

OpenEye
SCIENTIFIC

Quacpac TK – Java

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Cadence Design Systems, Inc.

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CHAPTER

ONE

THEORY

1.1 Introduction to Quacpac TK

The chemistry of molecular interactions is a matter of shape and electrostatics, but doing electrostatics poorly is worse than doing none at all; accurate charges are required. Even the best charge models are useless if protonation states are wrong. Quacpac TK attempts to offer everything necessary to do charges correctly. It includes pKa and tautomer enumeration in order to get correct protonation states, partial charges using multiple models that cover a range of speed and accuracy, and electrostatic potential map construction and storage.

1.2 *tautomers*

When dealing with tautomers there are four primary tasks to be addressed. These include:

- Generating a single representative tautomer suitable for molecular visualization
- Generating a list of tautomers expected to be present in aqueous phase
- Generating a unique (canonical) representation for a set of tautomers
- Generating a substantial list of most possible tautomers suitable for input to further calculations.

Each of these four tasks is covered in a section below. In every case, the tautomerization can be handled alone, but it is generally more useful to handle tautomerization in conjunction with ionization. Each function includes the potential for pKa normalization alongside the tautomer normalization or enumeration.

1.2.1 Visualization

While the unique or canonical tautomer generated above is useful for storage in a database, they do not necessarily represent a low-energy tautomer suitable for visualization by modelers and chemists. In order to generate a structure suitable for visualization, we recommend you use the function *OEGetReasonableProtomer*. This function sets the molecule into a low-energy, neutral-pH, aqueous-phase tautomeric state that should be pleasing for visualization in a scientific setting.

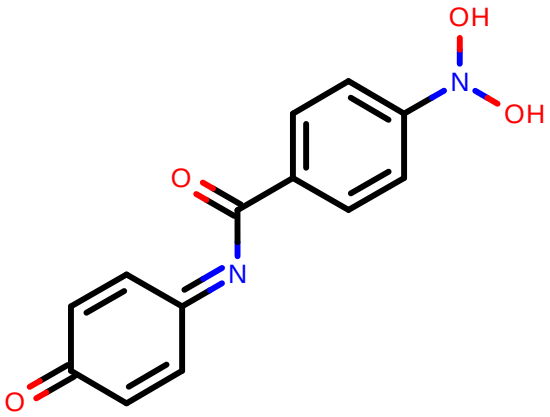
1.2.2 Reasonable Tautomer Ensemble

In the course of molecular modeling, it is often desirable to generate a small ensemble of low-energy, neutralpH, aqueous-phase tautomers. The function *OEGetReasonableTautomers* returns such an ensemble. In order to generate low-energy tautomers reliably, the function works with a form of the molecule that has formal charges removed. By default, each tautomer's ionization state is set to a neutral pH form, but ionization states are not enumerated.

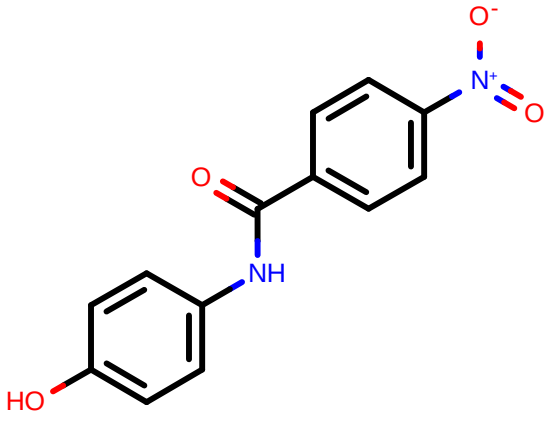
The following depictions show some examples of tautomers that are favored as "reasonable":

- Conversion of carboxylates to diols and nitros to di-hydroxy amines is very unfavorable.

disfavored

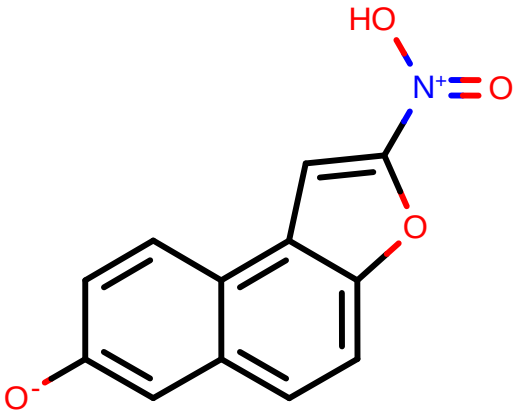


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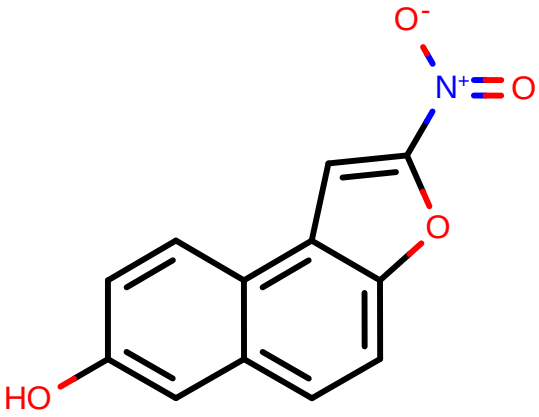


- Generation of unnecessary, non-dative, formal charges is unfavorable.

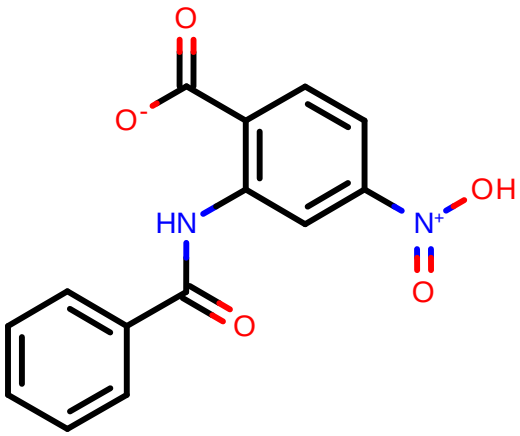
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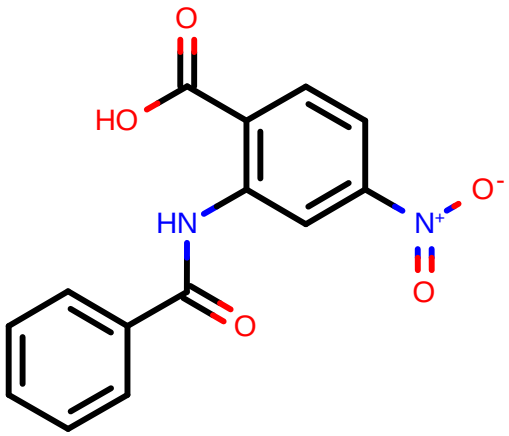
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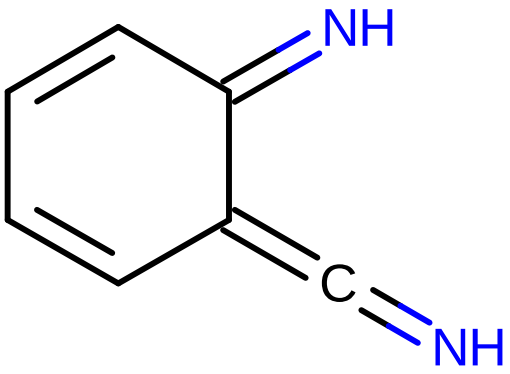


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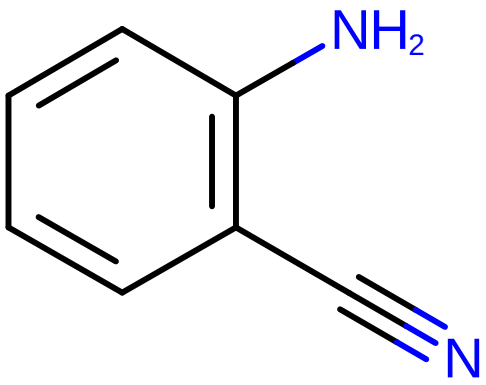


- Exocyclic bonds adjacent to aromatic rings are accounted for.

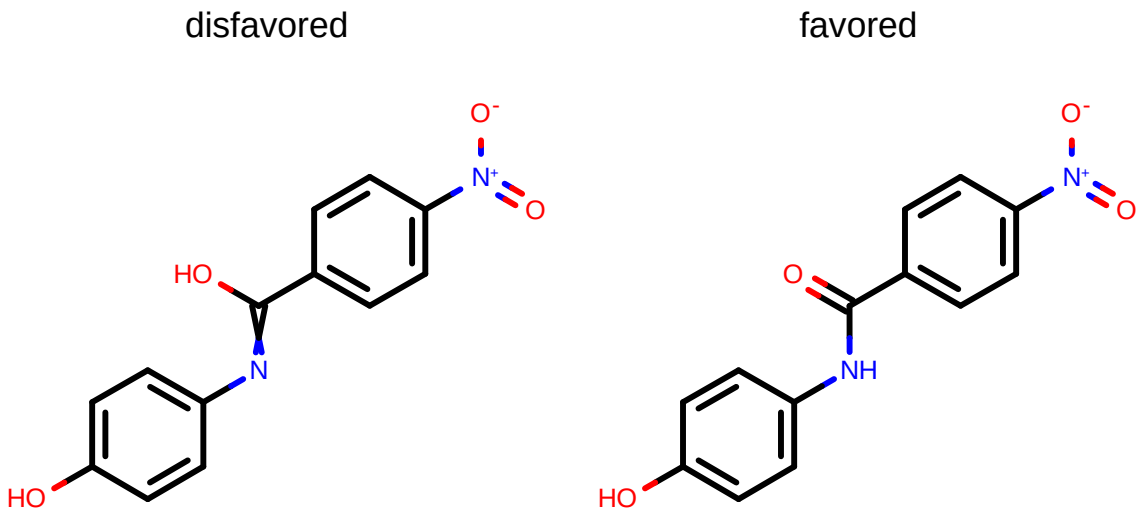
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- Priority is given to aliphatic double bond positions.



1.2.3 Canonicalization

The *OEGetUniqueProtomer* function is used for canonicalizing the tautomeric forms of a small molecule. Canonicalization converts any of the tautomeric forms of a given molecule into a single unique representation and removes all formal charges that can be appropriately neutralized. This is useful for database registration where alternate representations of tautomeric compounds often leads to duplicate entries in a database.

It is important to remember that a time limit cannot be used to control a canonical process as it might lead to hardware dependent behavior. Thus the identification of a unique protomer can take significant time when the size of the largest contiguous tautomeric atoms approaches or exceeds 30 atoms.

The tautomer returned by *OEGetUniqueProtomer* as the "canonical" representation often is not the physiologically preferred form. If a representative form is necessary, please use the functions referred to in the *Visualization* section above. If an ensemble of biologically relevant tautomers are necessary, please see the functions in the *Reasonable Tautomer Ensemble* section above.

OEGetUniqueProtomer is not a conformer generation function and will not create coordinates for molecules that are read in with no coordinates. When used on molecules with three-dimensional coordinates, *OEGetUniqueProtomer* attempts to place hydrogens in a reasonable manner. However, *OEGetUniqueProtomer* does not modify the heavy-atom coordinates of the molecule. In cases where the change in tautomer-state dictates a change in conformation, one will need to use a conformer-generation tool (such as OMEGA) to generate reasonable conformations for the output from *tautomers*. We recommend that in the preparation of small-molecules for study, charge-state and tautomer enumeration be performed before conformer generation.

1.2.4 Complete Enumeration

The *OEEnumerateTautomers* function is the core algorithm used to implement all functions listed above. It is useful for enumerating the tautomeric forms of a small molecule. Using the parameters in *OETautomerOptions* a user can control the behavior of the *OEEnumerateTautomers* to yield the behavior for their particular application.

It is recommended that before passing a molecule to *OEEnumerateTautomers* that first any dative bonds are normalized to the hypervalent form using *OEHypervalentNormalization* and second, formal charges are removed using *OERemoveFormalCharge*. These two steps improve the tautomers that are returned.

Tautomer generation is a combinatorial process and the time and memory requirements can grow quite rapidly. There are two mechanisms to help a use control this growth. First, the number of tautomers generated and the number of tautomers returned can be controlled with the *OETautomerOptions.SetMaxTautomersGenerated* and

OETautomerOptions.SetMaxTautomersToReturn respectively. Please be aware that if you require that few tautomers be generated, it is possible that no low energy tautomers will be generated. Second, one can limit the time the algorithm spends generating tautomers for each molecule using *OETautomerOptions.SetMaxSearchTime*.

OEEnumerateTautomers is not a conformer generation function and will not create coordinates for molecules that are read in with no coordinates. When used on molecules with three-dimensional coordinates, *OEEnumerateTautomers* attempts to place hydrogens in a reasonable manner. However, *OEEnumerateTautomers* does not modify the heavy-atom coordinates of the molecule. In cases where the change in tautomer-state dictates a change in conformation, one will need to use a conformer-generation tool (such as OMEGA) to generate reasonable conformations for the output from *tautomers*. We recommend that in the preparation of small-molecules for study, charge-state and tautomer enumeration be performed before conformer generation.

1.3 *pkatyper* - Ligand pKa

1.3.1 Introduction

Assessment of ligand pKas can be broken into two phases. The first phase is enumeration of the protonation states of interest, and the second phase is assigning a pKa value to each of these states. An intermediate phase of assigning microscopic pKas to each of the atomic-deprotonations may also be considered.

It is common in the course of modeling small-molecules to explore the conformational ensemble of the small molecule. Often structures as high as 5-8 kcal/mol above the aqueous ground-state can be important to biological processes. It is also appropriate to enumerate a protonation-state ensemble of the small molecule.

Similar to *tautomers*, OpenEye has a solution for enumerating reasonable protonation states, but not for assessing the energetics of the state (e.g. assigning a pKa value). OpenEye's solution for pKa enumeration seeks to enumerate all of the pKa states that fall roughly in the pH range of 2-14 in aqueous solvent. This range of pKa values generates an ensemble that includes the ground-state plus all charge states within 8 kcals/mol ΔG. This value was chosen to correspond to the similar range that is often used for generating conformational ensembles of small molecules.

1.3.2 Theory

pkatyper enumerates charge states based on primary, secondary and tertiary atom types of each atom in a molecule. The primary atom type is based on the atom's group and its valence. The primary atom-type defines the atom's basic propensity to support a formal charge. The secondary atom-type is defined by the atom-type of the neighbors for each atom. These secondary atom-types, such as aromaticity, alpha-beta unsaturation, or electronegative-groups, modulate each atom's basic propensity to support formal charges. The tertiary atom-types assess the effects of nearby formal charges on a given atom's formal charge. The combination of the primary, secondary and tertiary atom-types determine which formal charge states are allowed for each atom in a molecule. The primary and secondary atom-types are determined once, while the tertiary atom-types are determined as part of the enumeration process.

pkatyper is a rudimentary approach to pKa prediction. While pkatyper is not suited for prediction of absolute pKas, it is quite amenable to enumeration of all reasonable charge states of a very wide variety of small-molecule chemistries.

pkatyper is not a conformer generation program and will not create coordinates for molecules that are read in without coordinates. When used on molecules with three-dimensional coordinates, *pkatyper* attempts to place new hydrogens in a reasonable manner. However, *pkatyper* does not modify the heavy-atom coordinates of the molecule. In cases where the change in protonation-state dictates a change in conformation, one will need to use a conformer-generation tool (such as OMEGA) to generate reasonable conformations for the output from *pkatyper*. We recommend that in preparation of small-molecules for study, charge-state and tautomer enumeration be performed before conformer generation.

In the future, OpenEye will release a product which assigns a pKa value to each of the enumerated states.

1.4 *molcharge* - Partial Charges

1.4.1 Introduction

The assignment of appropriate atomic partial charges, both to small molecule ligands and to biopolymers (such as proteins and nucleic acids) is essential to getting meaningful results from any electrostatics calculation.

A molecule may be considered a collection of atomic nuclei and the electrons that surround them. The number of protons in each nucleus defines its atomic number/element. If the number of electrons exactly matches the number of protons in these nuclei, the molecule is neutral and has no net charge. If there are more electrons than protons, the molecule has a net negative charge, and if there are less, the molecule has a net positive charge.

It is both the atomic nuclei and the net charge that define the identity of a molecule. Indeed, this is a representation common to quantum chemistry. Adding or removing electrons (or atoms) from a molecule produces a different molecule.

In the discrete world of cheminformatics, valence bond theory allows the electrons present in a system to be represented in terms of bonds with formal bond orders, and formal charges assigned to particular atoms. The sum of the formal charges is equal to the net charge on the molecule, but which atoms are assigned which formal charges can be to some extent arbitrary due to resonance delocalization. In such cases the same molecule may be represented by similar connection tables, but with formal charges assigned to different sets of atoms.

For example, guanidinium may be expressed as either N[C+](N)N with the formal charge assigned to the carbon, or as [NH2+]=C(N)N with the formal charge assigned arbitrarily to one of the otherwise equivalent nitrogens. A similar example is a thiocarboxylate group, where either C(=O)[S-] or C(=S)[O-] are both equally appropriate representations of the same chemical functionality.

A zwitterion is an electrically neutral molecule that is represented as containing atoms with positive formal charge as well as atoms with negative formal charge.

Perhaps the most important fact to appreciate when considering formal charges on atoms is that they are all artificial constructs by chemists to accommodate a particular chemical model. A figment of a chemist's fevered imagination. Like valence bond theory, they are an exceptionally useful and powerful discretized model of the universe. But as with any model of reality, it has its limitations. Formal charges, for all their numerous benefits to mankind, unfortunately, are not localized on an atom.

The limitations of describing formal charges with valence bond theory is apparent even within cheminformatics. Sydnones, for example, are a class of heterocyclic compound that cannot be written using normal covalent bonds without introducing and arbitrarily assigning both positive and negative charges. Similarly, in inorganic chemistry, the ditechnetium cation, Te_2^{+5}, causes similar problems where the +5 formal charge cannot be assigned to both technetium atoms without breaking symmetry.

A better model, or approximation, of the wave function describing the distribution of electron density around a molecule is the use of atomic partial charges. A partial charge is a floating-point value assigned to each atomic center intended to model the distribution of electrons over a molecule.

Atomic partial charges are yet another approximation, much like the formal charges described above. However, partial charges provide a much better model to describe the electric field, dipole moment and other observable properties of a molecule.

A common limitation of the use of partial charges is the assumption that they are conformationally invariant. Unfortunately, the distribution of electrons around a molecule depends upon the spatial configuration of its nuclei. Some partial charge assignment algorithms, such as the method of Goddard and Rappé, consider these conformational effects, whilst others that are based on quantum mechanics, such as the RESP and AM1BCC methods of Bayly et al., go to great lengths to eliminate conformational effects, for example, by restraining and symmetrizing symmetric atom positions. This is necessary in order to be able to properly handle multiple conformations and changes in geometry (e.g. geometry optimization) with a single set of atomic charges.

1.4.2 Theory

Marsili-Gasteiger Partial Charges

Marsili-Gasteiger partial charges are assigned using a two stage algorithm. In the first stage, seed charges are assigned to each atom in the molecule. For example, carboxylate oxygens are each assigned the value -0.5. During the second stage, these initial charges are then shared across bonds, moving a certain amount of charge from one atom to another. The partial charge moved and its direction is determined by difference in electronegativities of the atoms on each end of the bond. The relaxation algorithm is then iterated several times (by default eight passes), attenuating the charge moved with each iteration. OpenEye does not recommend use of this charge model for intermolecular interactions; it was never intended for this purpose. The author of the method (Johann Gasteiger) developed it to compare relative reactivity of related organic chemical functional groups within different molecular contexts. Here it is included for comparison purposes.

MMFF94 Partial Charges

The partial charges used by the MMFF94 and MMFF94s force fields are assigned using a four stage algorithm. In the first stage, each atom of the molecule is assigned an MMFF94 atom type. In the second stage, an initial seed partial charge is assigned to each atom based upon its atom type. For a few atom types, the initial partial charge also depends upon the local environment. In the third stage, the initial charges assigned to aromatic rings are shared between all atoms of the aromatic ring. Finally, in the fourth stage, a table of bond charge increments (BCI) is used to move charges across bonds based upon the bond type of the bond (single, double, triple) and the atom types of the atoms at each end. Developed for the electrostatic interactions within the above-mentioned force fields, they are the appropriate charges to use with these force fields most notably for intramolecular interactions of pharmaceutical and bio-organic small molecules. They are less well-suited (but still passable) for intermolecular interactions using the common two-body additive Coulomb interactions as used in Amber, Charmm, Gromacs. For these better choices would be amber99sb charges on proteins and peptides, and am1bccsym charges on the ligand.

AM1 Charges

AM1 charges are a set of Mulliken-type charges derived from a semi-empirical quantum-mechanical calculation. For further discussion of this method, please see [Dewar-1985]. These should not be used for intermolecular interactions of force fields.

AM1BCC Charges

AM1BCC charges start with Mulliken-type partial charges derived from the AM1 semi-empirical quantum mechanical (QM) wave-function. In a second stage, bond-charge corrections (BCCs) are applied to the partial charges on each atom to generate new partial charges. Many different variants of AM1BCC charges are offered within our API because of the significant influences of several different factors on these QM-derived charges. Specifically, these factors are

- Optimization: whether or not the input geometry is optimized. QM wavefunctions in general are quite sensitive to geometry, especially bond lengths and bond angles, so this can markedly affect the partial charges. In general, optimizing the geometry is recommended. To avoid a collapse of the conformation due to strong intramolecular electrostatic interactions, light restraints to the starting geometry are applied.
- Symmetrization: whether or not topologically similar atoms (for example the two oxygens on a carboxylate) are constrained to have identical values. The true QM wavefunction is usually asymmetric around topologically similar atoms, leading to asymmetric partial charges. However, if the same partial charges are to be used on different conformers (as with general fixed-charge force fields) it is important that these charges be symmetrized or else interconverting between formally degenerate conformers (e.g. 180 degree rotation of the carboxylate) will have non-degenerate electrostatic energies. In general, if the partial charges are to be applied to more than the single conformer used to generate them, symmetrization is strongly recommended.

Another important issue with AM1BCC charges is if highly conformer-specific charges are generated which are unsuitable for other conformers, leading to undesirable perturbed electrostatic energies for those other conformers. To address this problem, we strongly recommend the ELF conformer selection protocol described below.

"Standard" AM1BCC includes both optimization and symmetrization.

OpenEye considers AM1BCC charges to be the best partial charge model currently available. For further discussion, please see the work of Christopher I. Bayly.

ELF Conformer Selection

ELF conformer selection is a method to select one or more conformers having Electrostatically Least-interacting Functional groups (ELF) from a large conformer database. The purpose of this method is to resolve important issues with QM-derived charges in general, including AM1BCC charges. The issue is that strong short-range intramolecular polarizations specific to a certain conformation, as with an intramolecular hydrogen bond or salt bridge, usually leads to strongly perturbed partial charges for the atoms involved. These charges can be very different from those found for other conformers which do not have that intramolecular polar interaction. If such partial charges are applied to all conformers, some of those other conformers are very likely to have wrongly over-stabilized solvation energies.

A second problem arising from this issue is the precision or sensitivity of the electrostatic energies resulting from QM-derived charges. By this we mean the variance in electrostatic relative energies between different conformers depending on what conformer is used for the QM-derived charges. Imagine two different sets of QM-derived partial charges for a molecule, each coming from a conformer having different strong intramolecular hydrogen bonds. Each set of partial charges will have strongly perturbed partial charges for the internally hydrogen bonded atoms, but they will be different. The relative energies between conformers will be different depending which partial charge set is used.

For these reasons it is important to avoid generating QM-derived partial charges from a conformer having electrostatically strongly interacting functional groups. This is what ELF conformer selection does.

ELF needs to start with enough conformers so that it can find a population of conformers that do not have strongly-interacting functional groups. In the first stage, the Coulomb electrostatic energy is calculated for every conformer using the absolute value of the MMFF94 partial charges (original negative charges are replaced with their absolute values). The electrostatic energies with such charges destabilize all strong polar interactions, and thus the lowest electrostatic energies correspond to the Electrostatically Least-interacting Functional groups. The lowest-energy 2% of conformers is selected as the 2% ELF population. We find that averaging 10 diverse conformers from the 2% ELF population is sufficient to provide a well-behaved set of QM-derived partial charges even for highly polar and charged molecules.

Amber ff94, ff96, ff99, ff99sb, and ff99sbc0 Partial Charges

The partial charges used by the AmberFF94 force field are based on fitting quantum mechanical electrostatic potentials (esp). They were developed to address two key issues with earlier esp-fit charge sets: unrealistically high charges on charge centers and the variation of atomic charges with conformation. While the latter should have some basis in electronic structure, numerical instability in the charge fitting process was the source of both these pathologies. AmberFF94 charge sets use restrained esp-fitting (RESP) to control the numerical instabilities and simultaneous multi-conformer fitting to lead to conformation-independent charges that are restricted to individual residues. Particular attention was given to ensure that backbone amides have consistent charges. The Amber force fields ff94, ff96, ff99, ff99sb, and ff99sbc0 all use the same set of RESP charges, they differ in other terms (mostly torsional).

1.5 Wiberg bond orders

1.5.1 Theory

The concept of bond order has been proposed by Wiberg [Wiberg-1966] as a calculated bond property using orthonormalized atomic orbitals which are a basis set for semi-empirical molecular orbitals. Originally it was formulated for the CNDO basis set, but it might be extended to AM1 or PM3 methods. Wiberg bond order is a measure of electron population overlap between two atoms:

$$W_{AB} = \sum_{\mu \in A} \sum_{\nu \in B} P_{\mu\nu}^2$$

where summation is over atomic orbitals μ on atom A and atomic orbitals ν on atom B, and $P_{\mu\nu}$ is the corresponding density matrix element. For non-bonded pairs of atoms in a molecule, W_{AB} is very low but always nonzero.

See also

- *OEAM1Results.GetBondOrder* method

CHAPTER

TWO

EXAMPLES

2.1 Quacpac TK Examples

The following table lists the currently available **Quacpac TK** examples:

Program	Description
assigncharges	assigning charges
neutralionization	setting a neutral ionization state
enumeratetautomers	enumerating tautomers
setreasonablechargestate	setting a reasonable charge state
wibergbondorders	obtaining Wiberg bond orders

Examples:

2.1.1 Assigning Charges

The following code example shows how to assign partial charges. The program reads all of the molecules in the input file, assigns partial charges to each based on the selected method (the default is `-method mmff94`), and writes each charged molecule to the output file.

Command Line Interface

A description of the command line interface can be obtained by executing the program with the –help argument.

```
prompt> java AssignCharges --help
```

will generate the following output:

```
Simple parameter list

 Charging options
   -method : which set of charges to apply

 input/output options
   -in : Input molecule
   -out : Output molecule (usually an oeb)
```

Code

```
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*/
package openeye.examples.oequacpac;

import java.io.IOException;
import java.net.URL;

import openeye.oequacpac.*;
import openeye.oechem.*;

public class AssignCharges {

    static boolean AssignChargesByName(OEMol mol, String name) {
      boolean optimize   = true;
      boolean symmetrize = true;

      if (name.equals( "noop"))
          return oequacpac.OEAssignCharges(mol, new OEChargeEngineNoOp());
      else if (name.equals( "mmff") || name.equals( "mmff94"))
          return oequacpac.OEAssignCharges(mol, new OEMMFF94Charges());
      else if (name.equals( "am1bcc"))
          return oequacpac.OEAssignCharges(mol, new OEAM1BCCCharges());
      else if (name.equals( "am1bccnosymspt"))
          return oequacpac.OEAssignCharges(mol, new OEAM1BCCCharges(!optimize,
                                                                    !symmetrize));
      else if (name.equals( "amber") || name.equals( "amberff94"))
          return oequacpac.OEAssignCharges(mol, new OEAmberFF94Charges());
      else if (name.equals( "am1bccelf10"))
          return oequacpac.OEAssignCharges(mol, new OEAM1BCCELF10Charges());
      return false;
    }

    public static void main(String[] argv) {
        URL fileURL = AssignCharges.class.getResource("AssignCharges.txt");
        OEInterface itf = null;
```

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```
        try {
            itf = new OEInterface();
            oechem.OEConfigureFromURL(itf, fileURL);
        } catch (IOException e) {
            oechem.OEThrow.Fatal("Unable to open interface file");
        }

        if (! oechem.OEParseCommandLine(itf, argv, "AssignCharges"))
            oechem.OEThrow.Fatal("Unable to interpret command line!");

        oemolistream ifs = new oemolistream();

        String inputFile = itf.GetString("-in");
        if (! ifs.open(inputFile))
            oechem.OEThrow.Fatal("Unable to open " + inputFile + " for reading");

        oemolostream ofs = new oemolostream();

        String outFile = itf.GetString("-out");
        if (! ofs.open(outFile))
            oechem.OEThrow.Fatal("Unable to open " + outFile + " for writing");

        String chargeName = itf.GetString("-method");

        OEMol mol = new OEMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
            if (! AssignChargesByName(mol, chargeName))
                oechem.OEThrow.Warning("Unable to assign " + chargeName +
                                       " charges to mol " + mol.GetTitle());

            oechem.OEWriteMolecule(ofs, mol);
        }

        ifs.close();
        ofs.close();
    }
}
```

with interface file

```
!BRIEF [-options] <inmol> [<outmol>]

!CATEGORY "input/output options :"
   !PARAMETER -in
      !ALIAS -i
      !TYPE string
      !BRIEF Input molecule
      !VISIBILITY simple
      !REQUIRED true
      !KEYLESS 1
   !END
```

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```
   !PARAMETER -out
      !ALIAS -o
      !TYPE string
      !DEFAULT oeassigncharges.oeb.gz
      !BRIEF Output molecule (usually an oeb)
      !VISIBILITY simple
      !REQUIRED false
      !KEYLESS 2
   !END
!END

!CATEGORY "Charging options :"
   !PARAMETER -method
      !TYPE string
      !LEGAL_VALUE noop
      !LEGAL_VALUE mmff
      !LEGAL_VALUE mmff94
      !LEGAL_VALUE am1bcc
      !LEGAL_VALUE am1bccnosymspt
      !LEGAL_VALUE amber
      !LEGAL_VALUE amberff94
      !LEGAL_VALUE am1bccelf10
      !DEFAULT mmff94
      !BRIEF which set of charges to apply
      !SIMPLE true
      !REQUIRED false
   !END
!END
```

See also

- *OEAssignCharges* function

2.1.2 Setting a Neutral Ionization State

This following example shows how to set a single dominant ionization state of a molecule at pH 7.4.

Command Line Interface

A description of the command line interface is shown as follows:

```
prompt> java NeutralIonization <mol-infile> <mol-outfile>
```

Code

```
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*/
package openeye.examples.oequacpac;

import openeye.oechem.*;
import openeye.oequacpac.*;

public class NeutralIonization {
    public void processFile(oemolistream ifs, oemolostream ofs) {
        OEGraphMol mol = new OEGraphMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
            if( oequacpac.OESetNeutralpHModel(mol))
                oechem.OEWriteMolecule(ofs, mol);
            else
            {
                String msg = "Unable to set a neutral pH model for molecule: "
                             + mol.GetTitle();
                oechem.OEThrow.Warning(msg);
            }
        }
    }

    private void displayUsage() {
        System.err.println("usage: NeutralIonization <mol-infile> <mol-outfile>");
        System.exit(1);
    }

    public static void main(String argv[]) {
        NeutralIonization app = new NeutralIonization();

        if (argv.length != 2)
            app.displayUsage();

        oemolistream ifs = new oemolistream();
        if (! ifs.open(argv[0]))
            oechem.OEThrow.Fatal("Unable to open " + argv[0] + " for reading");

        oemolostream ofs = new oemolostream();
        if (! ofs.open(argv[1]))
            oechem.OEThrow.Fatal("Unable to open " + argv[1] + " for writing");

        app.processFile(ifs, ofs);
```

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```
    }
}
```

See also

- *OESetNeutralpHModel* function

2.1.3 Enumerating Tautomers

This following example shows a fast informatics technique using tautomer enumeration which is capped at 200 states per molecule. Formal charge of each input molecule is removed first, and then tautomers are enumerated. The tautomers are saved to the output file after setting a favorable ionization state at neutral pH.

Command Line Interface

A description of the command line interface is shown as follows:

```
prompt> java EnumerateTautomers <mol-infile> <mol-outfile>
```

Code

```
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*/
package openeye.examples.oequacpac;

import openeye.oechem.*;
import openeye.oequacpac.*;

public class GetReasonableTautomers {
    public void processFile(oemolistream ifs, oemolostream ofs) {
        OETautomerOptions tautomerOptions = new OETautomerOptions();
        boolean pKaNorm = true;

        OEGraphMol mol = new OEGraphMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
```

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```
            for (OEMolBase tautomer : oequacpac.OEGetReasonableTautomers(mol,␣
↪tautomerOptions, pKaNorm)) {
                oechem.OEWriteMolecule(ofs, tautomer);
            }
        }
    }

    private void displayUsage() {
        System.err.println("usage: GetReasonableTautomers <mol-infile> <mol-outfile>");
        System.exit(1);
    }

    public static void main(String argv[]) {
        GetReasonableTautomers app = new GetReasonableTautomers();

        if (argv.length != 2)
            app.displayUsage();

        oemolistream ifs = new oemolistream();
        if (! ifs.open(argv[0]))
            oechem.OEThrow.Fatal("Unable to open " + argv[0] + " for reading");

        oemolostream ofs = new oemolostream();
        if (! ofs.open(argv[1]))
            oechem.OEThrow.Fatal("Unable to open " + argv[1] + " for writing");

        app.processFile(ifs, ofs);
    }
}
```

See also

- *OEGetReasonableTautomers* function

2.1.4 Setting a Reasonable Charge State

The following example shows how to use *OEGetReasonableProtomer* to set a favorable ionization state assuming pH=7.4.

Command Line Interface

A description of the command line interface is shown as follows:

```
prompt> java SetReasonableChargeState <mol-infile> <mol-outfile>
```

Code

```
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*/
package openeye.examples.oequacpac;

import openeye.oechem.*;
import openeye.oequacpac.*;

public class SetReasonableChargeState {
    public void processFile(oemolistream ifs, oemolostream ofs) {
        OEGraphMol mol = new OEGraphMol();
        while(oechem.OEReadMolecule(ifs, mol)){
          oequacpac.OEGetReasonableProtomer(mol);
          oechem.OEWriteMolecule(ofs, mol);
        }
    }

    private void displayUsage() {
        System.err.println("usage: SetReasonableChargeState <mol-infile> <mol-outfile>");
        System.exit(1);
    }

    public static void main(String argv[]) {
        SetReasonableChargeState app = new SetReasonableChargeState();

        if (argv.length != 2)
            app.displayUsage();

        oemolistream ifs = new oemolistream();
        if (! ifs.open(argv[0]))
            oechem.OEThrow.Fatal("Unable to open " + argv[0] + " for reading");

        oemolostream ofs = new oemolostream();
        if (! ofs.open(argv[1]))
            oechem.OEThrow.Fatal("Unable to open " + argv[1] + " for writing");

        app.processFile(ifs, ofs);
    }
}
```

See also

- *OEGetReasonableProtomer* function

2.1.5 Obtaining Wiberg bond orders

The following example shows how to obtain the Wiberg bond orders from an AM1 calculation.

Command Line Interface

A description of the command line interface is shown as follows:

```
prompt> java WibergBondOrders <mol-infile>
```

Code

```
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*/
package openeye.examples.oequacpac;

import openeye.oechem.*;
import openeye.oequacpac.*;

public class WibergBondOrders {

    public static void main(String[] args) {
        if (args.length!=1) {
            System.out.println("WibergBondOrders <infile>");
            System.exit(0);
        }

        oemolistream ifs = new oemolistream(args[0]);
        OEAM1 am1 = new OEAM1();
        OEAM1Results results = new OEAM1Results();
        OEMol mol = new OEMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
```

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```
            for (OEConfBase conf : mol.GetConfs()) {
                System.out.println(" molecule = "+mol.GetTitle());
                System.out.println(" conformer = "+conf.GetIdx());
                if (am1.CalcAM1(results, conf)) {
                    int nbonds = 0;
                    for (OEBondBase bond : mol.GetBonds(new OEIsRotor())) {
                        nbonds += 1;
                        System.out.println(results.GetBondOrder(bond.GetBgnIdx(), bond.
↪GetEndIdx()));
                    }
                    System.out.println(" Rotatable bonds: "+nbonds);
                }
            }
        }
    }
}
```

See also

- *OEAM1Results.GetBondOrder* method

2.1.6 Applying Charges to OEDesignUnit

The following code example shows how to apply charges to an OEDesignUnit. The program reads an OEDesignUnit as the input file, applies charges to it, and writes new OEDesignUnit to the specified output file.

Command Line Interface

A description of the command line interface is as follows.

Code

See also

- *OEDesignUnitCharges* class
- OEDesignUnit class

2.1.7 Enumerate ionization states at neutral pH using OEMultistatepKaModel and OEMultistatepKaModelOptions

The following code example shows how to use OEMultistatepKaModel and OEMultistatepKaModelOptions classes to enumerate ionization states at neutral pH. The program reads an input molecules file, create an instance of OEMultistatepKaModelOptions class. Use it in OEMultistatepKaModel class object and writes generated ionization states at neutral pH to specified output file.

Command Line Interface

A description of the command line interface is as following.

Code

See also

- *OEMultistatepKaModelOptions* class
- *OEMultistatepKaModel* class

CHAPTER

THREE

API

3.1 OEProton Classes

3.1.1 OEAM1BCCCharges

```
class OEAM1BCCCharges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign AM1 Mulliken-type partial charges with bond-charge corrections.

The input must be a 3D molecule with a number of atoms no larger than a defined maximum. The default is 300 atoms, see *constructors*. Parameters must be available for each atom and bond type. If permissive BCCs are requested, no correction is applied when a BCC is missing.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEAM1BCCCharges(bool optimize = true, bool symmetrize = true,
                bool permissiveBCCs = false,
                unsigned maxAtoms = 300)
```

Constructor. Parameters also have getter and setter methods.

GetOptimize

```
bool GetOptimize() const
```

Returns `true` if the geometry of the input molecule will be optimized during charge assignment.

GetPermissiveBCCs

```
bool GetPermissiveBCCs() const
```

Returns `true` if a missing BCC will be treated as a correction of zero rather than an error.

GetSizeLimit

```
unsigned GetSizeLimit() const
```

Returns the maximum number of atoms permitted.

GetSymmetrize

```
bool GetSymmetrize() const
```

Returns `true` if charges will be symmetrized with respect to bond-topologically equivalent atoms.

SetOptimize

```
void SetOptimize(bool optimize = true)
```

Defines whether the geometry of the input molecule will be optimized during charge assignment. Optimization is lightly restrained to starting coordinates.

SetPermissiveBCCs

```
void SetPermissiveBCCs(bool permissive = true)
```

Defines whether a missing BCC will be treated as a correction of zero or as an error.

SetSizeLimit

```
void SetSizeLimit(unsigned maxAtoms)
```

Defines the maximum number of atoms permitted in the input molecule.

SetSymmetrize

```
void SetSymmetrize(bool symmetrize = true)
```

Defines whether charges on the molecule are symmetrized with respect to bond-topologically equivalent atoms.

3.1.2 OEAM1BCCELF10Charges

```
class OEAM1BCCELF10Charges : public OEELFCharges
```

Charge engine input to *OEAssignCharges* to assign AM1 Mulliken-type partial charges with bond-charge corrections using the electrostatically least-interacting functional group (ELF) technique.

The input must be a 3D multi-conformer molecule with a number of atoms no larger than the default AM1BCC maximum. AM1BCC parameters must be available for each atom and bond type.

Equivalent to:

```
new OEELFCharges(new OEAM1BCCCharges(), 10)
```

The following methods are publicly inherited from *OEELFCharges*:

GetLimit	*GetPercentage*	*SetPercentage*
SetLimit	*GetReturnSelectedConfs*	*SetReturnSelectedConfs*

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEAM1BCCELF10Charges()
OEAM1BCCELF10Charges(const OEAM1BCCELF10Charges& rhs)
```

Constructor. There are no options for this charge engine.

3.1.3 OEAM1Charges

```
class OEAM1Charges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign AM1 Mulliken-type partial charges.

The input must be a 3D molecule with a number of atoms no larger than a defined maximum. The default is 300 atoms, see *constructors*. AM1 parameters must be available for each atom type.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEAM1Charges(bool optimize = true, bool symmetrize = false,
             unsigned maxAtoms = 300)
```

Constructor. Parameters also have getter and setter methods.

GetOptimize

```
bool GetOptimize() const
```

Returns `true` if the geometry of the input molecule will be optimized during charge assignment.

GetSizeLimit

```
unsigned GetSizeLimit() const
```

Returns the maximum number of atoms permitted.

GetSymmetrize

```
bool GetSymmetrize() const
```

Returns `true` if charges will be symmetrized with respect to bond-topologically equivalent atoms.

SetOptimize

```
void SetOptimize(bool optimize = true)
```

Defines whether the geometry of the input molecule will be optimized during charge assignment. Optimization is lightly restrained to starting coordinates.

SetSizeLimit

```
void SetSizeLimit(unsigned maxAtoms)
```

Defines the maximum number of atoms permitted in the input molecule.

SetSymmetrize

```
void SetSymmetrize(bool symmetrize = true)
```

Defines whether charges on the molecule are symmetrized with respect to bond-topologically equivalent atoms.

3.1.4 OEAmberFF94Charges

```
class OEAmberFF94Charges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign Amber force field 94 atomic partial charges to standard amino acids.

The input molecule must have explicit hydrogens and consist of only standard Amber amino acids. Residues must be perceived or repairs permitted. The amino acid name may be altered to match the Amber naming scheme, such as `HIP` for a protonated histidine. Currently OpenEye supports the following Amber amino acids: `ACE`, `ALA`, `ARG`, `ASH`, `ASN`, `ASP`, `CIM`, `CIP`, `CYM`, `CYS`, `CYX`, `GLH`, `GLN`, `GLU`, `GLY`, `HID`, `HIE`, `HIP`, `HIS`, `HOH`, `ILE`, `LEU`, `LYN`, `LYS`, `MET`, `NHE`, `NME`, `PHE`, `PRO`, `SER`, `THR`, `TRP`, `TYR`, `VAL`. Amber charges are graph-based and do not require 3D coordinates.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEAmberFF94Charges()
```

Constructor. There are no options for this charge engine.

3.1.5 OEChargeEngineBase

```
class OEChargeEngineBase
```

This is the abstract base class for all charge engines, containing methods used by the function *OEAssignCharges*.

The following charge engine classes derive from this base class:

- *OEAM1BCCCharges*
- *OEAM1BCCELF10Charges*
- *OEAM1Charges*
- *OEAmberFF94Charges*
- *OEChargeEngineNoOp*
- *OEClearCharges*
- *OECombineChargeEngines*
- *OEDesignUnitCharges*
- *OEELFCharges*
- *OEFormalToPartialCharges*
- *OEGasteigerCharges*
- *OEInitialCharges*
- *OEMMFF94Charges*

ApplyCharges

```
bool ApplyCharges(OEChem::OEMolBase& mol) const
bool ApplyCharges(OEChem::OEMCMolBase& mcMol) const
bool ApplyCharges(OEBio::OEDesignUnit& du) const
```

Assigns partial charges to the atoms of the molecule. The `OEMCMolBase` overload assigns charges using all conformers where applicable. The `OEDesignUnit` overload charges the small-molecule component of the design unit.

CheckCharges

```
bool CheckCharges(const OEChem::OEMolBase& mol) const
bool CheckCharges(const OEChem::OEMCMolBase& mcMol) const
bool CheckCharges(const OEBio::OEDesignUnit& du) const
```

Used by *OEAssignCharges* to determine if the charges on the molecule are as expected.

CreateCopy

```
OEChargeEngineBase* CreateCopy() const = 0
```

Deep copy of the charge engine.

GetExpectValidMol

```
bool GetExpectValidMol() const
```

Returns `true` if an input molecule must be valid before *OEAssignCharges* attempts to assign charges.

GetName

```
std::string GetName() const
```

Returns the name of the charge engine.

GetRepairRequestedHint

```
bool GetRepairRequestedHint() const
```

Returns `true` if *OEAssignCharges* is requested to repair the input molecule before assigning charges. Examples of repairing a molecule include adding explicit hydrogens and perceiving residues.

GetRequirements

```
unsigned GetRequirements() const
```

Returns a bit mask used by *OEAssignCharges* describing aspects of the input molecule required for this charging method. Examples include 3D coordinates, explicit hydrogens, and PDB order.

IsValid

```
bool IsValid(OEChem::OEMolBase& mol) const
bool IsValid(OEChem::OEMCMolBase& mcMol) const
bool IsValid(OEBio::OEDesignUnit& du) const
bool IsValid(const OEChem::OEMolBase& mol) const = 0
bool IsValid(const OEChem::OEMCMolBase& mcMol) const
bool IsValid(const OEBio::OEDesignUnit& du) const
```

Returns `true` if the input molecule appears to be valid for use with this method.

SetExpectValidMol

```
void SetExpectValidMol(bool expect = true)
```

Defines whether an input molecule must be valid before *OEAssignCharges* attempts to assign charges. If set to `false` and the molecule is not valid, then *OEAssignCharges* attempt to charge the molecule anyway.

SetRepairRequestedHint

```
void SetRepairRequestedHint(bool repair = true)
```

Define whether *OEAssignCharges* is requested to repair the input molecule before assigning charges. Examples of repairing a molecule include adding explicit hydrogens and perceiving residues. If set to `false` and the molecule requires repairs, then *OEAssignCharges* will fail and return `false`.

TransferCharge

```
bool TransferCharge(OEChem::OEAtomBase* dstAtom,
                    const OEChem::OEAtomBase* srcAtom) const
```

If *OEAssignCharges* must make a copy of the input molecule before charges can be applied, this method is used to transfer charges back to the input molecule.

3.1.6 OEChargeEngineNoOp

```
class OEChargeEngineNoOp : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* that does nothing to the input molecule, any existing charges are left untouched.

This charge engine can be used with any type of molecule.

Can be used as a pre-charging method for *OECombineChargeEngines*.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEChargeEngineNoOp()
```

Constructor. There are no options for this charge engine.

3.1.7 OEClearCharges

```
class OEClearCharges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to set partial charges on all atoms to zero. This charge engine is graph-based and does not require 3D coordinates.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEClearCharges()
```

Constructor. There are no options for this charge engine.

3.1.8 OECombineChargeEngines

```
class OECombineChargeEngines : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* that combines two user-specified charge engines into one. This is useful when the first charge engine is used to pre-charge a molecule and the second to adjust the charges. This allows more complicated charging schemes to be easily constructed.

The input molecule must conform to the requirements of the specified charge engines.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OECombineChargeEngines(const OECombineChargeEngines& rhs)
OECombineChargeEngines(const OEChargeEngineBase& preChargeEngine,
                       const OEChargeEngineBase& adjustmentEngine)
```

Constructors. The `preChargeEngine` is expected to set initial charges while the `adjustmentEngine` is expected to modify those charges.

3.1.9 OEDesignUnitCharges

> **Attention**
>
> This API is currently available in C++ and Python.

```
class OEDesignUnitCharges : public OEChargeEngineBase
```

This charge engine charges each component in the OEDesignUnit. The various components can be charged with different charging engines, and the default behavior is to do exactly that. The default behavior is for the protein engine to use *OEAmberFF94Charges* for the standard protein residues. It uses *OEAM1BCCCharges* for nonstandard residues. The nucleic acid component uses the *OEMMFF94Charges* charges. The ligand and or any other heterogen in the system (e.g cofactors), are charged using *OEAM1BCCCharges*. The solvent uses *OEAmberFF94Charges*, but by default uses the SZMAP water model, in which case it assigns the charges to match those described in The Szmap TK Standard Water Model. This is an option that can be turned off. Excipients are by default charged using the *OEMMFF94Charges* engine. The radii assigned are `OERadiiType.BondiVdw`, except in cases where AM1 charges have been used, in which case the radii is of the `OERadiiType.Zap9` type. Metals in the system (often in cofactors or otherCofactors) are initially charged with the *OEFormalToPartialCharges* engine, and in the last step of the calculation, the metal charges are spread in the system using the *OESpreadMetalCharges* as part of the finalization stage. Counter ions are charged with the same metal charge engine, but are not subsequently spread. The fall back engine is the same for all components; in case an engine fails, the method will try to charge a component with the fall back engine, which by default is *OEMMFF94Charges*.

Note

Currently, there is a hard limit of 100 atoms for molecules being charged with the *OEAM1BCCCharges* charging engine.

Warning

It is currently not possible to use *OEAM1BCCELF10Charges* for the ligand, cofactors, or other components. The method requires passing a conformer ensemble of the molecule to charge, which is currently not possible with an OEDesignUnit. If a user tries to use this type of charging engine, it will be downgraded to AM1BCC with a warning. Since the *OEAM1BCCELF10Charges* is recommended for the molecular dynamics type of simulations, we recommend charging the ligand independently and updating it in the DesignUnit using `OEUpdateDesignUnit`.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetExpectValidMol*	*SetExpectValidMol*
operator==	*GetName*	*SetRepairRequestedHint*
GetRepairRequestedHint	*TransferCharge*	
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	

Constructors

```
OEDesignUnitCharges()
OEDesignUnitCharges(const OEDesignUnitCharges& rhs)
```

Default and copy constructors.

ApplyCharges

```
bool ApplyCharges(OEBio::OEDesignUnit& du) const
```

Returns the boolean whether or not charges are able to be applied to the input OEDesignUnit argument (*du*).

CreateCopy

```
OEChargeEngineBase* CreateCopy() const
```

Creates a copy of the charge engine class. This class does not own the returned memory.

IsValid

```
bool IsValid(const OEChem::OEMolBase& mol) const
bool IsValid(const OEBio::OEDesignUnit& du) const
```

Returns the boolean whether or not the input OEMolBase or OEDesignUnit can be assigned partial charges from the charging engine.

SetCoFactorChargeEngine

```
void SetCoFactorChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets the charge engine for the `OEDesignUnitComponents.Cofactors` molecular component.

SetFallbackChargeEngine

```
void SetFallbackChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets a backup charge engine for any molecular component where the charge engine cannot be applied.

SetFinalizationChargeEngine

```
void SetFinalizationChargeEngine(const OEChargeEngineBase& chargeEngine)
```

SetLigandChargeEngine

```
void SetLigandChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets the charge engine for the `OEDesignUnitComponents.Ligand` molecular component.

SetMetalChargeEngine

```
void SetMetalChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets the charge engine for both the `OEDesignUnitComponents.Metals` and `OEDesignUnitComponents.CounterIons` molecular components.

SetNucleicChargeEngine

```
void SetNucleicChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets the charge engine for the `OEDesignUnitComponents.Nucleic` molecular component.

SetOtherChargeEngine

```
void SetOtherChargeEngine(const OEChargeEngineBase& chargeEngine)
```

SetProteinChargeEngine

```
void SetProteinChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets the charge engine for the `OEDesignUnitComponents.Protein` molecular component.

SetProteinNonStandardChargeEngine

```
void SetProteinNonStandardChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets the charge engine for any nonstandard amino acids in the `OEDesignUnitComponents.Protein` molecular component.

SetSolventChargeEngine

```
void SetSolventChargeEngine(const OEChargeEngineBase& chargeEngine)
```

Sets the charge engine for any solvent molecules in the `OEDesignUnitComponents.Solvent` molecular component.

TransferCharge

```
bool TransferCharge(OEChem::OEAtomBase* dstAtom,
                    const OEChem::OEAtomBase* srcAtom) const
```

Returns the boolean whether or not the transfer of charges from the source atom (*srcAtom*) to the destination atom (*dstAtom*) was successful.

UseSZMAPWaterModel

```
void UseSZMAPWaterModel(const bool value)
```

Sets the boolean of whether or not to use the Szmap water model within the context of charging the system (see Introduction for more information about the water model itself).

3.1.10 OEELF

```
class OEELF
```

This class defines an interface to select conformers from a given ensemble, using the electrostatically least-interacting functional group (ELF) technique.

The *OEELF* class defines the following public methods:

- *Select*

Constructors

```
OEELF(const OEELFOptions& opts = OEELFOptions())
OEELF(const OEELF&)
```

Default and copy constructors.

```
OEELF &operator=(const OEELF &)
```

The assignment operator.

Assignment operator.

Select

```
bool Select(OEChem::OEMCMolBase& mol) const
```

Selects the desired ELF population. Method discards the unwanted conformers in the input molecule.

3.1.11 OEELFCharges

```
class OEELFCharges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign charges with the user-specified charge engine using the electrostatically least-interacting functional group (ELF) technique.

The input must be a 3D multi-conformer molecule and conform to the requirements of the specified charge engine. Graph-based charge engines are not appropriate for use with ELF because they do not take 3D conformation into account.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

The following classes derive from this class:

- *OEAM1BCCELF10Charges*

Constructors

```
OEELFCharges(const OEELFCharges& rhs)
OEELFCharges(const OEChargeEngineBase& chargeEngine,
             unsigned limit = 10, double percentage = 2.0,
             bool selectedConfs = false)
```

Constructor. Parameters also have getter and setter methods.

GetLimit

```
unsigned GetLimit() const
```

Returns the number of diverse conformers to select from the least interacting conformers set.

GetPercentage

```
double GetPercentage() const
```

Returns the percentage of input conformers to select as the electrostatically least-interacting set.

GetReturnSelectedConfs

```
bool GetReturnSelectedConfs() const
```

Returns `true` if just the selected diverse conformers will be returned. Otherwise all the original conformers are returned.

SetLimit

```
void SetLimit(unsigned limit)
```

Sets the number of diverse conformers to select from the least interacting conformers set in the second step of the ELF algorithm.

SetPercentage

```
void SetPercentage(double pct)
```

Sets the percentage of input conformers to select as the electrostatically least-interacting set in the first step of the ELF algorithm.

SetReturnSelectedConfs

```
void SetReturnSelectedConfs(bool selected = true)
```

Determines whether only the selected diverse conformers will be returned.

3.1.12 OEELFOptions

```
class OEELFOptions : public OESystem::OEOptions
```

This class provides an interface to setup options required for *OEELF* calculations.

The *OEELFOptions* class defines the following public methods:

- *GetElfLimit* and *SetElfLimit*
- *GetPercent* and *SetPercent*

Constructors

```
OEELFOptions()
OEELFOptions(const OEELFOptions&)
```

Default and copy constructors.

GetElfLimit

```
unsigned GetElfLimit() const
```

See *SetElfLimit* method.

GetPercent

```
double GetPercent() const
```

See *SetPercent* method.

SetElfLimit

```
bool SetElfLimit(const unsigned)
```

Sets the **number of diverse conformers to select** from the least interacting conformers set. **Default: 10**

SetPercent

```
bool SetPercent(const double)
```

Sets the **percentage of input conformers to select** as the electrostatically least-interacting set. **Default: 2.0**

3.1.13 OEFormalChargeOptions

```
class OEFormalChargeOptions
```

This class is used for setting options during tautomer enumeration with *OEEnumerateFormalCharges*.

Constructors

```
OEFormalChargeOptions(const OEFormalChargeOptions& rhs)
OEFormalChargeOptions(unsigned int maxCount = 0u,
                      bool verbose = false, bool warts = true)
```

Default and copy constructors.

GetMaxCount

```
unsigned int GetMaxCount() const
```

Get the maximum number of charge states to be enumerated.

GetVerbose

```
bool GetVerbose() const
```

Get whether detailed info will be printed during charge enumeration.

GetWarts

```
bool GetWarts() const
```

Get whether to add `wart` to the title of each charge state.

SetMaxCount

```
void SetMaxCount(unsigned int max)
```

Set the maximum number of charge states to be enumerated.

SetVerbose

```
void SetVerbose(bool verbose)
```

Set whether detailed info is to be printed during charge enumeration. The default is `false`.

SetWarts

```
void SetWarts(bool warts)
```

Set whether to add `wart` to the title of each charge state. The default is `true`.

3.1.14 OEFormalToPartialCharges

```
class OEFormalToPartialCharges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign atomic partial charges equal to the atomic formal charges.

The input molecule must have explicit hydrogens. These charges are graph based and do not require 3D coordinates.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEFormalToPartialCharges()
```

Constructor. There are no options for this charge engine.

3.1.15 OEGasteigerCharges

```
class OEGasteigerCharges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign Marsili-Gasteiger atomic partial charges.

The input molecule must have explicit hydrogens. Gasteiger charges are graph based and do not require 3D coordinates.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEGasteigerCharges()
```

Constructor. There are no options for this charge engine.

3.1.16 OEInitialCharges

```
class OEInitialCharges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign atomic partial charges by smearing formal charges onto resonance shared atoms.

The input molecule must have explicit hydrogens. Initial charges are graph based and do not require 3D coordinates.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEInitialCharges()
```

Constructor. There are no options for this charge engine.

3.1.17 OEMMFF94Charges

```
class OEMMFF94Charges : public OEChargeEngineBase
```

Charge engine input to *OEAssignCharges* to assign MMFF94 atomic partial charges.

The input molecule must have explicit hydrogens and MMFF94 parameters must be available for each atom. MMFF charges are graph based and do not require 3D coordinates.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetName*	*SetRepairRequestedHint*
operator==	*GetRepairRequestedHint*	*TransferCharge*
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	
GetExpectValidMol	*SetExpectValidMol*	

Constructors

```
OEMMFF94Charges()
```

Constructor. There are no options for this charge engine.

3.1.18 OESpreadMetalCharges

```
class OESpreadMetalCharges : public OEChargeEngineBase
```

Charge engine derived from *OEChargeEngineBase* that spreads partial charges from a metal to its chelation bonding parters.

The following methods are publicly inherited from *OEChargeEngineBase*:

operator!=	*GetExpectValidMol*	*SetExpectValidMol*
operator==	*GetName*	*SetRepairRequestedHint*
GetRepairRequestedHint	*TransferCharge*	
CheckCharges	*GetRequirements*	
CreateCopy	*IsValid*	

Constructors

```
OESpreadMetalCharges(double chargeAliquot = 0.25,
                     double radiusMargin = 0.25,
                     double maxNbrDist = 6.0)
```

Constructor with input arguments of the incremental amount of charge that should be spread from the metal to each chelating atom (*chargeAliquot*), the distance beyond the radial-radial distance from which the nearest neighbors cutoff is defined (*radiusMargin*), and the maximum distance separating the metal and the chelating atoms (*maxNbrDist*). Parameters also have getter and setter methods.

CreateCopy

```
OEChargeEngineBase* CreateCopy() const
```

Creates a copy of the charge engine class. This class does not own the returned memory.

GetChargeAliquot

```
double GetChargeAliquot() const
```

Returns the amount of the charge that will be removed from the metal per chelating atom.

GetMaxNbrDist

```
double GetMaxNbrDist() const
```

Returns the maximum nearest neighbors distance (minus the *radiusMargin*) from the metal to the chelating atoms.

GetRadiusMargin

```
double GetRadiusMargin() const
```

Returns the extra marginal amount of distance such that two atoms can be considered chelators of each other.

SetChargeAliquot

```
void SetChargeAliquot(double aliquot)
```

Sets the amount of charge that should be spread from the metal to each chelating atom.

SetMaxNbrDist

```
void SetMaxNbrDist(double distance)
```

Sets the maximum nearest neighbors distance (minus the *radiusMargin*) from the metal to the chelating atoms.

SetRadiusMargin

```
void SetRadiusMargin(double distance)
```

Sets the extra marginal amount of distance that two atoms can be considered chelators of each other.

3.1.19 OETautomerOptions

```
class OETautomerOptions
```

This class is used for setting options during tautomer enumeration with *OEEnumerateTautomers*.

By default, *OEEnumerateTautomers* will return the "canonical" tautomer, regardless of the tautomer submitted to the function. This "canonical" tautomer is extremely useful for efficient and reliable tautomer cheminformatics, such as database searching. The *OETautomerOptions.SetRankTautomers* method can be used to make *OEEnumerateTautomers* generate a tautomer more "reasonable" for depiction for chemists.

Constructors

```
OETautomerOptions(unsigned int maxGenerated = 4096,
                  bool rank = true, bool warts = false,
                  unsigned int level = 0, bool carbonHybrid = true,
                  bool saveStereo = false,
                  unsigned int maxZoneSize = 35,
                  unsigned int maxTautomericAtoms = 70,
                  float maxTime = 120, bool kekule = false,
                  bool clearCoords = false,
                  unsigned int hybridLevel = OEHybridizationLevel::EnolEnamine,
                  unsigned int maxToReturn = 256,
                  unsigned int racemicType = OERacemicType::LocalSampled)
```

Default constructor.

```
OETautomerOptions(const OETautomerOptions& rhs)
```

Copy constructor.

GetApplyWarts

```
bool GetApplyWarts() const
```

Returns setting for warts application of {title}_1, {title}_2, etc., on tautomers.

GetCarbonHybridization

```
bool GetCarbonHybridization() const
```

Returns setting for whether or not carbon hybridization changes are allowed. Allowing sp2-sp3 changes of carbon atoms can significantly increase computation time.

GetClearCoordinates

```
bool GetClearCoordinates() const
```

Returns whether input coordinates are cleared. The default value is `false`.

GetHybridizationLevel

```
unsigned int GetHybridizationLevel() const
```

Returns setting for the level of hybridization changes allowed when carbon hybridization is allowed. Allowing carbon hybridization significantly increase computation time. The returned value is from the *OEHybridizationLevel* namespace.

See also

- *OEHybridizationLevel* namespace

GetKekule

```
bool GetKekule() const
```

Returns setting for whether or not generated tautomers are kekule or have aromaticity perceived.

GetLevel

```
unsigned int GetLevel() const
```

Returns level for tautomerization. Higher levels allow less likely atomic transitions to occur.

GetMaxSearchTime

```
float GetMaxSearchTime() const
```

Returns the maximum search time in seconds allowed for a molecule.

GetMaxTautomericAtoms

```
unsigned int GetMaxTautomericAtoms() const
```

Returns the maximum number of tautomeric atoms allowed in a molecule. The default value is 70.

GetMaxTautomersGenerated

```
unsigned int GetMaxTautomersGenerated() const
```

Returns setting for maximum number of tautomers that may be generated for each input molecule.

See also

- *OETautomerOptions.GetMaxTautomersToReturn* method

GetMaxTautomersToReturn

```
unsigned int GetMaxTautomersToReturn() const
```

Returns setting for maximum number of tautomers that may be returned for each input molecule.

See also

- *OETautomerOptions.GetMaxTautomersGenerated* method

GetMaxZoneSize

```
unsigned int GetMaxZoneSize() const
```

Returns setting for maximum number of atoms allowed in a continuous tautomerization zone. The default zone size is 35.

GetRacemicType

```
unsigned int GetRacemicType() const
```

Returns setting for the way to handle loss of stereocenters, if the *OETautomerOptions.GetSaveStereo* method returns `false`. If the *OETautomerOptions.GetSaveStereo* method returns `true`, this option is irrelevant. The returned value is from the *OERacemicType* namespace. The default value is *OERacemicType.LocalSampled*.

See also

- *OETautomerOptions.GetSaveStereo* method
- *OERacemicType* namespace

GetRankTautomers

```
bool GetRankTautomers() const
```

Returns setting for whether or not tautomers are ranked and ordered before being returned. By default, this is `false`, i.e., the canonical tautomer is returned as the first molecule in the iterator. As opposed to the most "reasonable" tautomer being returned first.

GetSaveStereo

```
bool GetSaveStereo() const
```

Returns setting for whether atoms and bonds with labeled stereochemistry are fixed or allowed to participate in tautomerization.

See also

- *OETautomerOptions.GetRacemicType* method

3.1.20 SetApplyWarts

```
void SetApplyWarts(bool warts)
```

Sets whether warts of {title}_1, {title}_2, etc., are added to tautomers.

3.1.21 SetCarbonHybridization

```
void SetCarbonHybridization(bool carbonHybrid)
```

Sets whether carbon hybridization changes are allowed. Allowing sp2-sp3 changes of carbon atoms can significantly increase computation time.

See also

- *OETautomerOptions.SetHybridizationLevel* method

3.1.22 SetClearCoordinates

```
bool SetClearCoordinates(bool clear_coordinates)
```

Sets whether input coordinates are cleared from generated tautomers.

3.1.23 SetHybridizationLevel

```
void SetHybridizationLevel(unsigned int level)
```

Sets level of hybridization changes allowed for carbon atoms if the *OETautomerOptions.GetCarbonHybridization* method returns `true`. If the *OETautomerOptions.GetCarbonHybridization* method returns `false`, this option is irrelevant.

level
: This value has to be from the *OEHybridizationLevel* namespace.

Note

The level of hybridization can have significantly impact on the computation time.

See also

- *OETautomerOptions.SetCarbonHybridization* method
- *OEHybridizationLevel* namespace

3.1.24 SetKekule

```
void SetKekule(bool kekule)
```

Sets whether tautomers are returned in kekule format or have aromaticity perceived.

3.1.25 SetLevel

```
void SetLevel(unsigned int level)
```

Sets level for tautomerization. Higher levels allow less likely atomic transitions to occur.

3.1.26 SetMaxSearchTime

```
void SetMaxSearchTime(float maxSearchTime)
```

Sets the maximum search time in seconds allowed for a molecule.

3.1.27 SetMaxTautomericAtoms

```
void SetMaxTautomericAtoms(unsigned int maxTautomerAtoms)
```

Sets the maximum number of tautomeric atoms allowed in a molecule.

3.1.28 SetMaxTautomersGenerated

```
void SetMaxTautomersGenerated(unsigned int max)
```

Sets the maximum number of tautomers that may be generated per input molecule.

See also

- *OETautomerOptions.SetMaxTautomersToReturn* method

3.1.29 SetMaxTautomersToReturn

```
void SetMaxTautomersToReturn(unsigned int max)
```

Sets the maximum number of tautomers that may be returned per input molecule.

See also

- *OETautomerOptions.SetMaxTautomersGenerated* method

3.1.30 SetMaxZoneSize

```
void SetMaxZoneSize(unsigned int maxZoneSize)
```

Sets the maximum number of atoms allowed in a continuous tautomerization zone.

3.1.31 SetRacemicType

```
void SetRacemicType(unsigned int racemicType)
```

Sets the racemic type for loss of stereocenters if the *OETautomerOptions.GetSaveStereo* method returns `false`. If the *OETautomerOptions.GetSaveStereo* method returns `true`, this option is irrelevant.

racemicType
This value has to be from the *OERacemicType* namespace.

See also

- *OETautomerOptions.SetSaveStereo* method
- *OERacemicType* namespace

3.1.32 SetRankTautomers

```
void SetRankTautomers(bool rank)
```

Sets whether or not tautomers are ranked and ordered before being returned. Setting this argument to `true` will cause the most "reasonable" tautomer to be returned as the first tautomer, opposed to the "canonical" tautomer being returned first.

The "canonical" tautomer may or may not be a suitable representative tautomer for depiction. To fill this role, the *SetRankTautomers(true)* provides "reasonable" tautomer forms for any input molecule.

3.1.33 SetSaveStereo

```
void SetSaveStereo(bool saveStereo)
```

Sets whether atoms and bonds with labeled stereochemistry are fixed or allowed to participate in tautomerization.

See also

- *OETautomerOptions.SetRacemicType* method

3.1.34 OETautomerMolFunction

```
class OETautomerMolFunction : public OEMolFunctionBase
```

Warning

This class is deprecated. Use *OETautomerOptions* instead.

Currently `OETautomerMolFunction` and *OETyperMolFunction* are similar, however it is expected that they will diverge more over time. They share the same first four arguments. The first argument is the oemolstream where the enumerated molecules will be placed. The second argument is a boolean indicating whether aromaticity should be calculated for the enumerated structure. The third argument is a boolean indicating whether the enumerated states should only be counted (rather than actually listed). The fourth argument is an unsigned int indicating the maximum number of states that should be enumerated for any single input molecule. The fifth argument for `OETautomerMolFunction` states whether a 'reasonable' type calculation is being setup and only the most aromatic tautomer should be stored. After the calculation, the most aromatic tautomer can be retrieved using *OETautomerMolFunction.GetMolecule*. The sixth argument will label the output tautomer titles with @`number` appended. When using the same `OETautomerMolFunction` instance for multiple tautomer runs, remember to call *OETautomerMolFunction.Reset* in between each run.

Constructors

```
OETautomerMolFunction(OEChem::oemolostream& ofp, bool arom,
                      bool ct = false, unsigned int max = 0,
                      bool mostAro = false, bool warts = true)
```

Default and copy constructors.

operator()

```
bool operator()(const OEChem::OEMolBase& inmol)
```

CreateCopy

```
base_type* CreateCopy() const
```

GetCount

```
unsigned int GetCount() const
```

Returns the number of tautomers generated. Calling *OETautomerMolFunction.Reset* will reset this number to zero.

GetMolecule

```
const OEChem::OEMolBase& GetMolecule() const
```

This method is used in conjunction with the mostAro flag to retrieve a reasonable looking tautomer.

Reset

```
void Reset()
```

This method resets the count to zero and clears the stored molecule that *OETautomerMolFunction.GetMolecule* has access to.

3.1.35 OETyperMolFunction

```
class OETyperMolFunction : public OEMolFunctionBase
```

Currently OETyperMolFunction and *OETautomerMolFunction* are similar, however it is expected that they will diverge more over time. They share the same first four arguments. The first argument is the oemolstream where the enumerated molecules will be placed. The second argument is a boolean indicating whether aromaticity should be calculated for the enumerated structure. The third argument is a boolean indicating whether the enumerated states should only be counted (rather than actually listed). The fourth argument is an unsigned int indicating the maximum number of states that should be enumerated for any single input molecule.

Constructors

```
OETyperMolFunction(OEChem::oemolostream& ofp, bool arom,
                   bool ct = false, unsigned int max = 0)
```

Default and copy constructors.

operator()

```
bool operator()(const OEChem::OEMolBase& inmol)
```

CreateCopy

```
base_type* CreateCopy() const
```

Reset

```
void Reset()
```

This method will reset the internal counter and should be called before reusing an *OETyperMolFunction* instance.

3.2 OEProton Constants

3.2.1 OECharges

This namespace contains constants used by the deprecated function *OEAssignPartialCharges* to define which charge model to apply. This function is being replaced by *OEAssignCharges* which uses an object that defines the charge model and any required pre-processing.

AM1

AM1 Mulliken-type charges. A full AM1 geometry optimization is done.

AM1BCC

AM1 Mulliken-type charges with bond-charge corrections. The AM1 optimization is lightly restrained to starting coordinates but no partial charge symmetrization is done (same as *OECharges.AM1BCCNoSym*).

> **Note**
>
> Note that this differs from the "standard" *AM1BCC* charging scheme as published, where symmetrization is done (same as *OECharges.AM1BCCSym*).

AM1BCCNoSym

AM1 Mulliken-type charges with bond-charge corrections. The AM1 optimization is lightly restrained to starting coordinates but no partial charge symmetrization is done.

AM1BCCNoSymSPt

AM1 Mulliken-type charges with bond-charge corrections. Neither AM1 geometry optimization nor partial charge symmetrization is done.

AM1BCCSPt

AM1 Mulliken-type charges with bond-charge corrections. Neither AM1 geometry optimization nor partial charge symmetrization is done. (same as *OECharges.AM1BCCNoSymSPt*).

AM1BCCSym

AM1 Mulliken-type charges with bond-charge corrections. The AM1 optimization is lightly restrained to starting coordinates and partial charges are symmetrized with respect to bond-topologically equivalent atoms.

AM1BCCSymSPt

AM1 Mulliken-type charges with bond-charge corrections; no AM1 geometry optimization is done. Partial charges are symmetrized with respect to bond-topologically equivalent atoms.

AM1SPt

AM1 Mulliken-type charges; no AM1 geometry optimization is done.

AmberFF94

Amber force field 94 charges for standard amino acids.

AmberFF99

Amber force field 99 charges (same charges as *OECharges.AmberFF94*).

AmberFF99SB

Amber force field 99SB charges (same charges as *OECharges.AmberFF94*).

AmberFF99bsc0

Amber force field 99bc0 charges (same charges as *OECharges.AmberFF94*).

Default

The current default charges, which are *OECharges.MMFF94*.

Formal

Copies the formal charge field of atoms into the partial charge field.

Gasteiger

Assigns Gasteiger partial charges.

Initial

Smears unit charges in the partial charge field onto resonance shared atoms.

MMFF94

Assigns MMFF94 partial charges.

Max

Number of charge type constants.

NoOp

No operation is performed. This setting is useful for indicating that charges originated elsewhere, such as user input, and have not been changed.

None

Remove all partial charges.

OPLS

OPLS protein dictionary charges.

> **Warning**
>
> This charging model is deprecated. The *OEAssignPartialCharges* function will throw a deprecated warning message when calling it with this charging model.

3.2.2 OEChargingRequirement

This namespace contains constants that describe requirements of charge model objects derived from the *OEChargeEngineBase* abstract base class.

AltersResidueName

BondedResidues

Compact

Coords3D

ExplicitHydrogens

MolComplexPrep

MultiConfOnly

Nothing

PDBOrder

Parameters

Precharged

ResPerceived

ReturnSelectedConfs

SetsAromaticity

SetsType

SizeWithinLimits

StandardResidues

3.2.3 OEHybridizationLevel

This namespace contains constants used by the class *OETautomerOptions* to store the level of carbon hybridization.

See also

- *OETautomerOptions* class
- *OETautomerOptions.GetHybridizationLevel* method
- *OETautomerOptions.SetHybridizationLevel* method

Default

The default value is *OEHybridizationLevel.EnolEnamine*.

Original

If carbon hybridization is set, then extensive carbon hybridization will take place.

DoubleBondNbr

If carbon hybridization is set, then only localized carbon hybridzation will take place, allowing generation of keto-enol tautomers without generating as many extreme tautomers as the default parameter.

EnolEnamine

If carbon hybridization is set, then local hybridization will take place to allow keto-enol and enol-enamine tautomerization while generating fewer tautomers than other options above.

3.2.4 OERacemicType

This namespace contains constants used by the class *OETautomerOptions* that stores the stereo loss behavior when the *OETautomerOptions.GetSaveStereo* method returns `false`.

Note

If the *OETautomerOptions.GetSaveStereo* method returns `true`, this flag is irrelevant.

See also

- *OETautomerOptions* class
- *OETautomerOptions.GetSaveStereo* method
- *OETautomerOptions.SetSaveStereo* method

Default

The default value is *OERacemicType.LocalSampled*.

None

This option indicates that no racemic type will be set.

LocalSampled

This option indicates that individual tautomers that have double bonds to tetrahedral stereocenters will have the stereo removed.

EverSampled

This option indicates that if an atom which are tetrahedral stereocenters has a double bonds in any of the tautomers returned by the function, then those tetrahedral stereocenters will have the stereo removed in ALL of the returned tautomers.

3.3 OEProton Functions

3.3.1 OEAssignCharges

```
bool OEAssignCharges(OEChem::OEMolBase& mol,
                     const OEChargeEngineBase& chargeEngine)
bool OEAssignCharges(OEChem::OEMCMolBase& mcMol,
                     const OEChargeEngineBase& chargeEngine)
```

Note

This function is designed to replace the legacy function *OEAssignPartialCharges*.

This function sets the charge of each atom in the molecule `mol` based on the specific nature of the *chargeEngine* object passed as the second argument. In general, charge engine implementations place scalar partial charges on atoms, but could be implemented to perform other roles such as assign multi-pole charges.

Listing 1: Assigning MMFF Partial Charges to a Molecule

```
if (oequacpac.OEAssignCharges(mol, new OEMMFF94Charges()))
    //...
```

Another example:

Listing 2: Assigning Unoptimized AM1 Partial Charges

```
boolean optimizationSetting = false;
if (oequacpac.OEAssignCharges(mol, new OEAM1Charges(optimizationSetting)))
    //...
```

The objects used by this function, derived from the abstract base class *OEChargeEngineBase*, can be thought of as "options objects" which describe the details of a specific charge model. *OEAssignCharges* analyzes these options and may need to add explicit hydrogens or perceive residues before assigning charges.

Listing 3: Assigning Non-symmetrized AM1BCC Partial Charges

```
OEAM1BCCCharges chargeEngine = new OEAM1BCCCharges();
chargeEngine.SetSymmetrize(false);
if (oequacpac.OEAssignCharges(mol, chargeEngine))
    //...
```

Some prerequisites, such as setting the aromaticity model, would alter the input molecule in ways that are incidental to the calculation. In this case, a copy of the input molecule is made before the alterations are made and the charges are transferred back to the input molecule after the calculation. This ensures that only charges, explicit hydrogens, residue perception, residue names, and the number of conformations returned can change on the input molecule.

This function returns `false` if does not succeed.

See also

- *OEAssignPartialCharges* function
- *OEChargeEngineBase* abstract base class
- *Assigning Charges* code example

3.3.2 OEAssignPartialCharges

```
bool OEAssignPartialCharges(OEChem::OEMolBase& mol,
                            unsigned int method = OECharges::Default,
                            bool noHydrogen = false,
                            bool debug = false, bool epsilon2 = false)
bool OEAssignPartialCharges(OEChem::OEMCMolBase& mol,
                            unsigned int method = OECharges::Default,
                            bool noHydrogen = false,
                            bool debug = false, bool epsilon2 = false)
```

Note

This deprecated function will not be developed further. It is being replaced by *OEAssignCharges* which provides more control and greater expandability.

This function sets the partial charge value of each atom in a molecule. The molecule to be charged is passed as the first argument. The second argument is the charge model to be used. These values should be selected from the *OECharges* namespace. The third argument is a boolean for whether the final molecule should have explicit hydrogens. If `noHydrogen` is set to true, all hydrogens will be made implicit, and the charge on each heavy atom with attached hydrogens will be adjusted to be the sum of its original partial charge and all of the attached hydrogen partial charges. The `debug` flag controls the volume of debug information written to standard error. This function returns a boolean value evaluating the success of the calculation.

This function is overloaded to accept an `OEMolBase` or an `OEMCMolBase`. Currently, only `AM1` and `AM1BCC` charges have specialized multiconformer implementations in the `OEMCMolBase` overload. For all other charges, the `OEMCMolBase` and `OEMolBase` implementations are identical. The `epsilon2` flag selects an alternative parameterization of the AM1-BCC charge model when set to `true`. [default = false]

See also

- *OEAssignCharges* function

3.3.3 OEEnumerateFormalCharges

```
OESystem::OEIterBase<OEChem::OEMolBase>* OEEnumerateFormalCharges(const␣
↪OEChem::OEMolBase& mol,
                                                                  const␣
↪OEFormalChargeOptions& formalChargeOptions = OEFormalChargeOptions())
OESystem::OEIterBase<OEChem::OEMolBase>* OEEnumerateFormalCharges(const␣
↪OEChem::OEMCMolBase& mol,
                                                                  const␣
↪OEFormalChargeOptions& formalChargeOptions = OEFormalChargeOptions())
```

This function takes a const input molecule and variants of that molecule different formal charges are returned as an `OESystem::OEIterBase<OEChem::OEMolBase> *`. Options are set with an *OEFormalChargeOptions*, a parameter that is not required. See the corresponding documentation for descriptions of options.

Warning

The following version of OEEnumerateFormalCharges is deprecated. Use the above *OEFormalChargeOptions* version instead.

```
unsigned int OEEnumerateFormalCharges(OEChem::OEMolBase& mol,
                                      OEMolFunctionBase& mfb,
                                      bool verbose = false)
```

This function has three arguments. The first is the non-const molecule whose formal charges are to be enumerated. For details of the enumeration process, please see *pkatyper - Ligand pKa*. The second argument is a functor call-back. The functor's `operator()` is called with each new protonation state enumerated. The enumeration will continue until the functor returns false or until the enumeration is complete. The third argument determines if verbose atom-type information should be written to standard out. The function will return the total number of states which were enumerated.

3.3.4 OEEnumerateTautomers

```
OESystem::OEIterBase<OEChem::OEMolBase>* OEEnumerateTautomers(const OEChem::OEMolBase&␣
↪mol,
                                                              const OETautomerOptions&␣
↪tautomerOptions)
OESystem::OEIterBase<OEChem::OEMCMolBase>* OEEnumerateTautomers(const␣
↪OEChem::OEMCMolBase& mol,
                                                                const OETautomerOptions&␣
↪tautomerOptions)
```

This function takes a const input molecule that is to be tautomerized and the tautomers are returned as an `OESystem::OEIterBase<OEChem::OEMolBase> *`. Options are set with an *OETautomerOptions*. See the corresponding documentation for descriptions of options. Aromaticity must be perceived on the input molecule before calling this function.

```
unsigned int OEEnumerateTautomers(OEChem::OEMolBase& mol,
                                  OEMolFunctionBase& mfb,
                                  unsigned int allflag = 0,
                                  bool ch3flag = false,
                                  bool saveStereo = false,
                                  float maxTime = 120)
```

Warning

This version of *OEEnumerateTautomers* is deprecated. Use the above *OETautomerOptions* version above instead.

This function has four arguments. The first argument in a non-const molecule that will be the basis for the tautomer enumeration. For details of the enumeration process, please see *tautomers*. The second argument is a functor call-back. The functor's `operator()` is called with each new tautomer state enumerated. The enumeration will continue until the functor returns false or until the enumeration is complete. The third argument is an `unsigned int` which indicates the maximum acceptable energetic category of enumerated tautomers. The function will return all categories of tautomers from the lowest available up to this cutoff. If the only available level is higher than the cutoff, that single level of tautomers will be enumerated. This control is in addition to the call-back control. Finally, the `bool ch3flag` argument controls whether tautomer enumeration should include tautomerization of methyl and methylene groups adjacent to a conjugated system. This allows cyclohexa-2,4-dien-1-one, `O=C1CC=CC=C1`, to be canonicalized as a tautomer of phenol, `Oc1ccccc1`. Unfortunately, the combinatorial explosion from tautomerizing across the alpha carbon of amino acids means that this option should not be used when enumerating the tautomers of proteins and large peptides. This function returns the total number of tautomers enumerated.

A setting of `saveStereo=true` will prevent associated atoms or bonds from taking part in tautomerization if they have stereochemistry set. Stereochemistry can naturally be lost with the creation and removal of double bonds.

3.3.5 OEGetChargeTypeName

```
const char* OEGetChargeTypeName(unsigned int chargeType)
```

This function returns the corresponding *OECharges* name for the *unsigned int chargeType* method.

3.3.6 OEGetReasonableProtomer

```
bool OEGetReasonableProtomer(OEChem::OEMolBase& mol)
bool OEGetReasonableProtomer(OEChem::OEMCMolBase& mol)
```

This function will attempt to produce a single protomer that will be a suitable representation of the molecule in a biological system. This state is defined as an aqueous environment with pH~7.4 and a tautomer from among the predominate tautomers that is favored by medicinal chemists. This function is intended to be suitable for preparing molecules to display to chemists. The molecules are quite consistent, but should not be considered a canonical form in this version.

See also

- *OEGetReasonableProtomers* function

3.3.7 OEGetReasonableProtomers

```
OESystem::OEIterBase<OEChem::OEMolBase>* OEGetReasonableProtomers(const␣
↪OEChem::OEMolBase& mol)
OESystem::OEIterBase<OEChem::OEMCMolBase>* OEGetReasonableProtomers(const␣
↪OEChem::OEMCMolBase& mol)
```

This function will attempt to produce a series of protomers that will be a suitable ensemble of the molecule in a biological system. This state is defined as an aqueous environment with pH~7.4. The tautomers of the molecule are enumerated. For each enumerated tautomer a single charge state representing the predominate ionization at pH 7.4 is chosen. Ionization states of each charge state are NOT enumerated in this version.

See also

- *OEGetReasonableProtomer* function
- *OEGetReasonableTautomers* function

3.3.8 OEGetReasonableTautomers

```
OESystem::OEIterBase<OEChem::OEMolBase>* OEGetReasonableTautomers(const␣
↪OEChem::OEMolBase& mol,
                                                                  const␣
↪OETautomerOptions& opts = OETautomerOptions(),
                                                                  bool pKaNorm = true)
OESystem::OEIterBase<OEChem::OEMCMolBase>* OEGetReasonableTautomers(const␣
↪OEChem::OEMCMolBase& mol,
                                                                    const␣
↪OETautomerOptions& opts = OETautomerOptions(),
                                                                    bool pKaNorm = true)
```

This function takes a const input molecule that is to be tautomerized and the tautomers are returned as an iterator over molecules. The function is overloaded to handle both single (OEMolBase) and multi-conformer (OEMCMolBase) molecules. Aromaticity must be perceived on the input molecule before calling this function.

mol
: The molecule being tautomerized.

opts
The *OETautomerOptions* object that stores properties that influence tautomerization process.

pKaNorm
This parameter determines whether to apply pKa normalization. If `true` the ionization state of each tautomer will be assigned to a predominate state at pH~7.4.

Example of tautomerizing a molecule

```
OETautomerOptions tautomer_options = new OETautomerOptions();
tautomer_options.SetMaxTautomersGenerated(4096);
tautomer_options.SetMaxTautomersToReturn(16);
tautomer_options.SetCarbonHybridization(true);
tautomer_options.SetMaxZoneSize(50);
tautomer_options.SetApplyWarts(true);

boolean pKaNorm = true;

while (oechem.OEReadMolecule(ifs, mol)) {
    for (OEMolBase tautomer : oequacpac.OEGetReasonableTautomers(mol, tautomer_options,␣
↪pKaNorm)) {
        // work with tautomer
```

See also

- *OEEnumerateTautomers* function
- *OEGetReasonableProtomer* function
- *OEGetReasonableProtomers* function
- *Enumerating Tautomers* code example

3.3.9 OEGetUniqueProtomer

```
bool OEGetUniqueProtomer(OEChem::OEMolBase& dst,
                         const OEChem::OEMolBase& mol)
bool OEGetUniqueProtomer(OEChem::OEMCMolBase& dst,
                         const OEChem::OEMCMolBase& mol)
```

This function will attempt to produce a single protomer that can be used to generate a canonical representation of all tautomers of this molecule. All charge states or tautomer representations of a molecule should generate the same unique tautomer.

Note

The unique protomer is NOT necessarily the low energy tautomer, or a scientifically reasonable tautomer. It is a tautomer useful for generating canonical hash strings. The unique protomer can be used to generate single or multiple protomers suitable for visualization by passing then through the *OEGetReasonableTautomers* functions.

See also

- *OEGetReasonableTautomers* function

3.3.10 OEHypervalentNormalization

```
void OEHypervalentNormalization(OEChem::OEMolBase& mol)
```

This function should be used in conjunction with *OERemoveFormalCharge* to prepare a molecule to be passed to the *OEEnumerateTautomers* function. These two normalization help the tautomer enumeration yield a higher proportion of lower-energy tautomers.

See also

- *OEEnumerateTautomers*
- *OERemoveFormalCharge*

3.3.11 OEQuacPacGetArch

```
const char* OEQuacPacGetArch()
```

Returns the architecture on which the release was built

3.3.12 OEQuacPacGetLicensee

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

Fills the parameter `string &licensee` with the licensee of the license file being used

3.3.13 OEQuacPacGetPlatform

```
const char* OEQuacPacGetPlatform()
```

Returns the platform on which the release of built

3.3.14 OEQuacPacGetRelease

```
const char* OEQuacPacGetRelease()
```

Returns the version number as a `const char*` in major.minor.bugfix form

3.3.15 OEQuacPacGetSite

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

Fills the parameter `string &licensee` with the site on the license file being used

3.3.16 OEQuacPacGetVersion

```
unsigned int OEQuacPacGetVersion()
```

Returns the build date of the release.

3.3.17 OEQuacPacIsLicensed

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

Determines 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 **Quacpac TK** functionality.

The 'feature' argument can be used to check for a valid license to **Quacpac TK** along with the following features: 'python', 'java', or 'clr' (for CSharp).

The 'expdate' argument can be used to obtain the expiration date of the current **Quacpac TK** license.

See also

- `OEChemIsLicensed` function

3.3.18 OERemoveFormalCharge

```
bool OERemoveFormalCharge(OEChem::OEMolBase& mol)
bool OERemoveFormalCharge(OEChem::OEMCMolBase& mol)
```

This function will attempt to remove all formal charges from `mol` in a manner that is consistent with adding and removing implicit or explicit protons. This method will not create radicals and will not attach more protons to an atom than is acceptable in that atom's standard valence form. The formal charge of quaternary amines is not removed because removing it would create a hypervalent nitrogen.

3.3.19 OESetNeutralpHModel

```
bool OESetNeutralpHModel(OEChem::OEMolBase& mol)
bool OESetNeutralpHModel(OEChem::OEMCMolBase& mol)
```

This function will attempt to set `mol` to the most energetically favorable ionization state for pH=7.4 using a rule-based system. This function does not enumerate multiple states for any molecule. In cases where the ionization is near 7.4 and could be represented by a mixture of states, the state that is likely to be most populated is chosen.

See also

- *Setting a Neutral Ionization State* code example

3.3.20 OETautomersLargestZoneSize

```
unsigned int OETautomersLargestZoneSize(const OEChem::OEMolBase& mol,
                                        const OETautomerOptions& tautomerOptions)
unsigned int OETautomersLargestZoneSize(const OEChem::OEMolBase& mol,
                                        unsigned maxZone = 0)
```

This function returns the largest number of atoms in a continuous tautomerization zone for the molecule and *OETautomerOptions* instance passed in as arguments. The later function provides a convenient function that relies on the default tautomer options other than potentially the maxZone size. The return value of this function plays a significant role in determining the upper bounds of the runtime for tautomer calculations on the molecule.

3.4 OEMolAM1 Classes

3.4.1 OEAM1

```
class OEAM1 : public OEMolPotential::OEMolFunc1
```

Note

This is a low level api class that allows access to advanced functionality from semi-empirical method calculations. It is recommended that you use the high level api method *OEAssignCharges* with *OEAM1Charges* options to assign AM1 charges on a molecule.

The *OEAM1* class calculates Mulliken-type partial charges and other relevant quantities in a molecule using AM1 type semi-empirical quantum mechanical methods.

The input must be a 3D molecule, and the AM1 parameters must be available for each atom type in the molecule.

The following methods are publicly inherited from OEFunc0:

- operator()
- GetFComponents
- NumVar

The following methods are publicly inherited from OEFunc1:

- operator()

The following methods are publicly inherited from OEMolFunc:

- GetInteractions
- Setup

The *OEAM1* class defines the following public methods:

- *CalcAM1*
- *GetOptions*
- *GetResults*

Constructors

```
OEAM1(const OEAM1Options& argOptions = OEAM1Options())
OEAM1(const OEAM1&)
```

Default and copy constructors.

Constructs an *OEAM1* instance using the specified set of parameters.

CalcAM1

```
bool CalcAM1(OEAM1Results&, const OEMolBase&)
```

Performs AM1 calculation on the specified molecule and fills up the specified *OEAM1Results* with calculated results. Returns `false` if calculation was not successful.

GetOptions

```
const OEAM1Options& GetOptions() const
```

Returns a reference to the *OEAM1Options* instance as currently set for this *OEAM1*.

GetResults

```
bool GetResults(OEAM1Results&) const
```

Fills up the specified *OEAM1Results* with results from the last calculation. Returns `false` if a valid set of results does not exist.

3.4.2 OEAM1Options

```
class OEAM1Options : public OESystem::OEOptions
```

This class provides an interface to setup options required for *OEAM1* calculations.

The *OEAM1Options* class defines the following public methods:

- *GetMaxScfIter*
- *GetNumericGradDelta*
- *GetSCFTolerance*
- *GetSemiMethod*
- *SetMaxScfIter*
- *SetNumericGradDelta*
- *SetSCFTolerance*
- *SetSemiMethod*

Constructors

```
OEAM1Options()
OEAM1Options(const OEAM1Options&)
```

Default and copy constructors.

GetMaxScfIter

```
unsigned int GetMaxScfIter() const
```

Gets the maximum number of self-consistent field iterations to be used.

GetNumericGradDelta

```
double GetNumericGradDelta() const
```

Gets the current value of the numerical gradients delta to be used for gradients calculation.

GetSCFTolerance

```
double GetSCFTolerance() const
```

Gets the current value of the self-consistent field calculation tolerance.

GetSemiMethod

```
unsigned int GetSemiMethod() const
```

Gets the current value of the semi-empirical method to be used.

SetMaxScfIter

```
bool SetMaxScfIter(const unsigned int)
```

Sets the maximum number of self-consistent field iterations to be used.

SetNumericGradDelta

```
bool SetNumericGradDelta(const double)
```

Sets the value of the numerical gradients delta to be used for gradients calculation.

SetSCFTolerance

```
bool SetSCFTolerance(const double)
```

Sets the value of the self-consistent field calculation tolerance.

SetSemiMethod

```
bool SetSemiMethod(const unsigned int)
```

Sets the semi-empirical method to be used for the calculations. The default is *OEMethodType.AM1*. Alternatives are defined in the *OEMethodType* namespace.

3.4.3 OEAM1Results

```
class OEAM1Results
```

This class represents *OEAM1* calculation results.

The *OEAM1Results* class defines the following public methods:

- *GetAtomicBondOrder*
- *GetBondOrder*
- *GetBondOrders*

- *GetCharges*
- *GetEnergy*
- *GetNumSCFCycles*
- *IsConverged*

Constructors

```
OEAM1Results()
OEAM1Results(const OEAM1Results&)
```

Default and copy constructors.

GetAtomicBondOrder

```
double GetAtomicBondOrder(const unsigned int index) const
```

Returns the atomic bond order of the atom with specified index.

GetBondOrder

```
double GetBondOrder(const unsigned int index1,
                    const unsigned int index2) const
```

Returns the bond order between the two atoms with specified indices.

See also

- *Wiberg bond orders* chapter

GetBondOrders

```
std::vector<double> GetBondOrders() const
```

Returns the bond orders on all bondss. Bond orders are stored in the vector according to the bond indices.

See also

- *Wiberg bond orders* chapter

GetCharges

```
std::vector<double> GetCharges() const
```

Returns the AM1 charges on all atoms. Charges are stored in the vector according to the atom indices.

GetEnergy

```
double GetEnergy() const
```

Returns the AM1 calculated energy of the molecule.

GetNumSCFCycles

```
unsigned int GetNumSCFCycles() const
```

Returns the number of self-consistent field cycles used during calculation.

IsConverged

```
bool IsConverged() const
```

Returns if the *OEAM1* self-consistent field calculation converged.

3.4.4 OEOptimizedAM1

```
class OEOptimizedAM1
```

> **Note**
>
> This is a low level api class that allows access to advanced functionality from semi-empirical method calculations. It is recommended that you use the high level api method *OEAssignCharges* with *OEAM1Charges* options to assign AM1 charges on a molecule.

The *OEOptimizedAM1* class optimizes *OEAM1* followed by calculation of Mulliken-type partial charges and other relevant quantities.

The input must be a 3D molecule, and the AM1 parameters must be available for each atom type in the molecule.

The *OEOptimizedAM1* class defines the following public methods:

- *CalcAM1*

Constructors

```
OEOptimizedAM1(unsigned int wvnFnType = OEMethodType::AM1)
OEOptimizedAM1(const OEOptimizedAM1&)
```

Default and copy constructors.

The wave functype could be any value defined in *OEMethodType* namespace.

CalcAM1

```
bool CalcAM1(OEAM1Results& results, const OEChem::OEMolBase& mol)
bool CalcAM1(OEAM1Results& results, const OEChem::OEMCMolBase& mol)
```

Optimizes and performs AM1 calculation on the specified molecule and fills up the specified *OEAM1Results* with calculated results. Returns `false` if calculation was not successful.

3.5 OEMolAM1 Constants

3.5.1 OEMethodType

This namespace contains constants which define the type of semi-empirical methods that can be used for *OEAM1* calculation.

AM1

AM1 semi-empirical method.

PM3

PM3 semi-empirical method.

3.6 OEMolAM1 Constants

3.6.1 OEBCCType

This namespace contains constants which define the type of bond charge correction models that can be used for *OEBCCPartialCharges* calculation.

AM1

AM1 semi-empirical method.

PM3

PM3 semi-empirical method.

3.7 OEAM1BCC Functions

3.7.1 OEBCCPartialCharges

```
bool OEBCCPartialCharges(OEChem::OEMolBase& mol,
                         unsigned int BCCModel = OEBCCType::AM1,
                         bool permissive = false, bool verbose = false)
```

This function calculates the bond correction partial charges on the specified molecule. Calculated charges are set as the partial charges of the molecule.

mol
: Molecule to calculate BCC partial charges.

BCCModel
: Bond charge correction semi-empirical model defined in *OEBCCType* namespace

permissive
: TODO - Need help.

verbose
: Flag if verbose information should be provided

3.7.2 OESymmetrizePartialCharges

```
bool OESymmetrizePartialCharges(OEChem::OEMolBase& mol)
```

This function makes the partial charges on the molecule symmetric based on molecule topology.

CHAPTER

FOUR

PRELIMINARY API

4.1 Preliminary OEProton Class

4.1.1 OEChargeParameter

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEChargeParameter : public OESystem::OEMultiParameter<OEProton::OEChargeEngineBase>
```

The *OEChargeParameter* represents parameter that has a value of type *OEChargeEngineBase*.

Following methods are publicly inherited from OEParameter:

- `AddAlias` and `GetAliases`
- `AddDetail` and `GetDetail`
- `AddIllegalRange` and `GetIllegalRanges`
- `AddIllegalValue` and `GetIllegalValues`
- `AddLegalRange` and `GetLegalRanges`
- `AddStringDefault` , `GetStringDefault` and `GetStringDefaults`
- `AddStringValue` , `GetStringValue` and `GetStringValues`
- `ClearDefaults`
- `ClearValues`
- `CreateCopy`
- `GetBrief` and `SetBrief`
- `GetHasDefault`
- `GetHasValue`
- `GetIsList` and `SetIsList`
- `GetKeyless` and `SetKeyless`
- `GetName` and `SetName`
- `GetOrderPriority` and `SetOrderPriority`

- `GetVisibility` and `SetVisibility`
- `IsLegalString`
- `IsSet` and `IsSetToString`

Following methods are publicly inherited from OEMultiParameter:

- `AddLegalEntry`
- `GetDefault` and `SetDefault`
- `GetSetting`
- `GetValue` and `SetValue`

Constructors

```
OEChargeParameter()
OEChargeParameter(const std::string& name)
OEChargeParameter(const OEChargeParameter&)
```

Default and copy constructors.

Constructs an *OEChargeParameter* instance using the specified set of parameters. The second argument in the second constructor represents if a custom forcefield can be used.

4.1.2 OEMultistatepKaModel

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEMultistatepKaModel
```

This class provides functionality to assess the atomic pKa of a given molecule and enumerate ionization states at neutral pH. The options required for this class can be set using the *OEMultistatepKaModelOptions* class.

See also

- *OEMultistatepKaModelOptions* class

The *OEMultistatepKaModel* class defines the following public methods:

- *Init*
- *CalculateNumOfMicrostates*
- *SetAllAtomspKaData*
- *GetModelMolecule*
- *GetAtompKaRange*
- *GenerateMicrostates*
- *GetMicrostates*
- *HasAdjTypeAtNeutralpH*

- *HaspKaRange*

Constructors

Constructors.

```
OEMultistatepKaModel()
OEMultistatepKaModel(const OEMultistatepKaModelOptions& opts)
OEMultistatepKaModel(OEChem::OEMolBase& mol,
                     const OEMultistatepKaModelOptions& opts =␣
↪OEMultistatepKaModelOptions())
```

Copy constructor.

```
OEMultistatepKaModel(const OEMultistatepKaModel& rhs)
```

Copy assignment constructor.

operator= :language: c++

```
OEMultistatepKaModel& operator=(const OEMultistatepKaModel &rhs)
Assignment operator.
```

Init

```
void Init(OEChem::OEMolBase& mol)
void Init(OEChem::OEMolBase& mol, OEMultistatepKaModelOptions& opts)
```

If a user has initialized the OEMultistatepKaModel instance with default constructor (without molecule and options object), they can add a molecule and *OEMultistatepKaModelOptions* instance later by the Init method.

CalculateNumOfMicrostates

```
int CalculateNumOfMicrostates()
```

This method calculates the number of microstates possible for given molecule. It uses the information (generic pKa data) assessed and set by the method SetAllAtomspKaData. It returns -1 if either OEMultistatepKaModel failed to assess all atomic pKa on the molecule (probably due to unknown atoms present), or it halted assessing pKa data because the projected number of microstates exceeded the provided limit of microstates to be generated.

GetModelMolecule

```
const OEChem::OEMolBase& GetModelMolecule()
```

This method returns the copy of the internal molecule object from the *OEMultistatepKaModel* class on which all atomic pKa data are assessed and set as generic data.

GetAtompKaRange

```
unsigned int GetAtompKaRange(const OEChem::OEAtomBase* atom)
```

This method allows a user to assess and get the pKa range (*OEpKaRange.Acidic*, *OEpKaRange.Neutral*, *OEpKaRange.Basic* or *OEpKaRange.Unidentified*) for an individual atom.

GetAtomAdjTypeAtNeutralpH

```
unsigned int GetAtomAdjTypeAtNeutralpH(const OEChem::OEAtomBase* atom)
```

This method allows a user to assess and get the adjustment type to be done at neutral pH (*OEAdjTypeAtNeutralpH.NoChange*, *OEAdjTypeAtNeutralpH.Protonation*, *OEAdjTypeAtNeutralpH.Deprotonation*, *OEAdjTypeAtNeutralpH.NoChangeAndProtonation*, *OEAdjTypeAtNeutralpH.NoChangeAndDeprotonation*) for an individual atom.

GenerateMicrostates

```
bool GenerateMicrostates()
```

This method generates all possible microstates (up to the limit specified by the options class). These generated microstates can be accessed by the method *GetMicrostates*.

GetMicrostates

```
OESystem::OEIterBase<OEChem::OEMolBase>* GetMicrostates()
```

Microstates generated by the method *GenerateMicrostates* can be accessed by this method. It returns an iterator over the generated microstates molecule objects.

HasAdjTypeAtNeutralpH

```
HasAdjTypeAtNeutralpH(unsigned AdjTypeAtNeutralpHID)
```

This is a predicate functor, which allows a user to filter atoms with the desired *OEAdjTypeAtNeutralpH* generic data attached.

HaspKaRange

```
HaspKaRange(unsigned pkarangeID)
```

This is a predicate functor, which allows a user to filter atoms with the desired *OEpKaRange* generic data attached.

SetAllAtomspKaData

```
bool SetAllAtomspKaData()
```

This method assesses the atomic pKa for all heavy/hetero atoms and sets generic pKa data for these atoms. If an OEMultistatepKaModelOptions class object is specified with the parameter processcarbons = true, it assesses all heavy atoms. If an OEMultistatepKaModelOptions class object is specified with the parameter processcarbons = false, then only hetero atoms are assessed.

4.1.3 OEMultistatepKaModelOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEMultistatepKaModelOptions
```

This class provides an interface to set up options required for *OEMultistatepKaModel*.

The *OEMultistatepKaModelOptions* class defines the following public methods:

- *GetpH* and *SetpH*
- *GetProcessCarbons* and *SetProcessCarbons*
- *GetMaxNumMicrostates* and *SetMaxNumMicrostates*

Constructors

```
OEMultistatepKaModelOptions()
OEMultistatepKaModelOptions(unsigned int maxnummicrostates,
                            bool processcarbons)
```

Copy constructor.

```
OEMultistatepKaModelOptions(const OEMultistatepKaModelOptions&)
```

Copy assignment constructor.

```
OEMultistatepKaModelOptions& operator=(const OEMultistatepKaModelOptions& rhs)
```

GetpH

```
unsigned int GetpH()
```

Gets the value of the pH parameters at which a user wants to assess ionization states of the molecule. Only a neutral pH can be set. This option is defined in anticipation of a wider pKa model at different pH environments.

SetpH

```
bool SetpH(unsigned ph)
```

Sets the pH to be used to assess the ionization states of the molecule. Only a neutral pH can be set. This option is defined in anticipation of a wider pKa model at different pH environments.

GetProcessCarbons

```
bool GetProcessCarbons()
```

Returns the parameter setting requesting the pKa assessment of carbon atoms. Default is true.

SetProcessCarbons

```
bool SetProcessCarbons(bool pc)
```

Sets whether a user wants to assess the pKa of carbon atoms, true or false.

GetMaxNumMicrostates

```
unsigned int GetMaxNumMicrostates()
```

Gets the value of maximum number of microstates to generate; the parameter is set by default or by the method *SetMaxNumMicrostates*.

SetMaxNumMicrostates

```
bool SetMaxNumMicrostates(unsigned int maxnummicrostates)
```

Sets the maximum number of microstates to generate. If the projected number of microstates is more than the maximum limit set by this function, the model will not generate any microstates.

4.2 Preliminary OEProton Constants

4.2.1 OEAdjTypeAtNeutralpH

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

This namespace contains constants used by the class *OEMultistatepKaModel* to define what adjustment is to apply to the atom according to the multistate model.

See also

- *OEMultistatepKaModel* class
- *OEpKaRange* constants namespace
- *OEMultistatepKaModelpH* constants namespace
- *OEGetAtomAdjTypeAtNeutralpHName* function
- *OEGetAtomAdjTypeAtNeutralpHType* function

Deprotonation

The atom with this tag will be deprotonated to generate a favored ionization state.

NoChange

The atom with this tag will not be modified in generated ionization state.

NoChangeAndDeprotonation

Two different ionization states will be generated for the atom with this tag. In one of them atom will not be changed and in another state the atom will be deprotonated.

NoChangeAndProtonation

Two different ionization states will be generated for the atom with this tag. In one of them atom will not be changed and in another state the atom will be protonated.

Protonation

The atom with this tag will be protonated to generate a favored ionization state.

Unknown

This constant represents an undefined or illegal context state.

4.2.2 OEMultistatepKaModelpH

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

This namespace contains constants used by the class *OEMultistatepKaModel* and *OEMultistatepKaModelOptions* to define the pH at which the multistate model assesses the pKa.

See also

- *OEMultistatepKaModelOptions* class
- *OEMultistatepKaModel* class
- *OEAdjTypeAtNeutralpH* constants namespace
- *OEMultistatepKaModelpH* constants namespace
- *OEGetMultistatepKaModelpHName* function
- *OEGetMultistatepKaModelpHType* function

Neutral

MultistatepKaModel assesses the pKa at Neutral pH (physiological pH i.e. 7.4).

Unknown

This constant represents an undefined or illegal context state.

4.2.3 OEpKaRange

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

This namespace contains constants used by the class *OEMultistatepKaModel* to define what is the assessed atomic pKa range of the atom according to the multistate model.

See also

- *OEMultistatepKaModel* class
- *OEAdjTypeAtNeutralpH* constants namespace
- *OEMultistatepKaModelpH* constants namespace
- *OEGetAtompKaRangeName* function
- *OEGetAtompKaRangeType* function

Acidic

The atom has Acidic pka range (<6.4).

Basic

The atom has Basic pka range (>8.4).

Neutral

The atom has Neutral pka range (between 6.4 and 8.4).

Unidentified

The atom's pKa range is unidentified by the multistate pka model.

Unknown

This constant represents an undefined or illegal context state.

4.3 Preliminary OEProton Functions

4.3.1 OEGetAtomAdjTypeAtNeutralpHName

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
std::string OEGetAtomAdjTypeAtNeutralpHName(const unsigned int adjTypeID)
```

This function returns a corresponding name for the given *adjTypeID* value from the *OEAdjTypeAtNeutralpH* namespace.

See also

- *OEGetAtomAdjTypeAtNeutralpHType* function

4.3.2 OEGetAtomAdjTypeAtNeutralpHType

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
unsigned int OEGetAtomAdjTypeAtNeutralpHType(const std::string& adjTypeName)
```

This function returns the constant from the *OEAdjTypeAtNeutralpH* namespace for the provided *adjTypeName*.

See also

- *OEGetAtomAdjTypeAtNeutralpHName* function

4.3.3 OEGetAtompKaRangeName

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
std::string OEGetAtompKaRangeName(const unsigned int pKaRangeID)
```

This function returns a corresponding name for the given *pKaRangeID* value from the *OEpKaRange* namespace.

See also

- *OEGetAtompKaRangeType* function

4.3.4 OEGetAtompKaRangeType

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
unsigned int OEGetAtompKaRangeType(const std::string& pKaRangeName)
```

This function returns the constant from the *OEpKaRange* namespace for the provided *pKaRangeName*.

See also

- *OEGetAtompKaRangeName* function

4.3.5 OEGetMultistatepKaModelpHName

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
std::string OEGetMultistatepKaModelpHName(const unsigned int pHType)
```

This function returns a corresponding name for the given *pHType* value from the *OEMultistatepKaModelpH* namespace.

See also

- *OEGetMultistatepKaModelpHType* function

4.3.6 OEGetMultistatepKaModelpHType

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
unsigned int OEGetMultistatepKaModelpHType(const std::string& pHName)
```

This function returns the constant from the *OEMultistatepKaModelpH* namespace for the provided *pHName*.

See also

- *OEGetMultistatepKaModelpHName* function

CHAPTER

FIVE

RELEASE HISTORY

5.1 Quacpac TK 2.3.0

Minor internal improvements have been made.

5.2 Quacpac TK 2.2.7

5.2.1 Minor Bug Fixes

- An issue that retained MDL-enhanced stereogroup information on stereocenters that are destroyed by protonation or bond order changes has been repaired.

5.3 Quacpac TK 2.2.6

Minor internal improvements have been made.

5.4 Quacpac TK 2.2.5

5.4.1 Minor bug fixes

- Some issues with primary amines processing in *OEMultistatepKaModel* have been fixed.

5.5 Quacpac TK 2.2.4

Minor internal improvements have been made.

5.6 Quacpac TK 2.2.3

Minor internal improvements have been made.

5.7 Quacpac TK 2.2.2

Minor internal improvements have been made.

5.8 Quacpac TK 2.2.1

Minor internal improvements have been made.

5.9 Quacpac TK 2.2.0

5.9.1 New features

- New preliminary API classes, *OEMultistatepKaModel* and *OEMultistatepKaModelOptions*, have been added to assess atomic pKa ranges for atoms of a given molecule, and to enumerate all possible ionization states of input molecules at neutral/physiological pH (7.4) based on a multistate heuristic pKa model.

5.10 Quacpac TK 2.1.4

5.10.1 New features

- [QUACPAC-599] New preliminary classes, *OEMultistatepKaModel* and *OEMultistatepKaModelOptions*, have been added to asses atomic pKa ranges for atoms of given molecule and enumerate all possible ionization states of input molecule at neutral/physiological pH (7.4) based on a heuristic pKa model.

5.10.2 Major bug fixes

5.10.3 Minor bug fixes

5.10.4 Python-specific changes

5.10.5 Java-specific changes

5.10.6 C#-specific changes

5.10.7 Documentation changes

5.11 Quacpac TK 2.1.3

Fall 2021

5.11.1 New features

- *OEChargeParameter* now accepts case-insensitive string input values.

5.12 Quacpac TK 2.1.2

July 2021

Minor internal improvements have been made.

5.13 Quacpac TK 2.1.1.2

March 2021

- *OEOptimizedAM1* no longer requires a special `am1bcc` license.
- The function *OEBCCPartialCharges* no longer requires a special `am1bcc` license.

5.14 Quacpac TK 2.1.1

Fall 2020

5.14.1 New features

- A new preliminary class, *OEChargeParameter*, has been added as part of the extended set of OEParameter classes. The new parameter class works with predefined charge engines using *OEChargeEngineBase* object.

5.15 Quacpac TK 2.1.0

5.15.1 New features

- The `OEDesignUnitComponents.CounterIons` molecule components are now charged with the metal charge engine for design unit charges.
- A new class, *OEOptimizedAM1*, has been added that obtains optimized *OEAM1* Mulliken-type partial charges.
- Two new classes, *OEELF* and *OEELFOptions*, have been added that allow selecting conformers from a given ensemble using the electrostatically least-interacting functional group (ELF) technique.
- A new method, *OEBCCPartialCharges*, has been added that calculates bond correction partial charges.
- A new method, *OESymmetrizePartialCharges*, has been added that makes partial charges symmetric based on molecule topology.
- A new method, *OEAM1Results.GetBondOrders*, has been added to *OEAM1Results* that provides access to all the bond orders in a list.

5.15.2 Minor bug fixes

- The following methods now return `bool` instead of a `void`:
  - *OEAM1Options.SetMaxScfIter*
  - *OEAM1Options.SetNumericGradDelta*
  - *OEAM1Options.SetSCFTolerance*
  - *OEAM1Options.SetSemiMethod*
- *OEAssignCharges* with *OEELFCharges* now outputs the correct set of conformers selected using the ELF technique.
- The number of diverse conformers needed to select and use for charge calculation is now automatically adjusted when the desired *OEELFOptions.SetElfLimit* is higher than the number of initial conformers selected based on *OEELFOptions.SetPercent* and the input number of conformers in the molecule.
- *OEEnumerateTautomers* no longer throws a fatal error when when no tautomers are found.

5.16 Quacpac TK 2.0.2

5.16.1 New features (Preliminary)

- A new preliminary class, *OEDesignUnitCharges*, has been added that charges an OEDesignUnit.

5.16.2 New features

- A new optional argument, `warts`, has been added to the *OEFormalChargeOptions* constructor. Two new methods, *OEFormalChargeOptions.GetWarts* and *OEFormalChargeOptions.SetWarts*, have also been added that control whether to add `wart` to the title of each charge state.

5.17 Quacpac TK 2.0.1

5.17.1 Minor bug fixes

- The definition of *OEHybridizationLevel.Default* has been changed from *OEHybridizationLevel.Original* to *OEHybridizationLevel.EnolEnamine* for consistency with the behavior of the default *OETautomerOptions* class constructor.
- *OEAssignCharges* no longer requires a `case` license when used with *OEELFCharges*.
- *OEEnumerateTautomers* has been fixed to output multiple tautomers when *OETautomerOptions.SetRankTautomers* is `false`.
- *OEAssignCharges* no longer crashes for molecules where the distance between atoms is less than 0.5 Angstrom.

5.18 Quacpac TK 2.0.0

5.18.1 New features

- A new *OEGetReasonableTautomers* function has been added that generates an ensemble of biologically relevant tautomers.
- A new *OEGetUniqueProtomer* function has been added that generates a canonical representation of a molecule.
- A new *OEGetReasonableProtomers* function has been added that generates an ensemble of reasonable protomers.
- The handling of keto-enol tautomerization by default has been improved. The improvement extends to include imine-enamine tautomerization and related analogs. The keto and imine forms are favored except in the case of 1,3 diketones, where the internal hydrogen bond can be formed.
- Controlling the interaction between tautomerization and tetrahedral stereochemistry has been improved. The method *OETautomerOptions.SetSaveStereo* can still be set to `true` in order to prevent any stereo atom from ever becoming an sp2 center. However, the behavior when the vale is set to `false` can now be controlled by passing a constant from the new *OERacemicType* namespace to the method *OETautomerOptions.SetRacemicType*. This functionality allows users to control which stereochemistry will be cleared on each generated tautomer.
- Reasonable tautomers for many simple and complex pyridone analogs, pyrrole analogs, and pyridine analogs have been improved.
- A new *OEHypervalentNormalization* function has been added to prepare molecules for tautomer enumeration (*OEEnumerateTautomers*).
- The user control of the algorithms memory and CPU usage by separately exposing the number of tautomers generated and the number of tautomers returned by the methods *OETautomerOptions.SetMaxTautomersGenerated* and *OETautomerOptions.SetMaxTautomersToReturn*, respectively, has been improved.
- The default parameters of the *OETautomerOptions* class have been updated to reflect the underlying improved tautomer generation algorithm.

5.18.2 Major bug fixes

- Several issues that caused double bonds and hydrogens to be allowed to move too far through a series of sp3 centers have been fixed.
- The default behavior of peptide tautomers and peptide stereochemistry has been improved.
- Keto-enol tautomerization by default has been added to improve the canonical grouping of unique molecules by their representative tautomers.

5.18.3 Minor bug fixes

- Aromatic bond count has been added to scoring to improve the handling of fused pyrrole and pyrazine chemistries when estimating low-energy tautomers.

5.18.4 Documentation changes

- The *tautomers* theory chapter has been rewritten to reflect common usages of the tautomer library.

5.19 Quacpac TK 1.9.3

5.19.1 New features

- A new class, *OEAM1*, has been added to provide AM1-like semi-empirical method functionality.
- A new class, *OEAM1Options*, has been added to set up *OEAM1* calculation options.
- A new class, *OEAM1Results*, has been added to obtain *OEAM1* calculation results.
- The class *OETautomerOptions* now exposes settings to allow control of Kekule results, clearing of coordinates, and the degree of carbon hybridization.

5.19.2 Documentation changes

- An example that displays obtaining Wiberg bond orders from an AM1 calculation has been added.

5.20 Quacpac TK 1.9.2

5.20.1 Minor bug fixes

- `OEAssignPartialCharges`, deprecated since the 2017.Feb release, now throws a deprecated warning.
- `OEEnumerateTautomers` now obeys the maximum tautomers option set in the *OETautomerOptions* class.

5.20.2 Documentation changes

- The functions `OEEnumerateTautomers` and `OEGetReasonableProtomer` remove molecule coordinates during their processing since changing the tautomer state may invalidate the 3D structure. This behavior change was introduced in the 2017.Feb release.

5.21 Quacpac TK 1.9.1

5.21.1 Documentation changes

- The behavior of the `OEChargeEngineBase.SetExpectValidMol` method is now documented correctly.
- Code examples in the *Quacpac TK Examples* chapter have been revised.

5.22 Quacpac TK 1.9.0

5.22.1 New features

- A new charging function, *OEAssignCharges*, has been developed to replace the more limited legacy function *OEAssignPartialCharges*. This new function uses *charge engines*, an open-ended options class, to define the charging method. Charge engines can be configured as required and new charge engines can be developed independently. Charge engines have been written for every supported charging method, as well as for the new method *OEAM1BCCELF10Charges*.

5.22.2 Minor bug fixes

- Warning messages from AM1BCC charging functions have been made more informative.

5.22.3 Documentation changes

- The documentation has been updated to describe the new *charge engine* approach to charging and to show examples of its use.

5.23 Quacpac TK 1.8.6

- Minor internal improvements have been made.

5.24 Quacpac TK 1.8.5

- Minor internal improvements have been made.

5.25 Quacpac TK 1.8.4

5.25.1 New features

- The number of *methods* available for use with *OEAssignPartialCharges* is now defined as *OECharges.Max*.
- A timer has been added to tautomer enumeration. *OETautomerOptions.SetMaxSearchTime* and *OETautomerOptions.GetMaxSearchTime* can be used to set and get a time limit for searching tautomers, respectively.

5.25.2 Major bug fixes

- Calling *OEAssignPartialCharges* on a molecule with no formal charges with the method *OECharges.Initial* no longer returns `false`.

5.25.3 Deprecated functionality

- *OECharges.OPLS* charging model is no longer supported with *OEAssignPartialCharges* function.

5.26 Quacpac TK 1.8.3

5.26.1 New features

- *OEGetReasonableProtomer* and *OEEnumerateTautomers* with *OETautomerOptions* with the *OETautomerOptions.SetRankTautomers* set to `true` have improved handling of diols and nitro groups in recognition of the most reasonable tautomers.

- *OEGetReasonableProtomer* and *OEEnumerateTautomers* with *OETautomerOptions* with the *OETautomerOptions.SetRankTautomers* set to `true` now employ a second-stage approach in cases where the first set of generated tautomers produces no desirable tautomeric states.

5.26.2 Major bug fixes

- *OEGetReasonableProtomer* will no longer have the side-effect of resetting the atomic coordinates to the origin.

5.27 Quacpac TK 1.8.2

5.27.1 Minor bug fixes

- *OESetNeutralpHModel* and *OERemoveFormalCharge* will now produce a planar geometry when deprotonating an N-protonated amide. Previously, this was incorrectly producing a pyrimidal geometry.
- *OECharges.AmberFF94* will no longer identify a CYS residue as anionic when it is bonded by a sulfur to something other than another CYS residue.
- *OEGetReasonableProtomer* will now preserve molecule title, SD data, and atom coordinates.

5.28 Quacpac TK 1.8.1

5.28.1 New features

- TIP3P water charges are now assigned when using Amber charge sets on molecules containing waters. The application of *OEAssignPartialCharges* using *OECharges.AmberFF94* or any of the other Amber charge sets to waters with explicit hydrogens will produce oxygen charges of -0.834 and hydrogen charges of +0.417.

5.28.2 Minor bug fixes

- The default behavior of *OETautomerOptions* has been changed from `true` to `false` when applying warts to titles.

5.28.3 Documentation fixes

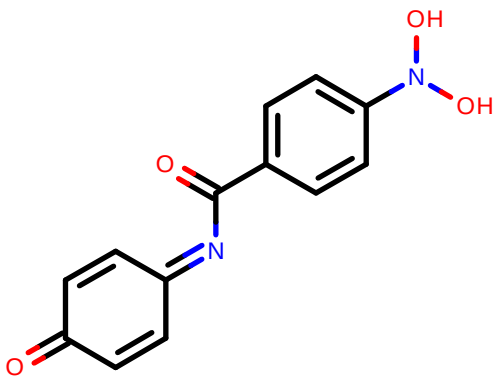
- *OEEnumerateTautomers* now includes a snippet of code in the documentation to make using the function easier.

5.29 Quacpac TK 1.8.0

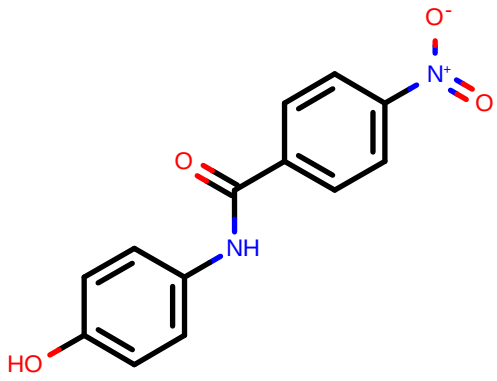
5.29.1 New features

- Passing `true` to *OETautomerOptions.SetRankTautomers* was dramatically improved to provide a low-energy, medicinally-relevant "reasonable" tautomeric form that is suitable for depiction for chemists. Significant improvements were made to the "reasonable" tautomer algorithm that effect the aliphatic and non-aromatic resonance portions of tautomers.
  - Made conversion of carboxylates to diols and nitros to di-hydroxy amines very unfavorable.

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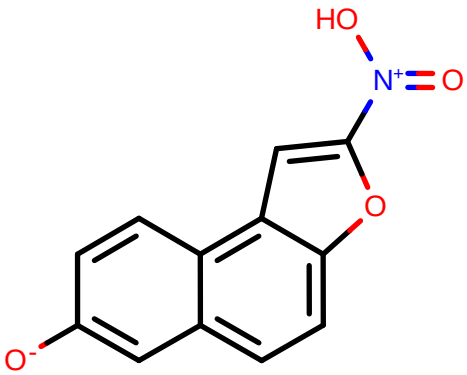


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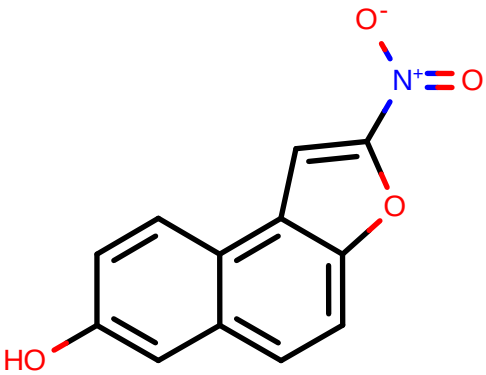


– Made generation of unnecessary, non-dative, formal charges unfavorable.

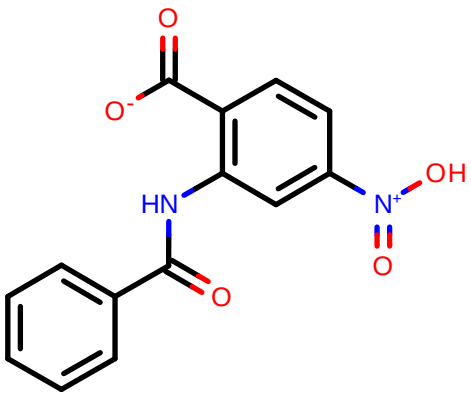
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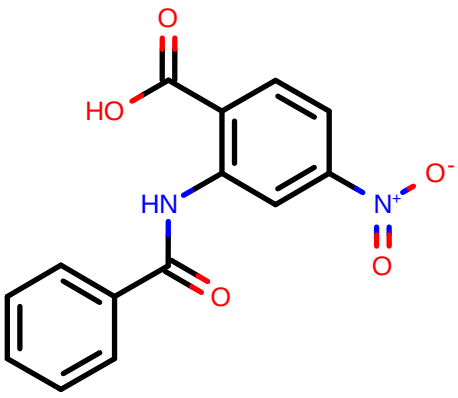
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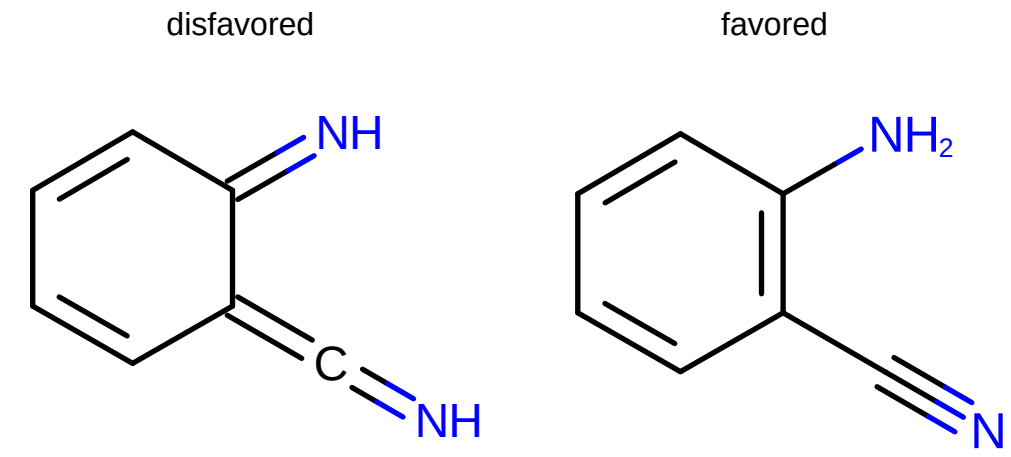
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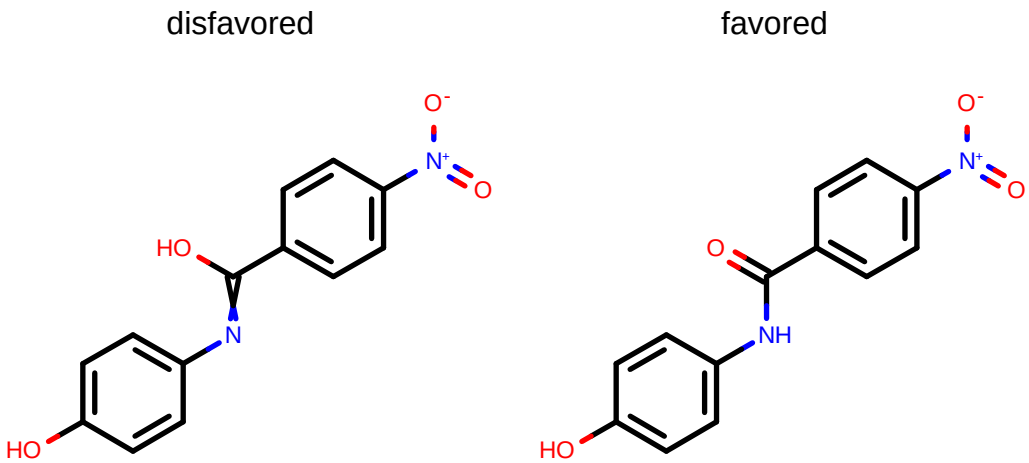
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- Improved accounting for exocyclic bonds adjacent to aromatic rings.



- Set priority for aliphatic double bond position that could be arbitrary in prior versions.



- `OEGetReasonableProtomer` added to provide a convenient "best practices" function to generate a most chemically reasonable tautomerization and ionization state for a molecule. The function yields a low-energy medicinally relevant protomer suitable for depiction for chemists.
- `OETautomersLargestZoneSize` now overloaded with a more convenient function that does not require constructing a *OETautomerOptions* object to explore the maximum zone size considered for tautomerization of a molecule.

5.29.2 Minor bug fixes

- `OESetNeutralpHModel` consistency has been improved by forcing the molecule to use the OpenEye aromaticity model before applying pH rules (pattern matching) to molecules from heterogeneous source or file formats.
- `OECharges.Default` constant is now the exact same value as `OECharges.MMFF94`. Previously, it was a different numerical value, making comparison un-necessarily difficult. Note, the default charging model is still the same.

5.29.3 Known bugs

- *OEGetReasonableProtomer* title warting is not working correctly. All titles will be output "_1". This will be fixed for the next release, 2015.Feb.

5.29.4 Documentation fixes

- The *tautomers* theory chapter has been made more specific to the toolkit.

5.30 Quacpac TK 1.7.2

5.30.1 New features

5.30.2 Minor bug fixes

- Calling *OEGetChargeTypeName* with the constant *OECharges.Default*, now returns the name of the default charge method, *OECharges.MMFF94*.

5.30.3 Documentation fixes

5.31 Quacpac TK 1.7.1

5.31.1 New features

- *OETyperMolFunction* and *OEFormalChargeOptions* is now the preferred way to set options for the *OEEnumerateFormalCharges* function. The new form of *OEEnumerateFormalCharges* returns an iterator of molecules.

5.31.2 Minor bug fixes

- Removed unbounded stack allocations.

5.31.3 Documentation fixes

- **Quacpac TK** examples have been renamed to more accurately reflect their function.
- Documented the Amber force field constants *OECharges.AmberFF94*, *OECharges.AmberFF99*, *OECharges.AmberFF99SB*, and *OECharges.AmberFF99bsc0*.
- Documented the AM1BCC constant *OECharges.AM1BCCSymSPt* and fixed a mistake in the description of the constant *OECharges.AM1BCCSPt*.

5.32 Quacpac TK 1.7.0

5.32.1 New features

- *OETautomerMolFunction* has been deprecated and *OETautomerOptions* is now the preferred way to set options for the *OEEnumerateTautomers* function. *OEEnumerateTautomers* will now return an iterator of molecules optionally ordered by favorableness of the tautomer. Therefore, the first tautomer in the iterator is the same as what was previously returned by *OETautomerMolFunction.GetMolecule*.
- A hard limit on the total number of atoms participating in tautomerization is now adjustable in *OETautomerOptions*. Additionally, an adjustable parameter `maxZoneSize` has been added for setting the maximum number of atoms that are allowed in a continuous tautomerization zone. Any molecule that exceeds either of these limits will cause *OEEnumerateTautomers* to return the input tautomer.

- *OETautomersLargestZoneSize* function added to return the largest number of atoms in a continuous tautomerization zone for a particular molecule.

5.33 Quacpac TK 1.6.4

5.33.1 New features

- The new function *OERemoveFormalCharge* has been added. This function sets the formal charges on a molecule to zero while maintaining a standard valence state.
- The new function *OEGetChargeTypeName* has been added. This function returns the corresponding *OECharges* name for the *unsigned int* passed in.

5.33.2 Minor bug fixes

- The wart symbol has been changed from @ to _ in order to help with parsing SMILES formatting.

5.34 Quacpac TK 1.6.2

5.34.1 Major bug fixes

- *OEEnumerateTautomers* was removing stereochemistry from all atoms that did not have a valence of 4. This has been fixed so that other types of atoms with legitimate stereochemistry, such as nitrogen and hypervalent atoms, no longer lose their stereochemistry information.
- *OEEnumerateFormalCharges* has been fixed to properly handle 3D input. Previously, 3D input would cause an incorrect number of hydrogen atoms and an incorrect valence state on adjusted heavy atoms.

5.34.2 Minor bug fixes

- *OESetNeutralpHModel* will no longer ionize difluoro, dichloro, and N-methyl acetamide.
- *OESetNeutralpHModel* will now use the molecule title when available instead of a smiles string for warning messages.
- *OESetNeutralpHModel* warning messages for bad valence have been clarified.
- *OEAssignPartialCharges* will no longer exit when using *OECharges.AM1BCCNoSym* with multiconformer molecules.

5.35 Quacpac TK 1.6.1

5.35.1 New features

- *OEEnumerateTautomers* will now allow interconversion of [NH2+]= and [NH3+]-.
- *OETautomerMolFunction* now has a warts option. Enabling this options will number the output molecules with an @ symbol.

5.35.2 Major bug fixes

5.35.3 Minor bug fixes

- *OEEnumerateTautomers* will now properly set stereochemistry on planar carbon to *OEAtomStereo::Undefined*. Previously, planar carbon could inherit stereochemistry from an input molecule with stereochemistry set on a tetrahedral carbon.

- A few bugs have been fixed in *OESetNeutralpHModel* involving quaternary nitrogen and protonated aromatic nitrogens.

5.36 Quacpac TK 1.6.0

5.36.1 New features

- The default AM1BCC charge model *OECharges.AM1BCC* now lightly restrains the AM1 geometry optimization to the starting coordinates. This allows the important relaxation of bond and angle degrees of freedom while greatly reducing the potential to alter the molecule's conformation away from its starting coordinates. AM1 geometry optimization can be suppressed with *OECharges.AM1BCCSPt* or *OECharges.AM1BCCNoSymSPt*.

5.36.2 Bug fixes

- The AM1BCC charge models *OECharges.AM1BCCSym* and *OECharges.AM1BCCSPt* now symmetrize the partial charges over bond-topologically equivalent atoms, e.g. methyl hydrogens, in keeping with the original model. This is especially important with conformationally flexible molecules. This behavior can be suppressed by using the default *OECharges.AM1BCC* or the non-default models *OECharges.AM1BCCNoSym* or *OECharges.AM1BCCNoSymSPt*.

5.37 Quacpac TK 1.5.2

5.37.1 New features

- Refined Neutral pH model (*OESetNeutralpHModel*) to reflect feedback from collaborators. In particular isoxazoles and oxadiazoles were added while pyrazoles and aryl sulfonamides were refined. Aryl sulfonamide refinement also incorporated changes based on newly obtained experimental data.

5.37.2 Minor bug fixes

- *OESetNeutralpHModel* now correctly addresses beta di-amino groups so that if all other considerations are equivalent, secondary amines are treated as most basic, followed by primary amines, with tertiary amine being treated as least basic.
- *OETautomerMolFunction.GetMolecule* has been fixed so that 3D molecules have 3D hydrogens instead of implicit hydrogens.
- *OEAssignPartialCharges* no longer inadvertently converts reduced cysteine residues (CYS) to the oxidized form (CYX) when *OECharges.AmberFF94* is used to assign Amber partial charges to protein residues.

5.38 Quacpac TK 1.5.1

5.38.1 Bug Fixes

- A bug has been fixed where tautomers were not guaranteed to be in a canonical form during output. In rare circumstances this could lead to tautomers with the same unique tautomer to print it in different non-canonical forms.

5.39 Quacpac TK 1.5.0

5.39.1 New Features

- Major improvement for carbon hybridization. Now carbon atoms with bonds to one, two, or three heavy atoms are able to change hybridization state. However, only carbons close to an appropriate heteroatom are allowed

to change hybridization state. Additionally, unreasonable charge states of carbon have been removed. Now the enabling the *ch3flag* option will only generate tautomers appropriate for the given level.

- Improvement of the *mostAro* option, particularly involving exocyclic heteroatoms.
- Added stereo preservation flag to *OEEnumerateTautomers* with a default of *false*. Stereo chemistry can be lost during creation and removal of double bonds, but if the user desires a certain stereo setting to be preserved this flag will prevent the associated atoms and bonds from taking part in tautomerization.
- Improvements to pka states.
- AmberFF94 charges can now be applied to standard protein residues.

5.40 Quacpac TK 1.4.1

5.40.1 Bug Fixes

- *OESetNeutralpHModel* has been added to the Java and Python wrappers.
- Bug has been fixed in *OEAssignPartialCharges* where it sometimes did not return false after a failure to assign charges. Now this function should always return false if charges are not set.
- Fixed tetronic acid rule in *OESetNeutralpHModel* to allow matching of aromatic bonds.

5.41 Quacpac TK 1.4.0

5.41.1 New features

- *OESetNeutralpHModel* has been added. This function may be used to set a molecule to an energetically favorable ionization state for pH=7.4. This is the same pH model that was available in the Filter application. Additionally, the perception of acceptable valence states has been improved to include phosphorus as well as aromatic oxygen and sulfur with +1 formal charge.
- *OEEnumerateFormalCharges* now implicitly uses the `mostAro=true` parameter on the *OETautomerMolFunction* it uses when choosing a tautomer. This provides a better reference tautomer when enumerating pKa states.
- Aromaticity settings on molecules are now unchanged when *OEAssignPartialCharges* is called. Aromaticity may be temporarily changed inside the function while charges are being calculated, but the molecule will have the same aromaticity after the function as before.

5.42 Quacpac TK 1.3.1

5.42.1 New features

- The distribution and installation of Quacpac has been modified. The Windows distribution is now a standard EXE installer, and the OS X distribution is a dmg containing a standard pkg installer. The executables are now scripts that chose the correct version of the program at runtime. Please see the Application Installation section for details.

5.42.2 Bug fixes

- The previous version had a license failure when AM1 charges were calculated. This bug has been fixed.

5.43 Quacpac TK 1.3.0

This release represents the first major reworking of the **Quacpac TK** and applications in several years. Any users of prior versions of Quacpac will quickly notice several significant changes. First, this version of Quacpac does not contain a new release of protein pKa program. We are in the midst of a major rewrite of the protein pKa program. We hope that this work will bring major improvements in the usability, science and analysis of the protein pKa program, yet we do not want to delay the release of the entire Quacpac package waiting for the protein pKa program. The current Quacpac release does not contain protein pKa, but it will be included in a future release when the rewrite is complete. In the interim, we hope you find the bug fixes and new features included in this release useful.

The preps and qpd programs will no longer be supported future versions of Quacpac.

5.43.1 New features

- A reasonable looking tautomer may be calculated by setting the `mostAro` boolean to `true` in *OETautomerMolFunction*. After the `max` number of tautomers have been attempted, the most aromatic looking molecule may be retrieved using the *`OETautomerMolFunction.GetMolecule`* method.
- An `OEMCMolBase` version of *`OEAssignPartialCharges`* has been added for calculating multiconformer AM1BCC charges

5.43.2 Bug fixes

- Library has changed names from liboeproton to liboequacpac
- Memory leak related to *OETyperMolFunction* and *OETautomerMolFunction* is fixed.
- SMILES map indexes and names are no longer lost when outputting molecules.

5.44 Quacpac TK 1.1.0

- Special Note: Version 1.4 of Molcharge and version 1.2b of the library have been released and inserted into version 1.1 of Quacpac. Both of these have removed support for the VC2003 partial charging method.
- Version 1.1 is the first full stable release of Quacpac. Quacpac remains a heterogeneous release including five primary applications and a programming library with a C++ api.
- Tautomers is in version 2.0. It provides enumeration of energetically reasonable tautomers of input molecules.
- pKaTyper is in version 1.1. pKaTyper provides enumeration of protonation states (pKa ~2-~14).
- Molcharge is in version 1.3. Molcharge provides MMFF, AM1, AM1BCC, VC2003 and other partial charges on small molecules.
- Protein_pka is in version 1.3. Protein pKa carries out PB calculations to assess the shifts in protein residue pKa's.
- This release includes the oeproton library. The oeproton library exposes the features of pKaTyper, tautomers and molcharge in three high level C++ api points. The version of the library in this release is 1.1b. However, the beta moniker signifies only that at this time, OpenEye reserves the right to modify this api. We believe the quality of the code in this library is very solid and the beta designation does not reflect its quality.

CHAPTER

SIX

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CHAPTER

SEVEN

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CHAPTER

EIGHT

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↪http://www.eyesopen.com.
```

The version number for a floe package is displayed on the first page of the package's release notes. For example: https://docs.eyesopen.com/floe/modules/large_scale_floes/docs/source/releasenotes_2025_1.html.

8.3 Toolkits and Applications

To cite OpenEye toolkits or applications used in your work, please use the following:

```
OpenEye Toolkits [or Applications] <version-number>. OpenEye, Cadence Molecular Sciences,
↪ Santa Fe, NM. http://www.eyesopen.com.
```

For example:

```
OpenEye Toolkits 2024.2.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
↪eyesopen.com.
```

The Applications and Toolkits are released as a package, multiple times per year. The first part of the version number designates the calendar year. The version number appears on the summary document for the package.

If you want to cite an individual application or toolkit, you can use the syntax:

```
<product name> <version-number>. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
↪http://www.eyesopen.com.
```

where <*product name*> is:

- Bioisostere TK
- OEChem TK
- OEDepict TK
- OEDocking TK
- OEFF TK
- Eon TK
- FastROCS TK
- Grapheme TK
- GraphSim TK
- Lexichem TK
- OEMedChem TK
- MolProp TK
- Omega TK
- Quacpac TK
- Shape TK
- Spicoli TK
- Spruce TK
- Szmap TK
- Szybki TK
- Zap TK
- AFITT Application
- BROOD Application
- OEDocking Application
- EON Application
- OMEGA Application
- PICTO Application
- pKa-Prospector Application
- QUACPAC Application

- ROCS Application
- SiteHopper Application
- SPRUCE Application
- SZMAP Application
- SZYBKI Application
- VIDA Application

You can use the version number of the individual Application or Toolkit. For example:

```
SZYBKI Application 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://
↪www.eyesopen.com.

Szybki TK 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
↪eyesopen.com.
```

The first documentation pages give the product names and version numbers, as in https://docs.eyesopen.com/applications/szybki/index.html and https://docs.eyesopen.com/toolkits/python/szybkitk/index.html.

8.4 Publications for Bibliographies

Please also cite these publications if the corresponding product was used in your research.

8.4.1 Orion

Sørensen, J., Bannan, C.C., Calabrò, G., Jain, V., Ovanesyan, G., Smith, A., Zhang, S., Bayly, C.I., Darden, T.A., Geballe, M.T., LeBard, D.N., McGann, M., Moon, J.B., Muddana, H.S., Shewmaker, A., LaFon, J., Tolbert, R.W., Skillman, A.G., Nicholls, A. Orion® A Cloud-Native Molecular Design Platform. In *Computational Drug Discovery*. V. Poongavanam and V. Ramaswamy, Eds. Wiley-VCH, 2024; pp. 579–615. DOI: 10.1002/9783527840748.ch24

8.4.2 AFITT and FLYNN Applications

Wlodek, S.; Skillman, A.G.; Nicholls, A. Automated Ligand Placement and Refinement with a Combined Force Field and Shape Potential. *Acta Crystallogr., Sect. D: Struct. Biol.* **2006**, *62* (7), 741–749. DOI: 10.1107/s0907444906016076

8.4.3 OEDocking Application and Toolkit

Kelley, B.P.; Brown, S.P.; Warren, G.L.; Muchmore, S.W. POSIT: Flexible Shape-Guided Docking For Pose Prediction. *J. Chem. Inf. Model.* **2015**, *55* (8), 1771-1780. DOI: 10.1021/acs.jcim.5b00142

McGann, M. FRED Pose Prediction and Virtual Screening Accuracy. *J. Chem. Inf. Model.* **2011**, *51* (3), 578-596. DOI: 10.1021/ci100436p

McGann, M. FRED and HYBRID Docking Performance on Standardized Datasets. *J. Comput.-Aided Mol. Des.* **2012**, *26* (8), 897-906. DOI: 10.1007/s10822-012-9584-8

8.4.4 OMEGA Application and Toolkit

If you are using OMEGA in torsion driving mode, please cite the following two publications.

Hawkins, P.C.D.; Skillman, A.G.; Warren, G.L.; Ellingson, B.A.; Stahl, M.T. Conformer Generation with OMEGA: Algorithm and Validation Using High Quality Structures from the Protein Databank and the Cambridge Structural Database. *J. Chem. Inf. Model.* **2010**, *50* (4), 572-584. DOI: 10.1021/ci100031x

Hawkins, P.C.D. and Nicholls, A. Conformer Generation with OMEGA: Learning from the Data Set and the Analysis of Failures. *J. Chem. Inf. Model.* **2012**, *52* (11), 2919–2936. DOI: /10.1021/ci300314k

If you are using OMEGA in macrocyle mode, please cite the following.

Hawkins, P.C.D. and Wlodek, S. Decisions with Confidence: Application to the Conformation Sampling of Molecules in the Solid State. *J. Chem. Inf. Model.* **2020**, *60* (7), 3518–3533. DOI: /10.1021/acs.jcim.0c00358

8.4.5 ROCS Application

Hawkins, P.C.D.; Skillman, A.G.; Nicholls, A. Comparison of Shape-Matching and Docking as Virtual Screening Tools. *J. Med. Chem.* **2007**, *50* (1), 74-82. DOI: 10.1021/jm0603365

8.5 OpenEye MMDS Web Service

To cite use of the Macromolecular Data Service (MMDS) web service, please use the syntax:

```
Macromolecular Data Service <version-number>. OpenEye, Cadence Molecular Sciences, Santa␣
↪Fe, NM. http://www.eyesopen.com.
```

For example:

```
Macromolecular Data Service 1.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
↪http://www.eyesopen.com.
```

The MMDS version number appears on the web service's release notes.

CHAPTER

NINE

TECHNOLOGY LICENSING

OpenEye products use the following technology under license.

Some of the open source technologies we use are licensed under the GNU Public License (GPL) version 2 or 3. In all instances, these technologies are communicated with using the "at arms length" principle, using pipes and command line arguments.

While the software is in some instances assembled into a container, that assembly does not invoke the GPL copyleft scope. For each Floe package where these are used, the environment log clearly details the installed programs and their version numbers. With the links below for each technology, the source for each of those programs is available.

Table 1: Licensed Technology

Name of Project	Website	License URL
_libgcc_mutex	https://github.com/conda-forge/_libgcc_mutex-feedstock	https://github.com/conda-forge/_libgcc_mutex-feedstock/blob/master/LICENSE.txt
_openmp_mutex	https://github.com/conda-forge/_openmp_mutex-feedstock	https://github.com/conda-forge/_openmp_mutex-feedstock/blob/main/LICENSE.txt
ablang2	https://github.com/TobiasHeOl/AbLang2	https://github.com/TobiasHeOl/AbLang2/blob/main/LICENSE
abseil-cpp	https://github.com/abseil/abseil-cpp	https://github.com/abseil/abseil-cpp/blob/master/LICENSE
absl-py	https://github.com/abseil/abseil-py	https://github.com/abseil/abseil-py/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
aiohappyeyeballs	https://github.com/aio-libs/aiohappyeyeballs	https://github.com/aio-libs/aiohappyeyeballs/blob/main/LICENSE
aiohttp	https://docs.aiohttp.org/en/stable/	https://github.com/aio-libs/aiohttp/blob/master/LICENSE.txt
aiosignal	https://github.com/aio-libs/aiosignal	https://github.com/aio-libs/aiosignal/blob/master/LICENSE
Amazon Linux 2	https://aws.amazon.com/amazon-linux-2	N/A
AmberUtils	http://ambermd.org	N/A
ambit	https://github.com/khimaros/ambit	https://github.com/khimaros/ambit/blob/master/LICENSE
amqp	https://github.com/celery/py-amqp	https://github.com/celery/py-amqp/blob/master/LICENSE
anaconda-anon-usage	https://github.com/anaconda/anaconda-anon-usage	https://github.com/anaconda/anaconda-anon-usage/blob/main/LICENSE
angular	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md
angular-animate	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md
angular-cache	https://github.com/jmdobry/angular-cache	https://github.com/jmdobry/angular-cache/raw/master/LICENSE
angular-cookies	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md

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Table 1 – continued from previous page

Name of Project	Website	License URL
angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger/raw/master/LICENSE.md
angular-mocks	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-resource	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch/blob/master/LICENSE
angular-ui-grid	https://github.com/angular-ui/ui-grid	https://github.com/angular-ui/ui-grid
angular-ui-router	https://github.com/angular-ui/ui-router	https://github.com/angular-ui/ui-router/raw/master/LICENSE
angular-ui-tree	https://github.com/angular-ui-tree/angular-ui-tree	https://github.com/angular-ui-tree/angular-ui-tree/raw/master/LICENSE
angular-vs-repeat	https://github.com/kamilkp/angular-vs-repeat	https://raw.githubusercontent.com/kamilkp/angular-vs-repeat/master/LICENSE
aniso8601	https://bitbucket.org/nielsenb/aniso8601	https://bitbucket.org/nielsenb/aniso8601/src/master/LICENSE
annotated-types	https://github.com/annotated-types/annotated-types	https://github.com/annotated-types/annotated-types/blob/main/LICENSE
antlr4-python3-runtime	http://www.antlr.org OR https://pypi.org/project/antlr4-python3-runtin	https://github.com/conda-forge/antlr4-python3-runtin/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
anyio	https://github.com/agronholm/anyio	https://github.com/agronholm/anyio/blob/master/LICENSE
appdirs	http://github.com/ActiveState/appdirs	http://github.com/ActiveState/appdirs/blob/master/LICENSE.txt
appengine	https://google.golang.org/appengine	https://github.com/golang/appengine/blob/master/LICENSE
arabic-reshaper	https://github.com/mpcabd/python-arabic-reshape	https://github.com/mpcabd/python-arabic-reshape/blob/master/LICENSE
archspec	https://github.com/archspec/archspec/blob/master/README.md	https://github.com/archspec/archspec/blob/master/COPYRIGHT
argon2-cffi	https://github.com/hynek/argon2-cffi	https://github.com/hynek/argon2-cffi/blob/master/LICENSE
argon2-cffi-bindings	https://github.com/hynek/argon2-cffi-bindings	https://github.com/hynek/argon2-cffi-bindings/blob/master/LICENSE
arpack	https://www.caam.rice.edu/software/ARPACK/	https://www.caam.rice.edu/software/ARPACK/
arrow	https://github.com/arrow-py/arrow	https://github.com/arrow-py/arrow?tab=Apache-2.0-1-ov-file#readme
ascii85	https://github.com/huandu/node-ascii85	https://github.com/huandu/node-ascii85/raw/master/LICENSE
ase	https://wiki.fysik.dtu.dk/ase/	https://wiki.fysik.dtu.dk/ase/development/licenseinfo.html#license-info
asgiref	https://github.com/django/asgiref/	https://github.com/django/asgiref/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
asn1crypto	https://github.com/wbond/asn1crypto	https://github.com/wbond/asn1crypto/blob/master/LICENSE
assertions go-render	https://github.com/smartystreets/assertions/internal/go-render/render	https://github.com/smartystreets/assertions/blob/master/internal/go-render/LICENSE
assertions oglmatchers	https://github.com/smartystreets/assertions/internal/oglematchers	https://github.com/smartystreets/assertions/blob/master/internal/oglematchers/LICENSE
assertions	https://github.com/smartystreets/assertions	https://github.com/smartystreets/assertions/blob/master/LICENSE.md
asttokens	https://github.com/gristlabs/asttokens	https://github.com/gristlabs/asttokens/blob/master/LICENSE
astunparse	https://github.com/simonpercivall/astunparse	https://github.com/simonpercivall/astunparse/blob/master/LICENSE
async-lru	https://github.com/aio-libs/async-lru	https://github.com/aio-libs/async-lru/blob/master/LICENSE
async-timeout	https://github.com/aio-libs/async-timeout	https://github.com/aio-libs/async-timeout/blob/master/LICENSE
atk-1.0	https://docs.gtk.org/atk/	https://gitlab.gnome.org/GNOME/atk/-/blob/master/COPYING
atomic	https://github.com/uber-go/atomic	https://github.com/uber-go/atomic/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
atomicwrites	https://github.com/untitaker/python-atomicwrites	https://github.com/untitaker/python-atomicwrites/blob/master/LICENSE
attrs	https://www.attrs.org/	https://github.com/python-attrs/attrs/blob/main/LICENSE
aws-sdk-go	https://github.com/aws/aws-sdk-go	https://github.com/aws/aws-sdk-go/blob/master/LICENSE.txt
babel	https://babel.pocoo.org/ OR https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE OR https://babel.pocoo.org/en/latest/license.html#babel-license
Babel	https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE
backcall	https://github.com/takluyver/backcall	https://github.com/takluyver/backcall/blob/master/LICENSE
backports	https://github.com/brandon-rhodes/backports	https://github.com/brandon-rhodes/backports/blob/master/LICENSE.TXT
backports.functools-lru-cache	https://github.com/jaraco/backports.functools_lru_cache	https://github.com/jaraco/backports.functools_lru_cache/blob/main/LICENSE
backports.zstd	https://github.com/rogdham/backports.zstd	https://github.com/rogdham/backports.zstd?tab=License-1-ov-file#readme
base62	https://github.com/kare/base62	https://github.com/kare/base62/blob/main/LICENSE
beautifulsoup4	https://www.crummy.com/software/BeautifulSoup/	https://www.crummy.com/software/BeautifulSoup/

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Table 1 – continued from previous page

Name of Project	Website	License URL
billiard	https://github.com/celery/billiard	https://github.com/celery/billiard/blob/master/LICENSE.txt
biopython	https://biopython.org	https://github.com/biopython/biopython/blob/master/LICENSE.rst
biotite	https://github.com/biotite-dev/biotite/blob/master/README.rst	https://github.com/biotite-dev/biotite/blob/master/LICENSE.rst
bitarray	https://github.com/ilanschnell/bitarray	https://github.com/ilanschnell/bitarray/blob/master/LICENSE
bitset	https://github.com/willf/bitset	https://github.com/willf/bitset/blob/master/LICENSE
blas	https://www.netlib.org/blas/	https://www.netlib.org/blas/#_licensing
bleach	https://github.com/mozilla/bleach	https://github.com/mozilla/bleach/blob/main/LICENSE
blessings	https://github.com/erikrose/blessings	https://github.com/erikrose/blessings/blob/master/LICENSE
blinker	https://pythonhosted.org/blinker/	https://github.com/pallets-eco/blinker/blob/master/LICENSE
bokeh	https://github.com/bokeh/bokeh	https://github.com/bokeh/bokeh/blob/branch-4.0/LICENSE.txt
blosc	https://github.com/Blosc/python-blosc	https://github.com/Blosc/python-blosc/blob/master/LICENSE.txt
blosc2	https://github.com/Blosc/python-blosc2	https://github.com/Blosc/c-blosc2/blob/main/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
boltons	https://github.com/mahmoud/boltons	https://github.com/mahmoud/boltons/blob/master/LICENSE
Boltz	https://boltz.bio	https://github.com/jwohlwend/boltz/blob/main/LICENSE
boost	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
boost-cpp	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue/raw/master/LICENSE
boto3	https://github.com/boto/boto3	https://github.com/boto/boto3/blob/develop/LICENSE
botocore	https://github.com/boto/botocore	https://github.com/boto/botocore/blob/develop/LICENSE.txt
Bottleneck	https://bottleneck.readthedocs.io/en/latest/index.html	https://bottleneck.readthedocs.io/en/latest/license.html
Brotli	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
brotli-bin	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
brotli-python	http://python-hyper.org/projects/brotlipy/en/latest/	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE
brotlicffi	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi?tab=MIT-1-ov-file#readme
brotlipy	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
bson	http://github.com/py-bson/bson	https://github.com/py-bson/bson/blob/master/LICENSE_APACHE
bytefmt	https://code.cloudfoundry.org/bytefmt	https://github.com/cloudfoundry/bytefmt/blob/master/LICENSE
bzip2	https://www.bzip.org	https://spdx.org/licenses/bzip2-1.0.6.html
c-ares	https://github.com/c-ares/c-ares	https://github.com/c-ares/c-ares/blob/main/LICENSE.md
ca-certificates	https://github.com/conda-forge/ca-certificates-feedsto	https://wiki.mozilla.org/CA/Included_Certificates
cached-property	https://github.com/pydanny/cached-property	https://github.com/pydanny/cached-property/blob/master/LICENSE
cachetools	https://github.com/tkem/cachetools/	https://github.com/tkem/cachetools/blob/master/LICENSE
cairo	https://pycairo.readthedocs.io/en/latest/	https://github.com/pygobject/pycairo/blob/master/COPYING
canvas	https://github.com/Automattic/node-canvas	https://github.com/Automattic/node-canvas
cctbx	https://github.com/cctbx/cctbx_project	https://github.com/cctbx/cctbx_project/blob/master/cctbx/LICENSE_2_0.txt
celery	https://github.com/celery/celery	https://github.com/celery/celery/blob/master/LICENSE
Cerberus	https://docs.python-cerberus.org/en/stable/	https://docs.python-cerberus.org/en/stable/license.html
certifi	https://certifiio.readthedocs.io/en/latest/	https://wiki.mozilla.org/index.php?title=CA/IncludedCertificates&redirect=no

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Table 1 – continued from previous page

Name of Project	Website	License URL
cffi	https://github.com/python-cffi	https://github.com/cffi/cffi/blob/master/COPYRIGHT
cftime	https://pypi.org/project/cftime/	https://github.com/Unidata/cftime/blob/master/LICENSE
chardet	https://github.com/chardet/chardet	https://github.com/chardet/chardet/blob/master/LICENSE
charset-normalizer	https://github.com/ousret/charset_normalizer	https://github.com/Ousret/charset_normalizer/blob/master/LICENSE
ChEMBL Structure Pipeline	https://github.com/chembl/ChEMBL_Structure_Pipeline/tree/master	https://github.com/chembl/ChEMBL_Structure_Pipeline/blob/master/LICENSE
choreographer	https://github.com/mazpie/choreographer	https://github.com/mazpie/choreographer/blob/main/LICENSE
chunkreader	https://github.com/jackc/chunkreader/v2	https://github.com/jackc/chunkreader/blob/master/LICENSE
click	https://palletsprojects.com/p/click/	https://github.com/pallets/click/blob/main/LICENSE.rst
click-completion	https://github.com/click-contrib/click-completion	https://github.com/click-contrib/click-completion/blob/master/LICENSE
click-didyoumean	https://github.com/click-contrib/click-didyoumean	https://github.com/click-contrib/click-didyoumean/blob/master/LICENSE
click-plugins	https://github.com/click-contrib/click-plugins	https://github.com/click-contrib/click-plugins/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
click-repl	https://github.com/untitaker/click-repl	https://github.com/click-contrib/click-repl/blob/master/LICENSE
cloudpickle	https://github.com/cloudpipe/cloudpickle	https://github.com/cloudpipe/cloudpickle/blob/master/LICENSE
cmake	https://cmake.org/	https://cmake.org/licensing/
colorama	https://github.com/tartley/colorama	https://github.com/tartley/colorama/blob/master/LICENSE.txt
comm	https://github.com/ipython/comm	https://github.com/ipython/comm/blob/master/LICENSE
compose	https://github.com/docker/compose	https://github.com/docker/compose/blob/v2/LICENSE
conda-content-trust	https://github.com/conda/conda-content-trust	https://github.com/conda/conda-content-trust/blob/main/LICENSE
conda-libmamba-solver	https://github.com/conda/conda-libmamba-solv	https://github.com/conda/conda-libmamba-solv/blob/main/LICENSE
conda-pack	https://conda.github.io/conda-pack/	https://github.com/conda/conda-pack/blob/main/LICENSE.txt
conda-package-handling	https://github.com/conda/conda-package-handli	https://github.com/conda/conda-package-handli/blob/main/LICENSE
conda-package-streaming	https://anaconda.org/conda-forge/conda-package-stream	https://github.com/conda/conda-package-stream/blob/main/LICENSE
conda-token	https://anaconda.org/anaconda/conda-token	https://anaconda.org/anaconda/conda-token

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Table 1 – continued from previous page

Name of Project	Website	License URL
conda_package_strear	https://github.com/conda/conda-package-streamtree/main/conda_package_streaming	https://github.com/conda/conda-package-streamtab=License-1-ov-file
confuse	https://github.com/beetbox/confuse	https://github.com/beetbox/confuse/blob/main/LICENSE
contourpy	https://github.com/contourpy/contourpy	https://github.com/contourpy/contourpy/blob/main/LICENSE
cpp-expected	https://github.com/TartanLlama/expected	https://github.com/TartanLlama/expected?tab=CC0-1.0-1-ov-file#readme
cpp-peglib	https://github.com/yhirose/cpp-peglib	https://github.com/yhirose/cpp-peglib/blob/master/LICENSE
cryptography	https://github.com/pyca/cryptography	https://github.com/pyca/cryptography/blob/main/LICENSE
cssselect2	https://github.com/Kozea/cssselect2/	https://github.com/Kozea/cssselect2/blob/master/LICENSE
cuda-bindings	https://nvidia.github.io/cuda-python/cuda-bindings/latest/install.html	https://github.com/NVIDIA/cuda-python/blob/main/cuda_bindings/LICENSE
cuda-pathfinder	https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/	https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/license.html
cudatoolkit	https://developer.nvidia.com/cuda-toolkit	https://docs.nvidia.com/cuda/eula/index.html
cuequivariance-ops-cu12	https://developer.nvidia.com/cuequivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
cuequivariance-ops-torch-cu12	https://developer.nvidia.com/cuequivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
cuequivariance-torch	https://docs.nvidia.com/cuda/cuequivariance/	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
cupy-cuda113	https://cupy.dev/	https://github.com/cupy/cupy/blob/main/LICENSE
cupy-cuda11x	https://cupy.dev/	https://github.com/cupy/cupy/?tab=MIT-1-ov-file#readme
curl	https://curl.se	https://curl.se/docs/copyright.html
cycler	https://github.com/matplotlib/cycler	https://github.com/matplotlib/cycler/blob/main/LICENSE
cyrus-sasl	https://github.com/cyrusimap/cyrus-sasl	https://github.com/cyrusimap/cyrus-sasl/blob/master/COPYING
Cython	https://cython.org	https://www.apache.org/licenses/LICENSE-2.0.html
d3	https://github.com/mbostock/d3	https://github.com/mbostock/d3/raw/master/LICENSE
dataclasses	https://github.com/ericvsmith/dataclasses	https://github.com/ericvsmith/dataclasses/blob/master/LICENSE.txt
ddsketch	http://github.com/datadog/sketches-py	https://github.com/DataDog/sketches-py/blob/master/LICENSE
debugpy	https://aka.ms/debugpy	https://github.com/microsoft/debugpy/blob/main/LICENSE

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Name of Project	Website	License URL
decimal	https://github.com/shopspring/decimal	https://github.com/shopspring/decimal/blob/master/LICENSE
decorator	https://github.com/micheles/decorator	https://github.com/micheles/decorator/blob/master/LICENSE.txt
deepdiff	https://github.com/seperman/deepdiff	https://github.com/seperman/deepdiff/blob/master/LICENSE
deeptime	https://github.com/deeptime-ml/deeptime	https://github.com/deeptime-ml/deeptime/blob/main/LICENSE.txt
defusedxml	https://github.com/tiran/defusedxml	https://github.com/tiran/defusedxml/blob/main/LICENSE
dftd3	https://github.com/dftd3/tad-dftd3	https://github.com/dftd3/tad-dftd3/blob/main/LICENSE
dill	https://github.com/uqfoundation/dill	https://github.com/uqfoundation/dill/blob/master/LICENSE
distlib	https://distlib.readthedocs.io/en/latest/	https://github.com/pypa/distlib/blob/master/LICENSE.txt
distro	https://github.com/python-distro/distro	https://github.com/python-distro/distro/blob/master/LICENSE
Django	https://www.djangoproject.com/	https://github.com/django/django/blob/main/LICENSE
django-classy-tags	https://github.com/django-cms/django-classy-tags	https://github.com/django-cms/django-classy-tags/blob/master/LICENSE
django-cors-headers	https://github.com/adamchainz/django-cors-headers	https://github.com/adamchainz/django-cors-headers/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
django-csp	https://github.com/mozilla/django-csp	https://github.com/mozilla/django-csp/blob/main/LICENSE
django-extensions	https://github.com/django-extensions/django-extensions	https://github.com/django-extensions/django-extensions/blob/main/LICENSE
django-filter	https://github.com/carltongibson/django-filter/tree/master	https://github.com/carltongibson/django-filter/blob/main/LICENSE
django-redis	https://github.com/jazzband/django-redis	https://github.com/jazzband/django-redis/blob/master/LICENSE
django-taggit	https://github.com/jazzband/django-taggit	https://github.com/jazzband/django-taggit/blob/master/LICENSE
django-taggit-serializer	https://github.com/glemmaPaul/django-taggit-serializ	https://github.com/glemmaPaul/django-taggit-serializ blob/master/LICENSE
django-taggit-templatetags2	https://github.com/fizista/django-taggit-templat	https://github.com/fizista/django-taggit-templat blob/master/LICENSE.txt
djangorestframework	https://www.django-rest-framewor org/	https://github.com/encode/django-rest-framewor blob/master/LICENSE.md
dkh	https://psicode.org/psi4manual/master/dkh.html	https://github.com/psi4/dkh/blob/master/COPYING.LESSER
dm-tree	https://github.com/deepmind/tree	https://github.com/deepmind/tree/blob/master/LICENSE
docker-py	https://github.com/docker/docker-py/	https://github.com/docker/docker-py/blob/master/LICENSE

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Name of Project	Website	License URL
docker-pycreds	https://github.com/shin-/dockerpy-creds	https://github.com/shin-/dockerpy-creds/blob/master/LICENSE
docopt	https://docopt.org	https://github.com/docopt/docopt/blob/master/LICENSE-MIT
docutils	https://docutils.sourceforge.io	https://docutils.sourceforge.io/COPYING.html
drf-dynamic-fields	https://github.com/dbrgn/drf-dynamic-fields	https://github.com/dbrgn/drf-dynamic-fields/blob/master/LICENSE
DuckDB	https://duckdb.org/	https://github.com/duckdb/duckdb?tab=MIT-1-ov-file#readme
edgembar	https://rutgerslbsr.gitlab.io/fe-toolkit/edgembar/index.html	https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE
editdistance	https://github.com/roy-ht/editdistance	https://github.com/roy-ht/editdistance/blob/master/LICENSE
eigen	https://eigen.tuxfamily.org/index.php?title=Main_Page	https://eigen.tuxfamily.org/index.php?title=Main_Page#License
einops	https://github.com/arogozhnikov/einops	https://github.com/arogozhnikov/einops/blob/master/LICENSE
einx	https://github.com/fferflo/einx	https://github.com/fferflo/einx/blob/master/LICENSE
entrypoints	https://github.com/takluyver/entrypoints	https://github.com/takluyver/entrypoints/blob/master/LICENSE
errors	https://github.com/pkg/errors	https://github.com/pkg/errors/blob/master/LICENSE

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Name of Project	Website	License URL
eslint-plugin	https://github.com/typescript-eslint/typescript-eslint	https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE
et_xmlfile	https://foss.heptapod.net/openpyxl/et_xmlfile	https://foss.heptapod.net/openpyxl/et_xmlfile/-/blob/branch/default/LICENCE.rst
exceptiongroup	https://github.com/agronholm/exceptiongroup	https://github.com/agronholm/exceptiongroup/blob/main/LICENSE
execnet	https://execnet.readthedocs.io/en/latest/	https://github.com/pytest-dev/execnet/blob/master/LICENSE
executing	https://github.com/alexmojaki/executing	https://github.com/alexmojaki/executing/blob/master/LICENSE.txt
expat	https://libexpat.github.io	https://github.com/libexpat/libexpat/blob/master/expat/COPYING
fairscale	https://github.com/facebookresearch/fairscale	https://github.com/facebookresearch/fairscale/blob/main/LICENSE
fairseq	https://github.com/pytorch/fairseq	https://github.com/facebookresearch/fairseq/blob/main/LICENSE
fastjsonschema	https://github.com/horejsek/python-fastjsonschem	https://github.com/horejsek/python-fastjsonschem/blob/master/LICENSE
fastrlock	https://github.com/scoder/fastrlock	https://github.com/scoder/fastrlock/blob/master/LICENSE
fftw	https://www.fftw.org	commercial license

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Name of Project	Website	License URL
filebuffer	https://github.com/mattetti/filebuffer	https://github.com/mattetti/filebuffer/blob/master/LICENSE
filelock	https://py-filelock.readthedocs.io/en/latest/index.html	https://github.com/tox-dev/py-filelock/blob/main/LICENSE
finufft	https://github.com/flatironinstitute/finufft	https://github.com/flatironinstitute/finufft/blob/master/LICENSE
Flask	https://flask.palletsprojects.com/en/2.1.x/	https://flask.palletsprojects.com/en/2.1.x/license/
flatbuffers	https://google.github.io/flatbuffers/	https://github.com/google/flatbuffers/blob/master/LICENSE.txt
flexcache	https://github.com/hgrecco/flexcache	https://github.com/hgrecco/flexcache/blob/main/LICENSE
flexparser	https://github.com/hgrecco/flexparser	https://github.com/hgrecco/flexparser/blob/main/LICENSE
flit-core	https://github.com/pypa/flit	https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md
FLTK	https://www.fltk.org/index.php	https://www.fltk.org/COPYING.php
fmt	https://fmt.dev/latest/index.html	https://github.com/fmtlib/fmt/blob/master/LICENSE.rst
font-awesome	https://github.com/FortAwesome/Font-Awesome	https://github.com/FortAwesome/Font-Awesome
font-ttf-dejavu-sans-mono	https://dejavu-fonts.github.io	https://dejavu-fonts.github.io/License.html
font-ttf-inconsolata	https://fonts.google.com/specimen/Inconsolata	https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL

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Name of Project	Website	License URL
font-ttf-source-code-pro	https://fonts.google.com/specimen/Source+Code+Pro	https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL
font-ttf-ubuntu	https://fonts.google.com/specimen/Ubuntu	https://ubuntu.com/legal/font-licence
fontconfig	https://www.freedesktop.org/wiki/Software/fontconfig/	https://gitlab.freedesktop.org/fontconfig/fontconfig/-/blob/main/COPYING
fonts-conda-ecosystem	https://anaconda.org/conda-forge/fonts-conda-ecosyster	https://docs.conda.io/en/latest/license.html
fonts-conda-forge	https://anaconda.org/conda-forge/fonts-conda-forge/	https://creativecommons.org/licenses/by/4.0/
fonttools	https://github.com/fonttools/fonttools	https://github.com/fonttools/fonttools/blob/main/LICENSE
forcebalance	https://simtk.org/home/forcebalance OR https://github.com/leeping/forcebalance	https://github.com/leeping/forcebalance/blob/master/LICENSE
fqdn	https://github.com/ypcrts/fqdn	https://github.com/ypcrts/fqdn?tab=MPL-2.0-1-ov-file#readme
freetype	https://freetype.org	https://freetype.org/license.html
freetype-py	https://github.com/rougier/freetype-py	https://github.com/rougier/freetype-py?tab=License-1-ov-file#readme
fribidi	https://github.com/fribidi/fribidi	https://github.com/fribidi/fribidi/blob/master/COPYING
frozendict	https://github.com/Marco-Sulla/python-frozendict	https://github.com/Marco-Sulla/python-frozendict/blob/master/LICENSE.txt
frozenlist	https://github.com/aio-libs/frozenlist	https://github.com/aio-libs/frozenlist/blob/master/LICENSE

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Name of Project	Website	License URL
fsmlite	https://github.com/tkem/fsmlite	https://github.com/tkem/fsmlite/blob/master/LICENSE
fsspec	https://github.com/fsspec/filesystem_spec	https://github.com/fsspec/filesystem_spec/blob/master/LICENSE
funcy	https://github.com/Suor/funcy	https://github.com/Suor/funcy/blob/master/LICENSE
gast	https://github.com/serge-sans-paille/gast/	https://github.com/serge-sans-paille/gast/blob/master/LICENSE
gau2grid	https://github.com/dgasmith/gau2grid	https://github.com/dgasmith/gau2grid/blob/master/LICENSE
gax-go	https://github.com/googleapis/gax-go/v2	https://github.com/googleapis/gax-go/blob/main/LICENSE
gdk-pixbuf	https://gitlab.gnome.org/GNOME/gdk-pixbuf	https://gitlab.gnome.org/GNOME/gdk-pixbuf/-/blob/master/COPYING
gemmi	https://gemmi.readthedocs.io/en/latest/	https://github.com/project-gemmi/gemmi/blob/master/LICENSE.txt
genproto	https://google.golang.org/genproto/googleapis	https://github.com/googleapis/go-genproto/blob/main/LICENSE
geometric	https://openbase.com/python/geometric	https://openbase.com/python/geometric
giflib	https://giflib.sourceforge.net	https://github.com/mirrorer/giflib/blob/master/COPYING
gitdb	https://github.com/gitpython-developers/gitdb	https://github.com/gitpython-developers/gitdb/blob/master/LICENSE
GitPython	https://github.com/gitpython-developers/GitPython	https://github.com/gitpython-developers/GitPython/blob/main/LICENSE

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Name of Project	Website	License URL
glib	https://docs.gtk.org/glib/	https://gitlab.gnome.org/GNOME/glib/-/blob/main/LICENSES/LGPL-2.1-or-later.txt
GLM Library	https://github.com/g-truc/glm	https://github.com/g-truc/glm/blob/master/manual.md#section0
gls	https://github.com/jtolds/gls	https://github.com/jtolds/gls/blob/master/LICENSE
gmpy2	https://github.com/aleaxit/gmpy	https://github.com/gmpy2/gmpy2/blob/master/COPYING.LESSER
go-cleanhttp	https://github.com/hashicorp/go-cleanhttp	https://github.com/hashicorp/go-cleanhttp/blob/master/LICENSE
go-connections	https://github.com/docker/go-connections	https://github.com/docker/go-connections/blob/master/LICENSE
go-cpio	https://github.com/cavaliercoder/go-cpio	https://github.com/cavaliercoder/go-cpio/blob/master/LICENSE
go-getter	https://github.com/hashicorp/go-getter	https://github.com/hashicorp/go-getter/blob/master/LICENSE
go-homedir	https://github.com/mitchellh/go-homedir	https://github.com/mitchellh/go-homedir/blob/master/LICENSE
go-ini	https://github.com/go-ini/ini	https://github.com/go-ini/ini/blob/master/LICENSE
go-jmespath	https://github.com/jmespath/go-jmespath	https://github.com/jmespath/go-jmespath/blob/master/LICENSE

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Name of Project	Website	License URL
go-junit-report	https://github.com/jstemmer/go-junit-report	https://github.com/jstemmer/go-junit-report/blob/master/LICENSE
go-netrc	https://github.com/bgentry/go-netrc/netrc	https://github.com/bgentry/go-netrc/blob/master/LICENSE
go-ole	https://github.com/go-ole/go-ole	https://github.com/go-ole/go-ole/blob/master/LICENSE
go-pg	https://github.com/go-pg/pg	https://github.com/go-pg/pg/blob/master/LICENSE
go-redis	https://github.com/go-redis/redis/v8	https://github.com/go-redis/redis/blob/master/LICENSE
go-rendezvous	https://github.com/dgryski/go-rendezvous	https://github.com/dgryski/go-rendezvous/blob/master/LICENSE
go-safetemp	https://github.com/hashicorp/go-safetemp	https://github.com/hashicorp/go-safetemp/blob/master/LICENSE
go-sysconf	https://github.com/tklauser/go-sysconf	https://github.com/tklauser/go-sysconf/blob/master/LICENSE
go-testing-interface	https://github.com/mitchellh/go-testing-interface	https://github.com/mitchellh/go-testing-interface/blob/master/LICENSE
go-units	https://github.com/docker/go-units	https://github.com/docker/go-units/blob/master/LICENSE
go-version	https://github.com/hashicorp/go-version	https://github.com/hashicorp/go-version/blob/master/LICENSE
go-zglob	https://github.com/mattn/go-zglob	https://github.com/mattn/go-zglob/blob/master/LICENSE

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Name of Project	Website	License URL
go.opencensus	https://go.opencensus.io	https://github.com/census-instrumentatio opencensus-go/blob/master/LICENSE
gobrake.v2	https://gopkg.in/airbrake/gobrake.v2	https://github.com/airbrake/gobrake/blob/v2.0.9/LICENSE
goconvey	https://github.com/smartystreets/goconvey	https://github.com/smartystreets/goconvey/blob/master/LICENSE.md
golden-layout	https://github.com/deepstreamIO/golden-layout	https://github.com/deepstreamIO/golden-layout/raw/master/LICENSE
google-auth	https://google-auth.readthedocs.io/en/master/	https://github.com/GoogleCloudPlatform google-auth-library-p blob/master/LICENSE
google-auth-oauthlib	https://github.com/googleapis/google-auth-library-p	https://github.com/googleapis/google-auth-library-p blob/main/LICENSE
google-cloud-go	https://cloud.google.com/go	https://github.com/googleapis/google-cloud-go/blob/main/LICENSE
google-cloud-go/storage	https://cloud.google.com/go/storage	https://github.com/googleapis/google-cloud-go/blob/main/LICENSE
google-pasta	https://github.com/google/pasta	https://github.com/google/pasta/blob/master/LICENSE
google.golang.org/api	https://google.golang.org/api	https://github.com/googleapis/google-api-go-client/blob/main/LICENSE
gopsutil	https://github.com/shirou/gopsutil	https://github.com/shirou/gopsutil/blob/master/LICENSE

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Name of Project	Website	License URL
gorilla websocket	https://github.com/gorilla/websocket	https://github.com/gorilla/websocket/blob/master/LICENSE
gpytorch	https://gpytorch.ai	https://github.com/cornellius-gp/gpytorch?tab=MIT-1-ov-file#readme
graphite2	https://github.com/silnrsi/graphite	https://github.com/silnrsi/graphite/blob/master/LICENSE
graphviz	https://graphviz.org/	https://graphviz.org/license/
greenlet	https://greenlet.readthedocs.io/en/latest/	https://github.com/python-greenlet/greenlet/blob/master/LICENSE
groupcache	https://github.com/golang/groupcache	https://github.com/golang/groupcache/blob/master/LICENSE
grpc	https://google.golang.org/grpc	https://github.com/grpc/grpc-go/blob/master/LICENSE
grpc-cpp	https://github.com/grpc/grpc	https://github.com/grpc/grpc/blob/master/LICENSE
grpcio	https://github.com/grpc/grpc.io/blob/main/LICENSE	https://github.com/grpc/grpc.io/blob/main/LICENSE
gtk2	https://gitlab.gnome.org/GNOME/gtk	https://gitlab.gnome.org/GNOME/gtk/-/blob/main/COPYING
gts	https://sourceforge.net/projects/gts/	https://www.gnu.org/licenses/lgpl-3.0.html
h11	https://github.com/python-hyper/h11	https://github.com/python-hyper/h11/blob/master/LICENSE.txt
h2	https://github.com/python-hyper/h2	https://github.com/python-hyper/h2?tab=MIT-1-ov-file#readme

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Name of Project	Website	License URL
h5py	https://www.h5py.org	https://docs.h5py.org/en/stable/licenses.html
harfbuzz	https://github.com/harfbuzz/harfbuzz	https://github.com/harfbuzz/harfbuzz/blob/main/COPYING
hdbscan	https://hdbscan.readthedocs.io/en/latest/	https://github.com/scikit-learn-contrib/hdbscan/blob/master/LICENSE
hdf4	https://www.hdfgroup.org/solutions/hdf4/	https://github.com/HDFGroup/hdf4/blob/master/COPYING
hdf5	https://www.hdfgroup.org/solutions/hdf5/	https://github.com/HDFGroup/hdf5/blob/master/COPYING
he	https://github.com/mathiasbynens/he	https://github.com/mathiasbynens/he/raw/master/LICENSE-MIT.txt
hpack	https://github.com/python-hyper/hpack	https://github.com/python-hyper/hpack?tab=MIT-1-ov-file#readme
html-loader	https://github.com/webpack-contrib/html-loader	https://github.com/webpack-contrib/html-loader/raw/master/LICENSE
html5lib	https://github.com/html5lib/html5lib-python	https://github.com/html5lib/html5lib-python/blob/master/LICENSE
htslib	https://www.htslib.org	https://github.com/samtools/htslib/blob/develop/LICENSE
httpcore	https://www.encode.io/httpcore/	https://github.com/encode/httpcore/blob/master/LICENSE.md
httpx	https://github.com/encode/httpx	https://github.com/encode/httpx/blob/master/LICENSE.md

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Name of Project	Website	License URL
humanize	https://github.com/jmoiron/humanize	https://github.com/jmoiron/humanize/blob/master/LICENCE
hydra-core	https://github.com/facebookresearch/hydra	https://github.com/facebookresearch/hydra/blob/main/LICENSE
hyperframe	https://github.com/python-hyper/hyperframe	https://github.com/python-hyper/hyperframe?tab=MIT-1-ov-file#readme
icu	https://github.com/unicode-org/icu	https://github.com/unicode-org/icu/blob/main/icu4c/LICENSE
idna	https://github.com/kjd/idna	https://github.com/kjd/idna/blob/master/LICENSE.md
ihm	https://github.com/ihmwg/python-ihm	https://github.com/ihmwg/python-ihm/blob/main/LICENSE
imageio	https://github.com/imageio/imageio	https://github.com/imageio/imageio/blob/master/LICENSE
imagesize	https://github.com/shibukawa/imagesize_py	https://github.com/shibukawa/imagesize_py/blob/master/LICENSE.rst
ImmuneBuilder	https://github.com/oxpig/ImmuneBuilder/tree/main	https://github.com/oxpig/ImmuneBuilder/blob/main/LICENSE
importlib-metadata	https://github.com/python/importlib_metadata	https://github.com/python/importlib_metadata/blob/main/LICENSE
importlib_metadata	https://github.com/python/importlib_metadata	https://github.com/python/importlib_metadata/blob/main/LICENSE

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Name of Project	Website	License URL
importlib_resources	https://github.com/python/importlib_resources	https://github.com/python/importlib_resources/blob/main/LICENSE
InChI	https://iupac.org/who-we-are/divisions/division-details/inchi/	https://iupac.org/wp-content/uploads/2021/06/iupac-inchi-license_2020.pdf
inflection	https://github.com/jinzhu/inflection	https://github.com/jinzhu/inflection/blob/master/LICENSE
ini.v1	https://gopkg.in/ini.v1	https://github.com/go-ini/ini/blob/v1.66.2/LICENSE
iniconfig	https://github.com/pytest-dev/iniconfig	https://github.com/pytest-dev/iniconfig/blob/main/LICENSE
innersvg-polyfill	https://github.com/dnozay/innersvg-polyfill	https://github.com/dnozay/innersvg-polyfill/raw/master/LICENSE
intel-openmp	https://github.com/hermitcore/libomp_oss	https://github.com/hermitcore/libomp_oss/blob/hermit/LICENSE.txt
ipykernel	https://ipython.org	https://ipython.org
ipython	https://ipython.org	https://github.com/ipython/ipython/blob/master/LICENSE
ipython-genutils	http://ipython.org	https://github.com/ipython/ipython_genutils/blob/master/COPYING.md
ipython_pygments_le	https://github.com/ipython/ipython-pygments-lex	https://github.com/ipython/ipython-pygments-lex blob/main/LICENSE
ipywidgets	http://jupyter.org	https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE

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Name of Project	Website	License URL
isodate	https://github.com/gweis/isodate/	https://github.com/gweis/isodate/blob/master/LICENSE
isoduration	https://github.com/bolsote/isoduration	https://github.com/bolsote/isoduration?tab=ISC-1-ov-file#readme
itsdangerous	https://palletsprojects.com/p/itsdangerous/	https://itsdangerous.palletsprojects.com/en/2.1.x/license/
jax	https://github.com/google/jax	https://github.com/google/jax/blob/main/LICENSE
jaxlib	https://github.com/google/jax	https://github.com/google/jax/blob/main/LICENSE
jaxtyping	https://github.com/patrick-kidger/jaxtyping	https://github.com/patrick-kidger/jaxtyping?tab=License-1-ov-file#readme
jedi	https://jedi.readthedocs.io/en/latest/	https://github.com/davidhalter/jedi/blob/master/LICENSE.txt
Jinja2	https://palletsprojects.com/p/jinja/	https://github.com/pallets/jinja/blob/main/LICENSE.rst
jmespath	https://github.com/jmespath/jmespath.py	https://github.com/jmespath/jmespath.py/blob/develop/LICENSE.txt
joblib	https://joblib.readthedocs.io/en/latest/	https://github.com/joblib/joblib/blob/master/LICENSE.txt
jpeg	https://www.ijg.org	https://www.ijg.org/files/README
json5	https://github.com/dpranke/pyjson5	https://github.com/dpranke/pyjson5/blob/main/LICENSE
jsonfield	https://github.com/dmkoch/django-jsonfield/	https://github.com/rpkilby/jsonfield/blob/master/LICENSE

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Name of Project	Website	License URL
jsonpatch	https://github.com/stefankoegl/python-json-patch	https://github.com/stefankoegl/python-json-patch/blob/master/LICENSE
jsonpickle	https://github.com/jsonpickle/jsonpickle	https://github.com/jsonpickle/jsonpickle/blob/main/LICENSE
jsonpointer	https://github.com/stefankoegl/python-json-pointer	https://github.com/stefankoegl/python-json-pointer/blob/master/LICENSE.txt
jsonschema	https://github.com/python-jsonschema/jsonschema	https://github.com/python-jsonschema/jsonschema/blob/master/COPYING
jsonschema-specifications	https://github.com/python-jsonschema/jsonschema-specificat	https://github.com/python-jsonschema/jsonschema-specificat blob/main/COPYING
jstat	https://github.com/jstat/jstat	https://www.opensource.org/licenses/mit-license.php
jupyter-client	https://jupyter.org	https://github.com/jupyter/jupyter_client/blob/main/COPYING.md
jupyter-core	https://jupyter.org	https://github.com/jupyter/jupyter_core/blob/master/COPYING.md
jupyter-events	https://github.com/jupyter/jupyter_events	https://github.com/jupyter/jupyter_events/blob/main/LICENSE
jupyter-lsp	https://github.com/jupyter-lsp/jupyterlab-lsp	https://github.com/jupyter-lsp/jupyterlab-lsp
jupyter-serverhttp://jupyter.or	https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE	
jupyter_client	http://jupyter.org	https://github.com/jupyter/jupyter_client/blob/main/LICENSE

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Name of Project	Website	License URL
jupyter_core	http://jupyter.org	https://github.com/jupyter/jupyter_core/blob/master/LICENSE
jupyter_server	https://github.com/jupyter-server/jupyter_server	https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE
jupyter_server_termin	https://github.com/jupyter-server/jupyter_server_terminals	https://github.com/jupyter-server/jupyter_server_terminals/blob/main/LICENSE
jupyterlab	https://github.com/jupyterlab/jupyterlab	https://github.com/jupyterlab/jupyterlab/blob/main/LICENSE
jupyterlab-pygments	http://jupyter.org	https://github.com/jupyterlab/jupyterlab_pygments/blob/main/LICENSE
jupyterlab-widgets	http://jupyter.org	https://github.com/jupyter-widgets/ipywidgets/blob/master/LICENSE
jupyter-lab_pygments	https://github.com/jupyterlab/jupyterlab_pygments	https://github.com/jupyterlab/jupyterlab_pygments?tab=BSD-3-Clause-1-ov-file#readme
jupyterlab_server	https://github.com/jupyterlab/jupyterlab_server	https://github.com/jupyterlab/jupyterlab_server/blob/main/LICENSE
jupyterlab_widgets	https://github.com/jupyter-widgets/ipywidgets	https://github.com/jupyter-widgets/ipywidgets?tab=BSD-3-Clause-1-ov-file#readme
kaleido	https://github.com/plotly/Kaleido	https://github.com/plotly/Kaleido/blob/master/LICENSE.txt
keras	https://github.com/keras-team/keras	https://github.com/keras-team/keras/blob/master/LICENSE

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Name of Project	Website	License URL
Keras-Preprocessing	https://github.com/keras-team/keras-preprocessing	https://github.com/keras-team/keras-preprocessing/blob/master/LICENSE
keras-tuner	https://github.com/keras-team/keras-tuner	https://github.com/keras-team/keras-tuner/blob/master/LICENSE
keyring	https://github.com/jaraco/keyring	https://github.com/jaraco/keyring/blob/main/LICENSE
keyutils	https://github.com/sassoftware/python-keyutils	https://github.com/sassoftware/python-keyutils/blob/master/LICENSE
kiwisolver	https://kiwisolver.readthedocs.io/en/latest/	https://github.com/nucleic/kiwi/blob/main/LICENSE
kombu	https://kombu.readthedocs.io	https://github.com/celery/kombu/blob/master/LICENSE
krb5	https://web.mit.edu/kerberos/	https://github.com/krb5/krb5/blob/master/src/lib/gssapi/LICENSE
kt-legacy	https://github.com/haifeng-jin/kt-legacy	https://github.com/haifeng-jin/kt-legacy/blob/main/LICENSE
lark	https://github.com/lark-parser/lark	https://github.com/lark-parser/lark?tab=MIT-1-ov-file#readme
lazy_loader	https://github.com/scientific-python/lazy_loader	https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md
lcms2	https://www.littlecms.com	https://github.com/sk1project/python-lcms2/blob/master/LICENSE
legacy-cgi	https://github.com/jackrosenthal/legacy-cgi	https://github.com/jackrosenthal/legacy-cgi?tab=License-1-ov-file#readme

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Name of Project	Website	License URL
lerc	https://github.com/Esri/lerc	https://github.com/Esri/lerc/blob/master/LICENSE
libarchive	http://www.libarchive.org	https://raw.githubusercontent.com/libarchive/libarchive/master/COPYING
libblas	https://www.netlib.org/blas/	https://www.netlib.org/blas/#_licensing
libbrotlicommon	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libbrotlidec	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libbrotlienc	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libcblas	https://anaconda.org/conda-forge/libcblas	N/A
libclang	https://github.com/sighingnow/libclang	https://github.com/sighingnow/libclang/blob/master/LICENSE.TXT
libcurl	https://curl.se/libcurl/	https://curl.se/docs/copyright.html
libcxx	https://github.com/llvm-mirror/libcxx	https://github.com/llvm-mirror/libcxx/blob/master/LICENSE.TXT
libdb	https://www.oracle.com/technology/software/products/berkeley-db/index.html	https://github.com/berkeleydb/libdb/blob/master/LEGAL
libdeflate	https://github.com/ebiggers/libdeflate	https://github.com/ebiggers/libdeflate/blob/master/COPYING
libedit	https://thrysoee.dk/editline/	http://www.netbsd.org/Goals/redistribution.html
libev	https://software.schmorp.de/pkg/libev.html	https://software.schmorp.de/pkg/libev.html

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Name of Project	Website	License URL
libexpat	https://libexpat.github.io/	https://github.com/libexpat/libexpat?tab=MIT-1-ov-file#readme
libffi	https://github.com/libffi/libffi	https://github.com/libffi/libffi/blob/master/LICENSE
libgcc	https://gcc.gnu.org/onlinedocs/gccint/Libgcc.html	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html
libgcrypt	https://gnupg.org/software/index.html	https://git.gnupg.org/cgi-bin/gitweb.cgi?p=libgcrypt.git;a=blob;f=COPYING.LIB;hb=HEAD
libgd	https://libgd.github.io	https://libgd.github.io/manuals/2.2.1/files/license-txt.html
libglib	https://github.com/PolMine/libglib	https://github.com/PolMine/libglib/blob/master/include/glib-2.0/glib.h
libiconv	https://www.gnu.org/software/libiconv/	https://www.gnu.org/software/libiconv/#downloading
libint	https://tinyurl.com/yvw97wbw	https://tinyurl.com/yvw97wbw
liblapack	http://www.netlib.org/lapack/	https://www.netlib.org/lapack/LICENSE.txt
liblapacke	https://anaconda.org/conda-forge/liblapacke	https://www.netlib.org/lapack/LICENSE.txt
liblzma	https://tukaani.org/xz/	https://git.tukaani.org/?p=xz.git;a=blob;f=COPYING.0BSD
libmamba	https://medium.com/@QuantStack/open-software-packag	https://github.com/mamba-org/mamba/blob/main/LICENSE

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Name of Project	Website	License URL
libmambapy	https://www.anaconda.com/blog/a-faster-conda-for-a-g	https://github.com/conda/conda-libmamba-solv/blob/main/LICENSE
libnetcdf	https://www.unidata.ucar.edu/software/netcdf/	https://www.unidata.ucar.edu/software/netcdf/copyright.html
libnghttp2	https://github.com/nghttp2/nghttp2	https://github.com/nghttp2/nghttp2/blob/master/COPYING
libnsl	https://github.com/thkukuk/libnsl	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html
libopenblas	https://www.openblas.net/	https://github.com/xianyi/OpenBLAS/blob/develop/LICENSE
libpng	https://www.libpng.org/pub/png/libpng.html	https://www.libpng.org/pub/png/src/libpng-LICENSE.txt
libpq	https://www.postgresql.org/	https://www.postgresql.org/about/licence/
librsvg	https://gitlab.gnome.org/GNOME/librsvg	https://gitlab.gnome.org/GNOME/librsvg/-/blob/main/COPYING.LIB
libsolv	https://github.com/openSUSE/libsolv	https://github.com/openSUSE/libsolv/blob/master/LICENSE.BSD
libsqlite	https://github.com/mackyle/sqlite	https://github.com/mackyle/sqlite?tab=License-1-ov-file#readme
libssh2	https://github.com/libssh2/libssh2	https://github.com/libssh2/libssh2/blob/master/COPYING
libstdcxx	https://gcc.gnu.org/	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html

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Name of Project	Website	License URL
libtiff	https://www.libtiff.org/	https://www.libtiff.org/misc.html
libtrust	https://github.com/docker/libtrust	https://github.com/docker/libtrust/blob/master/LICENSE
libuuid	https://sourceforge.net/projects/libuuid/	https://sourceforge.net/p/libuuid/code/ci/master/tree/COPYING
libuv	https://github.com/libuv/libuv	https://github.com/libuv/libuv/blob/v1.x/LICENSE
libwebp	https://chromium.googlesource.com/?format=HTML	https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE
libwebp-base	https://chromium.googlesource.com/?format=HTML	https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE
libxc	https://www.tddft.org/programs/libxc/	https://gitlab.com/libxc/libxc/-/blob/master/COPYING
libxcb	https://xcb.freedesktop.org	https://github.com/freedesktop/xcb-libxcb/blob/master/COPYING
libxcrypt	https://github.com/besser82/libxcrypt	https://github.com/besser82/libxcrypt?tab=LGPL-2.1-1-ov-file#readme
libxml2	https://git.gnome.org/browse/libxml2/	https://gitlab.gnome.org/GNOME/libxml2/-/blob/master/Copyright
libxmlsec1	https://github.com/lsh123/xmlsec	https://github.com/lsh123/xmlsec/blob/master/README
libxslt	https://gitlab.gnome.org/GNOME/libxslt/-/wikis/home	https://gitlab.gnome.org/GNOME/libxslt/-/blob/master/Copyright

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Name of Project	Website	License URL
libzlib	https://zlib.net	https://zlib.net/zlib_license.html
lightning-utilities	https://github.com/Lightning-AI/utilities	https://github.com/Lightning-AI/utilities?tab=Apache-2.0-1-ov-file#readme
lime	https://github.com/marcotcr/lime	https://github.com/marcotcr/lime/blob/master/LICENSE
linear-operator	https://github.com/cornellius-gp/linear_operator	https://github.com/cornellius-gp/linear_operator?tab=MIT-1-ov-file#readme
lit	http://llvm.org	https://releases.llvm.org/14.0.0/LICENSE.TXT
llvm-openmp	https://github.com/llvm-mirror/openmp	https://github.com/llvm-mirror/openmp/blob/master/LICENSE.txt
llvmlite	http://llvmlite.readthedocs.io	https://github.com/numba/llvmlite/blob/main/LICENSE
loader-utils	https://github.com/webpack/loader-utils	https://github.com/webpack/loader-utils/raw/master/LICENSE
logistro	https://github.com/geopozo/logistro	https://github.com/geopozo/logistro?tab=MIT-1-ov-file#readme
logomaker	https://logomaker.readthedocs.io/en/latest/	https://github.com/jbkinney/logomaker/blob/master/LICENSE
logrus	https://github.com/sirupsen/logrus	https://github.com/sirupsen/logrus/blob/master/LICENSE
logrus-airbrake-hook.v2	https://gopkg.in/gemnasium/logrus-airbrake-hook.v2	https://github.com/gemnasium/logrus-airbrake-hook/blob/v2.1.2/LICENSE
lxml	https://lxml.de	https://lxml.de/index.html#license

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Name of Project	Website	License URL
lz4-c	https://www.lz4.org/	https://github.com/lz4/lz4/blob/dev/LICENSE
lzo	https://www.oberhumer.com/opensource/lzo/	https://www.oberhumer.com/opensource/gpl.html
mamba	https://github.com/mamba-org/mamba	https://github.com/mamba-org/mamba?tab=BSD-3-Clause-1-ov-f readme
markdown	https://github.com/evilstreak/markdown-js	https://www.opensource.org/licenses/mit-license.php
markdown-it-py	https://github.com/executablebooks/markdown-it-py	https://github.com/executablebooks/markdown-it-py/blob/master/LICENSE
markupsafe	https://github.com/pallets/markupsafe/tree/main/src/markupsafe	https://github.com/pallets/markupsafe/tree/main?tab=BSD-3-Clause-1-ov-f
MarkupSafe	https://palletsprojects.com/p/markupsafe/	https://github.com/pallets/markupsafe/blob/main/LICENSE.rst
mashumaro	https://github.com/Fatal1ty/mashumaro	https://github.com/Fatal1ty/mashumaro
matplotlib	https://matplotlib.org	https://matplotlib.org/stable/users/project/license.html
matplotlib-base	https://matplotlib.org	https://matplotlib.org/stable/users/project/license.html
matplotlib-inline	https://github.com/ipython/matplotlib-inline	https://github.com/ipython/matplotlib-inline/blob/master/LICENSE
mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib/blob/main/LICENSE

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Name of Project	Website	License URL
mda_xdrlib	https://github.com/MDAnalysis/mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib?tab=License-1-ov-file#readme
mdtraj	https://www.mdtraj.org/	https://www.mdtraj.org/1.9.8.dev0/index.html#license
mdurl	https://github.com/markdown-it/mdurl	https://github.com/markdown-it/mdurl/blob/master/LICENSE
menuinst	https://github.com/conda/menuinst	https://github.com/conda/menuinst/blob/main/LICENSE.txt
mergo	https://github.com/imdario/mergo	https://github.com/imdario/mergo/blob/master/LICENSE
mistune	https://github.com/lepture/mistune	https://github.com/lepture/mistune/blob/master/LICENSE
mkl	https://github.com/rust-math/intel-mkl-src	https://github.com/rust-math/intel-mkl-src/blob/master/License.txt
mkl-fft	https://github.com/IntelPython/mkl_fft	https://github.com/IntelPython/mkl_fft/blob/master/LICENSE.txt
mkl-random	https://github.com/IntelPython/mkl_random	https://github.com/IntelPython/mkl_random/blob/master/LICENSE.txt
mkl-service	https://github.com/IntelPython/mkl-service	https://github.com/IntelPython/mkl-service/blob/master/LICENSE.txt
mkl_fft	http://github.com/IntelPython/mkl_fft	https://github.com/IntelPython/mkl_fft?tab=BSD-3-Clause-1-ov-file#readme

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Name of Project	Website	License URL
mkl_random	http://github.com/IntelPython/mkl_random	https://github.com/IntelPython/mkl_random?tab=BSD-3-Clause-1-ov-f readme
ml-dtypes	https://github.com/jax-ml/ml_dtypes	https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE
ml_dtypes	https://github.com/jax-ml/ml_dtypes	https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE
modelcif	https://github.com/ihmwg/python-modelcif	https://github.com/ihmwg/python-modelcif/blob/main/LICENSE
molecupy	https://molecupy.readthedocs.io/en/latest/	https://github.com/samirelanduk/atomium/blob/master/LICENSE
moment	https://github.com/moment/moment	https://github.com/moment/moment/raw/master/LICENSE
moment-precise-range-plugin	https://github.com/codebox/moment-precise-range	https://github.com/codebox/moment-precise-range raw/master/LICENSE.md
more-itertools	https://github.com/more-itertools/more-itertools	https://github.com/more-itertools/more-itertools/blob/master/LICENSE
mpiplus	https://github.com/choderalab/mpiplus	https://github.com/choderalab/mpiplus/blob/main/LICENSE
mpmath	http://mpmath.org/	https://github.com/mpmath/mpmath/blob/master/LICENSE
mrcfile	https://github.com/ccpem/mrcfile	https://github.com/ccpem/mrcfile/blob/master/LICENSE.txt

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Name of Project	Website	License URL
msgpack	https://msgpack.org/	https://github.com/msgpack/msgpack-python/blob/main/COPYING
multidict	https://github.com/aio-libs/multidict	https://github.com/aio-libs/multidict/blob/master/LICENSE
multierr	https://go.uber.org/multierr	https://github.com/uber-go/multierr/blob/master/LICENSE.txt
multiprocess	https://github.com/uqfoundation/multiprocess	https://github.com/uqfoundation/multiprocess/blob/master/LICENSE
munkres	https://software.clapper.org/munkres/	https://github.com/bmc/munkres/blob/master/LICENSE.md
myesui uuid	https://github.com/myesui/uuid	https://pkg.go.dev/github.com/myesui/uuid?tab=licenses
namex	https://github.com/bcgov/namex	https://github.com/bcgov/namex/blob/main/LICENSE
narwhals	https://github.com/narwhals-dev/narwhals	https://github.com/narwhals-dev/narwhals?tab=MIT-1-ov-file#readme
nbclassic	http://jupyter.org	https://github.com/jupyter/nbclassic/blob/main/LICENSE
nbclient	https://jupyter.org	https://github.com/jupyter/nbclient/blob/main/LICENSE
nbconvert	https://jupyter.org	https://github.com/jupyter/nbconvert/blob/main/LICENSE
nbformat	http://jupyter.org	https://github.com/jupyter/nbformat/blob/main/LICENSE

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Name of Project	Website	License URL
ncurses	https://invisible-island.net/ncurses/	https://invisible-island.net/ncurses/ncurses-license.html
ndfes	https://rutgerslbsr.gitlab.io/fe-toolkit/	https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE
ndindex	https://quansight-labs.github.io/ndindex/	https://github.com/Quansight-Labs/ndindex?tab=MIT-1-ov-file#readme
nest-asyncio	https://github.com/erdewit/nest_asyncio	https://github.com/erdewit/nest_asyncio/blob/master/LICENSE
nest_asyncio	https://github.com/erdewit/nest_asyncio	https://github.com/erdewit/nest_asyncio?tab=BSD-2-Clause-1-ov-f readme
netcdf-fortran	https://www.unidata.ucar.edu/software/netcdf/	https://www.unidata.ucar.edu/software/netcdf/copyright.html
netCDF4	http://github.com/Unidata/netcdf4-python	https://github.com/Unidata/netcdf4-python/blob/master/LICENSE
nettle	https://git.lysator.liu.se/nettle/nettle	https://git.lysator.liu.se/nettle/nettle/-/blob/master/AUTHORS?ref_type=heads
networkx	https://networkx.org	https://github.com/networkx/networkx/blob/main/LICENSE.txt
nfpm	https://github.com/goreleaser/nfpm	https://github.com/goreleaser/nfpm/blob/master/LICENSE.md
ng-tags-input	https://github.com/mbenford/ngTagsInput	https://github.com/mbenford/ngTagsInput
ng-toast	https://github.com/tameraydin/ngToast	https://github.com/tameraydin/ngToast

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Name of Project	Website	License URL
ngdraggable	https://github.com/fatlinesofcode/ngDraggable	https://github.com/fatlinesofcode/ngDraggable/raw/master/LICENSE.txt
ngVue	https://github.com/ngVue/ngVue	https://github.com/ngVue/ngVue/raw/master/LICENSE
nh3	https://nh3.readthedocs.io/en/latest/	https://github.com/messense/nh3/blob/main/LICENSE
nlohmann_json	https://github.com/nlohmann/json	https://github.com/nlohmann/json?tab=MIT-1-ov-file#readme
nlopt	https://nlopt.readthedocs.io/en/latest/NLopt_Python_Reference/	https://nlopt.readthedocs.io/en/latest/NLopt_License_and_Copyright/
nodejs	https://nodejs.org/en/	https://raw.githubusercontent.com/nodejs/node/master/LICENSE
nomkl	https://github.com/conda-forge/nomkl-feedstock	https://github.com/conda-forge/nomkl-feedstock/blob/main/LICENSE.txt
notebook	http://jupyter.org	https://github.com/jupyter/notebook/blob/main/LICENSE
notebook-shim	https://github.com/jupyter/notebook_shim	https://github.com/jupyter/notebook_shim
notebook_shim	http://jupyter.org	https://github.com/jupyter/notebook_shim/blob/main/LICENSE
numba	https://numba.pydata.org	https://github.com/numba/numba/blob/main/LICENSE
numcpus	https://github.com/tklauser/numcpus	https://github.com/tklauser/numcpus/blob/master/LICENSE

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Name of Project	Website	License URL
numexpr	https://github.com/pydata/numexpr	https://github.com/pydata/numexpr/blob/master/LICENSE.txt
numpy	https://numpy.org	https://github.com/numpy/numpy/blob/main/LICENSE.txt
numpy-base	https://numpy.org	https://github.com/numpy/numpy/blob/main/LICENSE.txt
numpydoc	https://numpydoc.readthedocs.io/en/latest/index.html	https://github.com/numpy/numpydoc/blob/main/LICENSE.txt
nvidia-cublas-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cublas-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-cupti-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-cupti-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-nvrtc-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-nvrtc-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-runtime-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-runtime-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cudnn-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/deeplearning/cudnn/sla/index.html
nvidia-cudnn-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/deeplearning/cudnn/sla/index.html

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Name of Project	Website	License URL
nvidia-cuEquivariance	https://github.com/NVIDIA/cuEquivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
nvidia-cufft-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cufft-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cufile-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html#
nvidia-curand-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-curand-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusolver-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusolver-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparse-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparse-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparselt-cu12	https://docs.nvidia.com/cuda/cusparselt/index.html	https://docs.nvidia.com/cuda/cusparselt/license.html
nvidia-ml-py	https://pypi.org/project/nvidia-ml-py/	https://pypi.org/project/nvidia-ml-py/
nvidia-nccl-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/hpc-sdk/eula/index.html
nvidia-nccl-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/hpc-sdk/eula/index.html
nvidia-nvjitlink-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html

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Name of Project	Website	License URL
nvidia-nvshmem-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-nvtx-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-nvtx-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
Oat++	https://oatpp.io/	https://github.com/oatpp/oatpp/blob/master/LICENSE
oauthlib	https://github.com/oauthlib/oauthlib	https://github.com/oauthlib/oauthlib/blob/master/LICENSE
ocl-icd	https://github.com/OCL-dev/ocl-icd	https://github.com/OCL-dev/ocl-icd/blob/master/COPYING
ocl-icd-system	https://github.com/conda-forge/ocl-icd-system-feedst	https://github.com/conda-forge/ocl-icd-system-feedst blob/main/LICENSE.txt
olefile	https://www.decalage.info/python/olefileio	https://olefile.readthedocs.io/en/latest/License.html
omegaconf	https://github.com/omry/omegaconf	https://github.com/omry/omegaconf/blob/master/LICENSE
OmegaFold	https://github.com/HeliXonProtein/OmegaFold/tree/main	https://github.com/HeliXonProtein/OmegaFold/blob/main/LICENSE
omnicanvas	https://omnicanvas.readthedocs.io/en/latest/	https://github.com/samirelanduk/omnicanvas/blob/master/LICENSE
OpenFF	https://openforcefield.org/	https://github.com/openforcefield/openff-forcefields
openff-amber-ff-ports	https://github.com/openforcefield/openff-amber-ff-ports	https://github.com/openforcefield/openff-amber-ff-ports blob/main/LICENSE

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Name of Project	Website	License URL
openff-forcefields	https://openforcefield.org	https://github.com/openforcefield/openff-forcefields/blob/master/LICENSE
openff-fragmenter	https://github.com/openforcefield/openff-fragmenter	https://github.com/openforcefield/openff-fragmenter/blob/main/LICENSE
openff-interchange	https://github.com/openforcefield/openff-interchange	https://github.com/openforcefield/openff-interchange/blob/main/LICENSE
openff-models	https://github.com/openforcefield/openff-models	https://github.com/openforcefield/openff-models/blob/main/LICENSE
openff-nagl	https://docs.openforcefield.org/projects/nagl/en/latest/?badge=latest	https://github.com/openforcefield/openff-nagl/blob/main/LICENSE
openff-nagl-models	https://github.com/openforcefield/openff-nagl-models	https://github.com/openforcefield/openff-nagl-models/blob/main/LICENSE
openff-toolkit	https://openforcefield.org	https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE
openff-toolkit-base	https://openforcefield.org	https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE
openff-units	https://github.com/openforcefield/openff-units	https://github.com/openforcefield/openff-units/blob/main/LICENSE
openff-utilities	https://github.com/openforcefield/openff-utilities	https://github.com/openforcefield/openff-utilities/blob/main/LICENSE
openjpeg	https://github.com/uclouvain/openjpeg	https://github.com/uclouvain/openjpeg/blob/master/LICENSE

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Name of Project	Website	License URL
openldap	https://www.openldap.org/software/repo.html	https://git.openldap.org/openldap/openldap/-/blob/master/LICENSE
OpenMM	https://openmm.org	https://docs.openmm.org/7.1.0/userguide/library.html#license
openmmtools	https://github.com/choderalab/openmmtools	https://github.com/choderalab/openmmtools/blob/main/LICENSE
openmoltools	https://github.com/choderalab/openmoltools	https://github.com/choderalab/openmoltools/blob/master/LICENSE
openpyxl	https://openpyxl.readthedocs.io/en/stable/	https://foss.heptapod.net/openpyxl/openpyxl/-/blob/branch/3.0/LICENCE.rst
openssl	https://www.openssl.org	https://github.com/openssl/openssl/blob/master/LICENSE.txt
opt-einsum	https://github.com/dgasmith/opt_einsum	https://github.com/dgasmith/opt_einsum/blob/master/LICENSE
opt_einsum	https://github.com/dgasmith/opt_einsum	https://github.com/dgasmith/opt_einsum/blob/main/LICENSE
OptKing	https://github.com/psi-rking/optking	https://github.com/psi-rking/optking/blob/master/LICENSE
optree	https://optree.readthedocs.io/en/latest/	https://github.com/metaopt/optree/blob/main/LICENSE
oscrypto	https://github.com/wbond/oscrypto	https://github.com/wbond/oscrypto/blob/master/LICENSE
overrides	https://github.com/mkorpela/overrides	https://github.com/mkorpela/overrides/blob/main/LICENSE

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Name of Project	Website	License URL
packaging	https://github.com/pypa/packaging	https://github.com/pypa/packaging/blob/main/LICENSE
packmol	https://leandro.iqm.unicamp.br/m3g/packmol/home.shtml	https://github.com/m3g/packmol/blob/master/LICENSE
packmol_memgen	http://cpclab.uni-duesseldorf.de/	https://gitlab.com/cbjh/memgen/py-memgen/-/blob/main/LICENSE
pandas	https://pandas.pydata.org	https://github.com/pandas-dev/pandas/blob/main/LICENSE
pandocfilters	http://github.com/jgm/pandocfilters	https://github.com/jgm/pandocfilters/blob/master/LICENSE
panedr	https://github.com/MDAnalysis/panedr	https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt
pango	https://pango.gnome.org	https://gitlab.gnome.org/GNOME/pango/-/blob/main/COPYING
ParmEd	https://parmed.github.io/ParmEd/html/index.html	https://github.com/ParmEd/ParmEd#license
parser	https://github.com/typescript-eslint/typescript-eslint	https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE
parso	https://parso.readthedocs.io/en/latest/	https://github.com/davidhalter/parso/blob/master/LICENSE.txt
pathos	https://github.com/uqfoundation/pathos	https://github.com/uqfoundation/pathos/blob/master/LICENSE
patsy	https://patsy.readthedocs.io/en/latest/	https://github.com/pydata/patsy/blob/master/LICENSE.txt

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Name of Project	Website	License URL
pbkdf2	https://golang.org/x/crypto/pbkdf2	https://cs.opensource.google/go/x/crypto/+/master:LICENSE
pbr	https://docs.openstack.org/pbr/latest/	https://opendev.org/openstack/pbr/src/branch/master/LICENSE
pcmsolver	https://pcmsolver.readthedocs.io/en/stable/	https://github.com/PCMSolver/pcmsolver/blob/master/LICENSE
pcre	https://www.pcre.org	https://www.pcre.org/licence.txt
pcre2	https://www.pcre.org	https://github.com/PCRE2Project/pcre2/blob/master/LICENCE
pdb4amber	https://github.com/Amber-MD/pdb4amber	https://github.com/Amber-MD/pdb4amber/blob/master/LICENSE
pdbfixer	https://github.com/openmm/pdbfixer	https://github.com/openmm/pdbfixer/blob/master/LICENSE
pexpect	https://pexpect.readthedocs.io/	https://github.com/pexpect/pexpect/blob/master/LICENSE
pgconn	https://github.com/jackc/pgconn	https://github.com/jackc/pgconn/blob/master/LICENSE
pgio	https://github.com/jackc/pgio	https://github.com/jackc/pgio/blob/master/LICENSE
pgpassfile	https://github.com/jackc/pgpassfile	https://github.com/jackc/pgpassfile/blob/master/LICENSE
pgproto3	https://github.com/jackc/pgproto3/v2	https://github.com/jackc/pgproto3/blob/master/LICENSE
pgtype	https://github.com/jackc/pgtype	https://github.com/jackc/pgtype/blob/master/LICENSE
pgx	https://github.com/jackc/pgx/v4	https://github.com/jackc/pgx/blob/v4.0.1/LICENSE

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Name of Project	Website	License URL
phonopy	https://github.com/phonopy/phono3py	https://github.com/phonopy/phono3py/blob/develop/LICENSE
pickleshare	https://github.com/pickleshare/pickleshare	https://github.com/pickleshare/pickleshare/blob/master/LICENSE
Pillow	https://python-pillow.org	https://github.com/python-pillow/Pillow/blob/main/LICENSE
Pint	https://pint.readthedocs.io/en/stable/	https://github.com/hgrecco/pint/blob/master/LICENSE
pip	https://pip.pypa.io/	https://github.com/pypa/pip/blob/main/LICENSE.txt
pip-licenses	https://github.com/raimon49/pip-licenses	https://github.com/raimon49/pip-licenses/blob/master/LICENSE
pixman	https://pixman.org	https://cgit.freedesktop.org/pixman/tree/COPYING
pkginfo	https://launchpad.net/pkginfo	https://bazaar.launchpad.net/~tseaver/pkginfo/trunk/view/head:/LICENSE.txt
pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme
pkgutil_resolve_name	https://github.com/graingert/pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme
platformdirs	https://github.com/platformdirs/platformdirs	https://github.com/platformdirs/platformdirs/blob/main/LICENSE

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Name of Project	Website	License URL
plotly	https://plotly.com/python/	https://github.com/plotly/plotly.py/blob/master/LICENSE.txt
plotly-orca	https://github.com/plotly/orca	https://github.com/plotly/orca/blob/master/LICENSE
plotly.js	https://github.com/plotly/plotly.js	https://github.com/plotly/plotly.js/raw/master/LICENSE
pluggy	https://pluggy.readthedocs.io/en/stable/index.html	https://github.com/pytest-dev/pluggy/blob/main/LICENSE
pooch	https://github.com/fatiando/pooch	https://github.com/fatiando/pooch/blob/main/LICENSE.txt
portalocker	https://github.com/WoLpH/portalocker	https://github.com/wolph/portalocker/blob/develop/LICENSE
pox	https://github.com/uqfoundation/pox	https://github.com/uqfoundation/pox/blob/master/LICENSE
ppft	https://github.com/uqfoundation/ppft	https://github.com/uqfoundation/ppft/blob/master/LICENSE
pq	https://github.com/lib/pq	https://github.com/lib/pq/blob/master/LICENSE.md
ProDy	http://www.csb.pitt.edu/ProDy	https://github.com/prody/ProDy/blob/master/LICENSE.rst
prometheus-client	https://github.com/prometheus/client_python	https://github.com/prometheus/client_python/blob/master/LICENSE
prometheus_client	https://github.com/prometheus/client_python	https://github.com/prometheus/client_python/blob/master/LICENSE
prompt-toolkit	https://python-prompt-toolkit.readthedocs.io/en/stable/	https://github.com/prompt-toolkit/python-prompt-toolkit/blob/master/LICENSE

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Name of Project	Website	License URL
prompt_toolkit	https://github.com/prompt-toolkit/python-prompt-toolki	https://github.com/prompt-toolkit/python-prompt-toolki tab=BSD-3-Clause-1-ov-f readme
propcache	https://github.com/aio-libs/propcache	https://github.com/aio-libs/propcache?tab=Apache-2.0-1-ov-file#readme
protobuf	https://google.golang.org/protobuf	https://github.com/protocolbuffers/protobuf-go/blob/master/LICENSE
psi4	https://psicode.org	https://github.com/psi4/psi4/blob/master/COPYING.LESSER
psutil	https://psutil.readthedocs.io/en/latest/	https://github.com/giampaolo/psutil/blob/master/LICENSE
psycopg2	https://psycopg.org/	https://github.com/psycopg/psycopg2/blob/master/LICENSE
PTable	https://github.com/kxxoling/PTable	https://github.com/kxxoling/PTable/blob/master/COPYING
pthread-stubs	https://xcb.freedesktop.org	https://github.com/freedesktop/xcb-pthread-stubs/blob/master/COPYING
ptyprocess	https://ptyprocess.readthedocs.io/en/latest/	https://github.com/pexpect/ptyprocess/blob/master/LICENSE
pure-eval	http://github.com/alexmojaki/pure_eval	http://github.com/alexmojaki/pure_eval/blob/master/LICENSE.txt
pure_eval	http://github.com/alexmojaki/pure_eval	https://github.com/alexmojaki/pure_eval?tab=MIT-1-ov-file#readme

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Name of Project	Website	License URL
py	https://py.readthedocs.io/en/latest/	https://github.com/pytest-dev/py/blob/master/LICENSE
py-cpuinfo	https://github.com/workhorsy/py-cpuinfo	https://github.com/workhorsy/py-cpuinfo/blob/master/LICENSE
pyasn1	https://github.com/etingof/pyasn1	https://github.com/etingof/pyasn1/blob/master/LICENSE.rst
pyasn1-modules	https://github.com/etingof/pyasn1-modules	https://github.com/etingof/pyasn1-modules/blob/master/LICENSE.txt
pyasn1_modules	https://pyasn1.readthedocs.io/en/latest/contents.html	https://github.com/pyasn1/pyasn1-modules?tab=BSD-2-Clause-1-ov-file#readme
pybind11	http://pybind11.readthedocs.io/en/stable/	https://github.com/pybind/pybind11/blob/master/LICENSE
pybind11-abi	https://github.com/pybind/pybind11	https://github.com/pybind/pybind11/blob/master/LICENSE
pybind11_global	http://pybind11.readthedocs.io/en/stable/	https://github.com/pybind/pybind11/blob/master/LICENSE
pycairo	https://pycairo.readthedocs.io/en/latest/index.html	https://github.com/pygobject/pycairo/blob/master/COPYING
pycosat	https://github.com/conda/pycosat	https://github.com/conda/pycosat/blob/main/LICENSE
pycparser	https://github.com/eliben/pycparser	https://github.com/eliben/pycparser/blob/master/LICENSE
pydantic	https://pydantic-docs.helpmanual.io	https://github.com/samuelcolvin/pydantic/blob/master/LICENSE

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Name of Project	Website	License URL
pydantic-core	https://github.com/pydantic/pydantic-core	https://github.com/pydantic/pydantic-core
pyedr	https://github.com/MDAnalysis/panedr	https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt
pyEMMA	http://github.com/markovmodel/PyEMMA	https://github.com/markovmodel/PyEMMA/blob/devel/LICENSE.txt
Pygments	https://pygments.org	https://github.com/pygments/pygments/blob/master/LICENSE
pygments	https://pygments.org/	https://github.com/pygments/pygments?tab=BSD-2-Clause-1-ov-file#readme
pygraphviz	https://pygraphviz.github.io	https://github.com/pygraphviz/pygraphviz/blob/main/LICENSE
pygtop	https://pygtop.readthedocs.io/en/latest/	https://github.com/samirelanduk/pygtop/blob/master/LICENSE
pyHanko	https://github.com/MatthiasValvekens/pyHanko	https://github.com/MatthiasValvekens/pyHanko/blob/master/LICENSE
pyhanko-certvalidator	https://github.com/MatthiasValvekens/certvalidator	https://github.com/MatthiasValvekens/certvalidator/blob/master/LICENSE
PyJWT	https://github.com/jpadilla/pyjwt	https://github.com/jpadilla/pyjwt/blob/master/LICENSE
pymbar	https://pymbar.org	https://github.com/choderalab/pymbar/blob/master/LICENSE
pynvml	https://github.com/gpuopenanalytics/pynvml	https://github.com/gpuopenanalytics/pynvml/blob/master/LICENSE.txt

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Name of Project	Website	License URL
pyOpenSSL	https://pyopenssl.org/	https://github.com/pyca/pyopenssl/blob/main/LICENSE
pyparsing	https://pyparsing-docs.readthedocs.io/en/latest/	https://github.com/pyparsing/pyparsing/blob/master/LICENSE
PyPDF3	https://github.com/sfneal/PyPDF3	https://github.com/sfneal/PyPDF3/blob/master/LICENSE
pyrsistent	http://github.com/tobgu/pyrsistent/	https://github.com/tobgu/pyrsistent/blob/master/LICENSE.mit
pysam	https://github.com/pysam-developers/pysam	https://github.com/pysam-developers/pysam/blob/master/COPYING
PySocks	https://github.com/Anorov/PySocks	https://github.com/Anorov/PySocks/blob/master/LICENSE
pytables	https://www.pytables.org	https://github.com/PyTables/PyTables/blob/master/LICENSE.txt
python	https://www.python.org/	https://docs.python.org/3/license.html
python-bidi	https://github.com/MeirKriheli/python-bidi	https://github.com/MeirKriheli/python-bidi/blob/master/COPYING
python-constraint	https://github.com/python-constraint/python-constraint	https://github.com/python-constraint/python-constraint/blob/master/LICENSE
python-dateutil	https://dateutil.readthedocs.io	https://github.com/dateutil/dateutil/blob/master/LICENSE
python-json-logger	http://github.com/madzak/python-json-logger	https://github.com/madzak/python-json-logger/blob/master/LICENSE

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Name of Project	Website	License URL
python-pptx	https://github.com/scanny/python-pptx	https://github.com/scanny/python-pptx/blob/master/LICENSE
python-ldap	https://www.python-ldap.org/	https://github.com/python-ldap/python-ldap/blob/python-ldap-3.4.0/LICENCE
python3-saml	https://github.com/onelogin/python3-saml	https://github.com/onelogin/python3-saml/blob/master/LICENSE
python_abi	https://github.com/conda-forge/python_abi-feedstock	https://github.com/conda-forge/python_abi-feedstock/blob/main/LICENSE.txt
pytorch-lightning	https://github.com/Lightning-AI/pytorch-lightning	https://github.com/Lightning-AI/pytorch-lightning/blob/master/LICENSE
pytz	https://pythonhosted.org/pytz	https://git.launchpad.net/pytz/tree/LICENSE.txt
pytz-deprecation-shim	https://github.com/pganssle/pytz-deprecation-shim	https://github.com/pganssle/pytz-deprecation-shim/blob/master/LICENSE
PyWavelets	https://github.com/PyWavelets/pywt	https://github.com/PyWavelets/pywt/blob/master/LICENSE
PyYAML	https://pyyaml.org/	https://github.com/yaml/pyyaml/blob/master/LICENSE
pyyml	No longer available	No longer available
pyzmq	https://pyzmq.readthedocs.io/en/latest/	https://github.com/zeromq/pyzmq/blob/main/COPYING.BSD
qcelemental	https://github.com/MolSSI/QCElemental	https://github.com/MolSSI/QCElemental/blob/master/LICENSE

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Name of Project	Website	License URL
qcengine	https://github.com/MolSSI/QCEngine	https://github.com/MolSSI/QCEngine/blob/master/LICENSE
qrcode	https://github.com/lincolnloop/python-qrcode	https://github.com/lincolnloop/python-qrcode/blob/main/LICENSE
ramda	https://github.com/ramda/ramda	https://github.com/ramda/ramda/raw/master/LICENSE.txt
rapidjson	https://rapidjson.org/	https://github.com/Tencent/rapidjson/blob/master/license.txt
rdkit	https://www.rdkit.org	https://github.com/rdkit/rdkit/blob/master/license.txt
re2	https://github.com/google/re2	https://github.com/google/re2/blob/main/LICENSE
readme-renderer	https://github.com/pypa/readme_renderer	https://github.com/pypa/readme_renderer/blob/main/LICENSE
redis-py	https://github.com/andymccurdy/redis-py	https://github.com/redis/redis-py/blob/master/LICENSE
referencing	https://github.com/python-jsonschema/referencing	https://github.com/python-jsonschema/referencing
regex	https://github.com/mrabarnett/mrab-regex	https://github.com/mrabarnett/mrab-regex/blob/hg/LICENSE.txt
reportlab	https://www.reportlab.com	https://www.reportlab.com/dev/docs/faq/#1.3
reproc	https://github.com/DaanDeMeyer/reproc	https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE
reproc-cpp	https://github.com/DaanDeMeyer/reproc	https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE

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Name of Project	Website	License URL
requests	https://requests.readthedocs.io	https://github.com/psf/requests/blob/main/LICENSE
requests-oauthlib	https://github.com/requests/requests-oauthlib	https://github.com/requests/requests-oauthlib/blob/master/LICENSE
requests-toolbelt	https://toolbelt.readthedocs.org	https://github.com/requests/toolbelt/blob/master/LICENSE
resumable	https://github.com/stevvooe/resumable	https://github.com/stevvooe/resumable/blob/master/LICENSE
retrying	https://github.com/rholder/retrying	https://github.com/rholder/retrying/blob/master/LICENSE
rfc3339-validator	https://github.com/naimetti/rfc3339-validator	https://github.com/naimetti/rfc3339-validator/blob/master/LICENSE
rfc3339_validator	https://github.com/naimetti/rfc3339-validator	https://github.com/naimetti/rfc3339-validator?tab=MIT-1-ov-file#readme
rfc3986	https://rfc3986.readthedocs.io/en/latest/	https://github.com/python-hyper/rfc3986/blob/main/LICENSE
rfc3986-validator	https://github.com/naimetti/rfc3986-validator	https://github.com/naimetti/rfc3986-validator/blob/master/LICENSE
rfc3987-syntax	https://github.com/willynilly/rfc3987-syntax	https://github.com/willynilly/rfc3987-syntax?tab=MIT-1-ov-file#readme
rich	https://github.com/Textualize/rich	https://github.com/Textualize/rich/blob/master/LICENSE

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Name of Project	Website	License URL
rich-argparse	https://github.com/hamdanal/rich-argparse	https://github.com/hamdanal/rich-argparse/blob/main/LICENSE
rlPyCairo	https://pypi.org/project/rlPyCairo/	https://hg.reportlab.com/hg-public/rlPyCairo/file/tip/rlPyCairo/LICENSE.txt
RocksDict	https://github.com/rocksdict/RocksDict	https://github.com/rocksdict/RocksDict?tab=MIT-1-ov-file#readme
roman-numerals	https://github.com/AA-Turner/roman-numerals	https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme
roman-numerals-py	https://github.com/AA-Turner/roman-numerals	https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme
rotary-embedding-torch	https://github.com/lucidrains/rotary-embedding-tor	https://github.com/lucidrains/rotary-embedding-tor blob/main/LICENSE
rpds-py	https://github.com/crate-py/rpds	https://github.com/crate-py/rpds
rpmpack	https://github.com/google/rpmpack	https://github.com/google/rpmpack/blob/master/LICENSE
rsa	https://stuvel.eu/rsa	https://github.com/sybrenstuvel/python-rsa/blob/main/LICENSE
ruamel-yaml	https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/	https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/LICENSE
ruamel.yaml.clib	https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/	https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/LICENSE

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Name of Project	Website	License URL
s3transfer	https://github.com/boto/s3transfer	https://github.com/boto/s3transfer/blob/develop/LICENSE.txt
sacrebleu	https://github.com/mjpost/sacrebleu	https://github.com/mjpost/sacrebleu/blob/master/LICENSE.txt
sapiens	https://github.com/Merck/Sapiens	https://github.com/Merck/Sapiens/blob/main/LICENSE
sasl	https://mellium.im/sasl	https://github.com/mellium/sasl/blob/main/LICENSE
scikit-gstat	https://mmaelicke.github.io/scikit-gstat/	https://github.com/mmaelicke/scikit-gstat/blob/main/LICENSE
scikit-image	https://scikit-image.org	https://scikit-image.org/docs/dev/license.html
scikit-learn	https://scikit-learn.org/stable/	https://github.com/scikit-learn/scikit-learn/blob/main/COPYING
scikit-learn-extra	https://github.com/scikit-learn-contrib/scikit-learn-extra	https://github.com/scikit-learn-contrib/scikit-learn-extra/blob/main/LICENSE
scikit-network	https://github.com/sknetwork-team/scikit-network	https://github.com/sknetwork-team/scikit-network?tab=License-1-ov-file#readme
scipy	https://scipy.org	https://github.com/scipy/scipy/blob/main/LICENSE.txt
seaborn	https://seaborn.pydata.org	https://github.com/mwaskom/seaborn/blob/master/LICENSE
seaborn-base	https://seaborn.pydata.org	https://github.com/mwaskom/seaborn/blob/master/LICENSE

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Name of Project	Website	License URL
semver	https://github.com/Masterminds/semver/v3	https://github.com/Masterminds/semver/blob/v3.0.3/LICENSE.txt
Send2Trash	https://github.com/arsenetar/send2trash	https://github.com/arsenetar/send2trash/blob/master/LICENSE
sentry-sdk	https://github.com/getsentry/sentry-python	https://github.com/getsentry/sentry-python/blob/master/LICENSE
setproctitle	https://github.com/dvarrazzo/py-setproctitle	https://github.com/dvarrazzo/py-setproctitle/blob/master/LICENSE
setuptools	https://github.com/pypa/setuptools	https://github.com/pypa/setuptools/blob/main/LICENSE
setuptools-scm	https://github.com/pypa/setuptools_scm/	https://github.com/pypa/setuptools_scm/blob/main/LICENSE
sh	https://github.com/amoffat/sh	https://github.com/amoffat/sh/blob/develop/LICENSE.txt
shellingham	https://github.com/sarugaku/shellingham	https://github.com/sarugaku/shellingham/blob/master/LICENSE
simdjson	https://github.com/simdjson/simdjson/tree/master	https://github.com/simdjson/simdjson/blob/master/LICENSE
simint	https://www.bennyp.org/research/simint/	https://github.com/simint-chem/simint-generator/blob/master/LICENSE
simplejson	https://github.com/simplejson/simplejson	https://github.com/simplejson/simplejson/blob/master/LICENSE.txt
six	https://github.com/benjaminp/six	https://github.com/benjaminp/six/blob/master/LICENSE

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Name of Project	Website	License URL
smirnoff99frosst	https://github.com/openforcefield/smirnoff99frosst	https://github.com/openforcefield/smirnoff99Frosst/blob/master/LICENSE
smmap	https://github.com/gitpython-developers/smmap	https://github.com/gitpython-developers/smmap/blob/master/LICENSE
snappy	https://github.com/google/snappy	https://github.com/google/snappy/blob/main/COPYING
sniffio	https://github.com/python-trio/sniffio	https://github.com/python-trio/sniffio/blob/master/LICENSE.MIT
snowballstemmer	https://github.com/snowballstem/snowball	https://github.com/snowballstem/snowball/blob/master/COPYING
soupsieve	https://github.com/facelessuser/soupsieve	https://github.com/facelessuser/soupsieve/blob/main/LICENSE.md
spdlog	https://github.com/gabime/spdlog	https://github.com/gabime/spdlog?tab=License-1-ov-file#readme
spglib	https://spglib.readthedocs.io/	https://github.com/spglib/spglib/blob/develop/COPYING
sphinx	https://github.com/sphinx-doc/sphinx	https://github.com/sphinx-doc/sphinx/blob/5.x/LICENSE
sphinxcontrib-applehelp	https://github.com/sphinx-doc/sphinxcontrib-applehe	https://github.com/sphinx-doc/sphinxcontrib-applehe blob/master/LICENSE
sphinxcontrib-devhelp	https://github.com/sphinx-doc/sphinxcontrib-devhelp	https://github.com/sphinx-doc/sphinxcontrib-devhelp blob/master/LICENSE
sphinxcontrib-htmlhelp	https://github.com/sphinx-doc/sphinxcontrib-htmlhel	https://github.com/sphinx-doc/sphinxcontrib-htmlhel blob/master/LICENSE

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Name of Project	Website	License URL
sphinxcontrib-jsmath	https://github.com/sphinx-doc/sphinxcontrib-jsmath	https://github.com/sphinx-doc/sphinxcontrib-jsmath/blob/master/LICENSE
sphinxcontrib-qthelp	https://github.com/sphinx-doc/sphinxcontrib-qthelp	https://github.com/sphinx-doc/sphinxcontrib-qthelp/blob/master/LICENSE
sphinxcontrib-serializinghtml	https://github.com/sphinx-doc/sphinxcontrib-serializ	https://github.com/sphinx-doc/sphinxcontrib-serializ blob/master/LICENSE
SQLAlchemy	https://www.sqlalchemy.org	https://docs.sqlalchemy.org/en/14/copyright.html
SQLAlchemy	https://www.sqlalchemy.org/	https://github.com/sqlalchemy/sqlalchemy?tab=MIT-1-ov-file#readme
sqlite	https://sqlite.org/index.html	https://sqlite.org/copyright.html
sqlparse	https://github.com/andialbrecht/sqlparse	https://github.com/andialbrecht/sqlparse/blob/master/LICENSE
stack-data	http://github.com/alexmojaki/stack_data	https://github.com/alexmojaki/stack_data/blob/master/LICENSE.txt
stack_data	http://github.com/alexmojaki/stack_data	https://github.com/alexmojaki/stack_data?tab=MIT-1-ov-file#readme
starfile	https://github.com/alisterburt/starfile	https://github.com/teamtomo/starfile/blob/main/LICENSE
statsmodels	https://github.com/statsmodels/statsmodels	https://github.com/statsmodels/statsmodels/blob/main/LICENSE.txt
structlog	https://www.structlog.org/	https://github.com/hynek/structlog/blob/main/LICENSE

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Name of Project	Website	License URL
streamlit	https://github.com/streamlit/streamlit	https://github.com/streamlit/streamlit/blob/develop/LICENSE
svglib	https://github.com/deeplook/svglib	https://github.com/deeplook/svglib/blob/master/LICENSE.txt
sympy	https://sympy.org	https://github.com/sympy/sympy/blob/master/LICENSE
tables	https://www.pytables.org/	https://github.com/PyTables/PyTables/blob/master/LICENSE.txt
tabulate	https://github.com/astanin/python-tabulate	https://github.com/astanin/python-tabulate/blob/master/LICENSE
tbb	https://github.com/oneapi-src/oneTBB	https://github.com/oneapi-src/oneTBB/blob/master/LICENSE.txt
tenacity	https://github.com/jd/tenacity	https://github.com/jd/tenacity/blob/master/LICENSE
tensorboard	https://github.com/tensorflow/tensorboard	https://github.com/tensorflow/tensorboard/blob/master/LICENSE
tensorboard-data-server	https://github.com/tensorflow/tensorboard	https://github.com/tensorflow/tensorboard/blob/master/LICENSE
tensorboard-plugin-wit	https://github.com/pair-code/what-if-tool	https://github.com/PAIR-code/what-if-tool/blob/master/LICENSE
tensorboardX	https://github.com/lanpa/tensorboardX	https://github.com/lanpa/tensorboardX/blob/master/LICENSE
tensorflow	https://github.com/tensorflow/tensorflow	https://github.com/tensorflow/tensorflow/blob/master/LICENSE

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Name of Project	Website	License URL
tensorflow-estimator	https://github.com/tensorflow/estimator	https://github.com/tensorflow/estimator/blob/master/LICENSE
tensorflow-io-gcs-filesystem	https://github.com/tensorflow/io	https://github.com/tensorflow/io/blob/master/LICENSE
tensorflow-probability	https://github.com/tensorflow/probability	https://github.com/tensorflow/probability/blob/main/LICENSE
termcolor	https://github.com/hugovk/termcolor	https://github.com/hugovk/termcolor/blob/main/COPYING.txt
terminado	https://github.com/jupyter/terminado	https://github.com/jupyter/terminado/blob/main/LICENSE
testpath	https://github.com/jupyter/testpath	https://github.com/jupyter/testpath/blob/master/LICENSE
textangular	https://github.com/fraywing/textAngular	https://github.com/fraywing/textAngular
texttable	https://github.com/foutaise/texttable/	https://github.com/foutaise/texttable/?tab=MIT-1-ov-file#readme
tf_keras	https://github.com/keras-team/keras-io	https://github.com/keras-team/keras-io/blob/master/LICENSE
tf_keras	https://github.com/keras-team/keras-io	https://github.com/keras-team/keras-io/blob/master/LICENSE
threadpoolctl	https://github.com/joblib/threadpoolctl	https://github.com/joblib/threadpoolctl/blob/master/LICENSE
three	https://github.com/mrdoob/three.js	https://github.com/mrdoob/three.js/raw/master/LICENSE

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Name of Project	Website	License URL
tifffile	https://github.com/cgohlke/tifffile/	https://github.com/cgohlke/tifffile/blob/master/LICENSE
tinycss2	https://github.com/Kozea/tinycss2/	https://github.com/Kozea/tinycss2/blob/master/LICENSE
tinyxml2	https://github.com/leethomason/tinyxml2	https://github.com/leethomason/tinyxml2/blob/master/LICENSE.txt
tk	https://www.tcl.tk/	https://www.tcl.tk/software/tcltk/license.html
toml	https://github.com/toml-lang/toml	https://github.com/toml-lang/toml/blob/main/LICENSE
tomli	https://github.com/hukkin/tomli	https://github.com/hukkin/tomli/blob/master/LICENSE
toolz	https://github.com/pytoolz/toolz	https://github.com/pytoolz/toolz/blob/master/LICENSE.txt
torch	https://pytorch.org/	https://pypi.org/project/torch/#license
torch-geometric	https://pyg.org/	https://github.com/pyg-team/pytorch_geometric?tab=MIT-1-ov-file#readme
torcheval	https://github.com/pytorch/torcheval	https://github.com/pytorch/torcheval?tab=License-1-ov-file#readme
torchmetrics	https://github.com/Lightning-AI/torchmetrics	https://github.com/Lightning-AI/torchmetrics?tab=Apache-2.0-1-ov-file#readme
tornado	https://www.tornadoweb.org	https://github.com/tornadoweb/tornado/blob/master/LICENSE

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Name of Project	Website	License URL		
tqdm	https://github.com/tqdm/tqdm	https://github.com/tqdm/tqdm/blob/master/LICENCE		
tracy	https://github.com/gear-genomics/tracy	https://github.com/gear-genomics/tracy/blob/main/LICENSE		
traitlets	https://github.com/ipython/traitlets	https://github.com/ipython/traitlets/blob/main/COPYING.md		
triton	https://github.com/openai/triton/	https://github.com/openai/triton/blob/main/LICENSE		
truststore	https://github.com/sethmlarson/trus	https://github.com/sethmlarson/truststore/blob/main/LICENSE		
truststore	https://github.com/sethmlarson/truststore	https://github.com/sethmlarson/truststore/blob/main/LICENSEtruststore	https://github.com/sethmlarson/truststore	https://github.com/sethmlarson/truststore/blob/main/LICENSE
ts-jest	https://github.com/kulshekhar/ts-jest	https://github.com/kulshekhar/ts-jest/raw/master/LICENSE.md		
ts-loader	https://github.com/TypeStrong/ts-loader	https://github.com/TypeStrong/ts-loader/raw/master/LICENSE		
twine	https://github.com/pypa/twine	https://github.com/pypa/twine/blob/main/LICENSE		
twinj uuid	https://github.com/twinj/uuid	https://github.com/twinj/uuid/blob/master/LICENSE		
types	https://github.com/babel/babel	https://github.com/babel/babel/raw/master/LICENSE		
types-python-dateutil	https://github.com/python/typeshed	https://github.com/python/typeshed?tab=License-1-ov-file#readme		
types-requests	https://pypi.org/project/types-requests/	https://github.com/python/typeshed/blob/main/LICENSE		

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Name of Project	Website	License URL
typescript	https://github.com/Microsoft/TypeScript	https://github.com/Microsoft/TypeScript/raw/master/LICENSE.txt
typing-inspection	https://github.com/pydantic/typing-inspection	https://github.com/pydantic/typing-inspection?tab=MIT-1-ov-file#readme
typing-utils	https://github.com/bojiang/typing_utils	https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme
typing_extensions	https://github.com/python/typing	https://github.com/python/typing/blob/master/LICENSE
typing_utils	https://github.com/bojiang/typing_utils	https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme
tzdata	https://github.com/python/tzdata	https://github.com/python/tzdata/blob/master/LICENSE
tzlocal	https://github.com/regebro/tzlocal	https://github.com/regebro/tzlocal/blob/master/LICENSE.txt
umf	https://github.com/oneapi-src/unified-memory-fram	https://github.com/oneapi-src/unified-memory-fram tab=License-1-ov-file#readme
umi-tools	https://github.com/CGATOxford/UMI-tools	https://github.com/CGATOxford/UMI-tools/blob/master/LICENSE
unicodedata2	https://github.com/fonttools/unicodedata2	https://github.com/fonttools/unicodedata2/blob/master/LICENSE
uri-template	https://gitlab.linss.com/open-source/python/uri-template	https://gitlab.linss.com/open-source/python/uri-template/-/blob/main/LICENSE
uritools	https://github.com/tkem/uritools/	https://github.com/tkem/uritools/blob/master/LICENSE

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Name of Project	Website	License URL		
urllib3	https://urllib3.readthedocs.io/	https://github.com/urllib3/urllib3/blob/main/LICENSE.txt		
vine	https://github.com/celery/vine	https://github.com/celery/vine/blob/master/LICENSE		
vue	https://github.com/vuejs/vue	https://github.com/vuejs/vue/raw/master/LICENSE		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readme		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readmewcwidth	https://github.com/jquast/wcwidth	https://github.com/jquast/wcwidth/blob/master/LICENSE
wandb	https://github.com/wandb/wandb	https://github.com/wandb/wandb/blob/main/LICENSE		
webcolors	https://github.com/ubernostrum/webcolors	https://github.com/ubernostrum/webcolors?tab=BSD-3-Clause-1-ov-file#readme		
webencodings	https://github.com/gsnedders/python-webencodings	https://github.com/gsnedders/python-webencodings/blob/master/LICENSE		
websocket-client	https://github.com/websocket-client/websocket-client.git	https://github.com/websocket-client/websocket-client/blob/master/LICENSE		
Werkzeug	https://palletsprojects.com/p/werkzeug/	https://werkzeug.palletsprojects.com/en/2.1.x/license/		
westpa	http://github.com/westpa/westpa	https://github.com/westpa/westpa/blob/westpa2/LICENSE		
wheel	https://github.com/pypa/wheel	https://github.com/pypa/wheel/blob/main/LICENSE.txt		

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Name of Project	Website	License URL
widgetsnbextension	https://github.com/jupyter-widgets/ipywidgets#readme	https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE
wrapt	https://github.com/GrahamDumpleton/wrapt	https://github.com/GrahamDumpleton/wrapt/blob/develop/LICENSE
wsutil	https://github.com/yhat/wsutil	https://github.com/yhat/wsutil/blob/master/LICENSE
x/lint	https://golang.org/x/lint	https://github.com/golang/lint/blob/master/LICENSE
x/mod	https://golang.org/x/mod/semver	https://cs.opensource.google/go/x/mod/+/master:LICENSE
x/net	https://golang.org/x/net	https://cs.opensource.google/go/x/net/+/master:LICENSE
x/oauth2	https://golang.org/x/oauth2	https://cs.opensource.google/go/x/oauth2/+/master:LICENSE
x/sys	https://golang.org/x/sys	https://cs.opensource.google/go/x/sys/+/master:LICENSE
x/text	https://golang.org/x/text	https://cs.opensource.google/go/x/text/+/master:LICENSE
x/tools	https://golang.org/x/tools	https://cs.opensource.google/go/x/tools/+/master:LICENSE
x/xerrors	https://golang.org/x/xerrors	https://cs.opensource.google/go/x/xerrors/+/master:LICENSE
xgboost	https://github.com/dmlc/xgboost	https://github.com/dmlc/xgboost/blob/master/LICENSE
xhtml2pdf	http://github.com/xhtml2pdf/xhtml2pdf	https://github.com/xhtml2pdf/xhtml2pdf/blob/master/LICENSE.txt

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Name of Project	Website	License URL
xlrd	https://github.com/python-excel/xlrd	https://github.com/python-excel/xlrd/blob/master/LICENSE
xlsxwriter	https://github.com/jmcnamara/XlsxWriter	https://github.com/jmcnamara/XlsxWriter/blob/main/LICENSE.txt
xmlsec	https://github.com/mehcode/python-xmlsec	https://github.com/mehcode/python-xmlsec/blob/master/LICENSE
xmltodict	https://github.com/martinblech/xmltodict	https://github.com/martinblech/xmltodict/blob/master/LICENSE
xorg-kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto/-/blob/master/COPYING
xorg-libice	https://gitlab.freedesktop.org/xorg/lib/libice	https://gitlab.freedesktop.org/xorg/lib/libice/-/blob/master/COPYING
xorg-libsm	https://gitlab.freedesktop.org/xorg/lib/libsm	https://gitlab.freedesktop.org/xorg/lib/libsm/-/blob/master/COPYING
xorg-libx11	https://gitlab.freedesktop.org/xorg/lib/libx11	https://gitlab.freedesktop.org/xorg/lib/libx11/-/blob/master/COPYING
xorg-libxau	https://gitlab.freedesktop.org/xorg/lib/libxau	https://gitlab.freedesktop.org/xorg/lib/libxau/-/blob/master/COPYING
xorg-libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp/-/blob/master/COPYING

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Name of Project	Website	License URL
xorg-libxext	https://gitlab.freedesktop.org/xorg/lib/libxext	https://gitlab.freedesktop.org/xorg/lib/libxext/-/blob/master/COPYING
xorg-libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender/-/blob/master/COPYING
xorg-libxt	https://gitlab.freedesktop.org/xorg/lib/libxt	https://gitlab.freedesktop.org/xorg/lib/libxt/-/blob/master/COPYING
xorg-renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto/-/blob/master/COPYING
xorg-xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto/-/blob/master/COPYING
xorg-xproto	https://gitlab.freedesktop.org/xorg/proto/xproto	https://gitlab.freedesktop.org/xorg/proto/xproto/-/blob/master/COPYING
xxhash	https://github.com/cespare/xxhash/v2	https://github.com/cespare/xxhash/blob/main/LICENSE.txt
xz	https://github.com/ulikunitz/xz	https://github.com/ulikunitz/xz/blob/master/LICENSE
yaml	https://pyyaml.org/	https://github.com/yaml/pyyaml/blob/master/LICENSE
yaml-cpp	https://github.com/jbeder/yaml-cpp	https://github.com/jbeder/yaml-cpp/blob/master/LICENSE
yaml.v2	https://gopkg.in/yaml.v2	https://github.com/go-yaml/yaml/blob/v2.4.0/LICENSE
yaml.v3	https://gopkg.in/yaml.v3	https://github.com/go-yaml/yaml/blob/v3/LICENSE

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Name of Project	Website	License URL
yarl	https://github.com/aio-libs/yarl/	https://github.com/aio-libs/yarl/blob/master/LICENSE
yaspin	https://github.com/pavdmyt/yaspin	https://github.com/pavdmyt/yaspin/blob/master/LICENSE
yfiles	https://www.yworks.com/products/yfiles	commercial license
yml	https://pypi.org/project/yml/	N/A
zap	https://go.uber.org/zap	https://github.com/uber-go/zap/blob/master/LICENSE.txt
zipp	https://github.com/jaraco/zipp	https://github.com/jaraco/zipp/blob/main/LICENSE
zlib	https://zlib.net/	https://zlib.net/zlib_license.html
zstandard	https://github.com/indygreg/python-zstandard	https://github.com/indygreg/python-zstandard/blob/main/LICENSE
zstd	https://facebook.github.io/zstd/	https://github.com/facebook/zstd/blob/dev/LICENSE
click-option-group	https://github.com/click-contrib/click-option-group	https://github.com/click-contrib/click-option-group/blob/master/LICENSE

9.1 GCC

On the Linux platform, The OpenEye toolkits are linked with the GCC libraries using an eligible compilation process under the terms of the GCC RUNTIME LIBRARY EXCEPTION (see below).

The OpenEye toolkits are NOT open source software and are NOT governed by GPL or other open source licenses. Your right to use the toolkits are governed by the OpenEye license which is binding to You.

For certain Linux distributions, GCC library components are included as object files. Your rights to use GCC library components (libstdc++, libgcc, and libgomp) included with these distributions are governed by the GPLv3 license as follows:

The components libstdc++, libgcc, and libgomp are part of GCC.

- GCC is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.
- GCC is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the

implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with GCC (see below). If not, see Licenses GNU Project .

Per GPLv3, section 6d, the source for GCC is available for download from the following location: GNU. The GCC library components included here are from version gcc-4.9.3 and are built using the standard instructions at Installing GCC.

9.1.1 GCC RUNTIME LIBRARY EXCEPTION

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Version 3.1, 31 March 2009

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When you use GCC to compile a program, GCC may combine portions of certain GCC header␣
↪files and runtime libraries with
the compiled program. The purpose of this Exception is to allow compilation of non-GPL␣
↪(including proprietary) programs
to use, in this way, the header files and runtime libraries covered by this Exception.

0. Definitions.

A file is an "Independent Module" if it either requires the Runtime Library for␣
↪execution after a Compilation Process,
or makes use of an interface provided by the Runtime Library, but is not otherwise based␣
↪on the Runtime Library.

"GCC" means a version of the GNU Compiler Collection, with or without modifications,␣
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↪use would permit combination with
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"Target Code" refers to output from any compiler for a real or virtual target processor␣
↪architecture, in executable
form or suitable for input to an assembler, loader, linker and/or execution phase.␣
↪Notwithstanding that, Target Code
does not include data in any format that is used as a compiler intermediate␣
↪representation, or used for producing a
compiler intermediate representation.
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The "Compilation Process" transforms code entirely represented in non-intermediate␣
↪languages designed for human-written
code, and/or in Java Virtual Machine byte code, into Target Code. Thus, for example, use␣
↪of source code generators and
preprocessors need not be considered part of the Compilation Process, since the␣
↪Compilation Process can be understood
as starting with the output of the generators or preprocessors.

A Compilation Process is "Eligible" if it is done using GCC, alone or with other GPL-
↪compatible software, or if it is
done without using any work based on GCC. For example, using non-GPL-compatible Software␣
↪to optimize any GCC intermediate
representations would not qualify as an Eligible Compilation Process.

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You have permission to propagate a work of Target Code formed by combining the Runtime␣
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↪Target Code was generated by
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↪your choice, consistent with the
licensing of the Independent Modules.

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The availability of this Exception does not imply any general presumption that third-
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See also

- http://www.gnu.org/licenses/gcc-exception.html

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  Some devices are designed to deny users access to install or run
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pattern of such abuse occurs in the area of products for individuals to
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stand ready to extend this provision to those domains in future versions
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  Finally, every program is threatened constantly by software patents.
States should not allow patents to restrict development and use of
software on general-purpose computers, but in those that do, we wish to
avoid the special danger that patents applied to a free program could
make it effectively proprietary.  To prevent this, the GPL assures that
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the interface presents a list of user commands or options, such as a
menu, a prominent item in the list meets this criterion.

  1. Source Code.

  The "source code" for a work means the preferred form of the work
for making modifications to it.  "Object code" means any non-source
form of a work.
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  A "Standard Interface" means an interface that either is an official
standard defined by a recognized standards body, or, in the case of
interfaces specified for a particular programming language, one that
is widely used among developers working in that language.

  The "System Libraries" of an executable work include anything, other
than the work as a whole, that (a) is included in the normal form of
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Component, and (b) serves only to enable use of the work with that
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"Major Component", in this context, means a major essential component
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  The "Corresponding Source" for a work in object code form means all
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work) run the object code and to modify the work, including scripts to
control those activities.  However, it does not include the work's
System Libraries, or general-purpose tools or generally available free
programs which are used unmodified in performing those activities but
which are not part of the work.  For example, Corresponding Source
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the work, and the source code for shared libraries and dynamically
linked subprograms that the work is specifically designed to require,
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   a) The work must carry prominent notices stating that you modified
   it, and giving a relevant date.

   b) The work must carry prominent notices stating that it is
   released under this License and any conditions added under section
   7.  This requirement modifies the requirement in section 4 to
   "keep intact all notices".
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    c) You must license the entire work, as a whole, under this
    License to anyone who comes into possession of a copy.  This
    License will therefore apply, along with any applicable section 7
    additional terms, to the whole of the work, and all its parts,
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works, which are not by their nature extensions of the covered work,
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"aggregate" if the compilation and its resulting copyright are not
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beyond what the individual works permit.  Inclusion of a covered work
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parts of the aggregate.

  6. Conveying Non-Source Forms.

  You may convey a covered work in object code form under the terms
of sections 4 and 5, provided that you also convey the
machine-readable Corresponding Source under the terms of this License,
in one of these ways:

  a) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by the
  Corresponding Source fixed on a durable physical medium
  customarily used for software interchange.

  b) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by a
  written offer, valid for at least three years and valid for as
  long as you offer spare parts or customer support for that product
  model, to give anyone who possesses the object code either (1) a
  copy of the Corresponding Source for all the software in the
  product that is covered by this License, on a durable physical
  medium customarily used for software interchange, for a price no
  more than your reasonable cost of physically performing this
  conveying of source, or (2) access to copy the
  Corresponding Source from a network server at no charge.

  c) Convey individual copies of the object code with a copy of the
  written offer to provide the Corresponding Source.  This
  alternative is allowed only occasionally and noncommercially, and
  only if you received the object code with such an offer, in accord
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   with subsection 6b.

   d) Convey the object code by offering access from a designated
   place (gratis or for a charge), and offer equivalent access to the
   Corresponding Source in the same way through the same place at no
   further charge.  You need not require recipients to copy the
   Corresponding Source along with the object code.  If the place to
   copy the object code is a network server, the Corresponding Source
   may be on a different server (operated by you or a third party)
   that supports equivalent copying facilities, provided you maintain
   clear directions next to the object code saying where to find the
   Corresponding Source.  Regardless of what server hosts the
   Corresponding Source, you remain obligated to ensure that it is
   available for as long as needed to satisfy these requirements.

   e) Convey the object code using peer-to-peer transmission, provided
   you inform other peers where the object code and Corresponding
   Source of the work are being offered to the general public at no
   charge under subsection 6d.

  A separable portion of the object code, whose source code is excluded
from the Corresponding Source as a System Library, need not be
included in conveying the object code work.

  A "User Product" is either (1) a "consumer product", which means any
tangible personal property which is normally used for personal, family,
or household purposes, or (2) anything designed or sold for incorporation
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doubtful cases shall be resolved in favor of coverage.  For a particular
product received by a particular user, "normally used" refers to a
typical or common use of that class of product, regardless of the status
of the particular user or of the way in which the particular user
actually uses, or expects or is expected to use, the product.  A product
is a consumer product regardless of whether the product has substantial
commercial, industrial or non-consumer uses, unless such uses represent
the only significant mode of use of the product.

  "Installation Information" for a User Product means any methods,
procedures, authorization keys, or other information required to install
and execute modified versions of a covered work in that User Product from
a modified version of its Corresponding Source.  The information must
suffice to ensure that the continued functioning of the modified object
code is in no case prevented or interfered with solely because
modification has been made.

  If you convey an object code work under this section in, or with, or
specifically for use in, a User Product, and the conveying occurs as
part of a transaction in which the right of possession and use of the
User Product is transferred to the recipient in perpetuity or for a
fixed term (regardless of how the transaction is characterized), the
Corresponding Source conveyed under this section must be accompanied
by the Installation Information.  But this requirement does not apply
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if neither you nor any third party retains the ability to install
modified object code on the User Product (for example, the work has
been installed in ROM).

  The requirement to provide Installation Information does not include a
requirement to continue to provide support service, warranty, or updates
for a work that has been modified or installed by the recipient, or for
the User Product in which it has been modified or installed.  Access to a
network may be denied when the modification itself materially and
adversely affects the operation of the network or violates the rules and
protocols for communication across the network.

  Corresponding Source conveyed, and Installation Information provided,
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