XyMJava System for World Wide Web Communication of Organic Chemical Structures

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The XyMJava system for drawing chemical structural formulas has been developed by using the Java language in order to enhance World Wide Web communication of chemical information, where the XyM notation system proposed previously has been adopted as a language for inputting structural data. The object-oriented technique, especially the design-pattern approach, is applied to parse a XyM notation in the XyMJava system. A chemical model is introduced to encapsulate information on chemical structural formulas and used to draw the formula on a CRT display. Thereby, an HTML document containing a XyM notation can be browsed by the XyMApplet of the XyM Java system.

Key Words: XyM Notation, Java, Structural Formula, WWW

Introduction

From the early stage in the history of organic chemistry, information on chemical structures has been communicated and stored by means of systematic diagrams, i.e. chemical structural formulas. They have been linked with conventional or systematic nomenclature systems to realize oral communication as well as documentation based on printed matters such as

journals and books. For example, the IUPAC nomenclature,^{1,2} the CAS nomenclature,³ and the HIRN nomenclature^{4,5} are representative as such traditional communication systems.

The exponential increase of information on chemical compounds during the two decades before 1980 had revealed the importance of chemical database, which in turn stimulated the progress of computer-manipulation of chemical structural formulas. This situation was typically exemplified by the fact that "Journal of Chemical Documentation" published by American Chemical Society was renamed into "Journal of

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Chemical Information and Computer Sciences" in 1961. Because of the shortage of computer capacity at that time, more effective representation systems than the nomenclatures were pursued in order to enhance data storage and retrieval by computer. Because of such restriction, linear notations were developed as compressed representation systems, as summarized in excellent reviews⁶⁻⁹ and books.¹⁰⁻¹³ Among them, the Dyson-IUPAC Notation,^{14, 15} the Wiswesser Line-Formula Notation (WLN),¹⁶ the Hayward Notation,¹⁷ and the Skolnik Notation¹⁸ should be referred to as representatives of such data-handling notations. Since these systems aimed at unique and unambiguous nature,¹⁰ their rules were so complicated as to require a specialist to give a correct name. According to advances in computer technology, more flexible approaches such as SMILES (Simplified Molecular Input Line Entry System),¹⁹⁻²¹ the (extended) Wilcox-Levinson System,^{22, 23} and SYBYL Line Notation²⁴ were reported as chemical notation systems.

As a result of the explosive development of computer hardware during 1980s, the restriction due to computer capacity was removed so that more informative representation systems (topological systems) were embodied, where connection tables²⁵⁻²⁷ or equivalents were used as a key technology.²⁸ They have been adopted by most database systems and application systems for manipulating chemical structures.^{29, 30}

Moreover, as computer hardware has further developed during the last decade (1990s), binary data or equivalent text data (e. g. Encapsulated PostScript data), which store chemical structures as image data, can be easily manipulated. Thereby, such data have been directly used in desktop publishing technique (DTP), as discussed in a review.³¹ In addition to the explosive development of computer hardware, the last decade has seen deep influences provided by the progress of the World Wide Web (WWW) system for the Internet, where browser techniques based on HTML (HyperText Markup Language) or XML (Extensible Markup Language) have played an important role.³² Beyond the preceding era of their storage and retrieval, the problem "how to communicate chemical structural formulas" has again attracted more and more attention as prerequisites to the WWW system. The XyM Markup Language (XyMML) has been reported by us^{33, 34} as an embodiment of the spirit of markup languages, where chemical meanings such as skeletons (e. g. benzene, naphthalene, and other aromatic rings; or pyridine, quinoline, and other heteroaromatic rings), functional groups, etc. can be obtained easily from the XyMML tags. Chemical Markup Language (CML)³⁵ has been proposed for communication in the WWW system. The CML contains chemical structural data in a format equivalent to a connection table in which such chemical meanings can be obtained only by some complicated algorithms that have been adopted in the chemical

database systems.

We developed the XyMTeX system for typesetting chemical structural formulas,³⁶⁻³⁹ where the XyMTeX commands were regarded as linear notation.⁴⁰ Although the XyMTeX command system was adopted in a WWW browsing system,⁴¹ it required layout data in complicated cases; hence it was insufficient to the WWW communication. To avoid the drawbacks of the XyMTeX command system, we have recently reported the XyM Notation system (the left branch of Fig. 1).⁴²

Figure 1 XyM Notation, XyMJava, and XyMTeX.

In the previous paper,⁴² we have shown that the XyM Notation system is one of dominant candidates capable of solving the problem "how to communicate chemical structural formulas" for the WWW communication. Since the XyM Notation system has been originally implemented as a typesetting system based on TeX/LaTeX,⁴³ a further device should be developed to spread the use of the XyM Notation system in the WWW. As clarified in the preceding paragraphs, our goal is the development of XyMJava³⁴ in which the XyM Notation system is implemented by the Java language to display chemical structural formulas on a CRT screen and to communicate them via WWW (the right branch of Fig. 1).

Minimum Features of the XyM Notation

Since the XyMJava system of the present paper is an implementation of the XyM Notation system by the Java language, essential items on the XyM notations shall be revisited briefly. The XyM Notation system is based on the methodology that each organic compound is regarded as a derivative of a mother skeleton, where such derivation processes are categorized into (1) substitution derivation, (2) atom derivation, or (3) bond derivation. The general formats of the XyM notations are represented as follows:

```

%GenSkel(SKBONDLIST)[BONDLIST]{ATOMLIST}{SUBSLIST}{OMITLIST}
%FuseSkel(SKBONDLIST)[BONDLIST]{ATOMLIST}{SUBSLIST}{FUSE}{OMITLIST}

```

where the symbol ¥GenSkel represents a mother skeleton and the symbol ¥FuseSkel represents a fusing skeleton for constructing fused rings. They take five or six arguments with parentheses, brackets and braces.

The name of each skeleton (¥sixheterov, ¥sixheterovi, etc.) or each fusing skeleton (¥sixfusev, ¥sixfusevi, etc.) consists of a backslash symbol (or a yen symbol in the Japanese character system) that represents the top of a XyM notation, a stem that comes from a ring size (sixhetero etc.) or a fusion mode (sixfuse etc.) and a suffix that represents the direction of drawing the skeleton structure (v, vi, vb, vt, h, and hi).

The arguments with braces are essential ones for the skeleton ¥GenSkel or the fusing skeleton ¥FuseSkel. Since they cannot be omitted in any situations, an empty pair of braces {} is necessary in an unspecified case.

1. The argument ATOMLIST is used to bring an atom derivation, which represents the replacement of vertices by appropriate hetero atoms. The ATOMLIST contains a semicolon for delimitating every replacement modes, each of which in turn contains a double equality symbol for separating a position number from a hetero atom to be replaced. For example, the argument {1==O;4==O} in the XyM notation of 1,4-dioxane, ¥sixheterov{1==O;4==O}{}, shows that positions 1 and 4 are replaced by oxygen atoms.
2. The argument SUBSLIST is to implement a substitution derivation. For example, the argument {1Sa==F;1Sb==F} for the XyM notation of 1,1-difluorocyclohexane, ¥sixheterov{{1Sa==F;1Sb==F}}, contains a semicolon to separate every substitution modes as well as a double equality symbol to distinguish between a substitution position (with a bond modifier such as 'Sa' and 'D' if necessary) and a substituent.
3. The argument FUSE represents a fusing bond (a lowercase or uppercase alphabet), which is omitted during a ring fusion. The usage of a lowercase or uppercase alphabet switches the normal or inverse node of the ring fusion.

The arguments with parentheses or brackets for the skeleton ¥GenSkel or the fusing skeleton ¥FuseSkel are optional ones that can be abbreviated if they are unnecessary:

1. Most important is the argument BONDLIST for introducing unsaturation of a skeleton as well as ring fusion (a bond derivation). The argument BONDLIST contains lowercase alphabets to designate such unsaturation, where an alphabet is assigned to each bond of the skeleton.
2. The top optional argument SKBONDLIST for treating stereochemical information. The

argument SKBONDLIST contains pairs of two alphabets in braces, where each pair consists of a bond specifier (a lowercase letter) and an uppercase letter (A or B).

3. The argument OMITLIST is a list of bond specifiers, each of which designates a bond to be deleted. As a matter of course, SKBONDLIST and OMITLIST take no common bond specifiers.

It should be noted here that any XyM notation contains arguments having specific chemical meanings such as aromatic or heteroaromatic rings (¥GenSkel and ATOMLIST), functional groups (SUBSLIST), and bond multiplicities (BONDLIST).

Any substituent can be derived from a skeleton (¥GenSkel) by adding the code (yl) with a locant number (n) to its SUBSLIST as follows:

```
¥GenSkel{BONDLIST}{ATOMLIST}{...;n==(yl);...}
```

where most useful arguments are selected and the other optional arguments are omitted for the sake of simplicity. This technique for generating a substituent is called "yl-function". The resulting notation for a substituent can be added to the SUBSLIST of any other skeleton. For example, cyclohexylcyclohexane is represented by the following XyM notation,

```
¥sixheterov{{1==¥sixheterov{{4==(yl)}}}}
```

where the cyclohexyl substituent is expressed by

```
¥sixheterov{{4==(yl)}}
```

A formula with a multi-nested substituent can be generated by using two or more yl-functions nested. For example, 4-(4-benzoylcyclohex-3-en-1-yl)-1-naphthol (Fig. 2) is drawn by the XyM notation:

```
¥decaheteroh{acfhk}{{1==HO;4==%
¥sixheteroh{c}{{1==(yl);4==%
¥tetrahedral{2==(yl);0==C;1D==O;%
4==¥sixheteroh{ace}{{1==(yl)}}}}
```

where a percent symbol is used to designate no space in the end of a line.

Figure 2. Formula with a multi-nested substituent.

The nesting is represented by the following scheme:
 (outer) ¥decaheteroh ← ¥sixheteroh ← ¥tetrahedral ← ¥sixheteroh (inner).

Two or more fusing skeletons `¥FuseSkel` can be nested to generate a multi-fused structural formula. The structural formula of a 7H-pyrazino[2,3-c]carbazole can be constructed by the nesting technique in the order of 6, 5 ← 6 ← 6 (Fig. 3):

```
¥nonaheterov[bejj{b¥sixfusev[ac{a¥sixfusev[bf]{6==N;3==N}{D}}
]{3==OH}{e}}{1==N}{1==H;4==OH}
```

Note that an uppercase letter 'D' in the FUSE argument is used in place of a lowercase letter 'd', since this usage determines the mode of fusion.

Figure 3. Multi-nested fused formula.

Development of the XyMJava System

Model-View-Controller for XyMJava

The XyMJava system for the WWW communication of information on chemical structural formulas has been developed by using the Java language. To realize an effective user interface for the XyMJava system, we have adopted the model-view-controller paradigm (MVC)^{44, 45} and design patterns for object-oriented programming.^{46, 47}

Table 1. Model-View-Controller (MVC) for XyMJava System

MVC	Class	Function
Model	<code>ChemStruct</code>	Representing chemical structures
	<code>Atom</code>	Representing atoms
	<code>Bond</code>	Representing bonds
View	<code>XyMApplet</code>	Displaying chemical structures via a WWW browser
Controller	<code>XyMJava</code>	Main Program
	<code>ChemStructCreator</code> (<code>XyMStructCreator</code>)	Extraction of chemical structures from XyM notations
	<code>XyMParser</code> (<code>XyMNotnParser</code>)	Parsing XyM notations Auxiliary for XyMParser

The Java classes of the XyMJava system are listed in Table 1 in terms of the MVC paradigm. The model

objects of the XyMJava system are based on a "chemical model" that is implemented as instances of the corresponding Java classes, i.e. the `ChemStruct` class for representing chemical structures, the `Atom` class for representing atoms, and the `Bond` class for representing bonds. The view object of the XyMJava system is based on the `XyMApplet` class for displaying chemical structures by using a WWW browser. The controller objects are derived from the main class `XyMJava`, the `XyMStructCreator` class for extracting chemical structures from XyM notations, the `XyMParser` class (and its extended class `XyMNotnParser`) for parsing XyM notations, and the `SubXyMParser` class (and its extended class `SubXyMNotnParser`) for supporting auxiliaries for `XyMParser`.

Parsing of XyM Notations for Encapsulated Structural Data

Chemical Model as Encapsulated Structural Data

We have introduced a chemical model for the XyMJava system in order to develop a common handling technique of structural data that are applicable to other types of software than WWW software. The chemical model is illustrated as a class diagram in Fig. 4 in terms of the unified modeling language (UML)⁴⁷ where a line with a rhombus represents an aggregation. For example, the `Bond` class multiply refers to the `Atom` class, while both of them are multiply referred to by the `ChemStruct` class.

Figure 4. Class Diagram for Chemical Model.

Atom Class. The `Atom` class (Fig. 4) encapsulates necessary and sufficient pieces of information on an atom or a functional group, e. g. x- and y-coordinates (and sometimes z-coordinate), an element symbol (String `ElementType`), a functional group (String `AtomGroup`), a flag for drawing the functional group (e.g. int `RIGHT` for -COOH or int `LEFT` for HOCO-), a flag for drawing a carbon atom (C) on each vertex

Figure 5. Class Diagram for Parsing a XyM Notation.

(boolean visible: 'false' for no drawing and 'true' for drawing C), and so on. Note that 'String' for character strings, 'int' for integers, and 'boolean' for boolean values are default classes provided by the Java packages.

Bond Class. The **Bond** class (Fig. 4) encapsulates necessary and sufficient pieces of information on a bond, e.g. a bond multiplicity (int `bondType`), terminal atoms (Atom `beginAtom` and Atom `endAtom`), incident positions (int `beginAtomConnectDirection` for a beginning atom and int `endAtomConnectDirection` for an ending atom), an adjustment flag for a double bond (int `right: 'rightHand'` for an endocyclic double bond), and so on.

ChemStruct. The **ChemStruct** class (Fig. 4) has no concrete information on atoms and bonds but contains a set of methods for referring to Atom objects (e.g. void `addAtom(:Atom)` for setting 'Atoms.addElement' to a Vector instance `Atoms`, an Enumeration instance `getAtomIterator()` for getting 'Atoms.elements()') as well as another set of methods for referring to Bond objects (e.g. void `connectAtom(:Atom, Atom)` for

setting 'Bonds.addElement' to a Vector instance `Bonds`, and an Enumeration instance `getBondIterator()` for getting 'Bonds.elements()').

Parsing of XyM Notations. To parse a XyM notation, the **XyMParser** class and its subclass **SubXyMParser** have been developed as interfaces (abstract classes), as shown in a class diagram based on UML (Fig. 5).

They have been respectively implemented as concrete classes, **XyMNotnParser** and **SubXyMNotnParser**, which contain concrete codes for parsing a XyM notation. According to the UML formats, an open triangle represents with a dotted line represents a *generalization* (inversely implementation), and an arrow with a solid line represents a *navigability*, and a solid triangle on the arrow line represents a relationship (e.g. **Requests-Creation**) between the roles of participant classes (e.g. **requestor** and **creator**).

The **XyMParser** class is an interface for dividing a XyM notation into a set of arguments, i.e., a skeleton name `¥GenSkel` or `¥GenFuse`, a bond list

(BONDLIST), an atom list (ATOMLIST), a substitution list (SUBSLIST), etc. This process is called a dividing process for the sake of simplicity. The `SubXyMParser` class is an interface for subdividing each of the components into sub-arguments, where the atom list, for example, is divided into a locant number, a bond modifier, an atom, etc. This process is called a subdividing process. Since the abstract classes, `XyMParser` and `SubXyMParser`, behave as interfaces, any change of the concrete classes, `XyMNotnParser` and `SubXyMNotnParser`, into other concrete classes (e.g. `XyMMLParser` for parsing XyM Markup Language) gives no influences on the `XyMStructCreator` class that creates structural formulas.

Figure 5 shows that the interfaces (`XyMParser` and `SubXyMParser`) and the concrete classes (`XyMNotnParser` and `SubXyMNotnParser`) for parsing a XyM notation can be regarded as a dual embodiment of the Factory-Method pattern.^{46, 47} This dual embodiment can be applied recursively to treat nesting structures in a substituent list (SUBSLIST) and in a bond list (BONDLIST). The Iterator pattern^{46, 47} is also used to treat branches in a tree structure produced from a XyM notation.

To parse the arguments of a XyM notation (a dividing process), the `XyMJava` class uses the `XyMParser` class as a Product, where the `XyMJava` class (as a requestor) is linked with the `SubXyMParser` class (as a creator) in a Requests-Creation fashion. Thereby, the `SubXyMParser` class as a FactoryIF (factory interface), or more precisely the corresponding concrete Factory `SubXyMNotnParser`, creates the `XyMParser` class as a 'Product'. As a result, the `XyMNotnParser` class is regarded as a concrete Product. As found in the code listed in Fig. 6, the `SubXyMParser` class contains the `getStruct()` method as a `XyMParser` instance in order to get a nested structure.

On the other hand, the `XyMJava` class uses the `SubXyMParser` class that is switched into a Product in a subdividing process designated with parentheses in Fig. 5. Thus, the `XyMJava` class (as a requestor) requests the creation of the `XyMParser` class (as a creator), which

acts as a FactoryIF (factory interface) in this process so as to make the corresponding concrete Factory `XyMNotnParser` create the `SubXyMParser` class as a 'Product'. As a result, the corresponding implement `SubXyMNotnParser` is now regarded as a concrete Product. As found in the code listed in Fig. 6, the `XyMParser` class contains the `getFuseStruct()` method as a `XyMParser` instance in order to get a fusing structure. The `XyMParser` class also contains the `nextAtom()` method for getting a next atom and the `nextSubs()` method for getting a next substituent, where both the methods are `SubXyMParser` instances.

```
abstract class XyMParser{
    public abstract String      getCommandName();//For getting a skeleton name.
    public abstract void        reset();// For resetting an iterator
    public abstract char        getSKBondType(char c);// SKBondType at vertex 'c'
    public abstract String      getLink();//For getting the SKBondlist
    public abstract String      getXyl();//For ryl and lyl.
    public abstract boolean     isDBLBond(char DBL);
                                // Flag for a double bond at edge 'DBL'
    public abstract void        setDoubleBond(char [] doubleBond);
                                // For setting a double bond at edge 'doubleBond'
    public abstract boolean     hasMoreFuse();//One more fusing atom?
    public abstract char        nextFuseLocant();//Locant no. for the fusing structure.
    public abstract XyMParser   getFuseStruct();//For getting a fusing structure.
    public abstract boolean     hasMoreAtom();//For getting the next atom;
    public abstract SubXyMParser nextAtom();// For getting the next atom.
    public abstract void        setAtom(int locant, String atomGroup);
                                //For setting 'atomGroup' at the position 'locant'
    public abstract boolean     hasMoreSubs();//One more substituent?
    public abstract SubXyMParser nextSubs();//One more substituent?
    public abstract int         getYlLocant();//For getting the locant no. of yl function.
    public abstract char        getFusingLocant();
                                //For getting the locant no. of a fusing position.
    public abstract void        makeOmit(char c);// Flag for bond deletion at edge 'c'.
    public abstract boolean     isOmit(char omit);//For deleting a bond at edge 'omit'.
}

abstract class SubXyMParser{
    abstract public boolean     isStruct();//Structure?
    abstract public XyMParser   getStruct();//For getting a structure.
    abstract public int         getLocant();//For getting a locant number.
    abstract public String      getMod();//For getting a bond modifier.
    abstract public String      getAtomicGroup();//For getting a functional group.
}
```

Figure 6. Codes of XyMParser and SubXyMParser Class.

Creation of a Chemical Model

The class diagram of the `XyMJava` package is shown in Fig. 7.

Figure 7. Class Diagram of the XyMJava Package.

The XyMStructCreator class leaves the parsing of a XyM notation to XyMParser and SubXyMParser and has access to a chemical model produced from the XyM notation. The XyMStructCreator class contains methods for creating respective skeletons (¥GenSkel) ; for example, the sixhetero method is to create ¥sixhetrov, ¥sixhetrovi, ¥sixhetroh, and ¥sixhetrohi. Each of these method calls the Struct method recursively to treat a nested structure of the XyM notation.

Displaying Structural Formulas

To display a chemical structural formula, we use the XyMApplet class that has been developed as an Applet instance of Java. The XyMApplet class uses the XyMJava class that has been collected with the other classes to give a package jp.ac.kit.chem.imt.XyMJava, as shown in Fig. 8.

Figure 8. Class Diagram of the XyMApplet.

The XyMApplet class works as follows:

1. It gets a XyM notation from a HTML document via a WWW browser.
2. It sends the XyM notation to the XyMJava class for parsing.
3. The resulting chemical model is used to display the corresponding chemical structural formula by means of a WWW browser.
4. The formula on display can be enlarged, reduced, and moved by mouse clipping or dragging.

Use of the XyMJava System

Figure 9 illustrates an example of a XyM notation in an HTML document.

```
<html>
<head>
<title>XyMJava</title>
</head>
<body>
<object code=XyMApplet.class name=XyMJava width="300" height="300">
<param name="xymnot"
value="Ysixheteroh[ace]{1==N}{4==Ysixheteroh[ace]{}{3==COOH;5==COOH
;1==(yl)}}">
<param name="xxym" value="50">
<param name="yxym" value="50">
<param name="input" value="Yes">
</object>
</body>
</html>
```

Figure 9. XyM Notation in an HTML Document.

The corresponding formula on a CRT display is shown in Fig. 10, which has been obtained by using the Internet Explorer Macintosh Edition (with MRJ version 1.2.2).

Figure 10. Structural formula on display.

The tags in the HTML document have the following meanings:

1. The Java main class `XyMApplet.class` is assigned to the attribute 'code' in an `<object>` tag, which also contains the attribute 'name' to specify the `XyMJava` class and the attributes 'width' and 'height' to set a drawing region for a formula to be drawn.
2. A `<param>` tag is to set other parameters. The attribute pair 'name=xxym' and 'value' and the pair 'name=yxym' and 'value' respectively specify the x- and y-coordinate of the bottom-left origin of the drawing region.

3. The attribute pair 'name=xymnot' and 'value' for in a `<param>` tag designates a XyM notation to be displayed.
4. The attribute pair 'name=input' and 'value=Yes' is used to open a window for key-inputting another XyM notation from a display.

```
<html>
<head>
<title>XyMJava</title>
</head>
<body>
<hr>
<applet
code=XyMApplet.class
name=XyMJava
width=600
height=600>
<param name=xymnot
value="Ysixheterov[ace]{}{1==Ytetrahedral{0==SOS_2S;3==(yl);1==Ytetrahedra
l{0==NH;3==(yl);1==Ysixheterov[ace]{bYsixfusev[ac]{}{1==OH;4==Ytetrahedral
{0==N;1==(yl);4D==Ytetrahedral{0==N;2==(yl);4==Ysixheteroh[ace]{}{1==(yl)
;2==SOS_2SCHS_3S;4==NOS_2S}}{E}}{}{4==(yl)}};3==Yryl{3==SOS_2S
NH}{4==Ysixheteroh[ace]{}{1==(yl);4==OCHS_2SCHS_2SO---RS^2S;5==Yryl{
3==SOS_2SNH}{6==Ysixheterov[ace]{}{6==(yl);1==OH;3==CHS_3S;4==OCS_
{16}SHS_{33}S---(n)}}{}{}">
<param name=input value="Yes">
</applet>
</body>
</html>
```

Figure 11. XyM Notation for a Cyan Dye Releaser in an HTML Document.

An HTML document for drawing a complicated example (a cyan dye releaser for instant color photography) is shown in Fig. 11.

The corresponding structural formula is created by using the Windows Internet Explorer 5.5, as shown in Fig. 12. Figures 10 and 12 exemplify a feature that the XyMJava system runs satisfactorily on such representative platforms as Macintosh and Windows machines by virtue of appropriate browser software.

Conclusion

The XyMJava system has been developed to draw a chemical structural formula by inputting a XyM notation. The object-oriented technique, especially the design-pattern approach, is applied to parse a XyM notation. An HTML document containing a XyM notation can be browsed by the XyMApplet of the XyMJava system, which produces a chemical model for encapsulating information on chemical structural formulas. The chemical model is then used for drawing formulas on a CRT display. Since the parsing class has been implemented as an interface in an abstract fashion, the parsing of any notation or language other than a XyM notation can be implemented without any change of the parsing class.

Figure 12. Structural Formula of a Cyan Dye Releaser on Display.

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化学構造式をワールドワイドウェブ伝達するための XyMJavaシステム

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インターネット上で化学構造式を伝達するための構造式描画システムとしてXyMJavaを開発した。これは、線形表現のXyM記法を入力言語としており、Javaアプレットとして実装されたシステムである。このシステムでは、XyM記法の解析段階で、オブジェクト指向技術、とくにデザインパターンの技術を応用している。さらに、構造式情報をカプセル化して画像表示するために、新たに考案した「化学モデル」を採用している。この結果、XyM記法をHTML文書の中に記入することによって、化学構造式をインターネットブラウザで表示することが可能になった。

キーワード: XyM記法, Java, 構造式, WWW

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