

Fragment-level replacement in organometallic complexes

User:

Given MoCl₃PNP.xyz, the PNP ligand is 2,6-bis(di-tert-butylphosphinomethyl)pyridine. Find all t-butyl groups attached to the phosphorus atoms. Replace them with hydrogen, methyl, and phenyl, creating separate XYZ files for each replacement.

⌚ Estructural

Tool used:

Tool Name: repl_tool

Arguments:

code =

import os

import shutil

```
project_dir = 'MoCl3PNP_derivatives_project'  
if not os.path.exists(project_dir):  
    os.makedirs(project_dir)
```

```
src = 'MoCl3PNP.xyz'  
dst = os.path.join(project_dir, 'MoCl3PNP.xyz')  
if os.path.exists(src):  
    shutil.copy(src, dst)  
    print(f"Copied {src} to {dst}")  
else:  
    print(f"{src} not found")
```

Tool Name: get_atomic_neighbors

Arguments:

target = P

file_path = MoCl3PNP_derivatives_project/MoCl3PNP.xyz

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Tool used:

Tool Name: get_atomic_neighbors

Arguments:

target = P

file_path = MoCl3PNP.xyz

Tool Name: repl_tool

Arguments:

code =

import os

print(os.listdir('MoCl3PNP_derivatives_project'))

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Tool used:

Tool Name: repl_tool

Arguments:

code =

```

import numpy as np

def read_xyz(path):
    with open(path, 'r') as f:
        lines = f.readlines()
    num_atoms = int(lines[0])
    atoms = []
    coords = []
    for line in lines[2:2+num_atoms]:
        parts = line.split()
        atoms.append(parts[0])
        coords.append([float(x) for x in parts[1:4]])
    return atoms, np.array(coords)

atoms, coords = read_xyz('MoCl3PNP.xyz')
targets = [7, 11, 15, 21, 22, 26]

for i in targets:
    c_neighbors = 0
    neighbor_indices = []
    for j, (atom, coord) in enumerate(zip(atoms, coords)):
        if i == j: continue
        dist = np.linalg.norm(coords[i] - coords[j])
        if dist < 1.7: # C-C is ~1.5, P-C is ~1.85. 1.7 should catch C-C but maybe exclude P-C?
            # Actually P-C is around 1.8. Let's strictly look for C neighbors.
            if atom == 'C':
                c_neighbors += 1
                neighbor_indices.append(j)

    print(f"Atom {i} ({atoms[i]}) has {c_neighbors} Carbon neighbors: {neighbor_indices}")

```

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Tool used:

Tool Name: replace_branch_with_predefined_FG

Arguments:

output_path = MoCl3PNP_derivatives_project/MoCl3PNP_H.xyz
 FG_name = H
 bond_pair = [[4, 7], [4, 11], [5, 22], [5, 26]]
 core_file_path = MoCl3PNP_derivatives_project/MoCl3PNP.xyz

Tool Name: replace_branch_with_predefined_FG

Arguments:

output_path = MoCl3PNP_derivatives_project/MoCl3PNP_Me.xyz
 FG_name = Me
 bond_pair = [[4, 7], [4, 11], [5, 22], [5, 26]]
 core_file_path = MoCl3PNP_derivatives_project/MoCl3PNP.xyz

Tool Name: replace_branch_with_predefined_FG

Arguments:

output_path = MoCl3PNP_derivatives_project/MoCl3PNP_Ph.xyz
 FG_name = Ph
 bond_pair = [[4, 7], [4, 11], [5, 22], [5, 26]]
 core_file_path = MoCl3PNP_derivatives_project/MoCl3PNP.xyz

Action:

Based on the analysis of the MoCl3PNP.xyz structure, I have successfully identified the *tert*-butyl groups attached to the Phosphorus atoms and generated the three requested derivative structures.

Execution Details:**1. Structure Analysis:**

- **Phosphorus Atoms:** Identified at indices **4** and **5**.
- **Ligand Topology:** By analyzing the coordination environment, I distinguished the *tert*-butyl groups from the pyridine-linker backbone:
 - **Linker Carbons:** Atoms **15** (connected to P4) and **21** (connected to P5) were identified as methylene bridges (-CH₂-) connecting to the pyridine ring.
 - **t-Butyl Quaternary Carbons:** Atoms **7, 11** (connected to P4) and **22, 26** (connected to P5) were identified as the anchor points for the *tert*-butyl groups.
- **Target Bonds:** The bonds selected for replacement were P(4)-C(7), P(4)-C(11), P(5)-C(22), and P(5)-C(26).

2. Modifications:

- Replaced the four *tert*-butyl branches with **Hydrogen (H)**.
- Replaced the four *tert*-butyl branches with **Methyl (Me)**.
- Replaced the four *tert*-butyl branches with **Phenyl (Ph)**.

3. File Generation: All files have been organized into the project folder MoCl3PNP_derivatives_project.

- MoCl3PNP_derivatives_project/MoCl3PNP_H.xyz
- MoCl3PNP_derivatives_project/MoCl3PNP_Me.xyz
- MoCl3PNP_derivatives_project/MoCl3PNP_Ph.xyz

The requested derivatives are now ready for use.