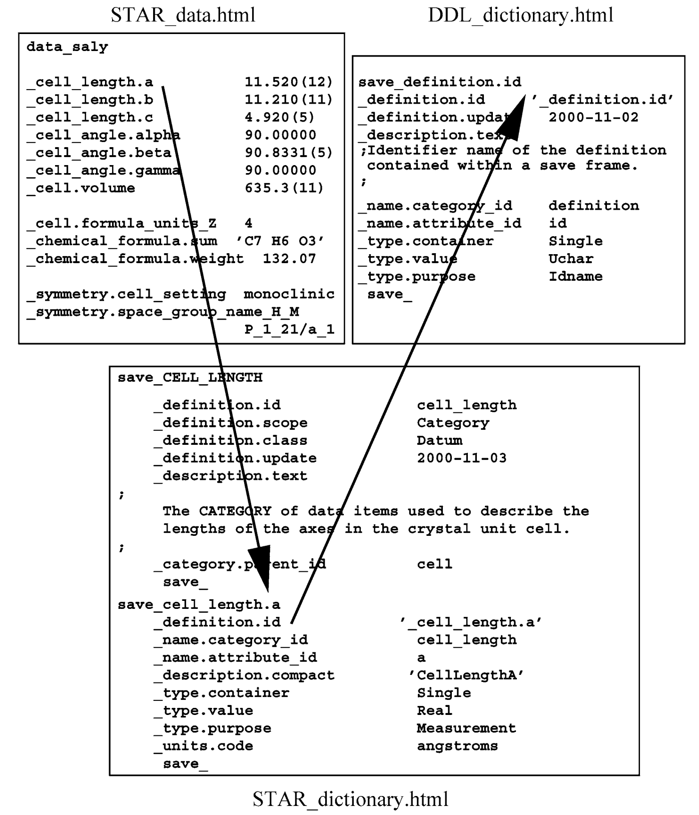
International Tables for Crystallography (2006). Vol. G, Section 5.2.6, pp. 495–497.



STAR_data.html

```
data_saly

_cell_length.a            11.520(12)
_cell_length.b            11.210(11)
_cell_length.c            4.920(5)
_cell_angle.alpha         90.00000
_cell_angle.beta          90.8331(5)
_cell_angle.gamma         90.00000
_cell.volume              635.3(11)

_cell.formula_units_Z    4
_chemical_formula.sum   'C7 H6 O3'
_chemical_formula.weight  132.07

_symmetry.cell_setting  monoclinic
_symmetry.space_group_name_H_M
                          P_1_21/a_1
```

DDL_dictionary.html

```
save_definition.id
_definition.id        '_definition.id'
_definition.update     2000-11-02
_description.text
;Identifier name of the definition
 contained within a save frame.
;
_name.category_id      definition
_name.attribute_id     id
_type.container        Single
_type.value            Uchar
_type.purpose          Idname
 save_
```

```
save_CELL_LENGTH

    _definition.id                  cell_length
    _definition.scope               Category
    _definition.class               Datum
    _definition.update              2000-11-03
    _description.text
;
     The CATEGORY of data items used to describe the
     lengths of the axes in the crystal unit cell.
;
    _category.parent_id             cell
     save_
save_cell_length.a
    _definition.id                 '_cell_length.a'
    _name.category_id               cell_length
    _name.attribute_id              a
    _description.compact           'CellLengthA'
    _type.container                 Single
    _type.value                     Real
    _type.purpose                   Measurement
    _units.code                     angstroms
     save_
```

STAR_dictionary.html

Fig. 5.2.5.1. Hyperlinking markup generated by *StarMarkUp*. The example is based on an extended relational dictionary definition language, StarDDL.

of the STAR File. The program understands only the rules of a legitimate STAR File.

StarMarkUp provides a number of hyperlinking facilities. During markup, it automatically hyperlinks frame-code values to the internal save-frame block to which they point. As part of the same process, *StarMarkUp* inserts anchors in all data and save-frame blocks. It does this in anticipation that there may be the need to hyperlink to these anchors from another STAR File. The most obvious application for this is in the marking up of the DDL dictionary. The list of anchors generated from this process can be passed on to the discipline dictionary during its markup phase (Fig. 5.2.5.1). In this way, the tags used in the discipline dictionary to define the data names can be made to point back to their entry in the DDL dictionary. At the same time that the discipline dictionary is being marked up, a list of its anchors is being generated (each anchor being to a data-item definition). This list is used when marking up an instance of the discipline STAR data file to hyperlink each data name back to its definition in the discipline dictionary.

StarMarkUp comprises a hand-crafted tokenizer employing a character buffer and one-character look-ahead to identify accepted tokens. *StarMarkUp* does not build an internal representation of the file, but functions as a streaming parser. The *GetToken()* function returns a structure consisting of the token type (an enumerated set) and the token value (the lexeme associated with that token). In most cases, the lexeme is marked up and injected into the output stream. If the token is associated with a STAR File block, the parser will recursively call a *MarkUpBlock()* function. A recursive descent parser makes it very easy to treat all STAR File blocks (`global_`, `data_` and `save_`) in identical fashion.

StarMarkUp is implemented in Tcl/Tk for novelty and not because of any particular superior qualities of the language and its API. It is, however, fast and sufficiently flexible, and extensions to the program can be rapidly implemented and tested.

5.2.6. Object-oriented STAR programming

The STAR File syntax is very simple but flexible, and suggests a number of well defined data structures. 'Scalar' values (*i.e.* single text strings identified by specific data names) are obvious, as are 'vectors' (multiple string values associated with a data name in a `loop_` declaration). 'Matrices' are constructed by associating identical-length vector items in the same `loop_` structure. Note that these data structures are not true matrices, but arrays or tables of column-addressable vectors. Column addressing arises from the need to associate each set of values with a distinct data name in the loop header declaration.

Through the nested loop construct in STAR, vector or matrix *elements* are permitted within vectors or matrices. Save frames provide addressable data structures containing one or more scalar, vector or matrix components; and data blocks contain similar data structures with the inclusion of embedded save frames.

This hierarchy of structure allows many other data models to be mapped onto the STAR syntax. For example, STAR does not in itself provide addressable *rows* in matrix structures, but such a concept may be achieved in application-specific ways. For example, the relational database structure of mmCIF and other DDL2 applications ensures that table rows can be identified by specific key values. Loops of multiple values associated with a single data name are similar to *lists* or one-dimensional *arrays* as defined in many computer languages. Simple *associative arrays*, or 'hashes', such as are used to great effect in Perl and Python, can be modelled by designating the first value of a two-item loop structure as the 'key' item, by analogy with the relational database example above (in such an application the key value of course needs to be unique). The hierarchy of nested loops can be used to model certain types of complex structures such as might be defined in a C-language 'struct', for example.

There is a natural possibility of representing particular well defined data structures as 'objects' and handling STAR Files by object-oriented programming techniques. Where applications associate properties of specific data items with external reference descriptions, as in the DDL dictionaries, the dictionary entries can be considered to express types, relationships and even methods associated with the object classes.

However, the versatility of the STAR syntax means that there are many ways of designing STAR objects and their relationships, and it is likely that the most useful efforts will be in designing applications for specific purposes or subject areas. Below we describe a number of prototypes and implementations of object-oriented STAR programming. Some are rather generic in outlook; others are informed by the crystallographic viewpoint embodied in CIF.

5.2.6.1. *OOSTAR*

The *OOSTAR* approach (Chang & Bourne, 1998) developed and tested an Objective-C (Pinson & Richard, 1991) toolset for STAR representation. The developers selected Objective-C over the more common C++ language because of its perceived advantages of (i) loose data typing, (ii) run-time type checking and (iii) message-passing ability. These were all seen to aid flexible software design, an asset for applications built on the very flexible structure of the STAR syntax itself.

Chang & Bourne constructed a set of classes built on the basic objects *item* and *value*. Their model builds upwards through a hierarchy of classes describing relationships between objects. The *ItemAssoc* class contains data members corresponding to the data item itself, its included value or set of values, and the data name that is used to reference the item; the class also has pointers to previous and next elements to allow iteration. The *StarAssoc* class contains methods for manipulating STAR objects through setting and retrieval of data names and assignment of values. *DataBlock* is the class containing all the lower-order items and associations, and one or more such *DataBlock* classes comprise the *StarFile* class.

The *OOSTAR* approach also provides *Dictionary* and *DictionaryElement* classes so that STAR applications that do describe element attributes in external dictionary files can make use of such information.

Some sample applications were built with the class libraries of the *OOSTAR* toolset, and they are described in Chang & Bourne (1998). They include: simple converters of STAR data files to HTML pages with hyperlinks to associated dictionary entries; a query tool for retrieving the data values for a specific item specified by name within a specific data block; and a query mechanism that retrieves a set of items from a STAR loop structure and represents their values in an array, *i.e.* flattening if necessary any nested loops into a purely tabular presentation. These query tools are different from *Star_Base* primarily in that they do not return the context in which the data are found in the original file – their interpretation depends on a detailed *a priori* understanding of the target file structure.

This approach is rather different from the canonical description of STAR given in this volume, and was never developed into full-blown applications (in part because the developers recognized that the Java language would provide a preferable platform for further development). Nevertheless, it provides interesting ideas for the developer considering building object-oriented applications for STAR Files.

5.2.6.2. *CIF++*

CIF++ was a small library of classes designed by Peter Murray-Rust during the time that DDL was being developed as a language for representing the properties and attributes of STAR data items (*e.g.* Murray-Rust, 1993). The purpose of this project was to demonstrate the design of data classes that represented real-world objects such as molecules and crystal cells. At a time when the structure of CIF was under intense discussion, many of the classes were potentially extensible to STAR features that were a superset of those found in CIF.

While these classes were never developed into fully functional applications, they demonstrated a potentially fruitful approach to model representation and gave rise to the idea of including methods in STAR dictionary definitions, thus allowing STAR applications to dynamically associate algorithmic relationships and operations with data objects by parsing the methods description in the dictionary definitions. This approach is currently being developed into a relational expression language for STAR called dREL (Spadaccini *et al.*, 2000).

The ideas behind *CIF++* were further developed in a class library for molecular representation called *Democritos*, and have informed the representation of molecular and crystal structure in Chemical Markup Language (CML) and in the structured document browser *Jumbo* (Murray-Rust, 1998).

The *CIF++* classes have been refactored into Java using the W3C document object model (W3C, 2004) and other DOM-like models. They are now based on an XML schema which is the abstraction of the formal DDL1 specification (Chapter 2.5).

These are available as part of the *Jumbo* distribution at http://cml.sf.net. The design involves an interface that would allow the C++ classes to be recreated from the Java.

5.2.6.3. *CIFOBJ*

The *CIFOBJ* class library (Schirripa & Westbrook, 1996) was developed to provide an object view of the mmCIF dictionary and to complement the relational *CIFLIB* class library (Westbrook *et al.*, 1997) for handling mmCIF data. As such, it is very much tuned to crystallographic applications and it handles only the subset of STAR features used in CIF dictionaries. This does, however, include some limited handling of save frames, and is therefore a little more complex than applications interested only in CIF data input/output processing.

CIFOBJ has two components. The first builds a persistent store of objects of types item, subcategory, category and dictionary. Each such object is a container for all relevant attributes permitted for that object type. The object store is populated from the mmCIF dictionary by the *CIFOBJ* loader class (using methods provided by *CIFLIB*). This loader class assembles the dictionary objects and passes them to an object-storage manager. The second component of the *CIFOBJ* class library provides the methods necessary for building dictionary objects from the persistent store and for passing attribute strings to procedures concerned with establishing the integrity of data values.

The main reason for discussing this implementation here is to indicate the rapid growth in complexity needed to impose an application-specific object view on even a relatively simple STAR data structure. In generic prototype STAR projects such as *OOSTAR*, half a dozen or so classes and associated methods suffice to represent the highest-level abstract concepts implied in STAR constructions. In *CIFOBJ*, however, dozens of methods are associated with dictionary access. Dictionary-driven validation of an mmCIF numerical data value can involve:

(i) retrieval from the dictionary of the extended type declaration associated with the data item;

(ii) validation of the basic type (*i.e.* that it is indeed numeric) against the primitive data types supported by the dictionary;

(iii) validation of the extended type by regular-expression matching of the string representation of the value against the allowed patterns stored in the dictionary;

(iv) retrieval of any existing range constraints specified in the dictionary and comparison with the data value;

(v) location and evaluation of any associated standard uncertainty;

(vi) identification of the units in which the physical quantity is expressed;

(vii) if necessary, conversion of the units according to the conversion tables stored in the dictionary.

More complexity arises from the relationships between data items expressed through dictionary attributes such as name aliasing, parent–child dependencies and category membership.

Nevertheless, the complexity of these relationships is an indication of the richness of the metadata available through the dictionary approach, and the availability of well defined object representations simplifies the construction of well designed large-scale application frameworks, such as underpin the Protein Data Bank (Berman, Battistuz *et al.*, 2002) and Nucleic Acid Database (Berman, Westbrook *et al.*, 2002).

5.2.6.4. *starlib*

BioMagResBank (BMRB) is a repository for NMR spectroscopy data on proteins, peptides and nucleic acids at the University of Wisconsin – Madison (Ulrich *et al.*, 1989). For some time, NMR data sets have been exchanged within this environment using STAR Files; an NMRStar data dictionary to define the data names used for tagging NMR data is under development

(BioMagResBank, 2004). The *starlib* class library was developed at BMRB for handling NMRStar files, but its initial application to such files independently of the prototype data dictionary means that it is applicable to any STAR File. It does not provide a relational database paradigm (although this is a long-term goal). However, it does provide objects and methods suitable for searching and manipulating STAR data.

Table 5.2.6.1 lists the top-level classes used in *starlib*. *ASTnode* is a formal base class, providing the types and methods that can be used in other derived classes. *StarFileNode* is the root parent of all other objects contained in an in-memory representation of a STAR File; in practice it contains a single *StarListNode*, which is the list of all items contained in the file. *BlockNode* is a class which contains a partition of the STAR File: the class handles both data blocks and global blocks. Data-block names are stored in instances of the *HeadingNode* object, which also holds save-frame identification codes and is therefore useful for accessing named portions of the file.

DataNode is a virtual class representing the types of data objects handled by the library (accessed directly as *DataItemNode*, *DataLoopNode* and *SaveFrameNode*).

Looped data items are handled by a number of objects. *DataLoopNameListNode* is a list of lists of names in a loop. The first list of names is the list of names for the outermost loop, the second list of names is the list of names for the next nesting level and so on. *LoopNameListNode* is a list of tag names representing one single nesting level of a loop's definition. *LoopTableNode* is a table of rows in a *DataLoopNode* (not itemized in Table 5.2.6.1; it is an object representing a list of tag names and their associated values, a particular case of *DataNode*). *starlib* views a loop in a STAR file as a table of values, with each iteration of the loop being a row of the table. Each row of the table can have another table under it (another nesting level), but such tables are the same structure as the outermost one. Thus *LoopTableNode* stores a table at some arbitrary nesting level in the loop. A simple singly nested loop will have only one loop table node, but a multiply nested loop will have a whole tree of loop tables. *LoopRowNode* is a single row of values in a loop.

DataNameNode holds the name of a tag/value pair or a loop tag name. *DataValueNode* is the type that holds a single string value from the STAR file and the delimiter type that is used to quote it.

DataListNode and *SaveFrameListNode* store lists of data within higher-order data objects or save frames, and are internal classes rarely invoked directly by a programmer.

A number of observations may be made regarding this approach. Firstly, the objects can be mapped with reasonable fidelity to the high-level Backus–Naur form representation of STAR (Chapter 2.1). Secondly, it is computationally convenient to abstract common features into parent classes, so that, for example, individual data items, looped data and save frames are represented as child objects of the *DataNode* object, and not themselves as first-generation children of the base class. Thirdly, the handling of nested loops may be achieved in different ways; *starlib* has chosen a particular view that is perhaps well suited to relational data models.

As expected within a programming toolkit, *starlib* offers a large number of methods for retrieving STAR data values, adding new data items, extending or re-ordering list structures, and performing structural transformations of the in-memory data representation. Unlike the stand-alone *Star_Base* application, it does not guarantee that output data will be in a STAR-conformant format; and the programmer is left with the responsibility of validating transformed data at a low level.

Table 5.2.6.1. *Object classes for manipulating STAR data in starlib*

ASTnode	The base class from which all other classes are derived
StarFileNode	The STAR File object
StarListNode	List of items contained in the STAR File
BlockNode	A data or global block
HeadingNode	Labels for major STAR File components
DataNode	General class for data objects
DataLoopNameListNode	List of lists of names in a loop
LoopNameListNode	List of tag names representing one nesting loop level
LoopTableNode	Table of rows in a loop
LoopRowNode	Single row of values in a loop
DataNameNode	A data name
DataValueNode	A single string value
DataListNode	List of data within a higher-order data object
SaveFrameListNode	List of data items allowed in a save frame

Nevertheless, this is a substantial and important library which, as with *CIFOBJ*, has played an important role in the functioning of a major public data repository. Development of the class libraries continues, with a Java version now available.

5.2.6.5. *StarDOM*

A convenience of well designed object representations is that effective transformation between different data representations may be possible. The *StarDOM* package (Linge *et al.*, 1999) demonstrates a transformation from STAR Files to an XML representation, where the tree structure of a STAR File as interpreted in the *starlib* view above is mapped to a document object model (DOM; W3C, 2004). This approach is similar to *Jumbo*, mentioned above in Section 5.2.6.2.

A demonstration of *StarDOM* is the transformation of the complete set of NMR data files at BioMagResBank to XML. The resultant files can then be interrogated using the *XQL* query language (Robie *et al.*, 1998). In this example implementation, the target XML document type definition (DTD) includes a small number of XML elements matching the STAR objects *global* and *data block*, *save frame*, *list*, *data item*, *data name* and *data value*. Particular data names are recorded as values of the <NAME> element. The authors of the *StarDOM* package are considering an extension in which named data items map directly to separate XML elements; the goal is to develop an NMR-specific DTD that is isomorphous to the emerging NMRStar data dictionary.

References

Berman, H. M., Battistuz, T., Bhat, T. N., Bluhm, W. F., Bourne, P. E., Burkhardt, K., Feng, Z., Gilliland, G. L., Iype, L., Jain, S., Fagan, P., Marvin, J., Padilla, D., Ravichandran, V., Schneider, B., Thanki, N., Weissig, H., Westbrook, J. D. & Zardecki, C. (2002). *The Protein Data Bank. Acta Cryst.* D**58**, 899–907.

Berman, H. M., Westbrook, J., Feng, Z., Iype, L., Schneider, B. & Zardecki, C. (2002). *The Nucleic Acid Database. Acta Cryst.* D**58**, 889–898.

BioMagResBank (2004). *NMR-STAR Dictionary*. Version 3.0. (Under development.) http://www.bmrb.wisc.edu/dictionary/3.0html/.

Chang, W. & Bourne, P. E. (1998). *CIF applications. IX. A new approach for representing and manipulating STAR files. J. Appl. Cryst.* **31**, 505–509.

Knuth, D. E. (1973). *The art of computer programming.* Vol. 3, *Sorting and searching*, pp. 422–447. Reading, MA: Addison-Wesley.

Linge, J. P., Nilges, M. & Ehrlich, L. (1999). *StarDOM: from STAR format to XML. J. Biomol. NMR*, **15**, 169–172.

Murray-Rust, P. (1993). *Analysis of the DDL/dictionary parsing problem. Proc. First Macromolecular Crystallographic Information File (CIF) Tools Workshop*, ch. 12. New York: Columbia University.