```
##############################################################################
#                                                                            #
#                       Image CIF Dictionary (imgCIF)                        #
#             and Crystallographic Binary File Dictionary (CBF)              #
#            Extending the Macromolecular CIF Dictionary (mmCIF)             #
#                                                                            #
#                              Version 1.5.4                                 #
#                              of 2007-07-28                                 #
#    ##################################################################      #
#    # *** WARNING *** THIS IS A DRAFT FOR DISCUSSSION *** WARNING *** #      #
#    #                 SUBJECT TO CHANGE WITHOUT NOTICE                 #      #
#    #       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         1.5.4
    _dictionary.datablock_id    cif_img.dic

##############################################################################
#    CONTENTS
#
#        CATEGORY_GROUP_LIST
#        SUB_CATEGORY
#
#        category  ARRAY_DATA
#
#                  _array_data.array_id
#                  _array_data.binary_id
#                  _array_data.data
#                  _array_data.header_contents
#                  _array_data.header_convention
#
#        category  ARRAY_ELEMENT_SIZE
#
#                  _array_element_size.array_id
```



```
#                  _array_element_size.index
#                  _array_element_size.size
#
#        category  ARRAY_INTENSITIES
#
#                  _array_intensities.array_id
#                  _array_intensities.binary_id
#                  _array_intensities.gain
#                  _array_intensities.gain_esd
#                  _array_intensities.linearity
#                  _array_intensities.offset
#                  _array_intensities.scaling
#                  _array_intensities.overload
#                  _array_intensities.undefined_value
#                  _array_intensities.pixel_fast_bin_size
#                  _array_intensities.pixel_slow_bin_size
#                  _array_intensities.pixel_binning_method
#
#        category  ARRAY_STRUCTURE
#
#                  _array_structure.byte_order
#                  _array_structure.compression_type
#                  _array_structure.compression_type_flag
#                  _array_structure.encoding_type
#                  _array_structure.id
#
#        category  ARRAY_STRUCTURE_LIST
#
#                  _array_structure_list.axis_set_id
#                  _array_structure_list.array_id
#                  _array_structure_list.dimension
#                  _array_structure_list.direction
#                  _array_structure_list.index
#                  _array_structure_list.precedence
#
#        category  ARRAY_STRUCTURE_LIST_AXIS
#
#                  _array_structure_list_axis.axis_id
#                  _array_structure_list_axis.axis_set_id
#                  _array_structure_list_axis.angle
#                  _array_structure_list_axis.angle_increment
#                  _array_structure_list_axis.displacement
#                  _array_structure_list_axis.fract_displacement
#                  _array_structure_list_axis.displacement_increment
#                  _array_structure_list_axis.fract_displacement_increment
#                  _array_structure_list_axis.angular_pitch
#                  _array_structure_list_axis.radial_pitch
#                  _array_structure_list_axis.reference_angle
#                  _array_structure_list_axis.reference_displacement
```

```
#
#         category  AXIS
#
#                   _axis.depends_on
#                   _axis.equipment
#                   _axis.id
#                   _axis.offset[1]
#                   _axis.offset[2]
#                   _axis.offset[3]
#                   _axis.type
#                   _axis.system
#                   _axis.vector[1]
#                   _axis.vector[2]
#                   _axis.vector[3]
#
#         category  DIFFRN_DATA_FRAME
#
#                   _diffrn_data_frame.array_id
#                   _diffrn_data_frame.binary_id
#                   _diffrn_data_frame.center_fast
#                   _diffrn_data_frame.center_slow
#                   _diffrn_data_frame.center_units
#                   _diffrn_data_frame.detector_element_id
#                   _diffrn_data_frame.id
#                   _diffrn_data_frame.details
#
#         category  DIFFRN_DETECTOR
#
#                   _diffrn_detector.details
#                   _diffrn_detector.detector
#                   _diffrn_detector.diffrn_id
#                   _diffrn_detector.dtime
#                   _diffrn_detector.id
#                   _diffrn_detector.number_of_axes
#                   _diffrn_detector.type
#
#         category  DIFFRN_DETECTOR_AXIS
#
#                   _diffrn_detector_axis.axis_id
#                   _diffrn_detector_axis.detector_id
#
#         category  DIFFRN_DETECTOR_ELEMENT
#
#                   _diffrn_detector_element.id
#                   _diffrn_detector_element.detector_id
#                   _diffrn_detector_element.reference_center_fast
#                   _diffrn_detector_element.reference_center_slow
#                   _diffrn_detector_element.reference_center_units
#
```



```
#         category  DIFFRN_MEASUREMENT
#
#                   _diffrn_measurement.diffrn_id
#                   _diffrn_measurement.details
#                   _diffrn_measurement.device
#                   _diffrn_measurement.device_details
#                   _diffrn_measurement.device_type
#                   _diffrn_measurement.id
#                   _diffrn_measurement.method
#                   _diffrn_measurement.number_of_axes
#                   _diffrn_measurement.sample_detector_distance
#                   _diffrn_measurement.sample_detector_voffset
#                   _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
#
#                   _diffrn_radiation.collimation
#                   _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
#                   _diffrn_radiation.polarizn_source_ratio
#                   _diffrn_radiation.probe
#                   _diffrn_radiation.type
#                   _diffrn_radiation.xray_symbol
#                   _diffrn_radiation.wavelength_id
#
#         category  DIFFRN_REFLN
#
#                   _diffrn_refln.frame_id
#
#         category  DIFFRN_SCAN
#
#                   _diffrn_scan.id
#                   _diffrn_scan.date_end
#                   _diffrn_scan.date_start
#                   _diffrn_scan.integration_time
```

```
#                 _diffrn_scan.frame_id_start
#                 _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
#
#       categor   MAP
#
#                 _map.details
#                 _map.diffrn_id
#                 _map.entry_id
#                 _map.id
#
#       categor   MAP_SEGMENT
#
```



```
#                 _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
#
#      ***DEPRECATED*** data items
#
#                 _diffrn_detector_axis.id
#                 _diffrn_detector_element.center[1]
#                 _diffrn_detector_element.center[2]
#                 _diffrn_measurement_axis.id
#
#      ***DEPRECATED*** category  DIFFRN_FRAME_DATA
#
#                 _diffrn_frame_data.array_id
#                 _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.

     It is recognized that the data in this category needs to be used in
     two distinct ways.  During a data collection the lack of ancillary
     data and timing constraints in processing data may dictate the
     need to make a 'miniCBF' nothing more than an essential minimum
     of information to record the results of the data collection.  In that
     case it is proper to use the ARRAY_DATA category as a
     container for just a single image and a compacted, beam-line
     dependent list of data collection parameter values.  In such
     a case, only the tags '_array_data.header_convention',
     '_array_data.header_contents' and '_array_data.data' need be
     populated.

     For full processing and archiving, most of the tags in this
     dictionary will need to be populated.
```



```
;
    _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: 1zsJjWPfol2GYl2V+QSXrw==

        ELhQAAAAAAAA...
        ...
        --CIF-BINARY-FORMAT-SECTION----
        ;
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
;
        Example 2 -

        This example shows a single image in a miniCBF, provided by
        E. Eikenberry.  The entire CBF consists of one data block
        containing one category and three tags.  The CBFlib
        program convert_miniCBF and a suitable template file
        can be used to convert this miniCBF to a full imgCIF
        file.
;
;
        ###CBF: VERSION 1.5
        # CBF file written by CBFlib v0.7.8

        data_insulin_pilatus6m

        _array_data.header_convention SLS_1.0
        _array_data.header_contents
        ;
        # Detector: PILATUS 6M SN: 60-0001
        # 2007/Jun/17 15:12:36.928
        # Pixel_size 172e-6 m x 172e-6 m
        # Silicon sensor, thickness 0.000320 m
        # Exposure_time 0.995000 s
        # Exposure_period 1.000000 s
        # Tau = 194.0e-09 s
        # Count_cutoff 1048575 counts
```



```
        # Threshold_setting 5000 eV
        # Wavelength 1.2398 A
        # Energy_range (0, 0) eV
        # Detector_distance 0.15500 m
        # Detector_Voffset -0.01003 m
        # Beam_xy (1231.00, 1277.00) pixels
        # Flux 22487563295 ph/s
        # Filter_transmission 0.0008
        # Start_angle 13.0000 deg.
        # Angle_increment 1.0000 deg.
        # Detector_2theta 0.0000 deg.
        # Polarization 0.990
        # Alpha 0.0000 deg.
        # Kappa 0.0000 deg.
        # Phi 0.0000 deg.
        # Chi 0.0000 deg.
        # Oscillation_axis  X, CW
        # N_oscillations 1
        ;

        _array_data.data
        ;
        --CIF-BINARY-FORMAT-SECTION--
        Content-Type: application/octet-stream;
             conversions="x-CBF_BYTE_OFFSET"
        Content-Transfer-Encoding: BINARY
        X-Binary-Size: 6247567
        X-Binary-ID: 1
        X-Binary-Element-Type: "signed 32-bit integer"
        X-Binary-Element-Byte-Order: LITTLE_ENDIAN
        Content-MD5: 8wO6i2+899lf5iO8QPdgrw==
        X-Binary-Number-of-Elements: 6224001
        X-Binary-Size-Fastest-Dimension: 2463
        X-Binary-Size-Second-Dimension: 2527
        X-Binary-Size-Padding: 4095

        ...

        --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.

              If not given, it defaults to 1.
;
    _item.name                  '_array_data.array_id'
    _item.category_id             array_data
    _item.mandatory_code          implicit
    _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
              for diffraction images in the ARRAY_DATA category.
              Note:  When appropriate in other categories, e.g. for
              photographs of crystals, more precise types, such as
              'image/jpeg', 'image/tiff', 'image/png', etc. should be used.

              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
0123456789012345678901234567890123456789012345678901234567890123
|         |         |         |         |         |         |
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_


save__array_data.header_contents
    _item_description.description
;
```

This item is an text field for use in minimal CBF files to carry
essential header information to be kept with image data
in _array_data.data when the tags that normally carry the
structured metadata for the image have not been populated.

Normally this data item should not appear when the full set
of tags have been populated and _diffrn_data_frame.details
appears.
;

```
    _item.name                  '_array_data.header_contents'
    _item.category_id            array_data
    _item.mandatory_code         no
    _item_type.code              text
     save_



save__array_data.header_convention
```

```
    _item_description.description
;             This item is an identifier for the convention followed in
              constructing the contents of _array_data.header_contents

              The permitted values are of the of an image creator identifier
              followed by an underscore and a version string.  To avoid
              confusion about conventions, all creator identifiers
              should be registered with the IUCr and the conventions
              for all identifiers and versions should be posted on
              the MEDSBIO.org web site.
;
    _item.name                  '_array_data.header_convention'
    _item.category_id            array_data
    _item.mandatory_code         no
    _item_type.code              code
     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          implicit
    _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          implicit
    _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.

                The type 'unsigned 1-bit integer' is used for
```

```
               packed Booleans arrays for masks.  Each element
               of the array corresponds to a single bit
               packed in unsigned 8-bit 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 1-bit integer'
                              '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.

               This item has been made implicit and given a default value of 1
               as a convenience in writing miniCBF files.  Normally an
               explicit name with useful content should be used.
;
    loop_
    _item.name
    _item.category_id
    _item.mandatory_code
             '_array_structure.id'              array_structure      implicit
             '_array_data.array_id'             array_data           implicit
             '_array_structure_list.array_id'   array_structure_list implicit
             '_array_intensities.array_id'      array_intensities    implicit
             '_diffrn_data_frame.array_id'      diffrn_data_frame    implicit
```



```
    _item_default.value           1
    _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          implicit
    _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'
```

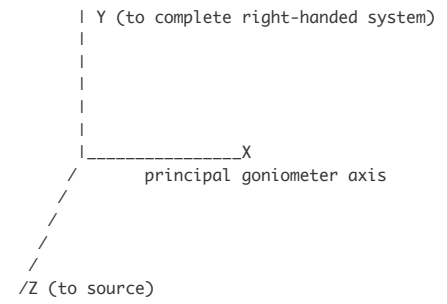


```
                scan with differing angular displacements between pixels,
                the value of this item may differ significantly from the
                value of _array_structure_list_axis.displacement_increment.
;
    _item.name               '_array_structure_list_axis.radial_pitch'
    _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 standard laboratory coordinate system is a right-handed
     orthogonal coordinate similar to the MOSFLM coordinate system,
     but imgCIF puts Z along the X-ray beam, rather than putting X along the
     X-ray beam as in MOSFLM.
```



```
     The vectors for the imgCIF standard laboratory coordinate system
     form 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
     be both in the sample and in the beam.  If the sample goniometer or other
     sample positioner has two axes the intersection of 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\%) or all obtuse (>=90\%)."

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(\a) 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          implicit
    _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.center_fast
     _item_description.description
;             The value of _diffrn_data_frame.center_fast is
              the fast index axis beam center position relative to the detector
```



```
              element face in the units specified in the data item
              '_diffrn_data_frame.center_units' along the fast
              axis of the detector from the center of 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 the current setting of detector
              positioner given frame are used.

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

;
     _item.name '_diffrn_data_frame.center_fast'
     _item.category_id             diffrn_data_frame
     _item.mandatory_code          no
     _item_type.code               float

     save_


save__diffrn_data_frame.center_slow
     _item_description.description
;             The value of _diffrn_data_frame.center_slow is
              the slow index axis beam center position relative to the detector
              element face in the units specified in the data item
              '_diffrn_data_frame.center_units' along the slow
              axis of the detector from the center of 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 the current setting of detector
              positioner given frame are used.

              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_data_frame.center_slow'
     _item.category_id             diffrn_data_frame
     _item.mandatory_code          no
     _item_type.code               float

     save_


save__diffrn_data_frame.center_units
     _item_description.description
;             The value of _diffrn_data_frame.center_units
              specifies the units in which the values of
```

```
              '_diffrn_data_frame.center_fast' and
              '_diffrn_data_frame.center_slow'
              are presented.  The default is 'mm' for millimetres.  The
              alternatives are 'pixels' and 'bins'.  In all cases the
              center distances are measured from the center of the
              first pixel, i.e. in a 2x2 binning, the measuring origin
              is offset from the centers of the bins by one half pixel
              towards the first pixel.

              If 'bins' is specified, the data in
                  '_array_intensities.pixel_fast_bin_size',
                  '_array_intensities.pixel_slow_bin_size', and
                  '_array_intensities.pixel_binning_method'
              is used to define the binning scheme.


;
     _item.name '_diffrn_data_frame.center_units'
     _item.category_id             diffrn_data_frame
     _item.mandatory_code          no
     _item_type.code               code
      loop_
     _item_enumeration.value
     _item_enumeration.detail
                                   mm        'millimetres'
                                   pixels    'detector pixels'
                                   bins      'detector bins'

     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.

               Normally, when a conversion from a miniCBF has been done
               the data from '_array_data.header_convention'
               should be transferred to this data item and
               '_array_data.header_convention'
               should be removed.
;
```

```
    _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.  For each element, the detector
        face coordiate system, is assumed to have the fast axis
        running from left to right and the slow axis running from
        top to bottom with the origin at the top left corner.
;
;
        loop_
        _diffrn_detector_element.detector_id
        _diffrn_detector_element.id
        _diffrn_detector_element.reference_center_fast
        _diffrn_detector_element.reference_center_slow
        _diffrn_detector_element.reference_center_units
        d1     d1_ccd_1  201.5 201.5  mm
        d1     d1_ccd_2  -1.8  201.5  mm
        d1     d1_ccd_3  201.6  -1.4  mm
        d1     d1_ccd_4  -1.7   -1.5  mm
;
# - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
    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 the units specified in the data item
              '_diffrn_detector_element.reference_center_units' along the fast
              axis of the detector from the center of 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 for measurements in millimetres,
              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

     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 the units specified in the data item
              '_diffrn_detector_element.reference_center_units' along the slow
              axis of the detector from the center of 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

     save_


save__diffrn_detector_element.reference_center_units
     _item_description.description
;             The value of _diffrn_detector_element.reference_center_units
              specifies the units in which the values of
              '_diffrn_detector_element.reference_center_fast' and
              '_diffrn_detector_element.reference_center_slow'
              are presented.  The default is 'mm' for millimetres.  The
              alternatives are 'pixels' and 'bins'.  In all cases the
              center distances are measured from the center of the
```



```
              first pixel, i.e. in a 2x2 binning, the measuring origin
              is offset from the centers of the bins by one half pixel
              towards the first pixel.

              If 'bins' is specified, the data in
                  '_array_intensities.pixel_fast_bin_size',
                  '_array_intensities.pixel_slow_bin_size', and
                  '_array_intensities.pixel_binning_method'
              is used to define the binning scheme.


;
     _item.name '_diffrn_detector_element.reference_center_units'
     _item.category_id             diffrn_detector_element
     _item.mandatory_code          no
     _item_type.code               code
      loop_
     _item_enumeration.value
     _item_enumeration.detail
                                   mm        'millimetres'
                                   pixels    'detector pixels'
                                   bins      'detector bins'

     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_


#                  _diffrn_measurement.sample_detector_distance
#                  _diffrn_measurement.sample_detector_voffset

save__diffrn_measurement.sample_detector_distance
    _item_description.description
;              The value of _diffrn_measurement.sample_detector_distance gives
               the unsigned distance in millimetres from the sample to the
               detector along the beam.
;
    _item.name                  '_diffrn_measurement.sample_detector_distance'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
     loop_
    _item_range.maximum
    _item_range.minimum           .   0.0
    _item_type.code               float
    _item_units.code              mm
     save_

save__diffrn_measurement.sample_detector_voffset
    _item_description.description
;              The value of _diffrn_measurement.sample_detector_voffset gives
               the signed distance in millimetres in the vertical
               direction (positive for up) from the center of
               the beam to the center of the detector.
;
    _item.name                  '_diffrn_measurement.sample_detector_voffset'
    _item.category_id             diffrn_measurement
    _item.mandatory_code          no
     loop_
    _item_range.maximum
    _item_range.minimum           .   .
                                  .   .
    _item_type.code               float
    _item_units.code              mm
     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==

    AABRAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAZBQSr1sKNBOeOe9HITdMdDUnbq7bg
    ...
    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==

     AABRAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAZBQSr1sKNBOeOe9HITdMdDUnbq7bg
     ...
     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          implicit
    _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          implicit
    _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_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.

                Because of ambiguity about the setting used to determine this
                center, use of this data item is deprecated.  The data item
                _diffrn_data_frame.center_fast
                which is referenced to the detector coordinate system and not
                directly to the laboratory coordinate system should be used
                instead.

;
    _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.

              Because of ambiguity about the setting used to determine this
              center, use of this data item is deprecated. The data item
              _diffrn_data_frame.center_slow
              which is referenced to the detector coordinate system and not
              directly to the laboratory coordinate system should be used
              instead.

;
    _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_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          implicit
    _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

   1.5.4   2007-07-28

;  Typographics corrections (HJB)

     + Corrected embedded degree characters to \%
     + Corrected embedded Aring to \%A
     + Added trailing ^ for a power
     + Removed 2 cases of a space after an underscore
       in tag name.
;

   1.5.3   2007-07-08

;  Changes to support SLS miniCBF and suggestions
   from the 24 May 07 BNL imgCIF workshop (HJB)

     + Added new data items
       '_array_data.header_contents',
       '_array_data.header_convention',
       '_diffrn_data_frame.center_fast',
       '_diffrn_data_frame.center_slow',
       '_diffrn_data_frame.center_units',
       '_diffrn_measurement.sample_detector_distance',
       '_diffrn_measurement.sample_detector_voffset
     + Deprecated data items
       '_diffrn_detector_element.center[1]',
       '_diffrn_detector_element.center[2]'
     + Added comments and example on miniCBF
     + Changed all array_id data items to implicit
```



```
;

   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 definitions 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
```