NAME

SDFileIO

SYNOPSIS

use FileIO::SDFileIO;

use FileIO::SDFileIO qw(:all);

DESCRIPTION

SDFIleIO class provides the following methods:

new, GenerateMoleculeString, IsSDFile, ParseMoleculeString, ReadMolecule, ReadMoleculeString, WriteMolecule

The following methods can also be used as functions:

GenerateMoleculeString, IsSDFile, ParseMoleculeString

Data specific to SDFileIO 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 approptiate objects using following methods:

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

SD data label and values are attached to Molecule object as a refernece to a hash using SetDataFieldLabelAndValues and can be retrieved using GetDataFieldLabelAndValues method.

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

METHODS

new

```
$NewSDFileIO = new FileIO::SDFileIO(%NamesAndValues);
```

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

GenerateMoleculeString

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

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

IsSDFile

```
$Status = $SDFileIO->IsSDFile($FileName);
$Status = FileIO::SDFileIO::IsSDFile($FileName);
```

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

ParseMoleculeString

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

Parses *MoleculeString* and returns a Molecule object. SD data field label and value pairs are associated to Molecule object as a reference to a hash using:

```
$Molecule->SetDataFieldLabelAndValues(\%DataLabelsAndValues)
```

The reference to hash can be retrieved by:

```
$DataLabelsAndValues = $Molecule->GetDataFieldLabelAndValues();
for $DataLabel (sort keys %{$DataLabelsAndValues}) {
    $DataValue = $DataLabelsAndValues->{$DataLabel};
}
```

ReadMolecule

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

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

Molecule object.

ReadMoleculeString

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

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

WriteMolecule

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

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

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SEE ALSO

MoleculeFileIO.pm, MDLMolFileIO.pm

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