

# Multimodal reaction mechanism-guided structure generation

## User:

You are given an image file, mechanism.png, which depicts a chemical reaction mechanism. Based solely on the information shown in the image, generate three-dimensional molecular structures corresponding to each reaction intermediate and transition state depicted in the mechanism. Generate and save a separate XYZ file for each reaction intermediate and transition state.

## Estructural

### Action:

I'll start by viewing the mechanism.png image to understand the chemical reaction mechanism depicted and identify all the intermediates and transition states that need to be generated.

### Tool used:

Tool Name: view\_png\_file

Arguments:

png\_file\_relative\_path = mechanism.png

## Estructural

### Action:

Excellent! I can see this is a **migratory insertion mechanism** involving a zirconocene complex. The mechanism shows:

1. **Intermediate 1 (Left):**  $\text{Cp}_2\text{Zr}^+(\text{CH}_3)(\eta^2\text{-ethylene})$  - Zirconocene cation with a methyl group and coordinated ethylene
2. **Transition State (Middle):** 4-membered ring transition state showing the migratory insertion process with dashed bonds
3. **Intermediate 2 (Right):**  $\text{Cp}_2\text{Zr}^+(\text{n-propyl})$  - Zirconocene cation with a propyl group (product of insertion)

Let me start building these structures. First, let me check what predefined templates and fragments are available for zirconocene complexes.

### Tool used:

Tool Name: find\_available\_fragments

Arguments:

type = predefined\_organometallics

## Estructural

### Action:

Let me check for available ligands, specifically the cyclopentadienyl (Cp) ligand and other necessary fragments:

### Tool used:

Tool Name: find\_available\_fragments

Arguments:

name = Cp

## Estructural

### Tool used:

Tool Name: find\_available\_fragments

Arguments:

```
name = ethylene
```

## ⌚ Estructural

### Tool used:

Tool Name: find\_available\_fragments

Arguments:

```
name = Me
```

## ⌚ Estructural

### Action:

Now I have all the information I need. Let me build the three structures systematically.

### Building the structures:

**Structure 1 - Intermediate 1:**  $\text{Cp}_2\text{Zr}(\text{CH}_3)(\eta^2\text{-ethylene})^+$  **Structure 2 - Transition State:** 4-membered ring TS **Structure 3 - Intermediate 2:**  $\text{Cp}_2\text{Zr}(\text{n-propyl})^+$

Let me start by building **Intermediate 1** using the tetrahedral template with two Cp rings, a methyl group, and an ethylene ligand:

### Tool used:

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

Arguments:

```
coordination_geometry = tetrahedral
metal = Zr
ligand_bindings = [{"Cp": [1, 2]}, {"CH3": [3]}, {"ethylene": [4]}]
output_path = intermediate_1_Cp2Zr_CH3_ethylene.xyz
```

## ⌚ Estructural

### Action:

Intermediate 1 has been created. Let me visualize it to verify the structure:

### Tool used:

Tool Name: view\_molecule

Arguments:

```
xyz_file_relative_path = intermediate_1_Cp2Zr_CH3_ethylene.xyz
left_right_deg = 20
up_down_deg = 15
```

## ⌚ Estructural

### Action:

I can see Intermediate 1 with:

- Zr center (index 0)
- Two Cp rings (indices 2-11 and 12-21)
- Methyl group
- Ethylene ligand (C:25, C:26 at top)

Now let me build **Intermediate 2** (the product with propyl group). First, let me check if propyl is available in the fragment library:

### Tool used:

Tool Name: find\_available\_fragments

Arguments:

```
name = propyl
```

## Estructural

### Action:

Excellent! I found the propyl group (nPr). Now let me build **Intermediate 2** ( $\text{Cp}_2\text{Zr}$ -propyl):

### Tool used:

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

#### Arguments:

```
coordination_geometry = trigonal_planar
ligand_bindings = [{"Cp": [1, 2], "nPr": [3]}]
metal = Zr
output_path = intermediate_2_Cp2Zr_propyl.xyz
```

## Estructural

### Action:

Let me visualize Intermediate 2 to verify it:

### Tool used:

Tool Name: view\_molecule

#### Arguments:

```
left_right_deg = 20
up_down_deg = 15
xyz_file_relative_path = intermediate_2_Cp2Zr_propyl.xyz
```

## Estructural

### Action:

I can see Intermediate 2 with:

- Zr:0 at center
- Two Cp rings (C:2-6 and C:12-16 with their H atoms)
- Propyl group (C:1, C:23, C:24 chain with H atoms)

The propyl appears disconnected visually, but this is common for metal-organic bonds in the viewer.

Let me verify the Zr-C bond distance:

### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

```
input_path = intermediate_2_Cp2Zr_propyl.xyz
targets = [{"atom": [0], "atom": [1]}]
```

## Estructural

### Action:

The Zr-C distance is 2.475 Å, which is appropriate for a Zr-C bond. The structure is valid.

Now I need to construct the **Transition State** for the migratory insertion. Let me first analyze the atom connectivity in Intermediate 1 to understand the key atoms involved:

### Tool used:

Tool Name: get\_atomic\_neighbors

#### Arguments:

```
file_path = intermediate_1_Cp2Zr_CH3_ethylene.xyz
target = 0
```

## Estructural

**Action:**

Let me check the neighbors of the methyl carbon (which should be index 1 based on the bond pair info):

**Tool used:**

Tool Name: get\_atomic\_neighbors

Arguments:

file\_path = intermediate\_1\_Cp2Zr\_CH3\_ethylene.xyz

target = 1

 **Estructural****Action:**

Now I understand the structure:

- C:1 is the methyl carbon (bonded to Zr:0, H:22, H:23, H:24)
- C:25 and C:26 are the ethylene carbons

Let me check the ethylene carbon neighbors:

**Tool used:**

Tool Name: get\_atomic\_neighbors

Arguments:

file\_path = intermediate\_1\_Cp2Zr\_CH3\_ethylene.xyz

target = 25

 **Estructural****Tool used:**

Tool Name: get\_atomic\_neighbors

Arguments:

file\_path = intermediate\_1\_Cp2Zr\_CH3\_ethylene.xyz

target = 26

 **Estructural****Action:**

Now I have a clear picture of the structure:

- C:1 = methyl carbon (bonded to Zr:0)
- C:25 = ethylene carbon 1 (bonded to C:26, H:29, H:30, Zr:0)
- C:26 = ethylene carbon 2 (bonded to C:25, H:27, H:28, Zr:0)

For the **transition state**, I need to create a 4-membered ring: Zr-C25-C26-C1 (or similar). Let me get the current distances to plan the TS geometry:

**Tool used:**

Tool Name: repl\_tool

Arguments:

code =

```
# Get key distances in intermediate_1 for planning the TS
import subprocess
```

```
# Read the xyz file to understand the geometry
with open('intermediate_1_Cp2Zr_CH3_ethylene.xyz', 'r') as f:
    content = f.read()
print("Intermediate 1 structure:")
print(content[:2000])
```

## Estructural

### Action:

Now let me measure the key distances needed for the TS geometry:

#### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

```
input_path = intermediate_1_Cp2Zr_CH3_ethylene.xyz  
targets = [{"atom": [0]}, {"atom": [1]}]
```

## Estructural

#### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

```
input_path = intermediate_1_Cp2Zr_CH3_ethylene.xyz  
targets = [{"atom": [1]}, {"atom": [25]}]
```

## Estructural

#### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

```
input_path = intermediate_1_Cp2Zr_CH3_ethylene.xyz  
targets = [{"atom": [1]}, {"atom": [26]}]
```

## Estructural

#### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

```
input_path = intermediate_1_Cp2Zr_CH3_ethylene.xyz  
targets = [{"atom": [25]}, {"atom": [26]}]
```

## Estructural

### Action:

Now I have all the key distances:

- Zr-C1 (methyl): 2.475 Å
- C1-C25: 4.28 Å
- C1-C26: 3.90 Å
- C25-C26 (ethylene C=C): 1.33 Å

For the **transition state**, I need to bring the methyl carbon (C1) close to one of the ethylene carbons (C26) while allowing the rest of the structure to relax. I'll use constrained xTB optimization with a C1-C26 distance constraint of 2.1 Å (typical for a forming C-C bond in TS):

#### Tool used:

Tool Name: constraint\_xtb

#### Arguments:

```
input_xyz = intermediate_1_Cp2Zr_CH3_ethylene.xyz  
output_xyz = transition_state_migratory_insertion.xyz
```

```
distance_constraints = [{"atoms": [1, 26], "value": 2.1}]
force_constant = 1.0
charge = 1
gfn_method = gfn2
```

## ⌚ Estructural

### Action:

The transition state structure has been generated. Let me visualize it to verify the 4-membered ring geometry:

### Tool used:

Tool Name: view\_molecule

#### Arguments:

left\_right\_deg = 15

up\_down\_deg = 20

xyz\_file\_relative\_path = transition\_state\_migratory\_insertion.xyz

## ⌚ Estructural

### Action:

Excellent! The transition state structure shows the characteristic 4-membered ring geometry! I can see:

- Zr:0 at center
- Two Cp rings (top and right)
- The 4-membered ring on the left: C:1 (methyl) - C:26 - C:25 forming the insertion geometry

Let me verify the key distances in the transition state:

### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

input\_path = transition\_state\_migratory\_insertion.xyz

targets = [{"atom": [1], "atom": [26]}]

## ⌚ Estructural

### Action:

The C1-C26 distance is now 2.09 Å (forming C-C bond). Let me also check the Zr-C distances:

### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

input\_path = transition\_state\_migratory\_insertion.xyz

targets = [{"atom": [0], "atom": [1]}]

## ⌚ Estructural

### Tool used:

Tool Name: get\_distance\_angle\_dihedral

#### Arguments:

input\_path = transition\_state\_migratory\_insertion.xyz

targets = [{"atom": [0], "atom": [25]}]

## ⌚ Estructural

**Action:**

The Zr-C25 distance is 2.24 Å (forming new  $\sigma$ -bond to ethylene carbon).

The transition state shows excellent geometry for migratory insertion:

- **C1-C26:** 2.09 Å (forming C-C bond)
- **Zr-C1:** 2.43 Å (partially breaking Zr-methyl bond)
- **Zr-C25:** 2.24 Å (forming new Zr-C  $\sigma$ -bond)

Now let me view Intermediate 2 from a better angle to confirm the propyl structure:

**Tool used:**

Tool Name: view\_molecule

Arguments:

left\_right\_deg = -30

up\_down\_deg = 10

xyz\_file\_relative\_path = intermediate\_2\_Cp2Zr\_propyl.xyz

## ⌚ Estructural

**Action:**

I can clearly see Intermediate 2 with:

- Zr:0 at center
- Two Cp rings (C:12-16 and C:2-6)
- Propyl chain: C:1 (bonded to Zr) → C:24 → C:27 (terminal CH<sub>3</sub>)

**Summary: Generated XYZ Files for Migratory Insertion Mechanism**

Based on the mechanism image showing olefin insertion into a Zr-C bond, I have successfully generated three 3D molecular structures:

**1. Intermediate 1 (intermediate\_1\_Cp2Zr\_CH3\_ethylene.xyz)**

- **Structure:** Cp<sub>2</sub>Zr<sup>+</sup>(CH<sub>3</sub>)(η<sup>2</sup>-C<sub>2</sub>H<sub>4</sub>)
- **Description:** Zirconocene cation with methyl ligand and side-on coordinated ethylene
- **Key features:**
  - Zr-CH<sub>3</sub> bond: 2.48 Å
  - η<sup>2</sup>-ethylene coordination (both ethylene carbons bonded to Zr)
  - Tetrahedral-like geometry around Zr center

**2. Transition State (transition\_state\_migratory\_insertion.xyz)**

- **Structure:** 4-membered ring TS for migratory insertion
- **Description:** The methyl group migrates to ethylene while Zr forms a  $\sigma$ -bond
- **Key TS distances:**
  - C(methyl)-C(ethylene) forming bond: **2.09 Å**
  - Zr-C(methyl) elongating bond: **2.43 Å**
  - Zr-C(ethylene) forming  $\sigma$ -bond: **2.24 Å**

**3. Intermediate 2 (intermediate\_2\_Cp2Zr\_propyl.xyz)**

- **Structure:** Cp<sub>2</sub>Zr<sup>+</sup>(n-C<sub>3</sub>H<sub>7</sub>)
- **Description:** Zirconocene cation with n-propyl ligand (product of ethylene insertion)
- **Key features:**
  - Zr-C(propyl) bond: 2.48 Å
  - Propyl chain: -CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub> attached to Zr

All three XYZ files have been saved and represent the complete migratory insertion mechanism as depicted in the mechanism.png image.