

## Geometric operation on ferrocene

### User:

Generate an XYZ file for ferrocene. Then create and save separate XYZ files for the following structural modifications:

1. Stretch the distance between the Fe atom and one Cp ring to 4.5 Å
2. Change the Cp–Fe–Cp angle to 120°.

### Estructural

#### Tool used:

Tool Name: find\_available\_fragments

Arguments:

type = predefined\_organometallics

### Estructural

#### Tool used:

Tool Name: find\_available\_fragments

Arguments:

type = ligand

name = Cp

### Estructural

#### Tool used:

Tool Name: build\_tm\_complex\_from\_template

Arguments:

ligand\_bindings = [{"Cp": [1, 2]}]

output\_path = ferrocene\_mods\_project/ferrocene.xyz

coordination\_geometry = linear

metal = Fe

### Estructural

#### Tool used:

Tool Name: build\_tm\_complex\_from\_template

Arguments:

ligand\_bindings = [{"Cp": [1, 2]}]

output\_path = ferrocene\_project/ferrocene.xyz

coordination\_geometry = linear

metal = Fe

### Estructural

#### Tool used:

Tool Name: match\_smarts\_in\_xyz

Arguments:

file\_path = ferrocene\_project/ferrocene.xyz

smarts = c1ccccc1

### Estructural

**Tool used:**

Tool Name: match\_smarts\_in\_xyz  
Arguments:  
smarts = [#6]  
file\_path = ferrocene\_project/ferrocene.xyz

**⌚ Estructural****Tool used:**

Tool Name: get\_connected\_subgraph\_indices  
Arguments:  
exclude = 0  
file\_path = ferrocene\_project/ferrocene.xyz  
start\_index = 1

**⌚ Estructural****Tool used:**

Tool Name: get\_connected\_subgraph\_indices  
Arguments:  
exclude = 0  
file\_path = ferrocene\_project/ferrocene.xyz  
start\_index = 11

**⌚ Estructural****Tool used:**

Tool Name: set\_distance\_between\_fragments  
Arguments:  
input\_path = ferrocene\_project/ferrocene.xyz  
output\_path = ferrocene\_project/ferrocene\_dist\_4.5.xyz  
fragment\_indices = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]  
targets = [{"atom": [0]}, {"group": [1, 2, 3, 4, 5]}]  
distance = 4.5  
fragment\_mode = manual

**⌚ Estructural****Tool used:**

Tool Name: set\_angle\_between\_fragments  
Arguments:  
fragment\_indices = [11, 12, 13, 14, 15, 16, 17, 18, 19, 20]  
output\_path = ferrocene\_project/ferrocene\_angle\_120.xyz  
targets = [{"group": [1, 2, 3, 4, 5]}, {"atom": [0]}, {"group": [11, 12, 13, 14, 15]}]  
input\_path = ferrocene\_project/ferrocene.xyz  
angle = 120  
fragment\_mode = manual

**⌚ Estructural**

**Action:**

The requested XYZ files have been generated and saved in the `ferrocene_project` directory.

1. **Base Structure:** `ferrocene_project/ferrocene.xyz`
  - Generated using a linear iron template with two cyclopentadienyl (Cp) ligands.
2. **Distance Modification:** `ferrocene_project/ferrocene_dist_4.5.xyz`
  - The distance between the Iron atom and one Cp ring centroid was set to **4.5 Å**.
3. **Angle Modification:** `ferrocene_project/ferrocene_angle_120.xyz`
  - The Cp(centroid)-Fe-Cp(centroid) angle was adjusted to **120°**.