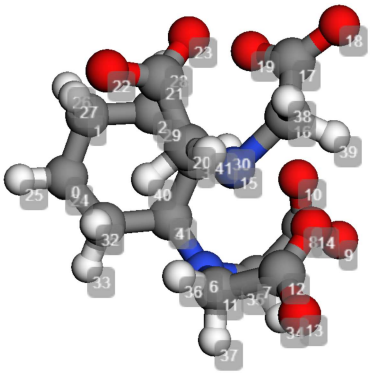
```
from architector import build_complex, view_structures
import pandas as pd # Pandas is used to read in the reference data
import numpy as np # Numpy is used for selecting from the database
import architector # Architector is used for importing the filepath to the reference data
from architector import smiles2Atoms


coreDict = {"metal":"Ba",
            "coreCN":6
            }
coreDict
```

```
     {'metal': 'Ba', 'coreCN': 6}
```

```
CyDTA=dict()
CyDTA['smiles']='C1CCC(C(C1)N(CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-]'
CyDTA['coordList']=[6,10,14,15,19,23]

CyDTA_atoms=smiles2Atoms(CyDTA['smiles'])
view_structures(CyDTA_atoms,labelinds=True,w=500,h=500)
```



```
# Initialize Parameters dictionary
parameters = dict()

# Specify oxidation state of 2 for the metal
parameters['metal_ox'] = 2
parameters['n_conformers']=40
parameters["relax"] =True
#parameters["crest_sampling"]= True
#parameters["crest_sampling_n_conformers"]=3

inputDict={
    'core':coreDict,
    'ligands':[CyDTA],
    'parameters':parameters
}

inputDict
```

```
     {'core': {'metal': 'Ba', 'coreCN': 6},
      'ligands': [{'smiles': 'C1CCC(C(C1)N(CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-]',
        'coordList': [6, 10, 14, 15, 19, 23]}],
      'parameters': {'metal_ox': 2, 'n_conformers': 40, 'relax': True}}
```

```
out = build_complex(inputDict)
```

```
ligType not specified for C1CCC(C(C1)N(CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-] - testing ligand placement to determine ligType!
Warning: can take a while depending on the size of the ligand.
Assigning lig C1CCC(C(C1)N(CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-] to ligType hexa_octahedral!
Shifting symmetries to match conformers.
ligType not specified for C1CCC(C(C1)N(CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-] - testing ligand placement to determine ligType!
Warning: can take a while depending on the size of the ligand.
Assigning lig C1CCC(C(C1)N(CC(=O)[O-])CC(=O)[O-])N(CC(=O)[O-])CC(=O)[O-] to ligType hexa_octahedral!
Shifting symmetries to match conformers.
```

```
view_structures(out)
```