

Organometallic complex construction with stereochemical and ligand variations

User:

Generate the following structures with their respective isomers: 1. cisplatin and transplatin 2. Δ -Fe(bpy)3 and Λ -Fe(bpy)3 3. fac-Ir(ppy)3 and mer-Ir(ppy)3

⌚ Estructural

Tool used:

Tool Name: find_available_fragments

Arguments:

type = ligand

Tool Name: find_available_fragments

Arguments:

type = bidentate_ligand

⌚ Estructural

Tool used:

Tool Name: repl_tool

Arguments:

code =

import os

os.makedirs('isomers_project', exist_ok=True)

print("Directory created")

⌚ Estructural

Tool used:

Tool Name: build_tm_complex_from_template

Arguments:

ligand_bindings = [{"NH3": [1, 2]}]

metal = Pt

coordination_geometry = square_planar

output_path = isomers_project/cisplatin.xyz

Tool Name: build_tm_complex_from_template

Arguments:

ligand_bindings = [{"NH3": [1, 3]}]

output_path = isomers_project/transplatin.xyz

coordination_geometry = square_planar

metal = Pt

Tool Name: build_tm_complex_from_template

Arguments:

ligand_bindings = [{"bpy": [[1, 4], [2, 3], [5, 6]]}]

metal = Fe

coordination_geometry = octahedral

output_path = isomers_project/delta_Fe_bpy3.xyz

Tool Name: build_tm_complex_from_template

Arguments:

ligand_bindings = [{"bpy": [[1, 5], [2, 6], [3, 4]]}]

metal = Fe

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coordination_geometry = octahedral
output_path = isomers_project/lambda_Fe_bpy3.xyz

Tool Name: build_tm_complex_from_template
Arguments:
ligand_bindings = [{"ppy": [[1, 5], [3, 4], [6, 2]]}]
metal = Ir
coordination_geometry = octahedral
output_path = isomers_project/fac_Ir_ppy3.xyz

Tool Name: build_tm_complex_from_template
Arguments:
ligand_bindings = [{"ppy": [[1, 5], [3, 4], [2, 6]]}]
metal = Ir
coordination_geometry = octahedral
output_path = isomers_project/mer_Ir_ppy3.xyz

```

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Action:

I have generated the requested structures and their isomers in the `isomers_project` folder.

1. Cisplatin and Transplatin ($\text{Pt}(\text{NH}_3)_2\text{Cl}_2$)

- **Cisplatin:** `isomers_project/cisplatin.xyz`
 - Generated using a square planar template with NH₃ ligands at cis positions (indices [1, 2]).
- **Transplatin:** `isomers_project/transplatin.xyz`
 - Generated using a square planar template with NH₃ ligands at trans positions (indices [1, 3]).

2. $\Delta\text{-Fe(bpy)}_3$ and $\Lambda\text{-Fe(bpy)}_3$

- **$\Delta\text{-Fe(bpy)}_3$:** `isomers_project/delta_Fe_bpy3.xyz`
 - Generated using an octahedral template with 2,2'-bipyridine (bpy) ligands arranged in the Delta (Δ) configuration (indices [[1, 4], [2, 3], [5, 6]]).
- **$\Lambda\text{-Fe(bpy)}_3$:** `isomers_project/lambda_Fe_bpy3.xyz`
 - Generated using an octahedral template with bpy ligands arranged in the Lambda (Λ) configuration (indices [[1, 5], [2, 6], [3, 4]]).

3. fac-Ir(ppy) $_3$ and mer-Ir(ppy) $_3$

- **fac-Ir(ppy) $_3$:** `isomers_project/fac_Ir_ppy3.xyz`
 - Generated using an octahedral template with 2-phenylpyridine (ppy) ligands in the facial (fac) arrangement (indices [[1, 5], [3, 4], [6, 2]]).
- **mer-Ir(ppy) $_3$:** `isomers_project/mer_Ir_ppy3.xyz`
 - Generated using an octahedral template with ppy ligands in the meridional (mer) arrangement (indices [[1, 5], [3, 4], [2, 6]]).