

Binding of reaction intermediates and ligands

User:

Given the cobalt-phthalocyanine complex (Co-Pc.xyz), bind the following ligands to the Co atom: CO₂, COOH, CO, H, OH, and H₂O.

⌚ Estructural

Tool used:

Tool Name: repl_tool

Arguments:

code =

import os

import shutil

```
project_dir = 'CoPc_ligand_binding_project'  
os.makedirs(project_dir, exist_ok=True)  
source_file = 'Co-Pc.xyz'  
target_file = os.path.join(project_dir, 'Co-Pc.xyz')  
  
if os.path.exists(source_file):  
    shutil.move(source_file, target_file)  
    print(f"Moved {source_file} to {target_file}")  
else:  
    print(f"{source_file} not found in root (it might have been moved already). Checking target...")  
    if os.path.exists(target_file):  
        print(f"Found {target_file}")  
    else:  
        print(f"Error: {source_file} missing.")
```

Tool Name: find_available_fragments

Arguments:

name = CO₂

Tool Name: find_available_fragments

Arguments:

name = COOH

Tool Name: find_available_fragments

Arguments:

name = CO

Tool Name: find_available_fragments

Arguments:

name = OH

Tool Name: find_available_fragments

Arguments:

name = H₂O

⌚ Estructural

Tool used:

Tool Name: bind_atom_ligands_library

Arguments:

output_path = CoPc_ligand_binding_project/CoPc_CO2.xyz

```

ligand_name = CO2
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz
Tool Name: bind_atom_ligands_library
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_COOH.xyz
ligand_name = COOH
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz
Tool Name: bind_atom_ligands_library
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_CO.xyz
ligand_name = CO
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = H
output_path = CoPc_ligand_binding_project/CoPc_H.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = OH
output_path = CoPc_ligand_binding_project/CoPc_OH.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = H2O
output_path = CoPc_ligand_binding_project/CoPc_H2O.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz

```

Estructural

Action:

I have successfully bound the requested ligands (CO₂, COOH, CO, H, OH, H₂O) to the Cobalt atom in the Co-Pc complex.

Action Summary:

- Project Organization:** Created a new directory CoPc_ligand_binding_project and moved the original Co-Pc.xyz file into it to keep the workspace organized.
- Ligand Binding:** Used the bind_atom_ligands_library tool to attach each specified ligand to the central Co atom (element 'Co'). The tool automatically handled the orientation and bonding.

Generated Files: All output files are located in the CoPc_ligand_binding_project directory:

- CoPc_CO2.xyz: Cobalt-phthalocyanine with a CO₂ ligand.
- CoPc_COOH.xyz: Cobalt-phthalocyanine with a Carboxyl (COOH) group.
- CoPc_CO.xyz: Cobalt-phthalocyanine with a Carbon Monoxide (CO) ligand.
- CoPc_H.xyz: Cobalt-phthalocyanine with a Hydride (H) ligand.
- CoPc_OH.xyz: Cobalt-phthalocyanine with a Hydroxyl (OH) group.
- CoPc_H2O.xyz: Cobalt-phthalocyanine with a Water (H₂O) ligand.

User:

To explore the axial ligand effect, take both the original Co-Pc.xyz (bare complex) and all the previously modified Co-Pc structures. For each structure, attach one of the following axial ligands to the Co atom: thiophene, pyridine, and Cl.

 **Estructural**

Tool used:

Tool Name: find_available_fragments

Arguments:

name = thiophene

Tool Name: find_available_fragments

Arguments:

name = pyridine

Tool Name: find_available_fragments

Arguments:

name = Cl

 **Estructural**

Tool used:

Tool Name: bind_atom_ligands_library

Arguments:

output_path = CoPc_ligand_binding_project/CoPc_thiophene.xyz

ligand_name = Thiophene

core_element = Co

core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz

Tool Name: bind_atom_ligands_library

Arguments:

output_path = CoPc_ligand_binding_project/CoPc_CO2_thiophene.xyz

ligand_name = Thiophene

core_element = Co

core_file_path = CoPc_ligand_binding_project/CoPc_CO2.xyz

Tool Name: bind_atom_ligands_library

Arguments:

output_path = CoPc_ligand_binding_project/CoPc_COOH_thiophene.xyz

ligand_name = Thiophene

core_element = Co

core_file_path = CoPc_ligand_binding_project/CoPc_COOH.xyz

Tool Name: bind_atom_ligands_library

Arguments:

output_path = CoPc_ligand_binding_project/CoPc_CO_thiophene.xyz

ligand_name = Thiophene

core_element = Co

core_file_path = CoPc_ligand_binding_project/CoPc_CO.xyz

Tool Name: bind_atom_ligands_library

Arguments:

output_path = CoPc_ligand_binding_project/CoPc_H_thiophene.xyz

ligand_name = Thiophene

core_element = Co

core_file_path = CoPc_ligand_binding_project/CoPc_H.xyz

```

Tool Name: bind_atom_ligands_library
Arguments:
    ligand_name = Thiophene
    output_path = CoPc_ligand_binding_project/CoPc_OH_thiophene.xyz
    core_element = Co
    core_file_path = CoPc_ligand_binding_project/CoPc_OH.xyz

Tool Name: bind_atom_ligands_library
Arguments:
    output_path = CoPc_ligand_binding_project/CoPc_H2O_thiophene.xyz
    ligand_name = Thiophene
    core_element = Co
    core_file_path = CoPc_ligand_binding_project/CoPc_H2O.xyz

```

Estructural

Tool used:

```

Tool Name: organic_molecules_xyz_generation
Arguments:
    filenames = ["CoPc_ligand_binding_project/thiophene.xyz"]
    smiles_list = ["c1ccsc1"]

```

Estructural

Tool used:

```

Tool Name: get_atomic_neighbors
Arguments:
    target = S
    file_path = CoPc_ligand_binding_project/thiophene.xyz

```

Estructural

Tool used:

```

Tool Name: bind_two_molecules
Arguments:
    output_path = CoPc_ligand_binding_project/CoPc_thiophene.xyz
    core_indices = [0]
    ligand_file_path = CoPc_ligand_binding_project/thiophene.xyz
    ligand_idx = 3
    ligand_type = ligand
    core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz

Tool Name: bind_two_molecules
Arguments:
    output_path = CoPc_ligand_binding_project/CoPc_CO2_thiophene.xyz
    core_indices = [0]
    ligand_file_path = CoPc_ligand_binding_project/thiophene.xyz
    ligand_idx = 3
    ligand_type = ligand
    core_file_path = CoPc_ligand_binding_project/CoPc_CO2.xyz

Tool Name: bind_two_molecules
Arguments:
    output_path = CoPc_ligand_binding_project/CoPc_COOH_thiophene.xyz
    core_indices = [0]

```

```

ligand_file_path = CoPc_ligand_binding_project/thiophene.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_COOH.xyz
ligand_type = ligand
ligand_idx = 3

Tool Name: bind_two_molecules
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_CO_thiophene.xyz
core_indices = [0]
ligand_file_path = CoPc_ligand_binding_project/thiophene.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_CO.xyz
ligand_type = ligand
ligand_idx = 3

Tool Name: bind_two_molecules
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_H_thiophene.xyz
core_indices = [0]
ligand_file_path = CoPc_ligand_binding_project/thiophene.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_H.xyz
ligand_type = ligand
ligand_idx = 3

Tool Name: bind_two_molecules
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_OH_thiophene.xyz
core_indices = [0]
ligand_file_path = CoPc_ligand_binding_project/thiophene.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_OH.xyz
ligand_type = ligand
ligand_idx = 3

Tool Name: bind_two_molecules
Arguments:
core_indices = [0]
output_path = CoPc_ligand_binding_project/CoPc_H2O_thiophene.xyz
ligand_file_path = CoPc_ligand_binding_project/thiophene.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_H2O.xyz
ligand_type = ligand
ligand_idx = 3

Tool Name: bind_atom_ligands_library
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_pyridine.xyz
ligand_name = Pyridine
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz

Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = Pyridine
output_path = CoPc_ligand_binding_project/CoPc_CO2_pyridine.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_CO2.xyz

Tool Name: bind_atom_ligands_library
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_COOH_pyridine.xyz
ligand_name = Pyridine

```

```

core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_COOH.xyz
Tool Name: bind_atom_ligands_library
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_CO_pyridine.xyz
ligand_name = Pyridine
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_CO.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = Pyridine
output_path = CoPc_ligand_binding_project/CoPc_H_pyridine.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_H.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = Pyridine
output_path = CoPc_ligand_binding_project/CoPc_OH_pyridine.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_OH.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = Pyridine
output_path = CoPc_ligand_binding_project/CoPc_H2O_pyridine.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_H2O.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = Cl
output_path = CoPc_ligand_binding_project/CoPc_Cl.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz
Tool Name: bind_atom_ligands_library
Arguments:
ligand_name = Cl
output_path = CoPc_ligand_binding_project/CoPc_CO2_Cl.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_CO2.xyz
Tool Name: bind_atom_ligands_library
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_COOH_Cl.xyz
ligand_name = Cl
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_COOH.xyz
Tool Name: bind_atom_ligands_library
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_CO_Cl.xyz
ligand_name = Cl
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_CO.xyz
Tool Name: bind_atom_ligands_library

```

Arguments:

```
output_path = CoPc_ligand_binding_project/CoPc_H_Cl.xyz
ligand_name = Cl
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_H.xyz
```

Tool Name: bind_atom_ligands_library

Arguments:

```
ligand_name = Cl
output_path = CoPc_ligand_binding_project/CoPc_OH_Cl.xyz
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_OH.xyz
```

Tool Name: bind_atom_ligands_library

Arguments:

```
output_path = CoPc_ligand_binding_project/CoPc_H2O_Cl.xyz
ligand_name = Cl
core_element = Co
core_file_path = CoPc_ligand_binding_project/CoPc_H2O.xyz
```

⌚ Estructural

Tool used:

Tool Name: organic_molecules_xyz_generation

Arguments:

```
filenames = ["CoPc_ligand_binding_project/pyridine.xyz"]
smiles_list = ["n1ccccc1"]
```

⌚ Estructural

Tool used:

Tool Name: get_atomic_neighbors

Arguments:

```
target = N
file_path = CoPc_ligand_binding_project/pyridine.xyz
```

⌚ Estructural

Tool used:

Tool Name: bind_two_molecules

Arguments:

```
output_path = CoPc_ligand_binding_project/CoPc_pyridine.xyz
core_indices = [0]
ligand_file_path = CoPc_ligand_binding_project/pyridine.xyz
core_file_path = CoPc_ligand_binding_project/Co-Pc.xyz
ligand_type = ligand
ligand_idx = 0
```

Tool Name: bind_two_molecules

Arguments:

```
core_indices = [0]
output_path = CoPc_ligand_binding_project/CoPc_CO2_pyridine.xyz
ligand_file_path = CoPc_ligand_binding_project/pyridine.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_CO2.xyz
```

```

ligand_type = ligand
ligand_idx = 0
Tool Name: bind_two_molecules
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_COOH_pyridine.xyz
core_indices = [0]
ligand_file_path = CoPc_ligand_binding_project/pyridine.xyz
ligand_idx = 0
ligand_type = ligand
core_file_path = CoPc_ligand_binding_project/CoPc_COOH.xyz
Tool Name: bind_two_molecules
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_CO_pyridine.xyz
core_indices = [0]
ligand_file_path = CoPc_ligand_binding_project/pyridine.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_CO.xyz
ligand_type = ligand
ligand_idx = 0
Tool Name: bind_two_molecules
Arguments:
core_indices = [0]
output_path = CoPc_ligand_binding_project/CoPc_H_pyridine.xyz
ligand_file_path = CoPc_ligand_binding_project/pyridine.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_H.xyz
ligand_type = ligand
ligand_idx = 0
Tool Name: bind_two_molecules
Arguments:
output_path = CoPc_ligand_binding_project/CoPc_OH_pyridine.xyz
core_indices = [0]
ligand_file_path = CoPc_ligand_binding_project/pyridine.xyz
core_file_path = CoPc_ligand_binding_project/CoPc_OH.xyz
ligand_type = ligand
ligand_idx = 0
Tool Name: bind_two_molecules
Arguments:
core_indices = [0]
output_path = CoPc_ligand_binding_project/CoPc_H2O_pyridine.xyz
ligand_file_path = CoPc_ligand_binding_project/pyridine.xyz
ligand_idx = 0
ligand_type = ligand
core_file_path = CoPc_ligand_binding_project/CoPc_H2O.xyz

```

Estructural

Action:

I have successfully generated all the requested structures to explore the axial ligand effect.

Task Summary: For each of the 7 core structures (original Co-Pc + 6 derivatives), I attached three different axial ligands: Thiophene, Pyridine, and Chloride (Cl), resulting in 21 new structures.

Execution Details:

1. **Thiophene:** Generated thiophene.xyz (SMILES: c1ccsc1), identified the Sulfur atom (index 3), and bound it to the Cobalt atom in each core structure.

2. **Pyridine:** Generated `pyridine.xyz` (SMILES: `n1ccccc1`), identified the Nitrogen atom (index 0), and bound it to the Cobalt atom in each core structure.
3. **Cl:** Used the `bind_atom_ligands_library` tool to bind a Chloride atom to the Cobalt atom in each core structure.

Generated Files (in `CoPc_ligand_binding_project`):

- **Thiophene Series:**

- `CoPc_thiophene.xyz`
- `CoPc_CO2_thiophene.xyz`
- `CoPc_COOH_thiophene.xyz`
- `CoPc_CO_thiophene.xyz`
- `CoPc_H_thiophene.xyz`
- `CoPc_OH_thiophene.xyz`
- `CoPc_H2O_thiophene.xyz`

- **Pyridine Series:**

- `CoPc_pyridine.xyz`
- `CoPc_CO2_pyridine.xyz`
- `CoPc_COOH_pyridine.xyz`
- `CoPc_CO_pyridine.xyz`
- `CoPc_H_pyridine.xyz`
- `CoPc_OH_pyridine.xyz`
- `CoPc_H2O_pyridine.xyz`

- **Chloride (Cl) Series:**

- `CoPc_Cl.xyz`
- `CoPc_CO2_Cl.xyz`
- `CoPc_COOH_Cl.xyz`
- `CoPc_CO_Cl.xyz`
- `CoPc_H_Cl.xyz`
- `CoPc_OH_Cl.xyz`
- `CoPc_H2O_Cl.xyz`

All files are neatly organized in the `CoPc_ligand_binding_project` folder.