

Construction of zirconocene-based complexes

User:

Generate XYZ files for the following zirconocene complexes:

1. Zirconocene dichloride, ZrCp_2Cl_2
2. A zirconocene complex with one methyl ligand and one η^2 -coordinated ethylene ligand, $\text{ZrCp}_2(\text{CH}_3)(\eta^2\text{-C}_2\text{H}_4)$

Estructural

Tool used:

Tool Name: find_available_fragments

Arguments:

```
type = predefined_organometallics  
name = zirconocene
```

Tool Name: find_available_fragments

Arguments:

```
type = ligand  
name = Cp
```

Tool Name: find_available_fragments

Arguments:

```
type = ligand  
name = ethylene
```

Estructural

Tool used:

Tool Name: build_tm_complex_from_template

Arguments:

```
ligand_bindings = [{"Cp": [1, 2]}]  
output_path = zirconocene_project/ZrCp2Cl2.xyz  
coordination_geometry = tetrahedral  
metal = Zr
```

Tool Name: build_tm_complex_from_template

Arguments:

```
ligand_bindings = [{"Cp": [1, 2]}, {"Me": [3]}, {"ethylene": [4]}]  
output_path = zirconocene_project/ZrCp2Me_ethylene.xyz  
coordination_geometry = tetrahedral  
metal = Zr
```

Estructural

Tool used:

Tool Name: repl_tool

Arguments:

```
code =  
import os  
os.makedirs('zirconocene_project', exist_ok=True)  
print("Directory created")
```

Estructural

Tool used:

Tool Name: build_tm_complex_from_template

Arguments:

```
ligand_bindings = [{"Cp": [1, 2]}]
metal = Zr
coordination_geometry = tetrahedral
output_path = zirconocene_project/ZrCp2Cl2.xyz
```

Tool Name: build_tm_complex_from_template

Arguments:

```
ligand_bindings = [{"Cp": [1, 2]}, {"Me": [3]}, {"ethylene": [4]}]
metal = Zr
coordination_geometry = tetrahedral
output_path = zirconocene_project/ZrCp2Me_ethylene.xyz
```

⌚ Estructural**Action:**

The XYZ files for the requested zirconocene complexes have been generated and saved in the zirconocene_project folder.

1. Zirconocene dichloride (ZrCp_2Cl_2)

- **File:** zirconocene_project/ZrCp2Cl2.xyz
- **Construction:** Built using a tetrahedral zirconium template with two cyclopentadienyl (Cp) ligands and two chloride ligands (default).

2. Zirconocene methyl ethylene complex ($\text{ZrCp}_2(\text{CH}_3)(\eta^2\text{-C}_2\text{H}_4)$)

- **File:** zirconocene_project/ZrCp2Me_ethylene.xyz
- **Construction:** Built using a tetrahedral zirconium template with two Cp ligands, one methyl (Me) ligand, and one ethylene ligand.
- **Note:** The ethylene ligand is attached using the standard fragment library definition. The " η^2 " coordination is implied by the binding mode in the template, though the exact hapticity depends on the predefined fragment's orientation relative to the metal center.