

## Symmetry-guided functionalization of a cobalt-porphyrin complex

User:

Given Co-porphyrin.xyz, find four hydrogens that are symmetry-equivalent. Replace these hydrogens with phenyl groups while keeping the rest of the hydrogens unchanged.

### ⌚ Estructural

**Tool used:**

Tool Name: repl\_tool

Arguments:

code =

```
import os
import shutil
```

```
project_dir = "porphyrin_phenyl_project"
if not os.path.exists(project_dir):
    os.makedirs(project_dir)

source_file = "Co-porphyrin.xyz"
dest_file = os.path.join(project_dir, "Co-porphyrin.xyz")

if os.path.exists(source_file):
    shutil.copy(source_file, dest_file)
    print(f"Copied {source_file} to {dest_file}")
else:
    print(f"{source_file} not found in root.")
```

### ⌚ Estructural

**Tool used:**

Tool Name: find\_pointgroup\_equivalent\_atoms

Arguments:

file\_path = porphyrin\_phenyl\_project/Co-porphyrin.xyz

### ⌚ Estructural

**Tool used:**

Tool Name: replace\_terminal\_atom\_with\_predefined\_FG

Arguments:

core\_indices = [33, 34, 35, 36]

FG\_name = Ph

output\_path = porphyrin\_phenyl\_project/Co-tetraphenylporphyrin.xyz

core\_file\_path = porphyrin\_phenyl\_project/Co-porphyrin.xyz

### ⌚ Estructural

**Action:**

The four symmetry-equivalent hydrogen atoms in Co-porphyrin.xyz were identified at indices **[33, 34, 35, 36]**. These correspond to the meso-positions of the porphyrin ring.

I have successfully replaced these hydrogens with phenyl groups (Ph) to generate the Co-tetraphenylporphyrin structure.

**Output File:** porphyrin\_phenyl\_project/Co-tetraphenylporphyrin.xyz