OpenFF Fragmenter Documentation

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The main purpose of `openff-fragmenter` is to fragment molecules for quantum chemical (QC) torsion drives.

Warning: `openff-fragmenter` is still pre-alpha. It is not fully tested and the API is still in flux.

Currently two fragmentation schemes are supported:

- a Wiberg Bond Order (WBO) sensitive fragmentation scheme [1] *(recommended)*
- the fragmentation schema detailed by Rai *et al* [2] reffered to in this package as the 'Pfizer' scheme.

CHAPTER

ONE

WBO SENSITIVE FRAGMENTATION

The assumption when fragmenting molecules is that the chemistry is localized and that removing or changing remote substituents (defined as substituents more than 2 bonds away from the central bond that is being driven in the torsion drive) will not change the torsion potential around the bond of interest. However, that is not always the case. `openff-fragmenter` uses the Wiberg Bond Order (WBO) as a surrogate signal to determine if the chemistry around the bond of interest was destroyed during fragmentation relative to the bond in the parent molecule.

The WBO is a measure of electronic population overlap between two atoms in a bond. It can be quickly calculated from an empirical QC calculation and is given by:

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

Where A and B are atoms A and B in a bond, D is the density matrix and μ and ν are occupied orbitals on atoms A and B respectively.

`openff-fragmenter` calculates the WBO of the parent molecules, then fragments according to a set of rules and then recalculates the WBO of the fragments. If the WBO for the fragment of the bond of interest changes more than a user's specified threshold, `openff-fragmenter` will add more substituents until the WBO of the bond of interest is within the user specified threshold.

CHAPTER

TWO

CONTRIBUTORS

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CHAPTER

THREE

ACKNOWLEDGMENT

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CHAPTER

FOUR

REFERENCES

4.1 Installation

4.1.1 Installing using conda

The recommended way to install `openff-fragmenter` is via the `conda` package manger:

```
conda install -c conda-forge openff-fragmenter
```

If you have access to the OpenEye toolkits (namely `oechem`, `oequacpac` and `oeomega`) we recommend installing these also as these can speed up fragmentation times significantly:

```
conda install -c openeye openeye-toolkits
```

4.1.2 Installing from source

To install `openff-fragmenter` from source begin by cloning the repository from github:

```
git clone https://github.com/openforcefield/fragmenter.git
cd fragmenter
```

Create a custom conda environment which contains the required dependencies and activate it:

```
conda env create --name fragmenter --file devtools/conda-envs/meta.yaml
conda activate fragmenter
```

Finally, install `openff-fragmenter` itself:

```
python setup.py develop
```

4.2 Fragmenting Molecules

This notebook aims to show how a drug-like molecule can be fragmented using this framework, and how those fragments can be easily visualised using its built-in helper utilities.

To begin with we load in the molecule to be fragmented. Here we load Cobimetinib directly using its SMILES representation using the Open Force Field toolkit:

[1]:
```
from openff.toolkit.topology import Molecule

parent_molecule = Molecule.from_smiles(
    "OC1(CN(C1)C(=O)C1=C(NC2=C(F)C=C(I)C=C2)C(F)=C(F)C=C1)[C@@H]1CCCCN1"
)
```

Next we create the fragmentation engine which will perform the actual fragmentation. Here we will use the recommended `WBOFragmenter` with default options:

[2]:
```
from openff.fragmenter.fragment import WBOFragmenter

frag_engine = WBOFragmenter()
# Export the engine's settings directly to JSON
frag_engine.json()
```

[2]:
```
'{"functional_groups": {"hydrazine": "[NX3:1][NX3:2]", "hydrazone": "[NX3:1][NX2:2]",
↪"nitric_oxide": "[N:1]-[O:2]", "amide": "[#7:1][#6:2](=[#8:3])", "amide_n": "[#7:1][#6:
↪2](-[O-:3])", "amide_2": "[NX3:1][CX3:2](=[OX1:3])[NX3:4]", "aldehyde": "[CX3H1:1](=[O:
↪2])[#6:3]", "sulfoxide_1": "[#16X3:1]=[OX1:2]", "sulfoxide_2": "[#16X3+:1][OX1-:2]",
↪"sulfonyl": "[#16X4:1](=[OX1:2])=[OX1:3]", "sulfinic_acid": "[#16X3:1](=[OX1:2])[OX2H,
↪OX1H0-:3]", "sulfinamide": "[#16X4:1](=[OX1:2])(=[OX1:3])([NX3R0:4])", "sulfonic_acid":
↪ "[#16X4:1](=[OX1:2])(=[OX1:3])[OX2H,OX1H0-:4]", "phosphine_oxide": "[PX4:1](=[OX1:
↪2])([#6:3])([#6:4])([#6:5])", "phosphonate": "[P:1](=[OX1:2])([OX2H,OX1-:3])([OX2H,OX1-
↪:4])", "phosphate": "[PX4:1](=[OX1:2])([#8:3])([#8:4])([#8:5])", "carboxylic_acid":
↪"[CX3:1](=[O:2])[OX1H0-,OX2H1:3]", "nitro_1": "[NX3+:1](=[O:2])[O-:3]", "nitro_2":
↪"[NX3:1](=[O:2])=[O:3]", "ester": "[CX3:1](=[O:2])[OX2H0:3]", "tri_halide": "[#6:1]([F,
↪Cl,I,Br:2])([F,Cl,I,Br:3])([F,Cl,I,Br:4])"}, "scheme": "WBO", "wbo_options": {"method":
↪ "am1-wiberg-elf10", "max_conformers": 800, "rms_threshold": 1.0}, "threshold": 0.03,
↪"heuristic": "path_length", "keep_non_rotor_ring_substituents": false}'
```

Use the engine to fragment the molecule:

[3]:
```
result = frag_engine.fragment(parent_molecule)
# Export the result directly to JSON
result.json()
```

[3]:
```
'{"parent_smiles": "[H:31][c:1]1[c:3]([c:9]([c:11]([c:8]([c:6]1[C:13](=[O:25])[N:23]2[C:
↪18]([C:21]([C:19]2([H:46])[H:47])([C@@:20]3([C:16]([C:14]([C:15]([C:17]([N:22]3[H:
↪49])([H:42])[H:43])([H:38])[H:39])([H:36])[H:37])([H:40])[H:41])[H:48])[O:26][H:
↪51])([H:44])[H:45])[N:24]([H:50])[c:7]4[c:2]([c:4]([c:12]([c:5]([c:10]4[F:28])[H:
↪35])[I:30])[H:34])[H:32])[F:29])[F:27])[H:33]", "fragments": [{"smiles": "[H:34][c:
↪4]1[c:12]([c:5]([c:10]([c:7]([c:2]1[H:32])[N:24]([H:50])[c:8]2[c:6]([c:1]([c:3]([c:
↪9]([c:11]2[F:29])[F:27])[H:33])[H:31])[C:13](=[O:25])[N:23]3[C:18]([C:21]([C:19]3([H:
↪46])[H:47])([H])[H])([H:44])[H:45])[F:28])[H:35])[H]", "bond_indices": [8, 24]}, {
↪"smiles": "[H:48][C@:20]1([C:16]([C:14]([C:15]([C:17]([N:22]1[H:49])([H:42])[H:43])([H:
↪38])[H:39])([H:36])[H:37])([H:40])[H:41])[C:21]2([C:18]([N:23]([C:19]2([H:46])[H:
↪47])[C:13](=[O:25])[C:6]([H])([H])[H])([H:44])[H:45])[O:26][H:51]", "bond_indices":
↪[20, 21]}, {"smiles": "[H:34][c:4]1[c:12]([c:5]([c:10]([c:7]([c:2]1[H:32])[N:24]([H:
↪50])[c:8]2[c:6]([c:1]([c:3]([c:9]([c:11]2[F:29])[H])[H:33])[H:31])[C:13](=[O:25])[N:
↪23]3[C:18]([C:21]([C:19]3([H:46])[H:47])([H])[H])([H:44])[H:45])[F:28])[H:35])[H]",
↪"bond_indices": [7, 24]}, {"smiles": "[H:33][c:3]1[c:9]([c:11]([c:8]([c:6]([c:1]1[H:
↪31])[C:13](=[O:25])[N:23]2[C:18]([C:21]([C:19]2([H:46])[H:47])([H])[H])([H:44])[H:
↪45])[N:24]([H:50])[C:7]([H])([H])[H])[H])[H]", "bond_indices": [13, 23]}, {"smiles":
↪"[H:33][c:3]1[c:1]([c:6]([c:8]([c:11]([c:9]1[H])[F:29])[N:24]([H:50])[C:
```

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Any generated fragments will be returned in a `FragmentationResult` object. We can loop over each of the generated fragments and print both the SMILES representation of the fragment as well as the map indices of the bond that the fragment was built around:

[4]:
```
for fragment in result.fragments:
    print(f"{fragment.bond_indices}: {fragment.smiles}")
```

```
(8, 24): [H:34][c:4]1[c:12]([c:5]([c:10]([c:7]([c:2]1[H:32])[N:24]([H:50])[c:8]2[c:6]([c:
↪1]([c:3]([c:9]([c:11]2[F:29])[F:27])[H:33])[H:31])[C:13](=[O:25])[N:23]3[C:18]([C:
↪21]([C:19]3([H:46])[H:47])([H])[H])([H:44])[H:45])[F:28])[H:35])[H]
(20, 21): [H:48][C@:20]1([C:16]([C:14]([C:15]([C:17]([N:22]1[H:49])([H:42])[H:43])([H:
↪38])[H:39])([H:36])[H:37])([H:40])[H:41])[C:21]2([C:18]([N:23]([C:19]2([H:46])[H:
↪47])[C:13](=[O:25])[C:6]([H])([H])[H])([H:44])[H:45])[O:26][H:51]
(7, 24): [H:34][c:4]1[c:12]([c:5]([c:10]([c:7]([c:2]1[H:32])[N:24]([H:50])[c:8]2[c:6]([c:
↪1]([c:3]([c:9]([c:11]2[F:29])[H])[H:33])[H:31])[C:13](=[O:25])[N:23]3[C:18]([C:21]([C:
↪19]3([H:46])[H:47])([H])[H])([H:44])[H:45])[F:28])[H:35])[H]
(13, 23): [H:33][c:3]1[c:9]([c:11]([c:8]([c:6]([c:1]1[H:31])[C:13](=[O:25])[N:23]2[C:
↪18]([C:21]([C:19]2([H:46])[H:47])([H])[H])([H:44])[H:45])[N:24]([H:50])[C:
↪7]([H])([H])[H])[H])[H]
(6, 13): [H:33][c:3]1[c:1]([c:6]([c:8]([c:11]([c:9]1[H])[F:29])[N:24]([H:50])[C:
↪7]([H])([H])[H])[C:13](=[O:25])[N:23]2[C:18]([C:21]([C:19]2([H:46])[H:47])([H])[H])([H:
↪44])[H:45])[H:31]
```

Finally, we can visualize the produced fragments:

[5]:
```
from openff.fragmenter.depiction import depict_fragmentation_result

depict_fragmentation_result(result=result, output_file="example_fragments.html")

from IPython.core.display import HTML

with open("example_fragments.html") as file:
    display(HTML(file.read()))
```

```
<IPython.core.display.HTML object>
```

4.3 API

Below is an outline of the API for the main functions of `openff-fragmenter` See the examples for details on how to use these objects.

Warning: The `openff-fragmenter` package is still pre-alpha so the API is still in flux.

4.3.1 Fragmentation Engines

pydantic model `openff.fragmenter.fragment.`**`Fragmenter`**

The base class that all fragmentation engines should inherit from.

```
{
   "title": "Fragmenter",
   "description": "The base class that all fragmentation engines should inherit␣
↪from.",
   "type": "object",
   "properties": {
      "functional_groups": {
         "title": "Functional Groups",
         "description": "A dictionary of SMARTS of functional groups that should␣
↪not be fragmented, indexed by an informative name, e.g. 'alcohol': '[#6]-[#8X2H1]
↪'.",
         "type": "object",
         "additionalProperties": {
            "type": "string"
         }
      }
   }
}
```

Fields

- *functional_groups (Dict[str, str])*

field functional_groups: Dict[str, str] [Optional]

A dictionary of SMARTS of functional groups that should not be fragmented, indexed by an informative name, e.g. 'alcohol': '[#6]-[#8X2H1]'.

classmethod find_rotatable_bonds(*molecule: Molecule, target_bond_smarts: Optional[List[str]]*) → List[Tuple[int, int]]

Finds the rotatable bonds in a molecule *including* rotatable double bonds.

Parameters

- **molecule** – The molecule to search for rotatable bonds.
- **target_bond_smarts** – An optional list of SMARTS patterns that should be used to identify the bonds within the parent molecule to grow fragments around. Each SMARTS pattern should include **two** indexed atoms that correspond to the two atoms involved in the central bond.

  If no pattern is provided fragments will be constructed around all 'rotatable bonds'. A 'rotatable bond' here means any bond matched by a *[!$(*#*)&!D1:1]-,=;!@[!$(*#*)&!D1:2]* SMARTS pattern with the added constraint that the **heavy** degree (i.e. the degree excluding hydrogen) of both atoms in the bond must be >= 2.

Returns

- *A list of the **map** indices of the atoms that form the rotatable*
- bonds, `[(m1, m2),...]`.

fragment(*molecule: Molecule, target_bond_smarts: Optional[List[str]] = None, toolkit_registry: Optional[Union[openff.toolkit.utils.ToolkitRegistry, openff.toolkit.utils.ToolkitWrapper]] = None*) → *FragmentationResult*

Fragments a molecule according to this class' settings.

Notes

- This method is currently *not* guaranteed to be thread safe as it uses and modifies the OpenFF toolkits' `GLOBAL_TOOLKIT_REGISTRY`.

Parameters

- **molecule** – The molecule to fragment.
- **target_bond_smarts** – An optional list of SMARTS patterns that should be used to identify the bonds within the parent molecule to grow fragments around. Each SMARTS pattern should include **two** indexed atoms that correspond to the two atoms involved in the central bond.

  If no pattern is provided fragments will be constructed around all 'rotatable bonds'. A 'rotatable bond' here means any bond matched by a *[!$(*#*)&!D1:1]-,=;!@[!$(*#*)&!D1:2]* SMARTS pattern with the added constraint that the **heavy** degree (i.e. the degree excluding hydrogen) of both atoms in the bond must be >= 2. Note this will not find terminal rotatable bonds such as -OH, -NH2 -CH3.
- **toolkit_registry** – The underlying cheminformatics toolkits to use for things like conformer generation, WBO computation etc. If no value is provided, the current `GLOBAL_TOOLKIT_REGISTRY` will be used. See the OpenFF toolkit documentation for more information.

Returns

- *The results of the fragmentation including the fragments and provenance*
- *about the fragmentation.*

WBO

pydantic model `openff.fragmenter.fragment.`**WBOFragmenter**

Fragment engine for fragmenting molecules using Wiberg Bond Order.

```
{
   "title": "WBOFragmenter",
   "description": "Fragment engine for fragmenting molecules using Wiberg Bond␣
↪Order.",
   "type": "object",
   "properties": {
      "functional_groups": {
         "title": "Functional Groups",
         "description": "A dictionary of SMARTS of functional groups that should␣
↪not be fragmented, indexed by an informative name, e.g. 'alcohol': '[#6]-[#8X2H1]
↪'.",
```

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```
            "type": "object",
            "additionalProperties": {
               "type": "string"
            }
         },
         "scheme": {
            "title": "Scheme",
            "default": "WBO",
            "enum": [
               "WBO"
            ],
            "type": "string"
         },
         "wbo_options": {
            "title": "Wbo Options",
            "description": "The options to use when computing the WBOs.",
            "default": {
               "method": "am1-wiberg-elf10",
               "max_conformers": 800,
               "rms_threshold": 1.0
            },
            "allOf": [
               {
                  "$ref": "#/definitions/WBOOptions"
               }
            ]
         },
         "threshold": {
            "title": "Threshold",
            "description": "The threshold for the central bond WBO. If the fragment␣
↪WBO is below this threshold, fragmenter will grow out the fragment one bond at a␣
↪time via the path specified by the heuristic option",
            "default": 0.03,
            "type": "number"
         },
         "heuristic": {
            "title": "Heuristic",
            "description": "The path fragmenter should take when fragment needs to be␣
↪grown out. The options are ``['wbo', 'path_length']``.",
            "default": "path_length",
            "enum": [
               "path_length",
               "wbo"
            ],
            "type": "string"
         },
         "keep_non_rotor_ring_substituents": {
            "title": "Keep Non Rotor Ring Substituents",
            "description": "Whether to always keep all non rotor substituents on rings.
↪ If ``False``, rotor substituents on rings will only be retained if they are␣
↪ortho to the central bond or if it's needed for WBO to be within the threshold.",
            "default": false,
```

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```
            "type": "boolean"
         }
      },
      "definitions": {
         "WBOOptions": {
            "title": "WBOOptions",
            "description": "A set of options for controlling how Wiberg Bond Orders␣
↪are computed.",
            "type": "object",
            "properties": {
               "method": {
                  "title": "Method",
                  "description": "The method to use when computing the WBOs.",
                  "default": "am1-wiberg-elf10",
                  "enum": [
                     "am1-wiberg-elf10"
                  ],
                  "type": "string"
               },
               "max_conformers": {
                  "title": "Max Conformers",
                  "description": "The maximum number of conformers to average the WBOs␣
↪over.",
                  "default": 800,
                  "type": "integer"
               },
               "rms_threshold": {
                  "title": "Rms Threshold",
                  "description": "The minimum RMS value [Angstrom] at which two␣
↪conformers are considered redundant and one is deleted.",
                  "default": 1.0,
                  "type": "number"
               }
            }
         }
      }
}
```

Fields

- *heuristic (typing_extensions.Literal[path_length, wbo])*
- *keep_non_rotor_ring_substituents (bool)*
- *scheme (typing_extensions.Literal[WBO])*
- *threshold (float)*
- *wbo_options (openff.fragmenter.fragment.WBOOptions)*

field scheme: typing_extensions.Literal[WBO] = 'WBO'

field wbo_options: *WBOOptions* = WBOOptions(method='am1-wiberg-elf10', max_conformers=800, rms_threshold=1.0)

The options to use when computing the WBOs.

field threshold: float = 0.03

The threshold for the central bond WBO. If the fragment WBO is below this threshold, fragmenter will grow out the fragment one bond at a time via the path specified by the heuristic option

field heuristic: typing_extensions.Literal[path_length, wbo] = 'path_length'

The path fragmenter should take when fragment needs to be grown out. The options are `['wbo', 'path_length']`.

field keep_non_rotor_ring_substituents: bool = False

Whether to always keep all non rotor substituents on rings. If `False`, rotor substituents on rings will only be retained if they are ortho to the central bond or if it's needed for WBO to be within the threshold.

pydantic model `openff.fragmenter.fragment.`**WBOOptions**

A set of options for controlling how Wiberg Bond Orders are computed.

```
{
   "title": "WBOOptions",
   "description": "A set of options for controlling how Wiberg Bond Orders are␣
↪computed.",
   "type": "object",
   "properties": {
      "method": {
         "title": "Method",
         "description": "The method to use when computing the WBOs.",
         "default": "am1-wiberg-elf10",
         "enum": [
            "am1-wiberg-elf10"
         ],
         "type": "string"
      },
      "max_conformers": {
         "title": "Max Conformers",
         "description": "The maximum number of conformers to average the WBOs over.
↪",
         "default": 800,
         "type": "integer"
      },
      "rms_threshold": {
         "title": "Rms Threshold",
         "description": "The minimum RMS value [Angstrom] at which two conformers␣
↪are considered redundant and one is deleted.",
         "default": 1.0,
         "type": "number"
      }
   }
}
```

Fields

- *max_conformers (int)*
- *method (typing_extensions.Literal[am1-wiberg-elf10])*
- *rms_threshold (float)*

field method: typing_extensions.Literal[am1-wiberg-elf10] = 'am1-wiberg-elf10'

The method to use when computing the WBOs.

field max_conformers: int = 800

The maximum number of conformers to average the WBOs over.

field rms_threshold: float = 1.0

The minimum RMS value [Angstrom] at which two conformers are considered redundant and one is deleted.

Pfizer

pydantic model openff.fragmenter.fragment.**PfizerFragmenter**

Fragment engine for fragmenting molecules using Pfizer's protocol (doi: 10.1021/acs.jcim.9b00373)

```
{
   "title": "PfizerFragmenter",
   "description": "Fragment engine for fragmenting molecules using Pfizer's␣
↪protocol\n(doi: 10.1021/acs.jcim.9b00373)",
   "type": "object",
   "properties": {
      "functional_groups": {
         "title": "Functional Groups",
         "description": "A dictionary of SMARTS of functional groups that should␣
↪not be fragmented, indexed by an informative name, e.g. 'alcohol': '[#6]-[#8X2H1]
↪'.",
         "type": "object",
         "additionalProperties": {
            "type": "string"
         }
      },
      "scheme": {
         "title": "Scheme",
         "default": "Pfizer",
         "enum": [
            "Pfizer"
         ],
         "type": "string"
      }
   }
}
```

Fields

- *scheme (typing_extensions.Literal[Pfizer])*

field scheme: typing_extensions.Literal[Pfizer] = 'Pfizer'

4.3.2 Fragmentation Outputs

pydantic model openff.fragmenter.fragment.**Fragment**

An object which stores minimal information about a molecules fragment.

```
{
   "title": "Fragment",
   "description": "An object which stores minimal information about a molecules␣
↪fragment.",
   "type": "object",
   "properties": {
      "smiles": {
         "title": "Smiles",
         "description": "A mapped SMILES pattern describing the fragment. The map␣
↪indices assigned to each atom in the pattern will correspond to the map index of␣
↪the corresponding parent atom. If an atom does not have a map index it is likely␣
↪that the atom was added (either H, or C) to ensure every atom in the fragment has␣
↪a sensible valence.",
         "type": "string"
      },
      "bond_indices": {
         "title": "Bond Indices",
         "description": "The map indices of the atoms involved in the bond that the␣
↪fragment was built around.",
         "type": "array",
         "minItems": 2,
         "maxItems": 2,
         "items": [
            {
               "type": "integer"
            },
            {
               "type": "integer"
            }
         ]
      }
   },
   "required": [
      "smiles",
      "bond_indices"
   ]
}
```

Fields

- *bond_indices (Tuple[int, int])*
- *smiles (str)*

field smiles: str [Required]

A mapped SMILES pattern describing the fragment. The map indices assigned to each atom in the pattern will correspond to the map index of the corresponding parent atom. If an atom does not have a map index it is likely that the atom was added (either H, or C) to ensure every atom in the fragment has a sensible valence.

field bond_indices: Tuple[int, int] [Required]

The map indices of the atoms involved in the bond that the fragment was built around.

property molecule: Molecule

The fragment represented as an OpenFF molecule object.

pydantic model openff.fragmenter.fragment.**FragmentationResult**

An object which stores the results of fragmenting a molecule.

```
{
   "title": "FragmentationResult",
   "description": "An object which stores the results of fragmenting a molecule.",
   "type": "object",
   "properties": {
      "parent_smiles": {
         "title": "Parent Smiles",
         "description": "A mapped SMILES pattern describing the parent molecule␣
↪that was fragmented.",
         "type": "string"
      },
      "fragments": {
         "title": "Fragments",
         "description": "The generated fragments.",
         "type": "array",
         "items": {
            "$ref": "#/definitions/Fragment"
         }
      },
      "provenance": {
         "title": "Provenance",
         "description": "A dictionary storing provenance information about how the␣
↪fragments were generated.",
         "type": "object"
      }
   },
   "required": [
      "parent_smiles",
      "fragments",
      "provenance"
   ],
   "definitions": {
      "Fragment": {
         "title": "Fragment",
         "description": "An object which stores minimal information about a␣
↪molecules fragment.",
         "type": "object",
         "properties": {
            "smiles": {
               "title": "Smiles",
               "description": "A mapped SMILES pattern describing the fragment. The␣
↪map indices assigned to each atom in the pattern will correspond to the map index␣
↪of the corresponding parent atom. If an atom does not have a map index it is␣
↪likely that the atom was added (either H, or C) to ensure every atom in the␣
↪fragment has a sensible valence.",
```

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```
                "type": "string"
            },
            "bond_indices": {
                "title": "Bond Indices",
                "description": "The map indices of the atoms involved in the bond␣
↪that the fragment was built around.",
                "type": "array",
                "minItems": 2,
                "maxItems": 2,
                "items": [
                    {
                        "type": "integer"
                    },
                    {
                        "type": "integer"
                    }
                ]
            }
        },
        "required": [
            "smiles",
            "bond_indices"
        ]
    }
  }
}
```

Fields

- *fragments (List[openff.fragmenter.fragment.Fragment])*
- *parent_smiles (str)*
- *provenance (Dict[str, Any])*

field parent_smiles: str [Required]

A mapped SMILES pattern describing the parent molecule that was fragmented.

field fragments: List[*Fragment*] [Required]

The generated fragments.

field provenance: Dict[str, Any] [Required]

A dictionary storing provenance information about how the fragments were generated.

property parent_molecule: Molecule

The parent molecule represented as an OpenFF molecule object.

property fragment_molecules: Dict[Tuple[int, int], Molecule]

A dictionary of the fragment molecules represented as OpenFF molecule objects, indexed by the map indices of the bond that each fragment was built around.

property fragments_by_bond: Dict[Tuple[int, int], *Fragment*]

Returns a dictionary of fragments indexed by the bond (defined in terms of the map indices of the atoms that form it) that the fragment was built around.

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[2] Brajesh K. Rai, Vishnu Sresht, Qingyi Yang, Ray Unwalla, Meihua Tu, Alan M. Mathiowetz, and Gregory A. Bakken. Comprehensive assessment of torsional strain in crystal structures of small molecules and protein–ligand complexes using ab initio calculations. *Journal of Chemical Information and Modeling*, 59(10):4195–4208, 2019. PMID: 31573196. URL: https://doi.org/10.1021/acs.jcim.9b00373, arXiv:https://doi.org/10.1021/acs.jcim.9b00373, doi:10.1021/acs.jcim.9b00373.

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