

3. CIF DATA DEFINITION AND CLASSIFICATION

3.7.2.2. Array elements

Data items in this category are as follows:

```
ARRAY_ELEMENT_SIZE
• _array_element_size.array_id
  → _array_structure.id
• _array_element_size.index
  → _array_structure_list.index
  _array_element_size.size
```

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item.

The value of the `_array_element_size.size` data item is a size in metres of an image element (a pixel or voxel). The direction of the measurement is given in each dimension by `_array_element_size.index`. The array structure specifying the organization of the dimensions is referenced by the value of `_array_element_size.array_id`, which is a pointer to `_array_structure.id`. The value of `_array_element_size.index` is a pointer to `_array_structure_list.index`. For data organized into rectangular arrays of pixels or voxels, this gives the spatial dimensions of the individual image elements.

3.7.2.3. Intensities

Data items in this category are as follows:

```
ARRAY_INTENSITIES
• _array_intensities.array_id
  → _array_structure.id
• _array_intensities.binary_id
  → _array_data.binary_id
  _array_intensities.gain
  _array_intensities.gain_esd
  _array_intensities.linearity
  _array_intensities.offset
  _array_intensities.overload
  _array_intensities.scaling
  _array_intensities.undefined_value
```

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item.

The relationship between the data values for individual image elements and the number of incident photons can be complex. The data items in the `ARRAY_INTENSITIES` category provide information about this relationship. The value of `_array_intensities.linearity` states the type of relationship, and the values of `_array_intensities.array_id` and `_array_intensities.binary_id` identify the array structure and the image being discussed. The other items are used in different ways depending on the relationship. If the value of `_array_intensities.linearity` is `raw`, then the image elements hold uninterpreted raw data values from the detector, *e.g.* for calibration. If the value of `_array_intensities.linearity` is `linear`, then the count in an image element is proportional to the incident number of photons by the value of `_array_intensities.gain`. The standard uncertainty (estimated standard deviation) of the gain may be given in `_array_intensities.gain_esd`. The value used for this should be estimated from a good understanding of the physical characteristics of the experimental apparatus. If the value of `_array_intensities.linearity` is `offset`, then the value of `_array_intensities.offset` should be added to the image element value. If the value of `_array_intensities.linearity` is `scaling`, `scaling_offset`, `sqrt_scaled` or `logarithmic_scaled`, the necessary scaling factor is given by the value of `_array_intensities.scaling`. In all cases, the scaling factor is applied to the image element value before the other operations are applied. In the first case, only simple scaling is used. In the second case, the value of `_array_intensities.offset` is added after

scaling. In the third case, the scaled value is squared. In the final case, 10 is taken to the power given by the scaled value.

3.7.2.4. Organization and encoding of array data

Data items in these categories are as follows:

```
(a) ARRAY_STRUCTURE
• _array_structure.id
  _array_structure.byte_order
  _array_structure.compression_type
  _array_structure.encoding_type

(b) ARRAY_STRUCTURE_LIST
• _array_structure_list.array_id
• _array_structure_list.index
  → _array_structure.id
  _array_structure_list.axis_set_id
  _array_structure_list.dimension
  _array_structure_list.direction
  _array_structure_list.precedence

(c) ARRAY_STRUCTURE_LIST_AXIS
• _array_structure_list_axis.axis_id
  → _axis.id
• _array_structure_list_axis.axis_set_id
  → _array_structure_list.axis_set_id
  _array_structure_list_axis.angle
  _array_structure_list_axis.angle_increment
  _array_structure_list_axis.angular_pitch
  _array_structure_list_axis.displacement
  _array_structure_list_axis.displacement_increment
  _array_structure_list_axis.radial_pitch
```

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item.

The data items in the `ARRAY_STRUCTURE` category show how the stream of octets in a binary image is to be reorganized into words of an appropriate size. Each possible encoding is identified by a value of `_array_structure.id`. In most cases, large images will have been compressed. The type of compression used is given by `_array_structure.compression_type`. Once a stream of octets has been decompressed, it can be organized into words. The type of each word is given by the value of `_array_structure.encoding_type` and the order of mapping octets onto words, most significant octet first ('big-endian') or least significant octet first ('little-endian'), is given by the value of `_array_structure.byte_order`.

The data items in the `ARRAY_STRUCTURE_LIST` category show how the list of words defined by the `ARRAY_STRUCTURE` category should be organized into image arrays. The value of `_array_structure_list.array_id` is a pointer to `_array_structure.id`. Each dimension (row, column, sheet *etc.*) of the image is identified by an index, counting from 1, given by `_array_structure_list.index`. The order of nesting of the indices is given by the values of `_array_structure_list.precedence`, with the index of precedence 1 varying most rapidly (*i.e.* having values stored sequentially). The direction of index change for increasing memory location is given by the value of `_array_structure_list.direction`. For a given index, the number of image elements in that direction is given by the value of `_array_structure_list.dimension`.

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.