In [1]:
```
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]:
```
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]:
```
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]:

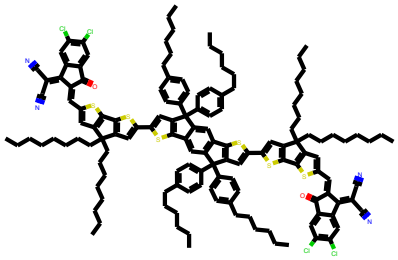
```
def view(data, i, _original):
    print('Original: {}'.format(_original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(_original[i])]))

    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 remaing 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 [ ]:

```
view(w_te_data, 7, original)
```

```
Original: CCCCCCC1=CC=C(C2(C3=CC=C(CCCCCC)C=C3)C4=CC(C(SC(C5=CC(C6(CCCCCCCC)CC
```

```
CCCCCC)=C(C7=C6C=C(/C=C(C8=O)/C(C9=CC(Cl)=C(Cl)C=C89)=C(C#N)/C#N)S7)S5)=C%10)=
C%10C%11(C%12=CC=C(CCCCCC)C=C%12)C%13=CC=C(CCCCCC)C=C%13)=C%11C=C4C%14=C2C=C(C
%15=CC(C%16(CCCCCCCC)CCCCCCCC)=C(C%17=C%16C=C(/C=C(C%18=O)/C(C%19=CC(Cl)=C(Cl)
C=C%18%19)=C(C#N)\C#N)S%17)S%15)S%14)C=C1
```

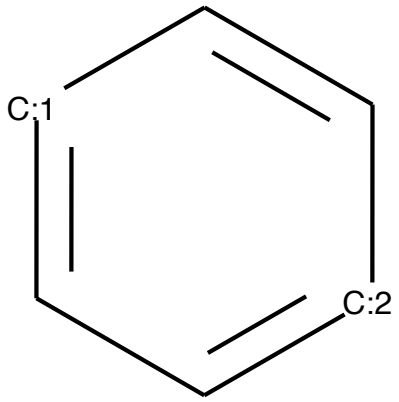


```
***************Sample 7th***************
-----Step-0-----
Root motif: C#N
Top 5 root motif configs: ('[N:1]#[CH:2]', tensor(19.6517))
('N#[CH:1]', tensor(-19.0220))
('C#[N:1]', tensor(-25.1142))
('C(N=[CH2:2])[CH3:1]', tensor(-972.3458))
('C(#C[CH3:2])[CH3:1]', tensor(-973.3757))
Displaying partial graph (aka molecule): C#N
```

```
------------------------------------------------------------
-----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=-5.960462772236497e-07
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-14.36723518371582
```

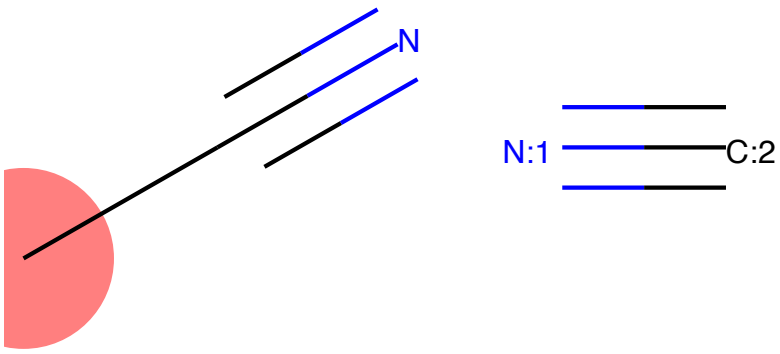
```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-17.00
7352828979492
```



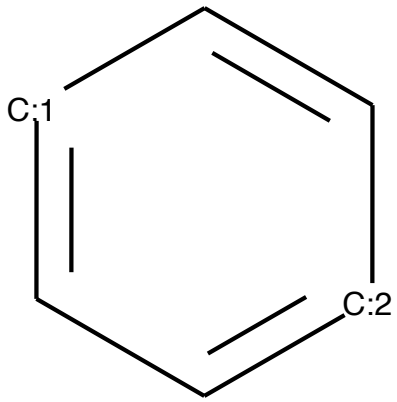

```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-17.76620864868164
```

```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-21.821922302246094
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC#N
Lastest graph (left) vs graph in last step (right)
```



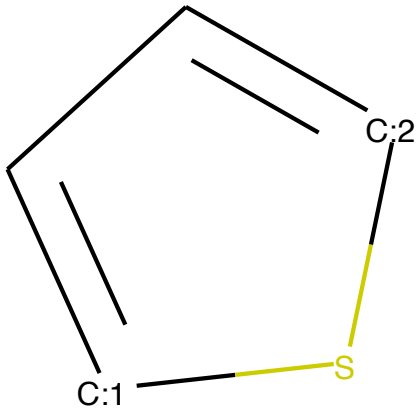

```
------------------------------------------------------------
-----Step-2-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.671
6226935386658
```




```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.7374266982078552
```

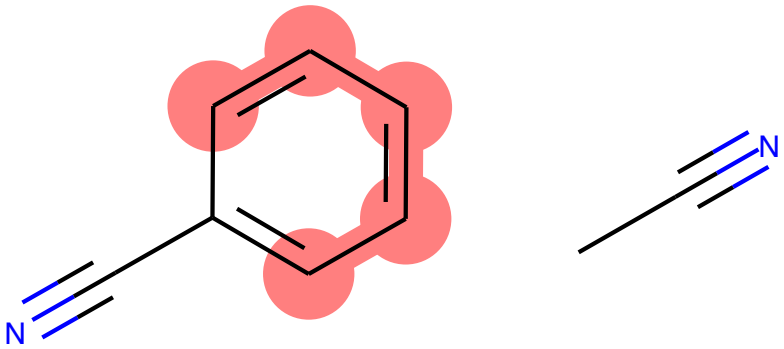
```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-4.924198150634766
```

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-5.6645574
56970215
```



Molecule C and its specific config C w/ p=-11.33038330078125

Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: N#Cc1ccccc1
Lastest graph (left) vs graph in last step (right)

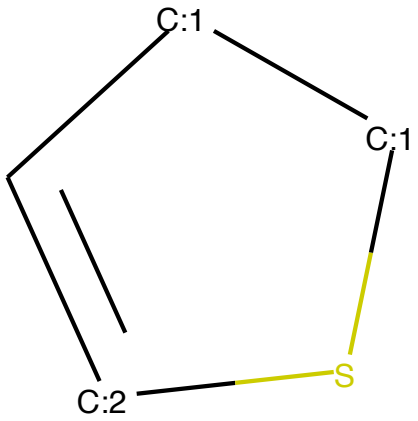


-----Step-3-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.002115513663738966

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-6.184431076049805
```

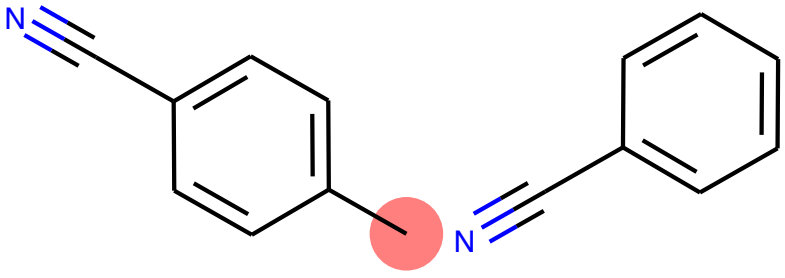
```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-10.497505187988281
```

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-10.8
19089889526367
```




```
------------------------------------------------------------
Molecule C[NH3+] and its specific config [NH3+:1][CH3:2] w/ p=-13.259058952331
543
```

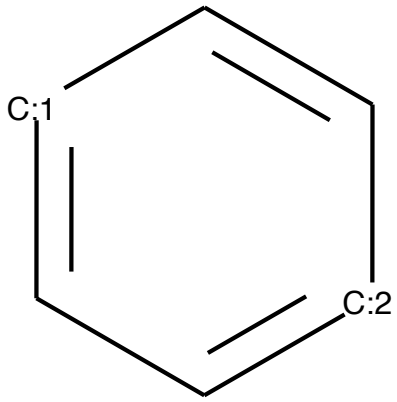
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(C#N)cc1
Lastest graph (left) vs graph in last step (right)
```



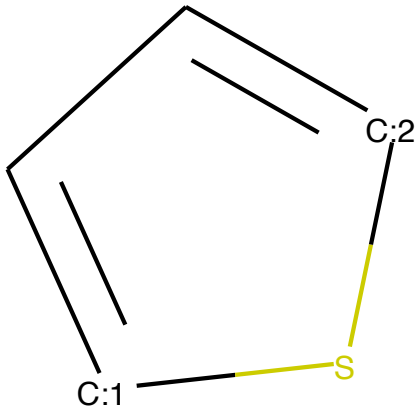

```
------------------------------------------------------------
-----Step-4-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.13669045269489288
```

Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-2.0976781845092773

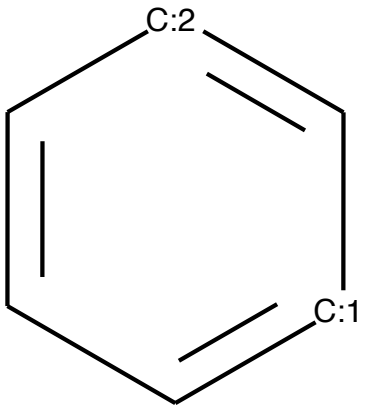
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-5.903273582458496



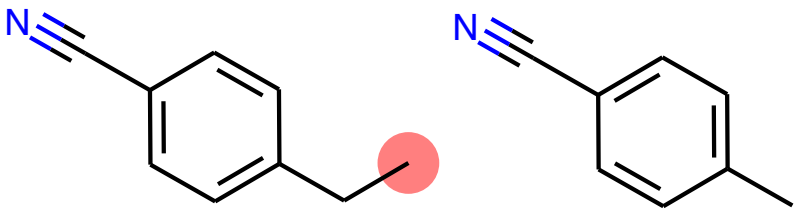
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-6.110535144805908




```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=C[CH:2]=C[CH:1]=C1 w/ p=-9.907
465934753418
```

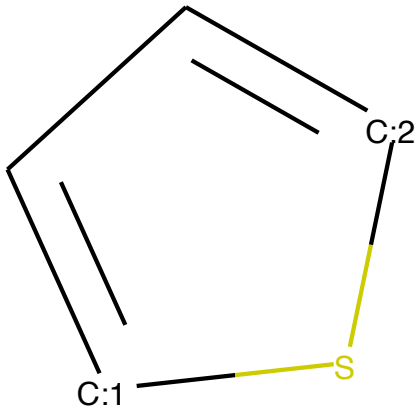



```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CCc1ccc(C#N)cc1
Lastest graph (left) vs graph in last step (right)
```

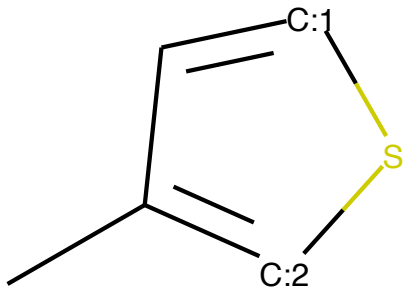



```
------------------------------------------------------------
-----Step-5-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.6420995593070984
```

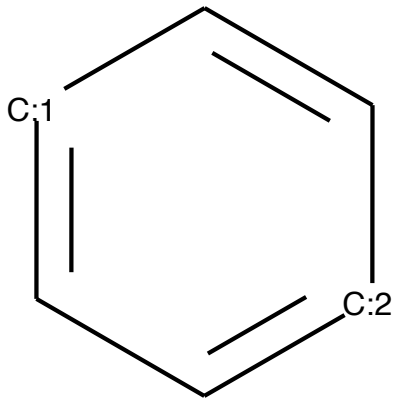
```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.8148662
447929382
```




```
------------------------------------------------------------
Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ p=-3.82005
52463531494
```

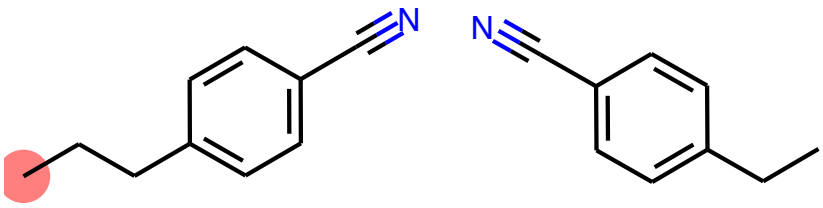



```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-4.876
8839836120605
```

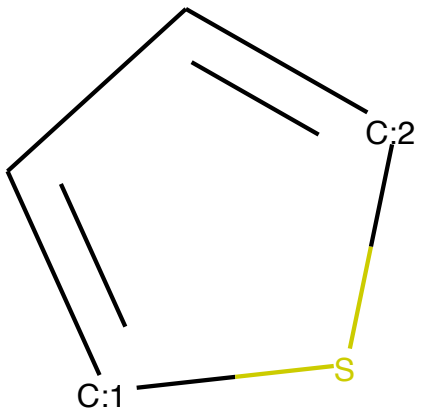



```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-6.933335781097412
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CCCc1ccc(C#N)cc1
Lastest graph (left) vs graph in last step (right)
```

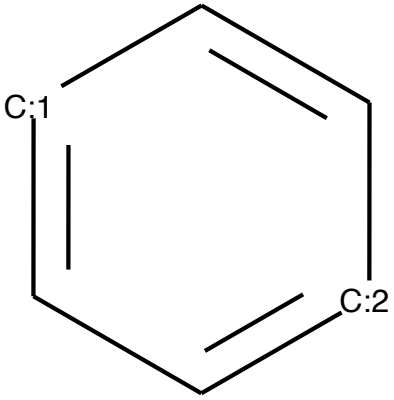



```
------------------------------------------------------------
-----Step-6-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.0203095
2088534832
```

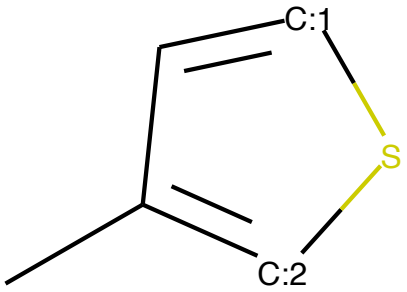


Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-3.92018461227417

Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-8.943048477172852

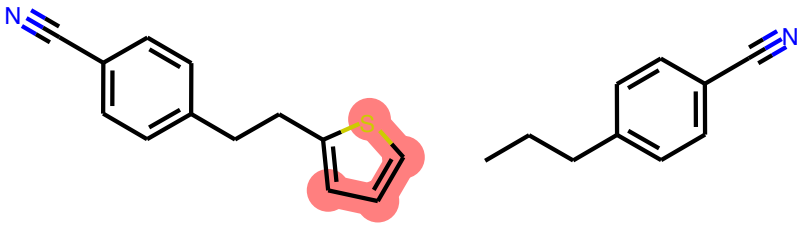


Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ p=-9.156630516052246




```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-11.249489784240723
```

```
------------------------------------------------------------
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: N#Cc1ccc(CCc2cccs2)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-7-----
Generate next fragment p = 0.9999597072601318
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=0.0
```

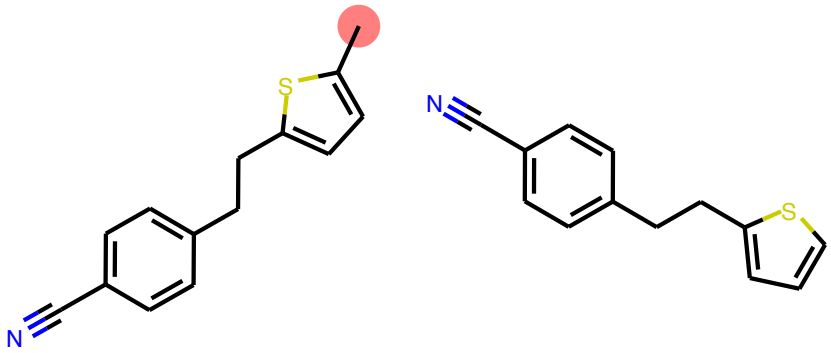
```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-16.7109375
```

```
------------------------------------------------------------
Molecule C=N and its specific config N=[CH2:1] w/ p=-21.7288761138916
```

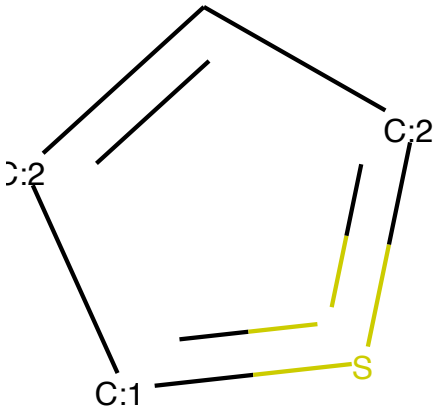
```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-22.081645965576172
```

```
------------------------------------------------------------
Molecule C=N and its specific config [NH:1]=[CH2:2] w/ p=-22.57670783996582
```

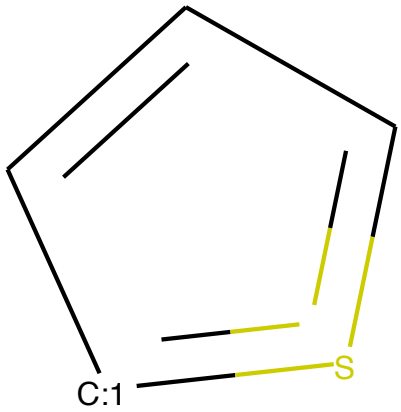
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(CCc2ccc(C#N)cc2)s1
Lastest graph (left) vs graph in last step (right)
```



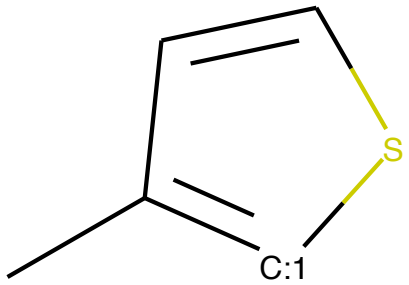

```
------------------------------------------------------------
-----Step-8-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:1]=S=[CH:2]1 w/ p=-0.
07804661989212036
```



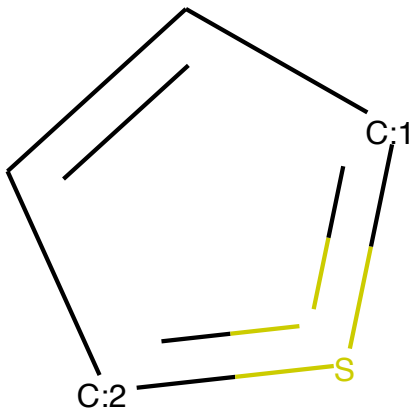
Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ p=-3.591478109359741



Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]SC=C1 w/ p=-4.145951747894287

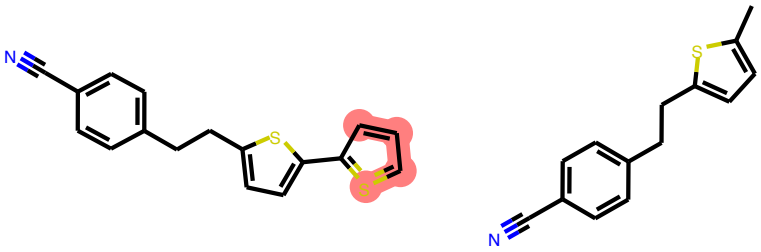


Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ p=-4.280362606048584



Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-4.622601509094238

Attaching fragment C1=[CH:2][CH:1]=S=[CH:2]1 of config ['C1=C[CH:1]=S=C1']
Latest partial graph: N#Cc1ccc(CCc2ccc(C3=S=CC=C3)s2)cc1
Lastest graph (left) vs graph in last step (right)



-----Step-9-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0005399914807640016

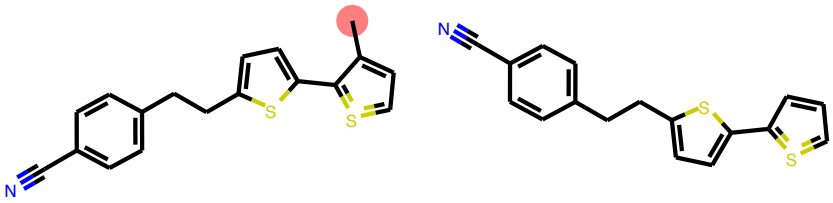
```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-7.524240493774414
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-26.357114791870117
```

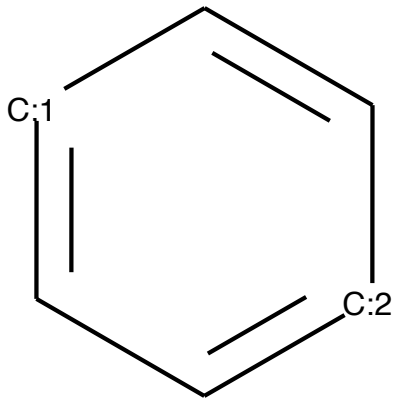
```
------------------------------------------------------------
Molecule CO and its specific config O[CH3:1] w/ p=-30.464248657226562
```

```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-32.347686767578125
```

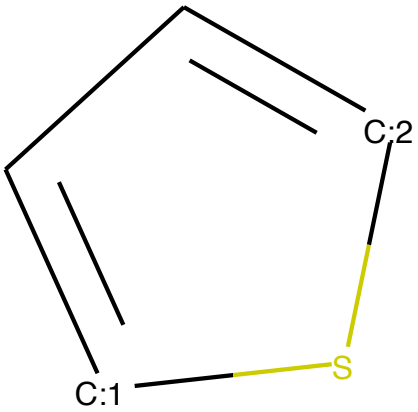
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC1=CC=S=C1c1ccc(CCc2ccc(C#N)cc2)s1
Lastest graph (left) vs graph in last step (right)
```



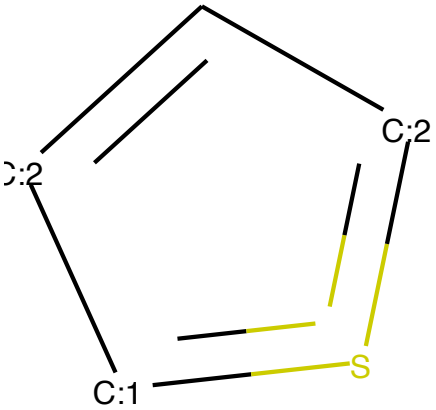

```
------------------------------------------------------------
-----Step-10-----
Generate next fragment p = 0.9998513460159302
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.537
3675227165222
```



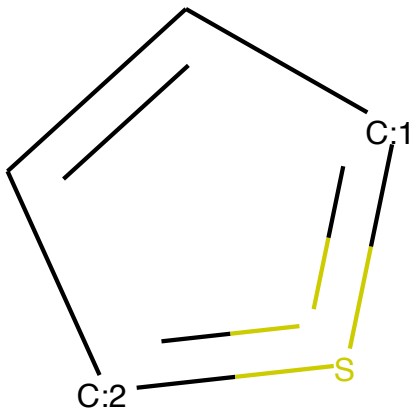
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-1.3620485067367554



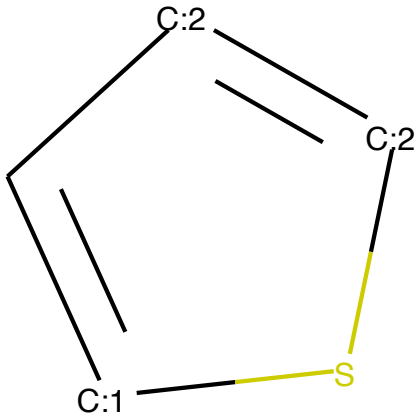
Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:1]=S=[CH:2]1 w/ p=-2.829477071762085



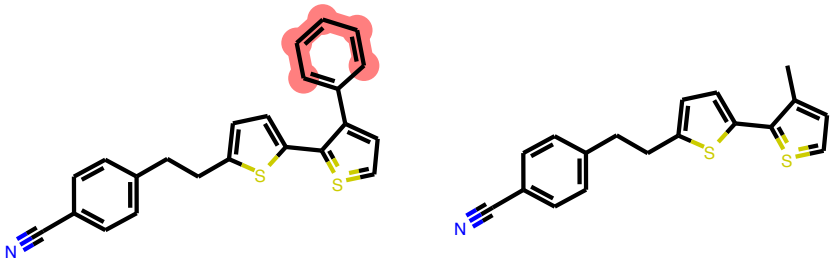
Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ p=-3.1695640087127686



Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-3.54
45308685302734



Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: N#Cc1ccc(CCc2ccc(C3=S=CC=C3c3ccccc3)s2)cc1
Lastest graph (left) vs graph in last step (right)

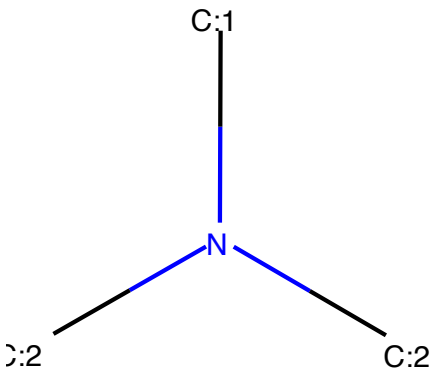


-----Step-11-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.7262435555458069

```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-0.8190346360206604
```

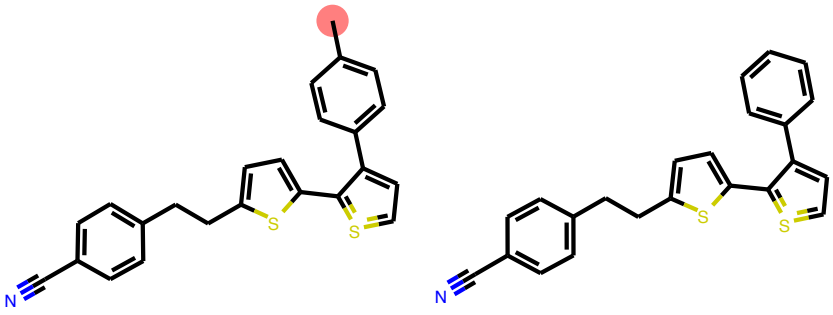
```
------------------------------------------------------------
Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-3.2060482501983
643
```

```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-3.826
5373706817627
```

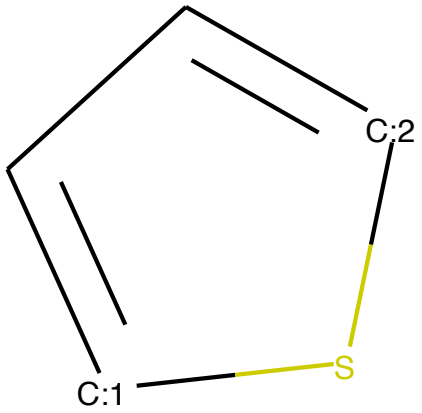



```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-4.873334884643555
```

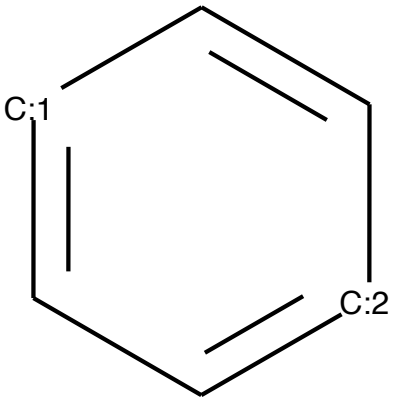
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(C2=CC=S=C2c2ccc(CCc3ccc(C#N)cc3)s2)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-12-----
Generate next fragment p = 0.9999996423721313
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.0039289
2025411129
```

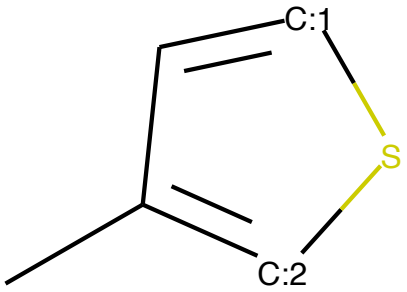


Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-5.551692485809326



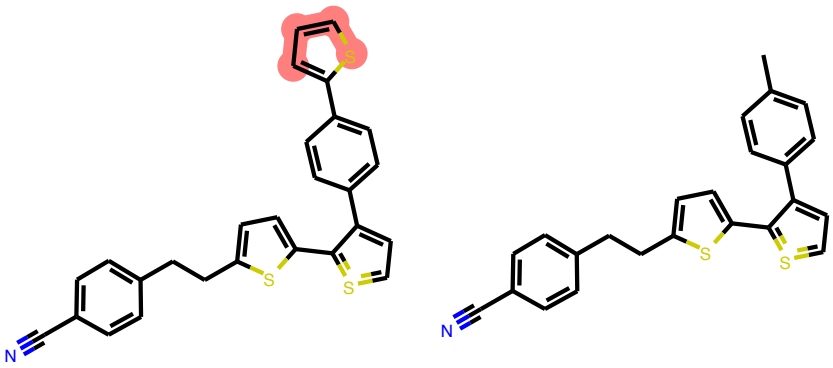
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-10.789213180541992

Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ p=-11.439164161682129



Molecule C#N and its specific config N#[CH:1] w/ p=-11.757345199584961

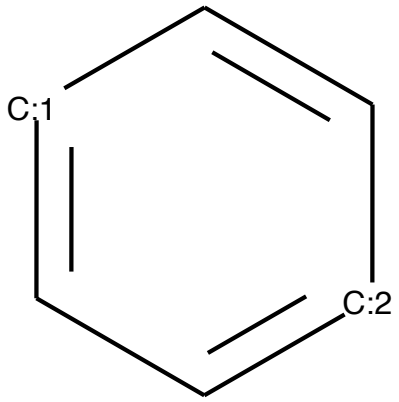
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: N#Cc1ccc(CCc2ccc(C3=S=CC=C3c3ccc(-c4cccs4)cc3)s2)cc1
Lastest graph (left) vs graph in last step (right)



-----Step-13-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config C[CH3:1] w/ p=-0.32609090209007263

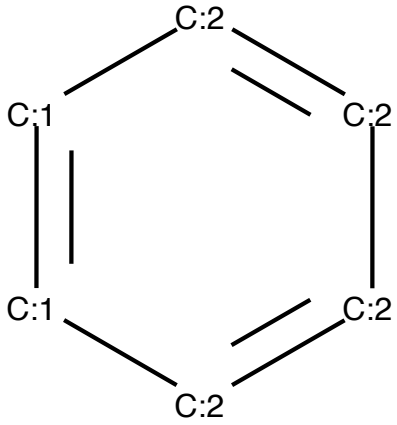
```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.2792088985443115
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-12.74
4547843933105
```

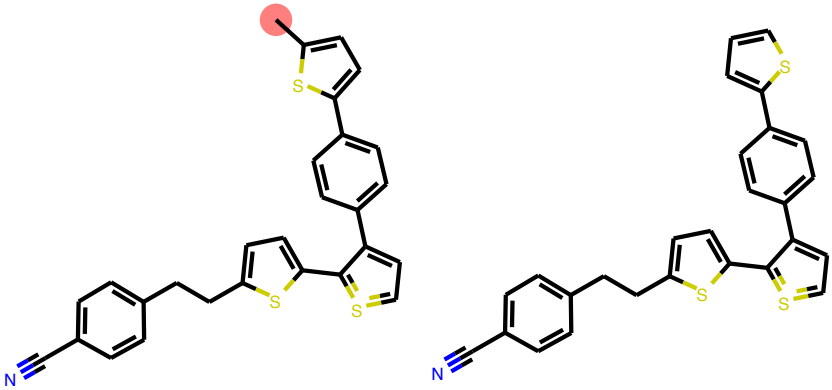



```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-15.83609390258789
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config [CH:1]1=[CH:1][CH:2]=[CH:2][CH:2]
=[CH:2]1 w/ p=-16.03433609008789
```



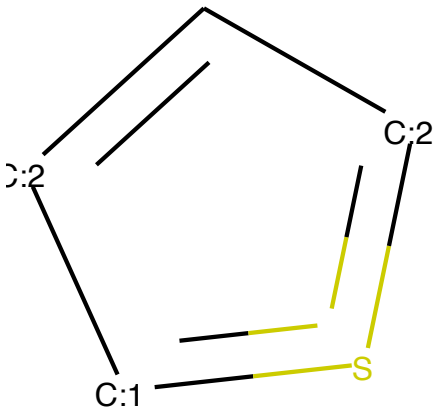

```
------------------------------------------------------------
Attaching fragment C[CH3:1] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)s1
Lastest graph (left) vs graph in last step (right)
```



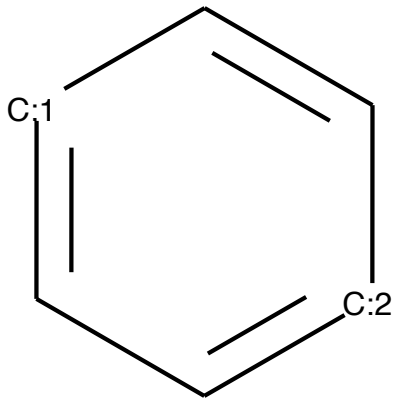

```
------------------------------------------------------------
-----Step-14-----
Generate next fragment p = 0.9981449842453003
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-0.00701524037867784
5
```

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.225250244140625
```

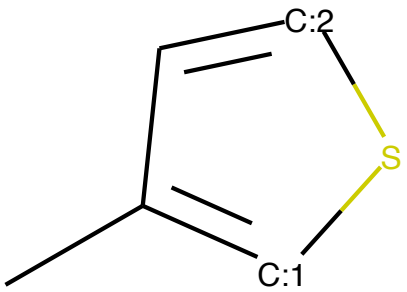
```
------------------------------------------------------------
Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:1]=S=[CH:2]1 w/ p=-7.
219426155090332
```




```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-7.761
297225952148
```



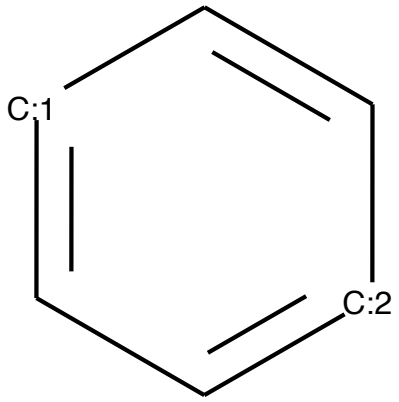
Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ p=-7.88810
96839904785



Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
-----Step-15-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config C[CH3:1] w/ p=-0.32609090209007263

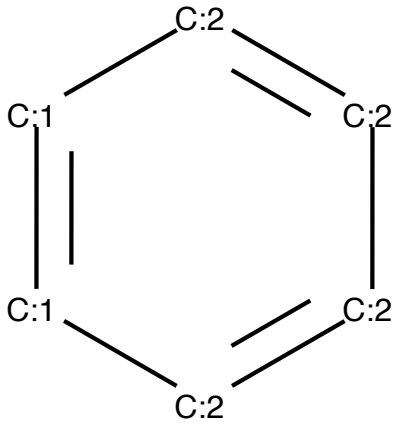
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.2792088985443115

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-12.74
4547843933105
```

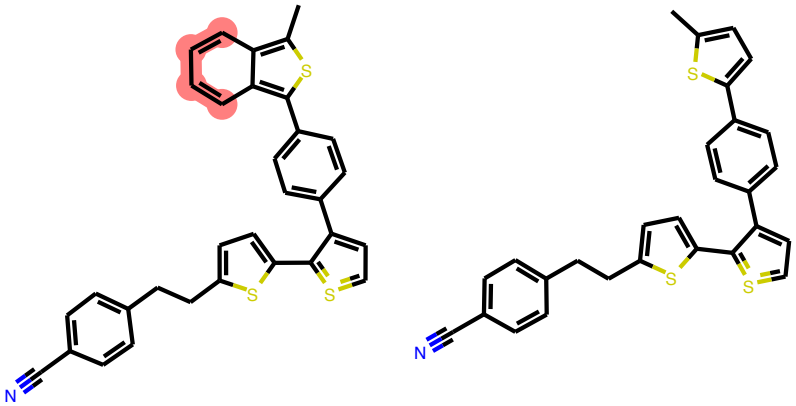



```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-15.83609390258789
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config [CH:1]1=[CH:1][CH:2]=[CH:2][CH:2]
=[CH:2]1 w/ p=-16.03433609008789
```

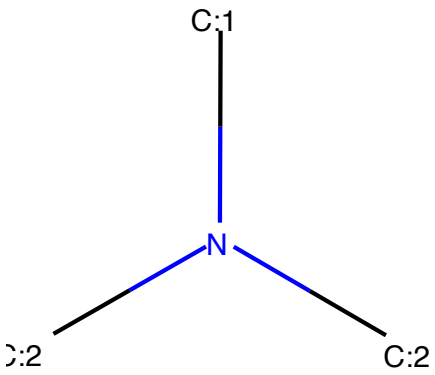



```
------------------------------------------------------------
Attaching fragment [CH:1]1=[CH:1][CH:2]=[CH:2][CH:2]=[CH:2]1 of config ['C1:C:
C:[CH:1]:C:C:1', 'C1:C:C:[CH:1]:C:C:1']
Latest partial graph: Cc1sc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)c2cc
ccc12
Lastest graph (left) vs graph in last step (right)
```

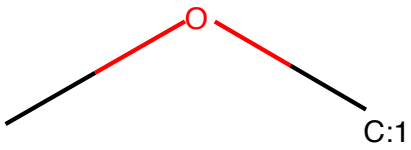



```
------------------------------------------------------------
-----Step-16-----
Generate next fragment p = 0.9999998807907104
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.1920928244535389e-0
7
```

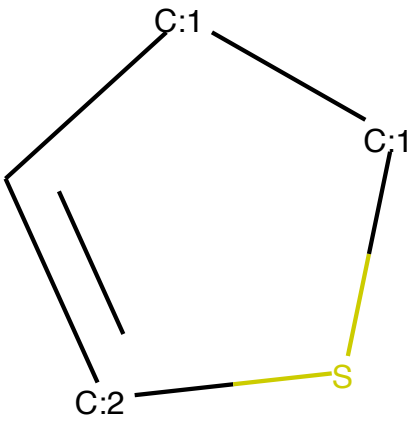
```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-16.55
008316040039
```




```
------------------------------------------------------------
Molecule COC and its specific config CO[CH3:1] w/ p=-18.543601989746094
```

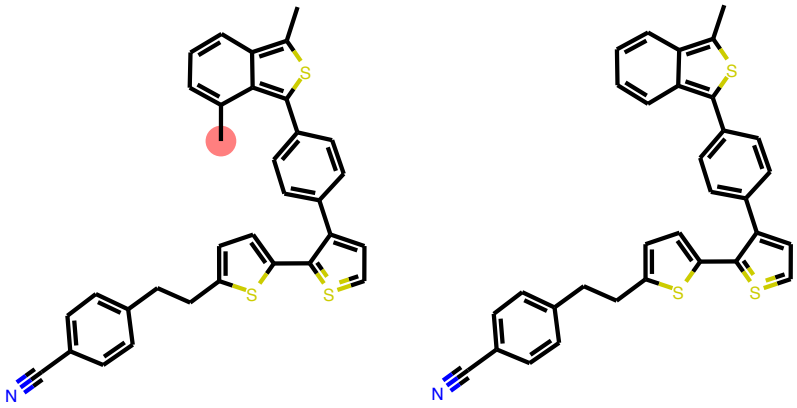



```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-20.3
3526039123535
```

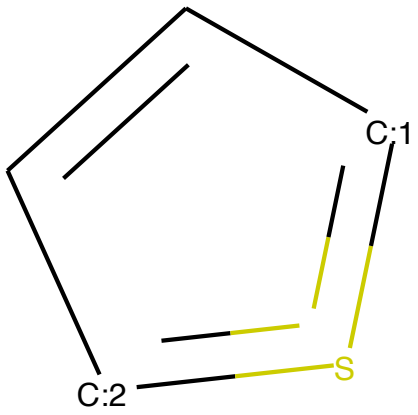



```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-21.73563003540039
```

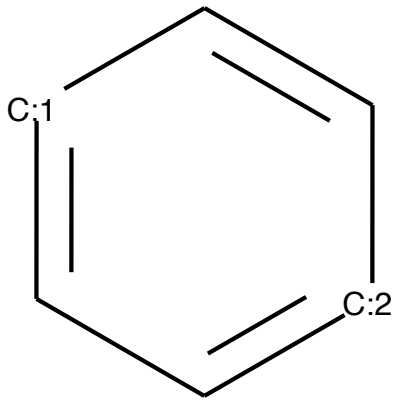
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1sc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)c2c(
C)cccc12
Lastest graph (left) vs graph in last step (right)
```



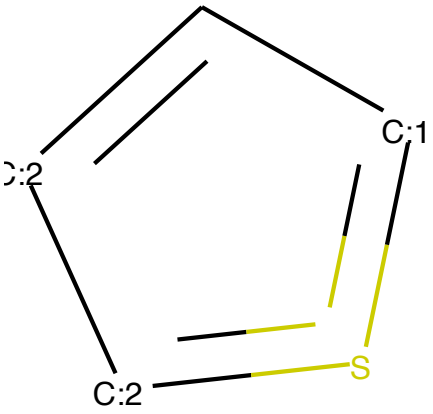

```
------------------------------------------------------------
-----Step-17-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ p=-0.10791
74280166626
```



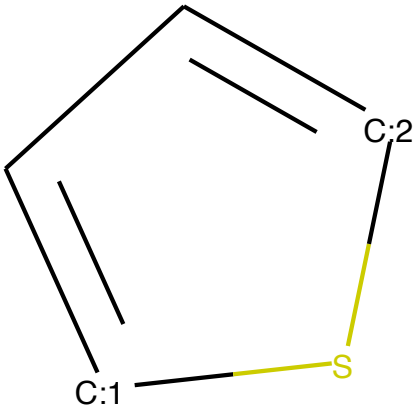

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-2.607
3691844940186
```



Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:2]=S=[CH:1]1 w/ p=-4.0261921882629395

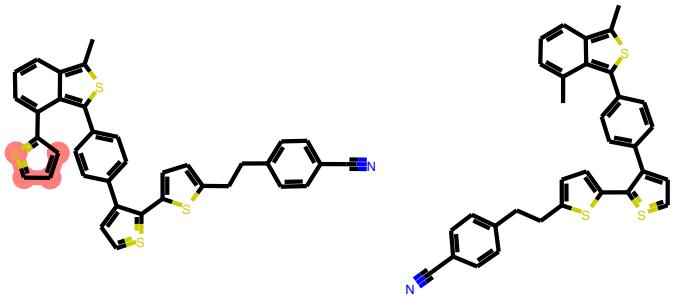


Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-5.211851119995117



Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.579514980316162

```
------------------------------------------------------------
Attaching fragment C1=C[CH:2]=S=[CH:1]1 of config ['C1=C[CH:1]=S=C1']
Latest partial graph: Cc1sc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)c2c(
C3=S=CC=C3)cccc12
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-18-----
Generate next fragment p = 0.9999998807907104
Top 5 next motifs to attach:
Molecule CC and its specific config C[CH3:1] w/ p=-2.109982233378105e-05
```

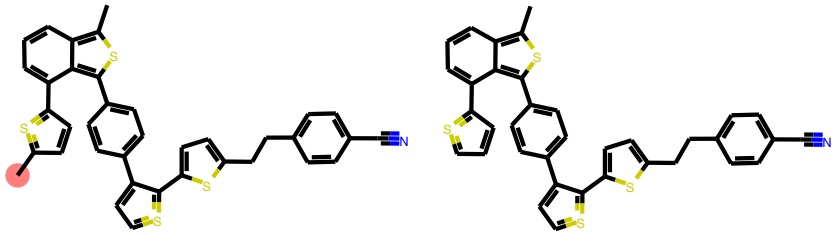
```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-10.766807556152344
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-31.469383239746094
```

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-34.28550720214844
```

```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-34.70173645019531
```

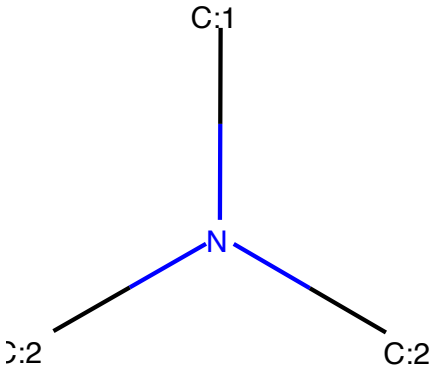
```
------------------------------------------------------------
Attaching fragment C[CH3:1] of config ['C[CH3:1]']
Latest partial graph: CC1=S=C(c2cccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N
)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



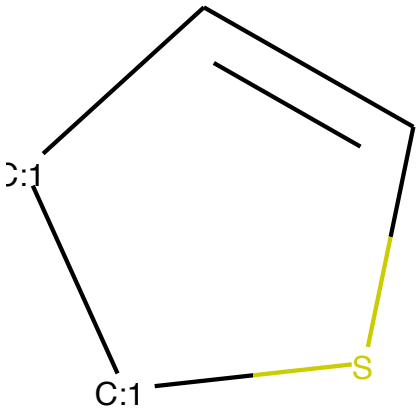
```
------------------------------------------------------------
-----Step-19-----
Generate next fragment p = 1.103717561790063e-08
-----Step-20-----
Generate next fragment p = 3.489583468763158e-05
-----Step-21-----
Generate next fragment p = 1.2617881726337075e-20
-----Step-22-----
Generate next fragment p = 0.9575585126876831
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-8.344646857949556e-07
```

Molecule CC and its specific config C[CH3:1] w/ p=-13.980932235717773

Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-16.98
9187240600586

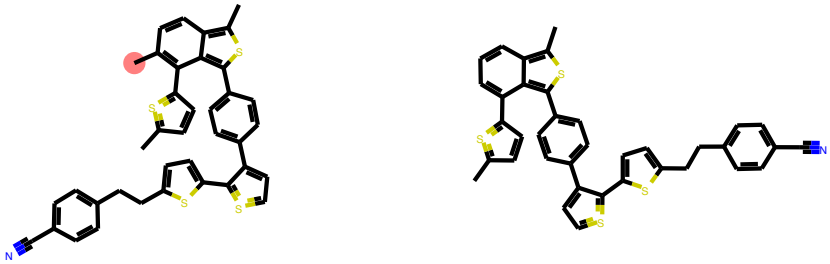


Molecule C1=CSCC1 and its specific config C1=C[CH2:1][CH2:1]S1 w/ p=-17.516544
342041016

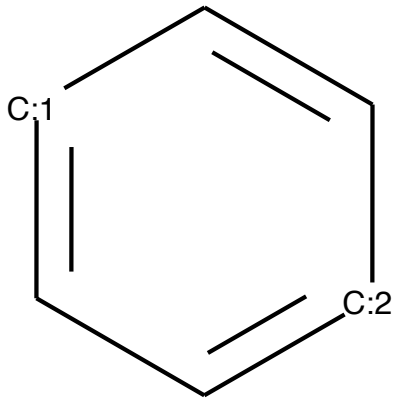


Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-19.952150344848633

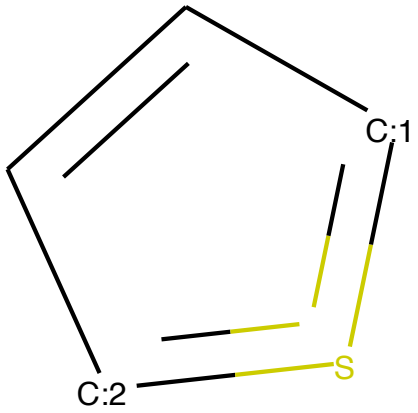
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC1=S=C(c2c(C)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(
C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



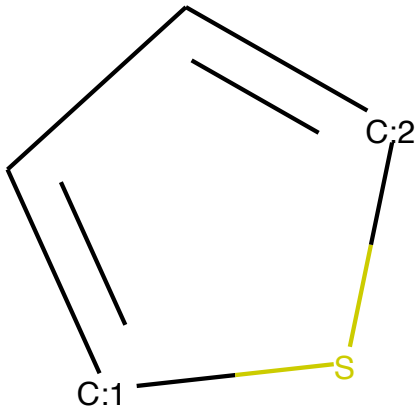
```
------------------------------------------------------------
-----Step-23-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.027
290765196084976
```




```
------------------------------------------------------------
Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ p=-4.42230
7968139648
```

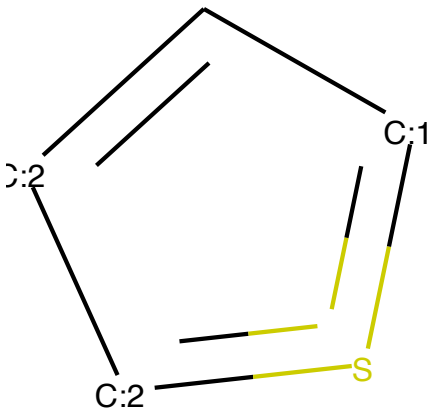


Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-4.5303835
86883545

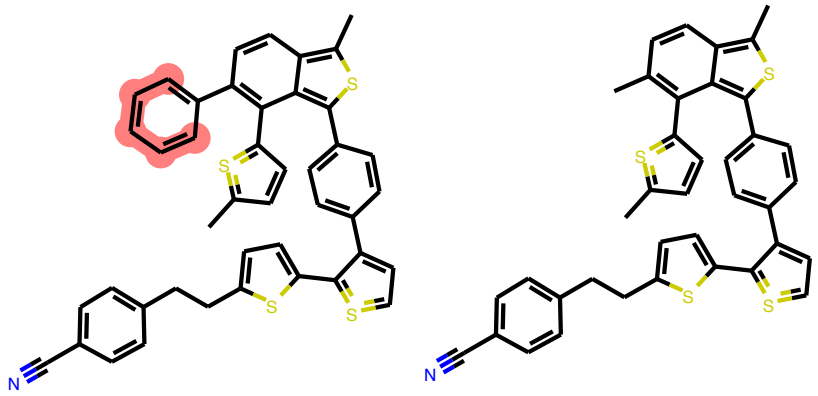


Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.7039713859558105

Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:2]=S=[CH:1]1 w/ p=-7.
235950469970703



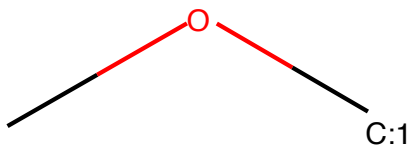
Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: CC1=S=C(c2c(-c3ccccc3)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(
CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)



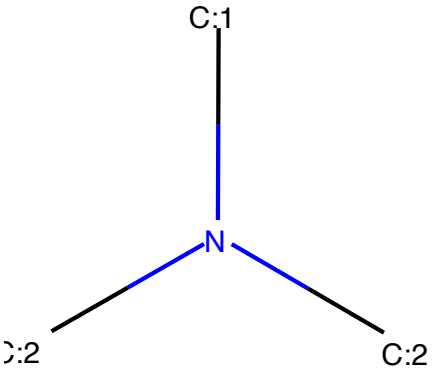
-----Step-24-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.25249555706977844

Molecule CC and its specific config C[CH3:1] w/ p=-1.4999552965164185

```
------------------------------------------------------------
Molecule COC and its specific config CO[CH3:1] w/ p=-15.377204895019531
```

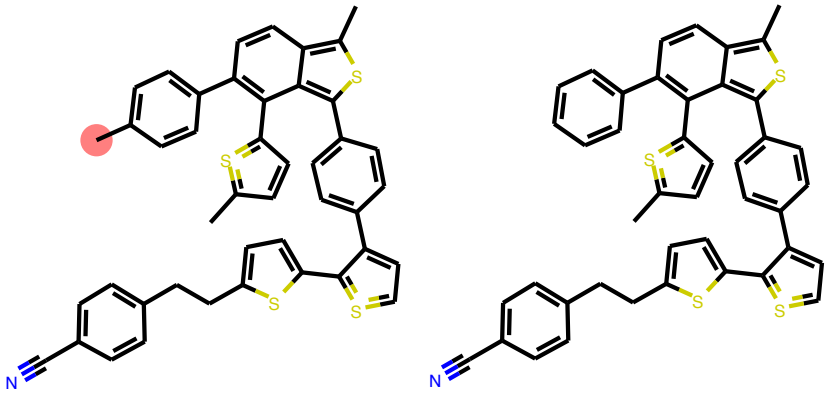



```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-18.22
846221923828
```

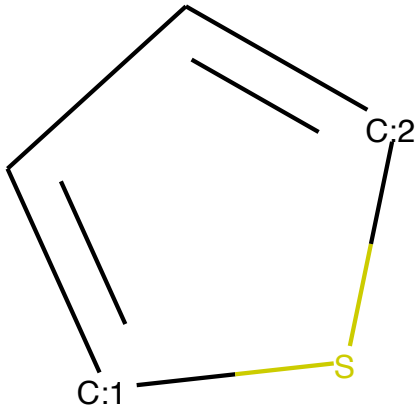



```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-19.656095504760742
```

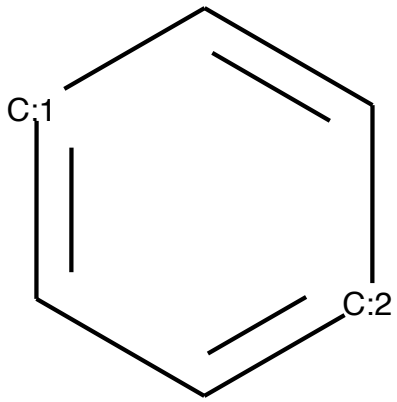
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC1=S=C(c2c(-c3ccc(C)cc3)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5c
cc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



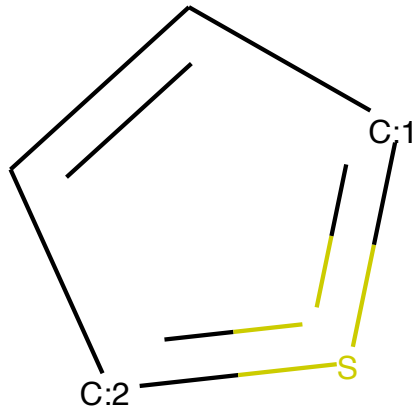

```
------------------------------------------------------------
-----Step-25-----
Generate next fragment p = 0.9999969005584717
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.0622238
3305430412
```




```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-2.835
22891998291
```

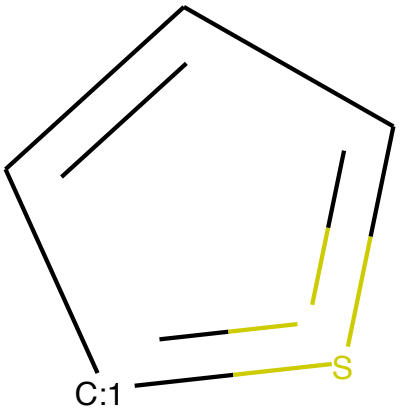


Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ p=-7.26152
8968811035

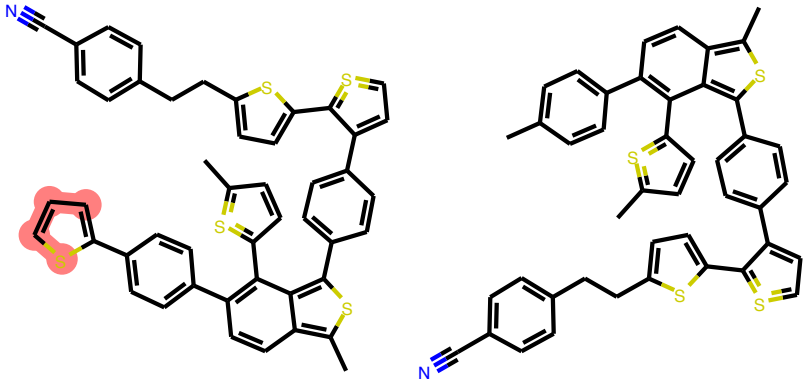


Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-7.4762797355651855

Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ p=-8.1165742874
1455



Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: CC1=S=C(c2c(-c3ccc(-c4cccs4)cc3)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)



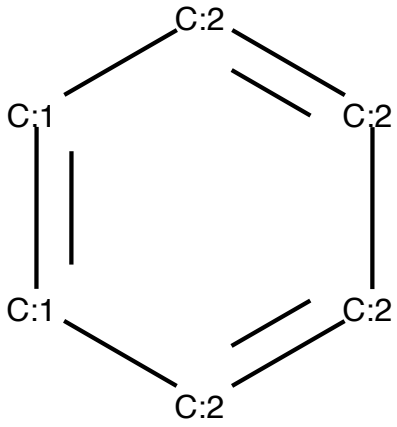
-----Step-26-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config C[CH3:1] w/ p=-0.002475176239386201

Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-6.002690315246582

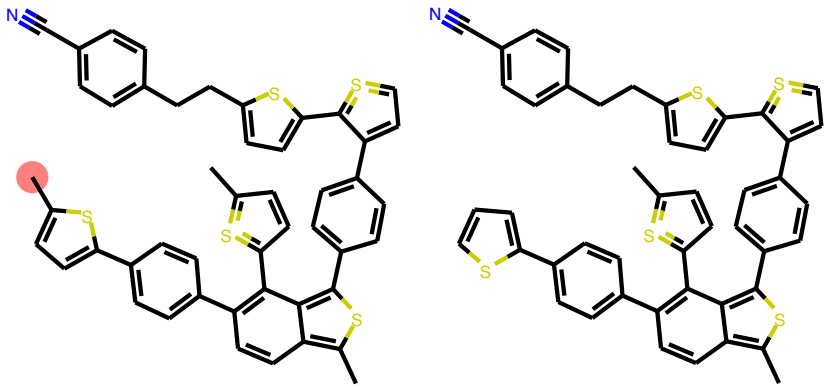
```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-22.822200775146484
```

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-23.828439712524414
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config [CH:1]1=[CH:1][CH:2]=[CH:2][CH:2]
=[CH:2]1 w/ p=-24.001911163330078
```

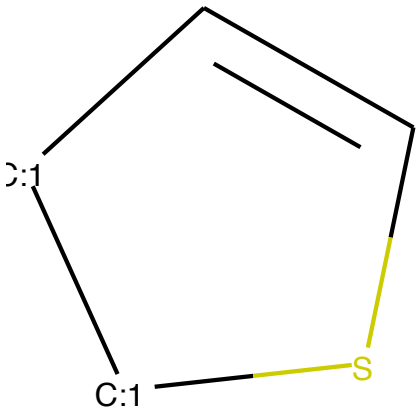



```
------------------------------------------------------------
Attaching fragment C[CH3:1] of config ['C[CH3:1]']
Latest partial graph: CC1=S=C(c2c(-c3ccc(-c4ccc(C)s4)cc3)ccc3c(C)sc(-c4ccc(C5=
CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



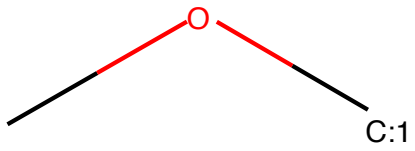
```
------------------------------------------------------------
-----Step-27-----
Generate next fragment p = 0.1861433982849121
-----Step-28-----
Generate next fragment p = 2.832648249295744e-07
-----Step-29-----
Generate next fragment p = 3.521837168062093e-24
-----Step-30-----
Generate next fragment p = 0.9999982118606567
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0969872921705246
```

Molecule C1=CSCC1 and its specific config C1=C[CH2:1][CH2:1]S1 w/ p=-2.7669434547424316

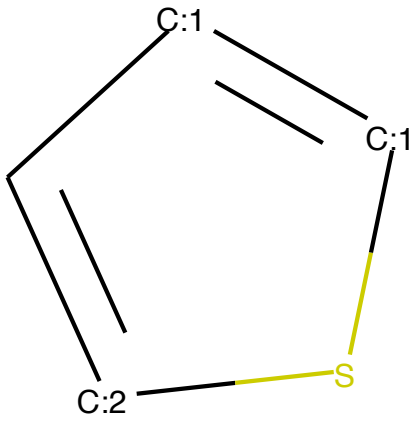


Molecule CC and its specific config C[CH3:1] w/ p=-3.8717174530029297

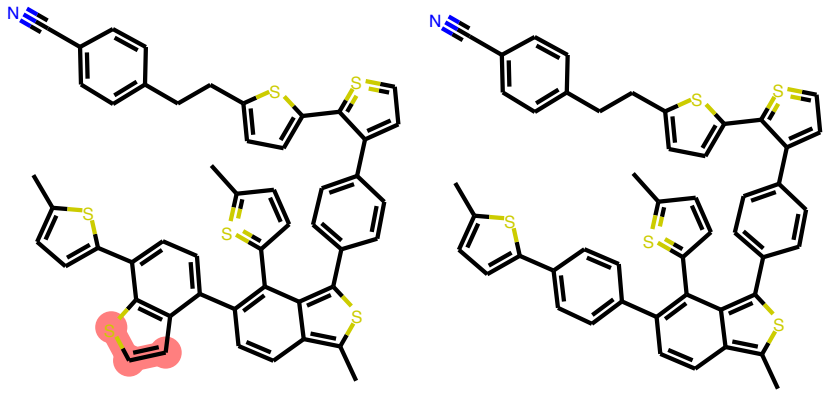
Molecule COC and its specific config CO[CH3:1] w/ p=-4.779026508331299



Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-8.568120956420898

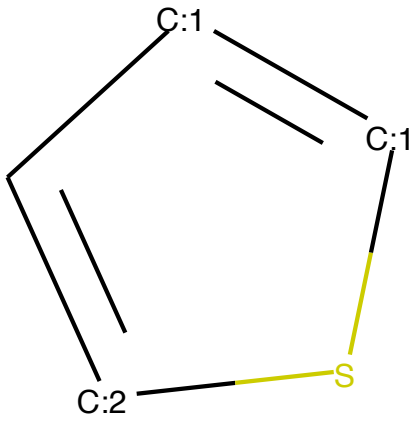



```
------------------------------------------------------------
Attaching fragment C1=C[CH2:1][CH2:1]S1 of config ['C1=C[CH2:1]CS1', 'C1=CS[CH
2:1]C1']
Latest partial graph: CC1=S=C(c2c(-c3ccc(-c4ccc(C)s4)c4sccc34)ccc3c(C)sc(-c4cc
c(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



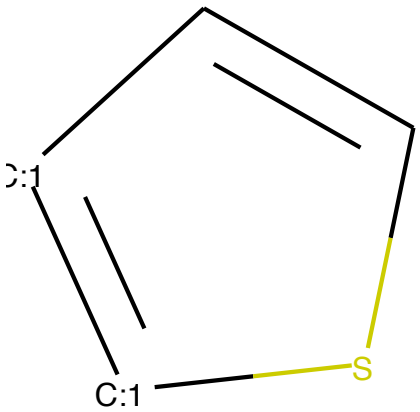
```
------------------------------------------------------------
-----Step-31-----
Generate next fragment p = 1.6251274246315006e-06
-----Step-32-----
Generate next fragment p = 0.9999061822891235
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-6.103341729613021e-05
```

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-9.75
3477096557617
```

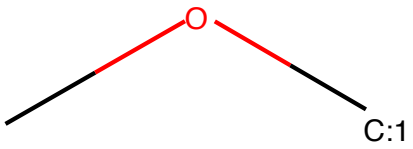



```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-13.044612884521484
```

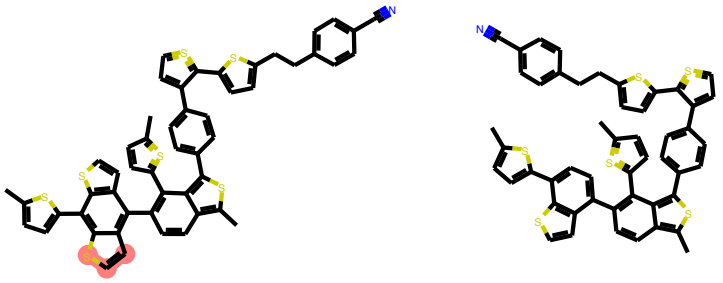
```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=C[CH:1]=[CH:1]S1 w/ p=-14.950750
350952148
```




```
------------------------------------------------------------
Molecule COC and its specific config CO[CH3:1] w/ p=-15.158754348754883
```



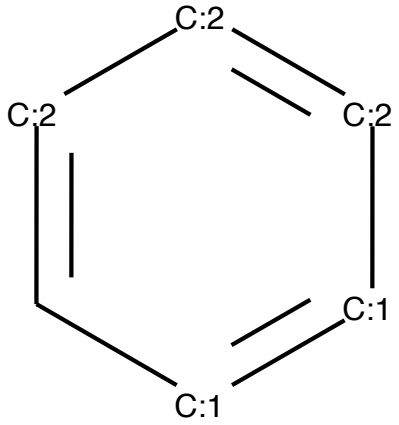

```
------------------------------------------------------------
Attaching fragment C1=[CH:2]S[CH:1]=[CH:1]1 of config ['C1:C:S:[CH:1]:C:1', 'C
1:C:[CH:1]:C:S:1']
Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sccc34)ccc3c(C)sc(
-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



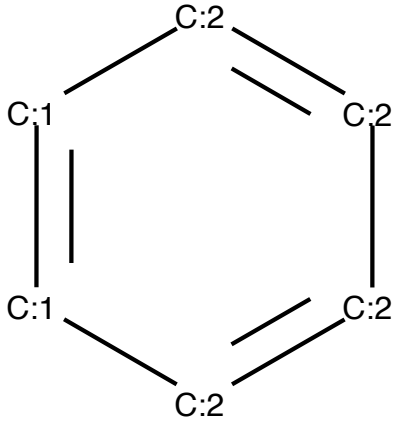
```
------------------------------------------------------------
-----Step-33-----
Generate next fragment p = 0.9991055130958557
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.10141272097826004
```

```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-2.338834762573242
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:2][CH:2]=[CH:2][CH:1]=[CH:
1]1 w/ p=-21.127647399902344
```

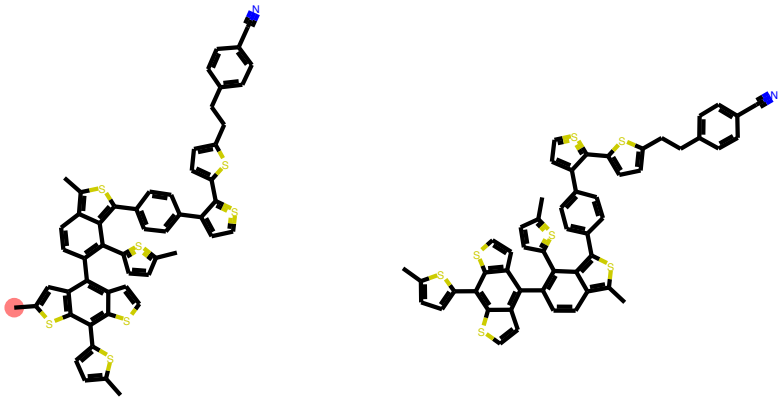



```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config [CH:1]1=[CH:1][CH:2]=[CH:2][CH:2]
=[CH:2]1 w/ p=-23.032691955566406
```

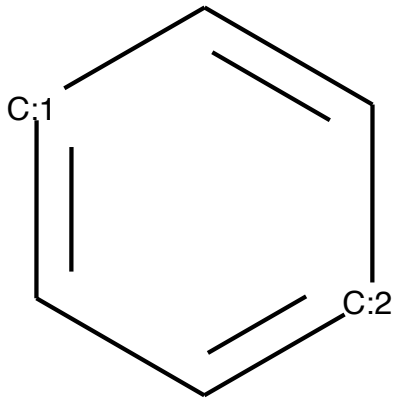



```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-24.913284301757812
```

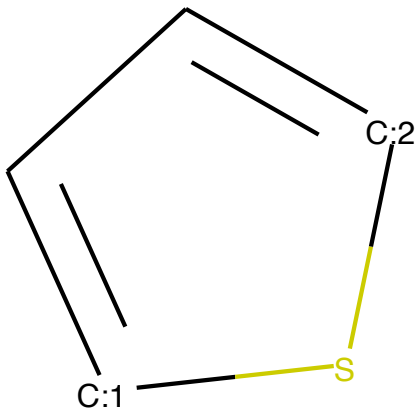
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sc(C)cc34)ccc3c(C)
sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



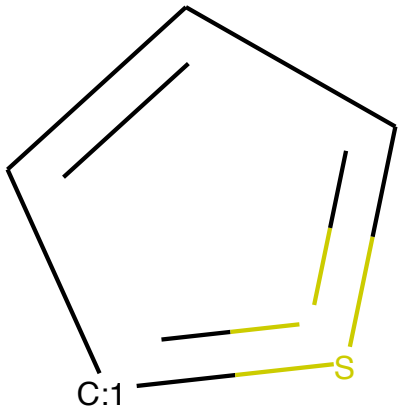
```
------------------------------------------------------------
-----Step-34-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.477
8480529785156
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-1.0630781
650543213
```

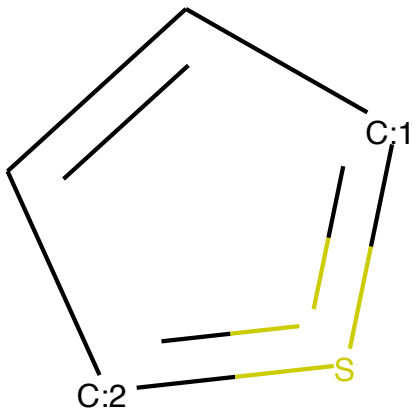


Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ p=-4.0439162254
3335

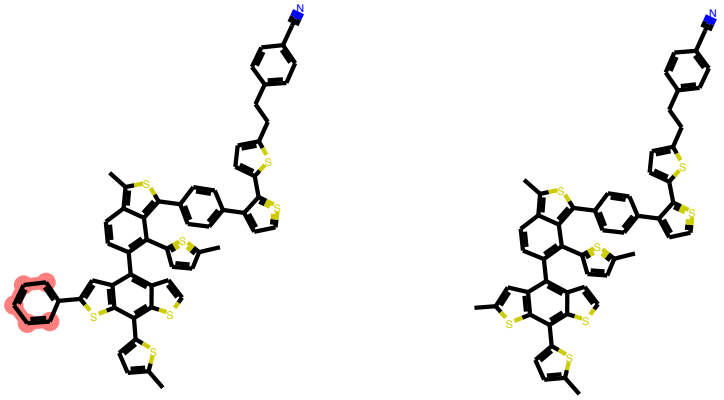


Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-4.756460189819336

Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ p=-4.95656
2042236328



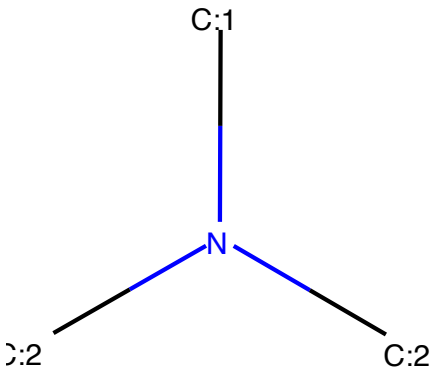
Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sc(-c5ccccc5)cc34)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)



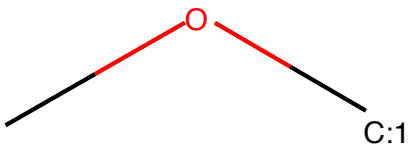
-----Step-35-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0049472046084702015

Molecule CC and its specific config C[CH3:1] w/ p=-5.316256999969482

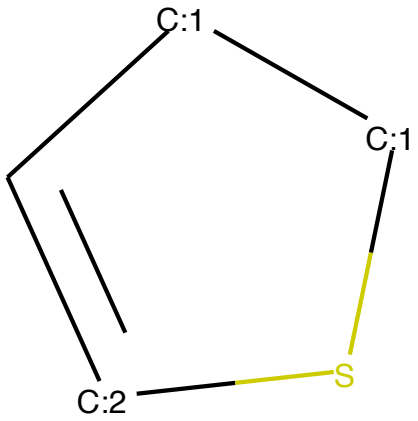
```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-10.64
2192840576172
```



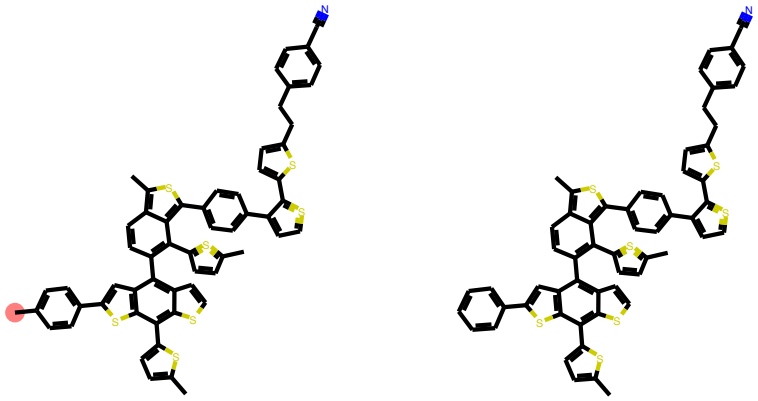

```
------------------------------------------------------------
Molecule COC and its specific config CO[CH3:1] w/ p=-19.70873260498047
```



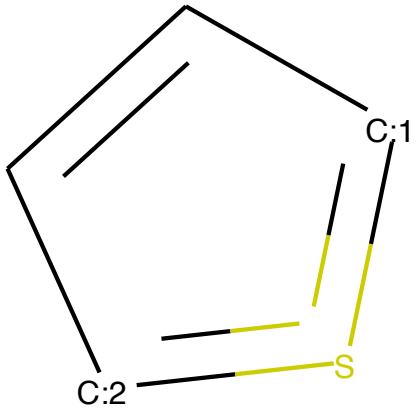

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-22.3
1403923034668
```



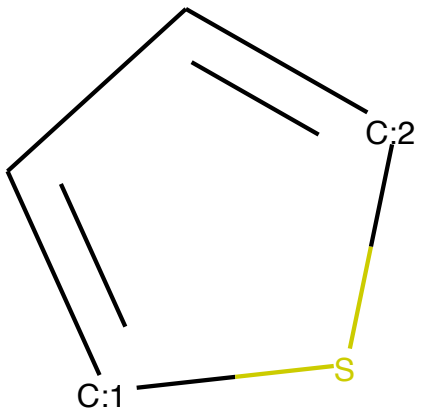

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sc(-c5ccc(C)cc5)cc
34)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-36-----
Generate next fragment p = 0.9999997615814209
Top 5 next motifs to attach:
Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ p=-0.98708
07528495789
```

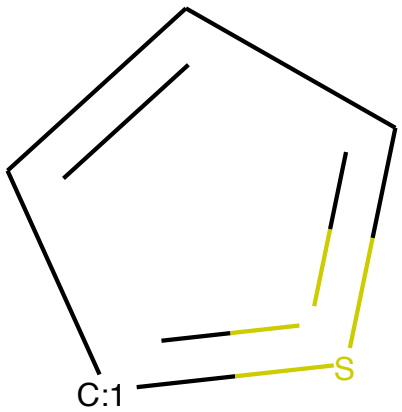



```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-1.1682732
105255127
```

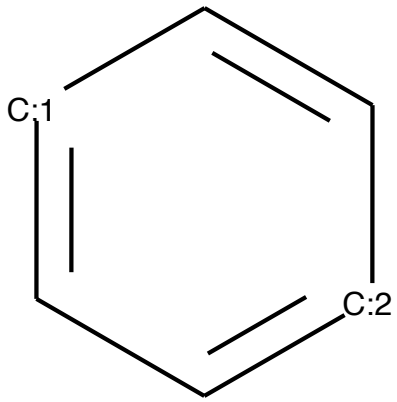


Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-1.210477590560913

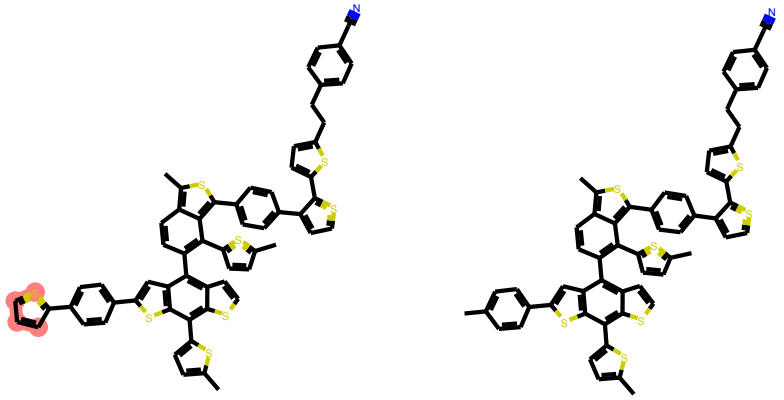
Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ p=-4.2015657424
92676



Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-6.060
859203338623




```
------------------------------------------------------------
Attaching fragment C1=C[CH:2]=S=[CH:1]1 of config ['C1=C[CH:1]=S=C1']
Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sc(-c5ccc(C6=S=CC=
C6)cc5)cc34)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-37-----
Generate next fragment p = 0.9999994039535522
Top 5 next motifs to attach:
Molecule CC and its specific config C[CH3:1] w/ p=-0.07598993927240372
```

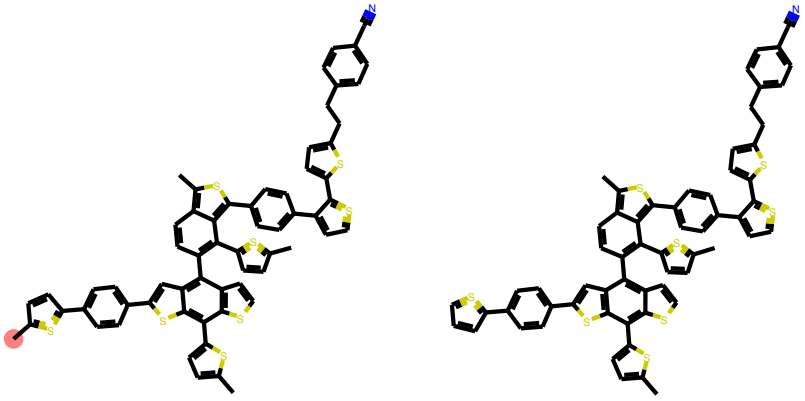
```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-2.6149091720581055
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-32.062870025634766
```

```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-40.745975494384766
```

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-41.10090637207031
```

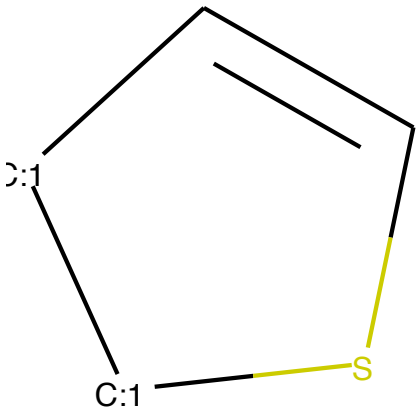
```
------------------------------------------------------------
Attaching fragment C[CH3:1] of config ['C[CH3:1]']
Latest partial graph: CC1=S=C(c2ccc(-c3cc4c(-c5ccc6c(C)sc(-c7ccc(C8=CC=S=C8c8c
cc(CCc9ccc(C#N)cc9)s8)cc7)c6c5C5=S=C(C)C=C5)c5ccsc5c(-c5ccc(C)s5)c4s3)cc2)C=C1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-38-----
Generate next fragment p = 1.1681968459242853e-07
-----Step-39-----
Generate next fragment p = 1.0555249900789931e-05
-----Step-40-----
Generate next fragment p = 2.803700798437766e-24
-----Step-41-----
Generate next fragment p = 0.0021140319295227528
-----Step-42-----
Generate next fragment p = 1.1969687327145323e-19
-----Step-43-----
Generate next fragment p = 4.590101085680254e-13
-----Step-44-----
Generate next fragment p = 7.515837822784184e-17
-----Step-45-----
Generate next fragment p = 8.215797001259585e-25
-----Step-46-----
Generate next fragment p = 1.8317692265898584e-14
-----Step-47-----
Generate next fragment p = 3.7074396330716297e-10
-----Step-48-----
Generate next fragment p = 8.661963293965297e-26
-----Step-49-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.3337589502334595
```

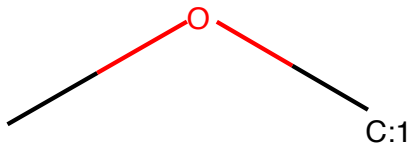
```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-1.4042267799377441
```

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=C[CH2:1][CH2:1]S1 w/ p=-3.8408818
24493408
```

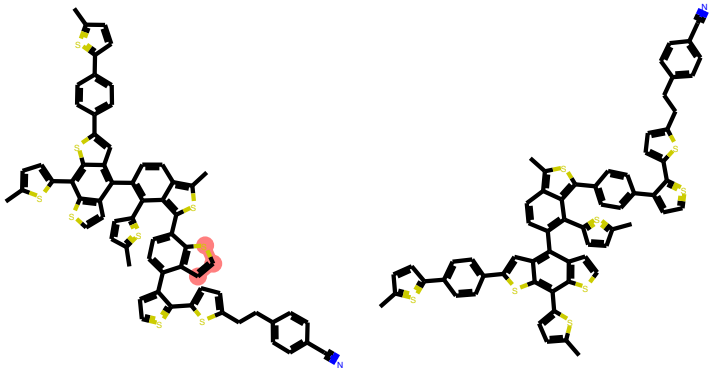



```
------------------------------------------------------------
Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-4.1856765747070
31
```

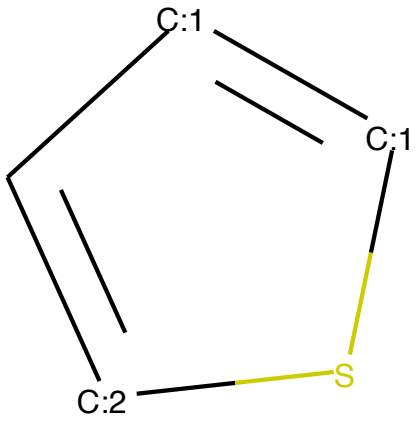
```
------------------------------------------------------------
Molecule COC and its specific config CO[CH3:1] w/ p=-7.125823020935059
```



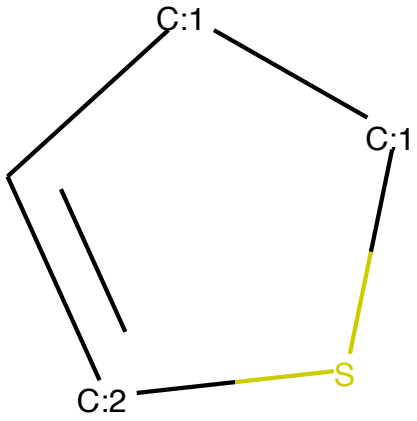

```
------------------------------------------------------------
Attaching fragment C1=C[CH2:1][CH2:1]S1 of config ['C1=C[CH2:1]CS1', 'C1=CS[CH
2:1]C1']
Latest partial graph: CC1=S=C(c2ccc(-c3cc4c(-c5ccc6c(C)sc(-c7ccc(C8=CC=S=C8c8c
cc(CCc9ccc(C#N)cc9)s8)c8ccsc78)c6c5C5=S=C(C)C=C5)c5ccsc5c(-c5ccc(C)s5)c4s3)cc2
)C=C1
Lastest graph (left) vs graph in last step (right)
```



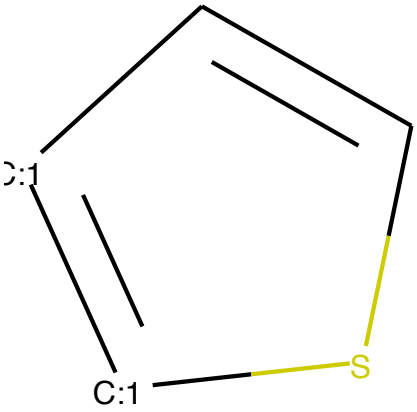
```
------------------------------------------------------------
-----Step-50-----
Generate next fragment p = 0.0001593736669747159
-----Step-51-----
Generate next fragment p = 0.9866913557052612
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.000364141829777509

------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-8.184357643127441

------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-9.87
5532150268555
```




```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-11.4
66437339782715
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=C[CH:1]=[CH:1]S1 w/ p=-11.515392
303466797
```



In [ ]: