

2.5. SPECIFICATION OF THE CORE CIF DICTIONARY DEFINITION LANGUAGE (DDL)

(a)

```

loop_
  _display_id
  _display_symbol
  _display_coord_x
  _display_coord_y
loop_
  _display_conn_id
  _display_conn_symbol
    1 1 180 110 2 1b stop_
    2 O 140 140 3 1b 4 1b stop_
    3 3 100 110 4 2b stop_
    4 4 120 60 5 1b stop_
    5 5 160 60 1 1b stop_
    6 S 205 140 1 2b stop_

```

(b)

```

data_display_coord_
  loop_ _name      '_display_coord_x'
        '_display_coord_y'
        _type          'numb'
        _list          'yes'
        _list_level   '1'
        _definition
; The projected coordinates of the display
object identified in _display_object and
_display_symbol.
;

data_display_conn_symbol_
  _name          '_display_conn_symbol'
  _type          'char'
  _list          'yes'
  _list_level   '2'
  _definition
; The symbol code for the bond connection to the
displayed objects identified by _display_id and
_display_conn_id. The symbol codes and
descriptions are stored in the validation file
'mif_core_bonds.val'.
;

```

Fig. 2.5.6.1. (a) Hypothetical example and (b) the typical definition of nested items.

by white space, quotation characters or, in the case of multi-line text, by semicolon characters in column 1 of a line.

The attribute `_type_conditions` is used to identify application-specific conditions that apply to the typing of data items. This attribute is used to alert parsing software of string constructions that may disrupt the normal identification and validation of data types. The permitted attribute states are `none`, `esd` (and its preferred synonym `su`) and `seq`. In the definition example in Fig. 2.5.5.3 the code `esd` signals that cell-length values are measurements and may have a standard uncertainty value appended in parentheses. Fig 2.5.5.8 indicates the use of the code `su` for the same purpose. A full description of `_type_conditions` states is given in the DDL1 dictionary in Chapter 4.9.

If a data item consists of a concatenation of values, the attribute `_type_construct` may be used to specify the encoding algorithm for the component values. The language used for this algorithm is POSIX regex (IEEE, 1991). The specification of `_type_construct` can include the data names of other defined items. Validation software interprets this attribute as format specifications and constraints, and expands the embedded data items according to their

```

data_publ_date
  _name          '_publ_date'
  _type          'char'
  _type_construct
    (_publ_year)/(_publ_month)/(_publ_day)
  _definition
; Specifies the syntax for declaring the
publication date.
;

data_publ_year
  _name          '_publ_year'
  _type          'char'
  _type_construct
    19|20[0-9][0-9]
  _definition
; Specifies how the publication year will
appear. Syntax is valid only for publication
in the 20th and 21st centuries!
;

```

Fig. 2.5.6.2. Definition example: type constructions.

separate definition. For example, the chronological date is a composite of day, month and year. These may be represented in many different ways and the `_type_construct` attribute enables a specific date representation to be defined. The two definitions shown in Fig. 2.5.6.2 illustrate how a date value of the construction '1995/03/25' may be embedded into the dictionary definitions (the month and day definitions have been omitted here for brevity).

Units attributes specify the measurement units permitted for a numerical data item. The attribute `_units` specifies a code that uniquely identifies the measurement units. A description of the units identified by the code is given by the attribute `_units_detail`. Typical uses of this attribute are shown in Fig. 2.5.5.8.

2.5.6.4. Relational attributes

This class of attributes is used to describe special relationships and dependencies between data items. These attributes are machine parsable and are formally defined in the DDL1 dictionary in Chapter 4.9. They are

```

_category
_list_link_child
_list_link_parent
_list_mandatory
_list_reference
_list_uniqueness
_related_item
_related_function

```

The attribute `_category` is used to specify to which group, or basis set, a data item belongs. The value of this attribute is a name string that identifies the group and it is usually the leading part of the tags for all items in this group. Data items in a list must have the same category value. Data items in the same category may, however, be divided into different lists, provided each list contains an appropriate key data item (see `_list_reference` below).

List-link attributes are used to specify dependencies between data items in different lists. The attribute `_list_link_parent` identifies an item in another list from which the defined item was derived. The parent data item, or items in the case of irreducible sets, must have a unique value within its own list. The `_list_link_child` attribute is declared in the definition of a parent item and identifies items in other lists that depend implicitly on the defined data item being present in the same data instantiation. The functionalities of these two attributes mirror each other. The parent item must be present in any data instantiation containing the child items, but not the converse. The definition examples in Figs 2.5.5.6 and 2.5.5.7 illustrate the use of these attributes.