In [1]:
```python
import pickle
from rdkit import Chem
from rdkit.Chem import Draw
from rdkit.Chem.Draw import IPythonConsole
from rdkit.Chem import rdFMCS
from rdkit.Chem.Draw import rdDepictor

from IPython.display import display
import matplotlib.pyplot as plt
from IPython.display import HTML
import pandas as pd

IPythonConsole.ipython_useSVG=True
rdDepictor.SetPreferCoordGen(True)
#IPythonConsole.drawOptions.minFontSize=20
```

In [2]:
```python
with open('predictions/w_logs.pkl', 'rb') as file: w_te_data = pickle.load(fi
with open('predictions/wo_logs.pkl', 'rb') as file: wo_te_data = pickle.load(
original = pd.read_csv('predictions/chem_departm_output_wo_tie_embedding/outp
```

In [3]:
```python
def view_difference(mol1, mol2):
    mcs = rdFMCS.FindMCS([mol1,mol2])
    mcs_mol = Chem.MolFromSmarts(mcs.smartsString)
    match1 = mol1.GetSubstructMatch(mcs_mol)
    target_atm1 = []
    for atom in mol1.GetAtoms():
        if atom.GetIdx() not in match1:
            target_atm1.append(atom.GetIdx())
    match2 = mol2.GetSubstructMatch(mcs_mol)
    target_atm2 = []
    for atom in mol2.GetAtoms():
        if atom.GetIdx() not in match2:
            target_atm2.append(atom.GetIdx())
    return Draw.MolsToGridImage([mol1, mol2],highlightAtomLists=[target_atm1,
```

Generation

Notes:

- Predict the next fragment when probability p > 0.5
- The logic takes top-5 attachments from combinations of top-5 motifs and its possible configs. E.g., motif C1=CC=CC=C1 has 2 possible configs, C1=[CH:1]C=C[CH:2]=C1 or C1=[CH:1]C=CC=C1. The first config could be connected to other motifs that the connections are marked by *:X*, X is a number. The second config is the end motif that couldn't connected to other motifs. Atoms marked by different mark numbers are connected together. No two atoms with same mark numbers are used for connection.
- For every attachment, it's checked for validity:
  - If the to-connect motif and to-be-connected (aka predicted motif) share common atoms for connections.
  - No self-loop.
  - If all atoms in the to-be-connected motif exist in the to-connect motif, no need to attach them.
- To view prediction logs of other molecules, subtract 2 from the molecule's index in Excel file.

In [4]:
```python
def view(data, i, _original):
    print('Original: {}'.format(_original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(_original[i])]))

    sample = data[i]
    # step 0
    step_f0 = sample[0]
    print('***************Sample {}th***************'.format(i))
    print('-----Step-0-----')
    print('Root motif: {}'.format(step_f0['root']))
    print('Top 5 root motif configs:', '\n'.join([str(x) for x in step_f0['to

    # display
    mol = Chem.MolFromSmiles(step_f0['top-5-root-attachments'][0][0])
    print('Displaying partial graph (aka molecule): {}'.format(step_f0['parti
    display(Draw.MolsToGridImage([mol]))
    print('----------------------------------------------------')


    # the remaining steps
    for i, step_f in enumerate(sample[1:]):
        print('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            print('Generate next fragment p = {}'.format(step_f['Generate fra
        else:
            print('Skip, current fragment has no next fragment to be attached
            continue

        if 'top-5-inter-cands' in step_f:
            print('Top 5 next motifs to attach:')
            for fragment in step_f['top-5-inter-cands']:
                print('Molecule {} and its specific config {} w/ p={}'.format
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                print('----------------------------------------------------
            if 'Attaching Fragment' in step_f:
                frag = step_f['Attaching Fragment']

                sub_mol = Chem.MolFromSmiles(step_f['partial-graph'])
                print('Attaching fragment {} of config {}'.format(frag[0], fr
                print('Latest partial graph: {}'.format(step_f['partial-graph
                print('Lastest graph (left) vs graph in last step (right)')
                display(view_difference(sub_mol, mol))
                mol = sub_mol
                print('----------------------------------------------------
            else:
                print("Skip, the best next fragment to be attached to the cur
```
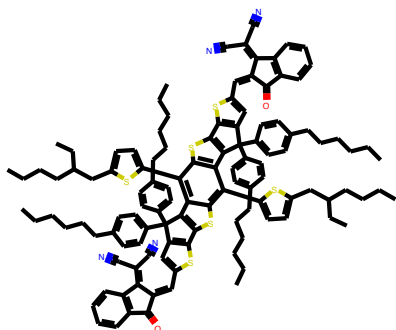
In [8]:
```python
view(w_te_data, 11, original)
```

Original: O=C(C(/C1=C(C#N)/C#N)=C\C2=CC(C(C3=CC=C(CCCCCC)C=C3)(C4=CC=C(CCCCCC)

```
C=C4)C5=C6SC7=C5C(C8=CC=C(CC(CC)CCCC)S8)=C(SC9=C%10C(C%11=CC=C(CCCCCC)C=C%11)(
C%12=CC=C(CCCCCC)C=C%12)C%13=C9SC(/C=C%14\C(C(C=CC=C%15)=C%15C%14=O)=C(C#N)\C#
N)=C%13)C%10=C7C%16=CC=C(CC(CC)CCCC)S%16)=C6S2)C%17=C1C=CC=C%17
```



```
***************Sample 11th***************
-----Step-0-----
Root motif: CN
Top 5 root motif configs: ('[CH3:1][NH2:2]', tensor(10.6275))
('[NH2:1][CH3:2]', tensor(-14.2601))
('N[CH3:1]', tensor(-24.1133))
('C[NH2:1]', tensor(-37.7583))
('CC([CH3:1])[CH3:2]', tensor(-953.2549))
Displaying partial graph (aka molecule): CN
```

```
----------------------------------------------------------
-----Step-1-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.30765676498413086
```
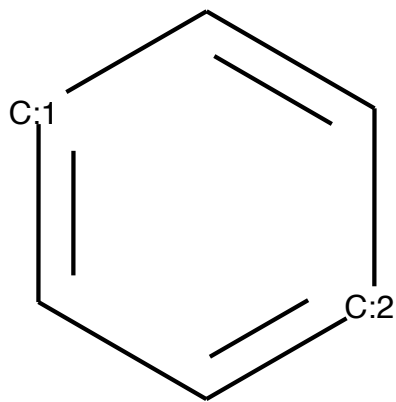

Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-1.497
5374937057495

C:1

C:2

Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-3.7784485816955566

Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-4.45
1709747314453
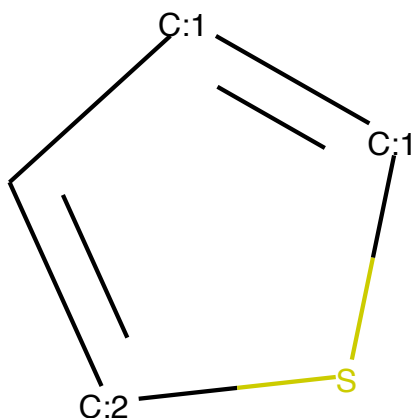
```
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```
Molecule C1=CC=CC=C1 and its specific config [CH:1]1=[CH:2][CH:2]=[CH:2][CH:2]
=[CH:2]1 w/ p=-5.410152435302734
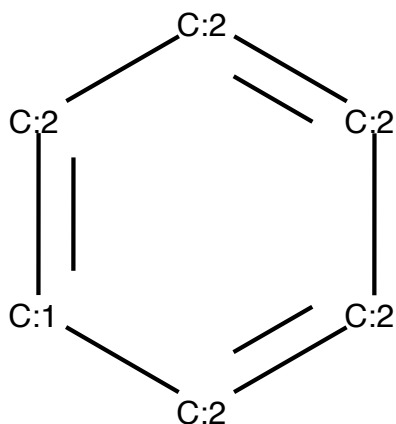

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ield a valid sub-molecule . Go back to the previous fragment.
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In [ ]: