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]:

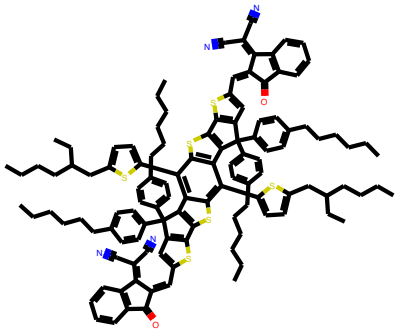
```
def view(data, i, _original):
    print('Original: {}'.format(_original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(_original[i])]))

    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 [12]:

```
view(wo_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)
```

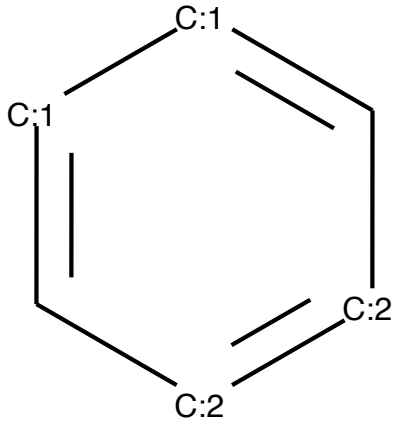
C=C4)C5=C6SC7=C5C(C8=CC=C(CC(CC)CCCC)S8)=C(SC9=C%10C(C%11=CC=C(CCCCCC)C=C%11)(C%12=CC=C(CCCCCC)C=C%12)C%13=C9SC(/C=C%14\C(C(C=CC=C%15)=C%15C%14=O)=C(C#N)\C#N)=C%13)C%10=C7C%16=CC=C(CC(CC)CCCC)S%16)=C6S2)C%17=C1C=CC=C%17



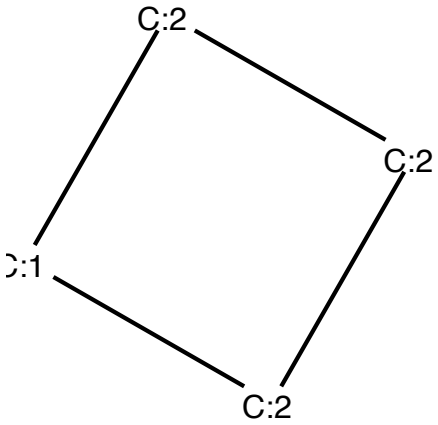
**********Sample 11th**********
-----Step-0-----
Root motif: C=C
Top 5 root motif configs: ('[CH2:1]=[CH2:2]', tensor(23.7334))
('C=[CH2:1]', tensor(-23.9553))
('C([OH:1])[CH3:2]', tensor(-964.8789))
('O([CH3:1])[CH3:2]', tensor(-970.5421))
('[O:1]=[CH2:2]', tensor(-970.8329))
Displaying partial graph (aka molecule): C=C

-----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=-0.0011457790387794375

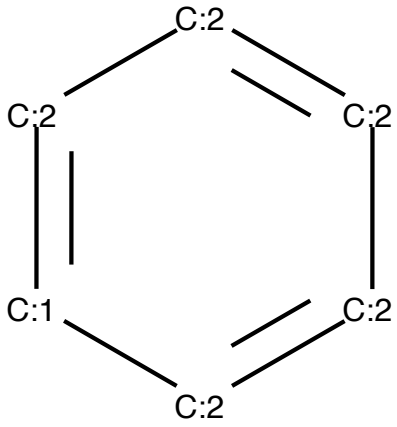
```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=[CH:2]1 w
/ p=-7.863254547119141
```




```
------------------------------------------------------------
Molecule C1CCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2]1 w/ p=-8
.10697078704834
```

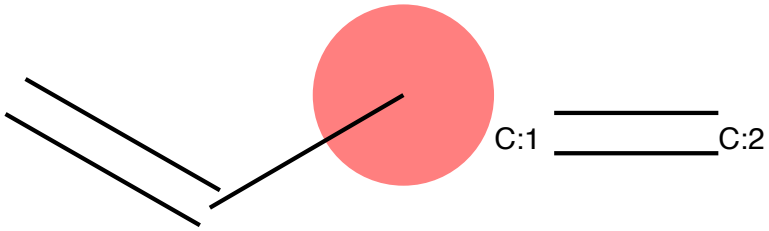



```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config [CH:1]1=[CH:2][CH:2]=[CH:2][CH:2]
=[CH:2]1 w/ p=-8.414703369140625
```

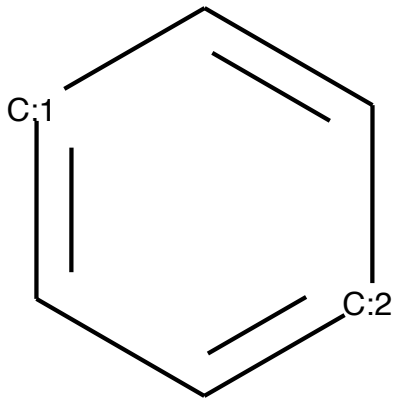



```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-8.76745891571045
```

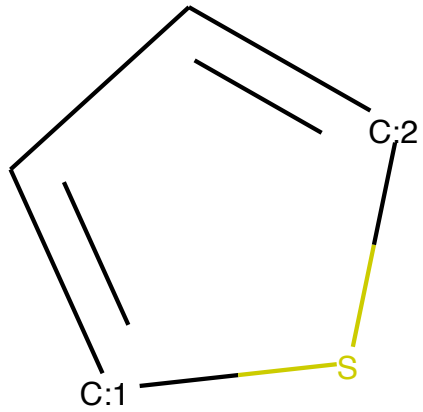
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=CC
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----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=-0.022
86357991397381
```

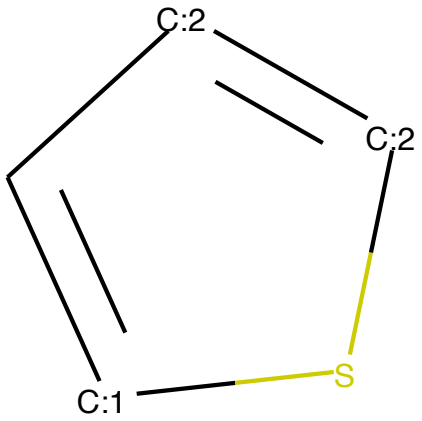


Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-4.2795324
32556152



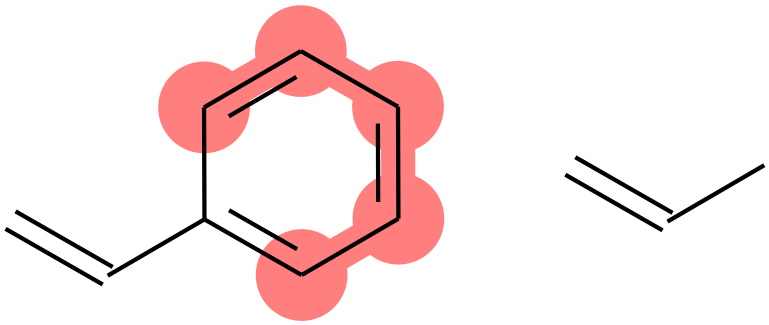
Molecule C#N and its specific config N#[CH:1] w/ p=-5.083974838256836

Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-6.99
843692779541

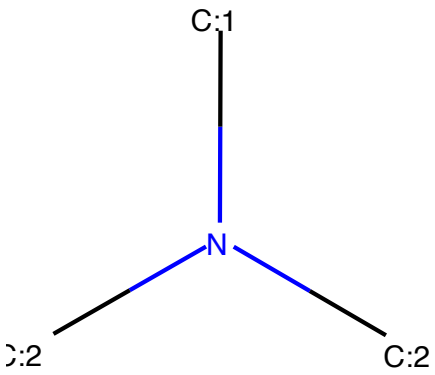


Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-7.2496418952941895

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

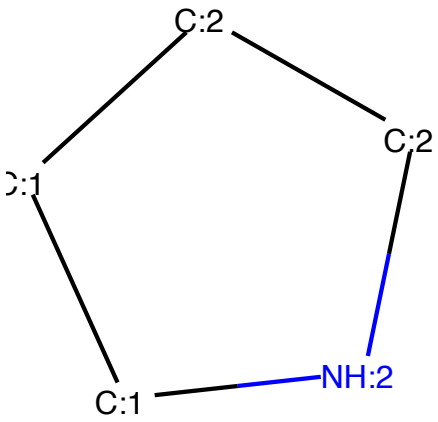


-----Step-3-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-0.484
2117428779602

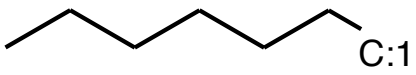



```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.2833836078643799
```

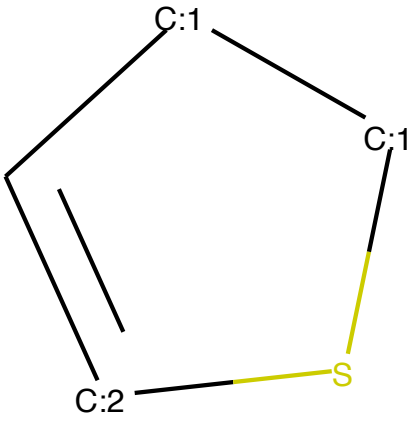
```
------------------------------------------------------------
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ p=-2.5312082767486572
```



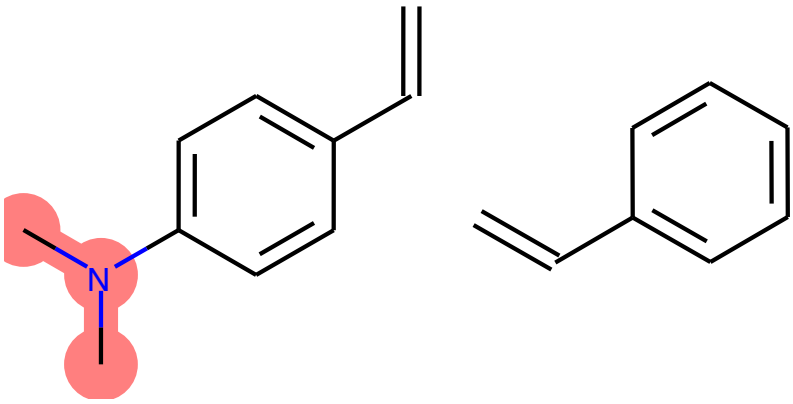

```
------------------------------------------------------------
Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ p=-4.782156944274902
```



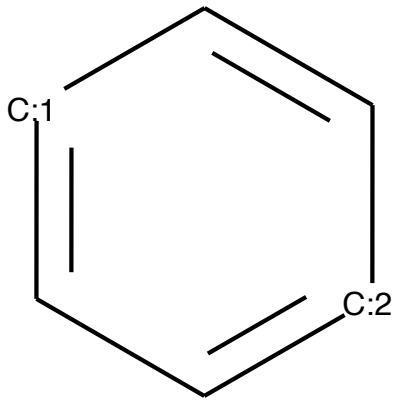

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-5.16
9488906860352
```



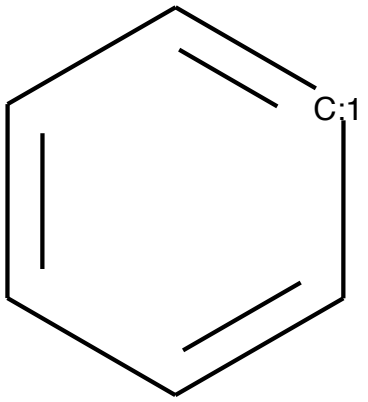

```
------------------------------------------------------------
Attaching fragment N([CH3:1])([CH3:2])[CH3:2] of config ['CN(C)[CH3:1]']
Latest partial graph: C=Cc1ccc(N(C)C)cc1
Lastest graph (left) vs graph in last step (right)
```



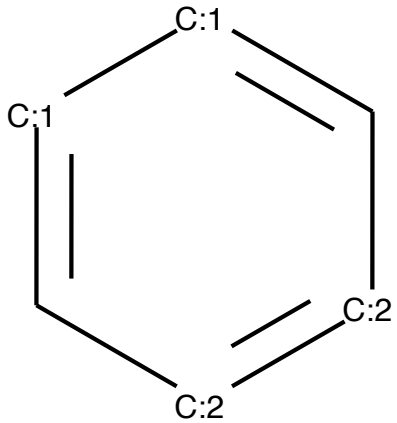

```
------------------------------------------------------------
-----Step-4-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.354
3316721916199
```



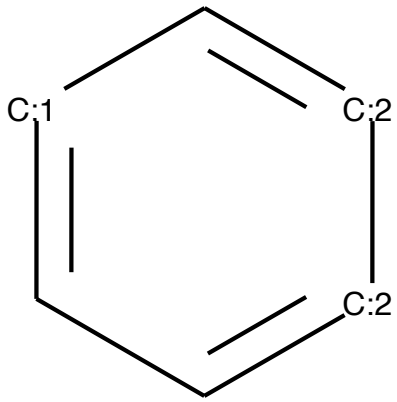
Molecule C1=CC=CC=C1 and its specific config C1=CC=[CH:1]C=C1 w/ p=-1.44056677
81829834



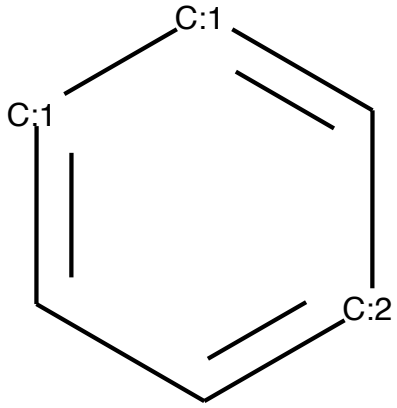
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=[CH:2]1 w
/ p=-3.485084295272827



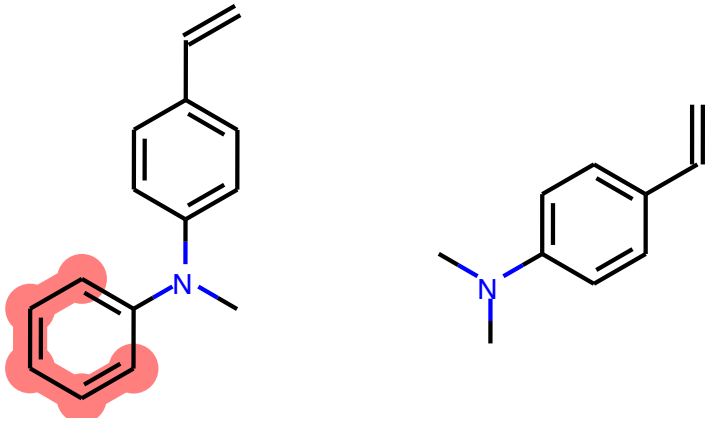
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=[CH:2][CH:2]=C1 w/ p=-
3.56367564201355




```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ p=-
6.2220940589904785
```



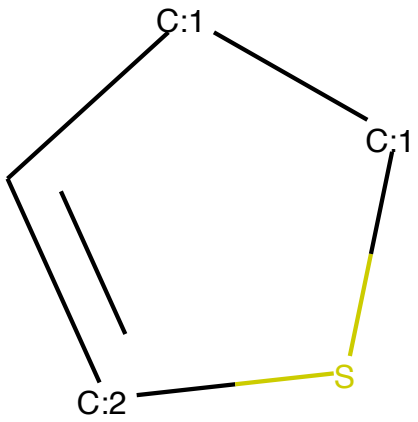

```
------------------------------------------------------------
Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: C=Cc1ccc(N(C)c2ccccc2)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-5-----
Generate next fragment p = 0.976083517074585
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.17526289820671082
```

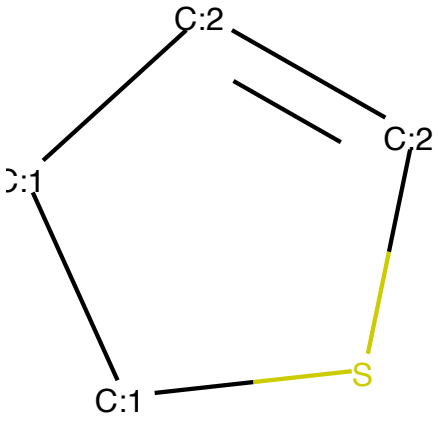
```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-2.208272695541382
```

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-3.20
7990884780884
```

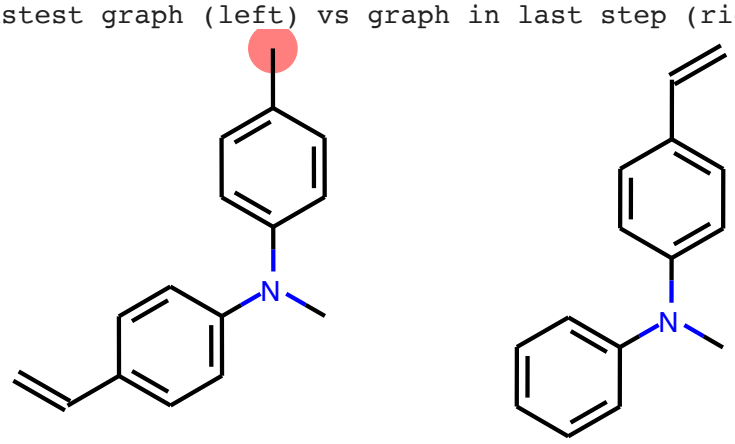



```
------------------------------------------------------------
Molecule [CH2-]C and its specific config [CH2-:1][CH3:2] w/ p=-5.4057230949401
855
```

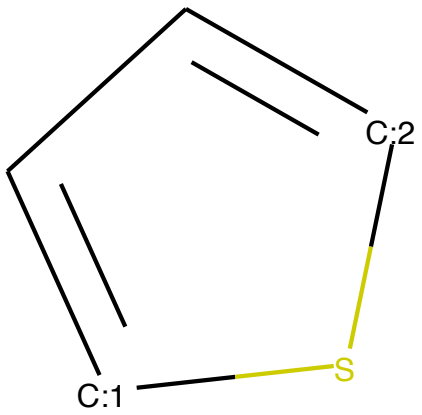
```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config S1[CH2:1][CH2:1][CH:2]=[CH:2]1 w/ p=
-6.09433650970459
```



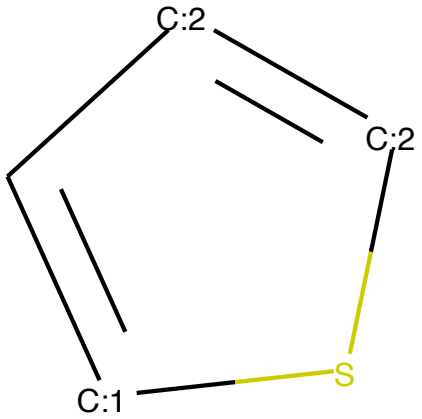

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(C)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----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=-0.9011122
584342957
```

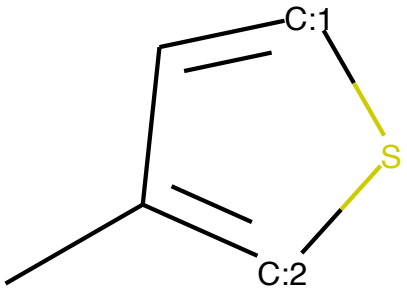


Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-1.11
5161657333374

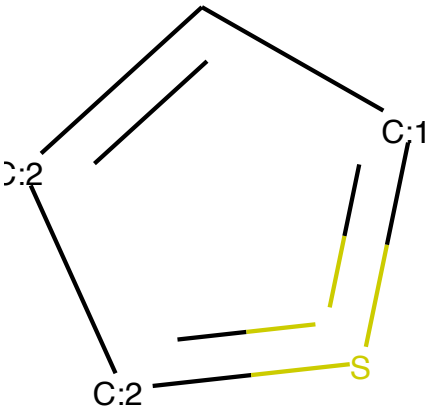


Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-1.3277950286865234

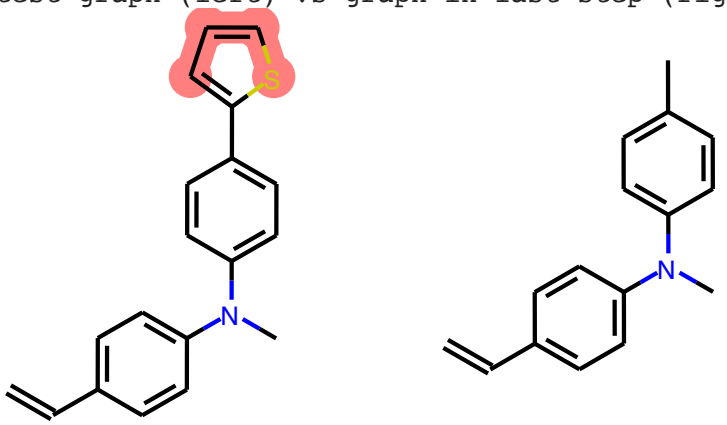
Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ p=-8.33792
5910949707



Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:2]=S=[CH:1]1 w/ p=-9.081652641296387

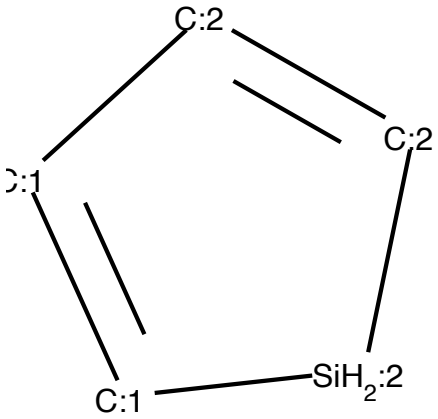


Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3cccs3)cc2)cc1
Lastest graph (left) vs graph in last step (right)

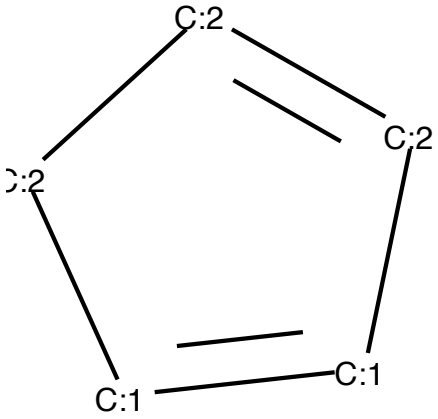


-----Step-7-----
Generate next fragment p = 0.9999912977218628
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.3353980779647827

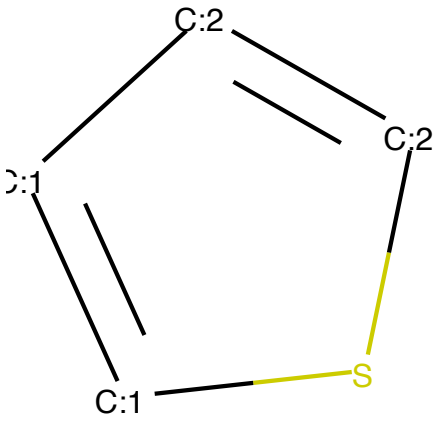
```
------------------------------------------------------------
Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:1][SiH2:2][CH:2]=[
CH:2]1 w/ p=-1.6166595220565796
```




```
------------------------------------------------------------
Molecule C1=CCC=C1 and its specific config [CH:1]1=[CH:1][CH2:2][CH:2]=[CH:2]1
w/ p=-2.5998778343200684
```

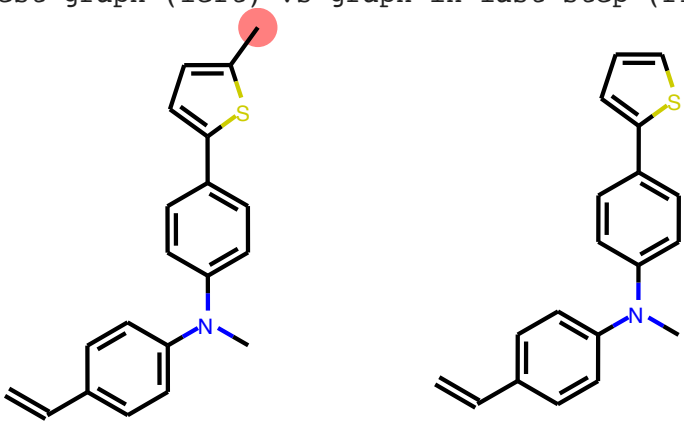



```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p=
-4.649660587310791
```



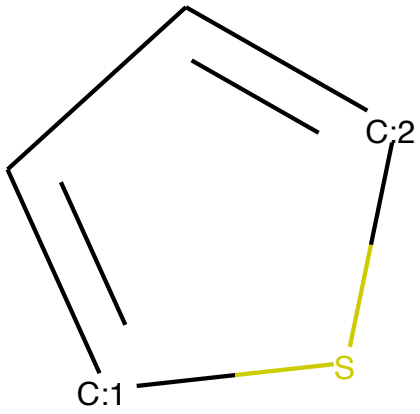

```
------------------------------------------------------------
Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ p=-6.8221774101257
32
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```

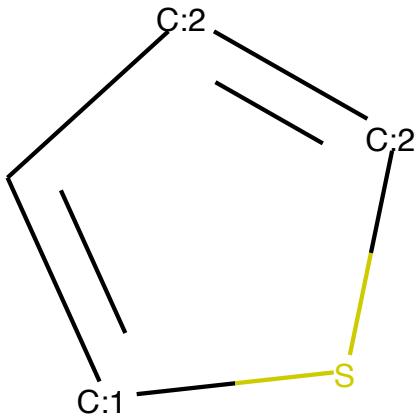



```
------------------------------------------------------------
-----Step-8-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-0.04345783218741417
```

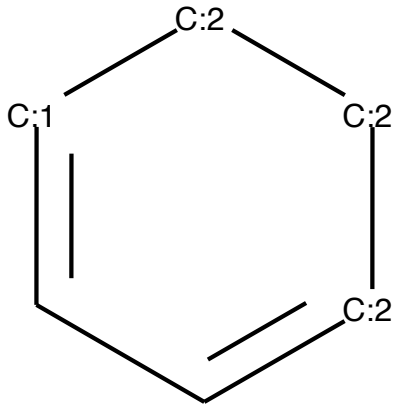
```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-3.9461703
300476074
```



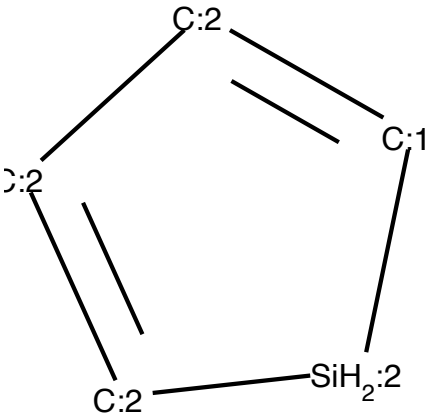

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-4.16
166353225708
```



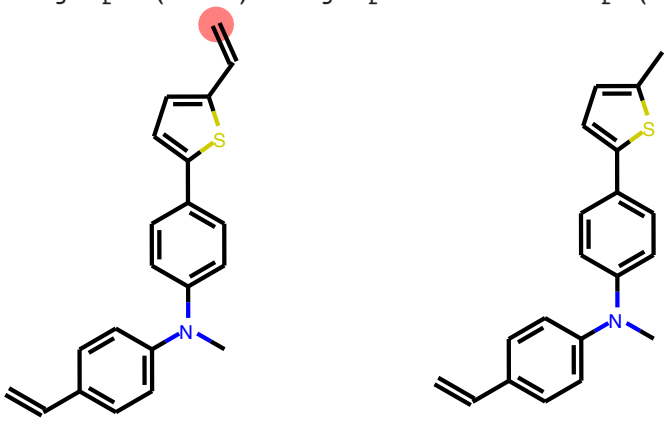

```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-5.0577592849731445
```



Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:2][CH:2]=[CH:2][Si
H2:2]1 w/ p=-8.179245948791504



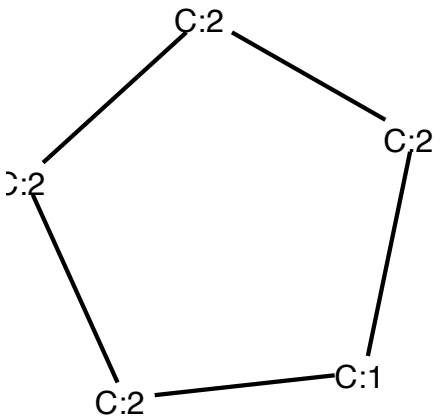
Attaching fragment [CH2:1]=[CH2:2] of config ['C=[CH2:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)



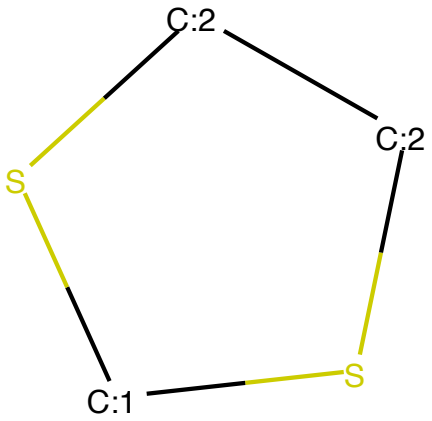
-----Step-9-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.14302974939346313

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-2.0491089820861816
```

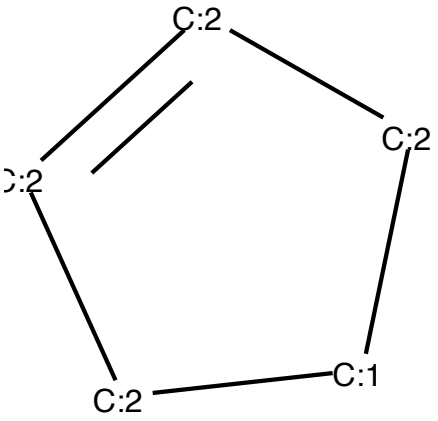
```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]1
w/ p=-5.688033580780029
```



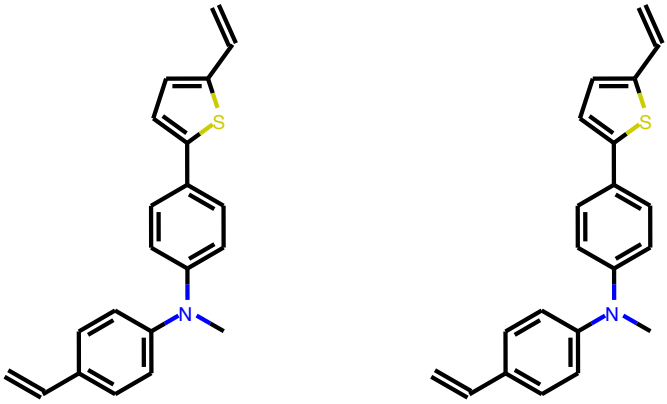

```
------------------------------------------------------------
Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ p=-7.512
922763824463
```




```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:2][CH:2]=[CH:2][CH2:2]1
w/ p=-8.504197120666504
```



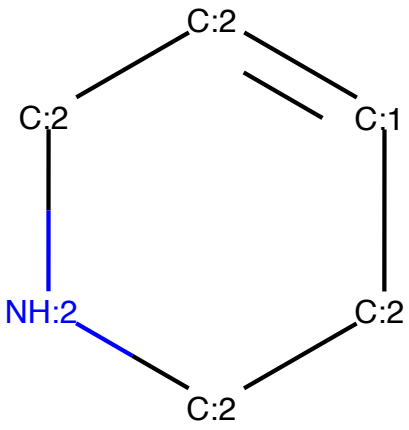

```
------------------------------------------------------------
Attaching fragment C of config ['[CH4:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-10-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=0.0
```

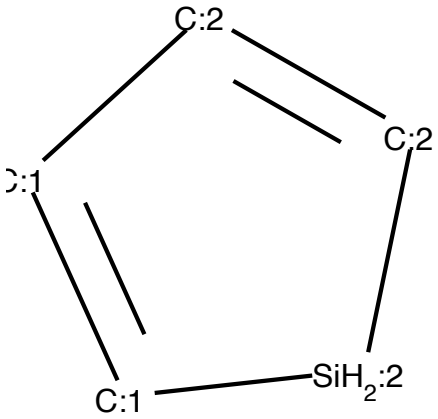
```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-17.890235900878906
```

```
------------------------------------------------------------
Molecule C1=CCNCC1 and its specific config [CH:1]1=[CH:2][CH2:2][NH:2][CH2:2][
CH2:2]1 w/ p=-18.23428726196289
```

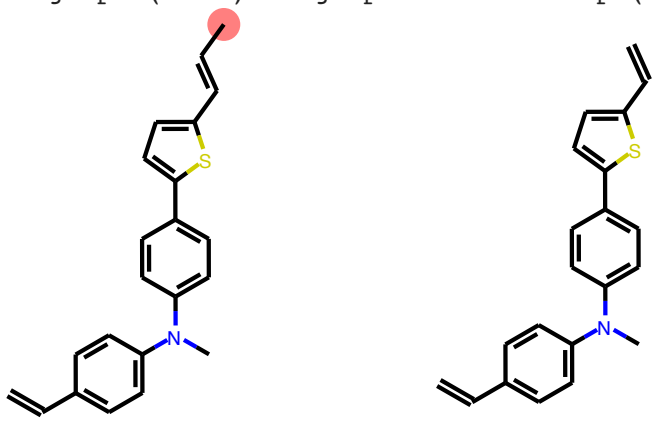



```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-18.619274139404297
```

```
------------------------------------------------------------
Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:1][SiH2:2][CH:2]=[
CH:2]1 w/ p=-20.469430923461914
```



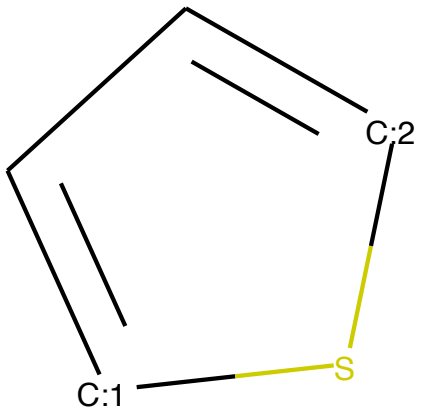

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=CC)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-11-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C#N and its specific config N#[CH:1] w/ p=-1.7762025890988298e-05
```

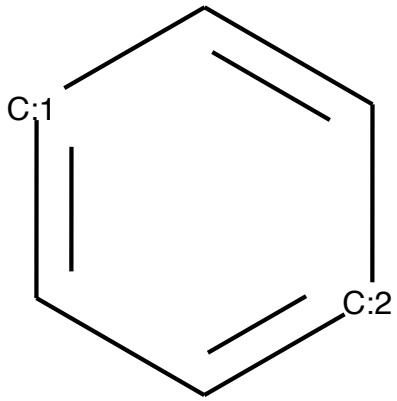
```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-11.711331367492676
```

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-12.286079
406738281
```

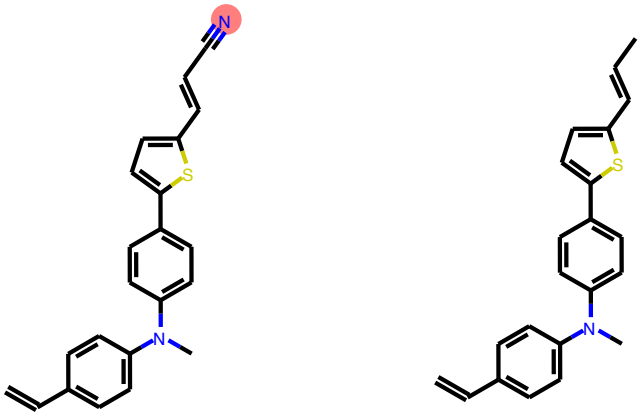



```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-12.406049728393555
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-14.15
0064468383789
```




```
------------------------------------------------------------
Attaching fragment N#[CH:1] of config ['N#[CH:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=CC#N)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```



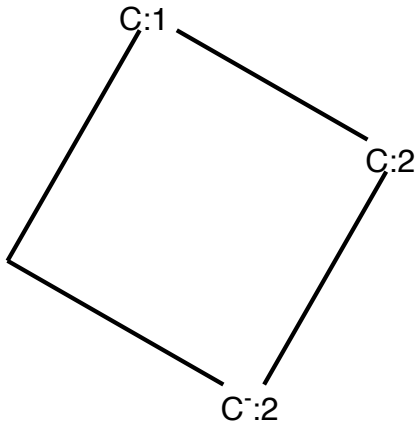
```
------------------------------------------------------------
-----Step-12-----
Generate next fragment p = 8.297082461528722e-26
-----Step-13-----
Generate next fragment p = 6.316603361514964e-15
-----Step-14-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.1920928244535389e-0
7
```

```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-16.106910705566406
```

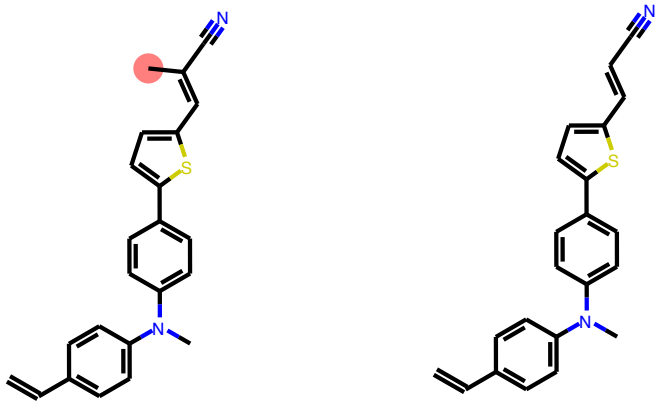
```
------------------------------------------------------------
Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ p=-19.303838729858
4
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-21.74822235107422
```

```
------------------------------------------------------------
Molecule [CH-]1CCC1 and its specific config C1[CH2:1][CH2:2][CH-:2]1 w/ p=-23.
587783813476562
```



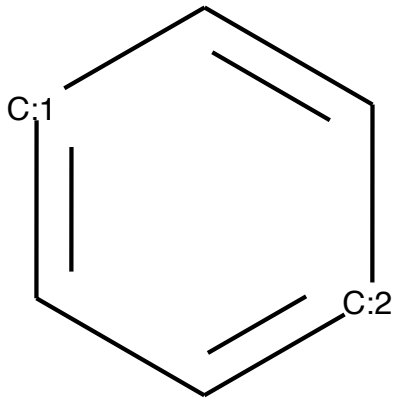

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C)C#N)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```



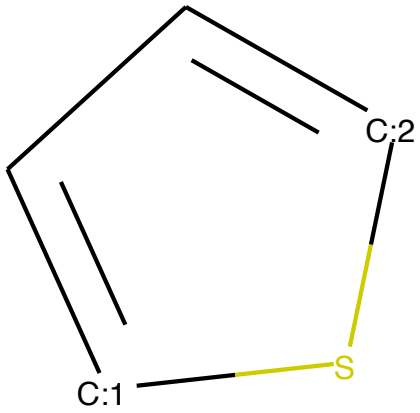

```
------------------------------------------------------------
-----Step-15-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.2121753990650177
```

Molecule C#N and its specific config N#[CH:1] w/ p=-1.7091403007507324

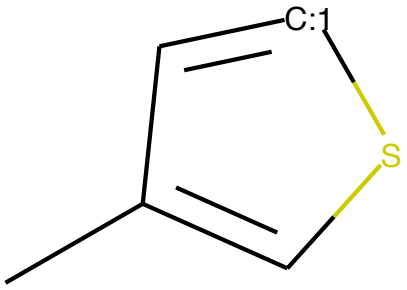
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-4.714538097381592



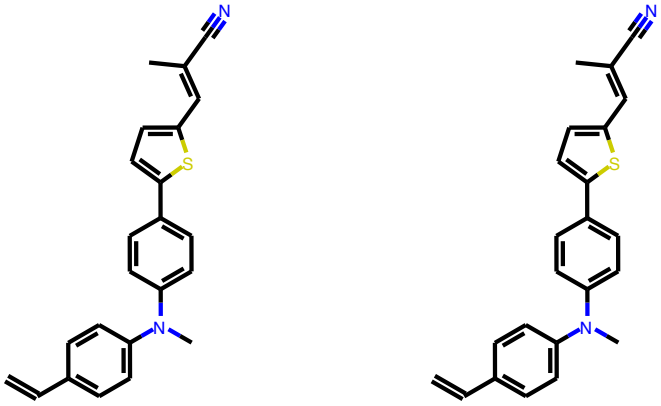
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-7.205321311950684



Molecule CC1=CSC=C1 and its specific config CC1=CS[CH:1]=C1 w/ p=-8.244633674621582



Attaching fragment C of config ['[CH4:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C)C#N)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)



-----Step-16-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=O and its specific config O=[CH2:1] w/ p=-1.1920928244535389e-07

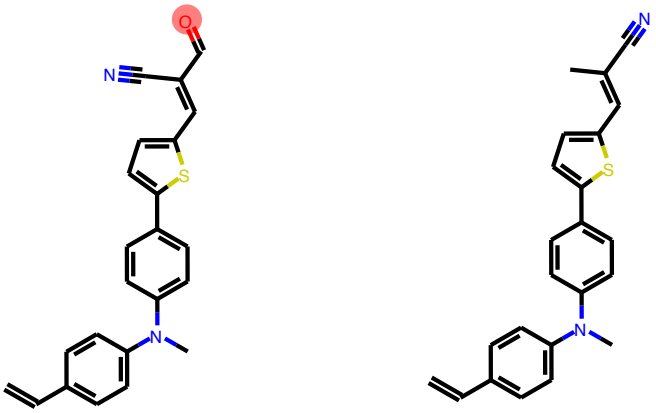
```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-15.93613052368164
```

```
------------------------------------------------------------
Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ p=-17.470401763916
016
```

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-17.63418197631836
```

```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-18.934730529785156
```

```
------------------------------------------------------------
Attaching fragment O=[CH2:1] of config ['O=[CH2:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C#N)C=O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-17-----
Generate next fragment p = 4.2734245125838786e-30
-----Step-18-----
Generate next fragment p = 0.9999843835830688
Top 5 next motifs to attach:
Molecule CO and its specific config O[CH3:1] w/ p=-0.06822425872087479
```

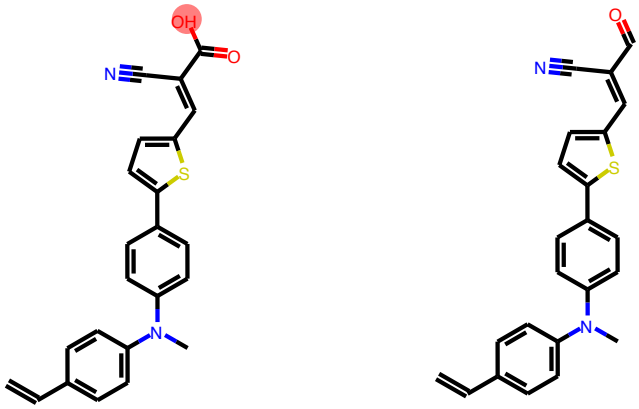
```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-3.1886191368103027
```

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-4.915480613708496
```

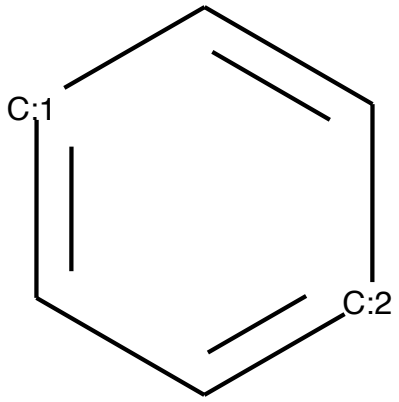
```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-5.206366539001465
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-5.31998348236084
```

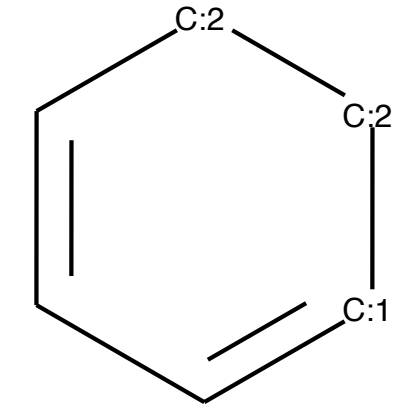
```
------------------------------------------------------------
Attaching fragment O[CH3:1] of config ['O[CH3:1]']
Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```



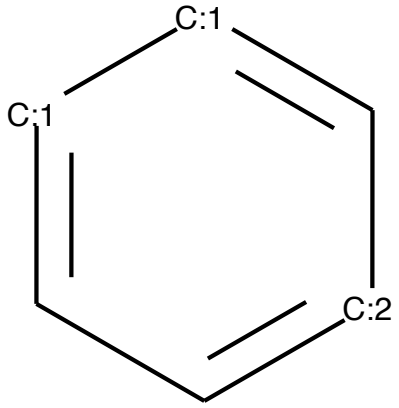
```
------------------------------------------------------------
-----Step-19-----
Generate next fragment p = 3.57101930603676e-06
-----Step-20-----
Generate next fragment p = 2.1999333910116547e-08
-----Step-21-----
Generate next fragment p = 7.065512619419678e-10
-----Step-22-----
Generate next fragment p = 7.199172387117869e-07
-----Step-23-----
Generate next fragment p = 4.2182819737224264e-12
-----Step-24-----
Generate next fragment p = 3.7500499091376507e-16
-----Step-25-----
Generate next fragment p = 0.004641843494027853
-----Step-26-----
Generate next fragment p = 3.592927233024611e-18
-----Step-27-----
Generate next fragment p = 8.48321506055072e-05
-----Step-28-----
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=-0.019
880110397934914
```



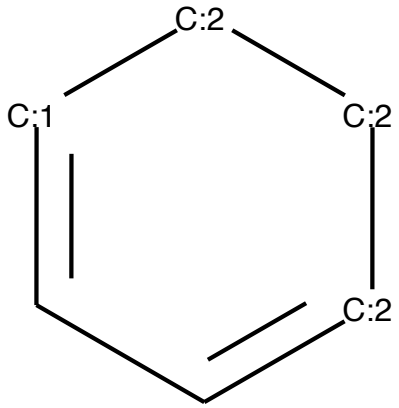

```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=C[CH2:2][CH2:2][CH:1]=C1 w/ p=-
4.1297407150268555
```



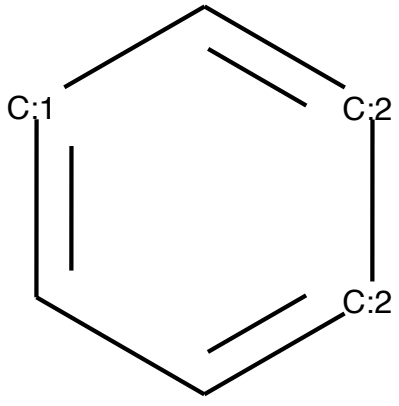
```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ p=-
6.395553112030029
```



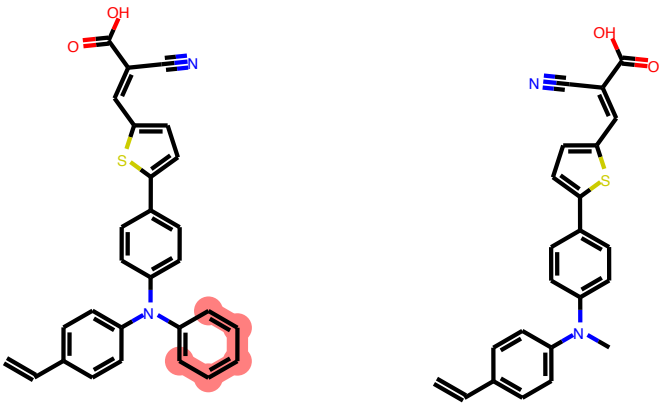

```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-6.8200578689575195
```




```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=[CH:2][CH:2]=C1 w/ p=-
7.765378475189209
```

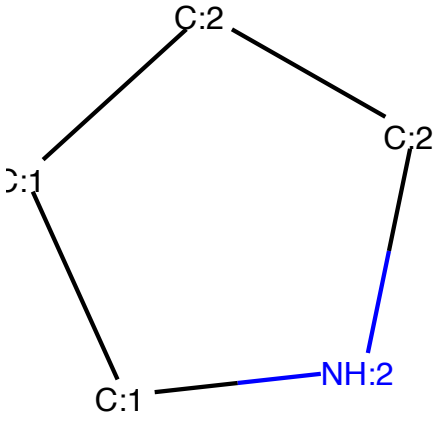



```
------------------------------------------------------------
Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: C=Cc1ccc(N(c2ccccc2)c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)cc2)c
c1
Lastest graph (left) vs graph in last step (right)
```

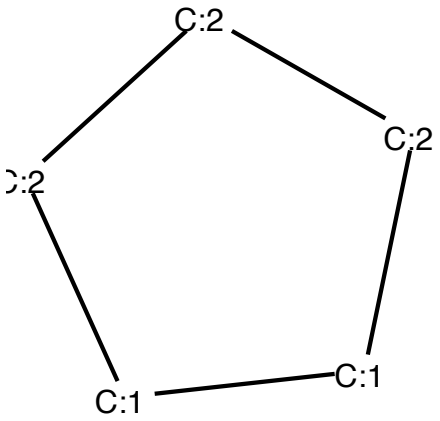



```
------------------------------------------------------------
-----Step-29-----
Generate next fragment p = 0.9999998807907104
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.3503771722316742
```

```
------------------------------------------------------------
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ p=-1.311802625656128
```

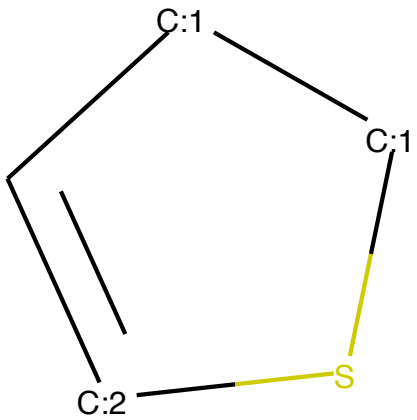



```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1
w/ p=-4.065310478210449
```

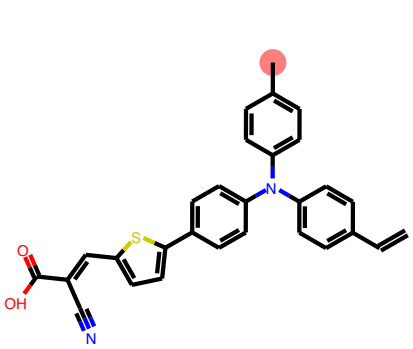


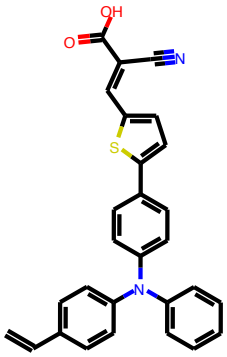

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-5.632542610168457
```

```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-6.00
679349899292
```

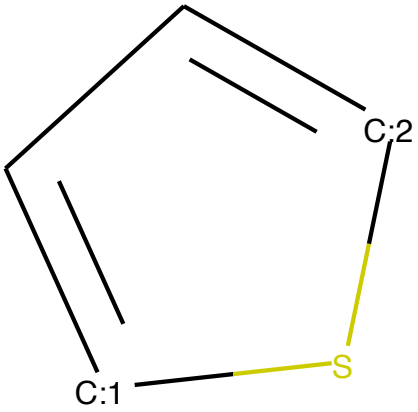



```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(C)cc2)c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)cc
2)cc1
Lastest graph (left) vs graph in last step (right)
```

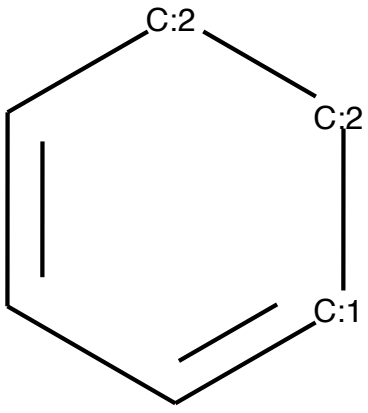




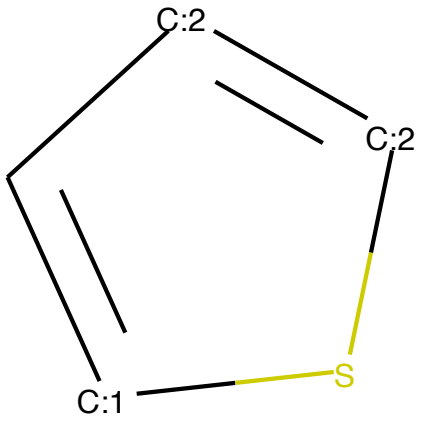

```
------------------------------------------------------------
-----Step-30-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.8655498
623847961
```




```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=C[CH2:2][CH2:2][CH:1]=C1 w/ p=-
0.9156503081321716
```

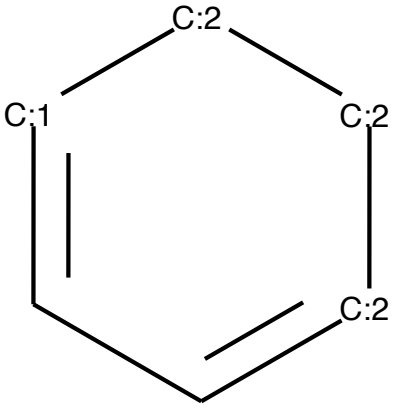



```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-2.59
64910984039307
```

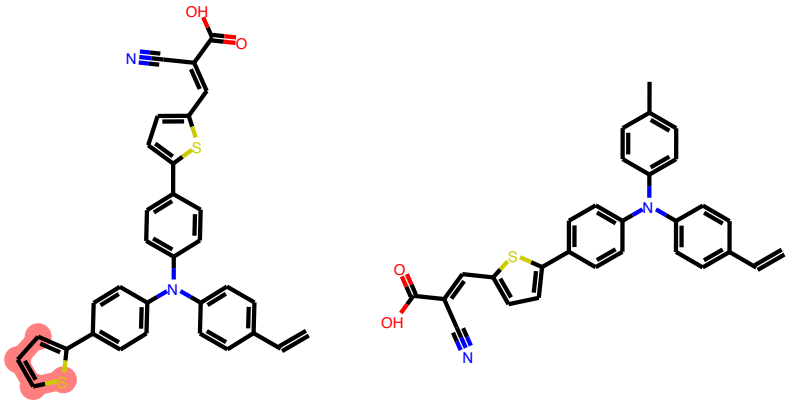



```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-3.4658820629119873
```

```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-4.144192695617676
```

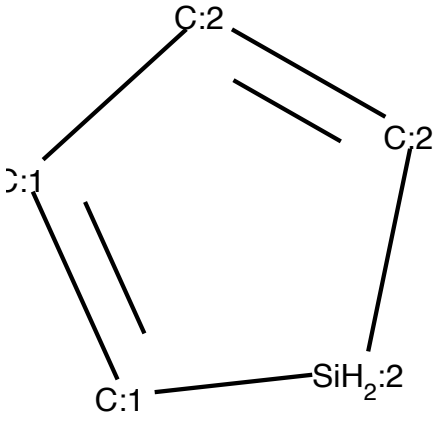



```
------------------------------------------------------------
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3cccs3)cc2)c2ccc(-c3ccc(C=C(C#N)C(=O)
O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```

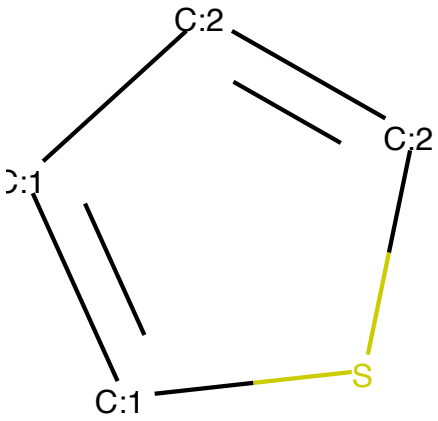



```
------------------------------------------------------------
-----Step-31-----
Generate next fragment p = 0.9997395873069763
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0018436607206240296
```

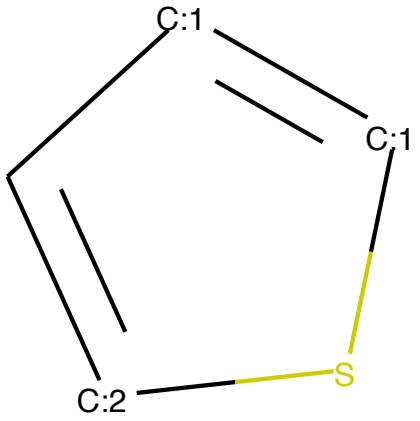
```
------------------------------------------------------------
Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:1][SiH2:2][CH:2]=[
CH:2]1 w/ p=-7.430148601531982
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p=
-7.491175651550293
```

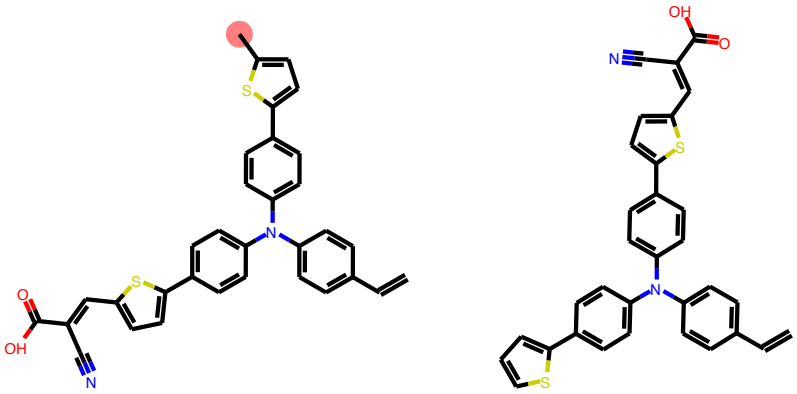



```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-8.09
8220825195312
```



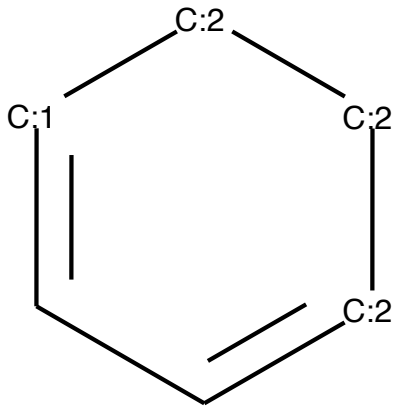

```
------------------------------------------------------------
Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-8.8334293365478
52
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C)s3)cc2)c2ccc(-c3ccc(C=C(C#N)C(
=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```

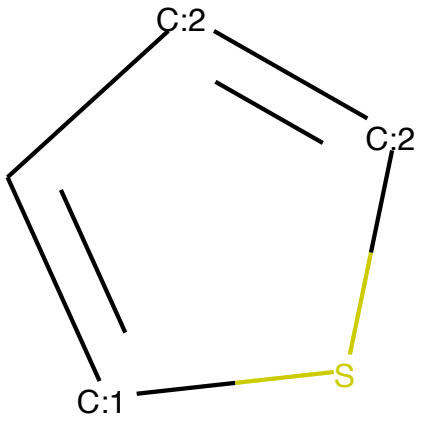


-----Step-32-----
Generate next fragment p = 0.9999994039535522
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-0.00562738487496972
1

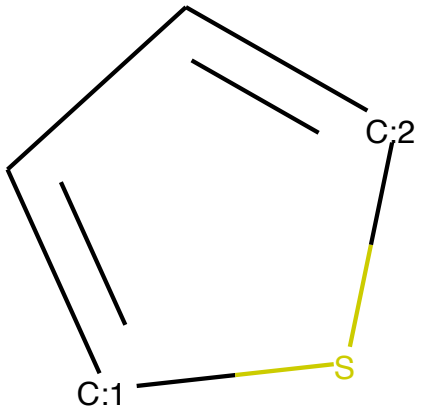
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-5.607522010803223



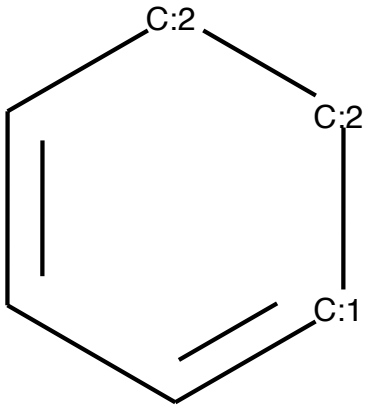
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-7.33
2898139953613



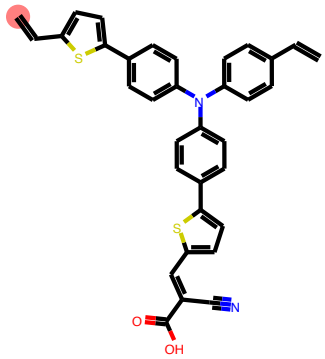
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-7.6666479
11071777

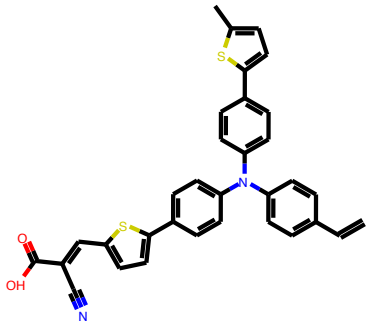


Molecule C1=CCCC=C1 and its specific config C1=C[CH2:2][CH2:2][CH:1]=C1 w/ p=-
7.793932914733887



Attaching fragment [CH2:1]=[CH2:2] of config ['C=[CH2:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C)s3)cc2)c2ccc(-c3ccc(C=C(C#N)
C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)

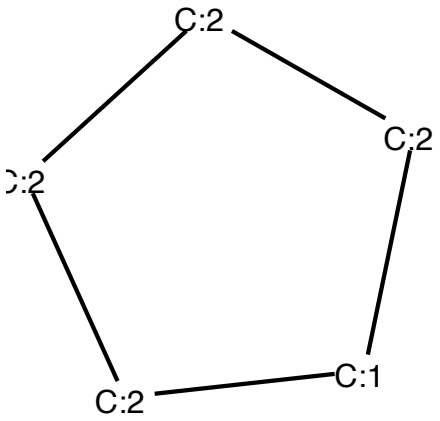




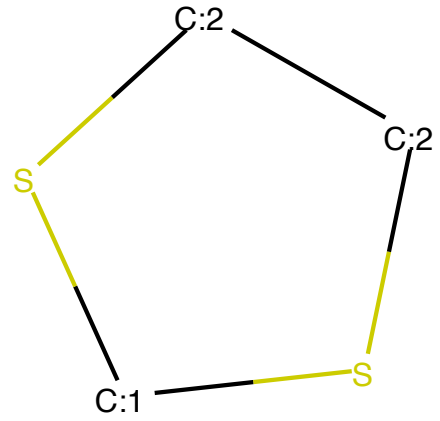
-----Step-33-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.13677558302879333

Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-2.2377471923828125

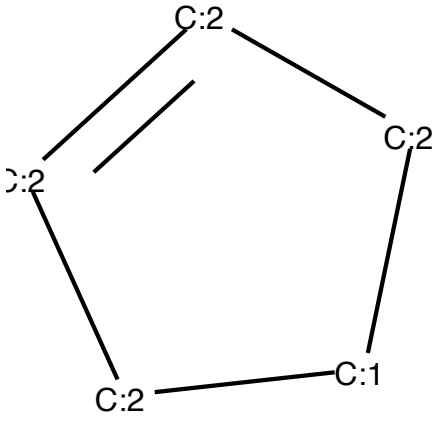
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]1 w/ p=-4.045051574707031



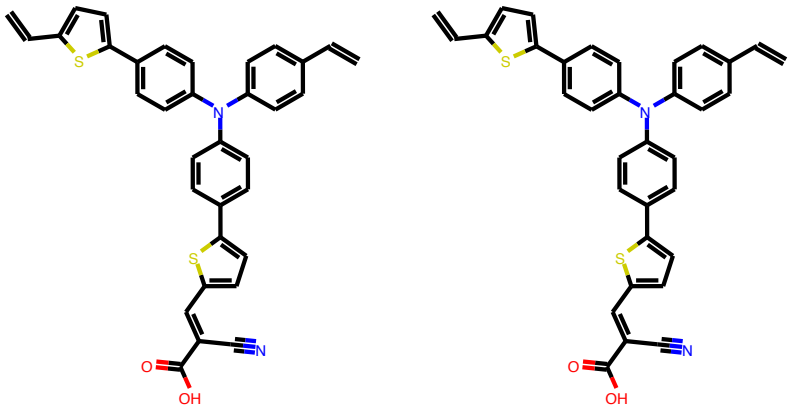

```
------------------------------------------------------------
Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ p=-6.126
567840576172
```




```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:2][CH:2]=[CH:2][CH2:2]1
w/ p=-6.613163948059082
```

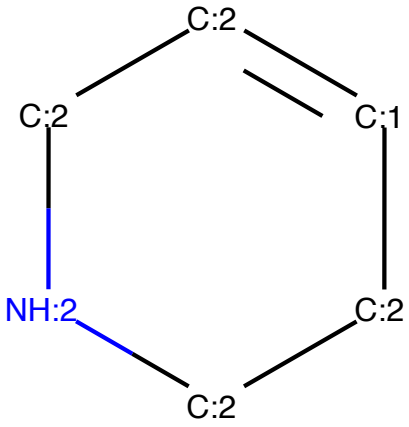



```
------------------------------------------------------------
Attaching fragment C of config ['[CH4:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C)s3)cc2)c2ccc(-c3ccc(C=C(C#N)
C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```



-----Step-34-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-3.576278118089249e-07

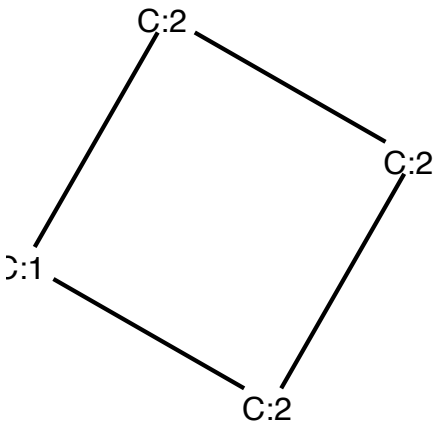
Molecule C1=CCNCC1 and its specific config [CH:1]1=[CH:2][CH2:2][NH:2][CH2:2][
CH2:2]1 w/ p=-15.156386375427246



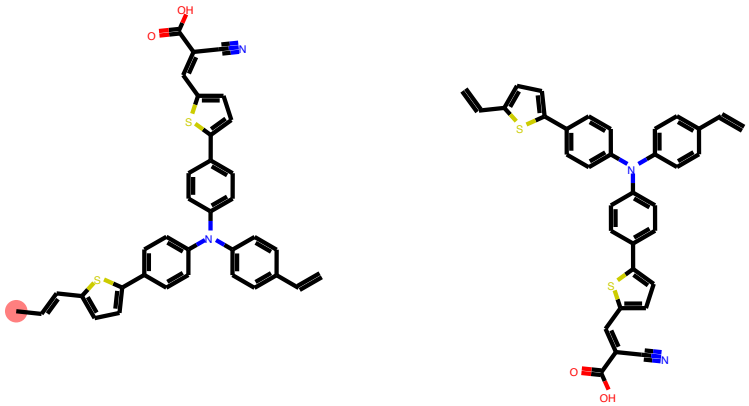
Molecule C=O and its specific config O=[CH2:1] w/ p=-16.070772171020508

```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-17.90203094482422
```

```
------------------------------------------------------------
Molecule C1CCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2]1 w/ p=-2
0.270742416381836
```




```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=CC)s3)cc2)c2ccc(-c3ccc(C=C(C#N
)C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```

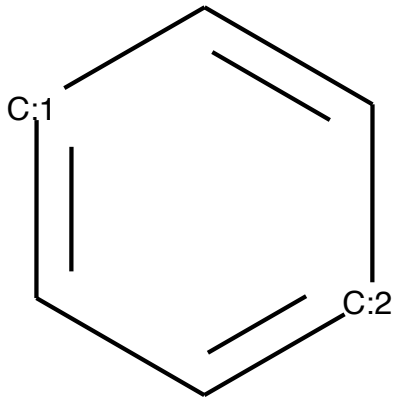


-----Step-35-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C#N and its specific config N#[CH:1] w/ p=-3.933898824470816e-06

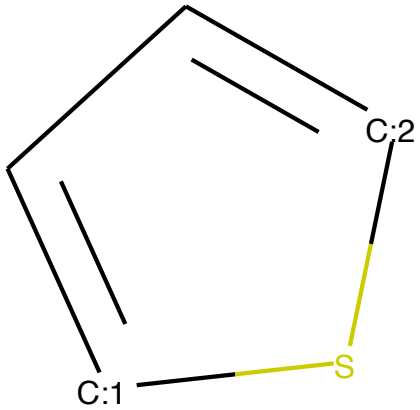
Molecule C and its specific config C w/ p=-13.240961074829102

Molecule C=O and its specific config O=[CH2:1] w/ p=-13.430374145507812

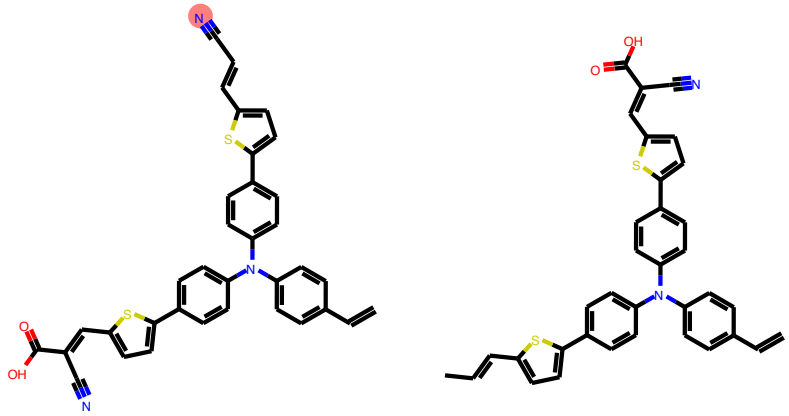
```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-14.62
369441986084
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-15.115761
756896973
```




```
------------------------------------------------------------
Attaching fragment N#[CH:1] of config ['N#[CH:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=CC#N)s3)cc2)c2ccc(-c3ccc(C=C(C
#N)C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-36-----
Generate next fragment p = 1.2988869673185622e-25
-----Step-37-----
Generate next fragment p = 1.3031530065113484e-13
-----Step-38-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=0.0
```

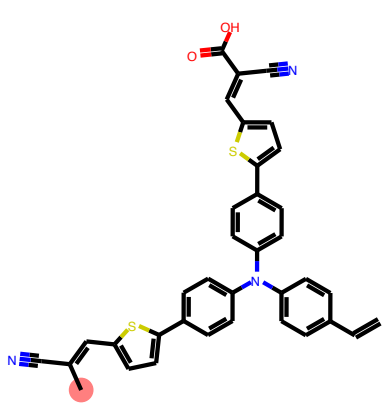
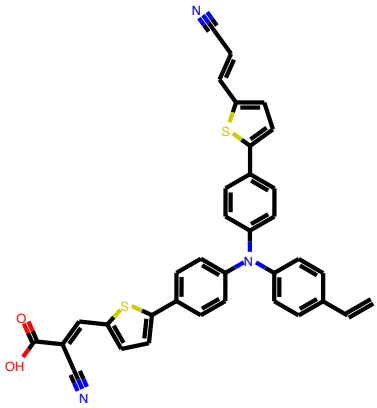
```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-17.414560317993164
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-20.953163146972656
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-21.039793014526367
```

```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-21.32840919494629
```

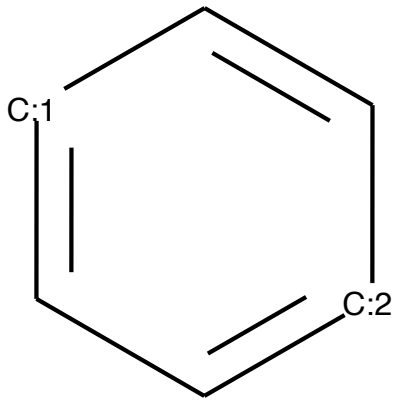
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C(C)C#N)s3)cc2)c2ccc(-c3ccc(C=
C(C#N)C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```

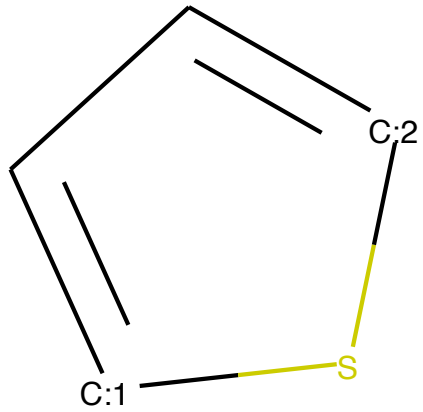
-----Step-39-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.46422889828681946

Molecule C#N and its specific config N#[CH:1] w/ p=-1.0358774662017822

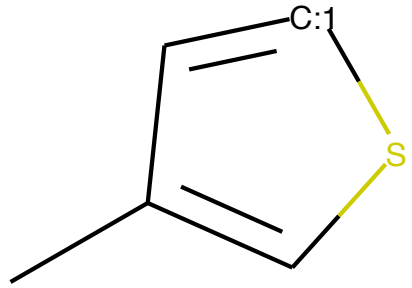
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-4.129965305328369



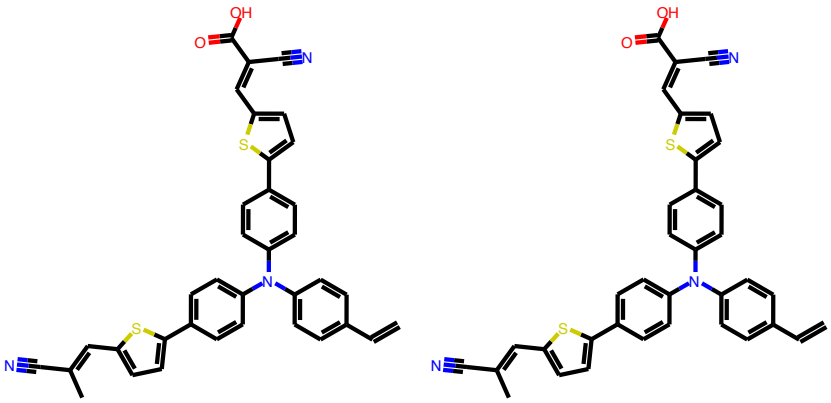
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-8.5757503
50952148



Molecule CC1=CSC=C1 and its specific config CC1=CS[CH:1]=C1 w/ p=-9.5103559494
01855



Attaching fragment C of config ['[CH4:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C(C)C#N)s3)cc2)c2ccc(-c3ccc(C=
C(C#N)C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)



-----Step-40-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=O and its specific config O=[CH2:1] w/ p=-1.1920928244535389e-07

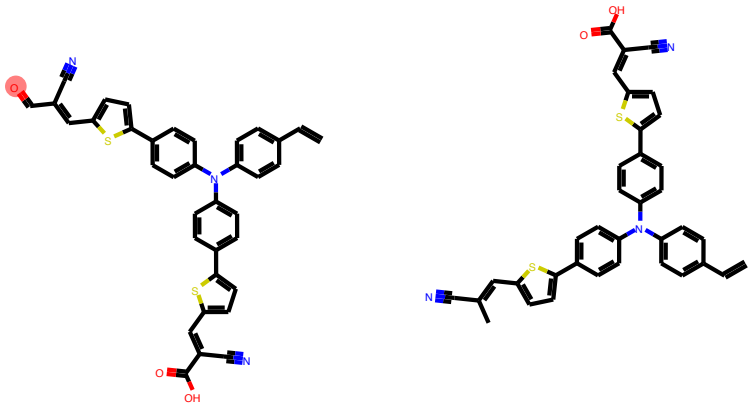
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-16.432518005371094

Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ p=-17.105947494506836

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-18.272764205932617
```

```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-18.63599967956543
```

```
------------------------------------------------------------
Attaching fragment O=[CH2:1] of config ['O=[CH2:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C(C#N)C=O)s3)cc2)c2ccc(-c3ccc(
C=C(C#N)C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```



-----Step-41-----
Generate next fragment p = 5.733921494370255e-21
-----Step-42-----
Generate next fragment p = 0.9999998807907104
Top 5 next motifs to attach:
Molecule CO and its specific config O[CH3:1] w/ p=-0.12501999735832214

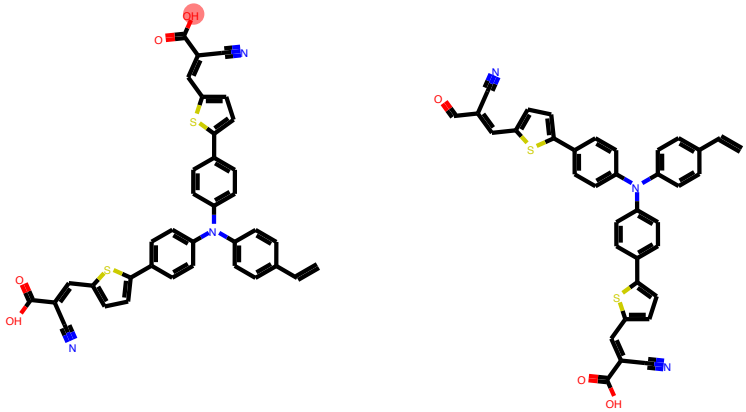
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-2.867701292037964

Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-2.9431989192962646

```
------------------------------------------------------------
Molecule CF and its specific config F[CH3:1] w/ p=-5.9173359870910645
```

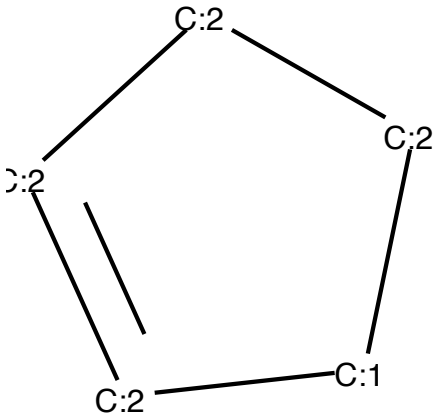
```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-5.969977378845215
```

```
------------------------------------------------------------
Attaching fragment O[CH3:1] of config ['O[CH3:1]']
Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)cc2)c2ccc(-c3c
cc(C=C(C#N)C(=O)O)s3)cc2)cc1
Lastest graph (left) vs graph in last step (right)
```

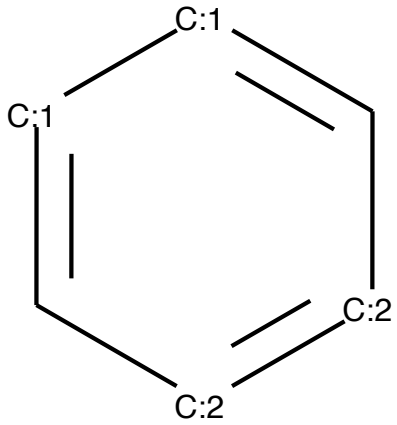


```
------------------------------------------------------------
-----Step-43-----
Generate next fragment p = 0.0005877779331058264
-----Step-44-----
Generate next fragment p = 4.1239500205847435e-06
-----Step-45-----
Generate next fragment p = 4.175789047877743e-09
-----Step-46-----
Generate next fragment p = 1.003355123430083e-07
-----Step-47-----
Generate next fragment p = 1.7379650236321043e-12
-----Step-48-----
Generate next fragment p = 1.6988516306605875e-16
-----Step-49-----
Generate next fragment p = 0.00016118038911372423
-----Step-50-----
Generate next fragment p = 8.228211122309318e-19
-----Step-51-----
Generate next fragment p = 3.517355651183607e-07
-----Step-52-----
Generate next fragment p = 9.966220362338436e-16
-----Step-53-----
Generate next fragment p = 6.167803601186961e-09
-----Step-54-----
Generate next fragment p = 3.2621559669038583e-15
-----Step-55-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-7.390948667307384e-06
```

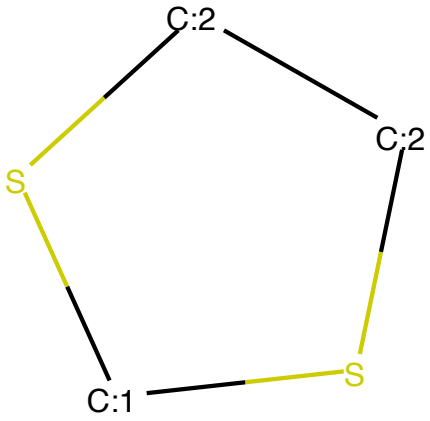
```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH:2]=[CH:2][CH2:2][CH2:2]1
w/ p=-13.064355850219727
```



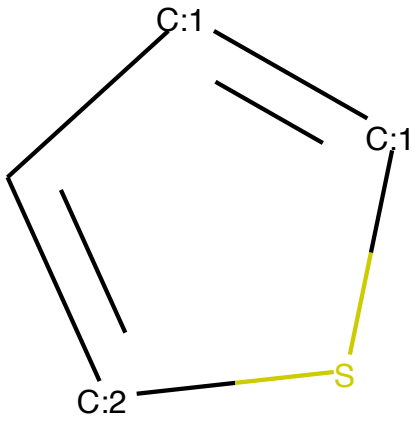

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=[CH:2]1 w
/ p=-13.119878768920898
```



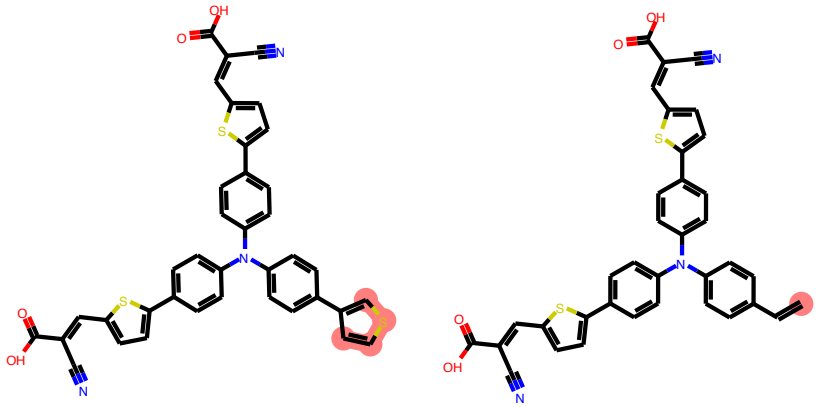

```
------------------------------------------------------------
Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ p=-13.66
5507316589355
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-14.9
61623191833496
```

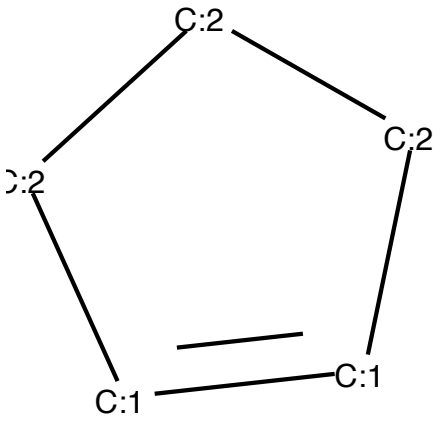


Attaching fragment C1=[CH:2]S[CH:1]=[CH:1]1 of config ['C1:C:S:[CH:1]:C:1', 'C1:C:[CH:1]:C:S:1']
Latest partial graph: N#CC(=Cc1ccc(-c2ccc(N(c3ccc(-c4ccsc4)cc3)c3ccc(-c4ccc(C=C(C#N)C(=O)O)s4)cc3)cc2)s1)C(=O)O
Lastest graph (left) vs graph in last step (right)

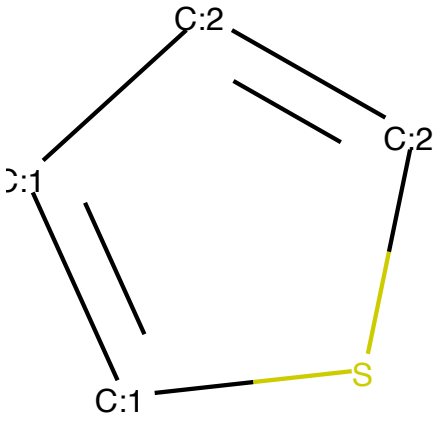


-----Step-56-----
Generate next fragment p = 0.9999998807907104
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.006059726700186729

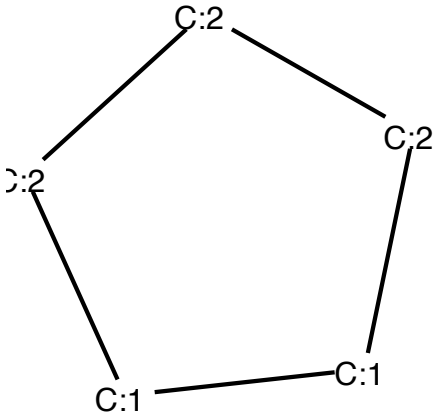
Molecule C1=CCCC1 and its specific config [CH:1]1=[CH:1][CH2:2][CH2:2][CH2:2]1 w/ p=-6.062966346740723



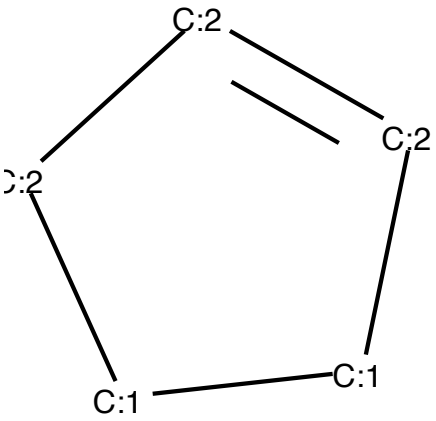
Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p=-7.047158718109131



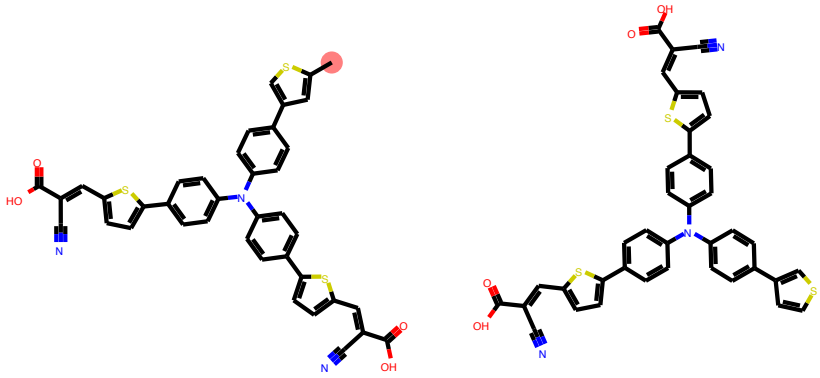
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1 w/ p=-7.105920791625977



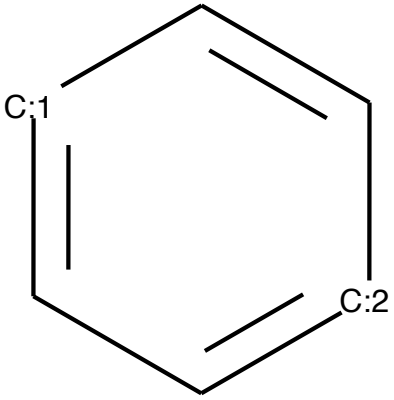
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH:2]=[CH:2]1 w/ p=-7.136292457580566



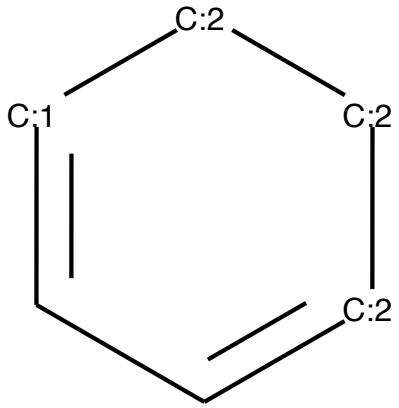

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1cc(-c2ccc(N(c3ccc(-c4ccc(C=C(C#N)C(=O)O)s4)cc3)c3ccc(
-c4ccc(C=C(C#N)C(=O)O)s4)cc3)cc2)cs1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-57-----
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=-0.979
3902635574341
```

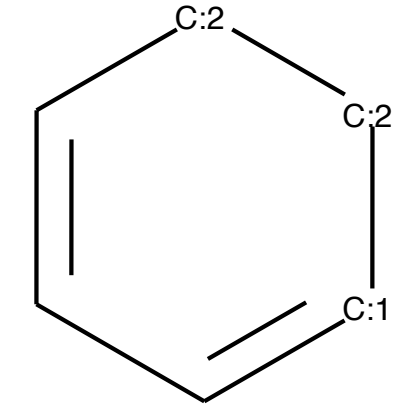



```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-1.162528395652771
```

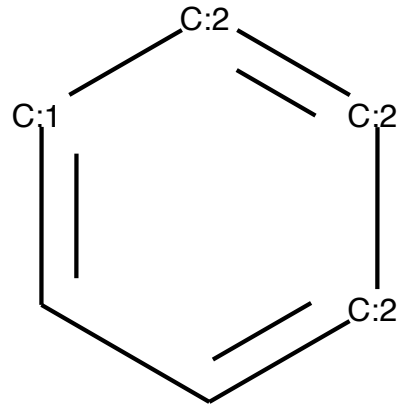



```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-1.3957931995391846
```

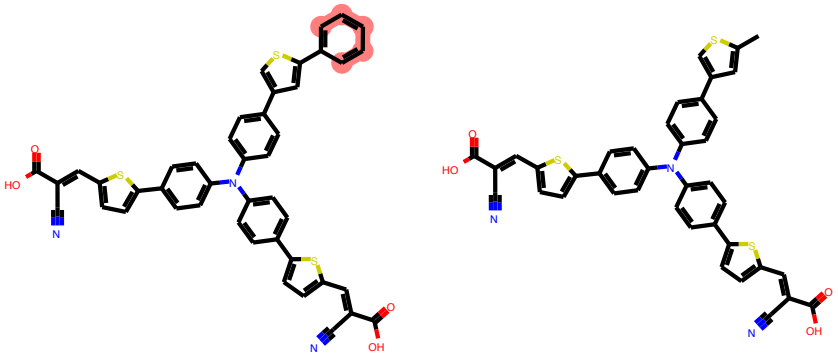
```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=C[CH2:2][CH2:2][CH:1]=C1 w/ p=-
3.6127207279205322
```



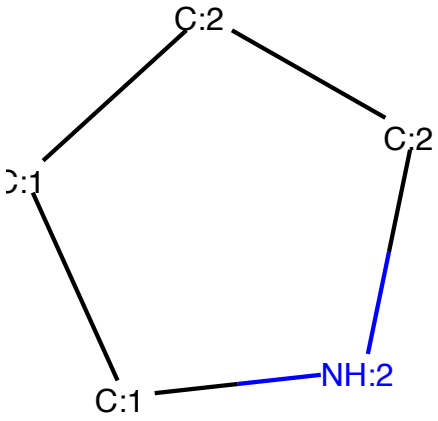

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:2]=[CH:2][CH:2]=C1 w
/ p=-4.562339782714844
```



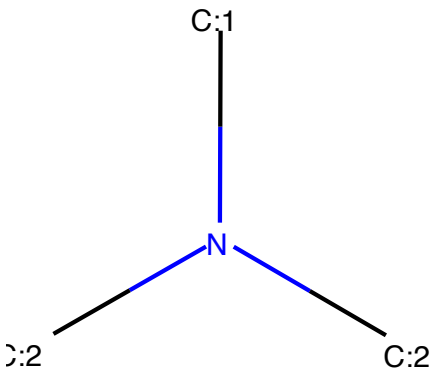

```
------------------------------------------------------------
Attaching fragment C1=[CH:1]C=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1']
Latest partial graph: N#CC(=Cc1ccc(-c2ccc(N(c3ccc(-c4csc(-c5ccccc5)c4)cc3)c3cc
c(-c4ccc(C=C(C#N)C(=O)O)s4)cc3)cc2)s1)C(=O)O
Lastest graph (left) vs graph in last step (right)
```



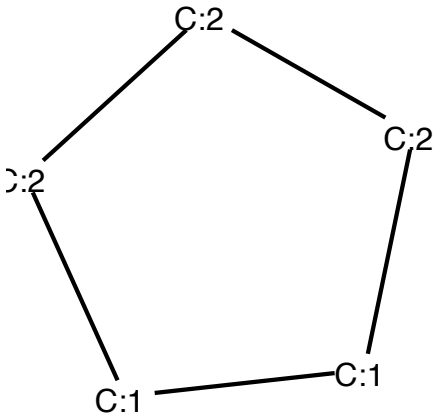
```
------------------------------------------------------------
-----Step-58-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ p=-0.13806338608264923
```



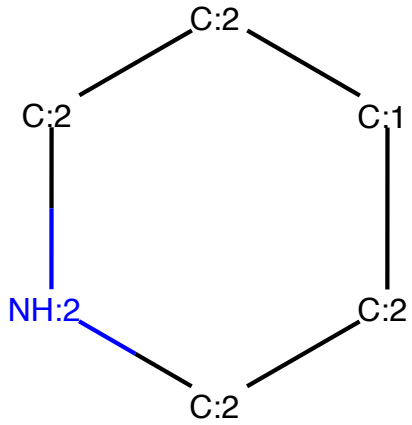

```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-2.325
024366378784
```



Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1 w/ p=-4.258026123046875

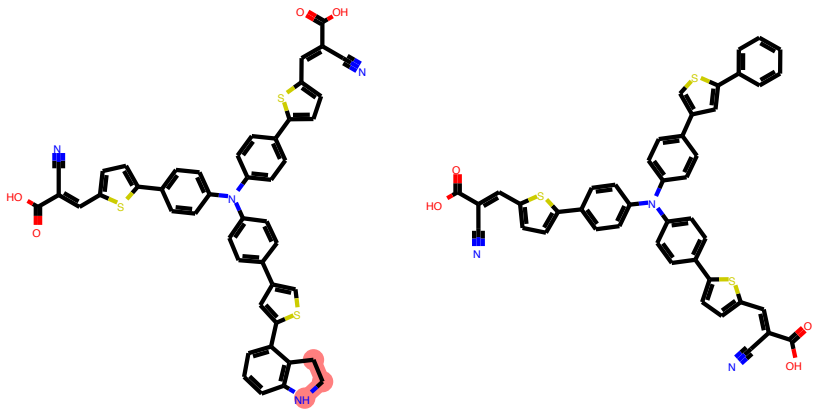


Molecule C1CCNCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2][CH2:2][CH2:2]1 w/ p=-4.540945053100586



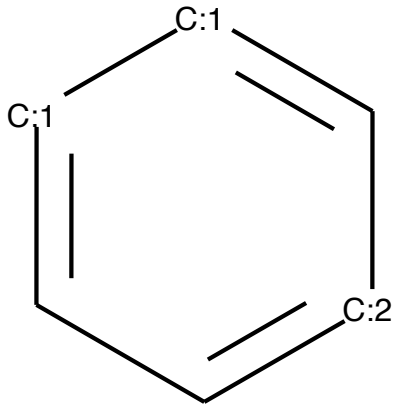
Molecule CBr and its specific config Br[CH3:1] w/ p=-6.290832996368408

```
------------------------------------------------------------
Attaching fragment [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1 of config ['C1C[CH2:1]
CN1', 'C1CN[CH2:1]C1']
Latest partial graph: N#CC(=Cc1ccc(-c2ccc(N(c3ccc(-c4csc(-c5cccc6c5CCN6)c4)cc3
)c3ccc(-c4ccc(C=C(C#N)C(=O)O)s4)cc3)cc2)s1)C(=O)O
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-59-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CN and its specific config C[NH2:1] w/ p=-0.7608727812767029
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ p=-
1.268972396850586
```

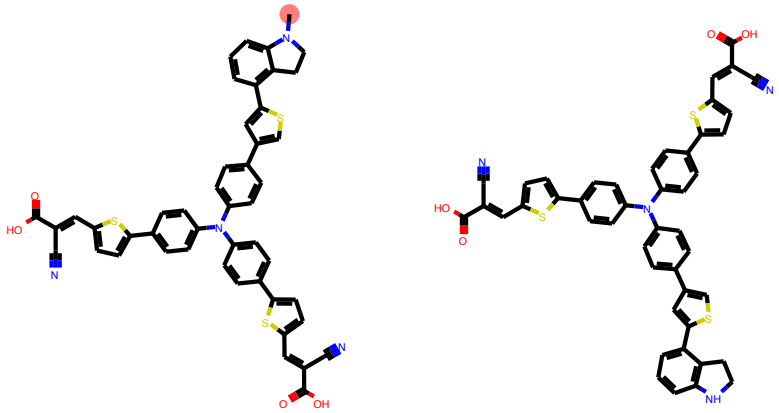



```
------------------------------------------------------------
Molecule N and its specific config N w/ p=-1.4923498630523682
```

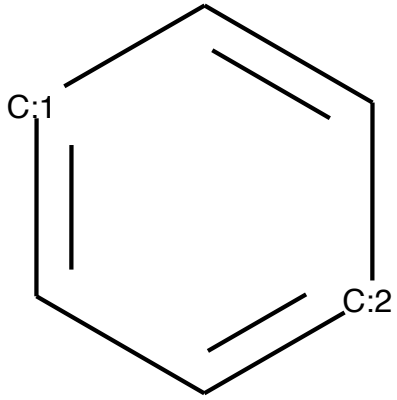
```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-4.306382179260254
```

```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-4.552807331085205
```

```
------------------------------------------------------------
Attaching fragment C[NH2:1] of config ['C[NH2:1]']
Latest partial graph: CN1CCc2c(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)c
c5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)cccc21
Lastest graph (left) vs graph in last step (right)
```



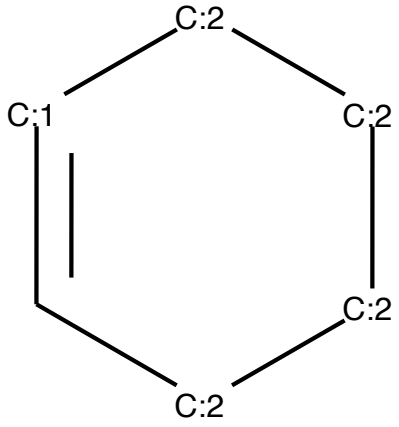
```
------------------------------------------------------------
-----Step-60-----
Generate next fragment p = 0.767174482345581
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.094
02607381343842
```



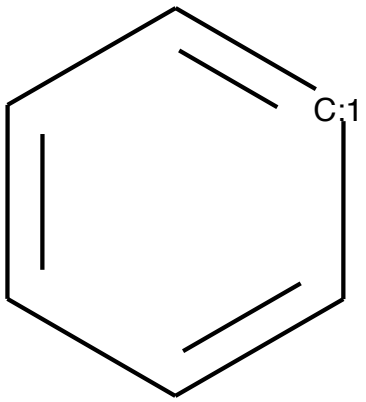

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-2.441336154937744
```

```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-6.683434963226318
```

```
------------------------------------------------------------
Molecule C1=CCCCC1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH2:2][CH2:
2]1 w/ p=-7.410592079162598
```

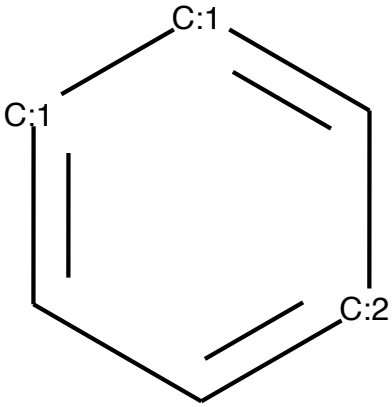



```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=CC=[CH:1]C=C1 w/ p=-7.66150808
3343506
```




```
------------------------------------------------------------
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-61-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CN and its specific config C[NH2:1] w/ p=-0.7608727812767029
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ p=-
1.268972396850586
```

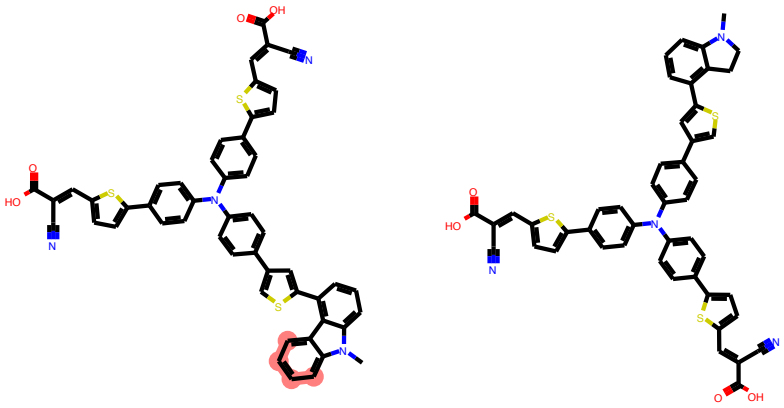



```
------------------------------------------------------------
Molecule N and its specific config N w/ p=-1.4923498630523682
```

```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-4.306382179260254
```

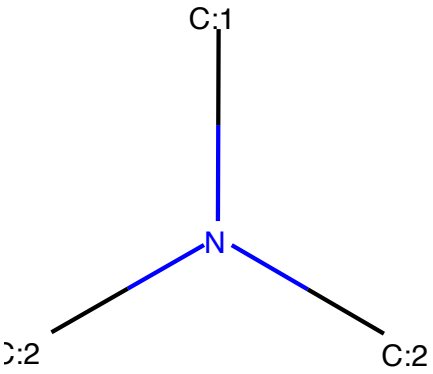
```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-4.552807331085205
```

```
------------------------------------------------------------
Attaching fragment C1=[CH:1][CH:1]=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1'
, 'C1:C:C:[CH:1]:C:C:1']
Latest partial graph: Cn1c2ccccc2c2c(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#N)C(=O)
O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)cccc21
Lastest graph (left) vs graph in last step (right)
```



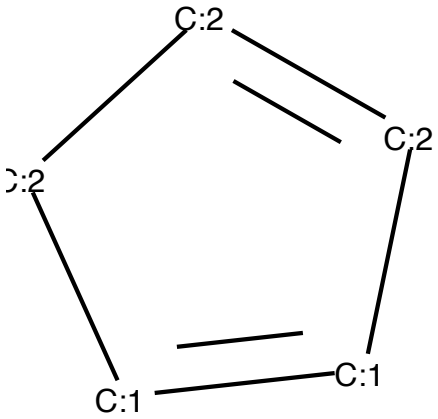
-----Step-62-----
Generate next fragment p = 0.9999222755432129
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.2408195436000824

Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-1.597
2133874893188

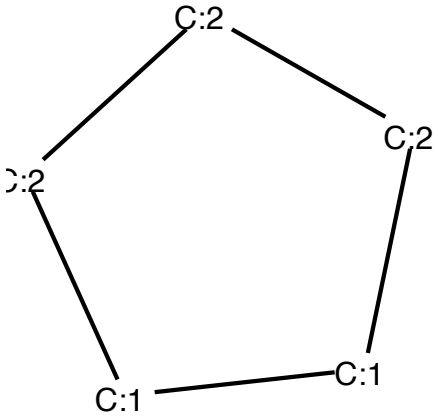


Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-5.819917678833008

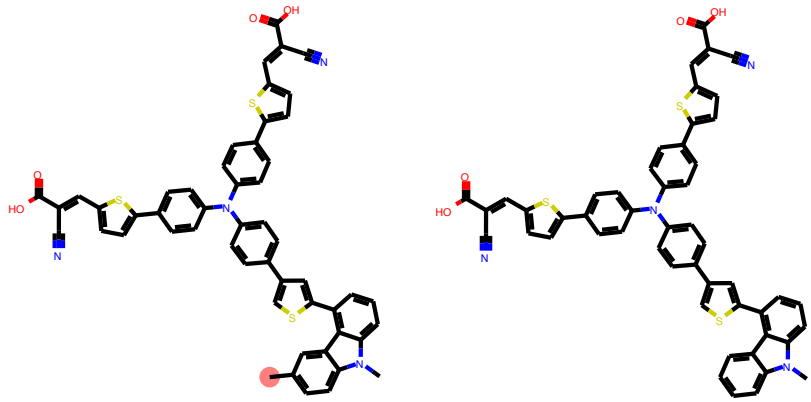
```
------------------------------------------------------------
Molecule C1=CCC=C1 and its specific config [CH:1]1=[CH:1][CH2:2][CH:2]=[CH:2]1
w/ p=-6.302859783172607
```




```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1
w/ p=-6.495670795440674
```

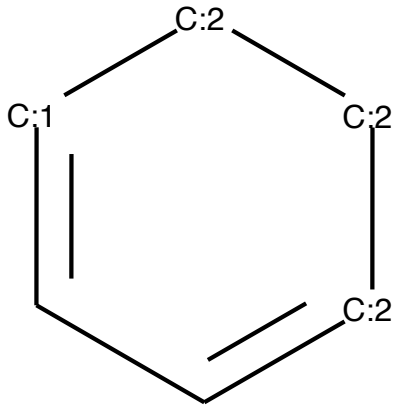



```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc2c(c1)c1c(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#N)C(=O
)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)cccc1n2C
Lastest graph (left) vs graph in last step (right)
```

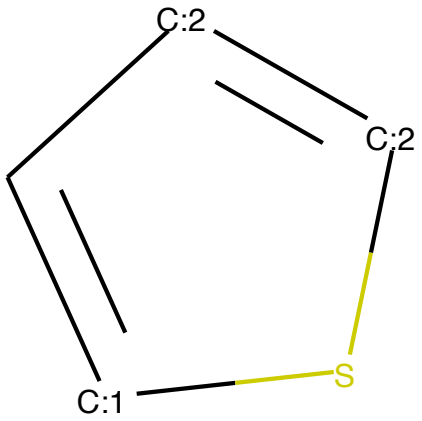


-----Step-63-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-1.1266475915908813

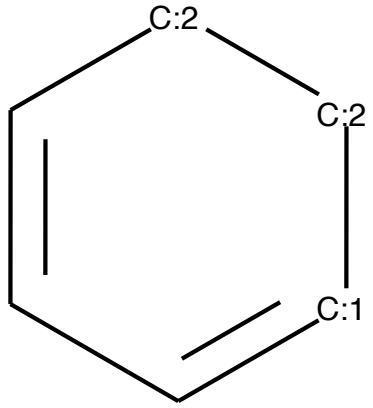
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-1.7038252353668213



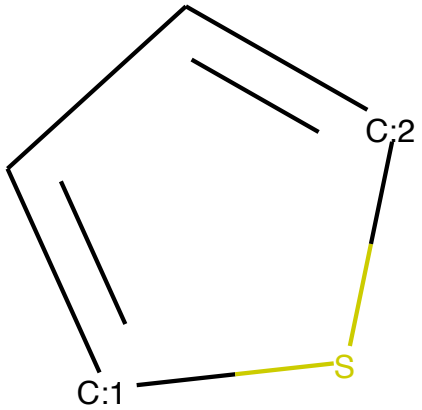
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-1.74
80614185333252



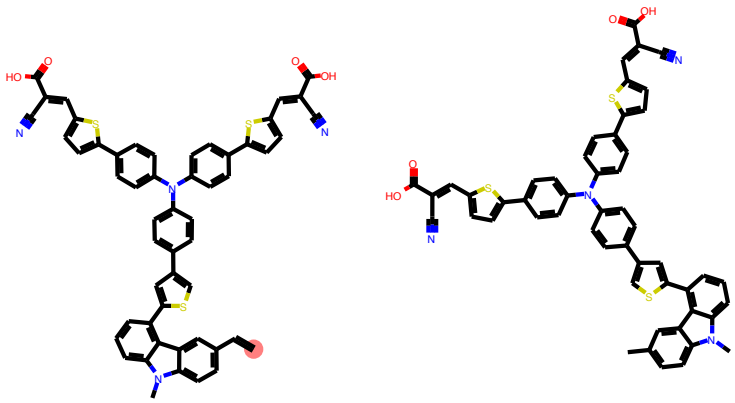
Molecule C1=CCCC=C1 and its specific config C1=C[CH2:2][CH2:2][CH:1]=C1 w/ p=-1.7600538730621338



Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-2.240104913711548



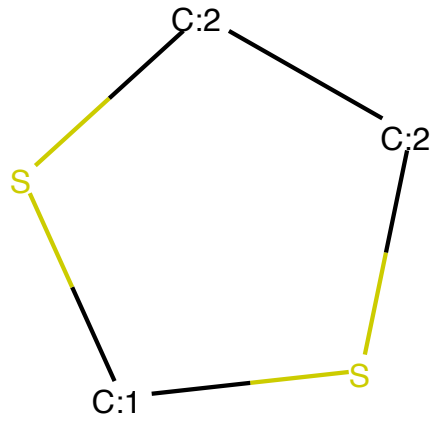
Attaching fragment [CH2:1]=[CH2:2] of config ['C=[CH2:1]']
Latest partial graph: C=Cc1ccc2c(c1)c1c(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)cccc1n2C
Lastest graph (left) vs graph in last step (right)



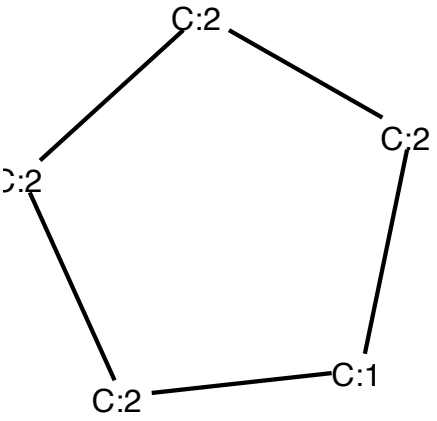
-----Step-64-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.5033437609672546

Molecule C and its specific config C w/ p=-1.5061886310577393

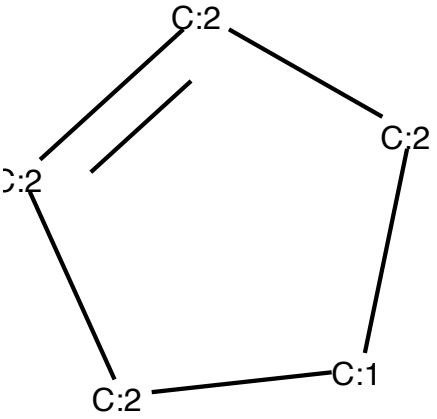
Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ p=-2.095
09015083313



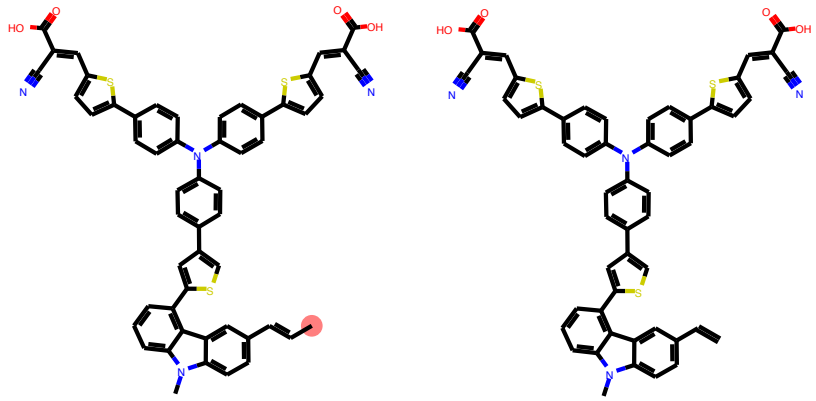
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]1
w/ p=-3.5078327655792236



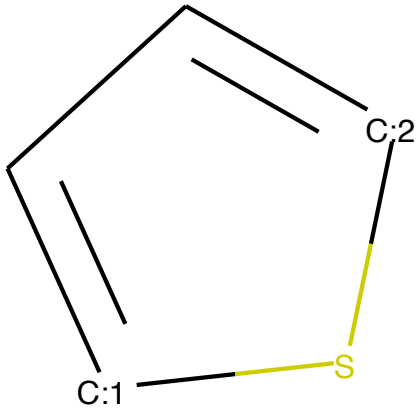
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:2][CH:2]=[CH:2][CH2:2]1
w/ p=-3.912304639816284



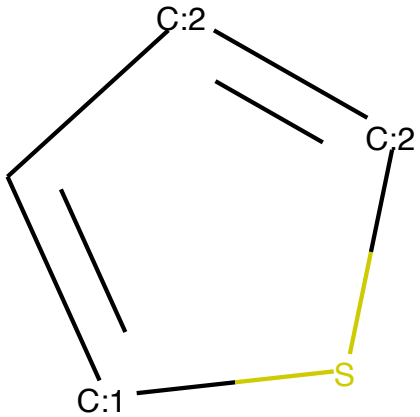
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC=Cc1ccc2c(c1)c1c(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#N)C
(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)cccc1n2C
Lastest graph (left) vs graph in last step (right)



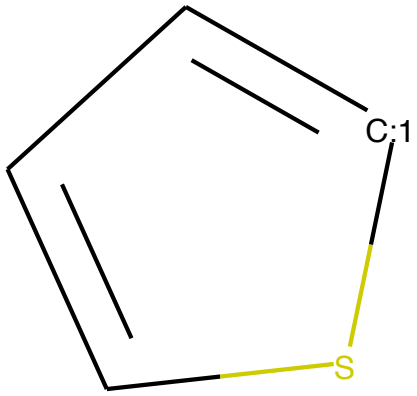
-----Step-65-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.1306476891040802



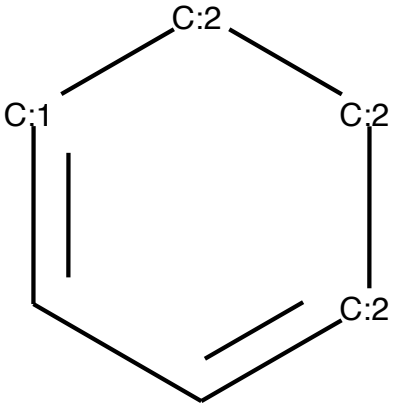
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-2.9443016052246094



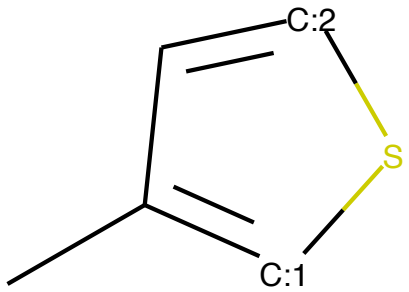
Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ p=-3.4541702270507812



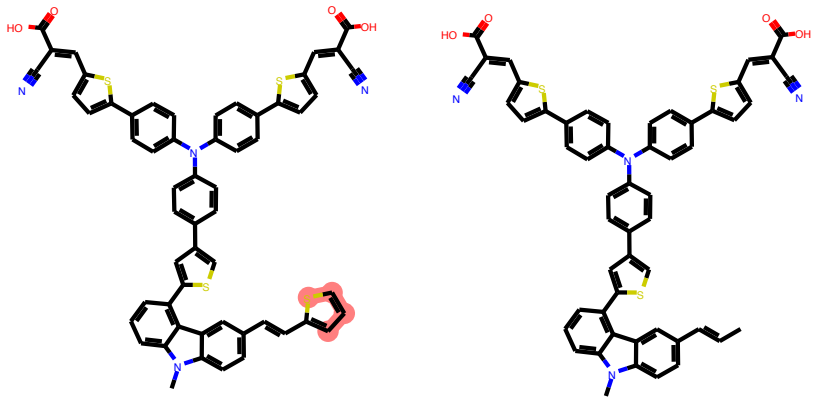
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-3.6914918422698975



Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ p=-4.74936
9144439697

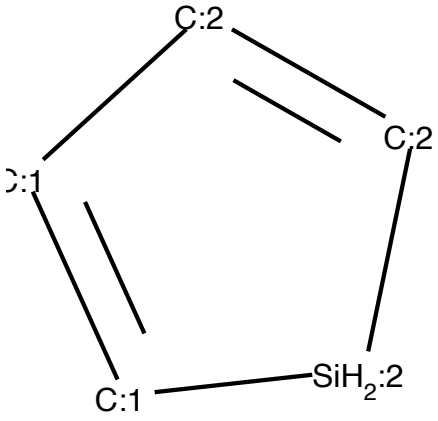


Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: Cn1c2ccc(C=Cc3cccs3)cc2c2c(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C
=C(C#N)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)cccc21
Lastest graph (left) vs graph in last step (right)



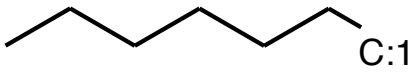
-----Step-66-----
Generate next fragment p = 0.871691882610321
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.06206965819001198

Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:1][SiH2:2][CH:2]=[CH:2]1 w/ p=-3.3673901557922363

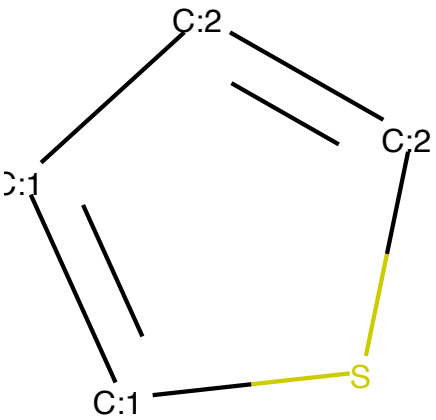


Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-4.4592947959899

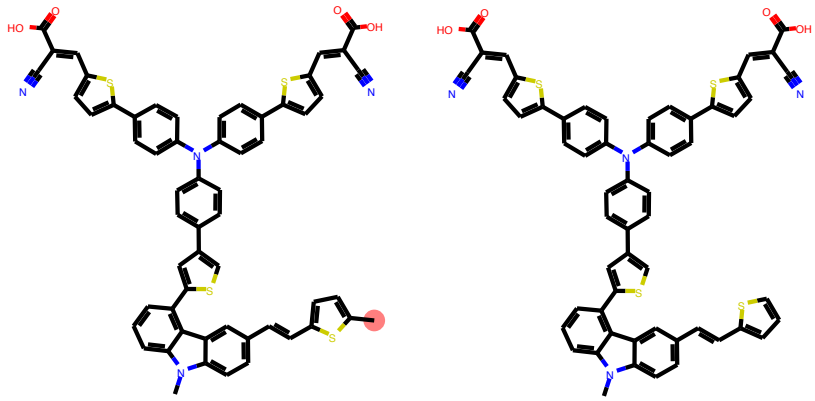
```
------------------------------------------------------------
Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ p=-4.933238506317139
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p=
-5.725491046905518
```

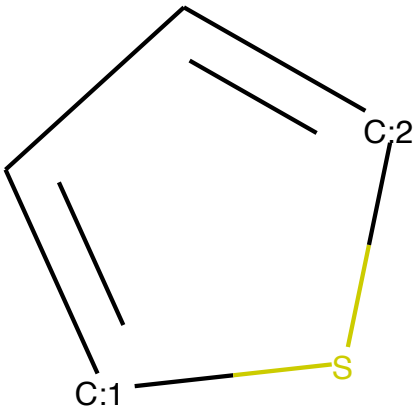



```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(C=Cc2ccc3c(c2)c2c(-c4cc(-c5ccc(N(c6ccc(-c7ccc(C=C
(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)cccc2n3C)s1
Lastest graph (left) vs graph in last step (right)
```

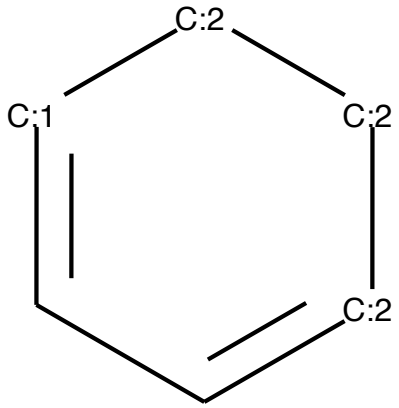


-----Step-67-----
Generate next fragment p = 0.9999935626983643
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-0.05087331682443619

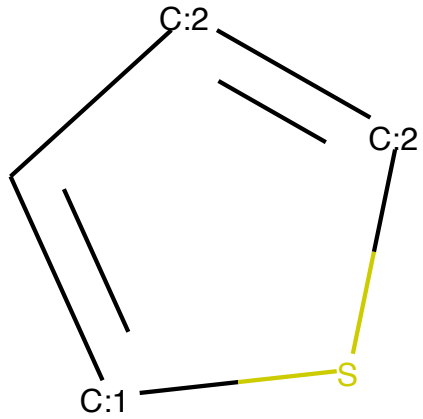
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-3.4192779
064178467



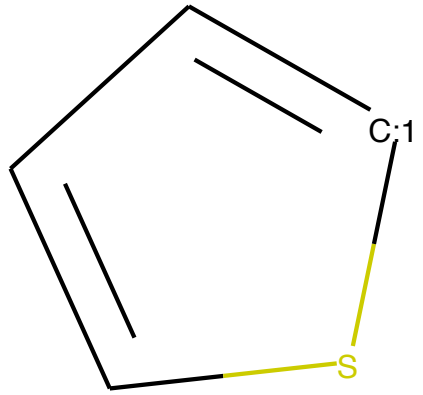
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-5.058685779571533



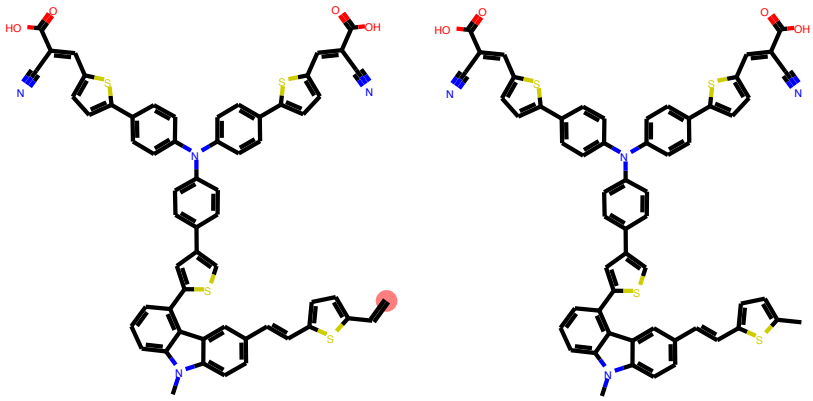
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-5.07
9668045043945



Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ p=-6.652697563171
387



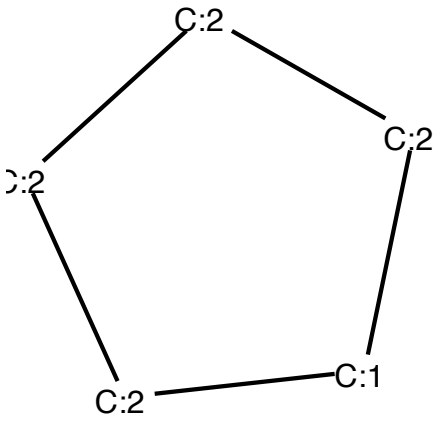
Attaching fragment [CH2:1]=[CH2:2] of config ['C=[CH2:1]']
Latest partial graph: C=Cc1ccc(C=Cc2ccc3c(c2)c2c(-c4cc(-c5ccc(N(c6ccc(-c7ccc(C
=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)cccc2n3C)s1
Lastest graph (left) vs graph in last step (right)



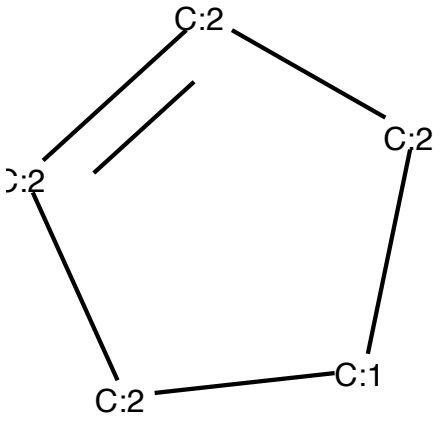
-----Step-68-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.008251977153122425

Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-4.8112382888793945

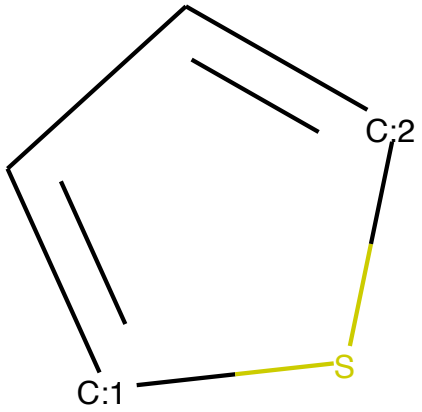
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]1 w/ p=-9.474623680114746



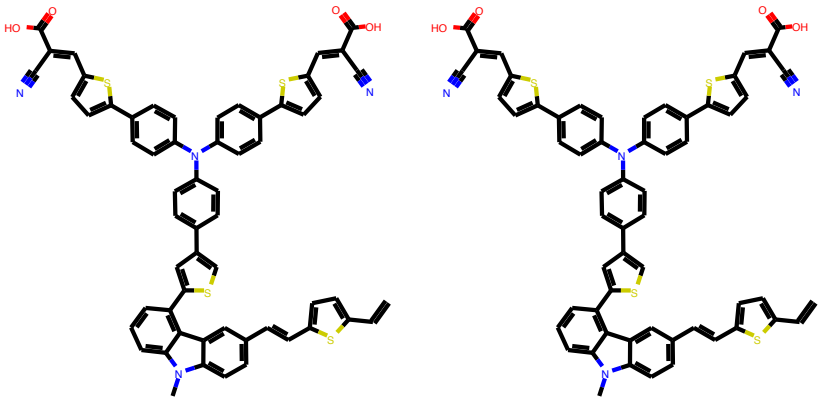

```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:2][CH:2]=[CH:2][CH2:2]1
w/ p=-13.712762832641602
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-14.705827
713012695
```




```
------------------------------------------------------------
Attaching fragment C of config ['[CH4:1]']
Latest partial graph: C=Cc1ccc(C=Cc2ccc3c(c2)c2c(-c4cc(-c5ccc(N(c6ccc(-c7ccc(C
=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)cccc2n3C)s1
Lastest graph (left) vs graph in last step (right)
```

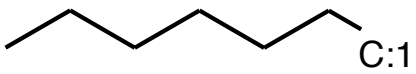


-----Step-69-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.722029527532868e-06

Molecule C=O and its specific config O=[CH2:1] w/ p=-12.142008781433105

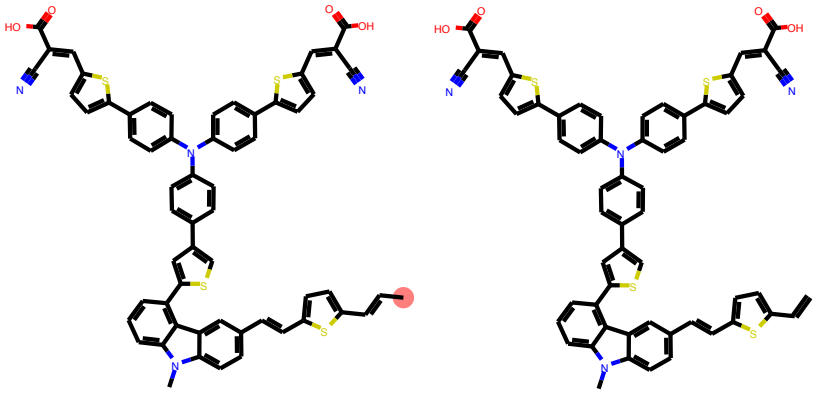
Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-16.139099121093
75

```
------------------------------------------------------------
Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ p=-16.46016502380371
```



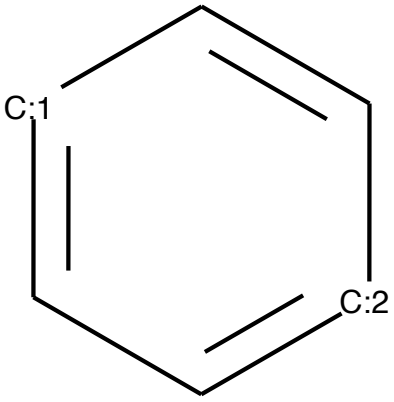

```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-16.62950325012207
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC=Cc1ccc(C=Cc2ccc3c(c2)c2c(-c4cc(-c5ccc(N(c6ccc(-c7ccc(
C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)cccc2n3C)s1
Lastest graph (left) vs graph in last step (right)
```



-----Step-70-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C#N and its specific config N#[CH:1] w/ p=-0.00012432756193447858

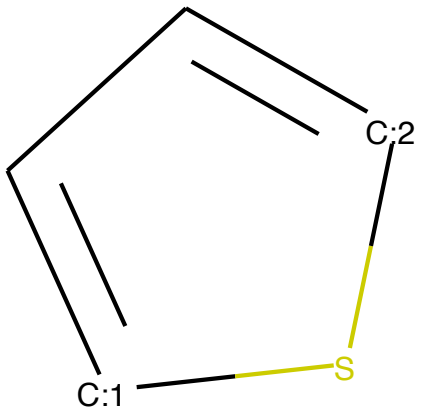
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-9.358192443847656



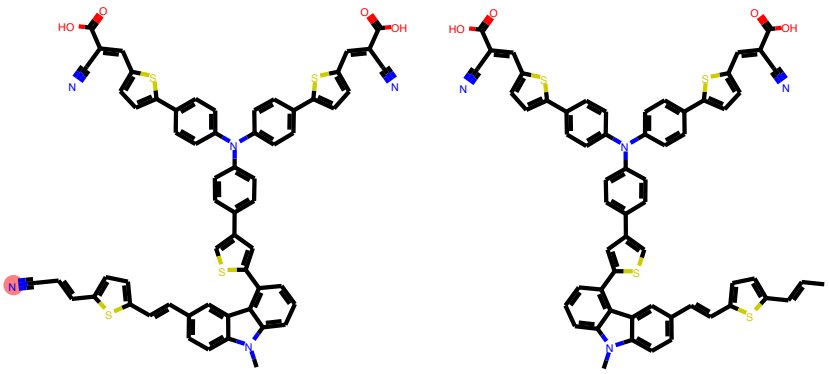
Molecule C and its specific config C w/ p=-10.463768005371094

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-11.708535194396973
```

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-13.973919
868469238
```




```
------------------------------------------------------------
Attaching fragment N#[CH:1] of config ['N#[CH:1]']
Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=CC#N)s3)cc2c2c(-c3cc(-c4ccc(N(c5ccc(
-c6ccc(C=C(C#N)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)cccc21
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-71-----
Generate next fragment p = 1.2375428747618282e-21
-----Step-72-----
Generate next fragment p = 1.074212333668223e-13
-----Step-73-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.6689286894688848e-0
6
```

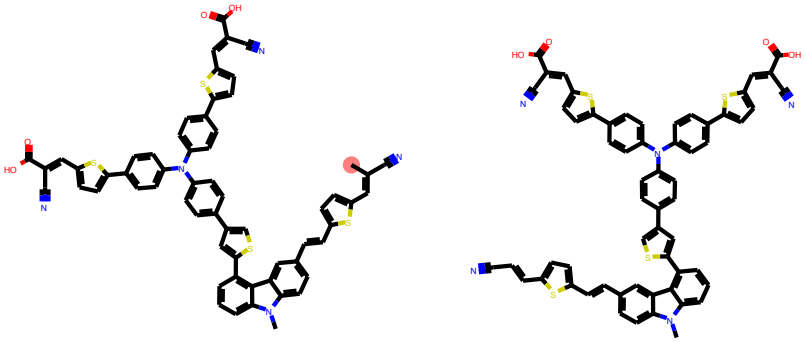
```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-14.100028991699219
```

```
------------------------------------------------------------
Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ p=-14.389986038208
008
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-14.865312576293945
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-17.095169067382812
```

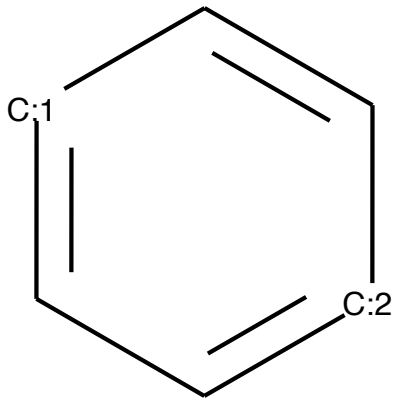
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC(C#N)=Cc1ccc(C=Cc2ccc3c(c2)c2c(-c4cc(-c5ccc(N(c6ccc(-c
7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)cccc2n3C
)s1
Lastest graph (left) vs graph in last step (right)
```



-----Step-74-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.33791378140449524

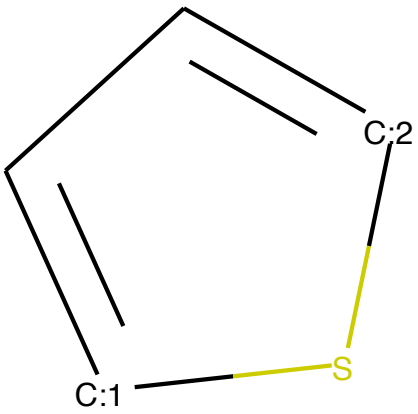
Molecule C#N and its specific config N#[CH:1] w/ p=-1.2967579364776611

Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-4.329936504364014

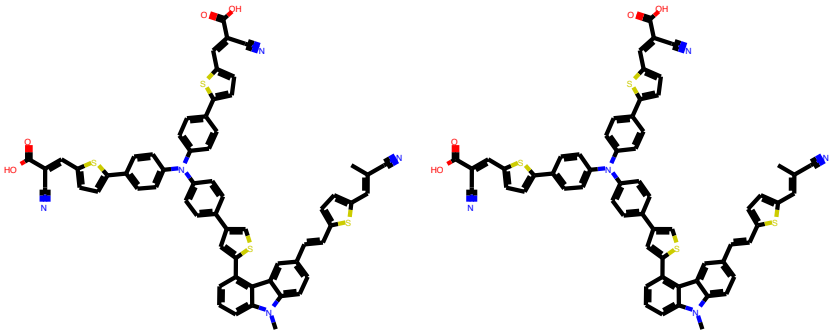



```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-9.103432655334473
```

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-10.106388
092041016
```




```
------------------------------------------------------------
Attaching fragment C of config ['[CH4:1]']
Latest partial graph: CC(C#N)=Cc1ccc(C=Cc2ccc3c(c2)c2c(-c4cc(-c5ccc(N(c6ccc(-c
7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)cccc2n3C
)s1
Lastest graph (left) vs graph in last step (right)
```



-----Step-75-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=O and its specific config O=[CH2:1] w/ p=-1.1920928244535389e-07

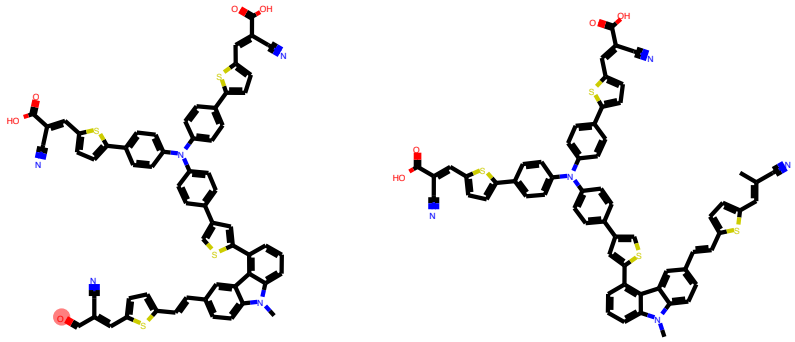
Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ p=-16.645597457885742

Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-17.349523544311523

```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-18.376365661621094
```

```
------------------------------------------------------------
Molecule CO and its specific config O[CH3:1] w/ p=-18.986194610595703
```

```
------------------------------------------------------------
Attaching fragment O=[CH2:1] of config ['O=[CH2:1]']
Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=C(C#N)C=O)s3)cc2c2c(-c3cc(-c4ccc(N(c
5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)c
ccc21
Lastest graph (left) vs graph in last step (right)
```

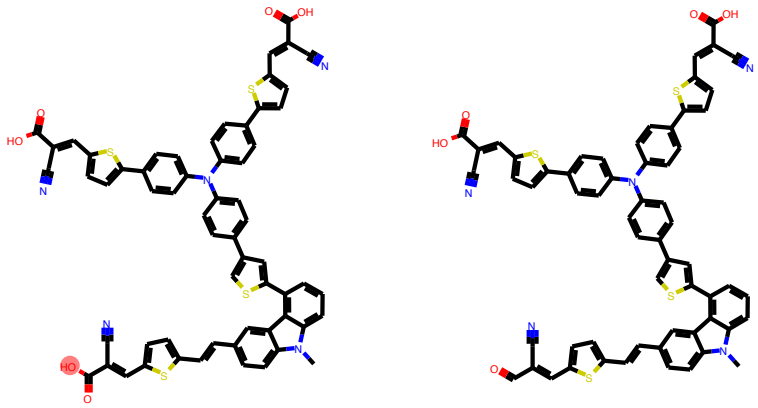


```
------------------------------------------------------------
-----Step-76-----
Generate next fragment p = 4.98099528597485e-21
-----Step-77-----
Generate next fragment p = 0.9999995231628418
Top 5 next motifs to attach:
Molecule CO and its specific config O[CH3:1] w/ p=-0.009655111469328403

------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-5.474306583404541

------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.6051836013793945
```

```
------------------------------------------------------------
Molecule CO and its specific config [CH3:1][OH:2] w/ p=-7.083941459655762
```

```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-7.425041198730469
```

```
------------------------------------------------------------
Attaching fragment O[CH3:1] of config ['O[CH3:1]']
Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=C(C#N)C(=O)O)s3)cc2c2c(-c3cc(-c4ccc(
N(c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs
3)cccc21
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-78-----
Generate next fragment p = 0.011908629909157753
-----Step-79-----
Generate next fragment p = 4.349339022269305e-08
-----Step-80-----
Generate next fragment p = 1.575442547618877e-05
-----Step-81-----
Generate next fragment p = 2.9677555968277147e-09
-----Step-82-----
Generate next fragment p = 1.1139944388228063e-15
-----Step-83-----
Generate next fragment p = 2.546456490590407e-17
-----Step-84-----
Generate next fragment p = 3.1717577257950325e-06
-----Step-85-----
Generate next fragment p = 6.617580609743468e-20
-----Step-86-----
Generate next fragment p = 2.0310472054196893e-11
-----Step-87-----
Generate next fragment p = 1.663748432588825e-19
-----Step-88-----
Generate next fragment p = 2.262406262332206e-08
-----Step-89-----
Generate next fragment p = 0.9998952150344849
Top 5 next motifs to attach:
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-0.023700183257460594
```

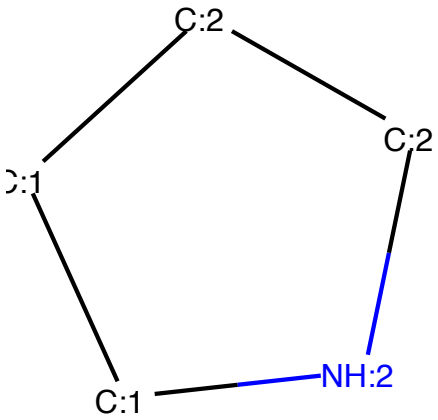
```
------------------------------------------------------------
Molecule CN and its specific config C[NH2:1] w/ p=-3.787357807159424
```

```
------------------------------------------------------------
Molecule N and its specific config N w/ p=-7.8594231605529785
```

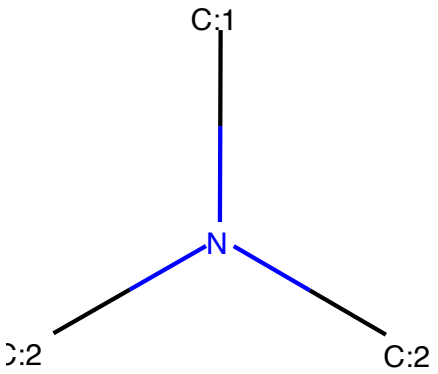
```
------------------------------------------------------------
Molecule [SiH4] and its specific config [SiH4] w/ p=-7.954206943511963
```

```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-11.697789192199707
```

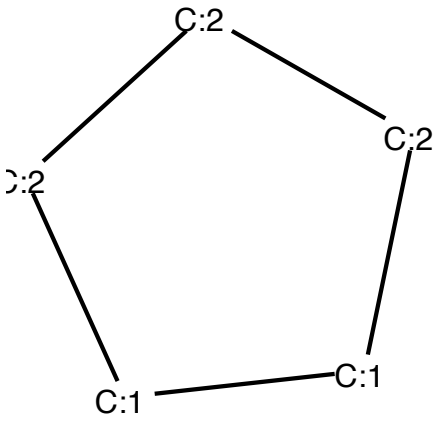
```
------------------------------------------------------------
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
-----Step-90-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ p=-0.13806328177452087
```



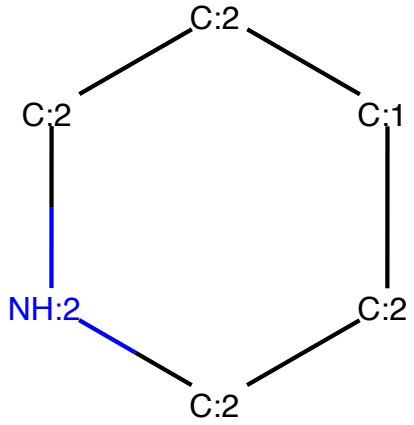

```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-2.325
0250816345215
```




```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1
w/ p=-4.258025169372559
```

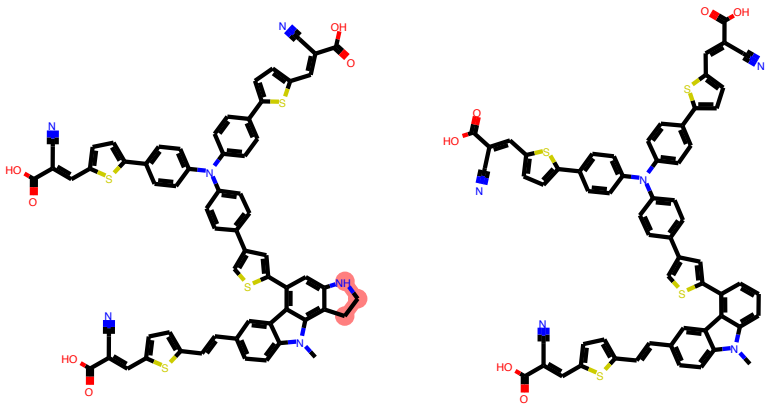



```
------------------------------------------------------------
Molecule C1CCNCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2][CH2:2][
CH2:2]1 w/ p=-4.540942192077637
```



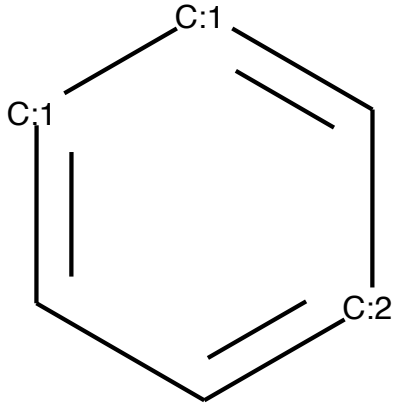

```
------------------------------------------------------------
Molecule CBr and its specific config Br[CH3:1] w/ p=-6.290830135345459
```

```
------------------------------------------------------------
Attaching fragment [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1 of config ['C1C[CH2:1]
CN1', 'C1CN[CH2:1]C1']
Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=C(C#N)C(=O)O)s3)cc2c2c(-c3cc(-c4ccc(
N(c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs
3)cc3c(c21)CCN3
Lastest graph (left) vs graph in last step (right)
```



-----Step-91-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CN and its specific config C[NH2:1] w/ p=-0.7608712911605835

Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ p=-1.2689768075942993

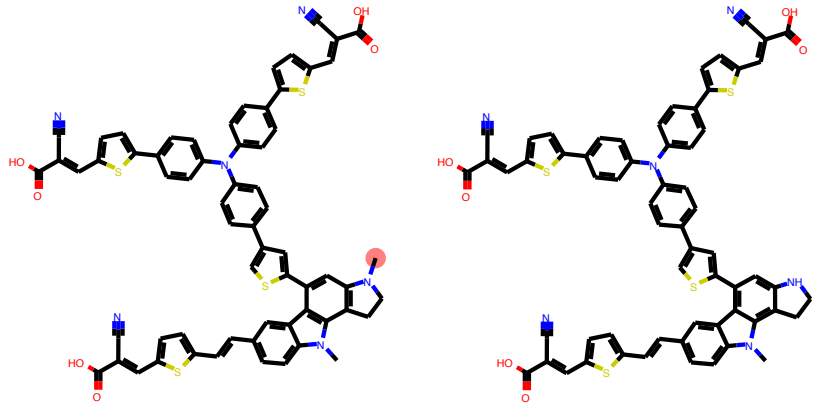


Molecule N and its specific config N w/ p=-1.4923474788665771

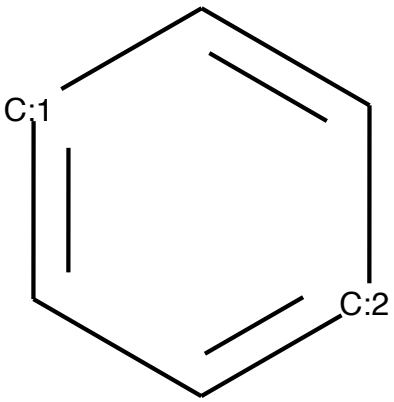
```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-4.306386470794678
```

```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-4.5528059005737305
```

```
------------------------------------------------------------
Attaching fragment C[NH2:1] of config ['C[NH2:1]']
Latest partial graph: CN1CCc2c1cc(-c1cc(-c3ccc(N(c4ccc(-c5ccc(C=C(C#N)C(=O)O)s
5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs1)c1c3cc(C=Cc4ccc(C=C(C#N)C(=O)
O)s4)ccc3n(C)c21
Lastest graph (left) vs graph in last step (right)
```



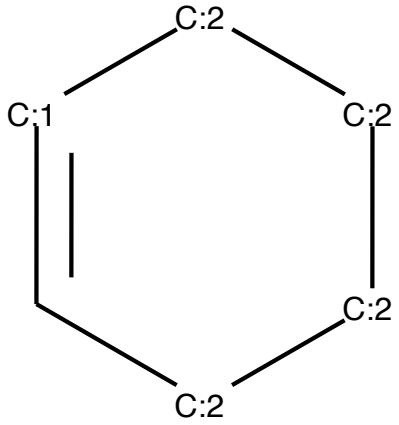
-----Step-92-----
Generate next fragment p = 0.7671745419502258
Top 5 next motifs to attach:
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-0.094
0258577466011



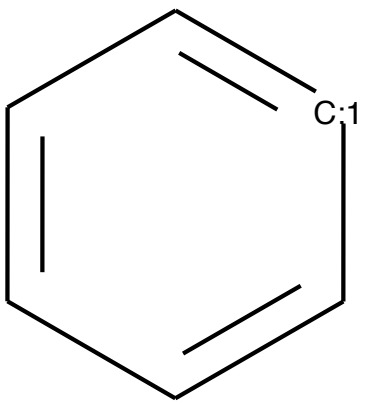
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-2.4413399696350098

Molecule C and its specific config C w/ p=-6.6834330558776855

```
------------------------------------------------------------
Molecule C1=CCCCC1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH2:2][CH2:
2]1 w/ p=-7.4105939865112305
```

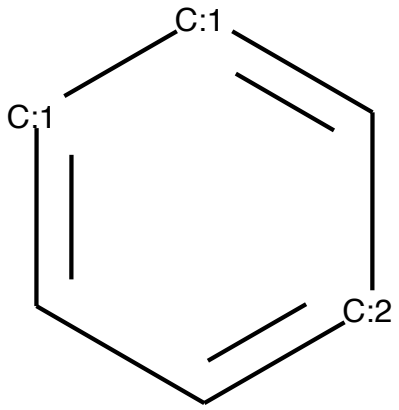



```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=CC=[CH:1]C=C1 w/ p=-7.66151380
5389404
```




```
------------------------------------------------------------
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-93-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CN and its specific config C[NH2:1] w/ p=-0.7608712911605835
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ p=-
1.2689768075942993
```

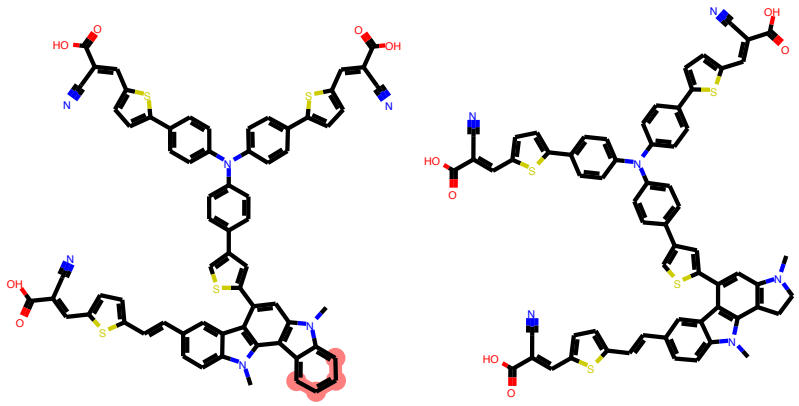



```
------------------------------------------------------------
Molecule N and its specific config N w/ p=-1.4923474788665771
```

```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-4.306386470794678
```

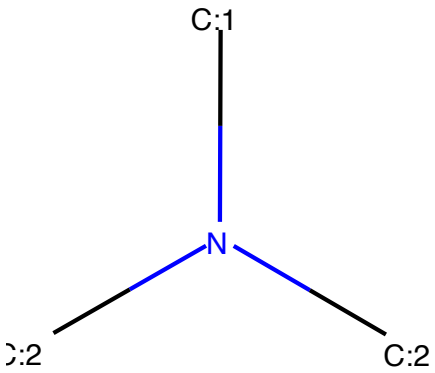
```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-4.5528059005737305
```

```
------------------------------------------------------------
Attaching fragment C1=[CH:1][CH:1]=C[CH:2]=C1 of config ['C1:C:C:[CH:1]:C:C:1'
, 'C1:C:C:[CH:1]:C:C:1']
Latest partial graph: Cn1c2ccccc2c2c1cc(-c1cc(-c3ccc(N(c4ccc(-c5ccc(C=C(C#N)C(
=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs1)c1c3cc(C=Cc4ccc(C=C(C#N
)C(=O)O)s4)ccc3n(C)c12
Lastest graph (left) vs graph in last step (right)
```



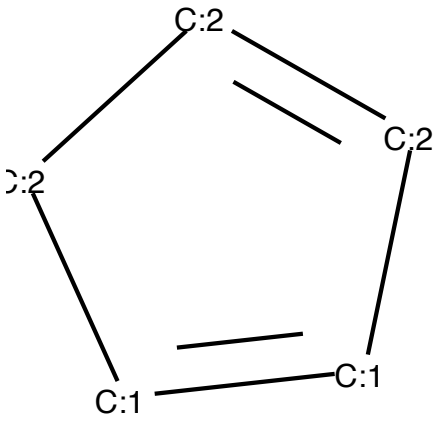
```
------------------------------------------------------------
-----Step-94-----
Generate next fragment p = 0.9999222755432129
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.24081973731517792
```

```
------------------------------------------------------------
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-1.597
212553024292
```

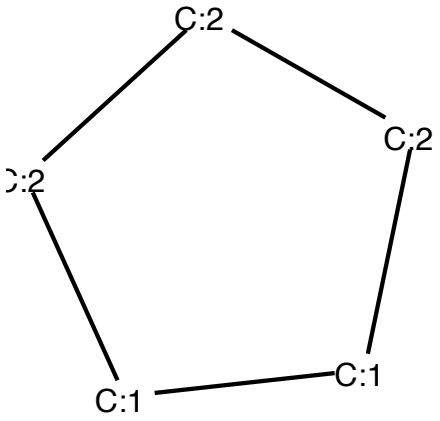



```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-5.8199143409729
```

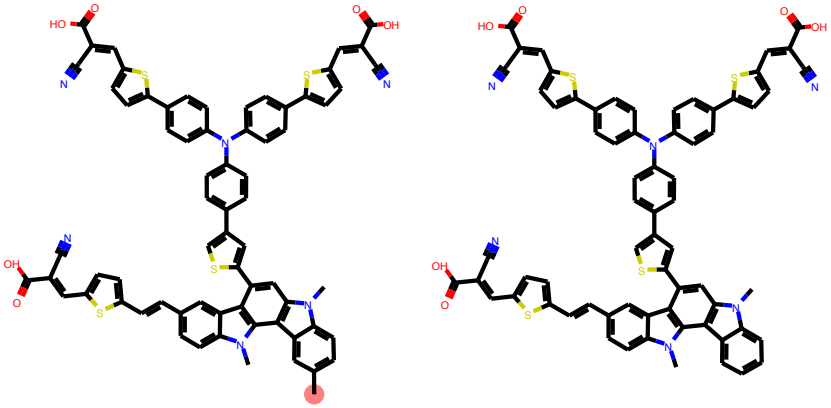
```
------------------------------------------------------------
Molecule C1=CCC=C1 and its specific config [CH:1]1=[CH:1][CH2:2][CH:2]=[CH:2]1
w/ p=-6.302864074707031
```




```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1
w/ p=-6.495669364929199
```

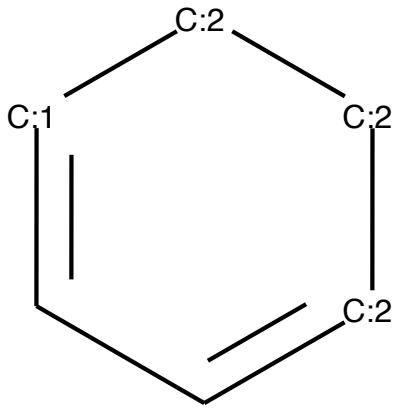



```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc2c(c1)c1c(cc(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#N)C
(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)c3c4cc(C=Cc5ccc(C=C(C#
N)C(=O)O)s5)ccc4n(C)c31)n2C
Lastest graph (left) vs graph in last step (right)
```

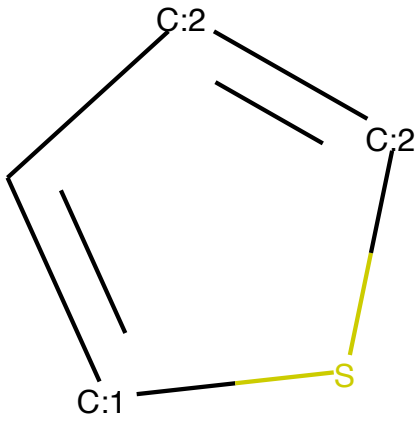


```
------------------------------------------------------------
-----Step-95-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-1.126648187637329
```

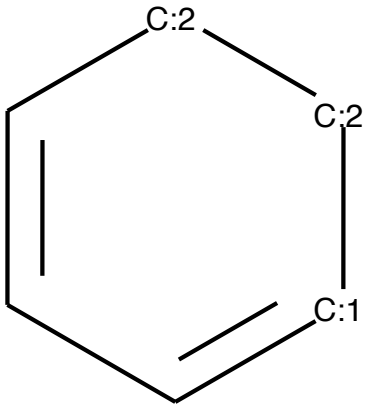
```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-1.7038220167160034
```



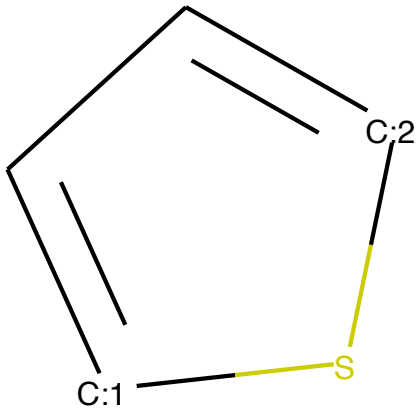

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-1.74
80615377426147
```



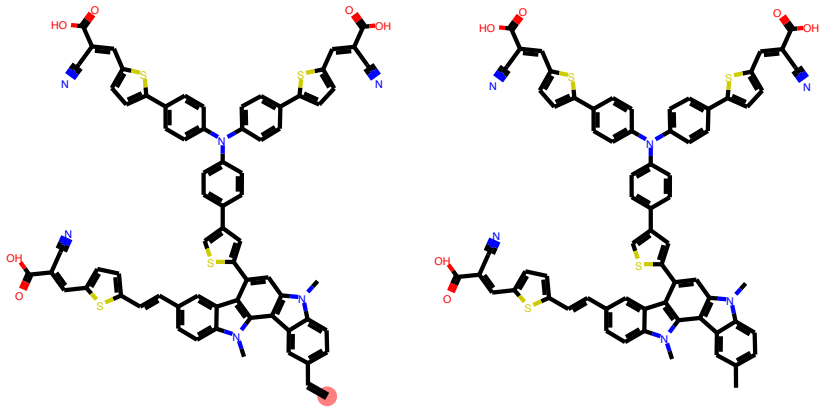

```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=C[CH2:2][CH2:2][CH:1]=C1 w/ p=-
1.7600525617599487
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-2.2401089
668273926
```



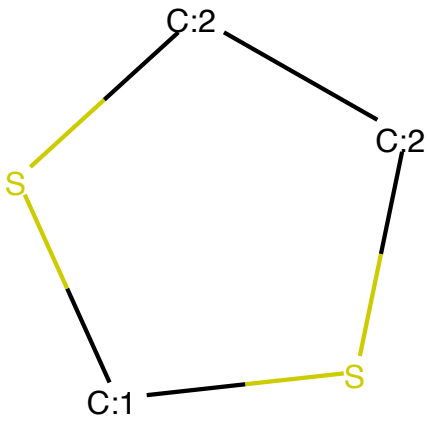

```
------------------------------------------------------------
Attaching fragment [CH2:1]=[CH2:2] of config ['C=[CH2:1]']
Latest partial graph: C=Cc1ccc2c(c1)c1c(cc(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#N
)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)c3c4cc(C=Cc5ccc(C=C(
C#N)C(=O)O)s5)ccc4n(C)c31)n2C
Lastest graph (left) vs graph in last step (right)
```



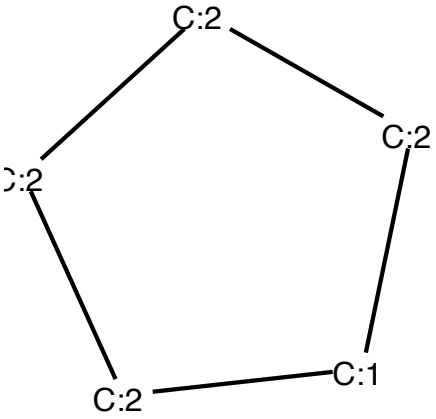
```
------------------------------------------------------------
-----Step-96-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.503343403339386
```

```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-1.506188154220581
```

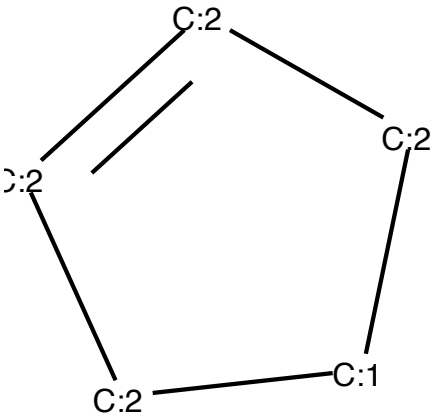
```
------------------------------------------------------------
Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ p=-2.095
0944423675537
```



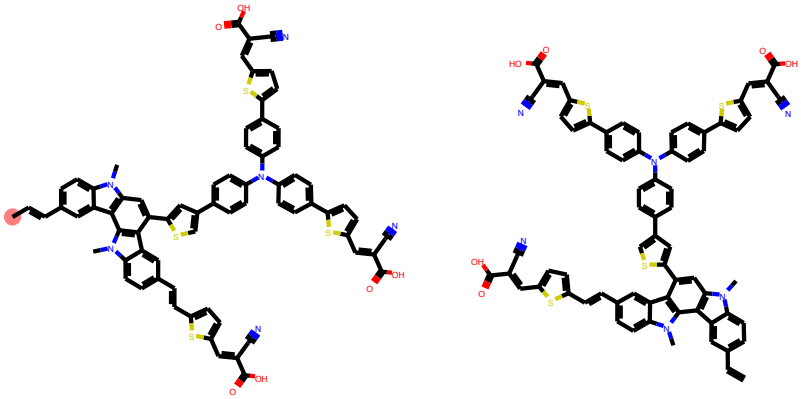

```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]1
w/ p=-3.5078275203704834
```



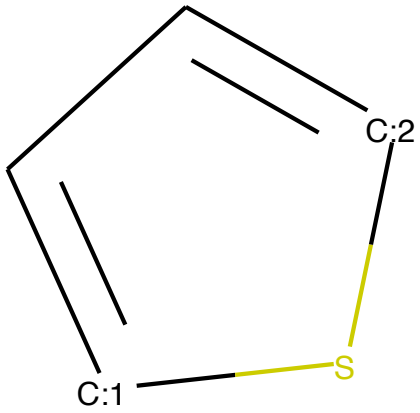

```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:2][CH:2]=[CH:2][CH2:2]1
w/ p=-3.9123003482818604
```



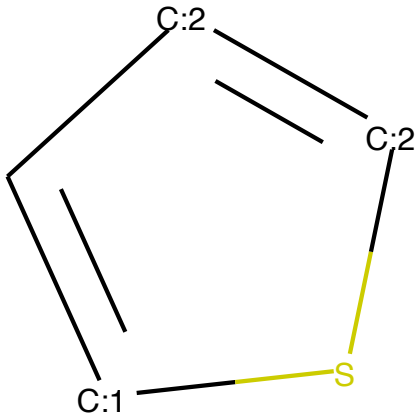

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC=Cc1ccc2c(c1)c1c(cc(-c3cc(-c4ccc(N(c5ccc(-c6ccc(C=C(C#
N)C(=O)O)s6)cc5)c5ccc(-c6ccc(C=C(C#N)C(=O)O)s6)cc5)cc4)cs3)c3c4cc(C=Cc5ccc(C=C
(C#N)C(=O)O)s5)ccc4n(C)c31)n2C
Lastest graph (left) vs graph in last step (right)
```



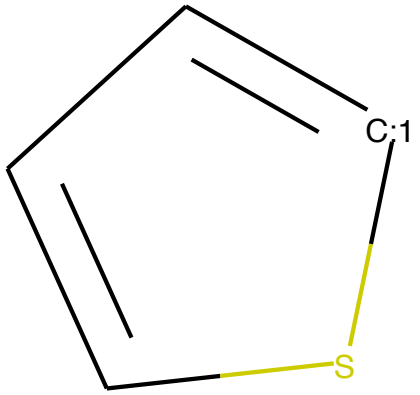
```
------------------------------------------------------------
-----Step-97-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.1306475
8479595184
```



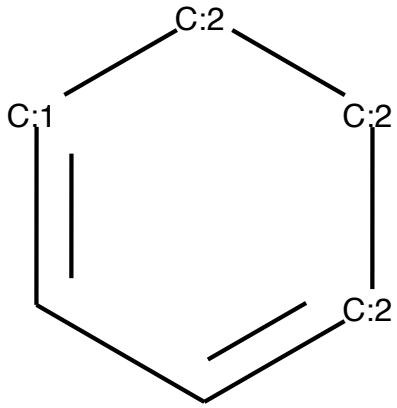
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-2.94429874420166



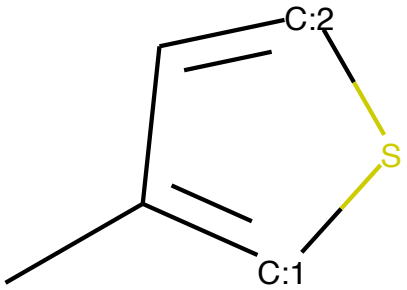
Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ p=-3.4541759490966797



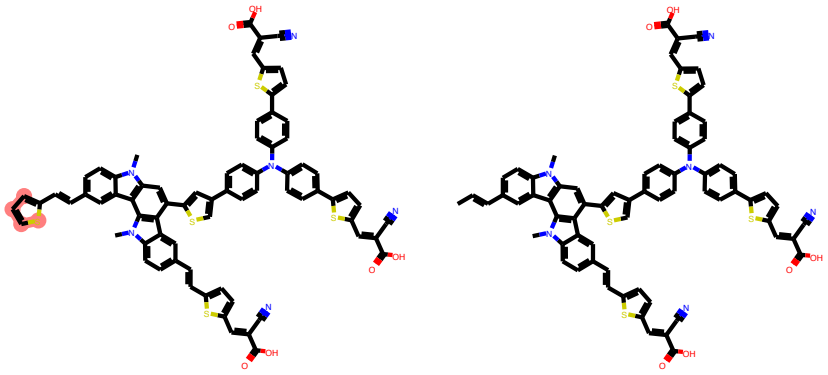
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w/ p=-3.6914896965026855



Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ p=-4.74936
9144439697

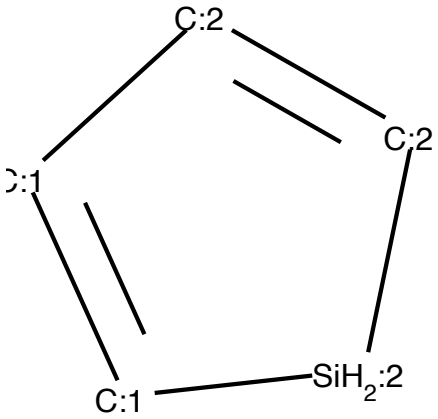


Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: Cn1c2ccc(C=Cc3cccs3)cc2c2c1cc(-c1cc(-c3ccc(N(c4ccc(-c5cc
c(C=C(C#N)C(=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs1)c1c3cc(C=Cc
4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12
Lastest graph (left) vs graph in last step (right)



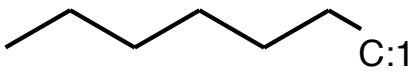
-----Step-98-----
Generate next fragment p = 0.8716926574707031
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.062069881707429886

```
------------------------------------------------------------
Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:1][SiH2:2][CH:2]=[
CH:2]1 w/ p=-3.3673901557922363
```

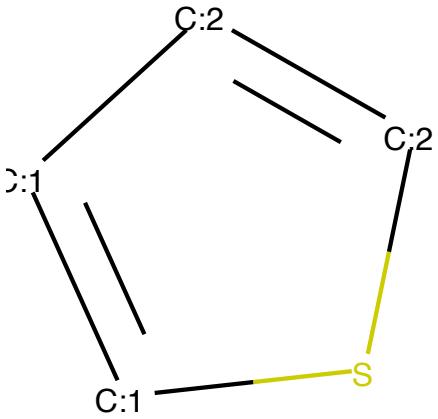



```
------------------------------------------------------------
Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-4.4592938423156
74
```

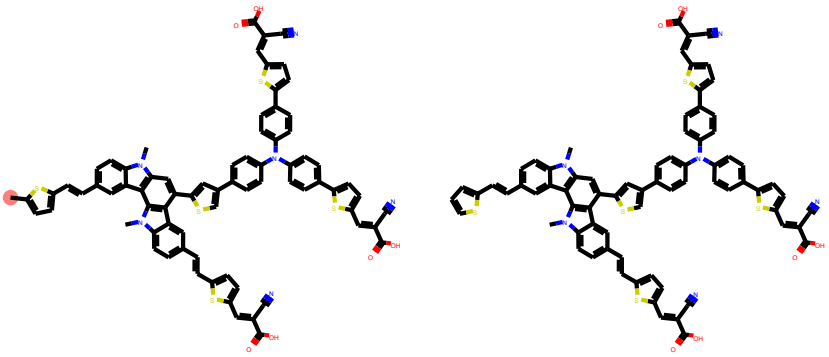
```
------------------------------------------------------------
Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ p=-4.933238506317139
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p=
-5.725485324859619
```

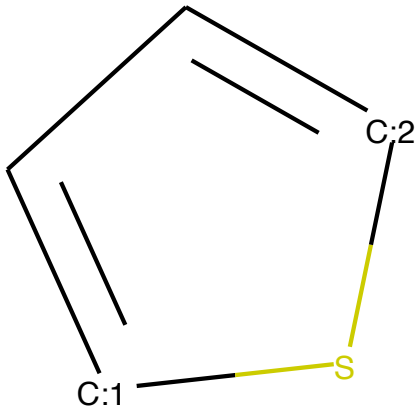



```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6ccc(-c7ccc(
C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5cc(C=Cc6c
cc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1
Lastest graph (left) vs graph in last step (right)
```

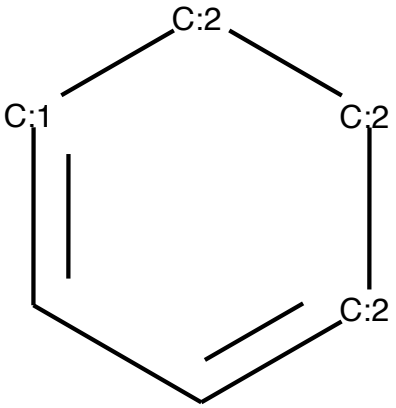


```
------------------------------------------------------------
-----Step-99-----
Generate next fragment p = 0.9999935626983643
Top 5 next motifs to attach:
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-0.05087331682443619
```

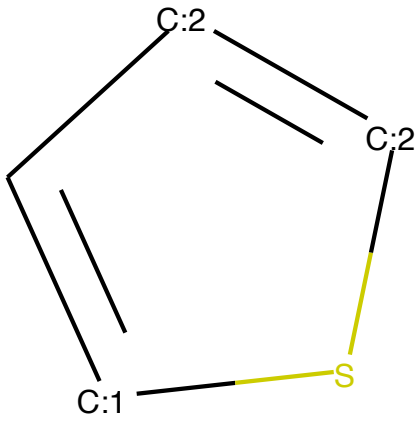
```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-3.4192769
527435303
```



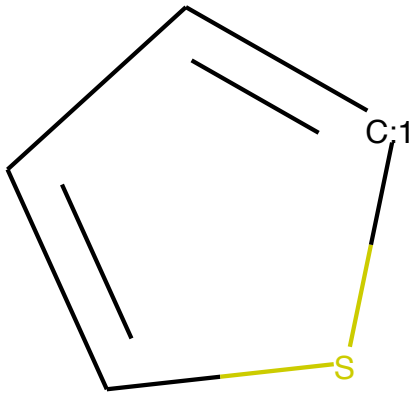

```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-5.058681011199951
```



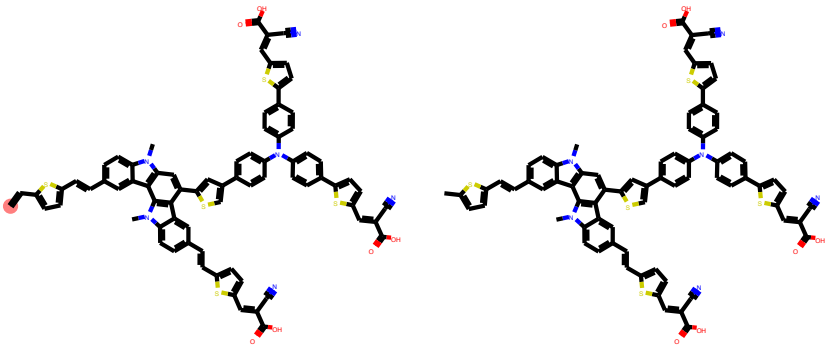

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-5.07
9664707183838
```



Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ p=-6.652697563171387



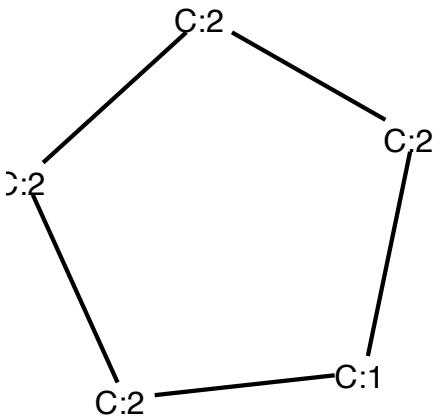
Attaching fragment [CH2:1]=[CH2:2] of config ['C=[CH2:1]']
Latest partial graph: C=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5cc(C=Cc6ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1
Lastest graph (left) vs graph in last step (right)



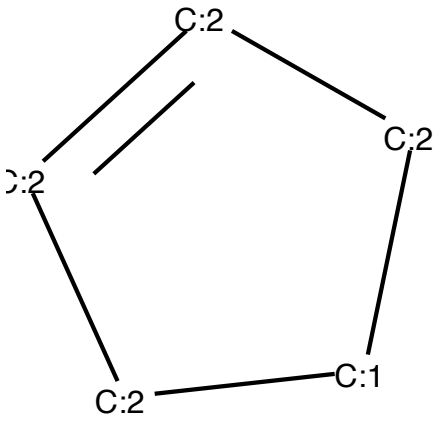
-----Step-100-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.008251977153122425

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-4.811239719390869
```

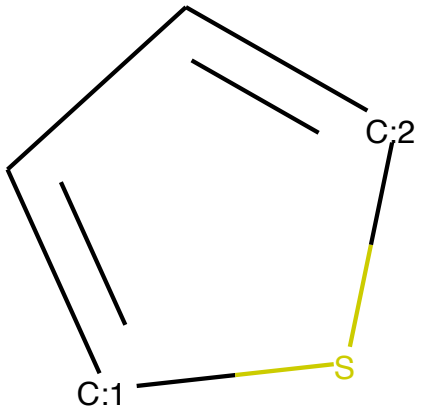
```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]1
w/ p=-9.474627494812012
```



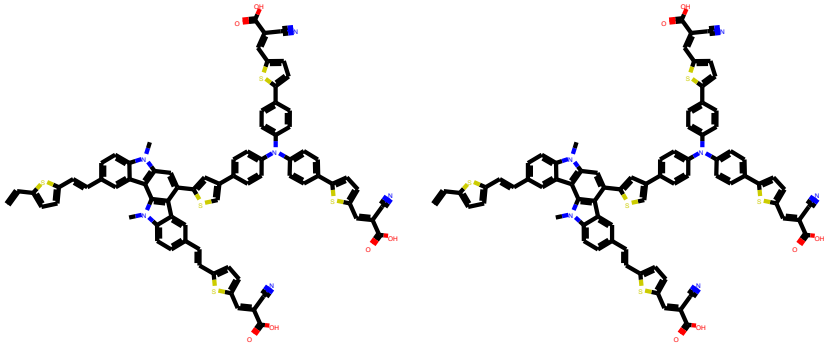

```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:2][CH:2]=[CH:2][CH2:2]1
w/ p=-13.712767601013184
```



Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-14.705822944641113



Attaching fragment C of config ['[CH4:1]']
Latest partial graph: C=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5cc(C=Cc6ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1
Lastest graph (left) vs graph in last step (right)

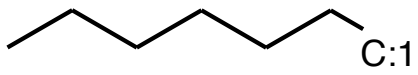


-----Step-101-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.722029527532868e-06

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-12.142010688781738
```

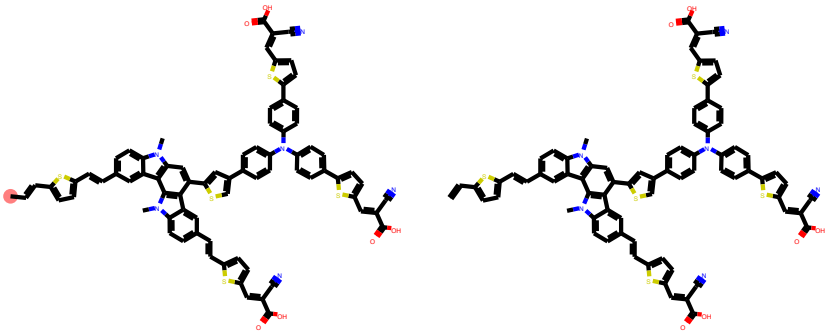
```
------------------------------------------------------------
Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-16.139101028442
383
```

```
------------------------------------------------------------
Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ p=-16.46015930175781
2
```



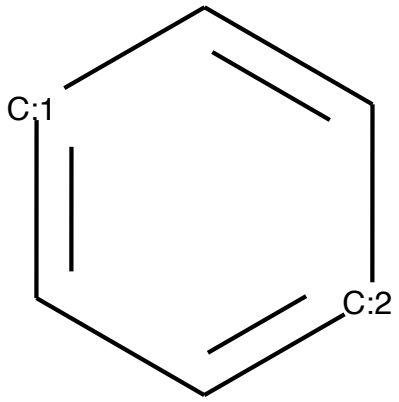

```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-16.629497528076172
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6ccc(-c7c
cc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5cc(C=C
c6ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-102-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C#N and its specific config N#[CH:1] w/ p=-0.00012432756193447858
```

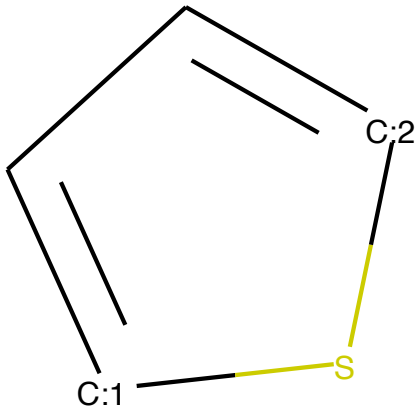
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-9.358190536499023



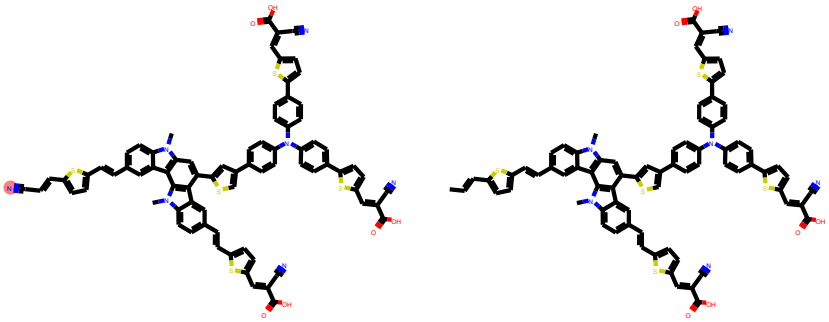
Molecule C and its specific config C w/ p=-10.463766098022461

Molecule C=O and its specific config O=[CH2:1] w/ p=-11.708536148071289

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-13.973914
14642334
```




```
------------------------------------------------------------
Attaching fragment N#[CH:1] of config ['N#[CH:1]']
Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=CC#N)s3)cc2c2c1cc(-c1cc(-c3ccc(N(c4c
cc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs1)c1c
3cc(C=Cc4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-103-----
Generate next fragment p = 1.2375334841616124e-21
-----Step-104-----
Generate next fragment p = 1.074206167268367e-13
-----Step-105-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.6689286894688848e-0
6
```

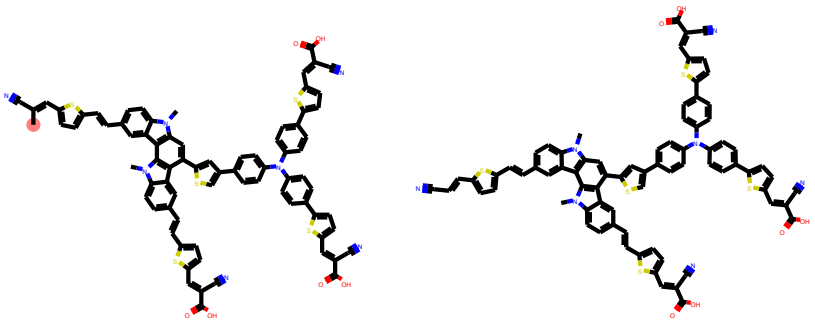
```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-14.100029945373535
```

```
------------------------------------------------------------
Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ p=-14.389986991882
324
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-14.865313529968262
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-17.095172882080078
```

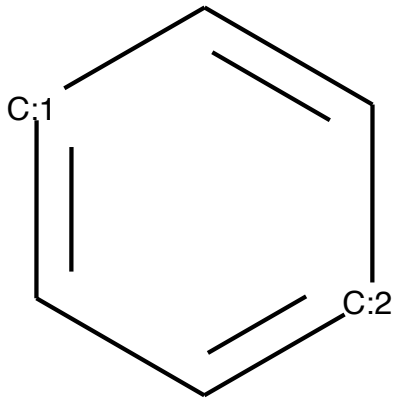
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CC(C#N)=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6ccc
(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5c
c(C=Cc6ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-106-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C and its specific config C w/ p=-0.3379138708114624
```

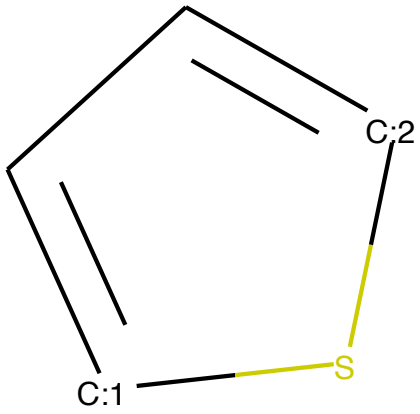
Molecule C#N and its specific config N#[CH:1] w/ p=-1.2967575788497925

Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-4.329935550689697

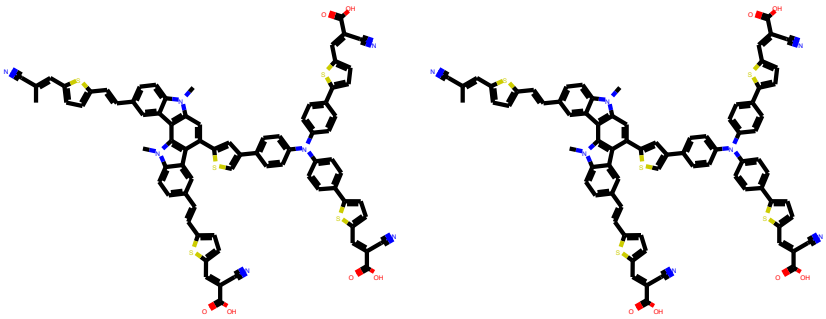


Molecule C=O and its specific config O=[CH2:1] w/ p=-9.10343074798584

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-10.106386
184692383
```




```
------------------------------------------------------------
Attaching fragment C of config ['[CH4:1]']
Latest partial graph: CC(C#N)=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6ccc
(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5c
c(C=Cc6ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-107-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C=O and its specific config O=[CH2:1] w/ p=-1.1920928244535389e-07
```

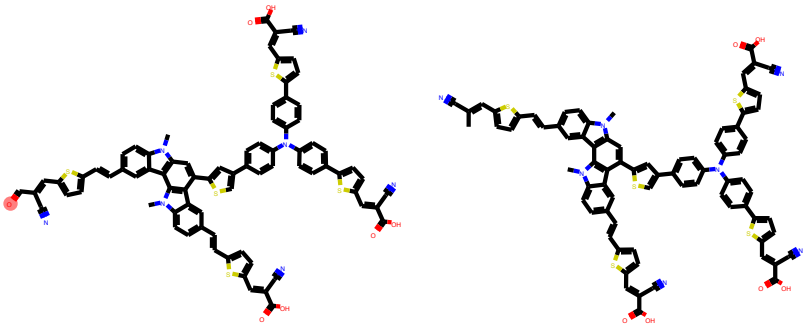
```
------------------------------------------------------------
Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ p=-16.645597457885
742
```

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-17.349519729614258
```

```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-18.376365661621094
```

```
------------------------------------------------------------
Molecule CO and its specific config O[CH3:1] w/ p=-18.986196517944336
```

```
------------------------------------------------------------
Attaching fragment O=[CH2:1] of config ['O=[CH2:1]']
Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=C(C#N)C=O)s3)cc2c2c1cc(-c1cc(-c3ccc(
N(c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs
1)c1c3cc(C=Cc4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-108-----
Generate next fragment p = 4.980957319677204e-21
-----Step-109-----
Generate next fragment p = 0.9999995231628418
Top 5 next motifs to attach:
Molecule CO and its specific config O[CH3:1] w/ p=-0.009655111469328403
```

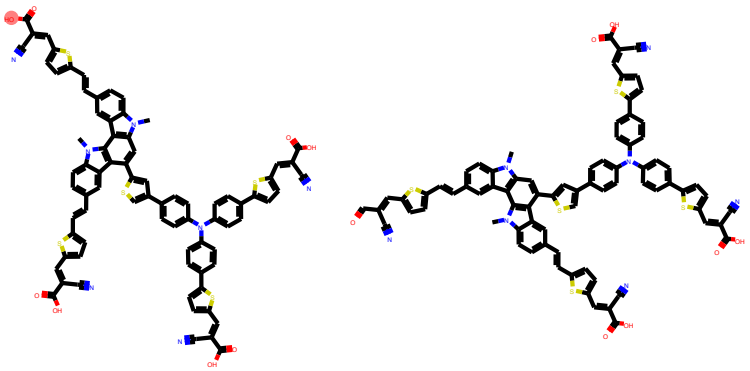
```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-5.474302291870117
```

```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-5.605182647705078
```

```
------------------------------------------------------------
Molecule CO and its specific config [CH3:1][OH:2] w/ p=-7.083941459655762
```

```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-7.4250383377075195
```

```
------------------------------------------------------------
Attaching fragment O[CH3:1] of config ['O[CH3:1]']
Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=C(C#N)C(=O)O)s3)cc2c2c1cc(-c1cc(-c3c
cc(N(c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3
)cs1)c1c3cc(C=Cc4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12
Lastest graph (left) vs graph in last step (right)
```



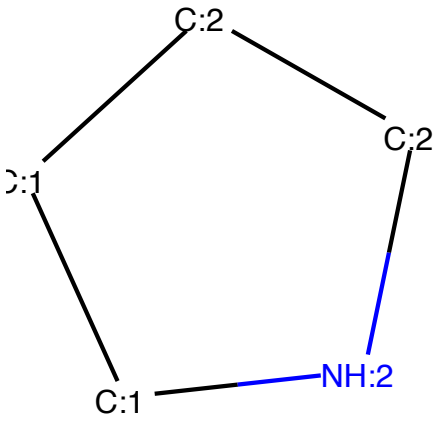
```
------------------------------------------------------------
-----Step-110-----
Generate next fragment p = 0.01190867368131876
-----Step-111-----
Generate next fragment p = 4.3493557200235955e-08
-----Step-112-----
Generate next fragment p = 1.575424539623782e-05
-----Step-113-----
Generate next fragment p = 2.967772472217689e-09
-----Step-114-----
Generate next fragment p = 1.11399020365807e-15
-----Step-115-----
Generate next fragment p = 2.546446729859179e-17
-----Step-116-----
Generate next fragment p = 3.1717604542791378e-06
-----Step-117-----
Generate next fragment p = 6.617605812902757e-20
-----Step-118-----
Generate next fragment p = 2.031031766380753e-11
-----Step-119-----
Generate next fragment p = 1.663748432588825e-19
-----Step-120-----
Generate next fragment p = 2.262406262332206e-08
-----Step-121-----
Generate next fragment p = 0.9998952150344849
Top 5 next motifs to attach:
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-0.023700183257460594









------------------------------------------------------------
Molecule CN and its specific config C[NH2:1] w/ p=-3.787360668182373
```

```
------------------------------------------------------------
Molecule N and its specific config N w/ p=-7.859424114227295
```

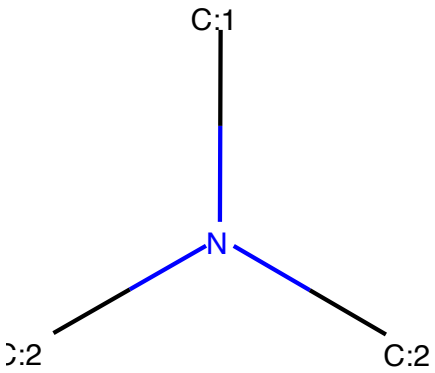
```
------------------------------------------------------------
Molecule [SiH4] and its specific config [SiH4] w/ p=-7.954198360443115
```

```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-11.69778823852539
```

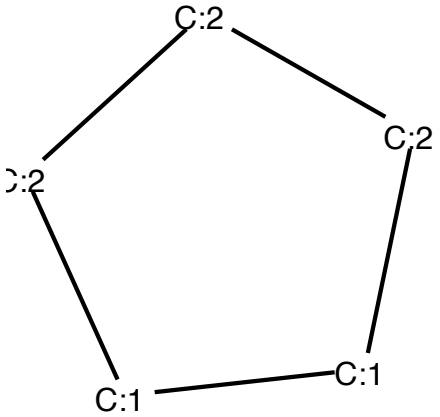
```
------------------------------------------------------------
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
-----Step-122-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ p=-0.13806338608264923
```



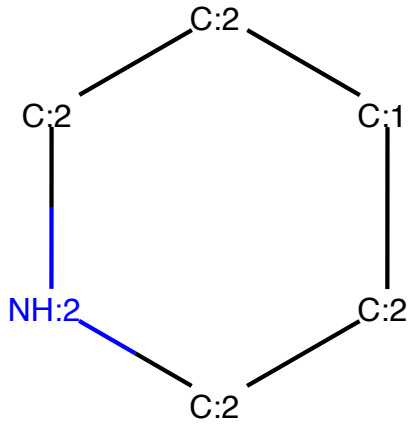
Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ p=-2.325
0234127044678



Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1
w/ p=-4.258027076721191

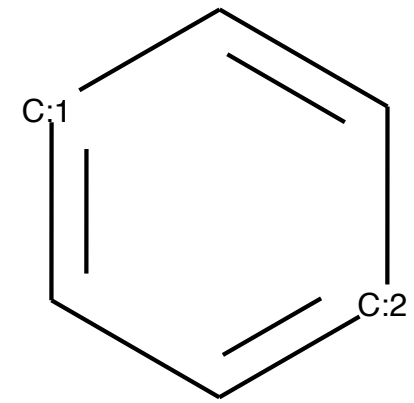


Molecule C1CCNCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2][CH2:2][
CH2:2]1 w/ p=-4.5409440994262695

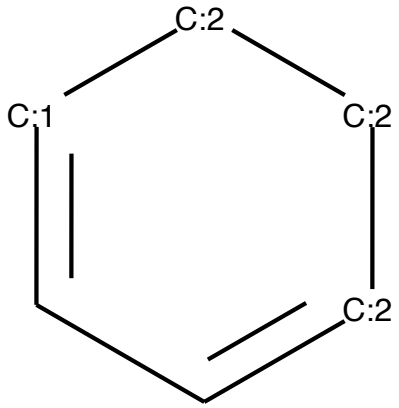



```
------------------------------------------------------------
Molecule CBr and its specific config Br[CH3:1] w/ p=-6.290830135345459
```

```
------------------------------------------------------------
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-123-----
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=-0.979
3890714645386
```

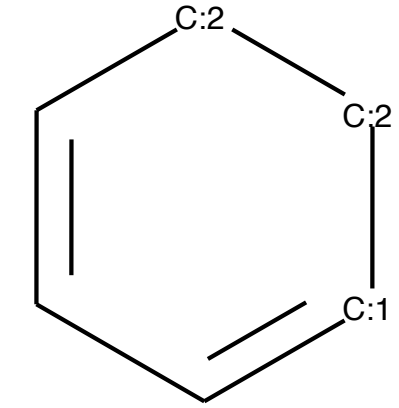



```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=[CH:1][CH2:2][CH2:2][CH:2]=C1 w
/ p=-1.16252863407135
```

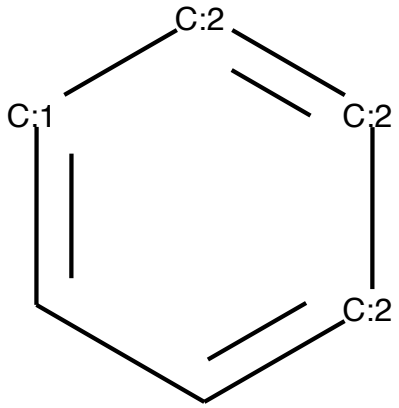



```
------------------------------------------------------------
Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ p=-1.39579439163208
```

```
------------------------------------------------------------
Molecule C1=CCCC=C1 and its specific config C1=C[CH2:2][CH2:2][CH:1]=C1 w/ p=-
3.6127209663391113
```

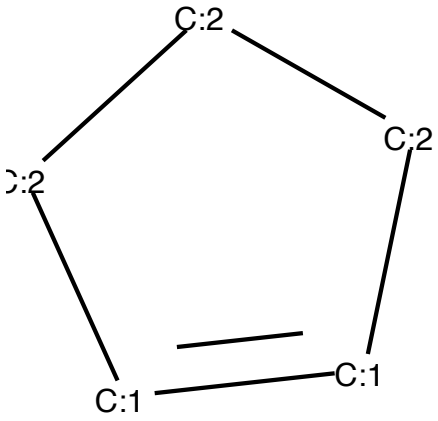



```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:2]=[CH:2][CH:2]=C1 w
/ p=-4.562343597412109
```

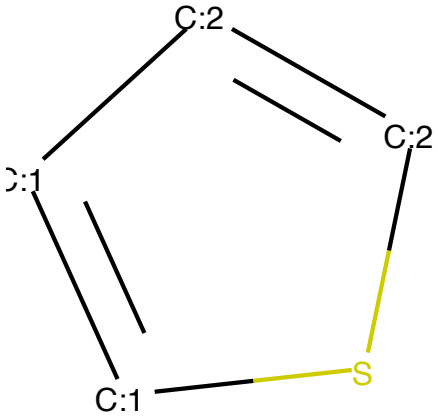



```
------------------------------------------------------------
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
-----Step-124-----
Generate next fragment p = 0.9999998807907104
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.006059726700186729
```

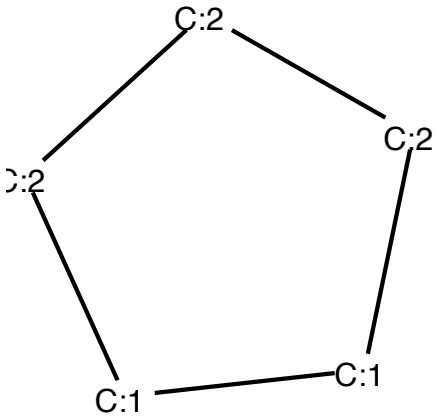
```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH:1]1=[CH:1][CH2:2][CH2:2][CH2:2]1
w/ p=-6.0629658699035645
```



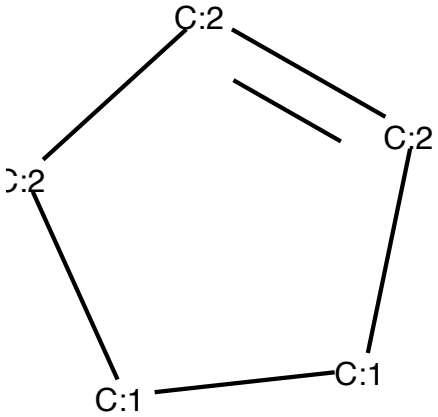

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p=
-7.047156810760498
```




```
------------------------------------------------------------
Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1
w/ p=-7.10591983795166
```

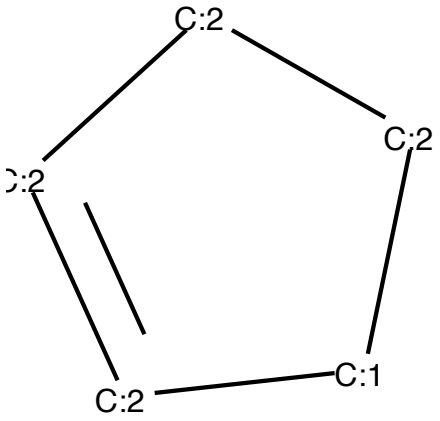



```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH:2]=[CH:2]1
w/ p=-7.136286735534668
```

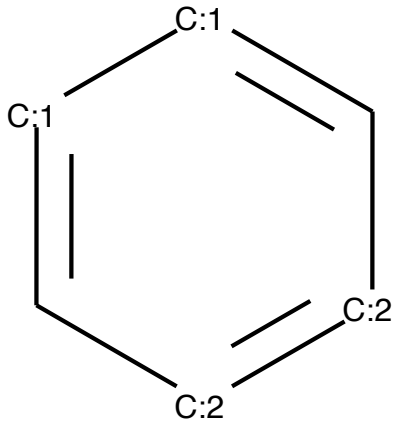



```
------------------------------------------------------------
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
-----Step-125-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-7.390948667307384e-06
```

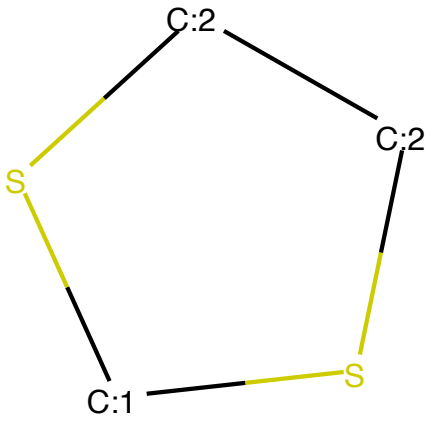
```
------------------------------------------------------------
Molecule C1=CCCC1 and its specific config [CH2:1]1[CH:2]=[CH:2][CH2:2][CH2:2]1
w/ p=-13.06435489654541
```



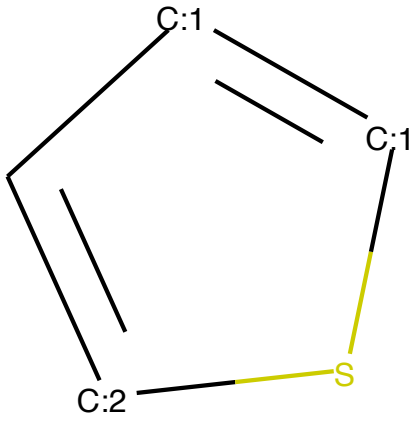

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=[CH:2]1 w
/ p=-13.119874954223633
```




```
------------------------------------------------------------
Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ p=-13.66
5506362915039
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-14.9
6162223815918
```




```
------------------------------------------------------------
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-126-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
```

In [ ]: