NAME

MDLMolFileIO

SYNOPSIS

use FileIO::MDLMolFileIO;

use FileIO::MDLMolFileIO qw(:all);

DESCRIPTION

MDLMolFIleIO class provides the following methods:

new, GenerateMoleculeString, IsMDLMolFile, ParseMoleculeString, ReadMolecule, ReadMoleculeString, WriteMolecule

The following methods can also be used as functions:

GenerateMoleculeString, IsMDLMolFile, ParseMoleculeString

Data specific to MDLMolFIleIO class not directly used by Molecule, Atom and Bond objects - data label/value pairs, atom SteroParity and so on - is associated to and retrieved from appropriate objects using following methods:

```
SetMDL<PropertyName>
GetMDL<PropertyName>.
```

MDLMolFIleIO class is derived from *FileIO* class and uses its methods to support generic file related functionality.

METHODS

new

```
$NewMDLMolFileIO = new FileIO::MDLMolFileIO(%NamesAndValues);
```

Using specified *MDLMolFileIO* property names and values hash, new method creates a new object and returns a reference to newly created MDLMolFIleIO object.

GenerateMoleculeString

```
$MoleculeString = $MDLMolFileIO->GenerateMoleculeString($Molecule);
$MoleculeString = FileIO::MDLMolFileIO::GenerateMoleculeString($Molecule);
```

Returns a MoleculeString in MDLMol format corresponding to *Molecule*.

IsMDLMolFile

```
$Status = $MDLMolFileIO->IsMDLMolFile($FileName);
$Status = FileIO::MDLMolFileIO::IsMDLMolFile($FileName);
```

Returns 1 or 0 based on whether *FileName* is a MDLMol file.

ParseMoleculeString

```
$Molecule = $MDLMolFileIO->ParseMoleculeString($MoleculeString);
$Molecule = FileIO::MDLMolFileIO::ParseMoleculeString($MoleculeString);
```

Parses *MoleculeString* and returns a Molecule object.

ReadMolecule

```
$Molecule = $MDLMolFileIO->ReadMolecule($FileHandle);
```

Reads data for the compound in a file using already opened *FileHandle*, creates, and returns a Molecule object.

ReadMoleculeString

```
$MoleculeString = $MDLMolFileIO->ReadMoleculeString($FileHandle);
```

Reads data for the compound in a file using already opened *FileHandle* and returns a MoleculeString corresponding to compound structure and other associated data.

WriteMolecule

```
$MDLMolFileIO->WriteMolecule($Molecule);
```

Writes *Molecule* data to a file in MDLMol format and returns MDLMolFIleIO.

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SEE ALSO

MoleculeFileIO.pm, SDFileIO.pm

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