Helium 0.2 Quick Reference Card

Molecule

Molecule()
Molecule(Molecule **mol**)
Molecule(Molecule **mol**, List<Bool> **atoms**,
List<Bool> **bonds**, Bool **adjustHydrogens**)
Int **numAtoms**()
Iter<Atom> **atoms**()
Atom **atom**(Int **index**)
Atom **addAtom**()
Void **removeAtom**(Atom **atom**)
Int **numBonds**()
Iter<Bond> **bonds**()
Bond **bond**(Int **index**)
Bond **bond**(Atom **source**, Atom **target**)
Bond **addBond**()
Void **removeBond**(Bond **bond**)
Void **clear**()

Bond

Int **index**()
Atom **source**()
Atom **target**()
Atom **other**(Atom **atom**)
Int **order**()
Bool **isAromatic**()
Void **setAromatic**(Bool **value**)
Void **setOrder**(Int **value**)

Ring

Int **size**()
List<Atom> **atoms**()
Atom **atom**(Int **index**)
Bool **containsAtom**(Atom **atom**)
List<Bond> **bonds**()
Bond **bond**(Int **index**)
Bool **containsBond**(Bond **bond**)

Fingerprint [python]

Fingerprint(Int **numWords**)
String **bin**(Bool **spaces** = true)
String **hex**()
Void **zero**()
Int **count**()
Int **count**(Int **begin**, Int **end**)
Bool **__getitem__**(Int **index**)
Void **__setitem__**(Int **index**, Bool **value**)
Int **numWords**()

Atom

Int **index**()
Int **degree**()
Iter<Bond> **bonds**()
Iter<Atom> **nbrs**()
Bool **isAromatic**()
Int **element**()
Int **mass**()
Int **hydrogens**()
Int **charge**()
Bool **isHydrogen**()
Bool **isCarbon**()
Bool **isNitrogen**()
Bool **isOxygen**()
Bool **isPhosphorus**()
Bool **isSulfur**()
Int **heavyDegree**()
Int **boSum**()
Int **valence**()
Int **connectivity**()
Void **setAromatic**(Bool **value**)
Void **setElement**(Int **value**)
Void **setMass**(Int **value**)
Void **setHydrogens**(Int **value**)
Void **setCharge**(Int **value**)

Element

String **element**(Int **element**) [static]
Int **averageMass**(Int **element**) [static]
Bool **addHydrogens**(Int **element**) [static]
Int **valence**(Int **element**, Int **charge**,
int **degree**) [static]

RingSet

RingSet(Molecule **mol**)
Int **size**()
List<Ring> **rings**()
Ring **ring**(Int **index**)
Bool **isAtomInRing**(Atom **atom**)
Bool **isAtomInRingSize**(Atom **atom**, Int **size**)
Int **numRingNbrs**(Atom **atom**)
Int **numRings**(Atom **atom**)
Bool **isBondInRing**(Bond **bond**)
Bool **isBondInRingSize**(Bond **bond**, Int **size**)

DistanceMatrix

String **__str__**() [python]
Int **dim**()
Int **infinity**() [static]
Int **operator()**(Int **i**, Int **j**) [C++]
Int **__call__**(Int **i**, Int **j**) [python]

Error

String **what**() [C++]
operator bool() [C++]
Bool **__nonzero__**() [python]
String **__str__**() [python]

Smiles

Enum **Flags**: None, Mass, Charge, Hydrogens, Order, All
Smiles()
Bool **read**(String **smiles**, Molecule **mol**)
String **write**(Molecule **mol**, Flags **flags** = All)
String **write**(Molecule **mol**, List<Index> **order**, Flags **flags** = All)
String **writeCanonical**(Molecule **mol**)
Error **error**()

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Smarts

Smarts()
Bool init(String **smarts**)
Error error()
Bool requiresCycles()
Bool requiresExplicitHydrogens()
Bool findMapping(Molecule **mol**, RingSet **rings**, Mapping **mapping**, Bool **uniqueComponents** = false)
Bool findMapping(Molecule **mol**, Mapping **mapping**, Bool **uniqueComponents** = false)
Bool find(Molecule **mol**, RingSet **rings**, Bool **uniqueComponents** = false)
Bool find(Molecule **mol**, Bool **uniqueComponents** = false)

Mapping implementations: NoMapping.match, CountMapping.count, SingleMapping.map, MappingList.maps

Smirks

Smirks()
Void setFixMass(Bool **value**)
Void setFixHydrogens(Bool **value**)
Bool init(String **smirks**)
Bool init(String **reactants**, String **products**)
SmirksError error()
Bool requiresCycles()
Bool requiresExplicitHydrogens()
Bool apply(Molecule **mol**, RingSet **rings**)
Bool apply(Molecule **mol**)

SmirksError

Enum Type: None, NoReaction, ReactantSmarts, ProductSmarts, AtomClassPairWise, ProductContainsOr, ProductContainsNot, InvalidProductBond, ProductConflict

Type type()
String what()

MemoryMappedMoleculeFile

MemoryMappedMoleculeFile()
MemoryMappedMoleculeFile(String **filename**)
Void load(String **filename**)
Int numMolecules()
Bool readMolecule(Int **index**, Molecule **mol**)

MoleculeFile

MoleculeFile()
MoleculeFile(String **filename**)
Void load(String **filename**)
Int numMolecules()
Bool readMolecule(Molecule **mol**)
Bool readMolecule(Int **index**, Molecule **mol**)
Void close()

Free Functions

HYDROGENS

Void make_hydrogens_explicit(Molecule **mol**)
Void make_hydrogens_implicit(Molecule **mol**)
Void reset_implicit_hydrogens(Molecule **mol**)
Void reset_implicit_hydrogens(Molecule **mol**, Atom **atom**)

FINGERPRINTS

Int BitePerWord
Int bitvec_num_words_for_bits(Int **bits**)
Void bitvec_zero(Fingerprint **fp**)
Fingerprint bitvec_copy(Fingerprint **fp**)
Bool bitvec_get(Int **index**, Fingerprint **fp**)
Void bitvec_set(Int **index**, Fingerprint **fp**)
Void bitvec_reset(Int **index**, Fingerprint **fp**)
Int bitvec_count(Fingerprint **fp**)
Int bitvec_count(Fingerprint **fp**, Int **begin**, Int **end**)
String bitvec_to_binary(Fingerprint **fp**)
String bitvec_to_hex(Fingerprint **fp**)
Fingerprint bitvec_from_binary(String **bin**)
Fingerprint bitvec_from_hex(String **hex**)
Int bitvec_union_count(Fingerprint **fp1**, Fingerprint **fp2**)
Bool bitvec_is_subset_superset(Fingerprint **subset**, Fingerprint **superset**)

Real bitvec_tanimoto(Fingerprint **fp1**, Fingerprint **fp2**)
Real bitvec_tanimoto(Fingerprint **fp1**, Fingerprint **fp2**, Int **count1**, Int **count2**)
Real bitvec_cosine(Fingerprint **fp1**, Fingerprint **fp2**)
Real bitvec_cosine(Fingerprint **fp1**, Fingerprint **fp2**, Int **count1**, Int **count2**)
Real bitvec_hamming(Fingerprint **fp1**, Fingerprint **fp2**)
Real bitvec_hamming(Fingerprint **fp1**, Fingerprint **fp2**, Int **count1**, Int **count2**)
Real bitvec_forbes(Fingerprint **fp1**, Fingerprint **fp2**)
Real bitvec_forbes(Fingerprint **fp1**, Fingerprint **fp2**, Int **count1**, Int **count2**)
Real bitvec_russell_rao(Fingerprint **fp1**, Fingerprint **fp2**)

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DFSVisitor [base class]

Void **initialize**(Molecule **mol**)
Void **component**(Int **component**)
Void **atom**(Molecule **mol**, Atom **prev**, Atom **atom**)
Void **bond**(Molecule **mol**, Atom **prev**, Bond **bond**)
Void **backtrack**(Molecule **mol**, Atom **atom**)
Void **back_bond**(Molecule **mol**, Bond **bond**)
Bool **stop**()

Default implementations: DFSAtomOrderVisitor, DFSBondOrderVisitor, DFSDebugVisitor, DFSClosureRecorderVisitor

BFSVisitor [base class]

Void **initialize**(Molecule **mol**)
Void **component**(Int **component**)
Void **depth**(Int **depth**)
Void **atom**(Molecule **mol**, Atom **prev**, Atom **atom**)
Void **bond**(Molecule **mol**, Atom **prev**, Bond **bond**)
Void **back_bond**(Molecule **mol**, Bond **bond**)
Bool **stop**()

Default implementations: BFSAtomOrderVisitor, BFSBondOrderVisitor, BFSDebugVisitor, BFSClosureRecorderVisitor

AtomInvariant [base class]

Int **operator()**(Molecule **mol**, Atom **atom**) [C++]
Int **__call__**(Molecule **mol**, Atom **atom**) [python]

BondInvariant [base class]

Int **operator()**(Molecule **mol**, Bond **bond**) [C++]
Int **__call__**(Molecule **mol**, Bond **bond**) [python]

DefaultAtomInvariant

Enum **Invariants**: None, Element, Mass, Charge, Degree, Aromatic, All
DefaultAtomInvariant(Invariants **invariants** = All)

DefaultBondInvariant

Enum **Invariants**: None, Order, Aromatic, All
DefaultAtomInvariant(Invariants **invariants** = All)

Dijkstra

Dijkstra(Molecule **mol**, Atom **source**, Bool **preferSmallerIndexPaths** = false)
Int **infinity**()
Int **distance**(Atom **target**)
List<Atom> **path**(Atom **target**)

SubgraphCallback [base class]

Void **operator()**(Subgraph **subgraph**) [C++]
Void **__call__**(Subgraph **subgraph**) [python]

Subgraph

List<Bool> **hashable**()
List<Bool> **atoms**, **bonds**

Algorithms

DEPTH-FIRST SEARCH

Void **depth_first_search**(Molecule **mol**, DFSVisitor **visitor**)
Void **depth_first_search_mask**(Molecule **mol**, DFSVisitor **visitor**, List<Bool> **atomMask**)
Void **depth_first_search_mask**(Molecule **mol**, DFSVisitor **visitor**, List<Bool> **atomMask**, List<Bool> **bondMask**)
Void **depth_first_search**(Molecule **mol**, Atom **atom**, DFSVisitor **visitor**)
Void **depth_first_search_mask**(Molecule **mol**, Atom **atom**, DFSVisitor **visitor**, List<Bool> **atomMask**)
Void **depth_first_search_mask**(Molecule **mol**, Atom **atom**, DFSVisitor **visitor**, List<Bool> **atomMask**, List<Bool> **bondMask**)
Void **ordered_depth_first_search**(Molecule **mol**, List<Int> **order**, DFSVisitor **visitor**)
Void **exhaustive_depth_first_search**(Molecule **mol**, Atom **atom**, DFSVisitor **visitor**)

BREADTH-FIRST SEARCH

Void **breadth_first_search**(Molecule **mol**, BFSVisitor **visitor**)
Void **breadth_first_search_mask**(Molecule **mol**, BFSVisitor **visitor**, List<Bool> **atomMask**)
Void **breadth_first_search_mask**(Molecule **mol**, BFSVisitor **visitor**, List<Bool> **atomMask**, List<Bool> **bondMask**)
Void **breadth_first_search**(Molecule **mol**, Atom **atom**, BFSVisitor **visitor**)
Void **breadth_first_search_mask**(Molecule **mol**, Atom **atom**, BFSVisitor **visitor**, List<Bool> **atomMask**)
Void **breadth_first_search_mask**(Molecule **mol**, Atom **atom**, BFSVisitor **visitor**, List<Bool> **atomMask**, List<Bool> **bondMask**)

COMPONENTS

List<Int> **connected_bond_components**(Molecule **mol**)
List<Int> **connected_atom_components**(Molecule **mol**)
Int **num_connected_components**(Molecule **mol**)

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Algorithms (contd.)

CYCLES (RINGS)

Int **cyclomatic_number**(Molecule **mol**)
Int **cyclomatic_number**(Molecule **mol**, Int **numComponents**)
(List<Int, List<Int>) **cycle_membership**(Molecule **mol**) [python]
Void **cycle_membership**(Molecule **mol**, List<Bool> **cyclicAtoms**, List<Bool> **cyclicBonds**) [C++]
RingSet **relevant_cycles**(Molecule **mol**)
RingSet **relevant_cycles**(Molecule **mol**, List<Bool> **cyclicAtoms**, List<Bool> **cyclicBonds**)

FLOYD-WARSHALL SHORTEST PATH

DistanceMatrix **floyd_warshall**(Molecule **mol**)

MORGAN'S EXTENDED CONNECTIVITIES

List<Int> **extended_connectivities**(Molecule **mol**, AtomInvariant **invariant**)

CANONICALIZATION

(List<Int>, List<Int>) **canonicalize_component**(Molecule **mol**, List<Int> **symmetry**,
AtomInvariant **atomInvariant**, BondInvariant **bondInvariant**)
(List<Int>, List<Int>) **canonicalize**(Molecule **mol**, List<Int> **symmetry**,
AtomInvariant **atomInvariant**, BondInvariant **bondInvariant**,
List<Int> **atomComponents**, List<Int> **bondComponents**)

ENUMERATION

List<List<Int>> **enumerate_paths**(Molecule **mol**, Int **maxSize**)
Void **enumerate_subgraphs**(Molecule **mol**, SubgraphCallback **callback**, Int **maxSize**, Bool **onlyTrees**)

FINGERPRINTS

Fingerprint **path_fingerprint**(Molecule **mol**, Int **maxSize** = 7, Int **numWords** = 16, Int **hashPrime** = 1021)
Fingerprint **tree_fingerprint**(Molecule **mol**, Int **maxSize** = 7, Int **numWords** = 16, Int **hashPrime** = 1021)
Fingerprint **subgraph_fingerprint**(Molecule **mol**, Int **maxSize** = 7, Int **numWords** = 16,
Int **hashPrime** = 1021)