

## 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
```

## Estructural

### 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...")
```

## Estructural

### Tool used:

```
Tool Name: get_atomic_neighbors
Arguments:
target = 5
file_path = isomers_and_enantiomers_project/L-alanine.xyz
```

## Estructural

### Tool used:

```
Tool Name: get_atomic_neighbors
Arguments:
target = 3
file_path = isomers_and_enantiomers_project/L-alanine.xyz
```

## Estructural

### 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
```

## ⌚ Estructural

### 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.