

Molecular fragment operations and fragment analysis

User:

You are given trans-stilbene.xyz and L-alanine.xyz. 1. Make edits to trans-stilbene.xyz to create its photoisomerization TS and also cis-stilbene. 2. Make edits to L-alanine.xyz to generate its enantiomer.

 **Estructural**

Tool used:

Tool Name: repl_tool

Arguments:

```
code =
import os
import shutil

project_dir = "isomers_and_enantiomers_project"
os.makedirs(project_dir, exist_ok=True)

shutil.copy("trans-stilbene.xyz", os.path.join(project_dir, "trans-stilbene.xyz"))
shutil.copy("L-alanine.xyz", os.path.join(project_dir, "L-alanine.xyz"))

print(f"Created {project_dir} and copied files.")
```

 **Estructural**

Tool used:

Tool Name: match_smarts_in_xyz

Arguments:

```
file_path = isomers_and_enantiomers_project/trans-stilbene.xyz
smarts = C=C
```

Tool Name: match_smarts_in_xyz

Arguments:

```
file_path = isomers_and_enantiomers_project/L-alanine.xyz
smarts = C(N)(C)C(=O)O
```

 **Estructural**

Tool used:

Tool Name: get_atomic_neighbors

Arguments:

```
target = 2
file_path = isomers_and_enantiomers_project/trans-stilbene.xyz
```

Tool Name: get_atomic_neighbors

Arguments:

```
target = 3
file_path = isomers_and_enantiomers_project/trans-stilbene.xyz
```

Tool Name: get_atomic_neighbors

Arguments:

```
target = 0
file_path = isomers_and_enantiomers_project/L-alanine.xyz
```

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Tool used:

Tool Name: repl_tool

Arguments:

code =
import json

def parse_neighbors(output_str):

 # This is a dummy parser, I will just print the output in the next step
 pass

print("Checking neighbors for L-alanine atoms 1, 2, 3, 4, 5...")

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Tool used:

Tool Name: get_atomic_neighbors

Arguments:

target = 5
file_path = isomers_and_enantiomers_project/L-alanine.xyz

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Tool used:

Tool Name: get_atomic_neighbors

Arguments:

target = 3
file_path = isomers_and_enantiomers_project/L-alanine.xyz

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Tool used:

Tool Name: set_dihedral_between_fragments

Arguments:

input_path = isomers_and_enantiomers_project/trans-stilbene.xyz
output_path = isomers_and_enantiomers_project/stilbene_photoisomerization_TS.xyz
angle = 90
consider_fragments = True
atoms_list = [0, 2, 3, 1]

Tool Name: set_dihedral_between_fragments

Arguments:

input_path = isomers_and_enantiomers_project/trans-stilbene.xyz
output_path = isomers_and_enantiomers_project/cis-stilbene.xyz
angle = 0
consider_fragments = True
atoms_list = [0, 2, 3, 1]

Tool Name: rotate_substituents_around_bisector

Arguments:

center_idx = 3
output_path = isomers_and_enantiomers_project/D-alanine.xyz

```
fragment_mode = auto
base_vector_indices = [4, 6]
input_path = isomers_and_enantiomers_project/L-alanine.xyz
angle_deg = 180
```

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Action:

The requested edits have been performed on **trans-stilbene.xyz** and **L-alanine.xyz** to generate the specified isomers and enantiomers. The output files are saved in the **isomers_and_enantiomers_project** directory.

1. Stilbene Isomerization Using **trans-stilbene.xyz** as the starting structure, two new geometries were generated by modifying the C-C=C-C dihedral angle defined by the central double bond (atoms 2 and 3) and their phenyl attachments (atoms 0 and 1).

- **Photoisomerization Transition State (TS):**

- **File:** **isomers_and_enantiomers_project/stilbene_photoisomerization_TS.xyz**
- **Method:** The central dihedral angle was set to **90°** to approximate the perpendicular transition state characteristic of stilbene photoisomerization.

- **Cis-Stilbene:**

- **File:** **isomers_and_enantiomers_project/cis-stilbene.xyz**
- **Method:** The central dihedral angle was set to **0°**, converting the trans isomer (dihedral 180°) to the cis configuration.

2. L-Alanine Enantiomer Generation Using **L-alanine.xyz**, the D-alanine enantiomer was created by inverting the configuration at the chiral center.

- **D-Alanine:**

- **File:** **isomers_and_enantiomers_project/D-alanine.xyz**
- **Method:** The chiral center was identified at atom **C:3**. Its substituents, the methyl group (C:4) and the alpha-hydrogen (H:6), were swapped by rotating them 180° around their bisector axis. This operation inverted the stereocenter from L- to D-alanine.