the details about each frame of data.

              The items in this category are now in the
              DIFFRN_DATA_FRAME category.

              The items in the DIFFRN_FRAME_DATA category
              are now deprecated.  The items from this category
              are provided as aliases in the 1.0 dictionary
              or, in the case of _diffrn_frame_data.details,
              in the 1.4 dictionary.  THESE ITEMS SHOULD NOT
              BE USED FOR NEW WORK.

              The items from the old category are provided
              in this dictionary for completeness
              but should not be used or cited.  To avoid
              confusion, the example has been removed
              and the redundant parent-child links to other
              categories have been removed.
;
    _category.id                    diffrn_frame_data
    _category.mandatory_code        no
     loop_
    _category_key.name              '_diffrn_frame_data.id'
                                    '_diffrn_frame_data.detector_element_id'
    loop_
    _category_group.id              'inclusive_group'
                                    'array_data_group'
    loop_
    _category_examples.detail
    _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;
    THE DIFFRN_FRAME_DATA category is deprecated and should not be used.
;
;
       # EXAMPLE REMOVED #
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
    save_


save__diffrn_frame_data.array_id
    _item_description.description
;             This item is a pointer to _array_structure.id in the
              ARRAY_STRUCTURE category.

              DEPRECATED -- DO NOT USE
;
    _item.name                  '_diffrn_frame_data.array_id'
    _item.category_id             diffrn_frame_data
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__diffrn_frame_data.binary_id
    _item_description.description
;             This item is a pointer to _array_data.binary_id in the
              ARRAY_STRUCTURE category.

              DEPRECATED -- DO NOT USE
;
    _item.name                  '_diffrn_frame_data.binary_id'
    _item.category_id             diffrn_frame_data
    _item.mandatory_code          implicit
    _item_type.code               int
     save_


save__diffrn_frame_data.detector_element_id
    _item_description.description
```

```
;             This item is a pointer to _diffrn_detector_element.id
              in the DIFFRN_DETECTOR_ELEMENT category.

              DEPRECATED -- DO NOT USE
;
    _item.name                  '_diffrn_frame_data.detector_element_id'
    _item.category_id             diffrn_frame_data
    _item.mandatory_code          yes
    _item_type.code               code
     save_


save__diffrn_frame_data.id
    _item_description.description
;             The value of _diffrn_frame_data.id must uniquely identify
              each complete frame of data.

              DEPRECATED -- DO NOT USE
;
     loop_
    _item.name
    _item.category_id
    _item.mandatory_code
          '_diffrn_frame_data.id'        diffrn_frame_data  yes
    _item_type.code               code
     save_

save__diffrn_frame_data.details
     _item_description.description
;             The value of _diffrn_data_frame.details should give a
              description of special aspects of each frame of data.

              DEPRECATED -- DO NOT USE
;
     _item.name                 '_diffrn_frame_data.details'
     _item.category_id            diffrn_frame_data
     _item.mandatory_code         no
     _item_type.code              text
      save_

################ END DEPRECATED SECTION ###########


####################
## ITEM_TYPE_LIST ##
####################
#
#
#  The regular expressions defined here are not compliant
#  with the POSIX 1003.2 standard as they include the
#  '\n' and '\t' special characters.  These regular expressions
#  have been tested using version 0.12 of Richard Stallman's
#  GNU regular expression library in POSIX mode.
#  In order to allow presentation of a regular expression
#  in a text field concatenate any line ending in a backslash
#  with the following line, after discarding the backslash.
#
#  A formal definition of the '\n' and '\t' special characters
#  is most properly done in the DDL, but for completeness, please
#  note that '\n' is the line termination character ('newline')
#  and '\t' is the horizontal tab character.  There is a formal
#  ambiguity in the use of '\n' for line termination, in that
#  the intention is that the equivalent machine/OS-dependent line
#  termination character sequence should be accepted as a match, e.g.
#
#      '\r' (control-M) under MacOS
#      '\n' (control-J) under Unix
#      '\r\n' (control-M control-J) under DOS and MS Windows
#
     loop_
    _item_type_list.code
    _item_type_list.primitive_code
    _item_type_list.construct
    _item_type_list.detail
                code      char
                '[_,.;:"&<>()/\{}'`~!@#$%A-Za-z0-9*|+-]*'
;               code item types/single words ...
;
                ucode      uchar
                '[_,.;:"&<>()/\{}'`~!@#$%A-Za-z0-9*|+-]*'
;               code item types/single words (case insensitive) ...
;
                line      char
                '[][ \t_(),.;:"&<>/\{}'`~!@#$%?+=*A-Za-z0-9|^-]*'
;               char item types / multi-word items ...
;
                uline     uchar
                '[][ \t_(),.;:"&<>/\{}'`~!@#$%?+=*A-Za-z0-9|^-]*'
;               char item types / multi-word items (case insensitive)...
;
                text      char
              '[][ \n\t()_,.;:"&<>/\{}'`~!@#$%?+=*A-Za-z0-9|^-]*'
;               text item types / multi-line text ...
;
                binary    char
;\n--CIF-BINARY-FORMAT-SECTION--\n\
[][ \n\t()_,.;:"&<>/\{}'`~!@#$%?+=*A-Za-z0-9|^-]*\
\n--CIF-BINARY-FORMAT-SECTION----
;
;               binary items are presented as MIME-like ascii-encoded
                sections in an imgCIF.  In a CBF, raw octet streams
                are used to convey the same information.
;
                int       numb
                '-?[0-9]+'
;               int item types are the subset of numbers that are the negative
                or positive integers.
;
                float     numb
          '-?(([0-9]+)[.]?|([0-9]*[.][0-9]+))([][0-9]+[])?([eE][+-]?[0-9]+)?'
;               float item types are the subset of numbers that are the floating
                point numbers.
;
                any       char
                '.*'
;               A catch all for items that may take any form...
;
                yyyy-mm-dd  char
;\
[0-9]?[0-9]?[0-9][0-9]-[0-9]?[0-9]-[0-9]?[0-9]\
((T[0-2][0-9](:[0-5][0-9](:[0-5][0-9](.[0-9]+)?)?)?)?\
([+-][0-5][0-9]:[0-5][0-9]))?
;
;
                Standard format for CIF date and time strings (see
                http://www.iucr.org/iucr-top/cif/spec/datetime.html),
                consisting of a yyyy-mm-dd date optionally followed by
                the character 'T' followed by a 24-hour clock time,
                optionally followed by a signed time-zone offset.

                The IUCr standard has been extended to allow for an optional
                decimal fraction on the seconds of time.

                Time is local time if no time-zone offset is given.

                Note that this type extends the mmCIF yyyy-mm-dd type
                but does not conform to the mmCIF yyyy-mm-dd:hh:mm
                type that uses a ':' in place if the 'T' specified
                by the IUCr standard.  For reading, both forms should
                be accepted,  but for writing, only the IUCr form should
                be used.

                For maximal compatibility, the special time zone
                indicator 'Z' (for 'zulu') should be accepted on
```

```
              reading in place of '+00:00' for GMT.
;


####################
## ITEM_UNITS_LIST ##
####################

     loop_
    _item_units_list.code
    _item_units_list.detail
#
     'metres'                 'metres'
     'centimetres'            'centimetres (metres * 10^( -2)^)'
     'millimetres'            'millimetres (metres * 10^( -3)^)'
     'nanometres'             'nanometres  (metres * 10^( -9)^)'
     'angstroms'              '\%Angstroms   (metres * 10^(-10)^)'
     'picometres'             'picometres  (metres * 10^(-12)^)'
     'femtometres'            'femtometres (metres * 10^(-15)^)'
#
     'reciprocal_metres'      'reciprocal metres (metres^(-1)^)'
     'reciprocal_centimetres'
        'reciprocal centimetres ((metres * 10^( -2)^)^(-1)^)'
     'reciprocal_millimetres'
        'reciprocal millimetres ((metres * 10^( -3)^)^(-1)^)'
     'reciprocal_nanometres'
        'reciprocal nanometres  ((metres * 10^( -9)^)^(-1)^)'
     'reciprocal_angstroms'
        'reciprocal \%Angstroms   ((metres * 10^(-10)^)^(-1)^)'
     'reciprocal_picometres'
        'reciprocal picometres  ((metres * 10^(-12)^)^(-1)^)'
#
     'nanometres_squared'     'nanometres squared (metres * 10^( -9)^)^2^'
     'angstroms_squared'      '\%Angstroms squared  (metres * 10^(-10)^)^2^'
     '8pi2_angstroms_squared'
       '8\p^2^ * \%Angstroms squared (metres * 10^(-10)^)^2^'
     'picometres_squared'     'picometres squared (metres * 10^(-12)^)^2^'
#
     'nanometres_cubed'       'nanometres cubed (metres * 10^( -9)^)^3^'
     'angstroms_cubed'        '\%Angstroms cubed  (metres * 10^(-10)^)^3^'
     'picometres_cubed'       'picometres cubed (metres * 10^(-12)^)^3^'
#
     'kilopascals'            'kilopascals'
     'gigapascals'            'gigapascals'
#
     'hours'                  'hours'
     'minutes'                'minutes'
     'seconds'                'seconds'
     'microseconds'           'microseconds'
#
     'degrees'                'degrees (of arc)'
     'degrees_squared'        'degrees (of arc) squared'
#
     'degrees_per_minute'     'degrees (of arc) per minute'
#
     'celsius'                'degrees (of temperature) Celsius'
     'kelvins'                'degrees (of temperature) Kelvin'
#
     'counts'                 'counts'
     'counts_per_photon'      'counts per photon'
#
     'electrons'              'electrons'
#
     'electrons_squared'      'electrons squared'
#
     'electrons_per_nanometres_cubed'
; electrons per nanometres cubed (electrons/(metres * 10^( -9)^)^(-3)^)
;
     'electrons_per_angstroms_cubed'
; electrons per \%Angstroms cubed (electrons/(metres * 10^(-10)^)^(-3)^)
;
     'electrons_per_picometres_cubed'
; electrons per picometres cubed (electrons/(metres * 10^(-12)^)^(-3)^)
;
     'kilowatts'              'kilowatts'
     'milliamperes'           'milliamperes'
     'kilovolts'              'kilovolts'
#
     'pixels_per_element'     '(image) pixels per (array) element'
#
     'arbitrary'
; arbitrary system of units.
;
#


     loop_
    _item_units_conversion.from_code
    _item_units_conversion.to_code
    _item_units_conversion.operator
    _item_units_conversion.factor
###
     'metres'                   'centimetres'              '*'   1.0E+02
     'metres'                   'millimetres'              '*'   1.0E+03
     'metres'                   'nanometres'               '*'   1.0E+09
     'metres'                   'angstroms'                '*'   1.0E+10
     'metres'                   'picometres'               '*'   1.0E+12
     'metres'                   'femtometres'              '*'   1.0E+15
#
     'centimetres'              'metres'                   '*'   1.0E-02
     'centimetres'              'millimetres'              '*'   1.0E+01
     'centimetres'              'nanometres'               '*'   1.0E+07
     'centimetres'              'angstroms'                '*'   1.0E+08
     'centimetres'              'picometres'               '*'   1.0E+10
     'centimetres'              'femtometres'              '*'   1.0E+13
#
     'millimetres'              'metres'                   '*'   1.0E-03
     'millimetres'              'centimetres'              '*'   1.0E-01
     'millimetres'              'nanometres'               '*'   1.0E+06
     'millimetres'              'angstroms'                '*'   1.0E+07
     'millimetres'              'picometres'               '*'   1.0E+09
     'millimetres'              'femtometres'              '*'   1.0E+12
#
     'nanometres'               'metres'                   '*'   1.0E-09
     'nanometres'               'centimetres'              '*'   1.0E-07
     'nanometres'               'millimetres'              '*'   1.0E-06
     'nanometres'               'angstroms'                '*'   1.0E+01
     'nanometres'               'picometres'               '*'   1.0E+03
     'nanometres'               'femtometres'              '*'   1.0E+06
#
     'angstroms'                'metres'                   '*'   1.0E-10
     'angstroms'                'centimetres'              '*'   1.0E-08
     'angstroms'                'millimetres'              '*'   1.0E-07
     'angstroms'                'nanometres'               '*'   1.0E-01
     'angstroms'                'picometres'               '*'   1.0E+02
     'angstroms'                'femtometres'              '*'   1.0E+05
#
     'picometres'               'metres'                   '*'   1.0E-12
     'picometres'               'centimetres'              '*'   1.0E-10
     'picometres'               'millimetres'              '*'   1.0E-09
     'picometres'               'nanometres'               '*'   1.0E-03
     'picometres'               'angstroms'                '*'   1.0E-02
     'picometres'               'femtometres'              '*'   1.0E+03
#
     'femtometres'              'metres'                   '*'   1.0E-15
     'femtometres'              'centimetres'              '*'   1.0E-13
     'femtometres'              'millimetres'              '*'   1.0E-12
     'femtometres'              'nanometres'               '*'   1.0E-06
     'femtometres'              'angstroms'                '*'   1.0E-05
     'femtometres'              'picometres'               '*'   1.0E-03
###
     'reciprocal_centimetres'   'reciprocal_metres'        '*'   1.0E+02
     'reciprocal_centimetres'   'reciprocal_millimetres'   '*'   1.0E-01
     'reciprocal_centimetres'   'reciprocal_nanometres'    '*'   1.0E-07
     'reciprocal_centimetres'   'reciprocal_angstroms'     '*'   1.0E-08
```

```
     'reciprocal_centimetres'   'reciprocal_picometres'    '*'   1.0E-10
#
     'reciprocal_millimetres'   'reciprocal_metres'        '*'   1.0E+03
     'reciprocal_millimetres'   'reciprocal_centimetres'   '*'   1.0E+01
     'reciprocal_millimetres'   'reciprocal_nanometres'    '*'   1.0E-06
     'reciprocal_millimetres'   'reciprocal_angstroms'     '*'   1.0E-07
     'reciprocal_millimetres'   'reciprocal_picometres'    '*'   1.0E-09
#
     'reciprocal_nanometres'    'reciprocal_metres'        '*'   1.0E+09
     'reciprocal_nanometres'    'reciprocal_centimetres'   '*'   1.0E+07
     'reciprocal_nanometres'    'reciprocal_millimetres'   '*'   1.0E+06
     'reciprocal_nanometres'    'reciprocal_angstroms'     '*'   1.0E-01
     'reciprocal_nanometres'    'reciprocal_picometres'    '*'   1.0E-03
#
     'reciprocal_angstroms'     'reciprocal_metres'        '*'   1.0E+10
     'reciprocal_angstroms'     'reciprocal_centimetres'   '*'   1.0E+08
     'reciprocal_angstroms'     'reciprocal_millimetres'   '*'   1.0E+07
     'reciprocal_angstroms'     'reciprocal_nanometres'    '*'   1.0E+01
     'reciprocal_angstroms'     'reciprocal_picometres'    '*'   1.0E-02
#
     'reciprocal_picometres'    'reciprocal_metres'        '*'   1.0E+12
     'reciprocal_picometres'    'reciprocal_centimetres'   '*'   1.0E+10
     'reciprocal_picometres'    'reciprocal_millimetres'   '*'   1.0E+09
     'reciprocal_picometres'    'reciprocal_nanometres'    '*'   1.0E+03
     'reciprocal_picometres'    'reciprocal_angstroms'     '*'   1.0E+01
###
     'nanometres_squared'       'angstroms_squared'        '*'   1.0E+02
     'nanometres_squared'       'picometres_squared'       '*'   1.0E+06
#
     'angstroms_squared'        'nanometres_squared'       '*'   1.0E-02
     'angstroms_squared'        'picometres_squared'       '*'   1.0E+04
     'angstroms_squared'        '8pi2_angstroms_squared'   '*'   78.9568

#
     'picometres_squared'       'nanometres_squared'       '*'   1.0E-06
     'picometres_squared'       'angstroms_squared'        '*'   1.0E-04
###
     'nanometres_cubed'         'angstroms_cubed'          '*'   1.0E+03
     'nanometres_cubed'         'picometres_cubed'         '*'   1.0E+09
#
     'angstroms_cubed'          'nanometres_cubed'         '*'   1.0E-03
     'angstroms_cubed'          'picometres_cubed'         '*'   1.0E+06
#
     'picometres_cubed'         'nanometres_cubed'         '*'   1.0E-09
     'picometres_cubed'         'angstroms_cubed'          '*'   1.0E-06
###
     'kilopascals'              'gigapascals'              '*'   1.0E-06
     'gigapascals'              'kilopascals'              '*'   1.0E+06
###
     'hours'                    'minutes'                  '*'   6.0E+01
     'hours'                    'seconds'                  '*'   3.6E+03
     'hours'                    'microseconds'             '*'   3.6E+09
#
     'minutes'                  'hours'                    '/'   6.0E+01
     'minutes'                  'seconds'                  '*'   6.0E+01
     'minutes'                  'microseconds'             '*'   6.0E+07
#
     'seconds'                  'hours'                    '/'   3.6E+03
     'seconds'                  'minutes'                  '/'   6.0E+01
     'seconds'                  'microseconds'             '*'   1.0E+06
#
     'microseconds'             'hours'                    '/'   3.6E+09
     'microseconds'             'minutes'                  '/'   6.0E+07
     'microseconds'             'seconds'                  '/'   1.0E+06
###
     'celsius'                  'kelvins'                  '-'     273.0
     'kelvins'                  'celsius'                  '+'     273.0
###
     'electrons_per_nanometres_cubed'
     'electrons_per_angstroms_cubed'                       '*'   1.0E+03
     'electrons_per_nanometres_cubed'
     'electrons_per_picometres_cubed'                      '*'   1.0E+09
```

```
#
     'electrons_per_angstroms_cubed'
     'electrons_per_nanometres_cubed'                      '*'   1.0E-03
     'electrons_per_angstroms_cubed'
     'electrons_per_picometres_cubed'                      '*'   1.0E+06
#
     'electrons_per_picometres_cubed'
     'electrons_per_nanometres_cubed'                      '*'   1.0E-09
     'electrons_per_picometres_cubed'
     'electrons_per_angstroms_cubed'                       '*'   1.0E-06
###

########################
## DICTIONARY_HISTORY ##
########################

     loop_
    _dictionary_history.version
    _dictionary_history.update
    _dictionary_history.revision

   1.5.2   2007-05-06

;  Further clarifications of the coordinate system. (HJB)
;

   1.5.1   2007-04-26

;  Improve defintion of X-axis to cover the case of no goniometer
   and clean up more line folds (HJB)
;

   1.5     2007-07-25

;  This is a cummulative list of the changes proposed since the
   imgCIF workshop in Hawaii in July 2006.  It is the result
   of contributions by H. J. Bernstein, A. Hammersley,
   J. Wright and W. Kabsch.

   2007-02-19 Consolidated changes (edited by HJB)
     + Added new data items
       '_array_structure.compression_type_flag',
       '_array_structure_list_axis.fract_displacement',
       '_array_structure_list_axis.displacement_increment',
       '_array_structure_list_axis.reference_angle',
       '_array_structure_list_axis.reference_displacement',
       '_axis.system',
       '_diffrn_detector_element.reference_center_fast',
       '_diffrn_detector_element.reference_center_slow',
       '_diffrn_scan_axis.reference_angle',
       '_diffrn_scan_axis.reference_displacement',
       '_map.details', '_map.diffrn_id',
       '_map.entry_id', '_map.id',
       '_map_segment.array_id', '_map_segment.binary_id',
       '_map_segment.mask_array_id', '_map_segment.mask_binary_id',
       '_map_segment.id', '_map_segment.map_id',
       '_map_segment.details.
     + Change type of
       '_array_structure.byte_order' and
       '_array_structure.compression_type'
       to ucode to make these values case-insensitive
     + Add values 'packed_v2' and 'byte_offset' to enumeration of values for
       '_array_structure.compression_type'
     + Add to defintions for the binary data type to handle new compression types, maps,
       and a variety of new axis types.
    2007-07-25 Cleanup of typos for formal release (HJB)
     + Corrected text fields for reference_ tag descriptions that
       were off by one column
     + Fix typos in comments listing fract_ tags
     + Changed name of release from 1.5_DRAFT to 1.5
     + Fix unclosed text fields in various map definitions
```

```
;

   1.4     2006-07-04

;  This is a change to reintegrate all changes made in the course of
   publication of ITVG, by the RCSB from April 2005 through
   August 2008 and changes for the 2006 imgCIF workshop in
   Hawaii.

   2006-07-04 Consolidated changes for the 2006 imgCIF workshop (edited by HJB)
     + Correct type of '_array_structure_list.direction' from 'int' to 'code'.
     + Added new data items suggested by CN
       '_diffrn_data_frame.details'
       '_array_intensities.pixel_fast_bin_size',
       '_array_intensities.pixel_slow_bin_size and
       '_array_intensities.pixel_binning_method
     + Added deprecated item for completeness
       '_diffrn_frame_data.details'
     + Added entry for missing item in contents list
       '_array_structure_list_axis.displacement'
     + Added new MIME type X-BASE32K based on work by VL, KM, GD, HJB
     + Correct description of MIME boundary delimiter to start in
       column 1.
     + General cleanup of text fields to conform to changes for ITVG
       by removing empty lines at start and finish of text field.
     + Amend example for ARRAY_INTENSITIES to include binning.
     + Add local copy of type specification (as 'code') for all children
       of '_diffrn.id'.
     + For consistency, change all references to 'pi' to '\p' and all
       references to 'Angstroms' to '\%Angstroms'.
     + Clean up all powers to use IUCr convention of '^power^', as in
       '10^3^' for '10**3'.
     + Update 'yyyy-mm-dd' type regex to allow truncation from the right
       and improve comments to explain handling of related mmCIF
       'yyyy-mm-dd:hh:mm' type, and use of 'Z' for GMT time zone.

   2005-03-08 and
   2004-08-08 fixed cases where _item_units.code  used
              instead of _item_type.code (JDW)
   2004-04-15 fixed item ordering in
               _diffrn_measurement_axis.measurement_id
               added sub_category 'vector' (JDW)
;

   1.3.2   2005-06-25

;  2005-06-25 ITEM_TYPE_LIST: code, ucode, line, uline regexps updated
              to those of current mmCIF; float modified by allowing integers
              terminated by a point as valid. The 'time' part of
              yyyy-mm-dd types made optional in the regexp. (BM)

   2005-06-17 Minor corrections as for proofs for IT G Chapter 4.6
   (NJA)

   2005-02-21  Minor corrections to spelling and punctuation
   (NJA)

   2005-01-08 Changes as per Nicola Ashcroft.
   + Updated example 1 for DIFFRN_MEASUREMENT to agree with mmCIF.
   + Spelled out "micrometres" for "um" and "millimetres" for "mm".
   + Removed phrase "which may be stored" from ARRAY_STRUCTURE
     description.
   + Removed unused 'byte-offsets' compressions and updated
     cites to ITVG for '_array_structure.compression_type'.
   (HJB)
;

   1.3.1   2003-08-13
;
   Changes as per Frances C. Bernstein.
   + Identify initials.
   + Adopt British spelling for centre in text.
   + Set \p and \%Angstrom and powers.
   + Clean up commas and unclear wordings.
   + Clean up tenses in history.
   Changes as per Gotzon Madariaga.
   + Fix the ARRAY_DATA example to align '_array_data.binary_id'
   and X-Binary-ID.
   + Add a range to '_array_intensities.gain_esd'.
   + In the example of DIFFRN_DETECTOR_ELEMENT,
   '_diffrn_detector_element.id' and
   '_diffrn_detector_element.detector_id' interchanged.
   + Fix typos for direction, detector and axes.
   + Clarify description of polarisation.
   + Clarify axes in '_diffrn_detector_element.center[1]'
    '_diffrn_detector_element.center[2]'.
   + Add local item types for items that are pointers.
   (HJB)
;


   1.3.0   2003-07-24
;
   Changes as per Brian McMahon.
   + Consistently quote tags embedded in text.
   + Clean up introductory comments.
   + Adjust line lengths to fit in 80 character window.
   + Fix several descriptions in AXIS category which
     referred to '_axis.type' instead of the current item.
   + Fix erroneous use of deprecated item
     '_diffrn_detector_axis.id' in examples for
     DIFFRN_SCAN_AXIS.
   + Add deprecated items '_diffrn_detector_axis.id'
     and '_diffrn_measurement_axis.id'.
   (HJB)
;


   1.2.4   2003-07-14
;
   Changes as per I. David Brown.
   + Enhance descriptions in DIFFRN_SCAN_AXIS to make them less
     dependent on the descriptions in DIFFRN_SCAN_FRAME_AXIS.
   + Provide a copy of the deprecated DIFFRN_FRAME_DATA
     category for completeness.
   (HJB)
;


   1.2.3   2003-07-03
;
   Cleanup to conform to ITVG.
   + Correct sign error in ..._cubed units.
   + Correct '_diffrn_radiation.polarisn_norm' range.
   (HJB)
;


   1.2.2   2003-03-10
;
   Correction of typos in various DIFFRN_SCAN_AXIS descriptions.
   (HJB)
;


   1.2.1   2003-02-22
;
   Correction of ATOM_ for ARRAY_ typos in various descriptions.
   (HJB)
;


   1.2     2003-02-07
;
```

```
    Corrections to encodings (remove extraneous hyphens) remove
    extraneous underscore in '_array_structure.encoding_type'
    enumeration.  Correct typos in items units list.  (HJB)
;


    1.1.3   2001-04-19
;
    Another typo corrections by Wilfred Li, and cleanup by HJB.
;


    1.1.2   2001-03-06
;
    Several typo corrections by Wilfred Li.
;


    1.1.1   2001-02-16
;
    Several typo corrections by JW.
;


    1.1     2001-02-06
;
    Draft resulting from discussions on header for use at NSLS.  (HJB)

    + Change DIFFRN_FRAME_DATA to DIFFRN_DATA_FRAME.

    + Change '_diffrn_detector_axis.id' to '_diffrn_detector_axis.detector_id'.

    + Add '_diffrn_measurement_axis.measurement_device' and change
      '_diffrn_measurement_axis.id' to
      '_diffrn_measurement_axis.measurement_id'.

    + Add '_diffrn_radiation.div_x_source', '_diffrn_radiation.div_y_source',
     '_diffrn_radiation.div_x_y_source',
     '_diffrn_radiation.polarizn_source_norm',
    '_diffrn_radiation.polarizn_source_ratio', '_diffrn_scan.date_end',
    '_diffrn_scan.date_start', '_diffrn_scan_axis.angle_rstrt_incr',
    '_diffrn_scan_axis.displacement_rstrt_incr',
    '_diffrn_scan_frame_axis.angle_increment',
    '_diffrn_scan_frame_axis.angle_rstrt_incr',
    '_diffrn_scan_frame_axis.displacement',
    '_diffrn_scan_frame_axis.displacement_increment',and
    '_diffrn_scan_frame_axis.displacement_rstrt_incr'.

    + Add '_diffrn_measurement.device' to category key.

    + Update yyyy-mm-dd to allow optional time with fractional seconds
      for time stamps.

    + Fix typos caught by RS.

    + Add ARRAY_STRUCTURE_LIST_AXIS category, and use concept of axis sets to
      allow for coupled axes, as in spiral scans.

    + Add examples for fairly complete headers thanks to R. Sweet and P.
      Ellis.
;


    1.0     2000-12-21
;
    Release version - few typos and tidying up.  (BM & HJB)

    + Move ITEM_TYPE_LIST, ITEM_UNITS_LIST and DICTIONARY_HISTORY to end
    of dictionary.

    + Alphabetize dictionary.
;


    0.7.1   2000-09-29
;
    Cleanup fixes.  (JW)

    + Correct spelling of diffrn_measurement_axis in '_axis.id'

    + Correct ordering of uses of '_item.mandatory_code' and
    '_item_default.value'.
;


    0.7.0   2000-09-09
;
    Respond to comments by I. David Brown.  (HJB)

    + Add further comments on '\n' and '\t'.

    + Update ITEM_UNITS_LIST by taking section from mmCIF dictionary
      and adding metres.  Change 'meter' to 'metre' throughout.

    + Add missing enumerations to '_array_structure.compression_type'
      and make 'none' the default.

    + Remove parent-child relationship between
      '_array_structure_list.index' and '_array_structure_list.precedence'.

    + Improve alphabetization.

    + Fix '_array_intensities_gain.esd' related function.

    + Improve comments in AXIS.

    + Fix DIFFRN_FRAME_DATA example.

    + Remove erroneous DIFFRN_MEASUREMENT example.

    + Add '_diffrn_measurement_axis.id' to the category key.
;


    0.6.0   1999-01-14
;
    Remove redundant information for ENC_NONE data.  (HJB)

    + After the D5 remove binary section identifier, size and
      compression type.

    + Add Control-L to header.
;


    0.5.1   1999-01-03
;
    Cleanup of typos and syntax errors.  (HJB)

    + Cleanup example details for DIFFRN_SCAN category.

    + Add missing quote marks for '_diffrn_scan.id' definition.
;


    0.5   1999-01-01
;
    Modifications for axis definitions and reduction of binary header.  (HJB)

    + Restore '_diffrn_detector.diffrn_id' to DIFFRN_DETECTOR KEY.

    + Add AXIS category.

    + Bring in complete DIFFRN_DETECTOR and DIFFRN_MEASUREMENT categories
```

```
      from cif_mm.dic for clarity.

    + Change '_array_structure.encoding_type' from type code to uline and
      added X-Binary-Element-Type to MIME header.

    + Add detector beam centre '_diffrn_detector_element.center[1]' and
      '_diffrn_detector_element.center[2]'.

    + Correct item name of '_diffrn_refln.frame_id'.

    + Replace reference to '_array_intensities.undefined' by
      '_array_intensities.undefined_value'.

    + Replace references to '_array_intensity.scaling' with
      '_array_intensities.scaling'.

    + Add DIFFRN_SCAN... categories.
;


    0.4   1998-08-11
;
    Modifications to the 0.3 imgCIF draft.  (HJB)

    + Reflow comment lines over 80 characters and corrected typos.

    + Update examples and descriptions of MIME encoded data.

    + Change name to cbfext98.dic.
;


    0.3   1998-07-04
;
    Modifications for imgCIF.  (HJB)

    + Add binary type, which is a text field containing a variant on
      MIME encoded data.

    + Change type of '_array_data.data' to binary and specify internal
      structure of raw binary data.

    + Add '_array_data.binary_id', and make
      '_diffrn_frame_data.binary_id' and '_array_intensities.binary_id'
      into pointers to this item.
;


    0.2   1997-12-02
;
    Modifications to the CBF draft.  (JW)

    + Add category hierarchy for describing frame data developed from
      discussions at the BNL imgCIF Workshop Oct 1997.   The following
      changes are made in implementing the workshop draft.  Category
      DIFFRN_ARRAY_DATA is renamed to DIFFRN_FRAME_DATA.  Category
      DIFFRN_FRAME_TYPE is renamed to DIFFRN_DETECTOR_ELEMENT.   The
      parent item for '_diffrn_frame_data.array_id' is changed from
      '_array_structure_list.array_id' to '_array_structure.id'. Item
      '_diffrn_detector.array_id' is deleted.
    + Add data item '_diffrn_frame_data.binary_id' to identify data
      groups within a binary section.  The formal identification of the
      binary section is still fuzzy.
;


    0.1   1997-01-24
;
    First draft of this dictionary in DDL 2.1 compliant format by John
    Westbrook (JW).  This version is adapted from the Crystallographic
    Binary File (CBF) Format Draft Proposal provided by Andy Hammersley
    (AH).
```

```
    Modifications to the CBF draft.  (JW)

    + In this version the array description has been cast in the categories
      ARRAY_STRUCTURE and ARRAY_STRUCTURE_LIST.  These categories
      have been generalized to describe array data  of arbitrary dimension.

    + Array data in this description are contained in the category
      ARRAY_DATA.  This departs from the CBF notion of data existing
      in some special comment. In this description, data are handled as an
      ordinary data item encapsulated in a character data type.   Although
      data this manner deviates from CIF conventions, it does not violate
      any DDL 2.1 rules.  DDL 2.1 regular expressions can be used to define
      the binary representation which will permit some level of data
      validation.  In this version, the placeholder type code "any" has
      been used. This translates to a regular expression which will match
      any pattern.

      It should be noted that DDL 2.1 already supports array data objects
      although these have not been used in the current mmCIF dictionary.
      It may be possible to use the DDL 2.1 ITEM_STRUCTURE and
      ITEM_STRUCTURE_LIST categories to provide the information that is
      carried in by the ARRAY_STRUCTURE and ARRAY_STRUCTURE_LIST.  By
      moving the array structure to the DDL level it would be possible to
      define an array type as well as a regular expression defining the
      data format.

    + Multiple array sections can be properly handled within a single
      datablock.
;


#-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof-eof
```