1 mmCIF Dictionary Extensions

1.1 Types of Extensions

In order of increasing complexity, common types of dictionary extensions can be classified as the:

- addition of a data item which add a new property to an existing category.
- addition of a new category with no data items in common with any existing category.
- addition of a new category with data items in common with an existing category.
- addition of a data item to an existing category which changes the composition of the category key.

The following sections provide examples of how one might approach each of these cases.

1.2 Adding a new property to an existing category

This is the simplest type of modification in which a new data item definition is appended to an existing category. The first step in adding an item to a dictionary is to verify that the data item is not already defined within the current dictionary. If the item cannot be found in the mmCIF dictionary it may worthwhile to post a message to the mmCIF Discussion List (`mmciflist@ndbserver.rutgers.edu`) to verify that the item is indeed missing from the dictionary and that it has not already been defined locally by someone else.

After determining that the data item represents new content, the next step is to select an *appropriate* item name. In this example, the data item is being added to an existing category so that portion of the item name is fixed. The remaining portion should be chosen to be conforming with the style of other data item names within the category. At the moment, the recommended practice is to prefix local data items with an institutional acronym. These acronyms can be registered and reserved with the IUCr, which maintains the clearinghouse of these reserved prefixes.

Having chosen a data name, then the item definition can be constructed. In building the definition a description must be crafted and some consideration should be given to a default value, examples, and any range restrictions. Check the table of know data types in `ITEM_TYPE_LIST` and known units in `ITEM_UNITS_LIST` for an appropriate value. If an appropriate value cannot be found, then additional entries in these categories are required to create the new data type or system of units. Extending the list of know units also requires extensions to the table of unit conversions `ITEM_UNITS_CONVERSION`.

Here is template for the new item definition.

```
save__existing_category.acronym_new_item_name
    _item_description.description
;               Description goes here ...
;
    _item.name                   '_existing_category.acronym_new_item_name'
    _item.category_id              existing_category
    _item.mandatory_code           no
    _item_default.value            ?
     loop_
    _item_examples.case
    _item_examples.detail          ?  ?
```

```
     loop_
    _item_range.maximum
    _item_range.minimum           ?  ?
    _item_type.code               ?
    _item_units.code              ?
     save_
```

If the new data item can only have a discrete set of values then replace the data items in the ITEM_RANGE category in the above example with items from the ITEM_ENUMERATION category.

1.3 Adding a new category with no common items

All of the considerations associated with adding a new data item apply to the addition of a new category. In this case, multiple new data items will be created and a key consideration here is determining the key items for the new category. We restrict this example to the case where all of the data items in the category are newly created so that there are no interaction with existing categories.

The choice of the data items which compose the unique identifier for each row of the category is crucial. In most cases this should be a straightforward decision. However, when the choice is not clear it may indicate that multiple categories are required to properly represent the collection of data items.

Once the category key has been selected, an appropriate set of category and data item names must be chosen. In this case, the category name can carry the institutional prefix that will identify the category and its associated data items as locally developed. In building the category definition a description must be created and some examples of the full category should be developed. Some consideration should also be given to the membership of the new category in an existing category group.

Here is template for the new category definition.

```
save_ACRONYM_NEW_CATEGORY
    _category.description
;              Description goes here ...
;
    _category.id                   acronym_new_category
    _category.mandatory_code       no
     loop_
    _category_key.name           '_acronym_new_category.key_item_1'

     loop_
    _category_group.id            'inclusive_group'
                                  ?
     loop_
    _category_examples.detail
    _category_examples.case       ?   ?

     save_
```

A new category may contain subsets of items which have relationships which can be described in categories ITEM_RELATED and ITEM_DEPENDENT. Data items from these categories should be added to item definitions as required.

1.4 Adding a new category with some common items

The additional complexity in sharing items in a new category with those in an existing category arises from the additional parent-child relationships that are introduced in such an extension. It is generally possible to localize these additional relationships within the definition of the common items in the new category. Here is an example of a new category which includes a reference to the entity identifier which is has a parent definition in the existing ENTITY category.

```
save__acroynm_new_category.entity_id
    _item_description.description
;               This data item is a pointer to item _entity.id defined in
                the ENTITY category.
;
    _item.name                  '_acroynm_new_category.entity_id'
    _item.category_id             acronym_new_category
    _item.mandatory_code          yes
    _item_linked.parent_name    '_entity.id'
    _item_linked.child_name     '_acroynm_new_category.entity_id'
     save_
```

1.5 Adding a data item which changes the composition the key in an existing category

Changing the composition of an existing category key is can profoundly change the underlying organization of the a dictionary. Such a change should be considered as a last resort and only after careful consideration by the community of dictionary users.

mmCIF Dictionary Extensions

Table of Contents

1 mmCIF Dictionary Extensions 1
1.1 Types of Extensions 1
1.2 Adding a new property to an existing category 1
1.3 Adding a new category with no common items 2
1.4 Adding a new category with some common items 3
1.5 Adding a data item which changes the composition the key in an existing category . . . 3