

## 2. CONCEPTS AND SPECIFICATIONS

reference is provided as a convenience to avoid the redeclaration of the full data-type specification for each data item. The key item for this category is `_item_type.name`, which is defined in the parent category ITEM. Only one data type may be specified for a data item.

## 2.6.6.1.16. ITEM\_TYPE\_CONDITIONS

The category ITEM\_TYPE\_CONDITIONS defines special conditions applied to a data-item type. This category has been included in order to comply with previous applications of STAR and CIF. Since the constructions that are embodied in this category are antithetical to the data model that underlies DDL2, it is recommended that this category only be used for the purpose of parsing existing data files and dictionaries.

## 2.6.6.1.17. ITEM\_TYPE\_LIST

The ITEM\_TYPE\_LIST category holds the list of item data-type definitions. The key item in this category is `_item_type_list.code`. Data types are associated with data items by references to this key from the ITEM\_TYPE category. One of the data-type codes defined in this category must be assigned to each data item.

The definition of a data type consists of the specification of the item's primitive type and a regular expression that defines the pattern that must be matched by any occurrence of the item. The primitive type code, `_item_type_list.primitive_code`, can assume values of `char`, `uchar`, `numb` and `null`. This code is provided for backward compatibility with STAR and CIF applications that employ loose data typing. The data item `_item_type_list.construct` holds the regular expression that must be matched by the data type. Simple regular expressions can be used to define character fields of restricted width, floating-point and integer formats.

Molecular Information File (MIF) applications (Allen *et al.*, 1995) have extended the notion of the regular expression to include data-item components. This permits the construction of complex data items from one or more component data items using regular expression algebra. These extended regular expressions are defined in the category ITEM\_TYPE\_CONDITIONS.

Example 2.6.6.1 illustrates the data types that are defined within this DDL. The DDL uses a number of character data types which have subtly different definitions. For instance, the data type identified as `code` defines a single-word character string; `char` extends the `code` type with the addition of a white-space character; and `text` extends the `char` type with the addition of a newline character. Two special character data types `name` and `idname` are used to define the full STAR data name and the STAR name components, respectively. The data type `any` is used to match any potential data type. This type is used for data items that may hold a variety of data types. The data type `int` is defined as one or more decimal digits and the `yyyy-mm-dd` type defines a date string.

## 2.6.6.1.18. ITEM\_UNITS

The ITEM\_UNITS category holds a code that identifies the system of units in which a data item is expressed. The data item `_item_units.code` is a child of the item `_item_units_list.code`. Unit definitions are actually made in the ITEM\_UNITS\_LIST parent category. The item `_item_units.code` provides an indirect reference into the list of data-type definitions in category ITEM\_UNITS\_LIST. This indirect reference is provided as a convenience to avoid the redeclaration of the full data-type specification for each data item. The key item for this category is

Example 2.6.6.1. *The description of permitted data types in the DDL2 dictionary.*

```
#          DATA TYPE CONVERSION TABLE
#          -----
#
loop
  _item_type_list.code
  _item_type_list.primitive_code
  _item_type_list.detail
  _item_type_list.construct

code char 'A single word'           '[^\t\n ]*'
char char 'A single line of text'   '[^\n]*'
text char 'Text which may span lines' '.'*
int  numb 'Unsigned integer data'   '[0-9]+'
name uchar 'A data item name'
      '[_A-Za-z0-9]+[.][_A-Za-z0-9%/-]+'

idname uchar
      'A data item name component or identifier'
      '[_A-Za-z0-9]+'
any char 'Any data type'           '.'*
yyyy-mm-dd
      char 'A date format'
      '[0-9][0-9][0-9][0-9]-[0-9]?[0-9]-[0-9][0-9]'
```

`_item_units.name`, which is defined in the parent category ITEM. Only one type of unit may be specified for a data item.

## 2.6.6.1.19. ITEM\_UNITS\_CONVERSION

The ITEM\_UNITS\_CONVERSION category holds a table of conversion factors between the systems of units described in the ITEM\_UNITS\_LIST category. The systems of units are identified by a `*.from_code` and a `*.to_code`, which are both children of the item `_item_units_list.code`. The conversion is defined in terms of an arithmetic operator and a conversion factor, `_item_units_conversion.operator` and `_item_units_conversion.factor`, respectively.

## 2.6.6.1.20. ITEM\_UNITS\_LIST

The ITEM\_UNITS\_LIST category holds the descriptions of systems of physical units. The key item in this category is `_item_units_list.code`. Units are assigned to data items by references to this key from the ITEM\_UNITS category.

## 2.6.6.2. DDL2 definitions describing categories

In this section, the DDL definitions that describe the properties of categories, category groups and subcategories are presented. Fig. 2.6.4.2 illustrates the organization of these categories.

## 2.6.6.2.1. CATEGORY

The category named CATEGORY contains the data items that describe the properties of collections of related data items. A DDL category is essentially a table. In this category the characteristics of the table as a whole are defined. This category includes the data items `_category.id` to identify a category name; `_category.description` to describe a category; `_category.mandatory_code` to indicate whether the category must appear in a data block; and `_category.implicit_key`, which can be used to merge like categories between data blocks. The category identifier `_category.id` is a component of the key in most of the DDL categories in this section. The parent definition of the category identifier and all its child relationships are defined in this category.