IsoSpec

1.95

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3.1 Class List

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- class ConfEqual
- class ConfOrder
- class ConfOrderMarginal
- class ConfOrderMarginalDescending
- class DirtyAllocator
- class Iso

  The Iso class for the calculation of the isotopic distribution.
- class IsoGenerator

  The generator of isotopologues.
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- class IsoThresholdGenerator
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- class ReverseOrder
- class SSummator
- class Summator
- class TableOrder
- class Tabulator
- class ThreadSummator
- class TSummator

Typedefs

- typedef int * **Conf**

Functions

- template<typename T >
  void **copyConf** (const T *source, T *destination, int dim)
- double **RationalApproximation** (double t)
- double **NormalCDFInverse** (double p)
- double **NormalCDFInverse** (double p, double mean, double stdev)
- double **NormalCDF** (double x, double mean, double stdev)
- double **NormalPDF** (double x, double mean, double stdev)
- int **str_to_int** (const string &s)
- unsigned int **parse_formula** (const char *formula, std::vector< const double *> &isotope_masses, std::vector< const double *> &isotope_probabilities, int **isotopeNumbers, int **atomCounts, unsigned int *confSize)
- void **printConfigurations** (const std::tuple< double *, double *, int *, int > &results, int dimNumber, int *isotopeNumbers)
- Conf initialConfigure (const int atomCnt, const int isotopeNo, const double *probs, const double *lprobs)
- void **printMarginal** (const std::tuple< double *, double *, int *, int > &results, int dim)
- double * getMLogProbs (const double *probs, int isoNo)
- double **get_loggamma_nominator** (int x)
- Conf **initialConfigure** (int atomCnt, int isotopeNo, const double *probs)
- double **combinedSum** (const int *conf, const std::vector< double > **valuesContainer, int dimNumber)
- int * **getConf** (void *conf)
- double **getLProb** (void *conf)
- double **unnormalized_logProb** (const int *conf, const double *logProbs, int dim)
- double **mass** (const int *conf, const double *masses, int dim)
- bool **tupleCmp** (std::tuple< double, double, int *> t1, std::tuple< double, double, int *> t2)
- template<typename T >
  void **printArray** (const T *array, int size)
- template<typename T >
  void **printVector** (const std::vector< T > &vec)
- template<typename T >
  void **printNestedArray** (const T **array, const int *shape, int size)
- template<typename T >
  void **dealloc_table** (T *tbl, int dim)
- void **reallocate** (double **array, int new_size)

Variables

- const int **elem_table_atomicNo** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const double **elem_table_mass** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const int **elem_table_massNo** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const int **elem_table_extraNeutrons** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const char * **elem_table_element** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const char * **elem_table_symbol** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const bool **elem_table_Radioactive** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const double **elem_table_probability** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const double **elem_table_log_probability** [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]
- const double **pi** = 3.14159265358979323846264338328
- double * **g_lfact_table** = reinterpret_cast<double*>(calloc(ISOSPEC_G_FACT_TABLE_SIZE, sizeof(double)))

4.1.1 Detailed Description

4.1.2 Function Documentation

4.1.2.1 getMLogProbs()

```
double* IsoSpec::getMLogProbs (
            const double * probs,
            int isoNo )
```

Here we order the processor to round the numbers up rather than down. Rounding down could result in the algorithm falling in an infinite loop because of the numerical instability of summing.

4.1.2.2 initialConfigure()

```
Conf IsoSpec::initialConfigure (
            const int atomCnt,
            const int isotopeNo,
            const double * probs,
            const double * lprobs )
```

Here we perform hill climbing to the mode of the marginal distribution (the subisotopologue distribution). We start from the point close to the mean of the underlying multinomial distribution.

Chapter 5

Class Documentation

5.1 IsoSpec::Allocator< T > Class Template Reference

Public Member Functions

- **Allocator** (const int dim, const int tabSize=10000)
- void **shiftTables** ()
- T * **newConf** ()
- T * **makeCopy** (const T *conf)
- T * **makeExternalCopy** (const T *conf)

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/allocator.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/allocator.cpp

5.2 IsoSpec::ConfEqual Class Reference

Public Member Functions

- **ConfEqual** (int dim)
- bool **operator()** (const int *conf1, const int *conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.3 IsoSpec::IsoSpec::ConfEqual Class Reference

Public Member Functions

- **ConfEqual** (int dim)
- bool **operator()** (const int *conf1, const int *conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.4 IsoSpec::ConfOrder Class Reference

Public Member Functions

- bool **operator()** (void ∗conf1, void ∗conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.5 IsoSpec::IsoSpec::ConfOrder Class Reference

Public Member Functions

- bool **operator()** (void ∗conf1, void ∗conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.6 IsoSpec::ConfOrderMarginal Class Reference

Public Member Functions

- **ConfOrderMarginal** (const double ∗logProbs, int dim)
- bool **operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.7 IsoSpec::IsoSpec::ConfOrderMarginal Class Reference

Public Member Functions

- **ConfOrderMarginal** (const double ∗logProbs, int dim)
- bool **operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.8 IsoSpec::ConfOrderMarginalDescending Class Reference

Public Member Functions

- **ConfOrderMarginalDescending** (const double *logProbs, int dim)
- bool **operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.9 IsoSpec::IsoSpec::ConfOrderMarginalDescending Class Reference

Public Member Functions

- **ConfOrderMarginalDescending** (const double *logProbs, int dim)
- bool **operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.10 IsoSpec::DirtyAllocator Class Reference

Public Member Functions

- **DirtyAllocator** (const int dim, const int tabSize=10000)
- void **shiftTables** ()
- void * **newConf** ()
- void * **makeCopy** (const void *conf)
- void * **makeExternalCopy** (const void *conf)

The documentation for this class was generated from the following files:

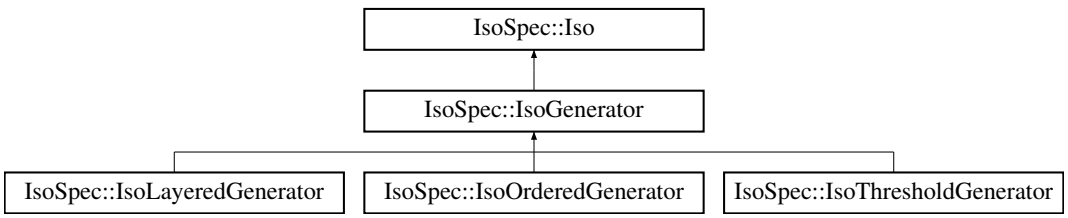
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/dirtyAllocator.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/dirtyAllocator.cpp

5.11 IsoSpec::Iso Class Reference

The Iso class for the calculation of the isotopic distribution.

`#include <isoSpec++.h>`

Inheritance diagram for IsoSpec::Iso:



Public Member Functions

- Iso (int _dimNumber, const int *_isotopeNumbers, const int *_atomCounts, const double *const *_isotope↩ Masses, const double *const *_isotopeProbabilities)

  General constructror.
- Iso (const char *formula)

  Constructor from the formula object.
- **Iso** (Iso &&other)
- **Iso** (const Iso &other, bool fullcopy)
- double getLightestPeakMass () const

  Get the mass of the lightest peak in the isotopic distribution.
- double getHeaviestPeakMass () const

  Get the mass of the heaviest peak in the isotopic distribution.
- double getModeLProb () const

  Get the log-probability of the mode-configuration (if there are many modes, they share this value).
- int getDimNumber () const

  Get the number of elements in the chemical formula of the molecule.
- int getAllDim () const

  Get the total number of isotopes of elements present in a chemical formula.
- PrecalculatedMarginal ** get_MT_marginal_set (double Lcutoff, bool absolute, int tabSize, int hashSize)

  Get the marginal distributions of subisotopologues.

Public Attributes

- bool disowned

Protected Attributes

- int dimNumber
- int * isotopeNumbers
- int * atomCounts
- unsigned int confSize
- int allDim
- Marginal ** marginals
- double modeLProb

5.11.1 Detailed Description

The Iso class for the calculation of the isotopic distribution.

It contains full description of the molecule for which one would like to calculate the isotopic distribution.

5.11.2 Constructor & Destructor Documentation

5.11.2.1 Iso()

```
IsoSpec::Iso::Iso (
            int _dimNumber,
            const int * _isotopeNumbers,
            const int * _atomCounts,
            const double *const * _isotopeMasses,
            const double *const * _isotopeProbabilities )
```

General constructror.

Parameters

_dimNumber	The number of elements in the formula, e.g. for C100H202 it would be 2, as there are only carbon and hydrogen atoms.
_isotopeNumbers	A table with numbers of isotopes for each element, e.g. for C100H202 it would be {2, 2}, because both C and H have two stable isotopes.
_atomCounts	Number of atoms of each element in the formula, e.g. for C100H202 corresponds to {100, 202}.
_isotopeMasses	A table of masses of isotopes of the elements in the chemical formula, e.g. {12.0, 13.003355, 1.007825, 2.014102} for C100H202.
_isotopeProbabilities	A table of isotope frequencies of the elements in the chemical formula, e.g. {.989212, .010788, .999885, .000115} for C100H202.

5.11.3 Member Function Documentation

5.11.3.1 get_MT_marginal_set()

```
PrecalculatedMarginal** IsoSpec::Iso::get_MT_marginal_set (
            double Lcutoff,
            bool absolute,
            int tabSize,
            int hashSize )
```

Get the marginal distributions of subisotopologues.

Parameters

Lcutoff	The logarithm of the cut off value.
absolute	Should the cutoff be in terms of absolute height of the peak, or relative to the height/probability of the mode.
tabSize	The size of the extension of the table with configurations.
hashSize	The size of the hash-table used to store subisotopologues and check if they have been already calculated.

5.11.4 Member Data Documentation

5.11.4.1 allDim

```
int IsoSpec::Iso::allDim  [protected]
```

The total number of isotopes of elements present in a chemical formula, e.g. for H20 it is 2+3=5.

5.11.4.2 atomCounts

```
int* IsoSpec::Iso::atomCounts  [protected]
```

A table with numbers of isotopes for each element.

5.11.4.3 confSize

```
unsigned int IsoSpec::Iso::confSize  [protected]
```

The number of bytes needed to represent the counts of isotopes present in the extended chemical formula.

5.11.4.4 dimNumber

```
int IsoSpec::Iso::dimNumber  [protected]
```

The number of elements in the chemical formula of the molecule.

5.11.4.5 disowned

```
bool IsoSpec::Iso::disowned
```

A variable showing if the Iso class was specialized by its child-class. If so, then the description of the molecules has been transfered there and Iso is a carcass class, dead as a dodo, an ex-class if you will.

5.11.4.6 isotopeNumbers

```
int* IsoSpec::Iso::isotopeNumbers  [protected]
```

A table with numbers of isotopes for each element.

5.11.4.7 marginals

```
Marginal** IsoSpec::Iso::marginals  [protected]
```

The table of pointers to the distributions of individual subisotopologues.

5.11.4.8 modeLProb

```
double IsoSpec::Iso::modeLProb  [protected]
```

The log-probability of the mode of the isotopic distribution.

The documentation for this class was generated from the following files:

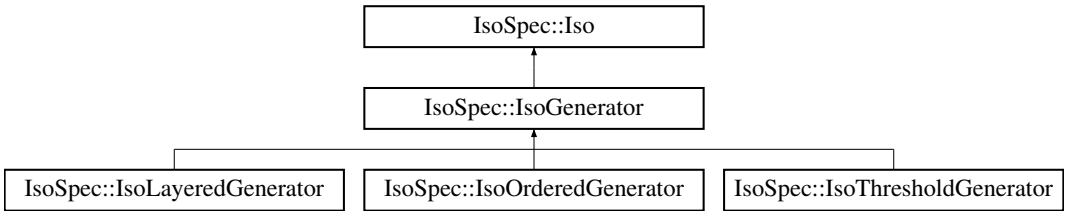
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.12 IsoSpec::IsoGenerator Class Reference

The generator of isotopologues.

`#include <isoSpec++.h>`

Inheritance diagram for IsoSpec::IsoGenerator:



Public Member Functions

- virtual bool advanceToNextConfiguration ()=0
- double **lprob** () const
- double **mass** () const
- double **eprob** () const
- virtual void **get_conf_signature** (int *space) const =0
- **IsoGenerator** (Iso &&iso)

Protected Attributes

- double * **partialLProbs**
- double * partialMasses
- double * partialExpProbs

Additional Inherited Members

5.12.1 Detailed Description

The generator of isotopologues.

This class provides the common interface for all isotopic generators.

5.12.2 Member Function Documentation

5.12.2.1 advanceToNextConfiguration()

```
virtual bool IsoSpec::IsoGenerator::advanceToNextConfiguration ( )  [pure virtual]
```

The prefix product of the probabilities of the current isotopologue.

Implemented in IsoSpec::IsoLayeredGenerator, IsoSpec::IsoThresholdGenerator, and IsoSpec::IsoOrderedGenerator.

5.12.3 Member Data Documentation

5.12.3.1 partialExpProbs

```
double* IsoSpec::IsoGenerator::partialExpProbs  [protected]
```

The prefix sum of the masses of the current isotopologue.

5.12.3.2 partialMasses

```
double* IsoSpec::IsoGenerator::partialMasses  [protected]
```

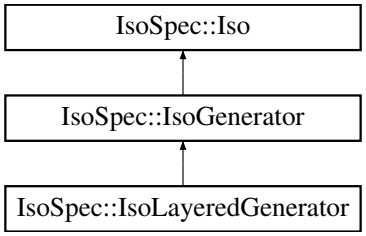
The prefix sum of the log-probabilities of the current isotopologue.

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.13 IsoSpec::IsoLayeredGenerator Class Reference

Inheritance diagram for IsoSpec::IsoLayeredGenerator:



Public Member Functions

- bool **advanceToNextConfiguration_internal** ()
- void **setup_delta** (double new_delta)
- bool advanceToNextConfiguration () override final
- bool **nextLayer** (double logCutoff_delta)
- **IsoLayeredGenerator** (Iso &&iso, double _delta=-3.0, int _tabSize=1000, int _hashSize=1000)
- void **get_conf_signature** (int *space) const override final
- void **terminate_search** ()

Additional Inherited Members

5.13.1 Member Function Documentation

5.13.1.1 advanceToNextConfiguration()

```
bool IsoSpec::IsoLayeredGenerator::advanceToNextConfiguration ( )  [inline], [final], [override],
[virtual]
```

The prefix product of the probabilities of the current isotopologue.

Implements IsoSpec::IsoGenerator.

The documentation for this class was generated from the following file:

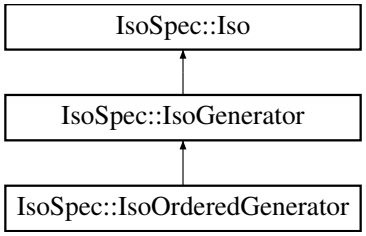
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h

5.14 IsoSpec::IsoOrderedGenerator Class Reference

The generator of isotopologues sorted by their probability of occurrence.

```
#include <isoSpec++.h>
```

Inheritance diagram for IsoSpec::IsoOrderedGenerator:



Public Member Functions

- bool advanceToNextConfiguration () override final
- void **get_conf_signature** (int *space) const override final
- **IsoOrderedGenerator** (Iso &&iso, int _tabSize=1000, int _hashSize=1000)

Additional Inherited Members

5.14.1 Detailed Description

The generator of isotopologues sorted by their probability of occurrence.

The subsequent isotopologues are generated with diminishing probability, starting from the mode. This algorithm take O(N*log(N)) to compute the N isotopologues because of using the Priority Queue data structure. Obtaining the N isotopologues can be achieved in O(N) if they are not required to be spit out in the descending order.

5.14.2 Member Function Documentation

5.14.2.1 advanceToNextConfiguration()

```
bool IsoSpec::IsoOrderedGenerator::advanceToNextConfiguration ( )  [final], [override], [virtual]
```

The prefix product of the probabilities of the current isotopologue.

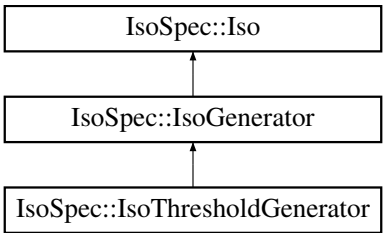
Implements IsoSpec::IsoGenerator.

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.15 IsoSpec::IsoThresholdGenerator Class Reference

Inheritance diagram for IsoSpec::IsoThresholdGenerator:



Public Member Functions

- bool advanceToNextConfiguration () override final
- void **get_conf_signature** (int *space) const override final
- **IsoThresholdGenerator** (Iso &&iso, double _threshold, bool _absolute=true, int _tabSize=1000, int _hash↩ Size=1000)
- void **terminate_search** ()

Additional Inherited Members

5.15.1 Member Function Documentation

5.15.1.1 advanceToNextConfiguration()

```
bool IsoSpec::IsoThresholdGenerator::advanceToNextConfiguration ( )  [final], [override],
[virtual]
```

The prefix product of the probabilities of the current isotopologue.

Implements IsoSpec::IsoGenerator.

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.16 IsoSpec::KeyHasher Class Reference

Public Member Functions

- **KeyHasher** (int dim)
- std::size_t **operator()** (const int *conf) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.17 IsoSpec::IsoSpec::KeyHasher Class Reference

Public Member Functions

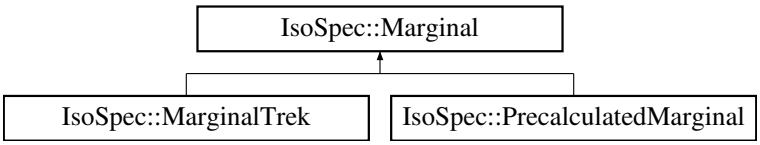
- **KeyHasher** (int dim)
- std::size_t **operator()** (const int *conf) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.18 IsoSpec::Marginal Class Reference

Inheritance diagram for IsoSpec::Marginal:



Public Member Functions

- **Marginal** (const double *_masses, const double *_probs, int _isotopeNo, int _atomCnt)
- **Marginal** (Marginal &other)=delete
- Marginal & **operator=** (const Marginal &other)=delete
- **Marginal** (Marginal &&other)
- int **get_isotopeNo** () const
- double **getLightestConfMass** () const
- double **getHeaviestConfMass** () const
- double **getModeLProb** () const
- double **getModeMass** () const
- double **getModeEProb** () const
- double **getSmallestLProb** () const
- double **logProb** (Conf conf) const

Protected Attributes

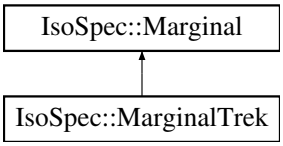
- const unsigned int **isotopeNo**
- const unsigned int **atomCnt**
- const double ∗const **atom_masses**
- const double ∗const **atom_lProbs**
- const double **loggamma_nominator**
- const Conf **mode_conf**
- const double **mode_lprob**
- const double **mode_mass**
- const double **mode_eprob**
- const double **smallest_lprob**

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.cpp

5.19 IsoSpec::MarginalTrek Class Reference

Inheritance diagram for IsoSpec::MarginalTrek:



Public Member Functions

- **MarginalTrek** (Marginal &&m, int tabSize=1000, int hashSize=1000)
- bool **probeConfigurationIdx** (int idx)
- int **processUntilCutoff** (double cutoff)
- const std::vector< double > & **conf_probs** () const
- const std::vector< double > & **conf_masses** () const
- const std::vector< int ∗ > & **confs** () const

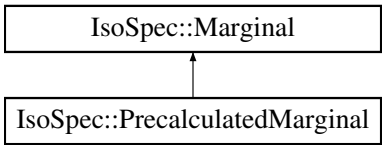
Additional Inherited Members

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.cpp

5.20 IsoSpec::PrecalculatedMarginal Class Reference

Inheritance diagram for IsoSpec::PrecalculatedMarginal:



Public Member Functions

- **PrecalculatedMarginal** (Marginal &&m, double lCutOff, bool sort=true, int tabSize=1000, int hash↩ Size=1000)
- bool **inRange** (unsigned int idx) const
- const double & **get_lProb** (int idx) const
- const double & **get_eProb** (int idx) const
- const double & **get_mass** (int idx) const
- const double ∗ **get_lProbs_ptr** () const
- const double ∗ **get_masses_ptr** () const
- const Conf & **get_conf** (int idx) const
- unsigned int **get_no_confs** () const

Protected Attributes

- std::vector< Conf > configurations
- Conf ∗ **confs**
- unsigned int **no_confs**
- double ∗ **masses**
- double ∗ **lProbs**
- double ∗ **eProbs**
- Allocator< int > **allocator**

5.20.1 Member Data Documentation

5.20.1.1 configurations

```
std::vector<Conf> IsoSpec::PrecalculatedMarginal::configurations  [protected]
```

This class serves to calculate a set of isotopologues that is defined by the minimal probability threshold.

This works faster than if you did not know the threshold. If you have no idea about the threshold, you would need to call us, to change encode the layered version of the marginal.

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.cpp

5.21 IsoSpec::IsoSpec::ReverseOrder< T > Class Template Reference

Public Member Functions

- bool **operator()** (const T a, const T b) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.22 IsoSpec::ReverseOrder< T > Class Template Reference

Public Member Functions

- bool **operator()** (const T a, const T b) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.23 IsoSpec::SSummator Class Reference

Public Member Functions

- **SSummator** (SSummator &other)
- void **add** (double x)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/summator.h

5.24 IsoSpec::Summator Class Reference

Public Member Functions

- void **add** (double what)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/summator.h

5.25 IsoSpec::TableOrder< T > Class Template Reference

Public Member Functions

- **TableOrder** (const T *_tbl)
- bool **operator()** (unsigned int i, unsigned int j)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.26 IsoSpec::IsoSpec::TableOrder< T > Class Template Reference

Public Member Functions

- **TableOrder** (const T *_tbl)
- bool **operator()** (unsigned int i, unsigned int j)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.27 IsoSpec::Tabulator< T > Class Template Reference

Public Member Functions

- **Tabulator** (T *generator, bool get_masses, bool get_probs, bool get_lprobs, bool get_confs)
- double * **masses** ()
- double * **lprobs** ()
- double * **probs** ()
- int * **confs** ()
- size_t **confs_no** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/tabulator.h

5.28 IsoSpec::ThreadSummator Class Reference

Public Member Functions

- void **add** (double what)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/summator.h

5.29 IsoSpec::TSummator Class Reference

Public Member Functions

- void **add** (double what)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/summator.h

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