```
##############################################################################
#                                                                            #
#                        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
    01234567890123456789012345678901234567890123456789012345678901234567890123
|         |         |         |         |         |         |
    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
```

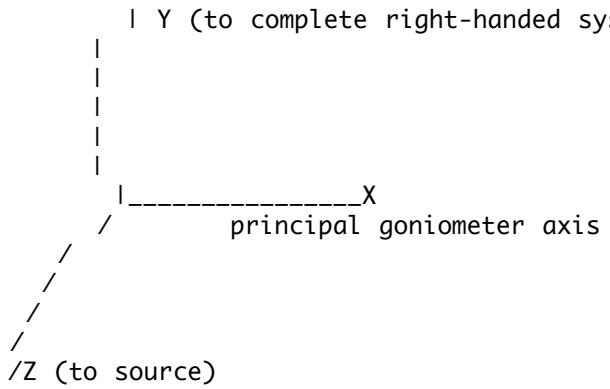
```
                    set of axes for which axis settings are being specified.

                    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
                'yes'
      loop_
      _item_linked.child_name
      _item_linked.parent_name
                '_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==

          AABRAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAZBQSr1sKNBOeOe9HITdMdDUnbq7bg
       ...
          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==

          AABRAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAZBQSr1sKNBOeOe9HITdMdDUnbq7bg
      ...
          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.
```