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Scientific Software

Lexichem TK – Java
Release 2.1.1

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FRONT MATTER

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THEORY

2.1 Input Name Representation

The *oeiupac* library currently processes NUL (zero) terminated ASCII character strings; therefore Greek characters, symbols, fonts and superscripts must be transliterated into the printable subset of ASCII. When parsing compound names, the *oeiupac* library considers both spaces and tab characters as interchangeable, and any number of consecutive 'whitespace' characters are treated as a single space.

Currently, the name parsing is case insensitive, allowing arbitrary mixing of upper and lower case characters, *e.g.* initial letter capitalization.

Greek characters are understood in a number of different representations. For example, the strings '\$a', '\${a}', 'alpha', '.alpha.', 'α', 'α' and 'α' are all understood to represent the Greek character *alpha*, (α).

There is no special representation for italic characters. Compound names such as '*tert*-butyl' and '*p*-aminobenzamidine' are represented as 'tert-butyl' and 'p-aminobenzamidine'. Both the long and short forms of prefixes can be used, allowing the above examples to also be written as 't-butyl' and 'para-aminobenzamidine'.

2.2 Output Name Representation

Unrecognized functional groups, linkers or ring systems are denoted in the generated name as the string '**BLAH**'. As much of the name as possible is generated resulting in compound names such as 'dichloroBLAHcarboxylic acid'. Generated compound names are entirely lower case, with no initial capitalization. Upper case characters are generated for locants and, as described above, for BLAH.

When generating Greek characters in compound names, the *oeiupac* library currently uses the dollar character followed by single letter representation. In this formalism, '\$a' represents the Greek character alpha, α , '\$b' the Greek character beta, β , '\$g' the Greek character gamma, γ and '\$l' the Greek character lambda, λ .

When generating superscripts, the *oeiupac* library currently uses the caret and curly braces representation. Hence '\$l^{5}' represents the Greek character lambda followed by a superscript five, *i.e.* λ^5 . Similarly, 'pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane' would be the von Baeyer system name for cubane, *i.e.*

pentacyclo [4.2.0.0^{2,5}.0^{3,8}.0^{4,7}] octane.

Multiple components in a disconnected molecule, apart from common salts and counter ions, are separated from each other by a semicolon followed by a space. Mixtures containing salts are written ordering the cations before the compound name, followed by anions, finally followed by any common neutral molecules (*e.g.* hydrate or hydrochloride).

2.3 Output Name Styles

The *LEXICHEM* compound naming functionality supports the generation of several *styles* of compound names. The currently predefined name styles are *OpenEye* (the default), IUPAC, CAS, Traditional and Systematic. *OpenEye* names loosely correspond to the kinds of names familiar to a medicinal chemist. These names are intended to be a subset of the IUPAC 2005 standard's acceptable names, but not necessarily the PIN (Preferred IUPAC Name). These correspond to the types of names found in a Sigma-Aldrich catalog or a Journal of Medicinal Chemistry article, for example.

IUPAC names are intended to follow the IUPAC 2005 recommendations for the Preferred IUPAC Name (PIN). Future releases of *LEXICHEM* may further refine this definition to provide IUPAC2005, IUPAC93 and IUPAC79 name styles that reflect the corresponding standard's preferred name.

The *LEXICHEM* CAS name style is intended to follow the Chemical Abstracts Service's naming conventions, where they differ from IUPAC's.

The Traditional name style corresponds to forms of compound naming that are now no longer acceptable to the IUPAC rules. The boundary between whether a trivial/common name is considered *OpenEye* or Traditional when it is acceptable to IUPAC but not preferred is blurred, with *OpenEye* attempting to follow the more prevalent usage.

Finally, Systematic names correspond to the fully systematic IUPAC names that the IUPAC preferred names are slowly converging towards.

2.4 Examples of Name Style Differences

Some of the concepts explained in the previous section are probably best clarified through some real examples.

2.4.1 Example *OpenEye* vs. IUPAC vs. Systematic Differences

- The SMILES string O is called 'water' by the *OpenEye* name style, but 'oxidane' by the IUPAC and Systematic name styles.
- The SMILES C#C is called 'acetylene' by the *OpenEye* and IUPAC name styles, but 'ethyne' by the Systematic name style.
- The SMILES prefix *Nc1ccccc1 is called 'anilino' by the *OpenEye* and IUPAC name styles, but 'phenylamino' by the Systematic name style.
- The SMILES prefix *O[N+]#[C-] is called 'fulminato' by the *OpenEye* name style, but 'isocyanooxy' by the IUPAC and Systematic name styles.
- The SMILES prefix *C(=O)C is called 'acetyl' in the *OpenEye* and IUPAC name styles, but 'ethanoyl' in the Systematic name style.
- The SMILES string CC(=O)C is called 'acetone' in the *OpenEye* name style, but 'propan-2-one' in the IUPAC and Systematic name styles.
- The SMILES string C(=O)O is called 'formic acid' in the *OpenEye* and IUPAC name styles, but 'methanoic acid' in the Systematic name style.

2.4.2 Example *OpenEye*/IUPAC vs. CAS Differences

- The SMILES string c1ccccc1CCCCCCC is named as '1-phenylheptane' by the *OpenEye* and IUPAC name styles, but as 'heptylbenzene' by the CAS name style.

- The SMILES prefix *[BH2] is called ‘boranyl’ by the *OpenEye* and IUPAC name styles, but as ‘boryl’ by the CAS name style.

2.4.3 Example OpenEye/IUPAC vs. Traditional Differences

- The SMILES prefix *S is called ‘sulfanyl’ by the *OpenEye* and IUPAC name styles, but as ‘mercapto’ by the Traditional name style.
- The SMILES string CCCCCCCCC(=O)O is called ‘nonanoic acid’ by the *OpenEye* and IUPAC name styles, but as ‘pelargonic acid’ by the Traditional name style.

EXAMPLES

3.1 Converting Molecules to Names

Converts a file of chemical structures (specified by *-in* option) into chemical names (*-out* option), in a choice of language (*-language* option), encodings (*-encoding* option) and styles (*-style* option).

Listing 1: Converting molecules to names

```
/*  
 * Copyright 2009 OpenEye Scientific Software, Inc.  
 */  
package openeye.examples.oeiupac;  
  
import java.net.URL;  
  
import openeye.oechem.*;  
import openeye.oeiupac.*;  
  
public class Mol2Nam_example {  
  
    private void Mol2Nam(OEInterface itf) {  
        oemolistream ifs = new oemolistream();  
        if (!ifs.open(itf.GetString("-in")))  
            oechem.OEThrow.Fatal("Unable to open input file: "+itf.GetString("-in"));  
  
        oemolostream ofs = new oemolostream();  
        String outname = null;  
        if (itf.HasString("-out")) {  
            outname = itf.GetString("-out");  
            if (!ofs.open(outname))  
                oechem.OEThrow.Fatal("Unable to open output file: "+outname);  
        }  
  
        int language = oeiupac.OEGetIUPACLanguage(itf.GetString("-language"));  
        int charset = oeiupac.OEGetIUPACCharSet(itf.GetString("-encoding"));  
        short [] style = oeiupac.OEGetIUPACNamStyle(itf.GetString("-style"));  
  
        OEGraphMol mol = new OEGraphMol();  
        while (oechem.OEReadMolecule(ifs, mol)) {  
            String name = oeiupac.OECreateIUPACName(mol, style);  
        }  
    }  
}
```

```

    if (language > 0)
        name = oeiupac.OEToLanguage(name, language);
    if (itf.GetBool("-capitalize"))
        name = oeiupac.OECapitalizeName(name);

    if (charset == OECharSet.ASCII)
        name = oeiupac.OEToASCII(name);
    else if (charset == OECharSet.UTF8)
        name = oeiupac.OEToUTF8(name);
    else if (charset == OECharSet.HTML)
        name = oeiupac.OEToHTML(name);
    else if (charset == OECharSet.SJIS)
        name = oeiupac.OEToSJIS(name);
    else if (charset == OECharSet.EUCJP)
        name = oeiupac.OEToEUCJP(name);

    if (outname != null) {
        if (itf.HasString("-delim"))
            name = mol.GetTitle() + itf.GetString("-delim") + name;
        if (itf.HasString("-tag"))
            oechem.OESetSDData(mol, itf.GetString("-tag"), name);
        mol.SetTitle(name);
        oechem.OEWriteMolecule(ofs, mol);
    } else {
        System.out.printf("%s\n", name);
    }
}

}

public static void main(String argv[]) {
    Mol2Nam_example app = new Mol2Nam_example();
    URL fileURL = app.getClass().getResource("Mol2Nam_example.txt");
    try {
        OEInterface itf = new OEInterface(fileURL, "Mol2Nam_example", argv);
        app.Mol2Nam(itf);
    } catch (java.io.IOException e) {
        System.err.println("Unable to open interface file");
    }
}
}

```

3.2 Converting Names to Molecules

Converts a file of chemical names (specified by the *-in* option) of a specific language (*-language* option) into a file of chemical structures (specified by the *-out* option).

Listing 2: Converting names to molecules

```

/*****
 * Copyright 2009 OpenEye Scientific Software, Inc.
 *****/
package openeye.examples.oeiupac;

```

```

import java.net.URL;

import openeye.oechem.*;
import openeye.oeiupac.*;

public class Nam2Mol_example {

    private void Nam2Mol(OEInterface itf) {
        oeifstream ifs = new oeifstream();
        if (!ifs.open(itf.GetString("-in")))
            oechem.OEThrow.Fatal("Unable to open input file: "+itf.GetString("-in"));

        oemolostream ofs = new oemolostream();
        if (!ofs.open(itf.GetString("-out")))
            oechem.OEThrow.Fatal("Unable to open output file: "+itf.GetString("-out"));

        int language = oeiupac.OEGetIUPACLanguage(itf.GetString("-language"));

        OEGraphMol mol = new OEGraphMol();
        StringBuffer name = new StringBuffer();
        while (ifs.getline(name)) {
            mol.Clear();

            // Speculatively reorder CAS permuted index names
            String str = oeiupac.OEReorderIndexName(name.toString());
            if (str.length() == 0)
                str=name.toString();

            if (language != OELanguage.AMERICAN) {
                str = oeiupac.OEFromUTF8(str);
                str = oeiupac.OELowerCaseName(str);
                str = oeiupac.OEFromLanguage(str, language);
            }

            boolean done = oeiupac.OEParseIUPACName(mol, str);

            if (!done && itf.GetBool("-empty")) {
                mol.Clear();
                done = true;
            }

            if (done) {
                if (itf.HasString("-tag"))
                    oechem.OESetSDDData(mol, itf.GetString("-tag"), name.toString());
                mol.SetTitle(name.toString());
                oechem.OEWriteMolecule(ofs, mol);
            }
        }
    }

    public static void main(String argv[]) {
        Nam2Mol_example app = new Nam2Mol_example();
        URL fileURL = app.getClass().getResource("Nam2Mol_example.txt");
        try {
            OEInterface itf = new OEInterface(fileURL, "Nam2Mol_example", argv);
            app.Nam2Mol(itf);
        } catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}

```

```
}  
  }  
}
```

4.1 OEIUPAC Constants

4.1.1 OEIUPAC

This namespace contains constants.

OENamStyleOpenEye

This constant is used to specify the (default) predefined OpenEye name style to the `OECreatIUPACName` function.

OENamStyleTraditional

This constant is used to specify the predefined traditional name style to the `OECreatIUPACName` function.

OENamStyleSystematic

This constant is used to specify the predefined systematic name style to the `OECreatIUPACName` function.

OENamStyleIUPAC

This constant is used to specify the predefined IUPAC 2005 name style to the `OECreatIUPACName` function.

OENamStyleCAS

This constant is used to specify the predefined Chemical Abstracts Service (CAS) name style to the `OECreatIUPACName` function.

OENamStyleCASIndex

This constant is used to specify the predefined Chemical Abstracts Service (CAS) permuted index name style to the `OECreatIUPACName` function.

OENamStyleAutoNom

This constant is used to specify the predefined MDL/Beilstein AutoNom name style to the `OECreatIUPACName` function.

OENamStyleIUPAC79

This constant is used to specify the predefined IUPAC 1979 name style to the `OECreatIUPACName` function.

OENamStyleIUPAC93

This constant is used to specify the predefined IUPAC 1993 name style to the `OECreatIUPACName` function.

OENamStyleACDName

This constant is used to specify the predefined ACD name style to the `OECreatIUPACName` function.

OE_LANG_ENGLISH

This constant is used to specify the American dialect of English to the `OEFromLanguage` and the `OEToLanguage` function. This is currently a synonym of the constant `OEIUPAC.OE_LANG_AMERICAN`.

OE_LANG_AMERICAN

This constant is used to specify the American dialect of English to the `OEFromLanguage` and the `OEToLanguage` function. This is currently a synonym of the constant `OEIUPAC.OE_LANG_ENGLISH`.

OE_LANG_BRITISH

This constant is used to specify the traditional British dialect of English to the `OEFromLanguage` and the `OEToLanguage` function.

OE_LANG_INTERNATIONAL

This constant is used to specify the international dialect of English to the `OEToLanguage` function.

OE_LANG_CHINESE

This constant is used to specify the Chinese language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_DANISH

This constant is used to specify the Danish language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_DUTCH

This constant is used to specify the Dutch language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_FRENCH

This constant is used to specify the French language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_GERMAN

This constant is used to specify the German language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_GREEK

This constant is used to specify the Greek language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_HUNGARIAN

This constant is used to specify the Hungarian language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_IRISH

This constant is used to specify the Irish language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_ITALIAN

This constant is used to specify the Italian language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_JAPANESE

This constant is used to specify the Japanese language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_POLISH

This constant is used to specify the Polish language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_PORTUGUESE

This constant is used to specify the Portuguese language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_ROMANIAN

This constant is used to specify the Romanian language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_RUSSIAN

This constant is used to specify the Russian language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_SLOVAK

This constant is used to specify the Slovak language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_SPANISH

This constant is used to specify the Spanish language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_SWEDISH

This constant is used to specify the Swedish language to the `OEFromLanguage` and the `OEToLanguage` functions.

OE_LANG_WELSH

This constant is used to specify the Welsh language to the `OEFromLanguage` and the `OEToLanguage` functions.

4.1.2 OELanguage

This namespace contains constants for defining which language to translate to/from using `OEFromLanguage` and `OEToLanguage`.

- ENGLISH
- AMERICAN
- BRITISH
- INTERNATIONAL
- CHINESE
- DANISH
- DUTCH
- FRENCH
- GERMAN
- GREEK
- HUNGARIAN
- IRISH

- ITALIAN
- JAPANESE
- POLISH
- PORTUGUESE
- ROMANIAN
- RUSSIAN
- SLOVAK
- SPANISH
- SWEDISH
- WELSH

4.2 OEIUPAC Functions

4.2.1 OECapitalizeName

```
std::string OECapitalizeName(const char *ptr)
```

Capitalize the appropriate first letter of a name generated by `OECreateIUPACName`. This function should be called after translating the name to a foreign language, but before converting the character set encoding.

4.2.2 OECreateIUPACName

```
std::string OECreateIUPACName(const OEChem::OEMolBase &mol,
                             const unsigned char *style=OENamStyleOpenEye)
```

This function attempts to generate a ‘reasonable’ IUPAC name for the given molecule, mol, and return the result in a C++ STL string. These ‘reasonable’ names attempts to be one of the recommended IUPAC names for a compound, however occasionally this function may fall back to using IUPAC ‘systematic’ naming for parts of a molecule. Any parts of a molecule that cannot be named, result in the substring BLAH appearing in the returned string.

The optional style argument can be used to control and customize the style of the names generated by this function. The nine currently predefined name styles are

- `OEIUPAC.OENamStyleOpenEye` (the default),
- `OEIUPAC.OENamStyleIUPAC`,
- `OEIUPAC.OENamStyleIUPAC79`,
- `OEIUPAC.OENamStyleIUPAC93`,
- `OEIUPAC.OENamStyleTraditional`,
- `OEIUPAC.OENamStyleAutoNom`,
- `OEIUPAC.OENamStyleCAS`,
- `OEIUPAC.OENamStyleCASIndex` and
- `OEIUPAC.OENamStyleSystematic`.

After the name has been generated it may be translated into one of several languages, for example using the `OEToGerman` or `OEToJapanese` functions, then optionally capitalized using `OECapitalizeName`, and finally converted into a final character encoding, for example using `OEToUTF8` or `OEToHTML`.

4.2.3 OEFromChinese

```
std::string OEFromChinese(const char *ptr)
```

Convert the chemical name specified by 'ptr' from simplified or traditional Chinese to English.

4.2.4 OEFromDanish

```
std::string OEFromDanish(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Danish to English.

4.2.5 OEFromDutch

```
std::string OEFromDutch(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Dutch to English.

4.2.6 OEFromFrench

```
std::string OEFromFrench(const char *ptr)
```

Convert the chemical name specified by 'ptr' from French to English.

4.2.7 OEFromGerman

```
std::string OEFromGerman(const char *ptr)
```

Convert the chemical name specified by 'ptr' from German to English.

4.2.8 OEFromGreek

```
std::string OEFromGreek(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Greek to English.

4.2.9 OEFromHungarian

```
std::string OEFromHungarian(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Hungarian to English.

4.2.10 OEFromIrish

```
std::string OEFromIrish(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Irish to English.

4.2.11 OEFromItalian

```
std::string OEFromItalian(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Italian to English.

4.2.12 OEFromJapanese

```
std::string OEFromJapanese(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Japanese to English.

4.2.13 OEFromKOI8R

```
std::string OEFromKOI8R(const char *ptr)
```

Convert the string 'ptr' from the Russian KOI-8 character encoding to *Lexichem*'s default encoding using `\u` escapes to represent non-ASCII unicode characters.

4.2.14 OEFromLanguage

```
std::string OEFromLanguage(const char *ptr, unsigned int lang)
```

This is a helper wrapper function that can be used to convert the chemical name specified by 'ptr' from the language specified by 'lang' to English. The languages are specified by the constants with the `OE_LANG_` prefix described in the `OEIUPAC` namespace.

4.2.15 OEFromPolish

```
std::string OEFromPolish(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Polish to English.

4.2.16 OEFromRomanian

```
std::string OEFromRomanian(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Romanian to English.

4.2.17 OEFromRussian

```
std::string OEFromRussian(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Russian to English.

4.2.18 OEFromSlovak

```
std::string OEFromSlovak(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Slovak to English.

4.2.19 OEFromSpanish

```
std::string OEFromSpanish(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Spanish to English.

4.2.20 OEFromSwedish

```
std::string OEFromSwedish(const char *ptr)
```

Convert the chemical name specified by 'ptr' from Swedish to English.

4.2.21 OEFromUTF8

```
std::string OEFromUTF8(const char *ptr)
```

Convert the string 'ptr' from the UTF-8 character encoding to *Lexichem*'s default encoding using 'u' escapes to represent non-ASCII unicode characters.

4.2.22 OEFromWelsh

```
std::string OEFromWelsh(const char *ptr)
```

Convert the chemical name specified by 'ptr' from simplified or traditional Welsh to English.

4.2.23 OEGetCIPStereo

```
char OEGetCIPStereo(const OEChem::OEMolBase &mol,  
                   const OEChem::OEAtomBase *atm)  
char OEGetCIPStereo(const OEChem::OEMolBase &mol,  
                   const OEChem::OEBondBase *bnd)
```

These functions return the Cahn-Ingold-Prelog descriptor for the given atom or bond stereo center, from the stereochemistry set on the `OEMolBase`. For chiral atom centers, the `OEAtomBase` form of this function returns either 'R' or 'S' for specified CIP stereo centers, 'N' for CIP stereo centers that don't have stereo specified (*i.e.* `OEAtomBase.HasStereoSpecified` returns `false`), and 'X' for atoms that are not CIP stereo centers. For double bonds, the `OEBondBase` form of this function returns either 'E' or 'Z' specified CIP stereo centers, 'N' for CIP stereo centers that don't have stereo specified (*i.e.* `OEBondBase.HasStereoSpecified` returns `false`), and 'X' for bonds that are not CIP stereo centers.

4.2.24 OEIUPACGetArch

```
const char *OEIUPACGetArch()
```

Returns the system architecture.

4.2.25 OEIUPACGetLicensee

```
bool OEIUPACGetLicensee(std::string &licensee)
```

Determines the valid licensee.

4.2.26 OEIUPACGetPlatform

```
const char *OEIUPACGetPlatform()
```

Returns the system platform.

4.2.27 OEIUPACGetRelease

```
const char *OEIUPACGetRelease()
```

Returns the *Lexichem* toolkit release number.

4.2.28 OEIUPACGetSite

```
bool OEIUPACGetSite(std::string &site)
```

Determines whether a valid site is present.

4.2.29 OEIUPACGetVersion

```
unsigned int OEIUPACGetVersion()
```

Returns *Lexichem* toolkit build date.

4.2.30 OEIUPACIsLicensed

```
bool OEIUPACIsLicensed(const char *feature=0, unsigned int *expdate=0)
```

Determine whether a valid license file is present. This function may be called without a legitimate run-time license to determine whether it is safe to call any of OEIUPAC's functionality.

The 'features' argument can be used to check for a valid license to OEIUPAC along with that feature. For example, to verify that OEIUPAC can be used from Python:

```
if (!OEIUPACIsLicensed("python"))
    OEThrow.Warning("OEIUPAC is not licensed for the python feature");
```

The second argument can be used to get the expiration date of the license. This is an array of size three with the date returned as {day, month, year}. Even if the function returns `false` due to an expired license, the `expdate` will show that expiration date. A value of a zero implies that no license or date was found.

```
unsigned int expdate[3];
if (OEIUPACIsLicensed(0, expdate))
{
    OEThrow.Info("License expires: day: %d month: %d year: %d",
                expdate[0], expdate[1], expdate[2]);
}
```

4.2.31 OELowerCaseName

```
std::string OELowerCaseName(const char *ptr)
```

Convert the specified compound name to lower-case. This function understands chemical nomenclature and foreign alphabets. This function should be called prior to translating a name from a foreign language, as the language translation routines assume that the name is lower-case.

4.2.32 OENameLocant

```
std::string OENameLocant(unsigned int loc, bool iupac=false)
```

Generate the lexical form of a *Lexichem* locant index. The molecules created by the function `OEParseIUPACName` are annotated with locant information in each atom's integer atom type field. These locant indices may be retrieved using *OEChem*'s `OEAtomBase.GetIntType` method.

4.2.33 OEParseIUPACName

```
bool OEParseIUPACName(OEChem::OEMolBase &mol, const char *name)
```

This function parses the compound name (not necessarily a systematic or preferred IUPAC name) from the NULL-terminated string given by `name`, and places the processed molecule in `mol`. This function returns `true` if the name could be parsed without problems. When returning `false`, the contents of `mol` contain as much of the name as could be processed.

4.2.34 OEReorderIndexName

```
std::string OEReorderIndexName(const char *ptr)
```

Attempt to reorder the specified permuted index name. This permute strings such as “benzene, chloro-” into the form “chloro-benzene” which can then be processed by *Lexichem*'s `OEParseIUPACName` function.

This function returns an empty string (or the original input string) if its argument is not recognized as a permuted index name.

4.2.35 OESetCIPStereo

```
bool OESetCIPStereo(OEChem::OEMolBase &mol, OEChem::OEAtomBase *atm, char s)
```

```
bool OESetCIPStereo(OEChem::OEMolBase &mol, OEChem::OEBondBase *bnd, char s)
```

These functions set the internal *OEChem* stereochemistry from the given CIP stereo descriptor. For the `OEAtomBase` form, the descriptor `s` must be either ‘R’ or ‘S’, and for the `OEBondBase` form, the descriptor `s` must be either ‘E’ or ‘Z’. This function returns `true` if the stereochemistry was successfully set, and `false` otherwise: *i.e.* the descriptor was invalid or the specified atom or bond was not a CIP stereo center.

4.2.36 OEToASCII

```
std::string OEToASCII(const char *ptr)
```

Convert the string ‘ptr’, typically the output of the function `OECreatIUPACName` post-processed by a language translation function, from the default ISO-8859-1 encoding, which includes 8-bit European characters, into a reduced 7-bit ASCII representation by stripping the accents off of the 8-bit characters.

4.2.37 OEToBritish

```
std::string OEToBritish(const char *ptr, bool sulph)
```

Convert the string ‘ptr’, typically the output of the function `OECreatIUPACName`, from the default American output, to either British spelling (when ‘sulph’ is `true`) or IUPAC international spelling (when ‘sulph’ is `false`).

4.2.38 OEToChinese

```
std::string OEToChinese(const char *ptr)
```

Convert the string ‘ptr’, typically the output of the function `OECreatIUPACName`, from English to simplified Chinese.

4.2.39 OEToDanish

```
std::string OEToDanish(const char *ptr)
```

Convert the string ‘ptr’, typically the output of the function `OECreatIUPACName`, from English to Danish.

4.2.40 OEToDutch

```
std::string OEToDutch(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Dutch.

4.2.41 OEToEUCJP

```
std::string OEToEUCJP(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName` post-processed by a call to `OEToJapanese`, from the default encoding which uses 'u' escapes to represent unicode characters to instead use the EUC-JP character encoding for Japanese characters.

4.2.42 OEToFrench

```
std::string OEToFrench(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to French.

4.2.43 OEToGerman

```
std::string OEToGerman(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to German.

4.2.44 OEToGreek

```
std::string OEToGreek(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Greek.

4.2.45 OEToHTML

```
std::string OEToHTML(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName` possibly post-processed by a language translation function, from the default encoding to use HTML mark-up to represent accented characters, unicode characters and superscripts.

4.2.46 OEToHungarian

```
std::string OEToHungarian(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Hungarian.

4.2.47 OEToIrish

```
std::string OEToIrish(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Irish.

4.2.48 OEToItalian

```
std::string OEToItalian(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Italian.

4.2.49 OEToJapanese

```
std::string OEToJapanese(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Japanese.

4.2.50 OEToLanguage

```
std::string OEToLanguage(const char *ptr, unsigned int lang)
```

This is a helper wrapper function that can be used to convert the chemical name specified by 'ptr' from English to the language specified by 'lang'. The languages are specified by the constants with the `OE_LANG_` prefix described in the `OEIUPAC` namespace.

4.2.51 OEToPolish

```
std::string OEToPolish(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Polish.

4.2.52 OEToRomanian

```
std::string OEToRomanian(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Romanian.

4.2.53 OEToRussian

```
std::string OEToRussian(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatIUPACName`, from English to Russian.

4.2.54 OEToSJIS

```
std::string OEToSJIS(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatelUPACName` post-processed by a call to `OEToJapanese`, from the default encoding which uses 'u' escapes to represent unicode characters to instead use the Shift-JIS character encoding for Japanese characters.

4.2.55 OEToSlovak

```
std::string OEToSlovak(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatelUPACName`, from English to Slovak.

4.2.56 OEToSpanish

```
std::string OEToSpanish(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatelUPACName`, from English to Spanish.

4.2.57 OEToSwedish

```
std::string OEToSwedish(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatelUPACName`, from English to Swedish.

4.2.58 OEToUTF8

```
std::string OEToUTF8(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatelUPACName` post-processed by a language translation function, from the default ISO-8859-1 encoding which uses 'u' escapes to represent unicode characters to instead use the UTF-8 character encoding for accented and other characters.

4.2.59 OEToWelsh

```
std::string OEToWelsh(const char *ptr)
```

Convert the string 'ptr', typically the output of the function `OECreatelUPACName`, from English to Welsh.

RELEASE NOTES

5.1 Lexichem TK 2.1.1

5.1.1 Bug fixes

- Fixed a bug with structure generation for tetramethylammonium pyrrolidine-2-carboxylate trihydrate.
- Components of salts are now separated by semi-colons.
- Added numerous dictionary entries.
- Added additional ring templates.
- Fixed a bug with names including benzene) or benzene}, the appropriate substitution should have been phenyl.
- Fixed an issue when incorrect von Baeyer names are parsed to Lexichem, Lexichem now fails silently.
- Fixed dictionary lookup algorithm.
- Fixed a crash in Mol2Nam when a H-atom was part of the main ring system in simple spiro compounds.
- Fixed a bug in names like sulfuric acid mono(x) ester.

5.2 LEXICHEM 2.1.0

- Performance benchmark results: conversion of canonical isomeric smiles to names and back to the same canonical isomeric smiles. Size of the databases are given in brackets after the name.

	v2.0.2	v2.1.0
Database	Round Tripping	Round Tripping
Maybridge (63872)	88.94%	98.69%
MDDR (111171)	48.69%	88.54%
NCI (250251)	84.54%	92.32%
Wombat (53214)	52.80%	89.54%

5.2.1 New features

- Added support for converting von Baeyer names to structures e.g. tricyclo[5.2.2.0^{3,5}]undecane is converted to :C1CC2CCC1CC3CC3C2.
- Added basic support for a number of steroid, alkaloid and terpene parent structures.
- Added support for L/D-amino acids.

- Added support for R-groups for name to structure conversion.
- Added support for both linear and branched polyspiro alicyclic hydrocarbons.
- Activated stereochemistry support for name to structure.
- Added a number of dictionary entries.
- Added a number of ring templates.
- Added partial support for von Baeyer name generation from structures.

5.2.2 Bug fixes

- Added support for names: 2H-imidazol-4-thiol and 1,2-dihydroimidazole-5-imine.
- Added support for barium(2+), sodium(1+).
- *LEXICHEM* now understands trifluoroneodymium.
- Added support for dihydrides e.g. calcium dihydride, magnesium dihydride.
- *LEXICHEM* now supports multi-ammonium salts and multi-derivative ethynyl pyridines.
- Added support for oxoarsinite based compounds.
- Added support for a number of additional metal linking groups e.g. Mg, K, La, Dy, Er, V, Ni etc.
- Fixed a bug in the name: 3-acetyl-8-bromo-1,2,3,6-tetrahydro-azepino[4,5-b]indole-2,5-dicarboxylic acid diethyl ester.
- Corrected unicode conversion for: acetate, glycinate, nitrite and iodide.

5.3 Lexichem TK 2.0.2

- Updated ring numbering templates that catch a significant fraction of ring naming failures in the NCBI's PubChem database.
- Updated the rules we use for naming the prefix "2-carboxyethyl" and friends, which we'd previously name "3-hydroxy-3-oxopropyl" (or similar).
- Added parsing support for the traditional prefix "phenethoxy".
- Removed the insertion of a single explicit space after a semi-colon. We now prefer to preserve the original input string, rather than beautify it. This also plays nicer with HTML style input, where "λ" really doesn't need an explicit space character after it.
- Added several minor tweaks to AutoNom-style naming, such as "isophthalic acid" and "benzene-1,2-carbaldehyde".
- Updated some erroneous SMILES in the dictionary including sulfamethoxazole and tinidazole.

5.4 Lexichem TK 2.0.0

- The applications have a new, standardized command line interface. Please have a look at the updated documentation for *mol2nam*, *nam2mol* and *translate*.
- This release includes the ability to parse stereo on input names. Previously it was read and ignored.
- Fixed a bug where, in rare cases, the output name depended on input atom ordering.

- Fixed a crash in determining CIP stereo for very large, pathological molecules.

5.5 Lexichem TK 1.9

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 234297 structures (93.62%) to names without BLAH. Of these 234297 names, `nam2mol` is able to convert 231566 (98.83%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. Several bugs have also been fixed. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now up to 95.24%.
- Several improvements have been made to the specification of CIP stereochemistry during name generation. For example, previously linking groups such as `amidino`, `carbamimidoyl` and `diazenyl` would forget to specify E/Z descriptors if they contained a chiral double bond with specified stereochemistry. We would also fail to place some chiral prefixes such as (E)-`styr1` and (Z)-`cinnamyl` in brackets which can lead to ambiguity when interpreting the generated name.

5.6 Lexichem TK 1.8

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 234296 structures (93.62%) to names without BLAH. Of these 234296 names, `nam2mol` is able to convert 228102 (97.36%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. Several bugs have also been fixed. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now up to 95.12%.
- One of the major parsing improvements in this release is the much improved support for handling von Baeyer ring nomenclature. We can now parse names such as:
 - '1,4-dithioniabicyclo[2.2.2]octane',
 - 'bicyclo[4.2.0]octa-1(6),2,4-triene' and
 - '2,4-diazaspiro[4.4]nonane-1,3-dione'.

5.7 Lexichem TK 1.7

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 234155 structures (93.57%) to names without BLAH. Of these 234155 names, `nam2mol` is able to convert 223246 (95.34%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. Several bugs have also been fixed. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now up to 93.81%.
- A new `OELowerCaseName` function has been added to the *Lexichem* toolkit API. This function converts the input chemical name to lower-case, whilst preserving the case sensitive aspects of IUPAC names. This functionality allows uppercase and mixed case names to be translated into English, as the `OEFROM<FOO>` functions assume their input is lowercase. For example, this feature allows AGUA to be recognized via `OEFROMSpanish`.

- A new `OEReorderIndexName` function has been added to the *Lexichem* toolkit API. This function attempts to reorder the given permuted index name into a form that can be handled by the `OEParseIUPACName` function. For example, this will convert the string ‘benzene, chloro-’ into ‘chloro-benzene’.
- A number of improvements and bug fixes have been made to *Lexichem*’s naming styles. For example, AutoNom and CAS permuted index styles are now far more AutoNom-like and CAS-like respectively. Naming of metallocenes and fullerenes is much improved.
- Some dramatic improvements have been made with foreign language support. On the 250251 compounds in the NCI00 database mentioned above, we now round-trip 100% to German and back without any differences. Japanese, Spanish and Swedish rates are all currently above 99%. Support for Hungarian and Polish has been dramatically improved.

5.8 Lexichem TK 1.6

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 233010 structures (93.11%) to names without BLAH. Of these 233010 names, `nam2mol` is able to convert 221331 (94.99%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. For example, both name generation and parsing now do a much better job on ring fusion nomenclature, for names like ‘5,6,7,8-tetrahydro[1,2,4]triazolo[4,3-a]pyridine’. There’s also much improved handling of charged ring systems. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now 93.25% in v1.6, up from 80.80% in v1.5.
- In name generation, new naming styles have been added for MDL/Beilstein AutoNom style names, for CAS permuted index style names (and there are new placeholder styles for IUPAC79 and IUPAC93 naming). A large number of improvements have been made to names generated using the ‘traditional’ naming style. A new `OECapitalizeName` API function is available to capitalizing the appropriate first letter of a generated name, such as ‘p-tert-Butylbenzoic acid’.
- Several bug fixes have been made to the Cahn-Ingold-Prelog (CIP) chirality perception implementation.
- The `OEParseIUPACName` function is now able return supplementary locant annotations for each atom. This function now stores an integer locant code/identifier in the integer atom type field of each atom, which may be retrieved using the `OEAtomBase.GetIntType` method and converted into a readable/displayable string using the recently exposed `OENameLocant` function. This functionality is a recent addition (obviously), and most but not all supported ring systems and parents have locant annotations in this initial release.
- Finally, for the adventurous, new APIs for translating compound names from foreign languages into English are available as the experimental `OEFromJapanese`, `OEFromSwedish` and `OEFromSpanish` functions. Additionally, a `OEFromUTF8` function is available for converting UTF-8 encoded strings into the escaped sequences expected by these functions (effectively the inverse of `OEToUTF8`).

5.9 Lexichem TK 1.5

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 223066 structures (89.14%) to names without BLAH. Of these 223066 names, `nam2mol` is able to convert 192487 (86.29%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. For example, `nam2mol` now supports more numbered locants, such as ‘N1-methylaniline’ and for ‘Maybridge-style’ locant names such as N’1 (interpreted as the more common N1’). These and similar changes have increased the conversion rate for the 71367 compound names in the 2003 Maybridge catalog, from 69.51% in v1.4 to 80.80% in v1.5.

- This release includes the ability to generate compound names in Japanese, and much improved Spanish and Polish naming support. In order to better support internationalization, APIs are now available to map from the default ISO-8859-1 output to either 7-bit ASCII, UTF-8, HTML and for Japanese locales, Shift-JIS or EUC-JP.
- Although impossible in the general case, several improvements have been made to *Lexichem*'s compound naming such that the assigned names are now more stable under arbitrary input ordering of atoms and bonds.

5.10 Lexichem TK 1.4

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 221254 structures (88.41%) to names without BLAH. Of these 221254 names, `nam2mol` is able to convert 192345 (86.93%) back into structures.
- *Lexichem* v1.4 is predominantly a maintenance to provide a version of the *oeiupac* library that is compatible with *OEChem* v1.4. However, there have been a number of significant improvements to name parsing, and minor improvements to name generation since last month's v1.3 release.
- This release also includes the ability to generate compound names in several languages. In addition, to British spellings, *Lexichem* can now generate German, Italian, French, Spanish, Swedish, Dutch and Polish names. Whilst the translations for German, Italian, Swedish and Polish are quite comprehensive, those for French, Spanish and Dutch are less complete.
- A potential ambiguity with the ring names 'oxazole' and 'thiazole' has also been resolved. The IUPAC documentation states that it is permissible to omit locants from Hantzsch-Widman names when the locants are consecutive, *i.e.* '1,2,3,4-tetrazole' may be written as 'tetrazole', and '1,2-oxazirene' is preferred as 'oxazirene'. Unfortunately, this conflicts with the traditional interpretations of 'oxazole' as meaning '1,3-oxazole' and 'thiazole' as '1,3-thiazole'. Instead the traditional names 'isoxazole' and 'isothiazole' denote the '1,2-' forms. This ambiguity, that affected IUPAC-style (but not OpenEye-style) names, has been resolved by preserving the locants, so that the IUPAC names '1,2-oxazole', '1,3-oxazole', '1,2-thiazole' and '1,3-thiazole' are now generated for 'isoxazole', 'oxazole', 'isothiazole' and 'thiazole' respectively.

5.11 Lexichem TK 1.3

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 221205 structures (88.39%) to names without BLAH. Of these 221205 names, `nam2mol` is able to convert 183444 (82.93%) back into structures.
- The major announcement of this release is the support for stereochemistry in compound naming. The CIP rules for assigning R/S descriptors to tetrahedral chiral centers, and E/Z descriptors to double bonds are used during name generation.

5.12 Lexichem TK 1.2

On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 220949 structures (88.29%) to names without BLAH. Of these 220949 names, `nam2mol` is able to convert 182438 (82.57%) back into structures.

5.13 Lexichem TK 1.2

On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 220949 structures (88.29%) to names without BLAH. Of these 220949 names, `nam2mol` is able to convert 182438 (82.57%) back into structures.

5.14 Lexichem TK 1.1

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 220924 structures (88.28%) to names without BLAH. Of these 220924 names, `nam2mol` is able to convert 177145 (80.18%) back into structures.
- A new `OEIUPACIsLicensed` API has been added so allow applications to check whether *Lexichem*'s parsing and naming functionality can safely be used.

5.14.1 OEParseIUPACName Improvements

The *Lexichem* name parsing routines now handle a small number of structural abbreviations when parsing names. For example, it can now handle names like '3-CF3-5-NO2-benzoic acid'. The usual improvements in name parsing, including more entries for common names in the Lexichem dictionary. Support for names containing multiple explicit hydrogen locants, such as 'pyrimidine-2,4(1H,3H)-dione' and '2,4(1H,3H)-pyrimidinedione'.

5.14.2 OECreatelUPACName Improvements

A serious bug that could cause a core dump when naming thioperoxoic acids has been fixed. The performance of compound naming has been improved. The usual improvements in the names generated (following the IUPAC standards more closely).

5.15 Lexichem TK 1.0

On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 220922 structures (88.28%) to names without BLAH. Of these 220922 names, `nam2mol` is able to convert 177032 (80.13%) back into structures.

5.15.1 OEParseIUPACName Improvements

In addition to a great many other improvements to the name parsing code, the *Lexichem* parser now contains an internal dictionary allowing the recognition of common non-systematic names, such as 'ranitidine' and 'zantac'.

5.15.2 OECreatelUPACName Improvements

In addition to a great many improvements to the name generation code, the *Lexichem* naming functionality now allows the specification of a naming style, allowing the compound to be named in either a traditional, OpenEye, IUPAC, CAS or systematic naming style.

5.16 Indices and tables

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