
ChemCoord Documentation

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CHAPTER 1

Features

- Molecules are reliably transformed between cartesian space and non redundant internal coordinates (Zmatrices). Dummy atoms are inserted and removed automatically on the fly if necessary.
- The created Zmatrix is not only a structure expressed in internal coordinates, it is a “chemical” Zmatrix. “Chemical” Zmatrix means, that e.g. distances are along bonds or dihedrals are defined as they are drawn in chemical textbooks (Newman projections).
- Analytical gradients for the transformations between the different coordinate systems are implemented.
- Performance intensive functions/methods are implemented with Fortran/C like speed using `numba`.
- Geometries may be defined with symbolic expressions using `sympy`
- Built on top of `pandas` with very similar syntax. This allows for example distinct label or row based indexing.
- It derived from my own work and I heavily use it during the day. So all functions are tested and tailored around the work flow in theoretical chemistry.
- The classes are safe to inherit from and can easily be customized.
- It is a python module ;)

2.1 Installation guide

A working python installation is required (2.7 and ≥ 3.5 are possible).

It is highly recommended to use this module in combination with [Ipython](#) and [jupyter](#). They come shipped by default with the [anaconda3](#) installer.

2.1.1 Unix

For the packaged versions, the following commands have to be executed in the terminal:

```
conda install -c mcocdawc chemcoord
```

or:

```
pip install chemcoord
```

For the up to date development version (experimental):

```
git clone https://github.com/mcocdawc/chemcoord.git
cd chemcoord
pip install .
```

2.1.2 Windows

Neither installation nor running the module are tested on windows. To the best of my knowledge it should work there as well. Just use the same steps as for UNIX.

2.2 Tutorial

Just follow the link to the example notebooks.

- Cartesian
- Zmat
- Transformation
- Gradients
- Advanced customisation

If you want to have an interactive session, just download the following [zip file](#), which contains all notebooks and coordinates.

2.3 Documentation

Contents:

2.3.1 Cartesian coordinates

Cartesian

The *Cartesian* class which is used to represent a molecule in cartesian coordinates.

<i>Cartesian</i> ([frame, atoms, coords, index, ...])	The main class for dealing with cartesian Coordinates.
---	--

chemcoord.Cartesian

```
class chemcoord.Cartesian (frame=None, atoms=None, coords=None, index=None, meta-  
                             data=None, _metadata=None)
```

The main class for dealing with cartesian Coordinates.

Mathematical Operations:

It supports binary operators in the logic of the scipy stack, but you need python3.x for using the matrix multiplication operator @.

The general rule is that mathematical operations using the binary operators + - * / @ and the unary operators + - abs are only applied to the ['x', 'y', 'z'] columns.

Addition/Subtraction/Multiplication/Division: If you add a scalar to a Cartesian it is added elementwise onto the ['x', 'y', 'z'] columns. If you add a 3-dimensional vector, list, tuple... the first element of this vector is added elementwise to the 'x' column of the Cartesian instance and so on. The last possibility is to add a matrix with `shape=(len(Cartesian), 3)` which is again added elementwise. The same rules are true for subtraction, division and multiplication.

Matrixmultiplication: Only leftsided multiplication with a matrix of `shape=(n, 3)`, where n is a natural number, is supported. The usual usecase is for example `np.diag([1, 1, -1]) @ cartesian_instance` to mirror on the x-y plane.

Indexing:

The indexing behaves like Indexing and Selecting data in [Pandas](#). You can slice with `loc()`, `iloc()` and `Cartesian[...]`. The only question is about the return type. If the information in the columns is enough to draw a molecule, an instance of the own class (e.g. `Cartesian`) is returned. If the information in the columns is not enough to draw a molecule, there are two cases to consider:

- A `Series` instance is returned for one dimensional slices.
- A `DataFrame` instance is returned in all other cases.

This means that:

```
molecule.loc[:, ['atom', 'x', 'y', 'z']] returns a Cartesian.
molecule.loc[:, ['atom', 'x']] returns a pandas.DataFrame.
molecule.loc[:, 'atom'] returns a pandas.Series.
```

Comparison:

Comparison for equality with `==` is supported. It behaves exactly like the equality comparison of DataFrames in [pandas](#). Amongst other things this means that the index has to be the same and the comparison of floating point numbers is exact and not numerical. For this reason you rarely want to use `==`. Usually the question is “are two given molecules chemically the same”. For this comparison you have to use the function `allclose()`, which moves to the barycenter, aligns along the principal axes of inertia and compares numerically.

Chemical Methods

<code>__init__</code> (frame, atoms, coords, index, ...)	How to initialize a Cartesian instance.
<code>get_bonds</code> (self_bonding_allowed, offset, ...)	Return a dictionary representing the bonds.
<code>restrict_bond_dict</code> (bond_dict)	Restrict a bond dictionary to self.
<code>get_fragment</code> (list_of_indextuples[, ...])	Get the indices of the atoms in a fragment.
<code>fragmentate</code> (give_only_index, use_lookup)	Get the indices of non bonded parts in the molecule.
<code>get_without</code> (fragments[, use_lookup])	Return self without the specified fragments.
<code>add_data</code> (new_cols)	Adds a column with the requested data.
<code>get_total_mass</code> ()	Returns the total mass in g/mol.
<code>get_electron_number</code> ([charge])	Return the number of electrons.
<code>get_coordination_sphere</code> (index_of_atom, ...)	Return a Cartesian of atoms in the n-th coordination sphere.
<code>partition_chem_env</code> (n_sphere, use_lookup)	This function partitions the molecule into subsets of the same chemical environment.

chemcoord.Cartesian.__init__

`Cartesian.__init__`(frame=None, atoms=None, coords=None, index=None, metadata=None, _metadata=None)

How to initialize a Cartesian instance.

Parameters

- **frame** (`pd.DataFrame`) – A Dataframe with at least the columns ['atom', 'x', 'y', 'z']. Where 'atom' is a string for the elementsymbol.
- **atoms** (`sequence`) – A list of strings. (Elementsymbols)
- **coords** (`sequence`) – A `n_atoms * 3` array containing the positions of the atoms. Note that atoms and coords are mutually exclusive to frame. Besides atoms and coords have to be both either None or not None.

Returns A new cartesian instance.

Return type *Cartesian*

chemcoord.Cartesian.get_bonds

`Cartesian.get_bonds` (*self_bonding_allowed=False*, *offset=3*, *modified_properties=None*, *use_lookup=False*, *set_lookup=True*, *atomic_radius_data=None*)

Return a dictionary representing the bonds.

Warning: This function is **not sideeffect free**, since it assigns the output to a variable `self._metadata['bond_dict']` if `set_lookup` is `True` (which is the default). This is necessary for performance reasons.

`.get_bonds()` will use or not use a lookup depending on `use_lookup`. Greatly increases performance if `True`, but could introduce bugs in certain situations.

Just imagine a situation where the *Cartesian* is changed manually. If you apply later on a method e.g. `get_zmat()` that makes use of `get_bonds()` the dictionary of the bonds may not represent the actual situation anymore.

You have two possibilities to cope with this problem. Either you just re-execute `get_bonds` on your specific instance, or you change the `internally_use_lookup` option in the settings. Please note that the internal use of the lookup variable greatly improves performance.

Parameters

- **modified_properties** (*dic*) – If you want to change the van der Waals radius of one or more specific atoms, pass a dictionary that looks like:

```
modified_properties = {index1: 1.5}
```

For global changes use the constants module.

- **offset** (*float*) –
- **use_lookup** (*bool*) –
- **set_lookup** (*bool*) –
- **self_bonding_allowed** (*bool*) –
- **atomic_radius_data** (*str*) – Defines which column of constants elements is used. The default is `atomic_radius_cc` and can be changed with `settings['defaults']['atomic_radius_data']`. Compare with `add_data()`.

Returns Dictionary mapping from an atom index to the set of indices of atoms bonded to.

Return type `dict`

chemcoord.Cartesian.restrict_bond_dict

`Cartesian.restrict_bond_dict` (*bond_dict*)

Restrict a bond dictionary to self.

Parameters **bond_dict** (*dict*) – Look into `get_bonds()`, to see examples for a `bond_dict`.

Returns bond dictionary

chemcoord.Cartesian.get_fragment

`Cartesian.get_fragment` (*list_of_indextuples*, *give_only_index=False*,
use_lookup=None)

Get the indices of the atoms in a fragment.

The `list_of_indextuples` contains all bondings from the molecule to the fragment. `[(1, 3), (2, 4)]` means for example that the fragment is connected over two bonds. The first bond is from atom 1 in the molecule to atom 3 in the fragment. The second bond is from atom 2 in the molecule to atom 4 in the fragment.

Parameters

- `list_of_indextuples` (*list*) –
- `give_only_index` (*bool*) – If `True` a set of indices is returned. Otherwise a new `Cartesian` instance.
- `use_lookup` (*bool*) – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`

Returns A set of indices or a new `Cartesian` instance.

chemcoord.Cartesian.fragmentate

`Cartesian.fragmentate` (*give_only_index=False*, *use_lookup=None*)

Get the indices of non bonded parts in the molecule.

Parameters

- `give_only_index` (*bool*) – If `True` a set of indices is returned. Otherwise a new `Cartesian` instance.
- `use_lookup` (*bool*) – Use a lookup variable for `get_bonds()`.
- `use_lookup` – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`

Returns A list of sets of indices or new `Cartesian` instances.

Return type `list`

chemcoord.Cartesian.get_without

`Cartesian.get_without` (*fragments*, *use_lookup=None*)

Return self without the specified fragments.

Parameters

- `fragments` – Either a list of `Cartesian` or a `Cartesian`.
- `use_lookup` (*bool*) – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`

Returns List containing `Cartesian`.

Return type `list`

chemcoord.Cartesian.add_data

`Cartesian.add_data` (*new_cols=None*)

Adds a column with the requested data.

If you want to see for example the mass, the colormap used in jmol and the block of the element, just use:

```
['mass', 'jmol_color', 'block']
```

The underlying `pd.DataFrame` can be accessed with `constants.elements`. To see all available keys use `constants.elements.info()`.

The data comes from the module `mendelev` written by Lukasz Mentel.

Please note that I added three columns to the `mendelev` data:

```
['atomic_radius_cc', 'atomic_radius_gv', 'gv_color',  
 'valency']
```

The `atomic_radius_cc` is used by default by this module for determining bond lengths. The three others are taken from the MOLCAS grid viewer written by Valera Veryazov.

Parameters

- **new_cols** (*str*) – You can pass also just one value. E.g. 'mass' is equivalent to ['mass']. If `new_cols` is `None` all available data is returned.
- **inplace** (*bool*) –

Returns

Return type *Cartesian*

`chemcoord.Cartesian.get_total_mass`

`Cartesian.get_total_mass()`

Returns the total mass in g/mol.

Parameters `None` –

Returns

Return type `float`

`chemcoord.Cartesian.get_electron_number`

`Cartesian.get_electron_number(charge=0)`

Returns the number of electrons.

Parameters **charge** (*int*) – Charge of the molecule.

Returns

Return type `int`

`chemcoord.Cartesian.get_coordination_sphere`

`Cartesian.get_coordination_sphere(index_of_atom, n_sphere=1,
 give_only_index=False, only_surface=True,
 exclude=None, use_lookup=None)`

Return a Cartesian of atoms in the n-th coordination sphere.

Connected means that a path along covalent bonds exists.

Parameters

- **index_of_atom** (*int*) –
- **give_only_index** (*bool*) – If `True` a set of indices is returned. Otherwise a new Cartesian instance.
- **n_sphere** (*int*) – Determines the number of the coordination sphere.
- **only_surface** (*bool*) – Return only the surface of the coordination sphere.
- **exclude** (*set*) – A set of indices that should be ignored for the path finding.
- **use_lookup** (*bool*) – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`

Returns A set of indices or a new Cartesian instance.

chemcoord.Cartesian.partition_chem_env

`Cartesian.partition_chem_env` (*n_sphere=4, use_lookup=None*)

This function partitions the molecule into subsets of the same chemical environment.

A chemical environment is specified by the number of surrounding atoms of a certain kind around an atom with a certain atomic number represented by a tuple of a string and a frozenset of tuples. The `n_sphere` option determines how many branches the algorithm follows to determine the chemical environment.

Example: A carbon atom in ethane has bonds with three hydrogen (atomic number 1) and one carbon atom (atomic number 6). If `n_sphere=1` these are the only atoms we are interested in and the chemical environment is:

```
('C', frozenset([('H', 3), ('C', 1)]))
```

If `n_sphere=2` we follow every atom in the chemical environment of `n_sphere=1` to their direct neighbours. In the case of ethane this gives:

```
('C', frozenset([('H', 6), ('C', 1)]))
```

In the special case of ethane this is the whole molecule; in other cases you can apply this operation recursively and stop after `n_sphere` or after reaching the end of branches.

Parameters

- `n_sphere` (*int*) –
- `use_lookup` (*bool*) – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`

Returns

The output will look like this:

```
{ (element_symbol, frozenset([tuples])) : set([indices]) }
```

A dictionary mapping **from a** chemical environment to the **set** of indices of atoms **in** this environment.

Return type `dict`

Manipulate

<code>cut_cuboid</code> ([a, b, c, origin, ...])	Cut a cuboid specified by edge and radius.
<code>cut_sphere</code> ([radius, origin, outside_sliced, ...])	Cut a sphere specified by origin and radius.
<code>basistransform</code> (new_basis[, old_basis, ...])	Transform the frame to a new basis.
<code>align</code> (other[, indices, ignore_hydrogens])	Align two Cartesians.
<code>reindex_similar</code> (other[, n_sphere])	Reindex <code>other</code> to be similarly indexed as self.
<code>change_numbering</code> (rename_dict[, in-place])	Return the reindexed version of Cartesian.
<code>subs</code> (*args)	Substitute a symbolic expression in ['x', 'y', 'z']

chemcoord.Cartesian.cut_cuboid

Cartesian.**cut_cuboid**(*a=20, b=None, c=None, origin=None, outside_sliced=True, preserve_bonds=False*)

Cut a cuboid specified by edge and radius.

Parameters

- **a** (*float*) – Value of the a edge.
- **b** (*float*) – Value of the b edge. Takes value of a if None.
- **c** (*float*) – Value of the c edge. Takes value of a if None.
- **origin** (*list*) – Please note that you can also pass an integer. In this case it is interpreted as the index of the atom which is taken as origin.
- **outside_sliced** (*bool*) – Atoms outside/inside the sphere are cut away.
- **preserve_bonds** (*bool*) – Do not cut covalent bonds.

Returns

Return type *Cartesian*

chemcoord.Cartesian.cut_sphere

Cartesian.**cut_sphere**(*radius=15.0, origin=None, outside_sliced=True, preserve_bonds=False*)

Cut a sphere specified by origin and radius.

Parameters

- **radius** (*float*) –
- **origin** (*list*) – Please note that you can also pass an integer. In this case it is interpreted as the index of the atom which is taken as origin.
- **outside_sliced** (*bool*) – Atoms outside/inside the sphere are cut out.
- **preserve_bonds** (*bool*) – Do not cut covalent bonds.

Returns

Return type *Cartesian*

chemcoord.Cartesian.basistransform

Cartesian.**basistransform**(*new_basis, old_basis=None, orthonormalize=True*)

Transform the frame to a new basis.

This function transforms the cartesian coordinates from an old basis to a new one. Please note that *old_basis* and *new_basis* are supposed to have full Rank and consist of three linear independent vectors. If *rotate_only* is True, it is asserted, that both bases are orthonormal and right handed. Besides all involved matrices are transposed instead of inverted. In some applications this may require the function `xyz_functions.orthonormalize()` as a previous step.

Parameters

- **old_basis** (*np.array*) –
- **new_basis** (*np.array*) –
- **rotate_only** (*bool*) –

Returns The transformed molecule.

Return type *Cartesian*

chemcoord.Cartesian.align

Cartesian.**align**(*other, indices=None, ignore_hydrogens=False*)

Align two Cartesians.

Minimize the RMSD (root mean squared deviation) between `self` and `other`. Returns a tuple of copies of `self` and `other` where both are centered around their centroid and `other` is rotated unto `self`. The rotation minimises the distances between the atom pairs of same label. Uses the Kabsch algorithm implemented within `get_kabsch_rotation()`

Note: If `indices` is `None`, then `len(self) == len(other)` must be true and the elements in each index have to be the same.

Parameters

- **other** (*Cartesian*) –
- **indices** (*sequence*) – It is possible to specify a subset of indices that is used for the determination of the best rotation matrix:

```
[[i1, i2, ...], [j1, j2, ...]]
```

If `indices` is given in this form, the rotation matrix minimises the distance between `i1` and `j1`, `i2` and `j2` and so on.

- **ignore_hydrogens** (*bool*) –

Returns

Return type *tuple*

chemcoord.Cartesian.reindex_similar

`Cartesian.reindex_similar(other, n_sphere=4)`

Reindex `other` to be similarly indexed as `self`.

Returns a reindexed copy of `other` that minimizes the distance for each atom to itself in the same chemical environment from `self` to `other`. Read more about the definition of the chemical environment in `Cartesian.partition_chem_env()`

Note: It is necessary to align `self` and `other` before applying this method. This can be done via `align()`.

Note: It is probably necessary to improve the result using `change_numbering()`.

Parameters

- **other** (*Cartesian*) –
- **n_sphere** (*int*) – Wrapper around the argument for `partition_chem_env()`.

Returns Reindexed version of `other`

Return type *Cartesian*

chemcoord.Cartesian.change_numbering

`Cartesian.change_numbering(rename_dict, inplace=False)`

Return the reindexed version of `Cartesian`.

Parameters `rename_dict` (*dict*) – A dictionary mapping integers on integers.

Returns A renamed copy according to the dictionary passed.

Return type *Cartesian*

chemcoord.Cartesian.subs

Cartesian.**subs** (*args)

Substitute a symbolic expression in ['x', 'y', 'z']

This is a wrapper around the substitution mechanism of `sympy`. Any symbolic expression in the columns ['x', 'y', 'z'] of `self` will be substituted with value.

Parameters

- **symb_expr** (*sympy expression*) –
- **value** –
- **perform_checks** (*bool*) – If `perform_checks` is `True`, it is asserted, that the resulting Zmatrix can be converted to cartesian coordinates. Dummy atoms will be inserted automatically if necessary.

Returns Cartesian with substituted symbolic expressions. If all resulting `sympy` expressions in a column are numbers, the column is recasted to 64bit float.

Return type *Cartesian*

Geometry

<code>get_bond_lengths(indices)</code>	Return the distances between given atoms.
<code>get_angle_degrees(indices)</code>	Return the angles between given atoms.
<code>get_dihedral_degrees(indices[, start_row])</code>	Return the dihedrals between given atoms.
<code>get_barycenter()</code>	Return the mass weighted average location.
<code>get_inertia()</code>	Calculate the inertia tensor and transforms along rotation axes.
<code>get_centroid()</code>	Return the average location.
<code>get_distance_to(origin, other_atoms, sort)</code>	Return a Cartesian with a column for the distance from origin.
<code>get_shortest_distance(other)</code>	Calculate the shortest distance between self and other

chemcoord.Cartesian.get_bond_lengths

Cartesian.**get_bond_lengths** (*indices*)

Return the distances between given atoms.

Calculates the distance between the atoms with indices `i` and `b`. The indices can be given in three ways:

- As simple list [`i`, `b`]
- As list of lists: [`[i1, b1]`, `[i2, b2]`...]
- As `pd.DataFrame` where `i` is taken from the index and `b` from the respective column 'b'.

Parameters **indices** (*list*) –

Returns Vector of angles in degrees.

Return type `numpy.ndarray`

chemcoord.Cartesian.get_angle_degrees

Cartesian.**get_angle_degrees** (*indices*)

Return the angles between given atoms.

Calculates the angle in degrees between the atoms with indices *i*, *b*, *a*. The indices can be given in three ways:

- As simple list [*i*, *b*, *a*]
- As list of lists: [[*i*₁, *b*₁, *a*₁], [*i*₂, *b*₂, *a*₂]...]
- As `pd.DataFrame` where *i* is taken from the index and *b* and *a* from the respective columns '*b*' and '*a*'.

Parameters `indices` (*list*) –

Returns Vector of angles in degrees.

Return type `numpy.ndarray`

`chemcoord.Cartesian.get_dihedral_degrees`

`Cartesian.get_dihedral_degrees` (*indices*, *start_row=0*)

Return the dihedrals between given atoms.

Calculates the dihedral angle in degrees between the atoms with indices *i*, *b*, *a*, *d*. The indices can be given in three ways:

- As simple list [*i*, *b*, *a*, *d*]
- As list of lists: [[*i*₁, *b*₁, *a*₁, *d*₁], [*i*₂, *b*₂, *a*₂, *d*₂]...]
- As `pandas.DataFrame` where *i* is taken from the index and *b*, *a* and *d* from the respective columns '*b*', '*a*' and '*d*'.

Parameters `indices` (*list*) –

Returns Vector of angles in degrees.

Return type `numpy.ndarray`

`chemcoord.Cartesian.get_barycenter`

`Cartesian.get_barycenter` ()

Return the mass weighted average location.

Parameters `None` –

Returns

Return type `numpy.ndarray`

`chemcoord.Cartesian.get_inertia`

`Cartesian.get_inertia` ()

Calculate the inertia tensor and transforms along rotation axes.

This function calculates the inertia tensor and returns a 4-tuple.

The unit is `amu * length-unit-of-xyz-file**2`

Parameters `None` –

Returns

The returned dictionary has four possible keys:

`transformed_Cartesian`: A *Cartesian* that is transformed to the basis spanned by the eigenvectors of the inertia tensor. The x-axis is the axis with the lowest inertia moment, the z-axis the one with the highest. Contains also a column for the mass

`diag_inertia_tensor`: A vector containing the ascendingly sorted inertia moments after diagonalization.

`inertia_tensor`: The inertia tensor in the old basis.

`eigenvectors`: The eigenvectors of the inertia tensor in the old basis. Since the `inertia_tensor` is hermitian, they are orthogonal and are returned as an orthonormal righthanded basis. The *i*-th eigenvector corresponds to the *i*-th eigenvalue in `diag_inertia_tensor`.

Return type `dict`

`chemcoord.Cartesian.get_centroid`

`Cartesian.get_centroid()`

Return the average location.

Parameters `None` –

Returns

Return type `numpy.ndarray`

`chemcoord.Cartesian.get_distance_to`

`Cartesian.get_distance_to` (*origin=None, other_atoms=None, sort=False*)

Return a Cartesian with a column for the distance from origin.

`chemcoord.Cartesian.get_shortest_distance`

`Cartesian.get_shortest_distance` (*other*)

Calculate the shortest distance between self and other

Parameters `Cartesian` – other

Returns

Returns a tuple *i*, *j*, *d* with the following meaning:

i: The index on self that minimises the pairwise distance.

j: The index on other that minimises the pairwise distance.

d: The distance between self and other. (float)

Return type `tuple`

Conversion to internal coordinates

<code>get_zmat</code> ([<i>construction_table</i> , <i>use_lookup</i>])	Transform to internal coordinates.
<code>get_grad_zmat</code> (<i>construction_table</i> [, <i>as_function</i>])	Return the gradient for the transformation to a Zmatrix.
<code>get_construction_table</code> ([<i>fragment_list</i> , ...])	Create a construction table for a Zmatrix.
<code>check_dihedral</code> (<i>construction_table</i>)	Checks, if the dihedral defining atom is colinear.
<code>correct_dihedral</code> (<i>construction_table</i> [, ...])	Reindexe the dihedral defining atom if linear reference is used.
<code>check_absolute_refs</code> (<i>construction_table</i>)	Checks first three rows of <i>construction_table</i> for linear references

Continued on next page

Table 5 – continued from previous page

<code>correct_absolute_refs</code>	Reindex <code>construction_table</code> if linear reference in first three rows present.
<code>to_zmat(*args, **kwargs)</code>	Deprecated, use <code>get_zmat()</code>

chemcoord.Cartesian.get_zmat

`Cartesian.get_zmat` (*construction_table=None, use_lookup=None*)

Transform to internal coordinates.

Transforming to internal coordinates involves basically three steps:

1. Define an order of how to build and define for each atom the used reference atoms.
2. Check for problematic local linearity. In this algorithm an angle with $170 < \text{angle} < 10$ is assumed to be linear. This is not the mathematical definition, but makes it safer against “floating point noise”
3. Calculate the bond lengths, angles and dihedrals using the references defined in step 1 and 2.

In the first two steps a so called `construction_table` is created. This is basically a Zmatrix without the values for the bonds, angles and dihedrals hence containing only the information about the used references. ChemCoord uses a `pandas.DataFrame` with the columns ['b', 'a', 'd']. Look into `get_construction_table()` for more information.

It is important to know, that calculating the construction table is a very costly step since the algorithm tries to make some guesses based on connectivity to create a “chemical” zmatrix.

If you create several zmatrices based on the same references you can obtain the construction table of a zmatrix with `Zmat_instance.loc[:, ['b', 'a', 'd']]` If you then pass the buildlist as argument to `give_zmat`, the algorithm directly starts with step 3 (which is much faster).

If a `construction_table` is passed into `get_zmat()` the check for pathological linearity is not performed! So if a `construction_table` is either manually created, or obtained from `get_construction_table()` under the option `perform_checks = False`, it is recommended to use the following methods:

- `correct_dihedral()`
- `correct_absolute_refs()`

If you want to check for problematic indices in order to solve the invalid references yourself, use the following methods:

- `check_dihedral()`
- `check_absolute_refs()`

Parameters

- **construction_table** (*pandas.DataFrame*) –
- **use_lookup** (*bool*) – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`

Returns A new instance of `Zmat`.

Return type `Zmat`

chemcoord.Cartesian.get_grad_zmat

`Cartesian.get_grad_zmat` (*construction_table, as_function=True*)

Return the gradient for the transformation to a Zmatrix.

If `as_function` is `True`, a function is returned that can be directly applied onto instances of `Cartesian`, which contain the applied distortions in cartesian space. In this case the user does not have to worry about indexing and correct application of the tensor product. Basically this is the function `xyz_functions.apply_grad_zmat_tensor()` with partially replaced arguments.

If `as_function` is `False`, a $(3, n, n, 3)$ tensor is returned, which contains the values of the derivatives.

Since a $n \times 3$ matrix is derived after a $n \times 3$ matrix, it is important to specify the used rules for indexing the resulting tensor.

The rule is very simple: The indices of the numerator are used first then the indices of the denominator get swapped and appended:

$$\left(\frac{\partial \mathbf{Y}}{\partial \mathbf{X}}\right)_{i,j,k,l} = \frac{\partial \mathbf{Y}_{i,j}}{\partial \mathbf{X}_{l,k}}$$

Applying this rule to an example function:

$$f: \mathbb{R}^3 \rightarrow \mathbb{R}$$

Gives as derivative the known row-vector gradient:

$$(\nabla f)_{1,i} = \frac{\partial f}{\partial x_i} \quad i \in \{1, 2, 3\}$$

Note: The row wise alignment of the XYZ files makes sense for these CSV like files. But it is mathematically advantageous and sometimes (depending on the memory layout) numerically better to use a column wise alignment of the coordinates. In this function the resulting tensor assumes a $3 \times n$ array for the coordinates.

If

$$\begin{aligned} \mathbf{X}_{i,j} & \quad 1 \leq i \leq 3, \quad 1 \leq j \leq n \\ \mathbf{C}_{i,j} & \quad 1 \leq i \leq 3, \quad 1 \leq j \leq n \end{aligned}$$

denote the positions in cartesian and Zmatrix space,

The complete tensor may be written as:

$$\left(\frac{\partial \mathbf{C}}{\partial \mathbf{X}}\right)_{i,j,k,l} = \frac{\partial \mathbf{C}_{i,j}}{\partial \mathbf{X}_{l,k}}$$

Parameters

- `construction_table` (`pandas.DataFrame`) –
- `as_function` (`bool`) – Return a tensor or `xyz_functions.apply_grad_zmat_tensor()` with partially replaced arguments.

Returns Depending on `as_function` return a tensor or `apply_grad_zmat_tensor()` with partially replaced arguments.

Return type (`func`, `np.array`)

`chemcoord.Cartesian.get_construction_table`

`Cartesian.get_construction_table` (`fragment_list=None`, `use_lookup=None`, `perform_checks=True`)

Create a construction table for a Zmatrix.

A construction table is basically a Zmatrix without the values for the bond lengths, angles and dihedrals. It contains the whole information about which reference atoms are used by each atom in the Zmatrix.

The absolute references in cartesian space are one of the following magic strings:

```
['origin', 'e_x', 'e_y', 'e_z']
```

This method creates a so called “chemical” construction table, which makes use of the connectivity table in this molecule.

Parameters

- **fragment_list** (*sequence*) – There are four possibilities to specify the sequence of fragments:

1. A list of tuples is given. Each tuple contains the fragment with its corresponding construction table in the form of:

```
[(frag1, c_table1), (frag2, c_table2)...]
```

If the construction table of a fragment is not complete, the rest of each fragment’s construction table is calculated automatically.

2. It is possible to omit the construction tables for some or all fragments as in the following example:

```
[(frag1, c_table1), frag2, (frag3, c_table3)...]
```

3. If `self` contains more atoms than the union over all fragments, the rest of the molecule without the fragments is automatically prepended using `get_without()`:

```
self.get_without(fragments) + fragment_list
```

4. If `fragment_list` is `None` then fragmentation, etc. is done automatically. The fragments are then sorted by their number of atoms, in order to use the largest fragment as reference for the other ones.

- **use_lookup** (*bool*) – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`
- **perform_checks** (*bool*) – The checks for invalid references are performed using `correct_dihedral()` and `correct_absolute_refs()`.

Returns Construction table

Return type `pandas.DataFrame`

chemcoord.Cartesian.check_dihedral

Cartesian.**check_dihedral** (*construction_table*)

Checks, if the dihedral defining atom is colinear.

Checks for each index starting from the third row of the `construction_table`, if the reference atoms are colinear.

Parameters `construction_table` (*pd.DataFrame*) –

Returns A list of problematic indices.

Return type `list`

chemcoord.Cartesian.correct_dihedral

Cartesian.**correct_dihedral** (*construction_table*, *use_lookup=None*)

Reindexe the dihedral defining atom if linear reference is used.

Uses *check_dihedral()* to obtain the problematic indices.

Parameters

- **construction_table** (*pd.DataFrame*) –
- **use_lookup** (*bool*) – Use a lookup variable for *get_bonds()*. The default is specified in `settings['defaults']['use_lookup']`

Returns Appropriately renamed construction table.

Return type *pd.DataFrame*

chemcoord.Cartesian.check_absolute_refs

Cartesian.**check_absolute_refs** (*construction_table*)

Checks first three rows of *construction_table* for linear references

Checks for each index from first to third row of the *construction_table*, if the references are colinear. This case has to be specially treated, because the references are not only atoms (to fix internal degrees of freedom) but also points in cartesian space called absolute references. (to fix translational and rotational degrees of freedom)

Parameters **construction_table** (*pd.DataFrame*) –

Returns A list of problematic indices.

Return type *list*

chemcoord.Cartesian.correct_absolute_refs

Cartesian.**correct_absolute_refs** (*construction_table*)

Reindexe *construction_table* if linear reference in first three rows present.

Uses *check_absolute_refs()* to obtain the problematic indices.

Parameters **construction_table** (*pd.DataFrame*) –

Returns Appropriately renamed construction table.

Return type *pd.DataFrame*

chemcoord.Cartesian.to_zmat

Cartesian.**to_zmat** (**args, **kwargs*)

Deprecated, use *get_zmat()*

Symmetry

<i>get_pointgroup</i> ([tolerance])	Returns a PointGroup object for the molecule.
<i>get_equivalent_atoms</i> ([tolerance])	Returns sets of equivalent atoms with symmetry operations
<i>symmetrize</i> ([max_n, tolerance, epsilon])	Returns a symmetrized molecule
<i>get_asymmetric_unit</i> ([eq])	

chemcoord.Cartesian.get_pointgroup

`Cartesian.get_pointgroup` (*tolerance=0.3*)

Returns a PointGroup object for the molecule.

Parameters **tolerance** (*float*) – Tolerance to generate the full set of symmetry operations.

Returns *PointGroupOperations*

chemcoord.Cartesian.get_equivalent_atoms

`Cartesian.get_equivalent_atoms` (*tolerance=0.3*)

Returns sets of equivalent atoms with symmetry operations

Parameters **tolerance** (*float*) – Tolerance to generate the full set of symmetry operations.

Returns

The returned dictionary has two possible keys:

`eq_sets`: A dictionary of indices mapping to sets of indices, each key maps to indices of all equivalent atoms. The keys are guaranteed to be not equivalent.

`sym_ops`: Twofold nested dictionary. `operations[i][j]` gives the symmetry operation that maps atom `i` unto `j`.

Return type `dict`

chemcoord.Cartesian.symmetrize

`Cartesian.symmetrize` (*max_n=10, tolerance=0.3, epsilon=0.001*)

Returns a symmetrized molecule

The equivalent atoms obtained via `get_equivalent_atoms()` are rotated, mirrored... unto one position. Then the average position is calculated. The average position is rotated, mirrored... back with the inverse of the previous symmetry operations, which gives the symmetrized molecule. This operation is repeated iteratively `max_n` times at maximum until the difference between subsequently symmetrized structures is smaller than `epsilon`.

Parameters

- **max_n** (*int*) – Maximum number of iterations.
- **tolerance** (*float*) – Tolerance for detecting symmetry. Gets passed as Argument into `PointGroupAnalyzer`.
- **epsilon** (*float*) – If the elementwise absolute difference of two subsequently symmetrized structures is smaller epsilon, the iteration stops before `max_n` is reached.

Returns

The returned dictionary has three possible keys:

`sym_mol`: A symmetrized molecule *Cartesian*

`eq_sets`: A dictionary of indices mapping to sets of indices, each key maps to indices of all equivalent atoms. The keys are guaranteed to be not symmetry-equivalent.

`sym_ops`: Twofold nested dictionary. `operations[i][j]` gives the symmetry operation that maps atom `i` unto `j`.

Return type `dict`

chemcoord.Cartesian.get_asymmetric_unit

`Cartesian.get_asymmetric_unit` (*eq=None*)

IO

<code>to_xyz</code> ([buf, sort_index, index, header, ...])	Write xyz-file
<code>write_xyz</code> (*args, **kwargs)	Deprecated, use <code>to_xyz()</code>
<code>read_xyz</code> (buf[, start_index, get_bonds, ...])	Read a file of coordinate information.
<code>to_cjson</code> ([buf])	Write a cjson file or return dictionary.
<code>read_cjson</code> (buf)	Read a cjson file or a dictionary.
<code>view</code> ([viewer, use_curr_dir])	View your molecule.
<code>to_string</code> ([buf, columns, col_space, header, ...])	Render a DataFrame to a console-friendly tabular output.
<code>to_latex</code> ([buf, columns, col_space, header, ...])	Render a DataFrame to a tabular environment table.
<code>get_pymatgen_molecule</code> ()	Create a Molecule instance of the pymatgen library
<code>from_pymatgen_molecule</code> (molecule)	Create an instance of the own class from a pymatgen molecule
<code>get_ase_atoms</code> ()	Create an Atoms instance of the ase library
<code>from_ase_atoms</code> (atoms)	Create an instance of the own class from an ase molecule

chemcoord.Cartesian.to_xyz

`Cartesian.to_xyz` (*buf=None, sort_index=True, index=False, header=False, float_format=<built-in method format of str object>, overwrite=True*)

Write xyz-file

Parameters

- **buf** (*str*) – StringIO-like, optional buffer to write to
- **sort_index** (*bool*) – If `sort_index` is true, the `Cartesian` is sorted by the index before writing.
- **float_format** (*one-parameter function*) – Formatter function to apply to column's elements if they are floats. The result of this function must be a unicode string.
- **overwrite** (*bool*) – May overwrite existing files.

Returns string (or unicode, depending on data and options)

Return type formatted

chemcoord.Cartesian.write_xyz

`Cartesian.write_xyz` (**args, **kwargs*)

Deprecated, use `to_xyz()`

chemcoord.Cartesian.read_xyz

classmethod `Cartesian.read_xyz` (*buf*, *start_index=0*, *get_bonds=True*, *nrows=None*, *engine=None*)

Read a file of coordinate information.

Reads xyz-files.

Parameters

- **inputfile** (*str*) –
- **start_index** (*int*) –
- **get_bonds** (*bool*) –
- **nrows** (*int*) – Number of rows of file to read. Note that the first two rows are implicitly excluded.
- **engine** (*str*) – Wrapper for argument of `pandas.read_csv()`.

Returns

Return type *Cartesian*

chemcoord.Cartesian.to_cjson

`Cartesian.to_cjson` (*buf=None*, ***kwargs*)

Write a cjson file or return dictionary.

The cjson format is specified [here](#).

Parameters

- **buf** (*str*) – If it is a filepath, the data is written to filepath. If it is None, a dictionary with the cjson information is returned.
- **kwargs** – The keyword arguments are passed into the `dump` function of the `json` library.

Returns

Return type `dict`

chemcoord.Cartesian.read_cjson

classmethod `Cartesian.read_cjson` (*buf*)

Read a cjson file or a dictionary.

The cjson format is specified [here](#).

Parameters **buf** (*str*, *dict*) – If it is a filepath, the data is read from filepath. If it is a dictionary, the dictionary is interpreted as cjson.

Returns

Return type *Cartesian*

chemcoord.Cartesian.view

`Cartesian.view` (*viewer=None*, *use_curr_dir=False*)

View your molecule.

Note: This function writes a temporary file and opens it with an external viewer. If you modify your molecule afterwards you have to recall `view` in order to see the changes.

Parameters

- **viewer** (*str*) – The external viewer to use. If it is None, the default as specified in `cc.settings['defaults']['viewer']` is used.
- **use_curr_dir** (*bool*) – If True, the temporary file is written to the current directory. Otherwise it gets written to the OS dependent temporary directory.

Returns

Return type None

chemcoord.Cartesian.to_string

`Cartesian.to_string` (*buf=None, columns=None, col_space=None, header=True, index=True, na_rep='NaN', formatters=None, float_format=None, sparsify=None, index_names=True, justify=None, line_width=None, max_rows=None, max_cols=None, show_dimensions=False*)

Render a DataFrame to a console-friendly tabular output.

Wrapper around the `pandas.DataFrame.to_string()` method.

chemcoord.Cartesian.to_latex

`Cartesian.to_latex` (*buf=None, columns=None, col_space=None, header=True, index=True, na_rep='NaN', formatters=None, float_format=None, sparsify=None, index_names=True, bold_rows=True, column_format=None, longtable=None, escape=None, encoding=None, decimal='.', multicolumn=None, multicolumn_format=None, multirow=None*)

Render a DataFrame to a tabular environment table.

You can splice this into a LaTeX document. Requires `\usepackage{booktabs}`. Wrapper around the `pandas.DataFrame.to_latex()` method.

chemcoord.Cartesian.get_pymatgen_molecule

`Cartesian.get_pymatgen_molecule()`

Create a Molecule instance of the pymatgen library

Warning: The `pymatgen` library is imported locally in this function and will raise an `ImportError` exception, if it is not installed.

Parameters None –

Returns

Return type `pymatgen.core.structure.Molecule`

chemcoord.Cartesian.from_pymatgen_molecule

classmethod `Cartesian.from_pymatgen_molecule` (*molecule*)

Create an instance of the own class from a pymatgen molecule

Parameters *molecule* (`pymatgen.core.structure.Molecule`) –

Returns

Return type `Cartesian`

chemcoord.Cartesian.get_ase_atoms`Cartesian.get_ase_atoms()`

Create an Atoms instance of the ase library

Warning: The `ase` library is imported locally in this function and will raise an `ImportError` exception, if it is not installed.

Parameters None –**Returns****Return type** `ase.atoms.Atoms`**chemcoord.Cartesian.from_ase_atoms****classmethod** `Cartesian.from_ase_atoms(atoms)`

Create an instance of the own class from an ase molecule

Parameters `molecule` (`ase.atoms.Atoms`) –**Returns****Return type** `Cartesian`**Pandas DataFrame Wrapper**

<code>copy()</code>	
<code>index</code>	Returns the index.
<code>columns</code>	Returns the columns.
<code>replace([to_replace, value, inplace, limit, ...])</code>	Replace values given in 'to_replace' with 'value'.
<code>sort_index([axis, level, ascending, ...])</code>	Sort object by labels (along an axis)
<code>set_index(keys[, drop, append, inplace, ...])</code>	Set the DataFrame index (row labels) using one or more existing columns.
<code>append(other[, ignore_index])</code>	Append rows of <i>other</i> to the end of this frame, returning a new object.
<code>insert(loc, column, value[, ...])</code>	Insert column into molecule at specified location.
<code>sort_values(by[, axis, ascending, inplace, ...])</code>	Sort by the values along either axis
<code>loc</code>	Label based indexing
<code>iloc</code>	Label based indexing

chemcoord.Cartesian.copy`Cartesian.copy()`**chemcoord.Cartesian.index**`Cartesian.index`

Returns the index.

Assigning a value to it changes the index.

chemcoord.Cartesian.columns

Cartesian.**columns**

Returns the columns.

Assigning a value to it changes the columns.

chemcoord.Cartesian.replace

Cartesian.**replace** (*to_replace=None, value=None, inplace=False, limit=None, regex=False, method='pad', axis=None*)

Replace values given in 'to_replace' with 'value'.

Wrapper around the `pandas.DataFrame.replace()` method.

chemcoord.Cartesian.sort_index

Cartesian.**sort_index** (*axis=0, level=None, ascending=True, inplace=False, kind='quicksort', na_position='last', sort_remaining=True, by=None*)

Sort object by labels (along an axis)

Wrapper around the `pandas.DataFrame.sort_index()` method.

chemcoord.Cartesian.set_index

Cartesian.**set_index** (*keys, drop=True, append=False, inplace=False, verify_integrity=False*)

Set the DataFrame index (row labels) using one or more existing columns.

Wrapper around the `pandas.DataFrame.set_index()` method.

chemcoord.Cartesian.append

Cartesian.**append** (*other, ignore_index=False*)

Append rows of *other* to the end of this frame, returning a new object.

Wrapper around the `pandas.DataFrame.append()` method.

Parameters

- **other** (*Cartesian*) –
- **ignore_index** (*sequence, bool, int*) – If it is a boolean, it behaves like in the description of `pandas.DataFrame.append()`. If it is a sequence, it becomes the new index. If it is an integer, `range(ignore_index, ignore_index + len(new))` becomes the new index.

Returns

Return type *Cartesian*

chemcoord.Cartesian.insert

Cartesian.**insert** (*loc, column, value, allow_duplicates=False, inplace=False*)

Insert column into molecule at specified location.

Wrapper around the `pandas.DataFrame.insert()` method.

chemcoord.Cartesian.sort_values

`Cartesian.sort_values` (*by*, *axis=0*, *ascending=True*, *inplace=False*, *kind='quicksort'*, *na_position='last'*)

Sort by the values along either axis

Wrapper around the `pandas.DataFrame.sort_values()` method.

chemcoord.Cartesian.loc

`Cartesian.loc`

Label based indexing

The indexing behaves like Indexing and Selecting data in [Pandas](#). You can slice with `loc()`, `iloc()` and `Cartesian[...]`. The only question is about the return type. If the information in the columns is enough to draw a molecule, an instance of the own class (e.g. `Cartesian`) is returned. If the information in the columns is not enough to draw a molecule, there are two cases to consider:

- A `Series` instance is returned for one dimensional slices.
- A `DataFrame` instance is returned in all other cases.

This means that:

`molecule.loc[:, ['atom', 'x', 'y', 'z']]` returns a `Cartesian`.

`molecule.loc[:, ['atom', 'x']]` returns a `pandas.DataFrame`.

`molecule.loc[:, 'atom']` returns a `pandas.Series`.

chemcoord.Cartesian.iloc

`Cartesian.iloc`

Label based indexing

The indexing behaves like Indexing and Selecting data in [Pandas](#). You can slice with `loc()`, `iloc()` and `Cartesian[...]`. The only question is about the return type. If the information in the columns is enough to draw a molecule, an instance of the own class (e.g. `Cartesian`) is returned. If the information in the columns is not enough to draw a molecule, there are two cases to consider:

- A `Series` instance is returned for one dimensional slices.
- A `DataFrame` instance is returned in all other cases.

This means that:

`molecule.iloc[:, ['atom', 'x', 'y', 'z']]` returns a `Cartesian`.

`molecule.iloc[:, ['atom', 'x']]` returns a `pandas.DataFrame`.

`molecule.iloc[:, 'atom']` returns a `pandas.Series`.

Advanced methods

`_divide_et_impera`(*n_atoms_per_set*,
offset)

Continued on next page

Table 9 – continued from previous page

<code>_preserve_bonds(sliced_cartesian[, use_lookup])</code>	Is called after cutting geometric shapes.
--	---

chemcoord.Cartesian._divide_et_impera

`Cartesian._divide_et_impera (n_atoms_per_set=500, offset=3)`

chemcoord.Cartesian._preserve_bonds

`Cartesian._preserve_bonds (sliced_cartesian, use_lookup=None)`

Is called after cutting geometric shapes.

If you want to change the rules how bonds are preserved, when applying `Cartesian.cut_sphere()` this is the function you have to modify. e.g.

It is recommended to inherit from the Cartesian class to tailor it for your project, instead of modifying the source code of ChemCoord.

Parameters

- `sliced_frame (Cartesian)` –
- `use_lookup (bool)` – Use a lookup variable for `get_bonds()`. The default is specified in `settings['defaults']['use_lookup']`

Returns

Return type `Cartesian`

Attributes

<code>columns</code>	Returns the columns.
<code>index</code>	Returns the index.

xyz_functions

A collection of functions operating on instances of `Cartesian`.

<code>isclose(a, b[, align, rtol, atol])</code>	Compare two molecules for numerical equality.
<code>allclose(a, b[, align, rtol, atol])</code>	Compare two molecules for numerical equality.
<code>concat(cartesians[, ignore_index, keys])</code>	Join list of cartesians into one molecule.
<code>write_molden(*args, **kwargs)</code>	Deprecated, use <code>to_molden()</code>
<code>to_molden(cartesian_list[, buf, sort_index, ...])</code>	Write a list of Cartesians into a molden file.
<code>read_molden(inputfile[, start_index, get_bonds])</code>	Read a molden file.
<code>view(molecule[, viewer, use_curr_dir])</code>	View your molecule or list of molecules.
<code>dot(A, B)</code>	Matrix multiplication between A and B
<code>apply_grad_zmat_tensor(grad_C, ...)</code>	Apply the gradient for transformation to Zmatrix space onto <code>cart_dist</code> .

chemcoord.xyz_functions.isclose

`chemcoord.xyz_functions.isclose (a, b, align=False, rtol=1e-05, atol=1e-08)`

Compare two molecules for numerical equality.

Parameters

- **a** (*Cartesian*) –
- **b** (*Cartesian*) –
- **align** (*bool*) – a and b are prealigned along their principal axes of inertia and moved to their barycenters before comparing.
- **rtol** (*float*) – Relative tolerance for the numerical equality comparison look into `numpy.isclose()` for further explanation.
- **atol** (*float*) – Relative tolerance for the numerical equality comparison look into `numpy.isclose()` for further explanation.

Returns Boolean array.

Return type `numpy.ndarray`

`chemcoord.xyz_functions.allclose`

`chemcoord.xyz_functions.allclose(a, b, align=False, rtol=1e-05, atol=1e-08)`

Compare two molecules for numerical equality.

Parameters

- **a** (*Cartesian*) –
- **b** (*Cartesian*) –
- **align** (*bool*) – a and b are prealigned along their principal axes of inertia and moved to their barycenters before comparing.
- **rtol** (*float*) – Relative tolerance for the numerical equality comparison look into `numpy.allclose()` for further explanation.
- **atol** (*float*) – Relative tolerance for the numerical equality comparison look into `numpy.allclose()` for further explanation.

Returns

Return type `bool`

`chemcoord.xyz_functions.concat`

`chemcoord.xyz_functions.concat(cartesians, ignore_index=False, keys=None)`

Join list of cartesians into one molecule.

Wrapper around the `pandas.concat()` function. Default values are the same as in the pandas function except for `verify_integrity` which is set to true in case of this library.

Parameters

- **ignore_index** (*sequence, bool, int*) – If it is a boolean, it behaves like in the description of `pandas.DataFrame.append()`. If it is a sequence, it becomes the new index. If it is an integer, `range(ignore_index, ignore_index + len(new))` becomes the new index.
- **keys** (*sequence*) – If multiple levels passed, should contain tuples. Construct hierarchical index using the passed keys as the outermost level

Returns

Return type *Cartesian*

chemcoord.xyz_functions.write_molden

chemcoord.xyz_functions.**write_molden**(*args, **kwargs)
Deprecated, use `to_molden()`

chemcoord.xyz_functions.to_molden

chemcoord.xyz_functions.**to_molden**(cartesian_list, buf=None, sort_index=True, overwrite=True, float_format=<built-in method format of str object>)

Write a list of Cartesians into a molden file.

Note: Since it permanently writes a file, this function is strictly speaking **not sideeffect free**. The list to be written is of course not changed.

Parameters

- **cartesian_list** (*list*) –
- **buf** (*str*) – StringIO-like, optional buffer to write to
- **sort_index** (*bool*) – If sort_index is true, the Cartesian is sorted by the index before writing.
- **overwrite** (*bool*) – May overwrite existing files.
- **float_format** (*one-parameter function*) – Formatter function to apply to column's elements if they are floats. The result of this function must be a unicode string.

Returns string (or unicode, depending on data and options)

Return type formatted

chemcoord.xyz_functions.read_molden

chemcoord.xyz_functions.**read_molden**(inputfile, start_index=0, get_bonds=True)
Read a molden file.

Parameters

- **inputfile** (*str*) –
- **start_index** (*int*) –

Returns A list containing *Cartesian* is returned.

Return type list

chemcoord.xyz_functions.view

chemcoord.xyz_functions.**view**(molecule, viewer='gv.exe', use_curr_dir=False)
View your molecule or list of molecules.

Note: This function writes a temporary file and opens it with an external viewer. If you modify your molecule afterwards you have to recall view in order to see the changes.

Parameters

- **molecule** – Can be a cartesian, or a list of cartesians.
- **viewer** (*str*) – The external viewer to use. The default is specified in settings.viewer
- **use_curr_dir** (*bool*) – If True, the temporary file is written to the current directory. Otherwise it gets written to the OS dependent temporary directory.

Returns**Return type** None**chemcoord.xyz_functions.dot**`chemcoord.xyz_functions.dot` (*A*, *B*)

Matrix multiplication between A and B

This function is equivalent to $A @ B$, which is unfortunately not possible under python 2.x.**Parameters**

- **A** (*sequence*) –
- **B** (*sequence*) –

Returns**Return type** sequence**chemcoord.xyz_functions.apply_grad_zmat_tensor**`chemcoord.xyz_functions.apply_grad_zmat_tensor` (*grad_C*, *construction_table*, *cart_dist*)

Apply the gradient for transformation to Zmatrix space onto cart_dist.

Parameters

- **grad_C** (`numpy.ndarray`) – A (3, n, n, 3) array. The mathematical details of the index layout is explained in `get_grad_zmat()`.
- **construction_table** (`pandas.DataFrame`) – Explained in `get_construction_table()`.
- **cart_dist** (*Cartesian*) – Distortions in cartesian space.

Returns Distortions in Zmatrix space.**Return type** Zmat**Symmetry**

`PointGroupOperations`(sch_symbol, operations) Defines a point group as sequence of symmetry operations.

chemcoord.PointGroupOperations

class chemcoord.**PointGroupOperations** (*sch_symbol*, *operations*, *tolerance=0.1*)
Defines a point group as sequence of symmetry operations.

Parameters

- **sch_symbol** (*str*) – Schoenflies symbol of the point group.
- **operations** (*numpy.ndarray*) – Initial set of symmetry operations. It is sufficient to provide only just enough operations to generate the full set of symmetries.
- **tolerance** (*float*) – Tolerance to generate the full set of symmetry operations.

<i>AsymmetricUnitCartesian</i> ([<i>frame</i> , <i>atoms</i> , ...])	Manipulate cartesian coordinates while preserving the point group.
---	--

chemcoord.AsymmetricUnitCartesian

class chemcoord.**AsymmetricUnitCartesian** (*frame=None*, *atoms=None*, *coords=None*, *index=None*, *metadata=None*, *_metadata=None*)
Manipulate cartesian coordinates while preserving the point group.

This class has all the methods of a *Cartesian*, with one additional *get_cartesian()* method and contains only one member of each symmetry equivalence class.

<i>get_cartesian</i> ()	Return a <i>Cartesian</i> where all members of a symmetry equivalence class are inserted back in.
-------------------------	---

chemcoord.AsymmetricUnitCartesian.get_cartesian

AsymmetricUnitCartesian.**get_cartesian**()
Return a *Cartesian* where all members of a symmetry equivalence class are inserted back in.

Parameters *None* –

Returns A new cartesian instance.

Return type *Cartesian*

2.3.2 Internal coordinates

Zmat

The *Zmat* class which is used to represent a molecule in non redundant, internal coordinates.

<i>Zmat</i> (<i>frame</i> [, <i>metadata</i> , <i>_metadata</i>])	The main class for dealing with internal Coordinates.
---	---

chemcoord.Zmat

class chemcoord.**Zmat** (*frame*, *metadata=None*, *_metadata=None*)
The main class for dealing with internal Coordinates.

Rotational direction:

Chemcoord uses the [IUPAC definition](#). Note that this does not include the automatic choosing of the canonical equivalence class representation. An angle of -30° could be represented by 270° . Use `iupacify()` to choose also the IUPAC conform angle representation.

Mathematical Operations:

The general rule is that mathematical operations using the binary operators `+` `-` `*` `/` and the unary operators `+` `-` `abs` are only applied to the `['bond', 'angle', 'dihedral']` columns.

Addition/Subtraction/Multiplication/Division: The most common case is to add another `Zmat` instance. In this case it is tested, if the used references are the same. Afterwards the addition in the `['bond', 'angle', 'dihedral']` columns is performed. If you add a scalar to a `Zmat` it is added elementwise onto the `['bond', 'angle', 'dihedral']` columns. If you add a 3-dimensional vector, list, tuple... the first element of this vector is added elementwise to the `'bond'` column of the `Zmat` instance and so on. The third possibility is to add a matrix with `shape=(len(Zmat), 3)` which is again added elementwise. The same rules are true for subtraction, division and multiplication.

Indexing:

The indexing behaves like Indexing and Selecting data in [Pandas](#). You can slice with `loc()`, `iloc()`, and `Zmat[...]`. The only question is about the return type. If the information in the columns is enough to draw a molecule, an instance of the own class (e.g. `Zmat`) is returned. If the information in the columns is enough to draw a molecule, an instance of the own class (e.g. `Zmat`) is returned. If the information in the columns is not enough to draw a molecule, there are two cases to consider:

- A `Series` instance is returned for one dimensional slices.
- A `DataFrame` instance is returned in all other cases.

This means that:

```
molecule.loc[:, ['atom', 'b', 'bond', 'a', 'angle', 'd',
                  'dihedral']] returns a Zmat.

molecule.loc[:, ['atom', 'bond']] returns a pandas.DataFrame.

molecule.loc[:, 'atom'] returns a pandas.Series.
```

Comparison:

Comparison for equality with `==` is supported. It behaves exactly like the equality comparison of `DataFrames` in `pandas`. Amongst other things this means that the index has to be the same and the comparison of floating point numbers is exact and not numerical.

Chemical Methods

<code>__init__(frame[, metadata, _metadata])</code>	How to initialize a <code>Zmat</code> instance.
<code>add_data(new_cols)</code>	Adds a column with the requested data.
<code>change_numbering(new_index)</code>	Change numbering to a new index.
<code>has_same_sumformula(other)</code>	Determines if <code>other</code> has the same sumformula
<code>get_cartesian()</code>	Return the molecule in cartesian coordinates.
<code>get_grad_cartesian([as_function, chain, ...])</code>	Return the gradient for the transformation to a Cartesian.
<code>to_xyz(*args, **kwargs)</code>	Deprecated, use <code>get_cartesian()</code>
<code>get_total_mass()</code>	Returns the total mass in <code>g/mol</code> .
<code>get_electron_number([charge])</code>	Return the number of electrons.

Continued on next page

Table 16 – continued from previous page

<code>subs(*args, **kwargs)</code>	Substitute a symbolic expression in ['bond', 'angle', 'dihedral']
<code>iupacify()</code>	Give the IUPAC conform representation.
<code>minimize_dihedrals()</code>	Give a representation of the dihedral with minimized absolute value.

chemcoord.Zmat.__init__

`Zmat.__init__(frame, metadata=None, _metadata=None)`

How to initialize a Zmat instance.

Parameters

- **init** (*pd.DataFrame*) – A Dataframe with at least the columns ['atom', 'b', 'bond', 'a', 'angle', 'd', 'dihedral']. Where 'atom' is a string for the elementsymbol.
- **order_of_definition** (*list like*) – Specify in which order the Zmatrix is defined. If None it just uses `self.index`.

Returns A new zmat instance.

Return type *Zmat*

chemcoord.Zmat.add_data

`Zmat.add_data(new_cols=None)`

Adds a column with the requested data.

If you want to see for example the mass, the colormap used in jmol and the block of the element, just use:

```
['mass', 'jmol_color', 'block']
```

The underlying `pd.DataFrame` can be accessed with `constants.elements`. To see all available keys use `constants.elements.info()`.

The data comes from the module `mendeleev` written by Lukasz Mentel.

Please note that I added three columns to the `mendeleev` data:

```
['atomic_radius_cc', 'atomic_radius_gv', 'gv_color',
 'valency']
```

The `atomic_radius_cc` is used by default by this module for determining bond lengths. The three others are taken from the MOLCAS grid viewer written by Valera Veryazov.

Parameters

- **new_cols** (*str*) – You can pass also just one value. E.g. 'mass' is equivalent to ['mass']. If `new_cols` is None all available data is returned.
- **inplace** (*bool*) –

Returns

Return type *Cartesian*

chemcoord.Zmat.change_numbering`Zmat.change_numbering` (*new_index=None*)

Change numbering to a new index.

Changes the numbering of index and all dependent numbering (`bond_with...`) to a `new_index`.**The user has to make sure that the new_index consists of distinct** elements.**Parameters** `new_index` (*list*) – If `None` the `new_index` is taken from 1 to the number of atoms.**Returns** Reindexed version of the zmatrix.**Return type** *Zmat***chemcoord.Zmat.has_same_sumformula**`Zmat.has_same_sumformula` (*other*)Determines if `other` has the same sumformula**Parameters** `other` (*molecule*) –**Returns****Return type** `bool`**chemcoord.Zmat.get_cartesian**`Zmat.get_cartesian` ()

Return the molecule in cartesian coordinates.

Raises an *InvalidReference* exception, if the reference of the *i*-th atom is undefined.**Parameters** `None` –**Returns** Reindexed version of the zmatrix.**Return type** *Cartesian***chemcoord.Zmat.get_grad_cartesian**`Zmat.get_grad_cartesian` (*as_function=True, chain=True, drop_auto_dummies=True*)

Return the gradient for the transformation to a Cartesian.

If `as_function` is `True`, a function is returned that can be directly applied onto instances of *Zmat*, which contain the applied distortions in Zmatrix space. In this case the user does not have to worry about indexing and correct application of the tensor product. Basically this is the function `zmat_functions.apply_grad_cartesian_tensor()` with partially replaced arguments.If `as_function` is `False`, a $(3, n, n, 3)$ tensor is returned, which contains the values of the derivatives.Since a $n * 3$ matrix is derived after a $n * 3$ matrix, it is important to specify the used rules for indexing the resulting tensor.

The rule is very simple: The indices of the numerator are used first then the indices of the denominator get swapped and appended:

$$\left(\frac{\partial \mathbf{Y}}{\partial \mathbf{X}}\right)_{i,j,k,l} = \frac{\partial \mathbf{Y}_{i,j}}{\partial \mathbf{X}_{l,k}}$$

Applying this rule to an example function:

$$f: \mathbb{R}^3 \rightarrow \mathbb{R}$$

Gives as derivative the known row-vector gradient:

$$(\nabla f)_{1,i} = \frac{\partial f}{\partial x_i} \quad i \in \{1, 2, 3\}$$

Note: The row wise alignment of the zmat files makes sense for these CSV like files. But it is mathematically advantageous and sometimes (depending on the memory layout) numerically better to use a column wise alignment of the coordinates. In this function the resulting tensor assumes a 3 * n array for the coordinates.

If

$$\begin{aligned} \mathbf{C}_{i,j} & \quad 1 \leq i \leq 3, \quad 1 \leq j \leq n \\ \mathbf{X}_{i,j} & \quad 1 \leq i \leq 3, \quad 1 \leq j \leq n \end{aligned}$$

denote the positions in Zmatrix and cartesian space,

The complete tensor may be written as:

$$\left(\frac{\partial \mathbf{X}}{\partial \mathbf{C}}\right)_{i,j,k,l} = \frac{\partial \mathbf{X}_{i,j}}{\partial \mathbf{C}_{l,k}}$$

Parameters

- **construction_table** (*pandas.DataFrame*) –
- **as_function** (*bool*) – Return a tensor or *xyz_functions.apply_grad_zmat_tensor()* with partially replaced arguments.
- **chain** (*bool*) –
- **drop_auto_dummies** (*bool*) – Drop automatically created dummies from the gradient. This means, that only changes in regularly placed atoms are considered for the gradient.

Returns Depending on *as_function* return a tensor or *apply_grad_cartesian_tensor()* with partially replaced arguments.

Return type (*func, numpy.ndarray*)

chemcoord.Zmat.to_xyz

`Zmat.to_xyz(*args, **kwargs)`
 Deprecated, use *get_cartesian()*

chemcoord.Zmat.get_total_mass`Zmat.get_total_mass()`

Returns the total mass in g/mol.

Parameters `None` –**Returns****Return type** `float`**chemcoord.Zmat.get_electron_number**`Zmat.get_electron_number(charge=0)`

Return the number of electrons.

Parameters `charge (int)` – Charge of the molecule.**Returns****Return type** `int`**chemcoord.Zmat.subs**`Zmat.subs(*args, **kwargs)`

Substitute a symbolic expression in ['bond', 'angle', 'dihedral']

This is a wrapper around the substitution mechanism of `sympy`. Any symbolic expression in the columns ['bond', 'angle', 'dihedral'] of `self` will be substituted with value.

Note: This function is not side-effect free. If all symbolic expressions are evaluated and are concrete numbers and `perform_checks` is `True`, a check for the transformation to cartesian coordinates is performed. If no `InvalidReference` exceptions are raised, the resulting cartesian is written to `self._metadata['last_valid_cartesian']`.

Parameters

- **symb_expr** (*sympy expression*) –
- **value** –
- **perform_checks** (*bool*) – If `perform_checks` is `True`, it is asserted, that the resulting Zmatrix can be converted to cartesian coordinates. Dummy atoms will be inserted automatically if necessary.

Returns Zmatrix with substituted symbolic expressions. If all resulting sympy expressions in a column are numbers, the column is recasted to 64bit float.**Return type** `Zmat`**chemcoord.Zmat.iupacify**`Zmat.iupacify()`

Give the IUPAC conform representation.

Mathematically speaking the angles in a zmatrix are representations of an equivalence class. We will denote an equivalence relation with \sim and use α for an angle and δ for a dihedral angle. Then the following equations hold true.

$$\begin{aligned}(\alpha, \delta) &\sim (-\alpha, \delta + \pi) \\ \alpha &\sim \alpha \pmod{2\pi} \\ \delta &\sim \delta \pmod{2\pi}\end{aligned}$$

IUPAC defines a designated representation of these equivalence classes, by asserting:

$$\begin{aligned}0 &\leq \alpha \leq \pi \\ -\pi &\leq \delta \leq \pi\end{aligned}$$

Parameters None –

Returns Zmatrix with accordingly changed angles and dihedrals.

Return type *Zmat*

chemcoord.Zmat.minimize_dihedrals

`Zmat.minimize_dihedrals()`

Give a representation of the dihedral with minimized absolute value.

Mathematically speaking the angles in a zmatrix are representations of an equivalence class. We will denote an equivalence relation with \sim and use α for an angle and δ for a dihedral angle. Then the following equations hold true.

$$\begin{aligned}(\alpha, \delta) &\sim (-\alpha, \delta + \pi) \\ \alpha &\sim \alpha \pmod{2\pi} \\ \delta &\sim \delta \pmod{2\pi}\end{aligned}$$

This function asserts:

$$-\pi \leq \delta \leq \pi$$

The main application of this function is the construction of a transforming movement from `zmat1` to `zmat2`. This is under the assumption that `zmat1` and `zmat2` are the same molecules (regarding their topology) and have the same construction table (`get_construction_table()`):

```
with cc.TestOperators(False):
    D = zmat2 - zmat1
    zmat_s1 = [zmat1 + D * i / n for i in range(n)]
    zmat_s2 = [zmat1 + D.minimize_dihedrals() * i / n for i in range(n)]
```

The movement described by `zmat_s1` might be too large, because going from 5° to 355° is 350° in this case and not -10° as in `zmat_s2` which is the desired Δ in most cases.

Parameters None –

Returns Zmatrix with accordingly changed angles and dihedrals.

Return type *Zmat*

Selection of data

<code>loc</code>	Label based indexing for obtaining elements.
<code>safe_loc</code>	Label based indexing for obtaining elements and assigning values safely.
<code>unsafe_loc</code>	Label based indexing for obtaining elements and assigning values unsafely.
<code>iloc</code>	Integer position based indexing for obtaining elements.
<code>safe_iloc</code>	Integer position based indexing for obtaining elements and assigning values safely.
<code>unsafe_iloc</code>	Integer position based indexing for obtaining elements and assigning values unsafely.

chemcoord.Zmat.loc

Zmat.loc

Label based indexing for obtaining elements.

In the case of obtaining elements, the indexing behaves like Indexing and Selecting data in [Pandas](#).

For assigning elements it is necessary to make a explicit decision between safe and unsafe assignments. The differences are explained in the stub page of [safe_loc\(\)](#).

chemcoord.Zmat.safe_loc

Zmat.safe_loc

Label based indexing for obtaining elements and assigning values safely.

In the case of obtaining elements, the indexing behaves like Indexing and Selecting data in [Pandas](#).

chemcoord.Zmat.unsafe_loc

Zmat.unsafe_loc

Label based indexing for obtaining elements and assigning values unsafely.

In the case of obtaining elements, the indexing behaves like Indexing and Selecting data in [Pandas](#).

For assigning elements it is necessary to make a explicit decision between safe and unsafe assignments. The differences are explained in the stub page of [safe_loc\(\)](#).

chemcoord.Zmat.iloc

Zmat.iloc

Integer position based indexing for obtaining elements.

In the case of obtaining elements, the indexing behaves like Indexing and Selecting data in [Pandas](#).

For assigning elements it is necessary to make a explicit decision between safe and unsafe assignments. The differences are explained in the stub page of [safe_loc\(\)](#).

chemcoord.Zmat.safe_iloc

Zmat.safe_iloc

Integer position based indexing for obtaining elements and assigning values safely.

In the case of obtaining elements, the indexing behaves like Indexing and Selecting data in [Pandas](#).

For assigning elements it is necessary to make a explicit decision between safe and unsafe assignments. The differences are explained in the stub page of [safe_iloc\(\)](#).

chemcoord.Zmat.unsafe_iloc

Zmat.unsafe_iloc

Integer position based indexing for obtaining elements and assigning values unsafely.

In the case of obtaining elements, the indexing behaves like Indexing and Selecting data in [Pandas](#).

For assigning elements it is necessary to make a explicit decision between safe and unsafe assignments. The differences are explained in the stub page of [safe_iloc\(\)](#).

Pandas DataFrame Wrapper

<code>copy()</code>	
<code>index</code>	Returns the index.
<code>columns</code>	Returns the columns.
<code>Zmat.sort_index([axis, level, ascending, ...])</code>	Sort object by labels (along an axis)
<code>insert(loc, column, value[, ...])</code>	Insert column into molecule at specified location.
<code>sort_values(by[, axis, ascending, kind, ...])</code>	Sort by the values along either axis

chemcoord.Zmat.copy

Zmat.copy()

chemcoord.Zmat.index

Zmat.index

Returns the index.

Wrapper around the `pandas.DataFrame.index()` property.

chemcoord.Zmat.columns

Zmat.columns

Returns the columns.

Wrapper around the `pandas.DataFrame.columns()` property.

chemcoord.Zmat.sort_index

`Zmat.sort_index` (*axis=0, level=None, ascending=True, inplace=False, kind='quicksort', na_position='last', sort_remaining=True, by=None*)
Sort object by labels (along an axis)

Wrapper around the `pandas.DataFrame.sort_index()` method.

chemcoord.Zmat.insert

`Zmat.insert` (*loc, column, value, allow_duplicates=False, inplace=False*)
Insert column into molecule at specified location.

Wrapper around the `pandas.DataFrame.insert()` method.

chemcoord.Zmat.sort_values

`Zmat.sort_values` (*by, axis=0, ascending=True, kind='quicksort', na_position='last'*)
Sort by the values along either axis

Wrapper around the `pandas.DataFrame.sort_values()` method.

IO

<code>to_zmat</code> ([buf, upper_triangle, ...])	Write zmat-file
<code>write</code> (*args, **kwargs)	Deprecated, use <code>to_zmat()</code>
<code>read_zmat</code> (inputfile[, implicit_index])	Reads a zmat file.
<code>to_string</code> ([buf, format_abs_ref_as, ...])	Render a DataFrame to a console-friendly tabular output.
<code>to_latex</code> ([buf, upper_triangle])	Render a DataFrame to a tabular environment table.

chemcoord.Zmat.to_zmat

`Zmat.to_zmat` (*buf=None, upper_triangle=True, implicit_index=True, float_format=<built-in method format of str object>, overwrite=True, header=False*)
Write zmat-file

Parameters

- **buf** (*str*) – StringIO-like, optional buffer to write to
- **implicit_index** (*bool*) – If `implicit_index` is set, the zmat indexing is changed to `range(1, len(self) + 1)`. Using `change_numbering()` Besides the index is omitted while writing which means, that the index is given implicitly by the row number.
- **float_format** (*one-parameter function*) – Formatter function to apply to column's elements if they are floats. The result of this function must be a unicode string.
- **overwrite** (*bool*) – May overwrite existing files.

Returns string (or unicode, depending on data and options)

Return type formatted

chemcoord.Zmat.write

`Zmat.write(*args, **kwargs)`
Deprecated, use `to_zmat()`

chemcoord.Zmat.read_zmat

classmethod `Zmat.read_zmat(inputfile, implicit_index=True)`
Reads a zmat file.

Lines beginning with # are ignored.

Parameters

- **inputfile** (*str*) –
- **implicit_index** (*bool*) – If this option is true the first column
- **to be the element symbols for the atoms.** (*has*) – The row number is used to determine the index.

Returns

Return type *Zmat*

chemcoord.Zmat.to_string

`Zmat.to_string(buf=None, format_abs_ref_as='string', upper_triangle=True, header=True, index=True, **kwargs)`
Render a DataFrame to a console-friendly tabular output.

Wrapper around the `pandas.DataFrame.to_string()` method.

chemcoord.Zmat.to_latex

`Zmat.to_latex(buf=None, upper_triangle=True, **kwargs)`
Render a DataFrame to a tabular environment table.

You can splice this into a LaTeX document. Requires `\usepackage{booktabs}`. Wrapper around the `pandas.DataFrame.to_latex()` method.

Attributes

<i>columns</i>	Returns the columns.
<i>index</i>	Returns the index.
<i>shape</i>	Returns the shape.
<i>dtypes</i>	Returns the dtypes.

chemcoord.Zmat.shape

`Zmat.shape`
Returns the shape.

Wrapper around the `pandas.DataFrame.shape()` property.

chemcoord.Zmat.dtypes

Zmat.dtypes

Returns the dtypes.

Wrapper around the `pandas.DataFrame.dtypes()` property.

zmat_functions

A collection of functions operating on instances of *Zmat*.

Functions

<code>apply_grad_cartesian_tensor(grad_X, zmat_dist)</code>	Apply the gradient for transformation to cartesian space onto <code>zmat_dist</code> .
---	--

chemcoord.zmat_functions.apply_grad_cartesian_tensor

`chemcoord.zmat_functions.apply_grad_cartesian_tensor(grad_X, zmat_dist)`

Apply the gradient for transformation to cartesian space onto `zmat_dist`.

Parameters

- **grad_X** (`numpy.ndarray`) – A (3, n, n, 3) array. The mathematical details of the index layout is explained in `get_grad_zmat()`.
- **zmat_dist** (*Zmat*) – Distortions in Zmatrix space.

Returns Distortions in cartesian space.

Return type *Cartesian*

Contextmanagers

<code>DummyManipulation(dummy_manipulation_allowed)</code>	Contextmanager that controls the behaviour of <code>safe_loc()</code> and <code>safe_iloc()</code> .
--	--

<code>TestOperators(test_operators[, cls])</code>	Switch the validity testing of zmatrices resulting from operators.
---	--

chemcoord.zmat_functions.DummyManipulation

class `chemcoord.zmat_functions.DummyManipulation(dummy_manipulation_allowed, cls=None)`

Contextmanager that controls the behaviour of `safe_loc()` and `safe_iloc()`.

In the following examples it is assumed, that using the assignment with `safe_loc()` would lead to an invalid reference. Then there are two possible usecases:

```
with DummyManipulation(zmat, True):
    zmat.safe_loc[...] = ...
    # This inserts required dummy atoms and removes them,
    # if they are not needed anymore.
```

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```

# Removes only dummy atoms, that were automatically inserted.

with DummyManipulation(zmat, False):
    zmat.safe_loc[...] = ...
    # This raises an exception
    # :class:`~chemcoord.exceptions.InvalidReference`.
    # which can be handled appropriately.
    # The zmat instance is unmodified, if an exception was raised.

```

chemcoord.zmat_functions.TestOperators

class chemcoord.zmat_functions.**TestOperators** (*test_operators, cls=None*)

Switch the validity testing of zmatrices resulting from operators.

The following examples is done with + it is assumed, that adding zmat_1 and zmat_2 leads to a zmatrix with an invalid reference:

```

with TestOperators(True):
    zmat_1 + zmat_2
    # Raises InvalidReference Exception

```

2.3.3 Configuration of settings

The current settings of chemcoord can be seen with `cc.settings`. This is a dictionary that can be changed in place. If it is necessary to change these settings permanently there is the possibility to write a configuration file of the current settings, that is read automatically while importing the module. The configuration file is in the INI format and can be changed with any text editor.

The possible settings and their defaults are:

```
['defaults']
```

```
['atomic_radius_data'] = 'atomic_radius_cc' Determines which atomic radius is used
for calculating if atoms are bonded
```

```
['use_lookup_internally'] = True Look into get_bonds() for an explanation
```

```
['viewer'] = 'gv.exe' Which one is the default viewer used in chemcoord.Cartesian.view()
and chemcoord.xyz_functions.view().
```

```
write_configuration_file([filepath, over- Create a configuration file.
write])
```

```
read_configuration_file([filepath]) Read the configuration file.
```

chemcoord.configuration.write_configuration_file

chemcoord.configuration.**write_configuration_file** (*filepath='/home/docs/.chemcoordrc', overwrite=False*)

Create a configuration file.

Writes the current state of settings into a configuration file.

Note: Since a file is permanently written, this function is strictly speaking not sideeffect free.

Parameters

- **filepath** (*str*) – Where to write the file. The default is under both UNIX and Windows `~/.chemcoordrc`.
- **overwrite** (*bool*) –

Returns**Return type** `None`**chemcoord.configuration.read_configuration_file**

`chemcoord.configuration.read_configuration_file` (*filepath*='~/docs/.chemcoordrc')

Read the configuration file.

Note: This function changes `cc.settings` inplace and is therefore not sideeffect free.

Parameters **filepath** (*str*) – Where to read the file. The default is under both UNIX and Windows `~/.chemcoordrc`.

Returns**Return type** `None`**2.3.4 Exceptions**

<i>InvalidReference</i> ([message, i, b, a, d, ...])	Raised when the i-th atom uses an invalid reference.
<i>UndefinedCoordinateSystem</i> ([message])	Raised when there is no possibility to obtain a defined coordinate system for the chosen construction table.
<i>IllegalArgumentCombination</i>	Raised if the combination of correctly typed arguments is invalid.
<i>PhysicalMeaning</i> ([message])	Raised when data is corrupted in a way, that it can not carry any information of physical meaning.

chemcoord.exceptions.InvalidReference

exception `chemcoord.exceptions.InvalidReference` (*message*=None, *i*=None, *b*=None, *a*=None, *d*=None, *already_built_cartesian*=None, *zmat_after_assignment*=None)

Raised when the i-th atom uses an invalid reference.

May carry several attributes:

- *i*: Index of the atom with an invalid refernce.
- *b*, *a*, and *d*: Indices of reference atoms.
- *already_built_cartesian*: The cartesian of all atoms up to (*i*-1)

- `zmat_after_assignment`: Attached information if it was raised from the safe assignment methods (`Zmat.safe_loc()` and `Zmat.unsafe_loc()`).

chemcoord.exceptions.UndefinedCoordinateSystem

exception `chemcoord.exceptions.UndefinedCoordinateSystem` (*message=""*)

Raised when there is no possibility to obtain a defined coordinate system for the chosen construction table.

chemcoord.exceptions.IllegalArgumentCombination

exception `chemcoord.exceptions.IllegalArgumentCombination`

Raised if the combination of correctly typed arguments is invalid.

chemcoord.exceptions.PhysicalMeaning

exception `chemcoord.exceptions.PhysicalMeaning` (*message=""*)

Raised when data is corrupted in a way, that it can not carry any information of physical meaning.

2.4 References

2.5 Bugreports and Development

If you request new feautres or want to report bugs please open an issue on the [github project page](#).

If you want to contribute in the development, feel free to contact me as well over the [github project page](#).

2.6 Previous Contribution

- Main Work: Oskar Weser
- Python2 compatibility: Keld Lundgaard

2.7 License

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The changelog can be found [here](#).

Citation and mathematical background

If chemcoord is used in a project that leads to a scientific publication, please acknowledge this fact by citing Oskar Weser (2017) using this ready-made BibTeX entry:

```
@mastersthesis{OWeser2017,  
author = {Oskar Weser},  
title = {An efficient and general library for the definition and use of internal_  
↪coordinates in large molecular systems},  
school = {Georg August Universität Göttingen},  
year = {2017},  
month = {November},  
}
```

The master thesis including the derivation of implemented equations and the mathematical background can be found [here](#).

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