In [18]:
```
import pickle
from rdkit import Chem
from rdkit.Chem import Draw
from rdkit.Chem.Draw import IPythonConsole
from IPython.display import display
import matplotlib.pyplot as plt
from IPython.display import HTML
import pandas as pd

IPythonConsole.ipython_useSVG=True
```

In [68]:
```
with open('predictions/w_tie_embedding_logs.pkl', 'rb') as file: w_te_data = 
with open('predictions/wo_tie_embedding_logs.pkl', 'rb') as file: wo_te_data 
original = pd.read_csv('predictions/chem_departm_output_wo_tie_embedding/outp
```

In [69]:
```
def mol_with_atom_index(mol, indices=[]):
    new_idx = []
    for atom in mol.GetAtoms():
        #print(atom.GetIdx(), indices)
        idx = atom.GetIdx()
        if idx in indices:
            atom.SetAtomMapNum(idx)
        new_idx.append(idx)
    return mol, new_idx
```

Generation by wo-tie-embedding-motif-only

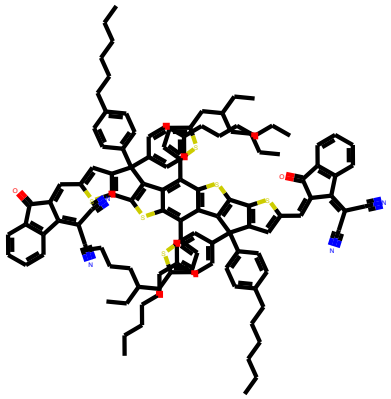
In [85]:

```
for i, sample in enumerate(wo_te_data):
    if i > 11:
        break
    elif i < 11:
        continue
    display('Original: {}'.format(original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(original[i])]))

    # step 0
    step_f0 = sample[0]
    display('***************Sample {}th***************'.format(i))
    display('-----Step-0-----')
    display(step_f0)
    mol = Chem.MolFromSmiles(step_f0['partial-graph'])
    display('Displaying partial graph (aka molecule): {}'.format(step_f0['par
            Draw.MolsToGridImage([mol]))
    display('------------------------------------------------------------', HTML
    num_atom = len(list(Chem.MolFromSmiles(step_f0['partial-graph']).GetAtoms
    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        display('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            display('Generate next fragment: {}'.format(step_f['Generate frag
        if 'top-5-inter-cands' in step_f:
            display('Top 5 next fragments to attach (current and potential gr
            for fragment in step_f['top-5-inter-cands']:
                display('Molecule {} and its specific config {} w/ probabilit
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                display('------------------------------------------------------
        if 'Attaching Fragment' in step_f:
            frag = step_f['Attaching Fragment'][0]

            mol, indices = mol_with_atom_index(Chem.MolFromSmiles(step_f['par
                                               list(range(num_atom)))
            display('Attaching fragment {}'.format(frag))
            display('Latest partial graph: {}'.format(step_f['partial-graph']
                    Draw.MolsToGridImage([mol]))
            num_atom = len(list(Chem.MolFromSmiles(step_f['partial-graph']).G
            display('------------------------------------------------------
```

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



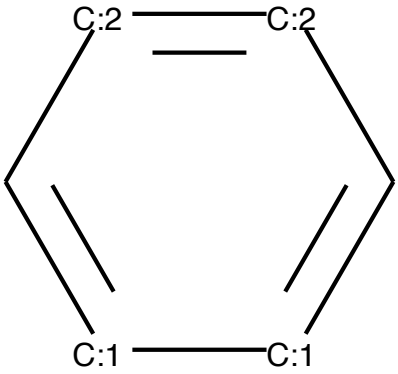
```
'***************Sample 11th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([570,  10, 653, 675, 714]),
 'super-root-idx': tensor(570),
 'top-5-root-fragment-cands': [('[CH2:1]=[CH2:2]', tensor(23.7334)),
  ('C=[CH2:1]', 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))],
 'Attaching Fragment': '[CH2:1]=[CH2:2]',
 'partial-graph': 'C=C'}
'Displaying partial graph (aka molecule): C=C'
```

```
'------------------------------------------------------------'

'-----Step-1-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00114577
90387794375'
```

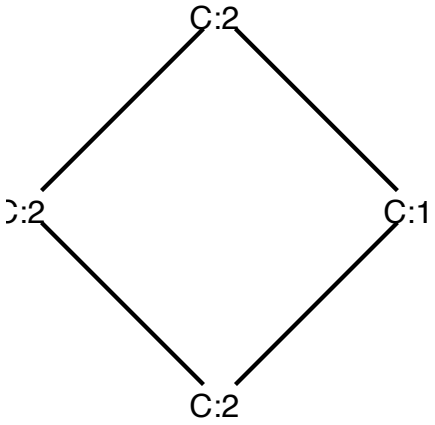
```
'------------------------------------------------------------'

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



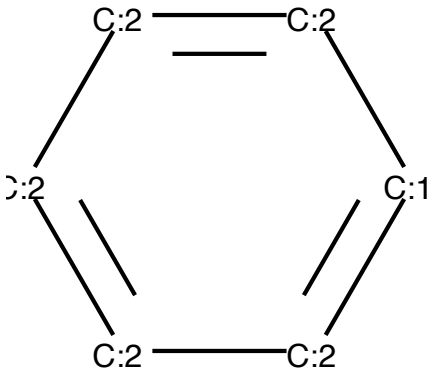

```
'------------------------------------------------------------'

'Molecule C1CCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2]1 w/ pro
bability -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/ probability -8.414703369140625'
```

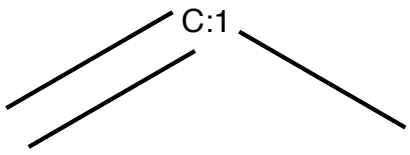



```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -8.767458
91571045'
```

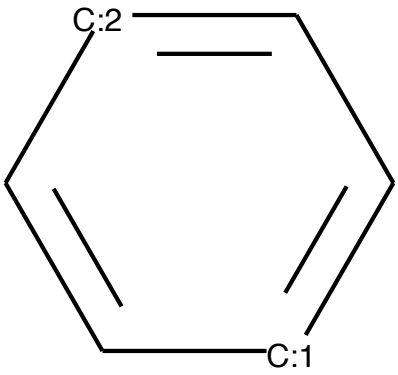
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=CC'
```



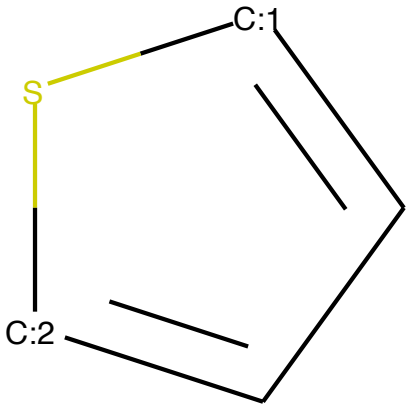

```
'------------------------------------------------------------'

'-----Step-2-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.02286357991397381'
```



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -4.279532432556152'

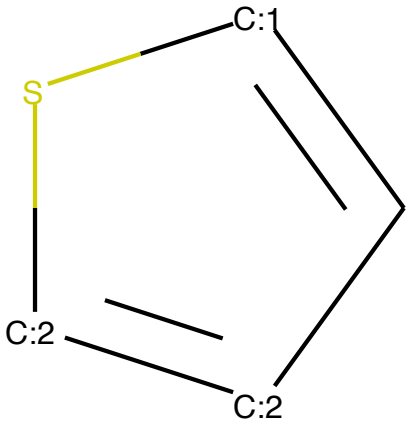


'--'

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

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probability -6.99843692779541'

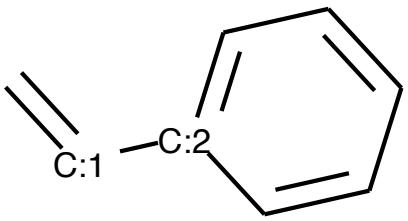



```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -7.249641
8952941895'
```

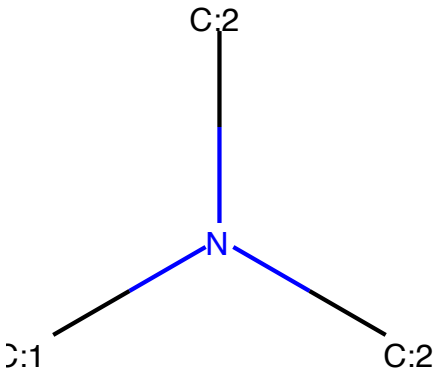
```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: C=Cc1ccccc1'
```




```
'------------------------------------------------------------'

'-----Step-3-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -0.4842117428779602'
```

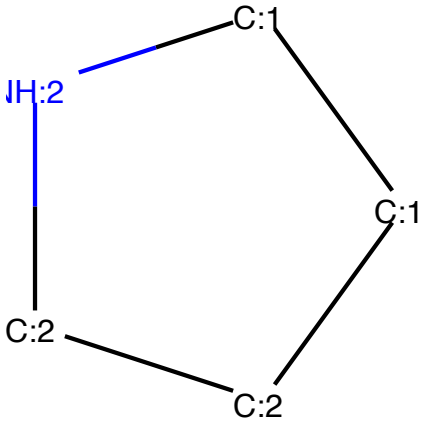



```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.28338360
78643799'
```

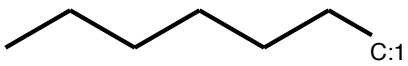
```
'------------------------------------------------------------'

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



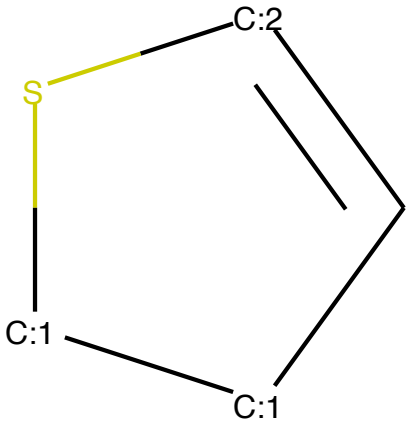

```
'------------------------------------------------------------'

'Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ probability -4.7821
56944274902'
```



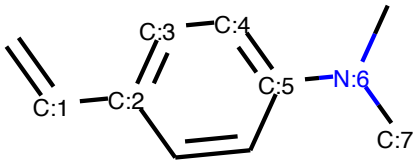
'--'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -5.169488906860352'



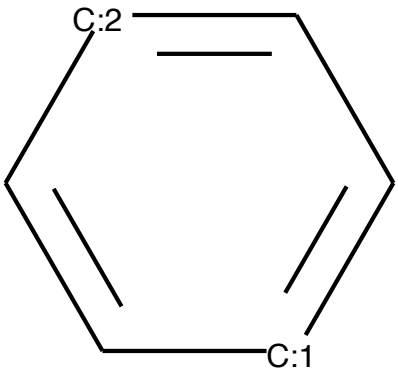
'--'

'Attaching fragment N([CH3:1])([CH3:2])[CH3:2]'
'Latest partial graph: C=Cc1ccc(N(C)C)cc1'



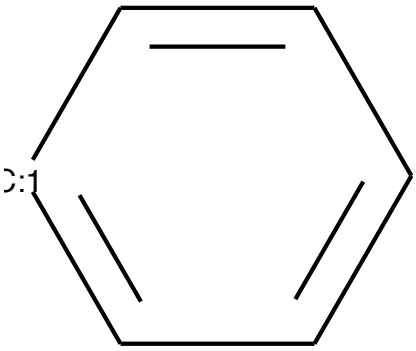
'--'

'-----Step-4-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.3543316721916199'



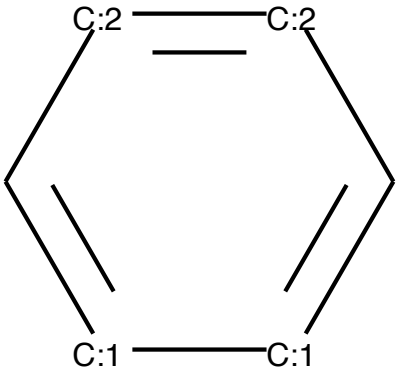
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=CC=[CH:1]C=C1 w/ probability -1.4405667781829834'



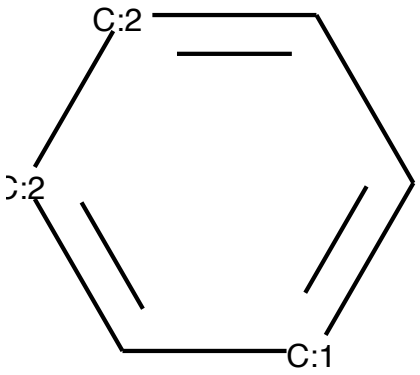
'--'

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



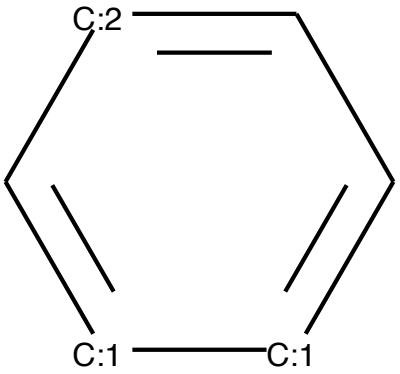
'--'

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



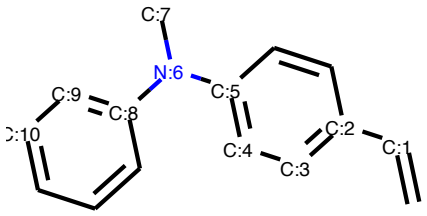
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ pr
obability -6.2220940589904785'



'--'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: C=Cc1ccc(N(C)c2ccccc2)cc1'



'--'

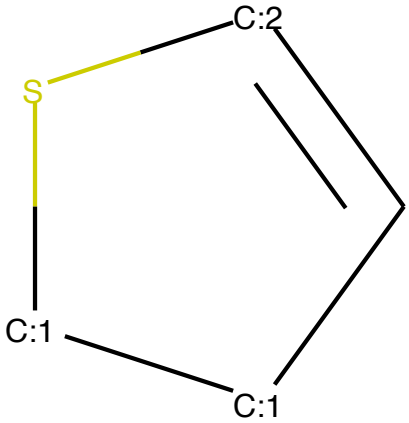
'-----Step-5-----'
'Generate next fragment: 0.976083517074585'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.17526289
820671082'

```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -2.20827269
5541382'
```

```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -3.207990884780884'
```

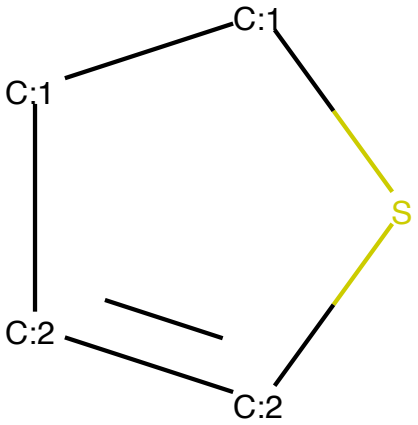



```
'------------------------------------------------------------'

'Molecule [CH2-]C and its specific config [CH2-:1][CH3:2] w/ probability -5.40
57230949401855'
```

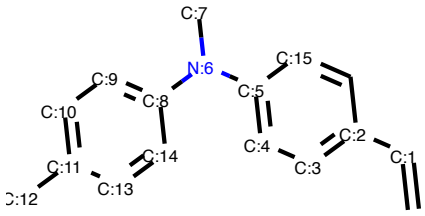
```
'------------------------------------------------------------'

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



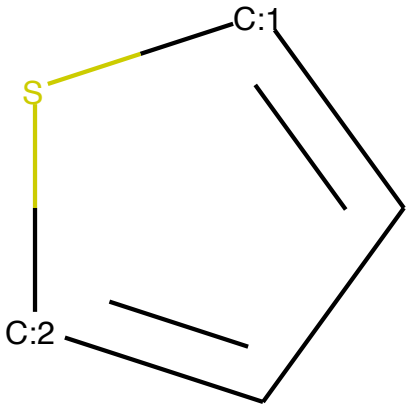

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(C)cc2)cc1'
```



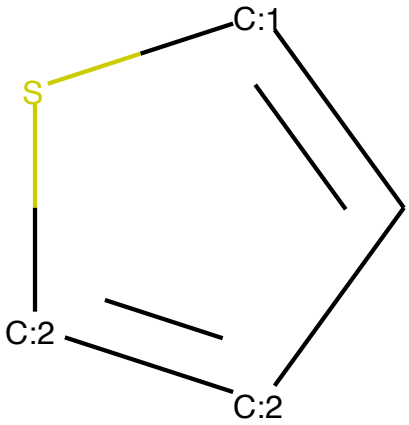

```
'------------------------------------------------------------'

'-----Step-6-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.9011122584342957'
```



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -1.115161657333374'

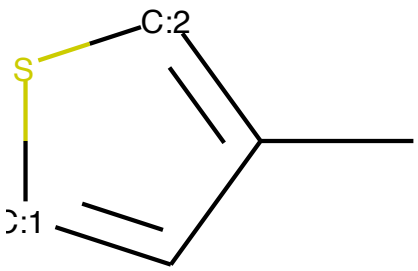


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -1.327795
0286865234'

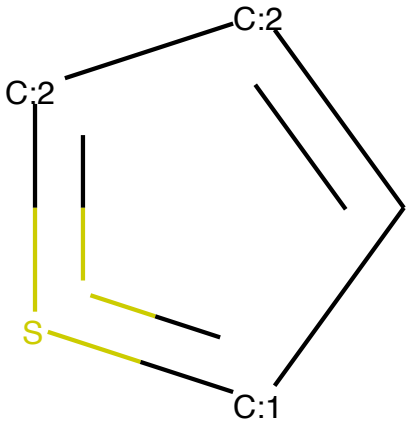
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ probabili
ty -8.337925910949707'



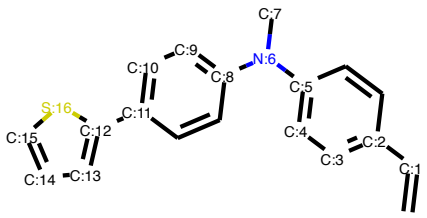

```
'-------------------------------------------------------------'

'Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:2]=S=[CH:1]1 w/ prob
ability -9.081652641296387'
```




```
'-------------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3cccs3)cc2)cc1'
```

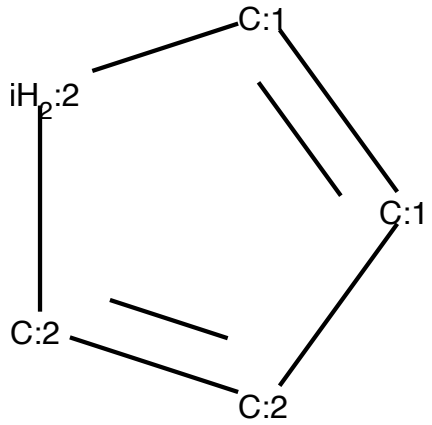



```
'-------------------------------------------------------------'

'-----Step-7-----'
'Generate next fragment: 0.9999912977218628'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.33539807
79647827'
```

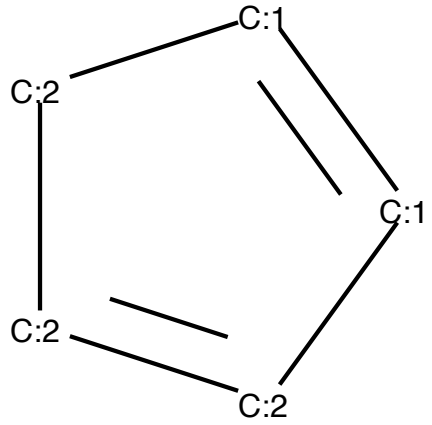
'--'

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



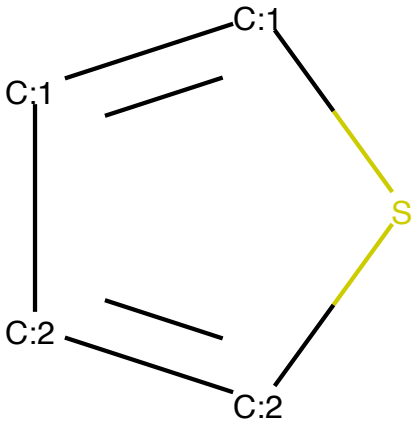
'--'

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



'--'

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

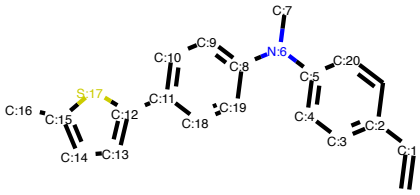



```
'------------------------------------------------------------'

'Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ probability -6.82
2177410125732'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C)s3)cc2)cc1'
```

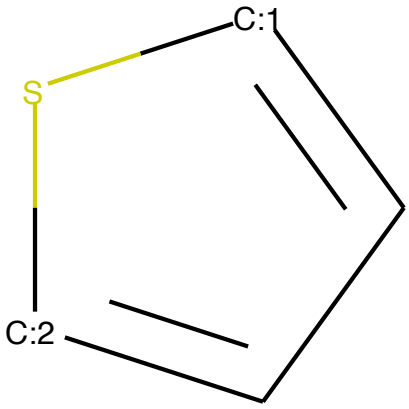



```
'------------------------------------------------------------'

'-----Step-8-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -0.043457
83218741417'
```

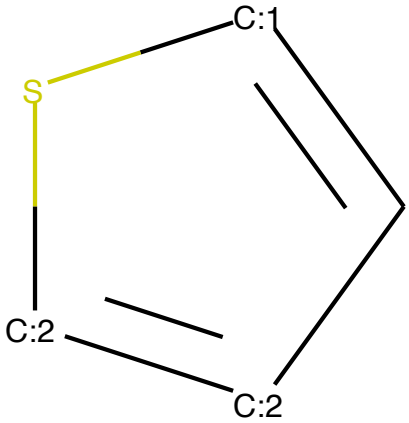
```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-3.9461703300476074'
```



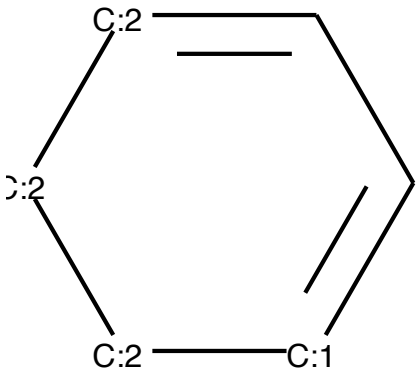

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -4.16166353225708'
```



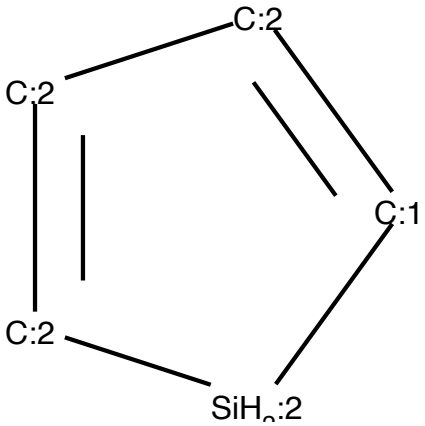

```
'------------------------------------------------------------'

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



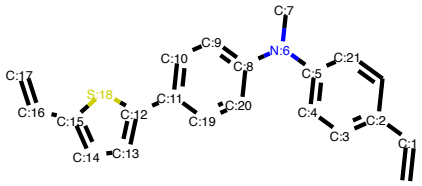
'--'

'Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:2][CH:2]=[CH:2][SiH2:2]1 w/ probability -8.179245948791504'



'--'

'Attaching fragment [CH2:1]=[CH2:2]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C)s3)cc2)cc1'



'--'

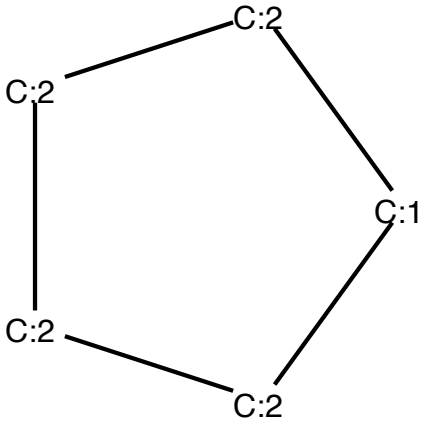
'-----Step-9-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.14302974939346313'

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -2.04910898
20861816'
```

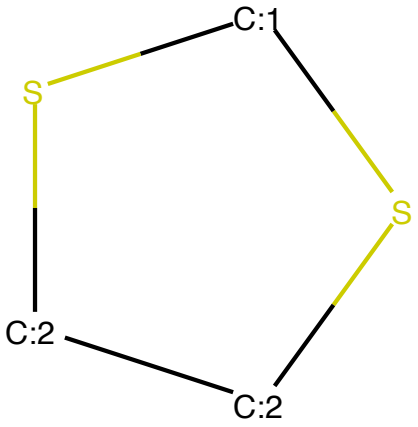
```
'------------------------------------------------------------'

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



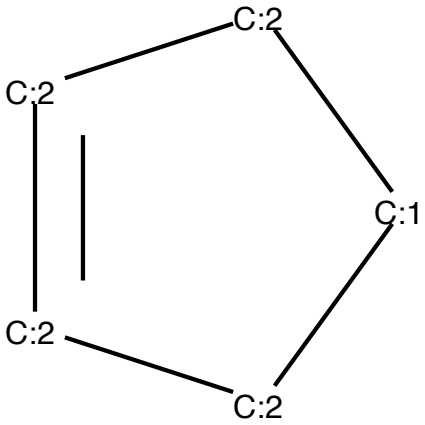

```
'------------------------------------------------------------'

'Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ probabi
lity -7.512922763824463'
```



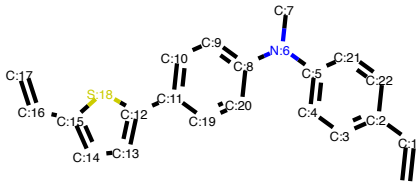
'--'

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



'--'

'Attaching fragment C'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C)s3)cc2)cc1'



'--'

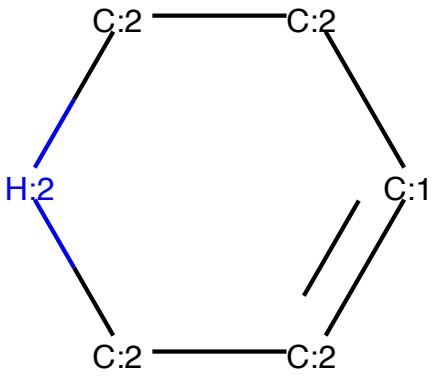
'-----Step-10-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability 0.0'

```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -17.89023
5900878906'
```

```
'------------------------------------------------------------'

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

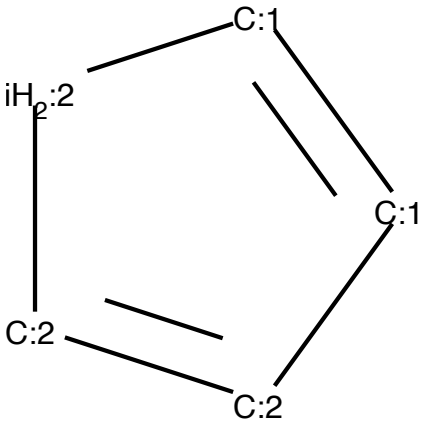



```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -18.61927413940
4297'
```

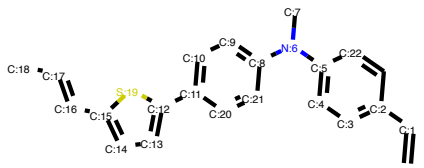
```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=CC)s3)cc2)cc1'
```




```
'------------------------------------------------------------'

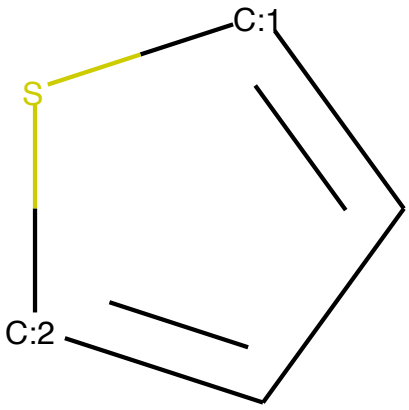
'-----Step-11-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C#N and its specific config N#[CH:1] w/ probability -1.7762025890988
298e-05'
```

```
'------------------------------------------------------------'

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

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -12.286079406738281'
```

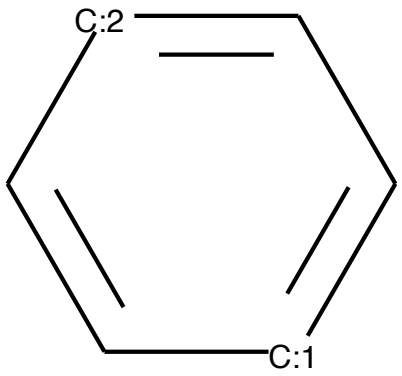



```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -12.406049728393555'
```

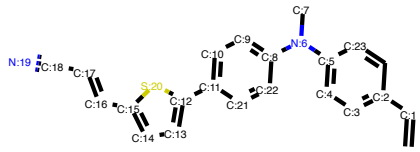
```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -14.150064468383789'
```




```
'------------------------------------------------------------'

'Attaching fragment N#[CH:1]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=CC#N)s3)cc2)cc1'
```




```
'------------------------------------------------------------'

'-----Step-12-----'
'-----Step-13-----'
'-----Step-14-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.19209282
44535389e-07'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -16.10691
0705566406'
```

```
'------------------------------------------------------------'
```

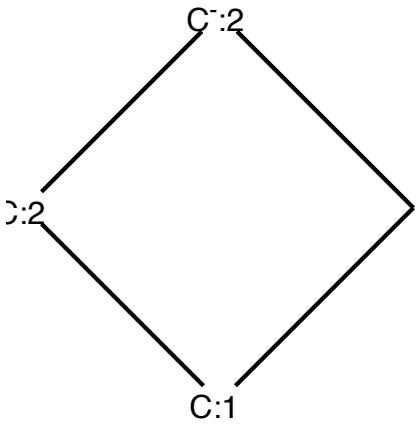
```
'Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ probability -19.3
038387298584'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -21.74822235107
422'
```

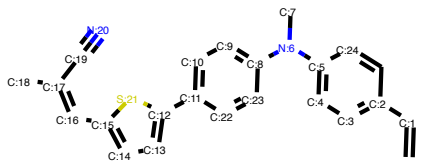
```
'-------------------------------------------------------------'

'Molecule [CH-]1CCC1 and its specific config C1[CH2:1][CH2:2][CH-:2]1 w/ proba
bility -23.587783813476562'
```




```
'-------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C)C#N)s3)cc2)cc1'
```




```
'-------------------------------------------------------------'

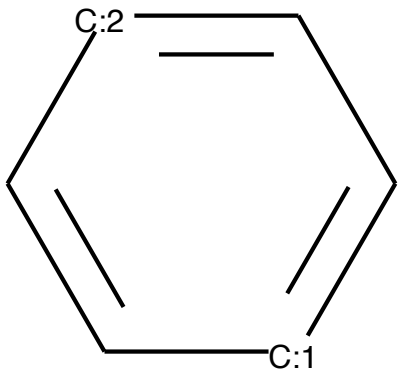
'-----Step-15-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.2121753990650177'
```

'--'

'Molecule C#N and its specific config N#[CH:1] w/ probability -1.7091403007507
324'

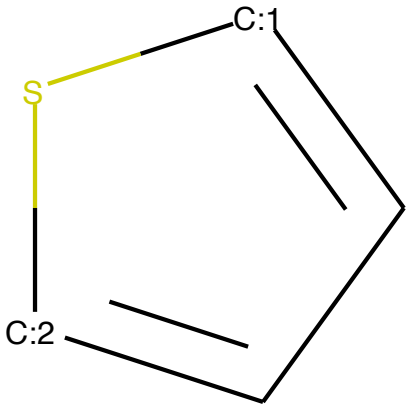
'--'

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



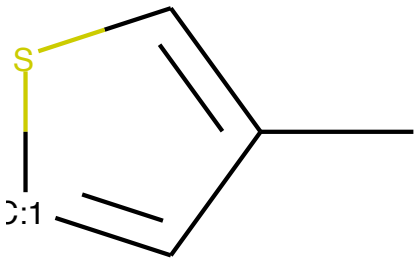
'--'

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



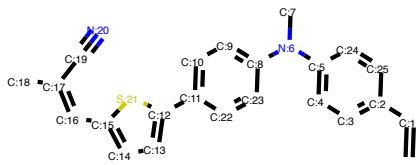
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=CS[CH:1]=C1 w/ probability -8
.244633674621582'



'--'

'Attaching fragment C'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C)C#N)s3)cc2)cc1'



'--'

'-----Step-16-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=O and its specific config O=[CH2:1] w/ probability -1.192092824453
5389e-07'

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -15.9361305
2368164'
```

```
'------------------------------------------------------------'

'Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ probability -17.4
70401763916016'
```

```
'------------------------------------------------------------'

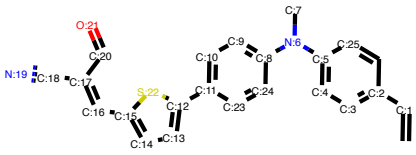
'Molecule CF and its specific config F[CH3:1] w/ probability -17.6341819763183
6'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config N[CH3:1] w/ probability -18.9347305297851
56'
```

```
'------------------------------------------------------------'

'Attaching fragment O=[CH2:1]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C#N)C=O)s3)cc2)cc1'
```




```
'------------------------------------------------------------'

'-----Step-17-----'
'-----Step-18-----'
'Generate next fragment: 0.9999843835830688'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CO and its specific config O[CH3:1] w/ probability -0.06822425872087
479'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -3.18861913
68103027'
```

```
'------------------------------------------------------------'

'Molecule CF and its specific config F[CH3:1] w/ probability -4.91548061370849
6'
```

```
'------------------------------------------------------------'

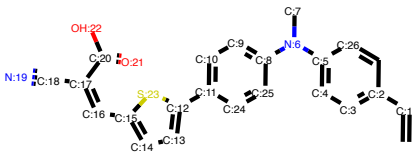
'Molecule CN and its specific config N[CH3:1] w/ probability -5.20636653900146
5'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -5.319983482360
84'
```

```
'------------------------------------------------------------'

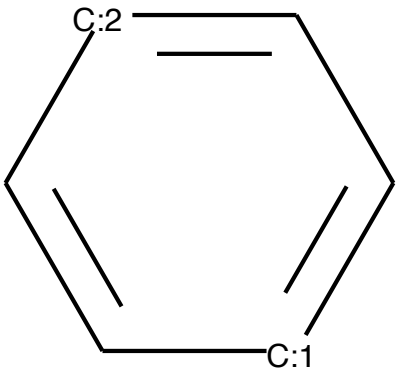
'Attaching fragment O[CH3:1]'
'Latest partial graph: C=Cc1ccc(N(C)c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)cc2)cc1'
```




```
'------------------------------------------------------------'

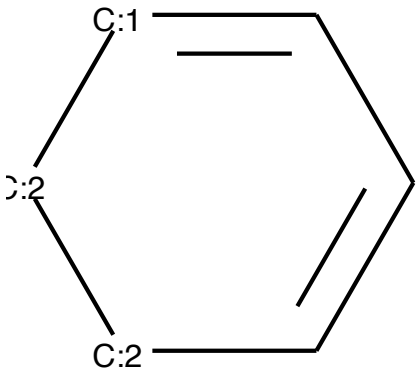
'-----Step-19-----'
'-----Step-20-----'
'-----Step-21-----'
'-----Step-22-----'
'-----Step-23-----'
'-----Step-24-----'
```

```
'-----Step-25-----'
'-----Step-26-----'
'-----Step-27-----'
'-----Step-28-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.019880110397934914'
```



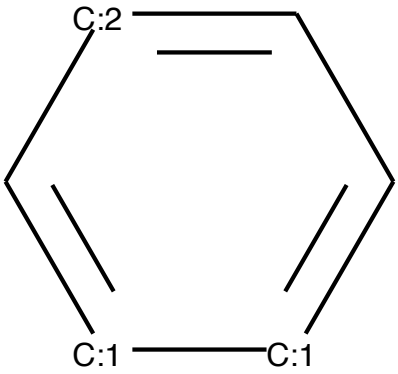

```
'------------------------------------------------------------'

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



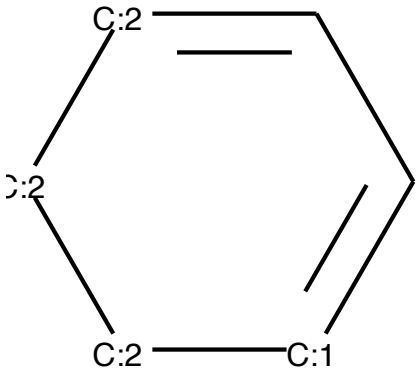

```
'------------------------------------------------------------'

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



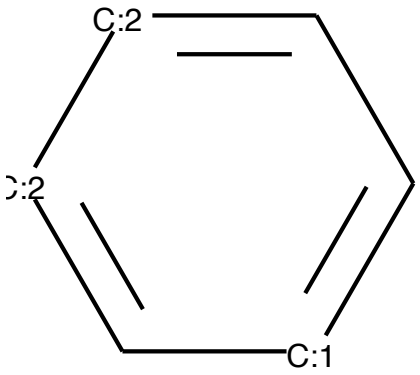
```
'------------------------------------------------------------'

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



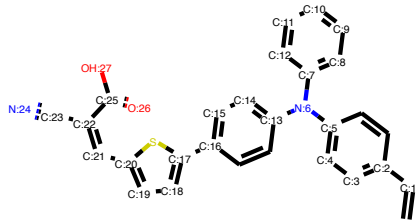

```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: C=Cc1ccc(N(c2ccccc2)c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)cc2)
cc1'
```



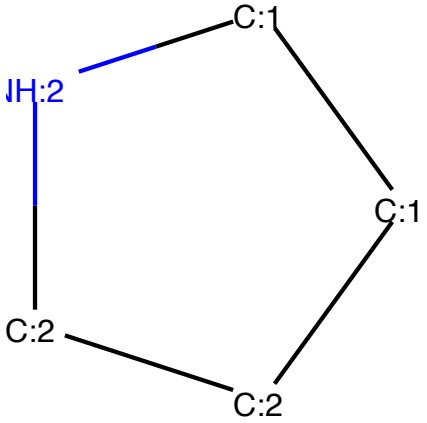

```
'------------------------------------------------------------'

'-----Step-29-----'
'Generate next fragment: 0.9999998807907104'
```

```
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.35037717
22316742'
```

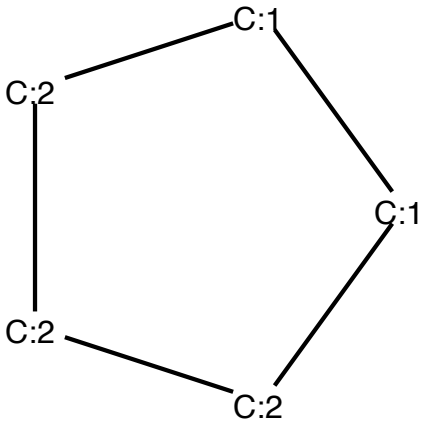
```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

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

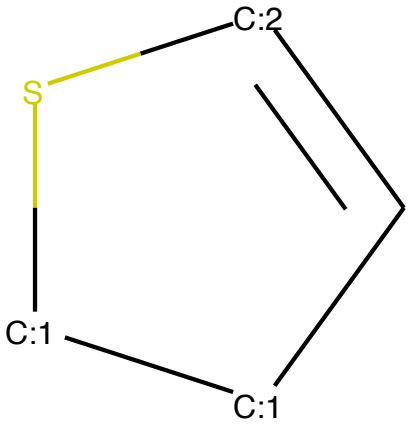



```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -5.63254261
0168457'
```

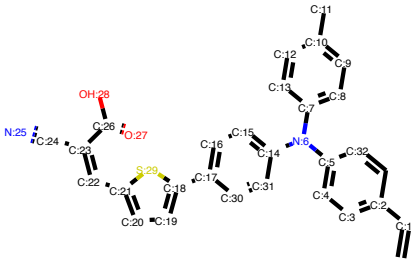
```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -6.00679349899292'
```



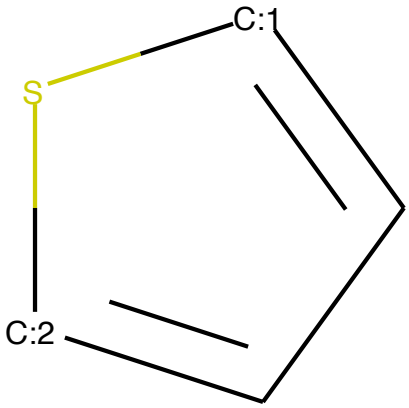

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=Cc1ccc(N(c2ccc(C)cc2)c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)c
c2)cc1'
```



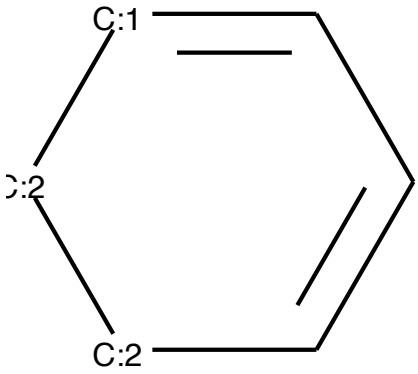

```
'------------------------------------------------------------'

'-----Step-30-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.8655498623847961'
```



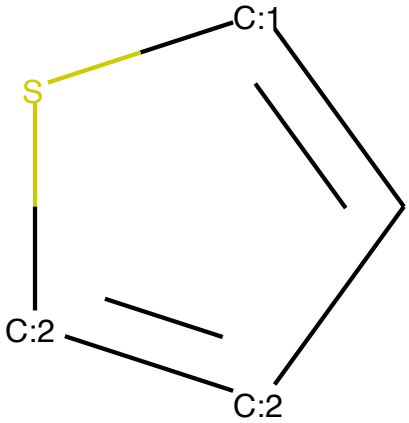
'--'

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



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -2.5964910984039307'

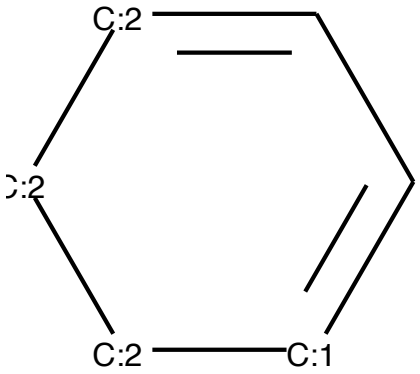


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -3.465882
0629119873'

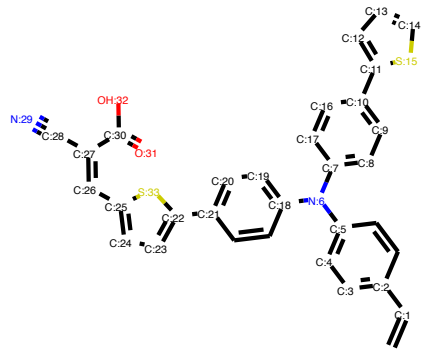
```
'-----------------------------------------------------------'

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




```
'-----------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: C=Cc1ccc(N(c2ccc(-c3cccs3)cc2)c2ccc(-c3ccc(C=C(C#N)C(=O
)O)s3)cc2)cc1'
```

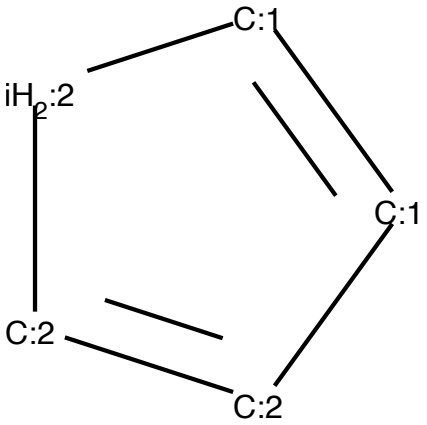



```
'-----------------------------------------------------------'

'-----Step-31-----'
'Generate next fragment: 0.9997395873069763'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00184366
07206240296'
```

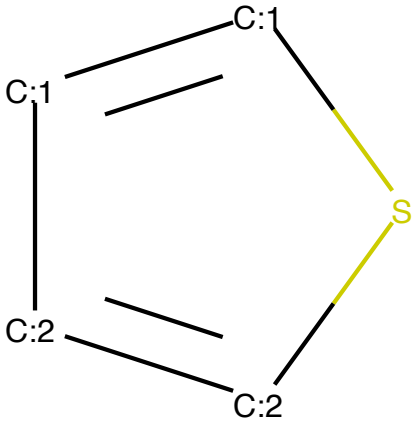
```
'------------------------------------------------------------'

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



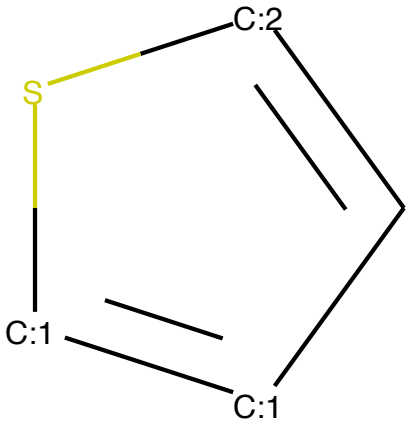

```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -8.098220825195312'
```

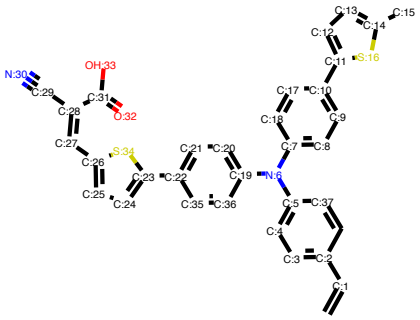


'--'

'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -8.83
3429336547852'

'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C)s3)cc2)c2ccc(-c3ccc(C=C(C#N)C
(=O)O)s3)cc2)cc1'

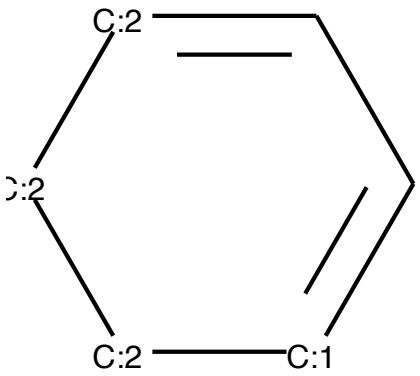


'--'

'-----Step-32-----'
'Generate next fragment: 0.9999994039535522'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -0.005627
384874969721'

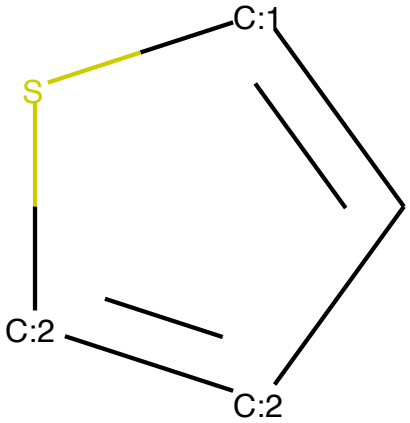
```
'------------------------------------------------------------'

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



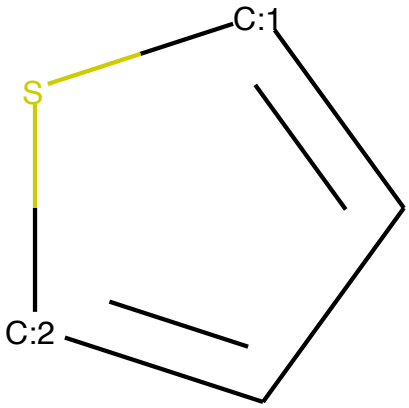

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -7.332898139953613'
```



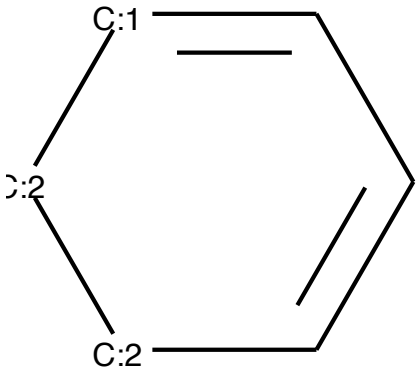

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-7.666647911071777'
```



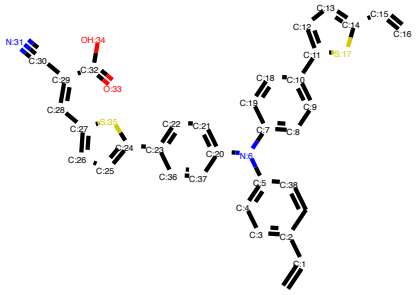
'--'

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



'--'

'Attaching fragment [CH2:1]=[CH2:2]'
'Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C)s3)cc2)c2ccc(-c3ccc(C=C(C#N
)C(=O)O)s3)cc2)cc1'



'--'

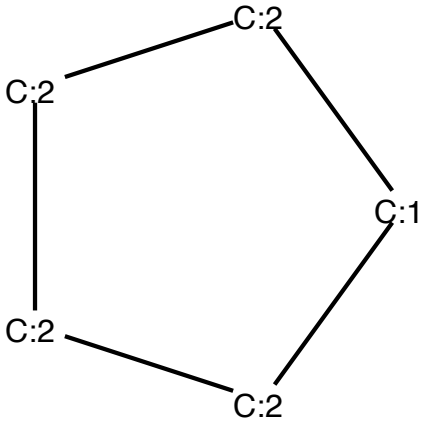
'-----Step-33-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.13677558302879333'

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -2.23774719
23828125'
```

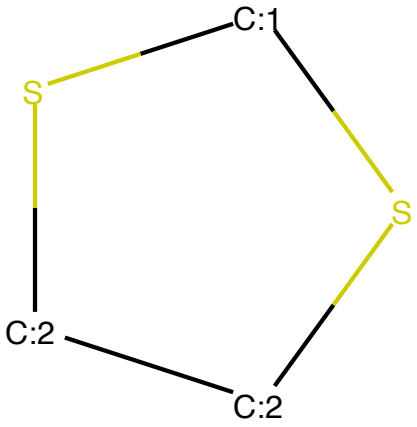
```
'------------------------------------------------------------'

'Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]
1 w/ probability -4.045051574707031'
```



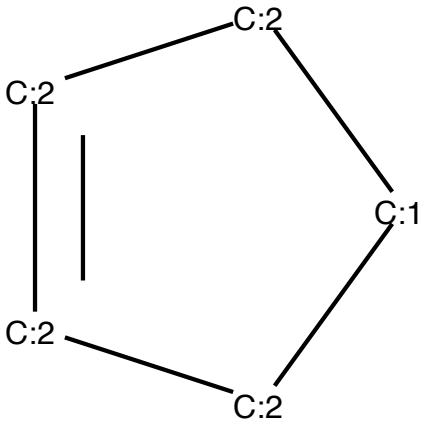

```
'------------------------------------------------------------'

'Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ probabi
lity -6.126567840576172'
```



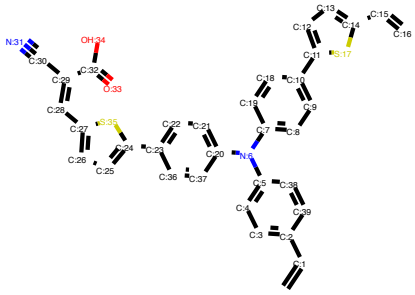
'--'

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



'--'

'Attaching fragment C'
'Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C)s3)cc2)c2ccc(-c3ccc(C=C(C#N
)C(=O)O)s3)cc2)cc1'

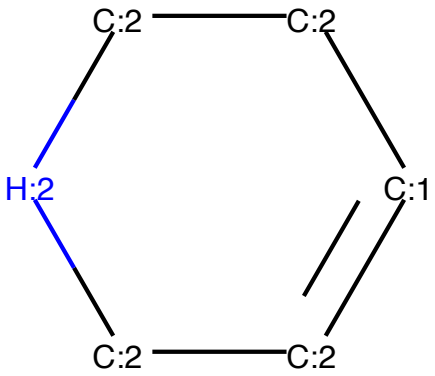


'--'

'-----Step-34-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -3.57627811
8089249e-07'

'--'

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



'--'

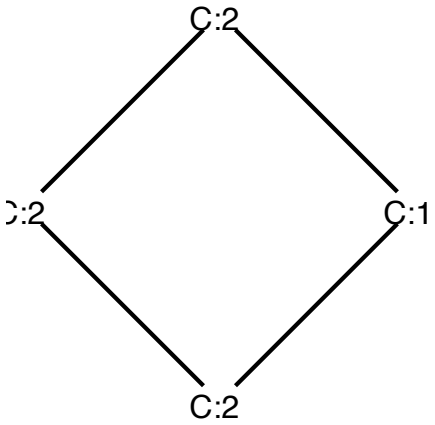
'Molecule C=O and its specific config O=[CH2:1] w/ probability -16.07077217102 0508'

'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -17.90203 094482422'

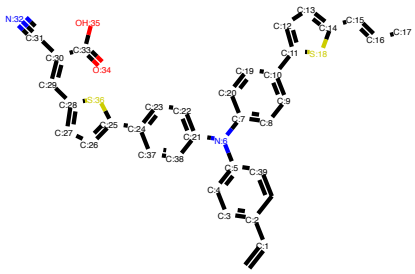
```
'------------------------------------------------------------'

'Molecule C1CCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2]1 w/ pro
bability -20.270742416381836'
```




```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=CC)s3)cc2)c2ccc(-c3ccc(C=C(C#
N)C(=O)O)s3)cc2)cc1'
```



```
'------------------------------------------------------------'

'-----Step-35-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C#N and its specific config N#[CH:1] w/ probability -3.9338988244708
16e-06'
```

```
'------------------------------------------------------------'

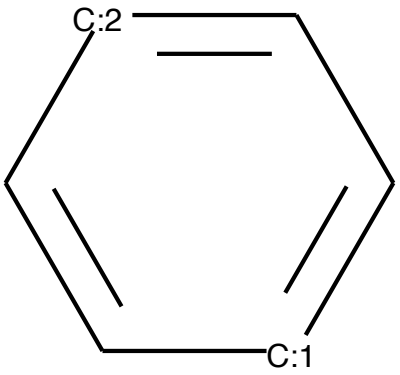
'Molecule C and its specific config C w/ probability -13.240961074829102'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -13.43037414550
7812'
```

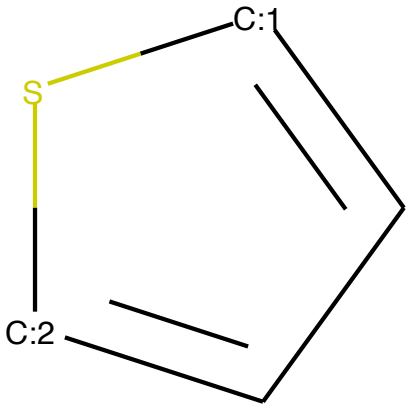
```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -14.62369441986084'
```



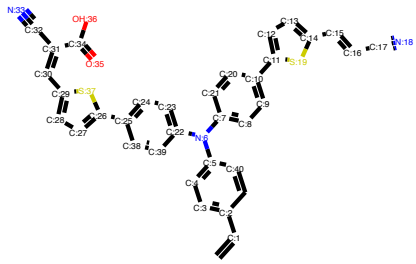
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -15.115761756896973'



'--'

'Attaching fragment 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'



'--'

'-----Step-36-----'
'-----Step-37-----'
'-----Step-38-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability 0.0'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -17.41456
0317993164'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -20.9531631
46972656'
```

```
'------------------------------------------------------------'
```

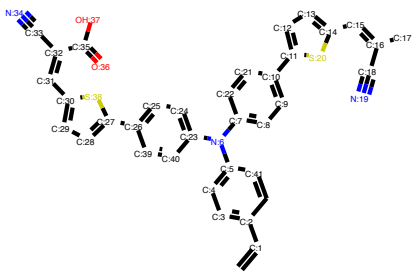
```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -21.03979301452
6367'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -21.3284091949462
9'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'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'
```




```
'------------------------------------------------------------'

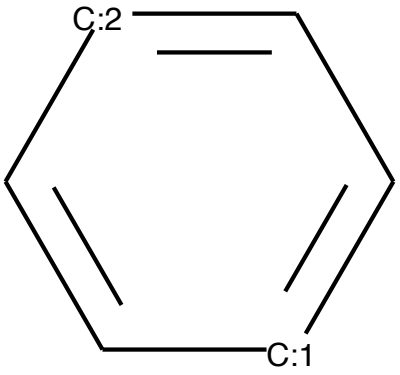
'-----Step-39-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.46422889828681946'
```

'--'

'Molecule C#N and its specific config N#[CH:1] w/ probability -1.0358774662017
822'

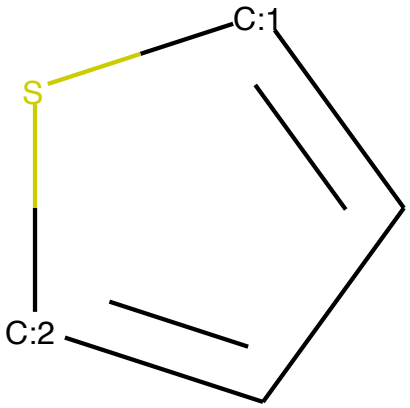
'--'

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



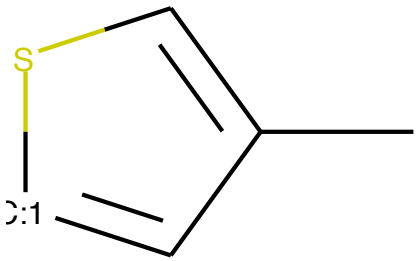
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-8.575750350952148'



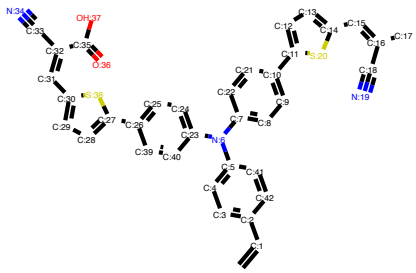
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=CS[CH:1]=C1 w/ probability -9
.510355949401855'



'--'

'Attaching fragment C'
'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'



'--'

'-----Step-40-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=O and its specific config O=[CH2:1] w/ probability -1.192092824453
5389e-07'

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -16.4325180
05371094'
```

```
'------------------------------------------------------------'

'Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ probability -17.1
05947494506836'
```

```
'------------------------------------------------------------'

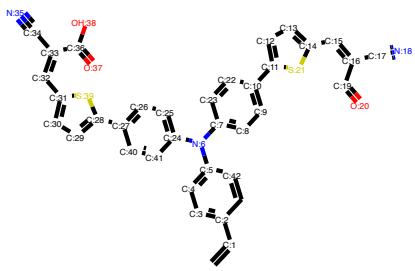
'Molecule CF and its specific config F[CH3:1] w/ probability -18.2727642059326
17'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config N[CH3:1] w/ probability -18.6359996795654
3'
```

```
'------------------------------------------------------------'

'Attaching fragment 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'
```




```
'------------------------------------------------------------'

'-----Step-41-----'
'-----Step-42-----'
'Generate next fragment: 0.9999998807907104'
'Top 5 next fragments to attach (current and potential graph)'
```

```
'Molecule CO and its specific config O[CH3:1] w/ probability -0.12501999735832
214'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -2.86770129
2037964'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -2.943198
9192962646'
```

```
'------------------------------------------------------------'
```

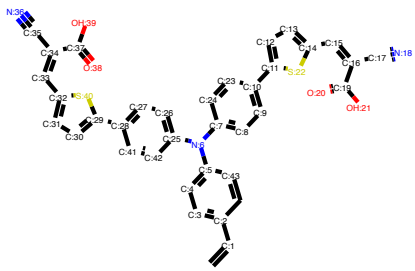
```
'Molecule CF and its specific config F[CH3:1] w/ probability -5.91733598709106
45'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -5.96997737
8845215'
```

```
'------------------------------------------------------------'

'Attaching fragment O[CH3:1]'
'Latest partial graph: C=Cc1ccc(N(c2ccc(-c3ccc(C=C(C#N)C(=O)O)s3)cc2)c2ccc(-c3
ccc(C=C(C#N)C(=O)O)s3)cc2)cc1'
```



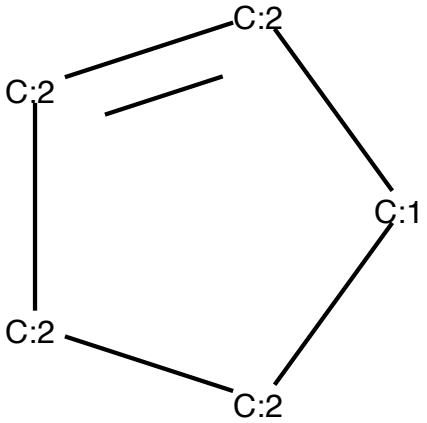

```
'------------------------------------------------------------'

'-----Step-43-----'
'-----Step-44-----'
'-----Step-45-----'
'-----Step-46-----'
'-----Step-47-----'
```

```
'-----Step-48-----'
'-----Step-49-----'
'-----Step-50-----'
'-----Step-51-----'
'-----Step-52-----'
'-----Step-53-----'
'-----Step-54-----'
'-----Step-55-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -7.39094866
7307384e-06'
```

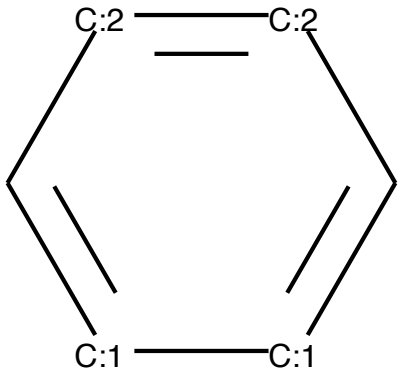
```
'------------------------------------------------------------'

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



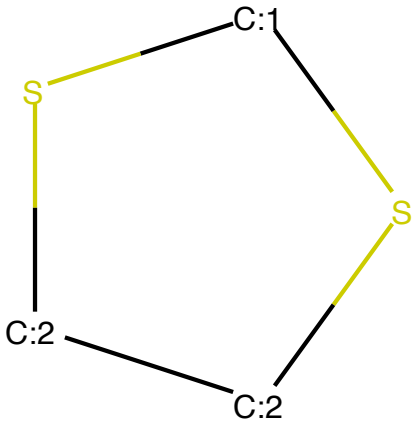

```
'------------------------------------------------------------'

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



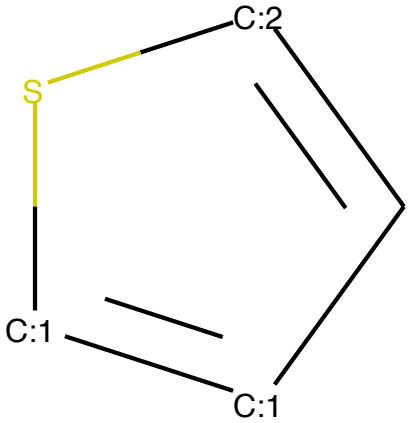

```
'------------------------------------------------------------'

'Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ probabi
lity -13.665507316589355'
```



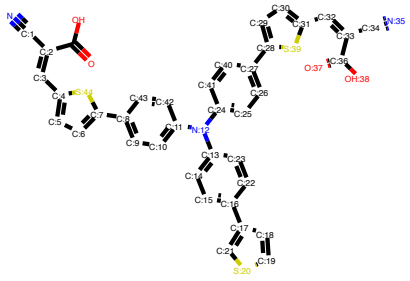

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -14.961623191833496'
```




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:2]S[CH:1]=[CH:1]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'
```

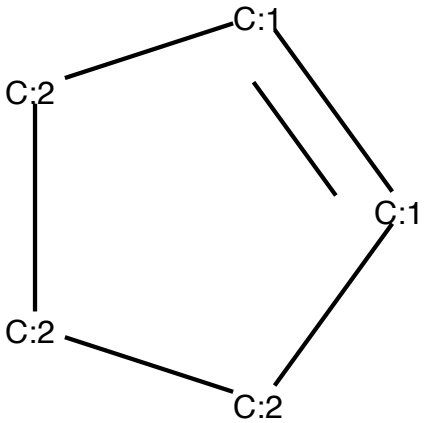


'--'

'-----Step-56-----'
'Generate next fragment: 0.9999998807907104'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00605972
6700186729'

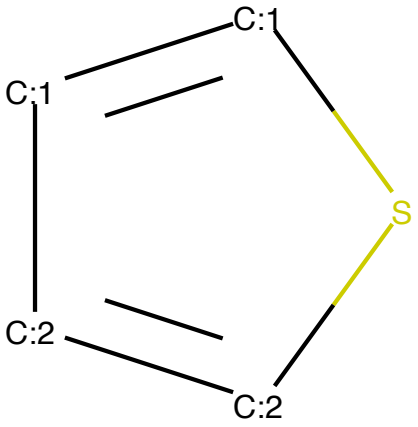
'--'

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



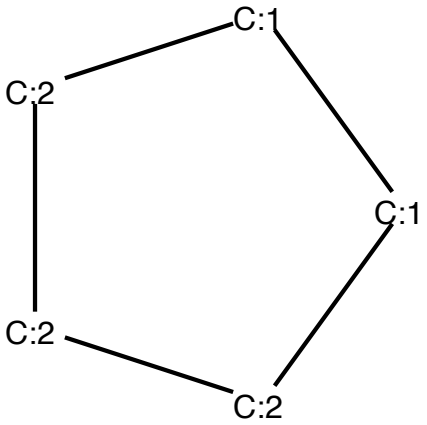
'--'

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



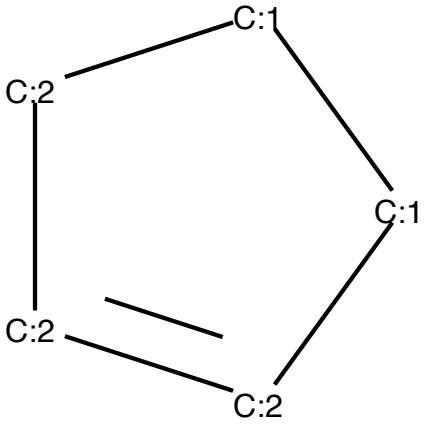
'--'

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



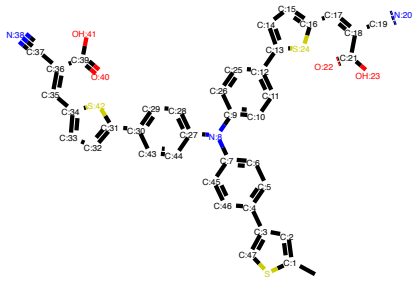
'--'

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



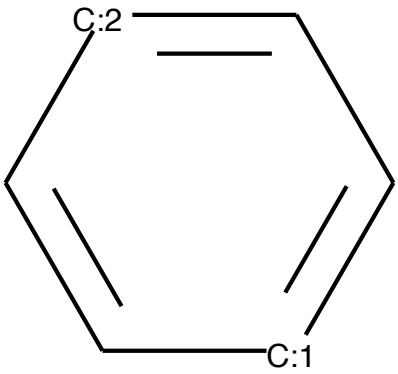
'--'

'Attaching fragment [CH3:1][CH3:2]'
'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'



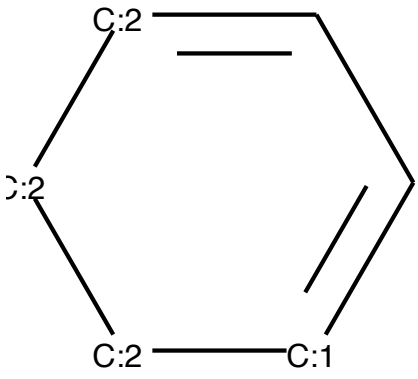
'--'

'-----Step-57-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.9793902635574341'



'--'

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

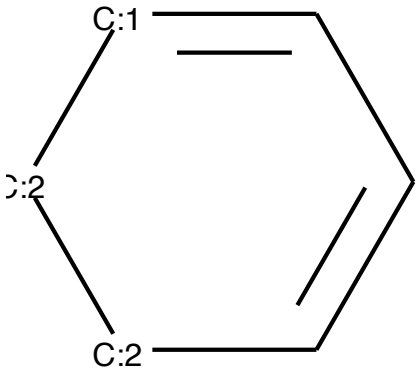


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -1.395793
1995391846'

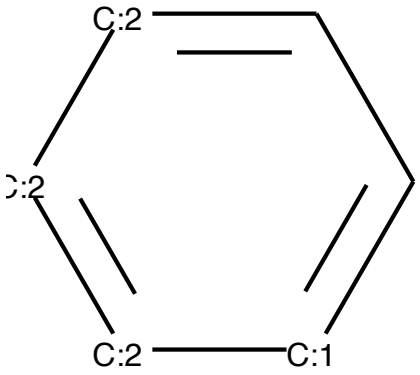
```
'------------------------------------------------------------'

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



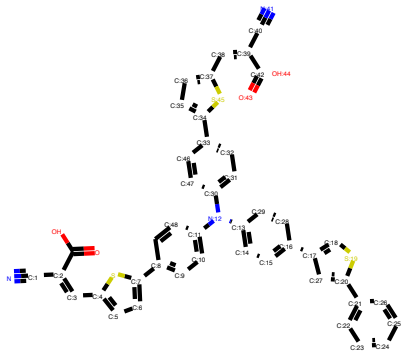

```
'------------------------------------------------------------'

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



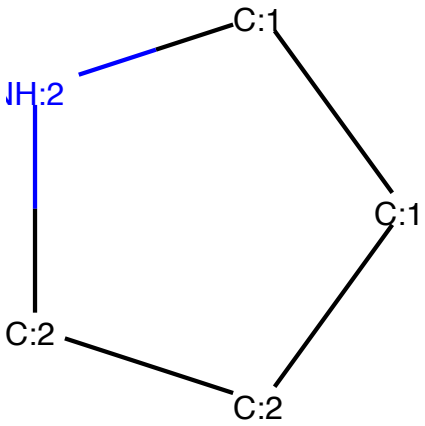

```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: N#CC(=Cc1ccc(-c2ccc(N(c3ccc(-c4csc(-c5ccccc5)c4)cc3)c3c
cc(-c4ccc(C=C(C#N)C(=O)O)s4)cc3)cc2)s1)C(=O)O'
```



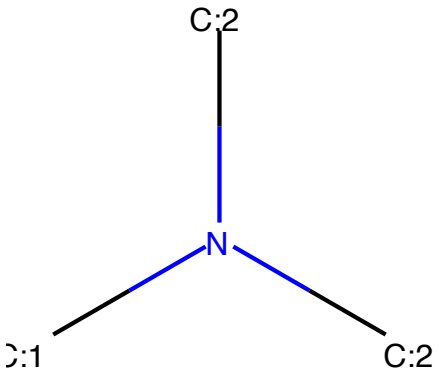
'--'

'-----Step-58-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ probability -0.13806338608264923'



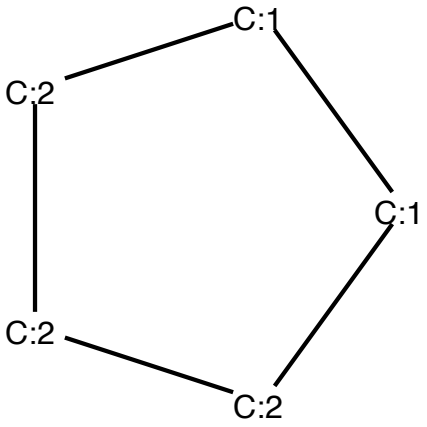
'--'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -2.325024366378784'



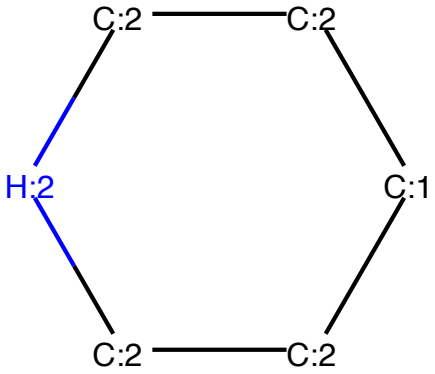
'--'

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




```
'-------------------------------------------------------------'

'Molecule C1CCNCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2][CH2:2]
[CH2:2]1 w/ probability -4.540945053100586'
```

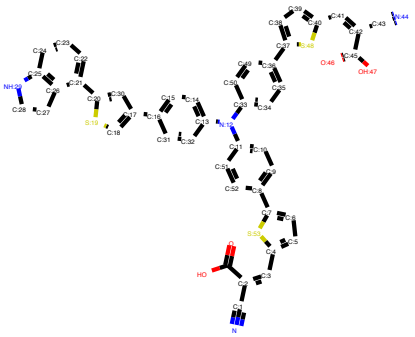



```
'-------------------------------------------------------------'

'Molecule CBr and its specific config Br[CH3:1] w/ probability -6.290832996368
408'
```

```
'-------------------------------------------------------------'

'Attaching fragment [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1'
'Latest partial graph: N#CC(=Cc1ccc(-c2ccc(N(c3ccc(-c4csc(-c5cccc6c5CCN6)c4)cc
3)c3ccc(-c4ccc(C=C(C#N)C(=O)O)s4)cc3)cc2)s1)C(=O)O'
```

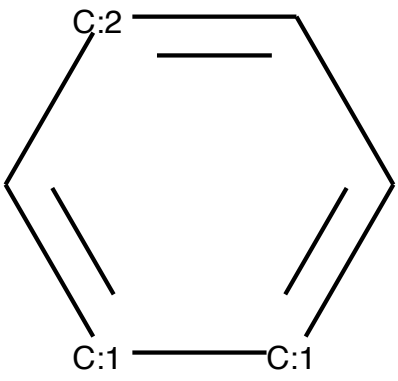


'--'

'-----Step-59-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CN and its specific config C[NH2:1] w/ probability -0.76087278127670
29'

'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ pr
obability -1.268972396850586'



'--'

'Molecule N and its specific config N w/ probability -1.4923498630523682'

```
'------------------------------------------------------------'

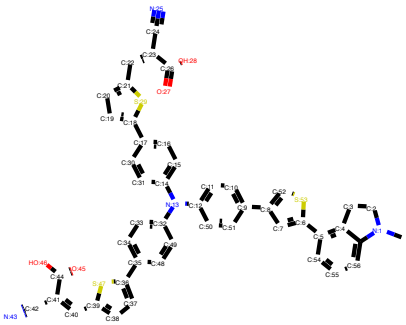
'Molecule C and its specific config C w/ probability -4.306382179260254'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -4.55280733
1085205'
```

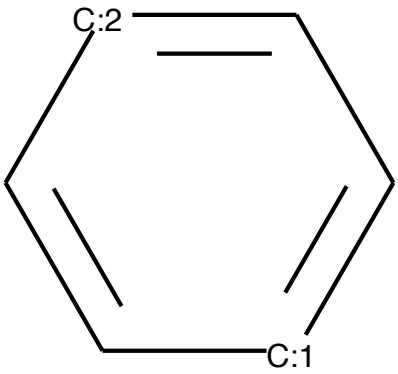
```
'------------------------------------------------------------'

'Attaching fragment C[NH2:1]'
'Latest partial graph: CN1CCc2c(-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'
```



'--'

'-----Step-60-----'
'Generate next fragment: 0.767174482345581'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.09402607381343842'



'--'

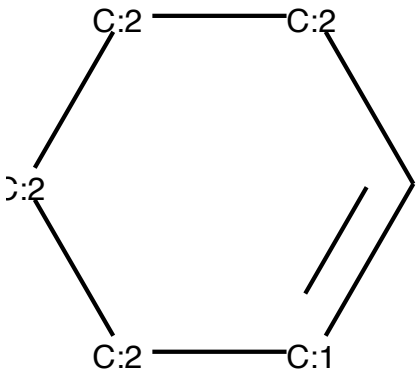
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -2.44133615
4937744'

'--'

'Molecule C and its specific config C w/ probability -6.683434963226318'

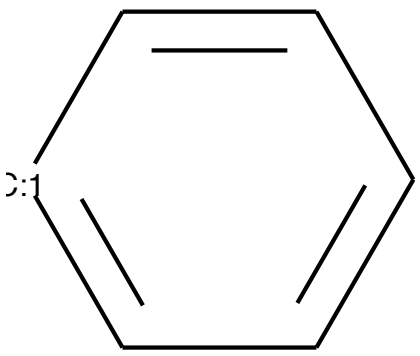
'--'

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



'--'

'Molecule C1=CC=CC=C1 and its specific config C1=CC=[CH:1]C=C1 w/ probability -7.661508083343506'

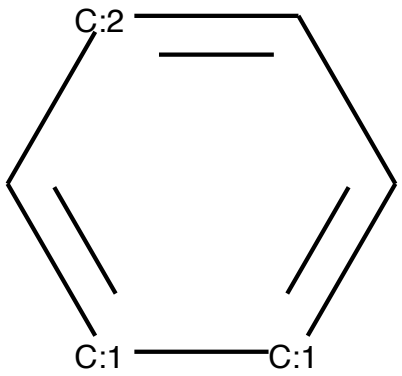


'--'

'-----Step-61-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CN and its specific config C[NH2:1] w/ probability -0.7608727812767029'

'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=C1 w/ pr
obability -1.268972396850586'



'--'

'Molecule N and its specific config N w/ probability -1.4923498630523682'

'--'

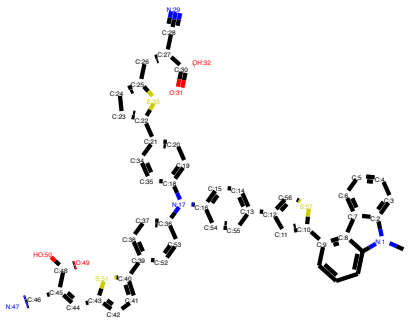
'Molecule C and its specific config C w/ probability -4.306382179260254'

```
'------------------------------------------------------------'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -4.55280733
1085205'
```

```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1][CH:1]=C[CH:2]=C1'
'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'
```

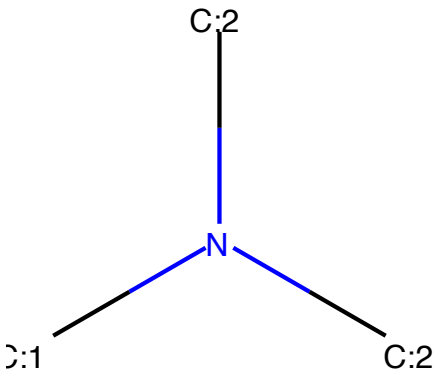


```
'------------------------------------------------------------'

'-----Step-62-----'
'Generate next fragment: 0.9999222755432129'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.24081954
36000824'
```

```
'------------------------------------------------------------'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -1.5972133874893188'
```

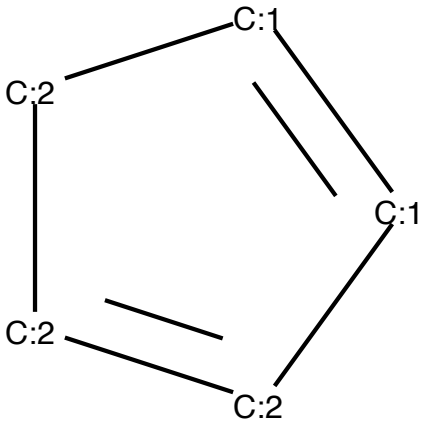



```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -5.81991767
8833008'
```

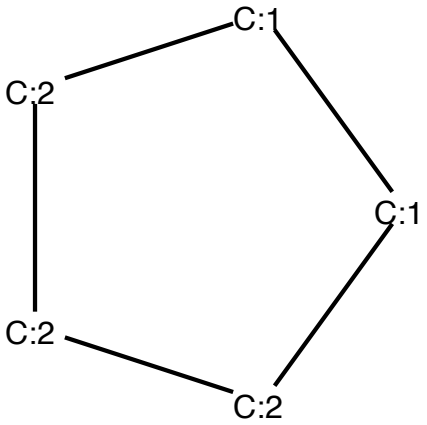
```
'------------------------------------------------------------'

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



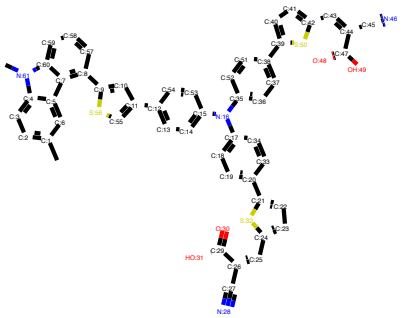
'--'

'Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]1 w/ probability -6.495670795440674'



'--'

'Attaching fragment [CH3:1][CH3:2]'
'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'

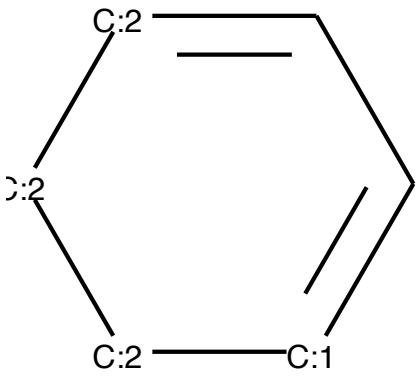


'--'

'-----Step-63-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -1.1266475915908813'

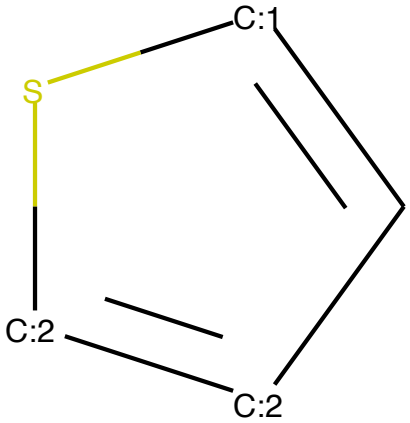
```
'------------------------------------------------------------'

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



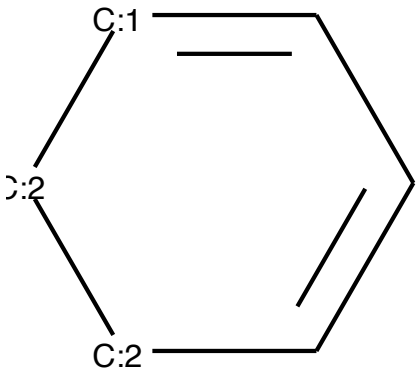

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -1.7480614185333252'
```



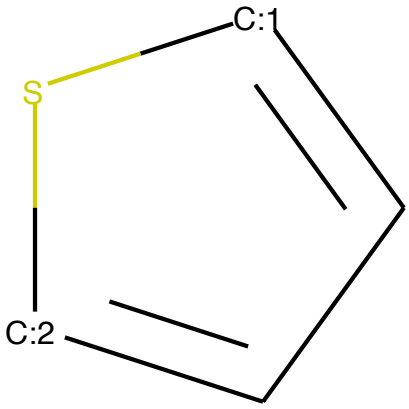

```
'------------------------------------------------------------'

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



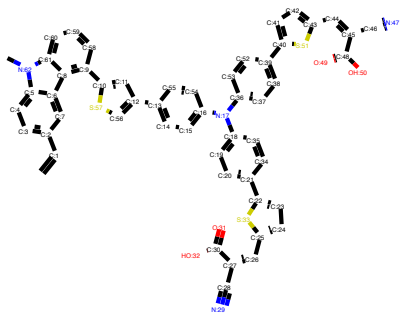
'--'

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



'--'

'Attaching fragment [CH2:1]=[CH2:2]'
'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'



'--'

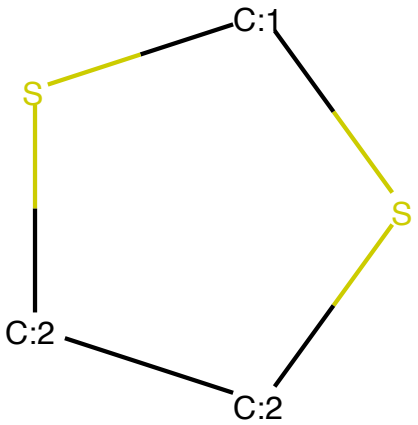
'-----Step-64-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.5033437609672546'

```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -1.5061886310577393'
```

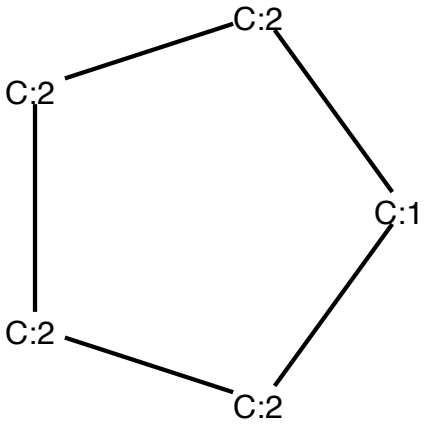
```
'------------------------------------------------------------'

'Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ probabi
lity -2.09509015083313'
```



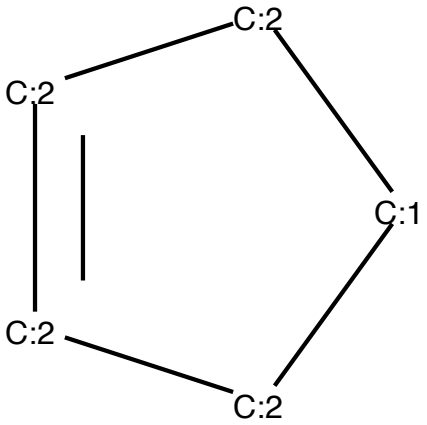

```
'------------------------------------------------------------'

'Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]
1 w/ probability -3.5078327655792236'
```



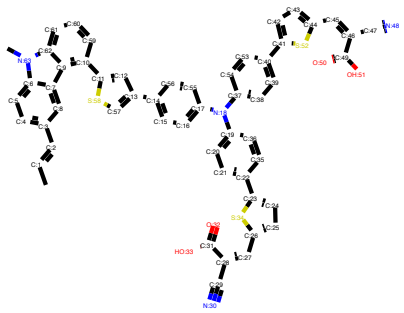
'--'

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



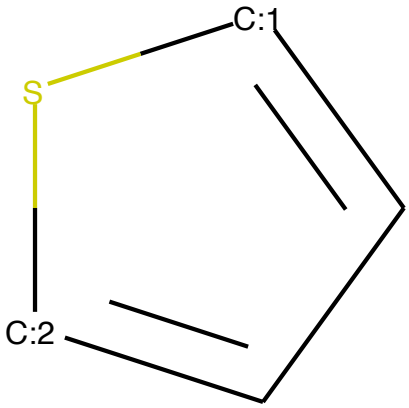
'--'

'Attaching fragment [CH3:1][CH3:2]'
'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'



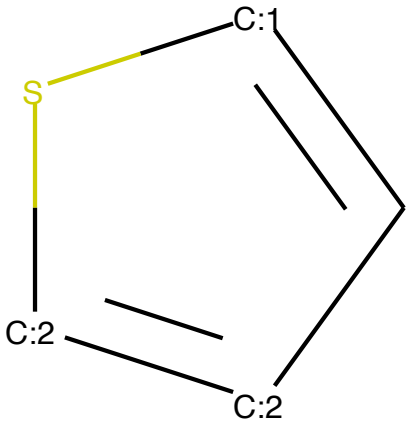
'--'

'-----Step-65-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.1306476891040802'



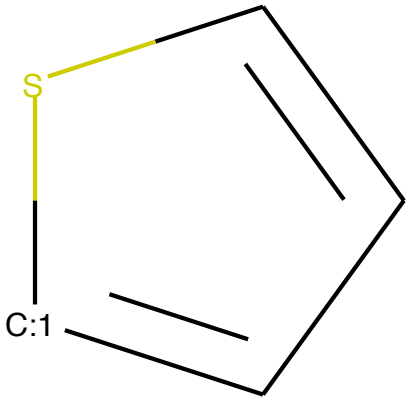
'--'

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



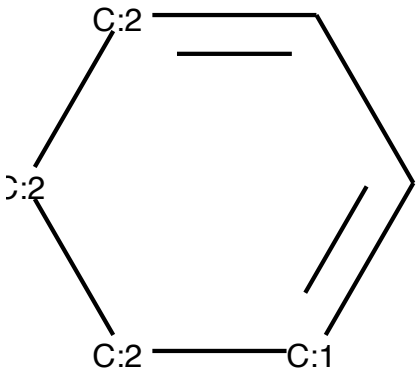
'--'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -3.4
541702270507812'



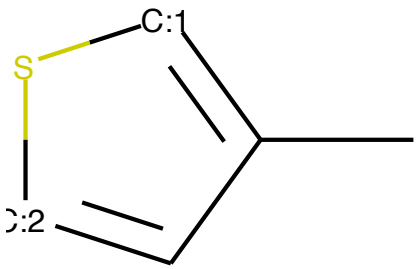
'--'

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



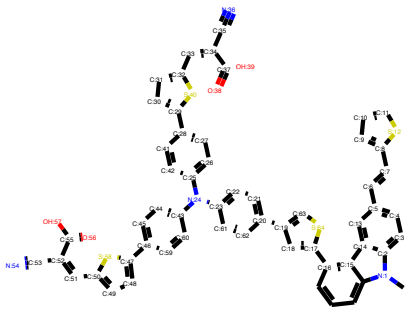
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -4.749369144439697'



'--'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'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'

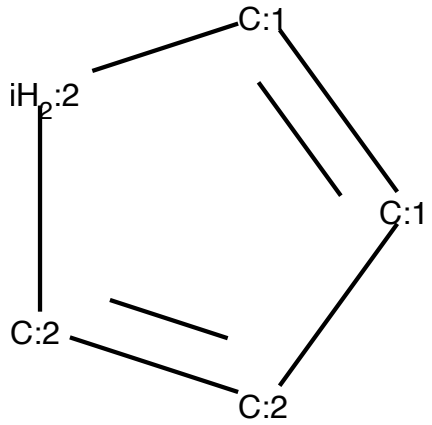


'--'

'-----Step-66-----'
'Generate next fragment: 0.871691882610321'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.06206965
819001198'

```
'------------------------------------------------------------'

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

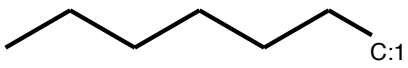



```
'------------------------------------------------------------'

'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -4.45
929479598999'

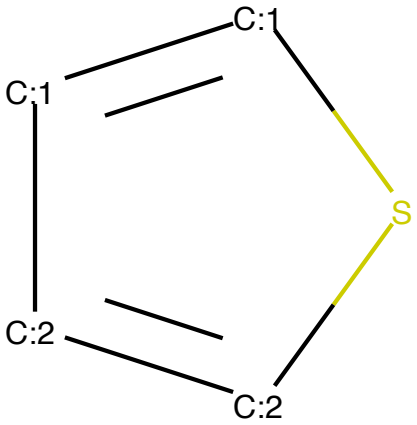
'------------------------------------------------------------'

'Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ probability -4.9332
38506317139'
```



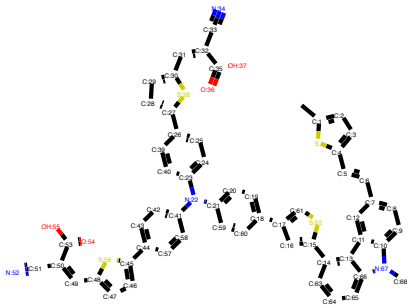
'--'

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



'--'

'Attaching fragment [CH3:1][CH3:2]'
'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'

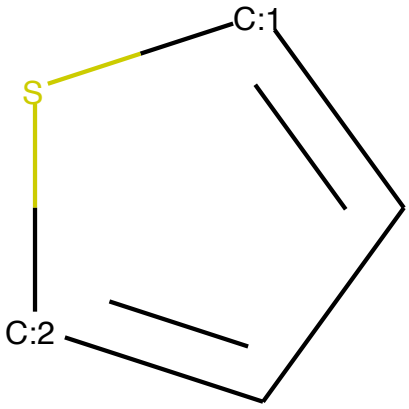


'--'

'-----Step-67-----'
'Generate next fragment: 0.9999935626983643'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -0.050873
31682443619'

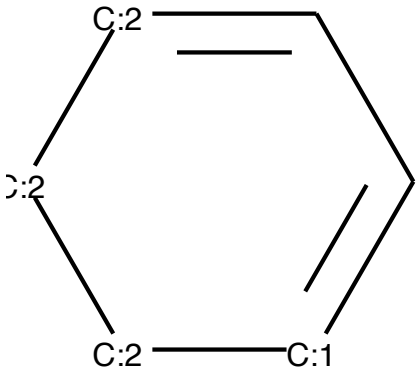
```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-3.4192779064178467'
```



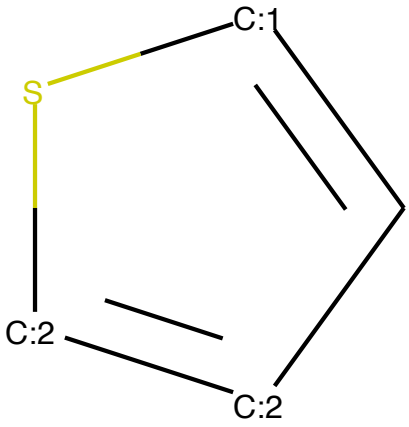

```
'------------------------------------------------------------'

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



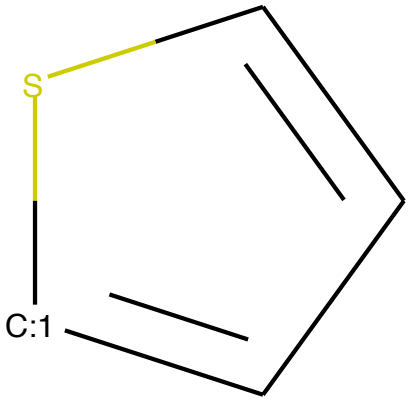

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -5.079668045043945'
```



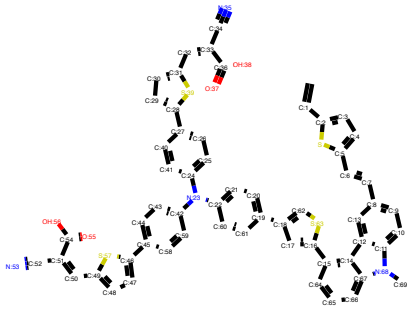
'--'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -6.6
52697563171387'



'--'

'Attaching fragment [CH2:1]=[CH2:2]'
'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'



'--'

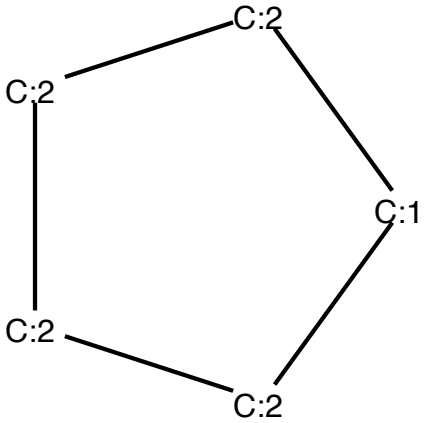
'-----Step-68-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.008251977153122425'

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -4.81123828
88793945'
```

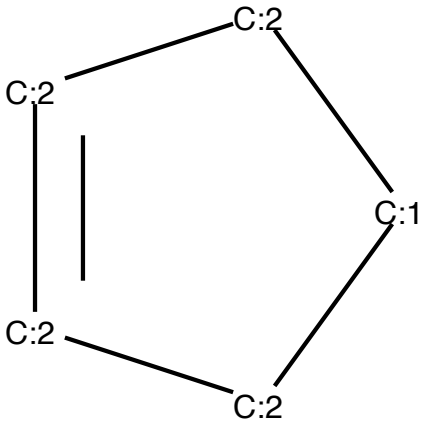
```
'------------------------------------------------------------'

'Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]
1 w/ probability -9.474623680114746'
```



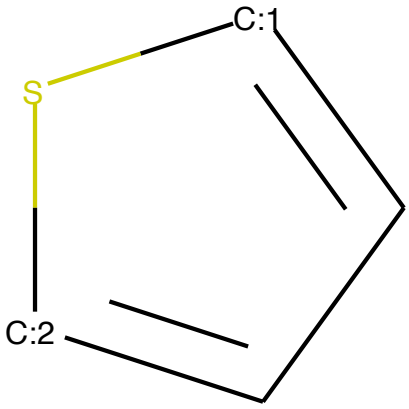

```
'------------------------------------------------------------'

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



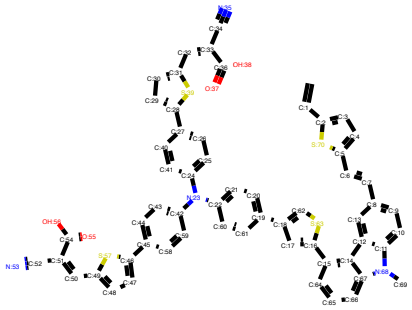
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -14.705827713012695'



'--'

'Attaching fragment C'
'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'



'--'

'-----Step-69-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.722029527532868e-06'

```
'------------------------------------------------------------'

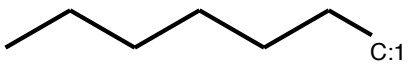
'Molecule C=O and its specific config O=[CH2:1] w/ probability -12.14200878143
3105'
```

```
'------------------------------------------------------------'

'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -16.1
3909912109375'
```

```
'------------------------------------------------------------'

'Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ probability -16.460
16502380371'
```

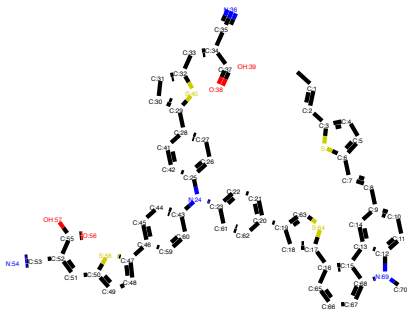


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -16.62950
325012207'

'--'

'Attaching fragment [CH3:1][CH3:2]'
'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'

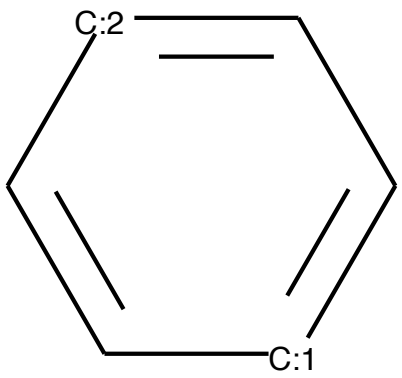


'--'

'-----Step-70-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C#N and its specific config N#[CH:1] w/ probability -0.0001243275619
3447858'

'--'

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



'--'

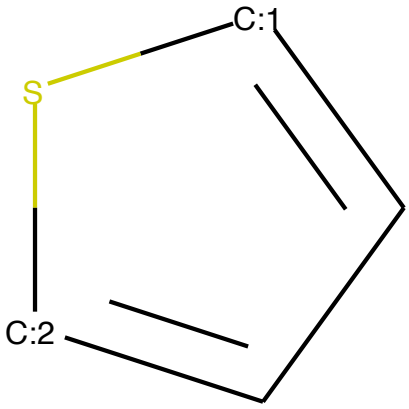
'Molecule C and its specific config C w/ probability -10.463768005371094'

'--'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -11.70853519439
6973'

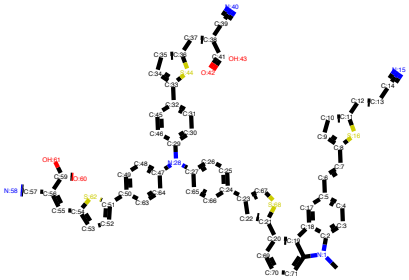
```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-13.973919868469238'
```




```
'------------------------------------------------------------'

'Attaching fragment 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)cccc2
1'
```



```
'------------------------------------------------------------'

'-----Step-71-----'
'-----Step-72-----'
'-----Step-73-----'
'Generate next fragment: 1.0'
```

```
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.66892868
94688848e-06'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -14.10002
8991699219'
```

```
'------------------------------------------------------------'
```

```
'Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ probability -14.3
89986038208008'
```

```
'------------------------------------------------------------'
```

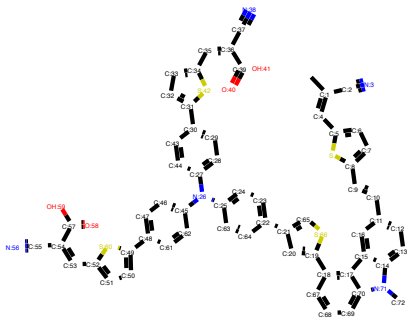
```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -14.86531257629
3945'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -17.0951690
67382812'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC(C#N)=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)cccc2n3
C)s1'
```



```
'------------------------------------------------------------'

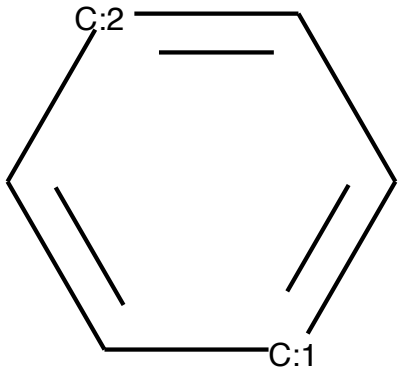
'-----Step-74-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.33791378140449524'
```

```
'------------------------------------------------------------'

'Molecule C#N and its specific config N#[CH:1] w/ probability -1.2967579364776
611'
```

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -4.329936504364014'
```

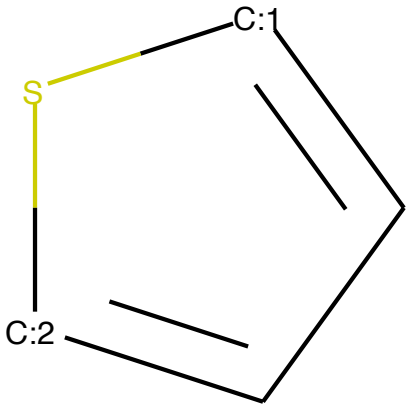



```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -9.103432655334
473'
```

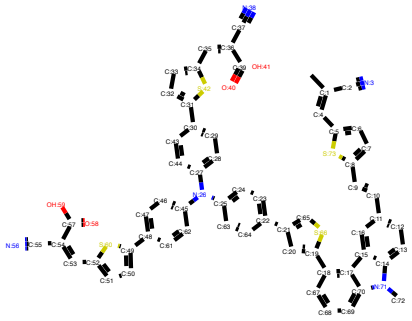
```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-10.106388092041016'
```




```
'------------------------------------------------------------'

'Attaching fragment C'
'Latest partial graph: CC(C#N)=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)cccc2n3
C)s1'
```



```
'------------------------------------------------------------'

'-----Step-75-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
```

```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -1.192092824453
5389e-07'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ probability -16.6
45597457885742'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -17.3495235
44311523'
```

```
'------------------------------------------------------------'
```

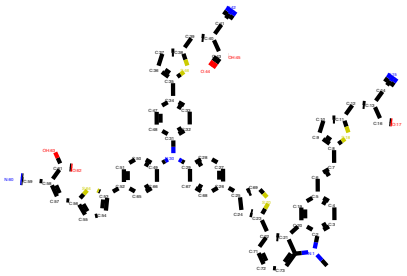
```
'Molecule CN and its specific config N[CH3:1] w/ probability -18.3763656616210
94'
```

```
'------------------------------------------------------------'

'Molecule CO and its specific config O[CH3:1] w/ probability -18.9861946105957
03'
```

```
'------------------------------------------------------------'

'Attaching fragment O=[CH2:1]'
'Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=C(C#N)C=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)cs3)
cccc21'
```



```
'------------------------------------------------------------'

'-----Step-76-----'
'-----Step-77-----'
'Generate next fragment: 0.9999995231628418'
'Top 5 next fragments to attach (current and potential graph)'
```

```
'Molecule CO and its specific config O[CH3:1] w/ probability -0.00965511146932
8403'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -5.47430658
3404541'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.60518360
13793945'
```

```
'------------------------------------------------------------'
```

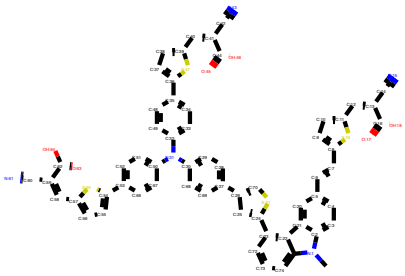
```
'Molecule CO and its specific config [CH3:1][OH:2] w/ probability -7.083941459
655762'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config N[CH3:1] w/ probability -7.42504119873046
9'
```

```
'------------------------------------------------------------'

'Attaching fragment 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)c
s3)cccc21'
```



```
'------------------------------------------------------------'

'-----Step-78-----'
'-----Step-79-----'
'-----Step-80-----'
'-----Step-81-----'
```

```
'-----Step-82-----'
'-----Step-83-----'
'-----Step-84-----'
'-----Step-85-----'
'-----Step-86-----'
'-----Step-87-----'
'-----Step-88-----'
'-----Step-89-----'
'Generate next fragment: 0.9998952150344849'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -0.02370018
3257460594'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config C[NH2:1] w/ probability -3.78735780715942
4'
```

```
'------------------------------------------------------------'

'Molecule N and its specific config N w/ probability -7.8594231605529785'
```

```
'------------------------------------------------------------'

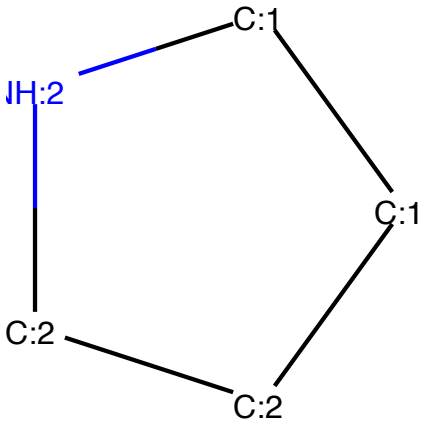
'Molecule [SiH4] and its specific config [SiH4] w/ probability -7.954206943511
963'
```

```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -11.697789192199707'
```

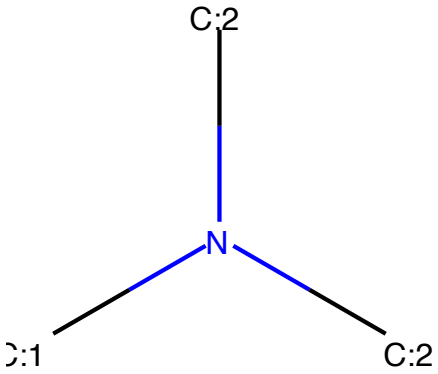
```
'------------------------------------------------------------'

'-----Step-90-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ probability -0.13806328177452087'
```



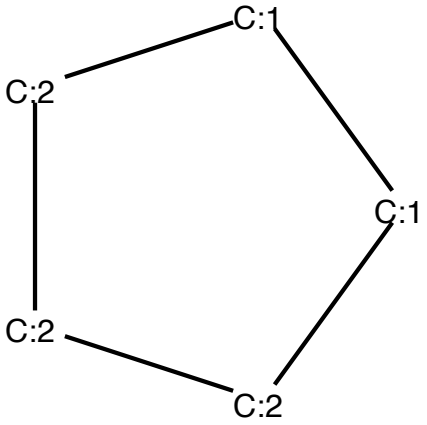
'--'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -2.3250250816345215'



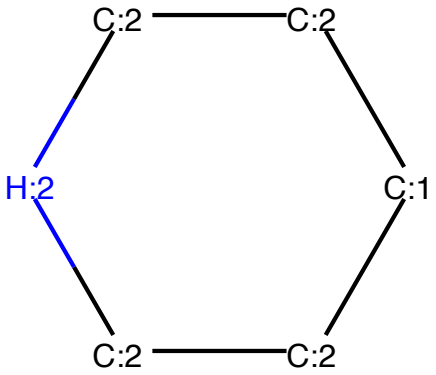
'--'

'Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]
1 w/ probability -4.258025169372559'



'--'

'Molecule C1CCNCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2][CH2:2]
[CH2:2]1 w/ probability -4.540942192077637'

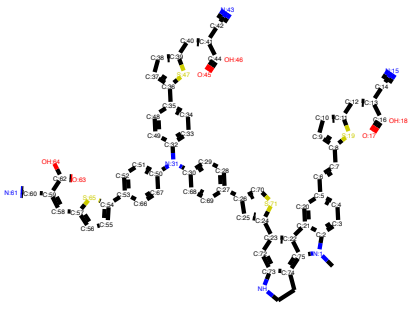



```
'------------------------------------------------------------'

'Molecule CBr and its specific config Br[CH3:1] w/ probability -6.290830135345
459'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]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)c
s3)cc3c(c21)CCN3'
```



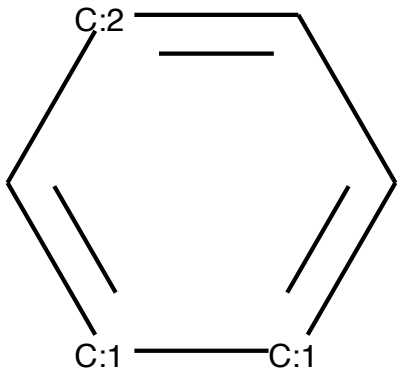
```
'------------------------------------------------------------'

'-----Step-91-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
```

'Molecule CN and its specific config C[NH2:1] w/ probability -0.76087129116058
35'

'--'

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



'--'

'Molecule N and its specific config N w/ probability -1.4923474788665771'

'--'

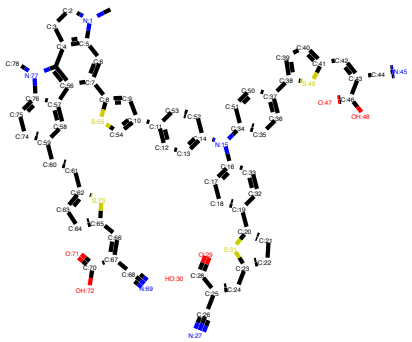
'Molecule C and its specific config C w/ probability -4.306386470794678'

```
'------------------------------------------------------------'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -4.55280590
05737305'
```

```
'------------------------------------------------------------'

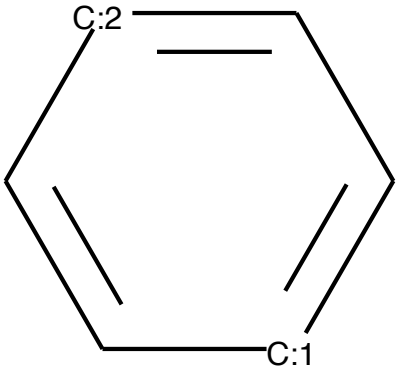
'Attaching fragment C[NH2:1]'
'Latest partial graph: CN1CCc2c1cc(-c1cc(-c3ccc(N(c4ccc(-c5ccc(C=C(C#N)C(=O)O)
s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs1)c1c3cc(C=Cc4ccc(C=C(C#N)C(=O
)O)s4)ccc3n(C)c21'
```



```
'------------------------------------------------------------'

'-----Step-92-----'
'Generate next fragment: 0.7671745419502258'
'Top 5 next fragments to attach (current and potential graph)'
```

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.0940258577466011'



'--'

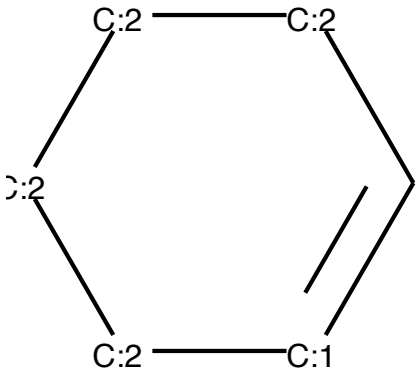
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -2.44133996
96350098'

'--'

'Molecule C and its specific config C w/ probability -6.6834330558776855'

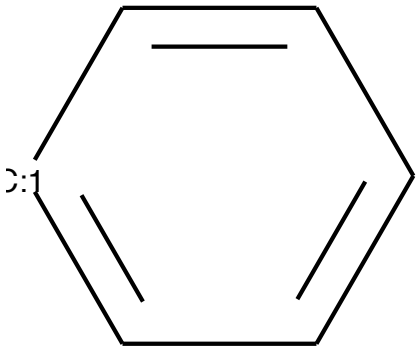
'--'

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



'--'

'Molecule C1=CC=CC=C1 and its specific config C1=CC=[CH:1]C=C1 w/ probability -7.661513805389404'

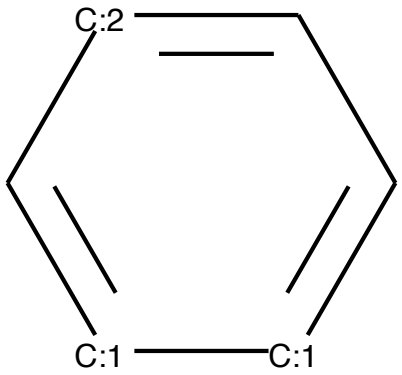


'--'

'-----Step-93-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CN and its specific config C[NH2:1] w/ probability -0.7608712911605835'

'--'

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




```
'------------------------------------------------------------'

'Molecule N and its specific config N w/ probability -1.4923474788665771'

'------------------------------------------------------------'

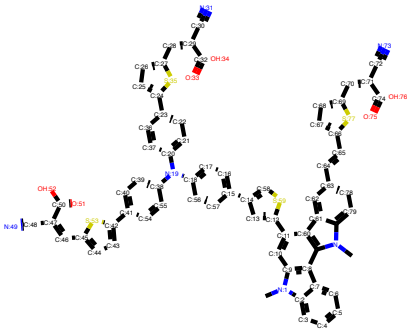
'Molecule C and its specific config C w/ probability -4.306386470794678'

'------------------------------------------------------------'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -4.55280590
05737305'
```

```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1][CH:1]=C[CH:2]=C1'
'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'
```

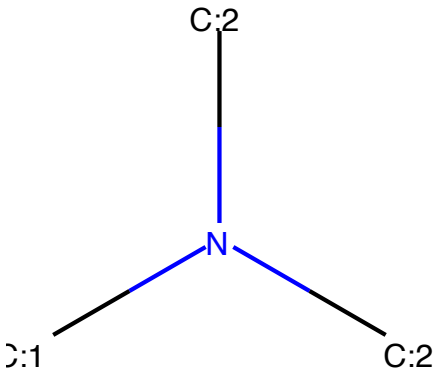


```
'------------------------------------------------------------'

'-----Step-94-----'
'Generate next fragment: 0.9999222755432129'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.24081973
731517792'
```

```
'------------------------------------------------------------'
```

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -1.597212553024292'

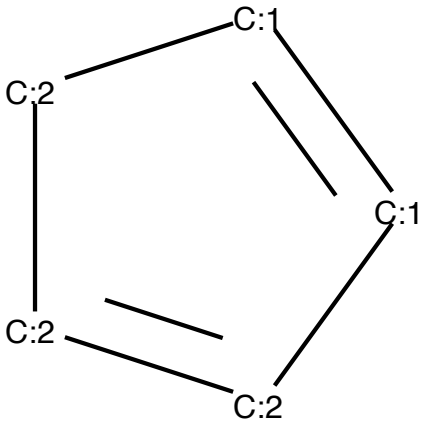


'--'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -5.81991434
09729'

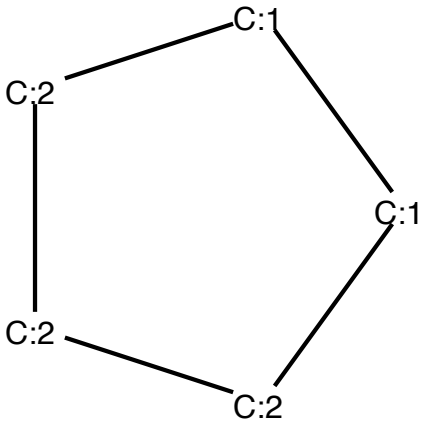
'--'

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



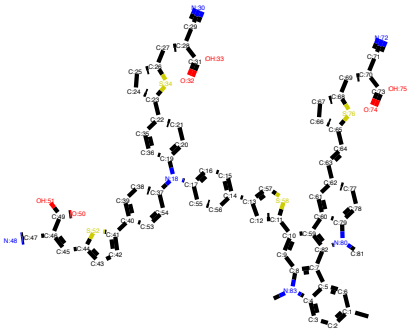
'--'

'Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:1][CH2:2][CH2:2][CH2:2]
1 w/ probability -6.495669364929199'




```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'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'
```

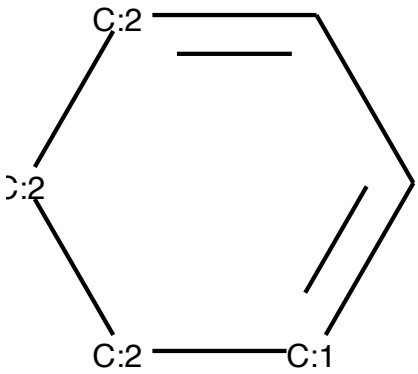


```
'------------------------------------------------------------'

'-----Step-95-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -1.126648
187637329'
```

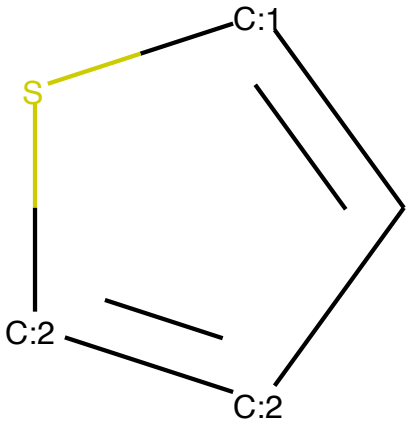
```
'------------------------------------------------------------'
```

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



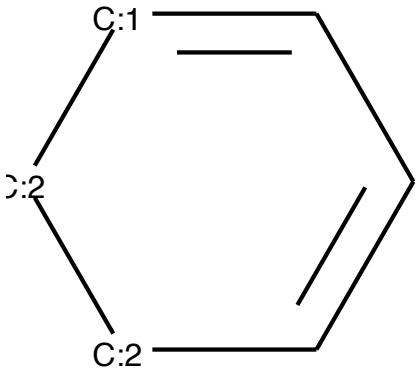

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -1.7480615377426147'
```



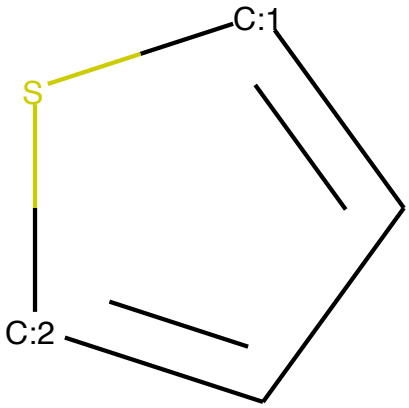

```
'------------------------------------------------------------'

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



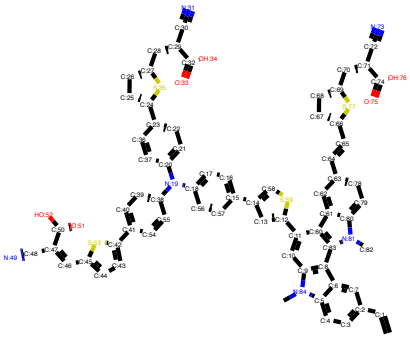

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-2.2401089668273926'
```




```
'------------------------------------------------------------'

'Attaching fragment [CH2:1]=[CH2:2]'
'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'
```



```
'------------------------------------------------------------'

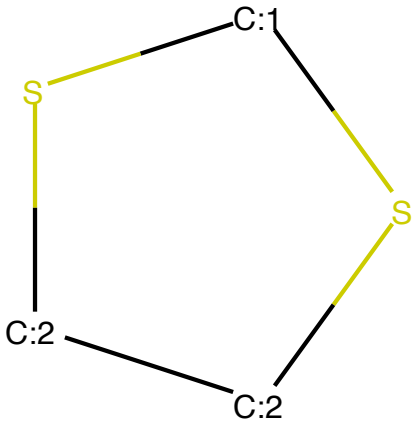
'-----Step-96-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.50334340
3339386'

'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -1.506188154220581'
```

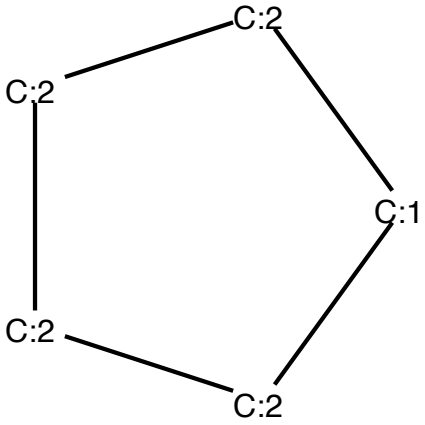
```
'-----------------------------------------------------------'

'Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ probabi
lity -2.0950944423675537'
```



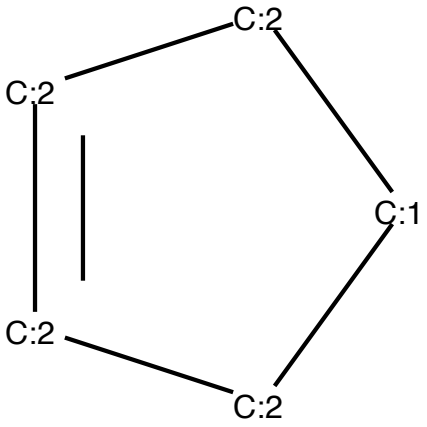

```
'-----------------------------------------------------------'

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



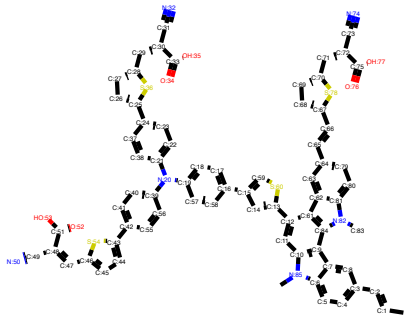

```
'-----------------------------------------------------------'

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



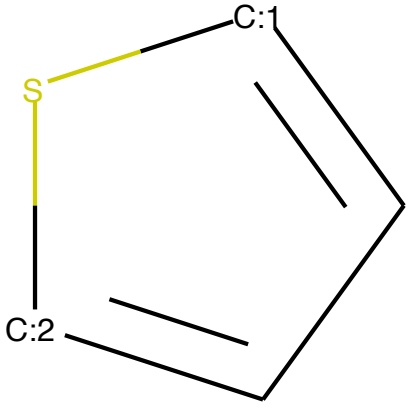
'--'

'Attaching fragment [CH3:1][CH3:2]'
'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'



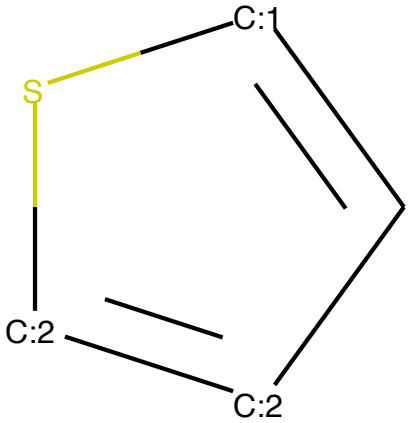
'--'

'-----Step-97-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.13064758479595184'



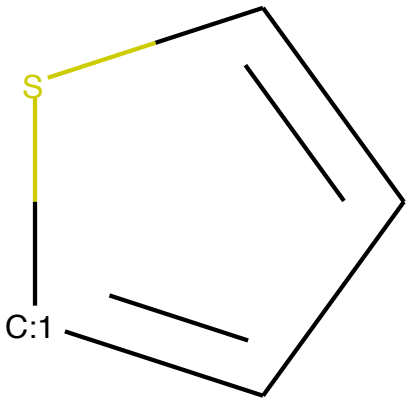
'--'

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



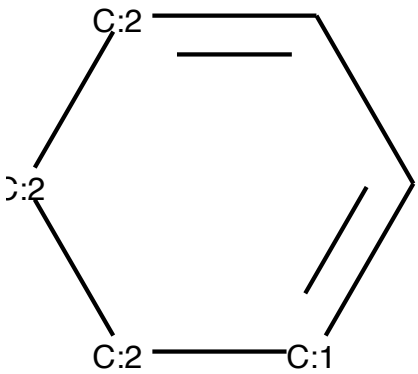
'--'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -3.4
541759490966797'



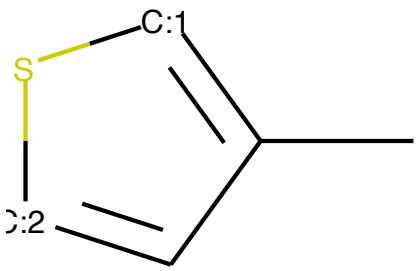
'--'

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



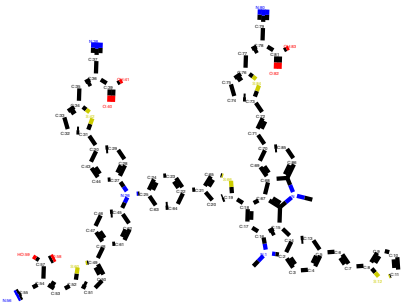
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -4.749369144439697'




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: Cn1c2ccc(C=Cc3cccs3)cc2c2c1cc(-c1cc(-c3ccc(N(c4ccc(-c5c
cc(C=C(C#N)C(=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs1)c1c3cc(C=C
c4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12'
```

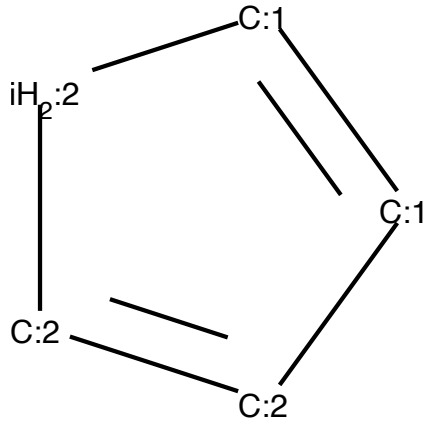


```
'------------------------------------------------------------'

'-----Step-98-----'
'Generate next fragment: 0.8716926574707031'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.06206988
1707429886'
```

```
'------------------------------------------------------------'
```

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

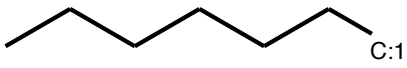


'--'

'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -4.459293842315674'

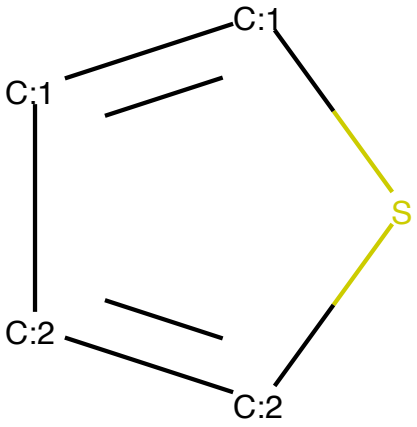
'--'

'Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ probability -4.933238506317139'



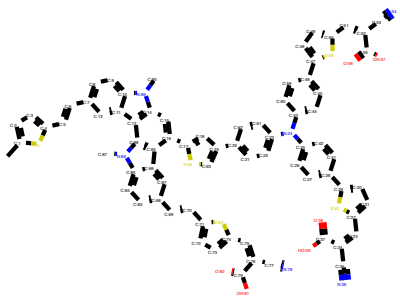
'--'

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




```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'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=Cc6
ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1'
```

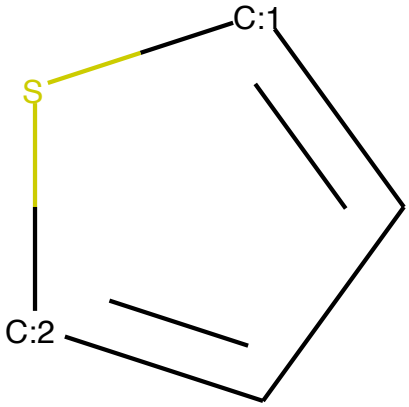


```
'------------------------------------------------------------'

'-----Step-99-----'
'Generate next fragment: 0.9999935626983643'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -0.050873
31682443619'
```

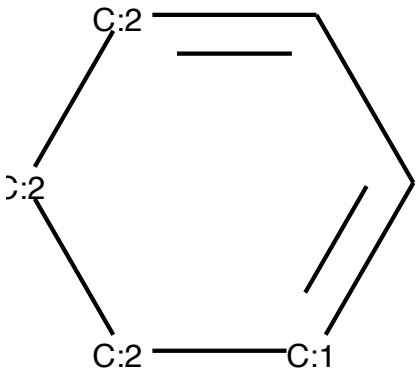
```
'------------------------------------------------------------'
```

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -3.4192769527435303'



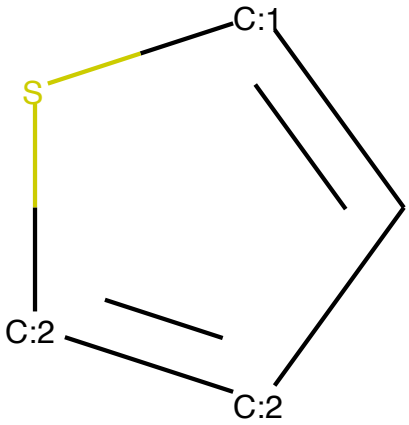
'--'

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



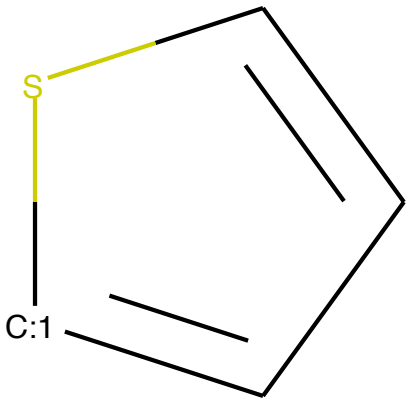
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probability -5.079664707183838'



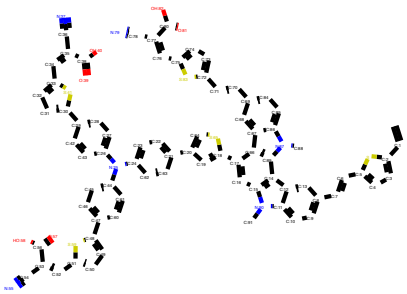
'--'

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




```
'------------------------------------------------------------'

'Attaching fragment [CH2:1]=[CH2:2]'
'Latest partial graph: C=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'
```



```
'------------------------------------------------------------'

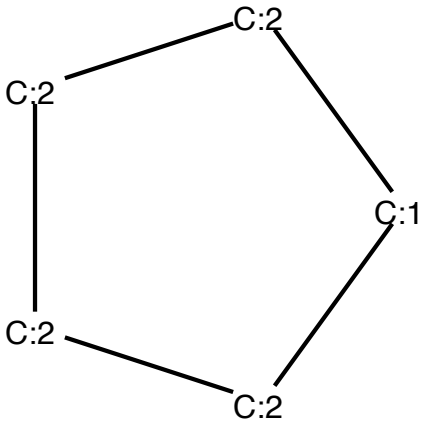
'-----Step-100-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.008251977153122425'

'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -4.81123971
9390869'
```

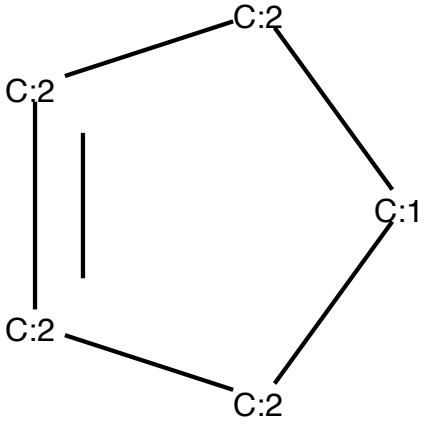
```
'------------------------------------------------------------'

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



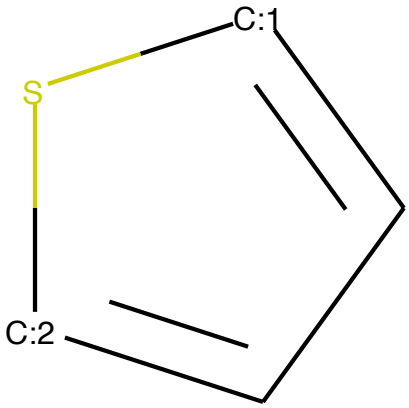

```
'------------------------------------------------------------'

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



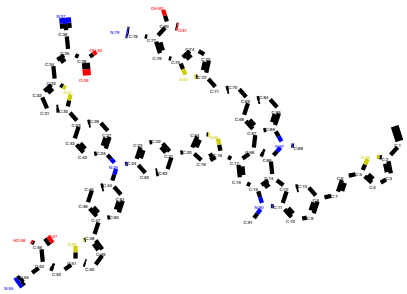

```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

'Attaching fragment C'
'Latest partial graph: C=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'
```



```
'------------------------------------------------------------'

'-----Step-101-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.72202952
7532868e-06'

'------------------------------------------------------------'
```

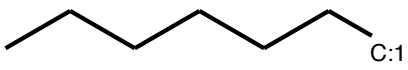
```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -12.14201068878
1738'
```

```
'------------------------------------------------------------'
```

```
'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -16.1
39101028442383'
```

```
'------------------------------------------------------------'
```

```
'Molecule CCCCCCC and its specific config CCCCCC[CH3:1] w/ probability -16.460
159301757812'
```

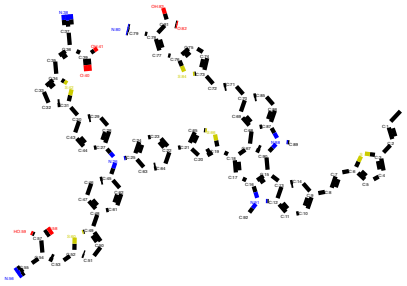



```
'------------------------------------------------------------'
```

```
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -16.62949
7528076172'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6ccc(-c7
ccc(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'
```

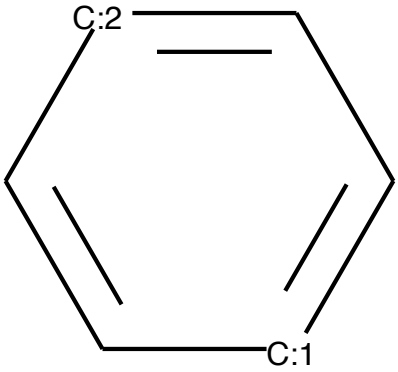


```
'------------------------------------------------------------'

'-----Step-102-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C#N and its specific config N#[CH:1] w/ probability -0.0001243275619
3447858'
```

```
'------------------------------------------------------------'
```

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



'--'

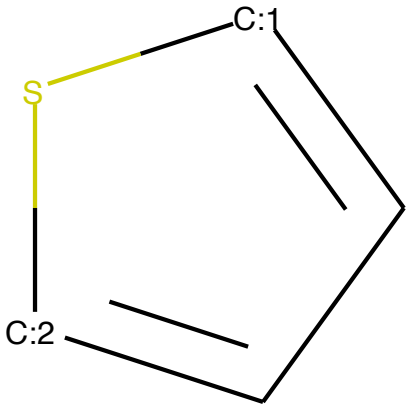
'Molecule C and its specific config C w/ probability -10.463766098022461'

'--'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -11.70853614807
1289'

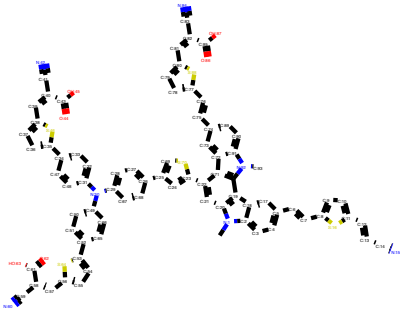
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-13.97391414642334'




```
'------------------------------------------------------------'

'Attaching fragment N#[CH:1]'
'Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=CC#N)s3)cc2c2c1cc(-c1cc(-c3ccc(N(c4
ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc3)cs1)c1
c3cc(C=Cc4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12'
```



```
'------------------------------------------------------------'

'-----Step-103-----'
'-----Step-104-----'
'-----Step-105-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.66892868
94688848e-06'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -14.10002
9945373535'
```

```
'------------------------------------------------------------'
```

```
'Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ probability -14.3
89986991882324'
```

```
'------------------------------------------------------------'
```

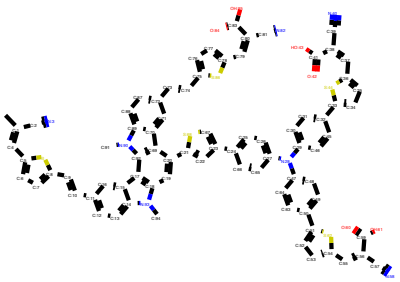
```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -14.86531352996
8262'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -17.0951728
82080078'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC(C#N)=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6cc
c(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5
cc(C=Cc6ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1'
```



```
'------------------------------------------------------------'

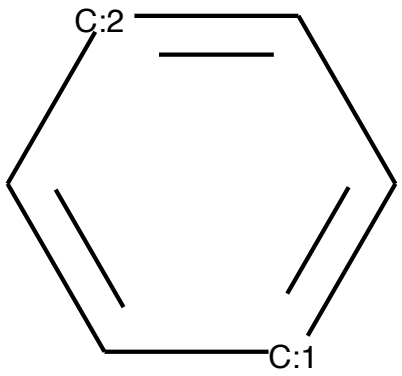
'-----Step-106-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.3379138708114624'
```

```
'------------------------------------------------------------'

'Molecule C#N and its specific config N#[CH:1] w/ probability -1.2967575788497
925'
```

'--'

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

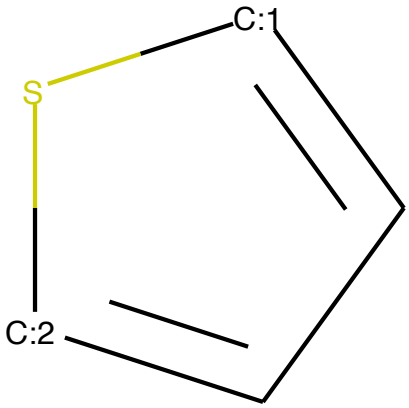


'--'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -9.103430747985
84'

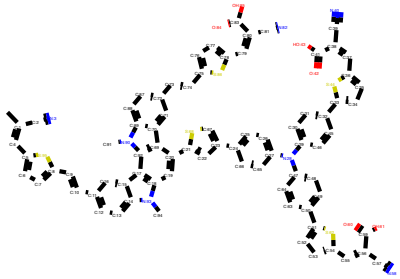
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-10.106386184692383'




```
'------------------------------------------------------------'

'Attaching fragment C'
'Latest partial graph: CC(C#N)=Cc1ccc(C=Cc2ccc3c(c2)c2c(cc(-c4cc(-c5ccc(N(c6cc
c(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)c6ccc(-c7ccc(C=C(C#N)C(=O)O)s7)cc6)cc5)cs4)c4c5
cc(C=Cc6ccc(C=C(C#N)C(=O)O)s6)ccc5n(C)c42)n3C)s1'
```



```
'------------------------------------------------------------'

'-----Step-107-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=O and its specific config O=[CH2:1] w/ probability -1.192092824453
5389e-07'

'------------------------------------------------------------'
```

```
'Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ probability -16.6
45597457885742'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -17.3495197
29614258'
```

```
'------------------------------------------------------------'
```

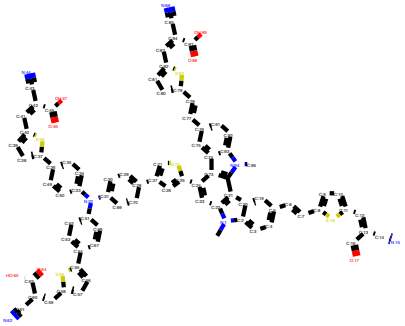
```
'Molecule CN and its specific config N[CH3:1] w/ probability -18.3763656616210
94'
```

```
'------------------------------------------------------------'
```

```
'Molecule CO and its specific config O[CH3:1] w/ probability -18.9861965179443
36'
```

```
'------------------------------------------------------------'

'Attaching fragment 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)c
s1)c1c3cc(C=Cc4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12'
```



```
'------------------------------------------------------------'

'-----Step-108-----'
'-----Step-109-----'
'Generate next fragment: 0.9999995231628418'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CO and its specific config O[CH3:1] w/ probability -0.00965511146932
8403'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -5.47430229
1870117'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.60518264
7705078'
```

```
'------------------------------------------------------------'
```

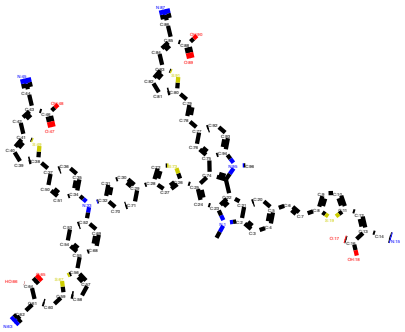
```
'Molecule CO and its specific config [CH3:1][OH:2] w/ probability -7.083941459
655762'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config N[CH3:1] w/ probability -7.42503833770751
95'
```

```
'------------------------------------------------------------'

'Attaching fragment O[CH3:1]'
'Latest partial graph: Cn1c2ccc(C=Cc3ccc(C=C(C#N)C(=O)O)s3)cc2c2c1cc(-c1cc(-c3
ccc(N(c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)c4ccc(-c5ccc(C=C(C#N)C(=O)O)s5)cc4)cc
3)cs1)c1c3cc(C=Cc4ccc(C=C(C#N)C(=O)O)s4)ccc3n(C)c12'
```



```
'------------------------------------------------------------'

'-----Step-110-----'
'-----Step-111-----'
'-----Step-112-----'
'-----Step-113-----'
'-----Step-114-----'
'-----Step-115-----'
'-----Step-116-----'
'-----Step-117-----'
'-----Step-118-----'
'-----Step-119-----'
'-----Step-120-----'
'-----Step-121-----'
'Generate next fragment: 0.9998952150344849'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -0.02370018
3257460594'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config C[NH2:1] w/ probability -3.78736066818237
3'
```

```
'------------------------------------------------------------'

'Molecule N and its specific config N w/ probability -7.859424114227295'
```

```
'------------------------------------------------------------'

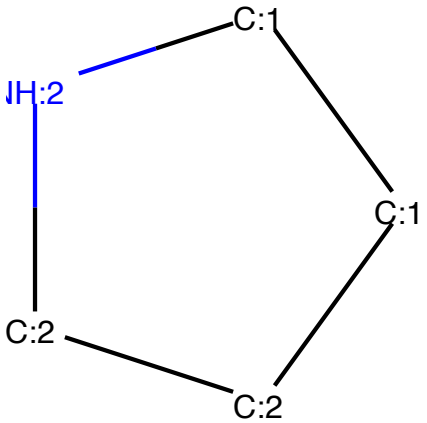
'Molecule [SiH4] and its specific config [SiH4] w/ probability -7.954198360443
115'
```

```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -11.69778823852539'
```

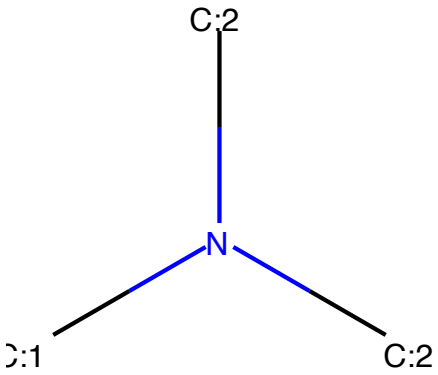
```
'------------------------------------------------------------'

'-----Step-122-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1
w/ probability -0.13806338608264923'
```



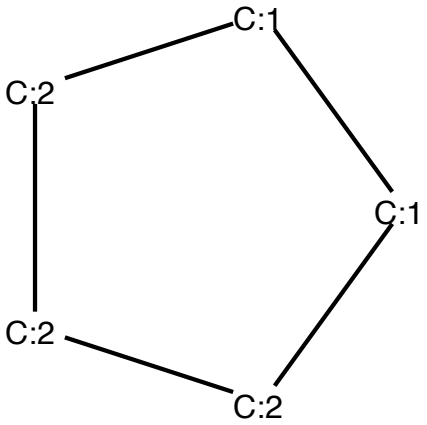

```
'------------------------------------------------------------'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -2.3250234127044678'
```



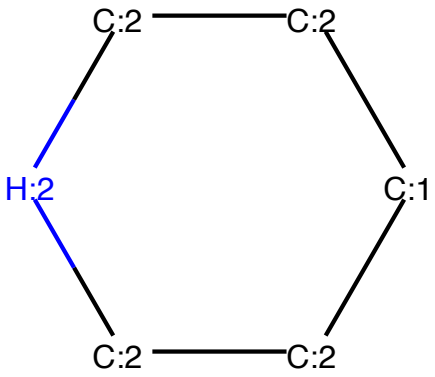
'--'

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



'--'

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

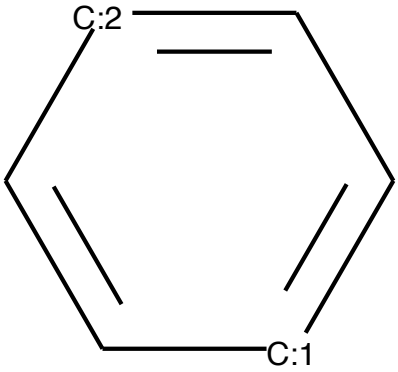


'--'

'Molecule CBr and its specific config Br[CH3:1] w/ probability -6.290830135345459'

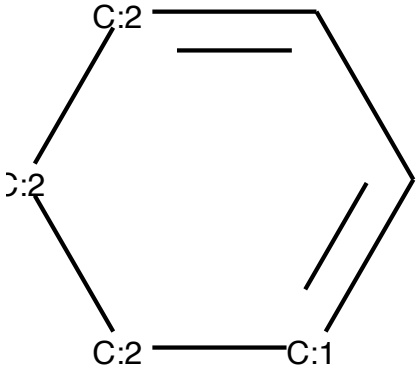
'--'

'-----Step-123-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.9793890714645386'



'--'

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

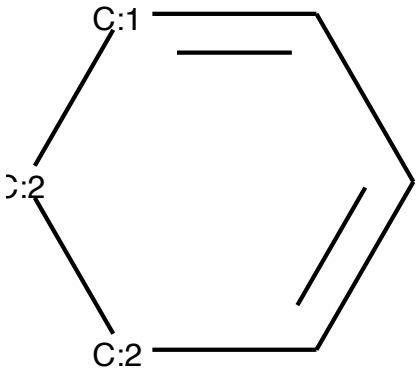


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -1.395794
39163208'

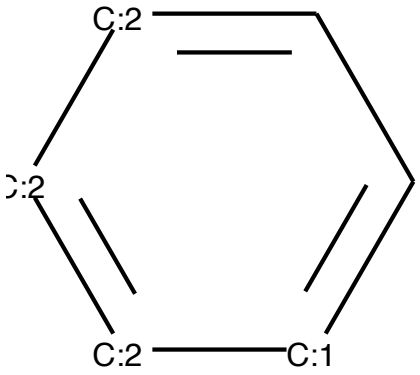
```
'-----------------------------------------------------------'

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




```
'-----------------------------------------------------------'

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

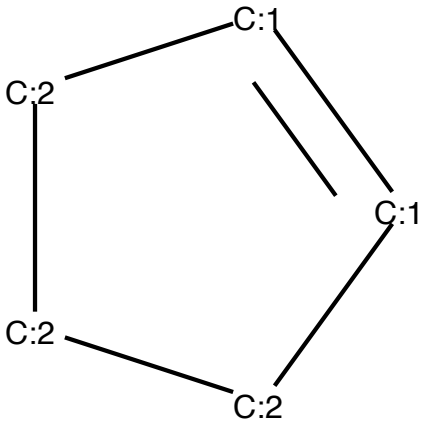



```
'-----------------------------------------------------------'

'-----Step-124-----'
'Generate next fragment: 0.9999998807907104'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00605972
6700186729'
```

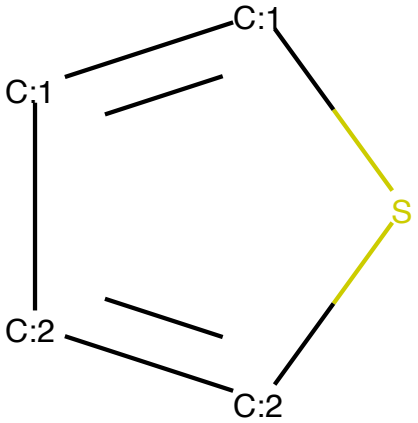
```
'-------------------------------------------------------------'

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



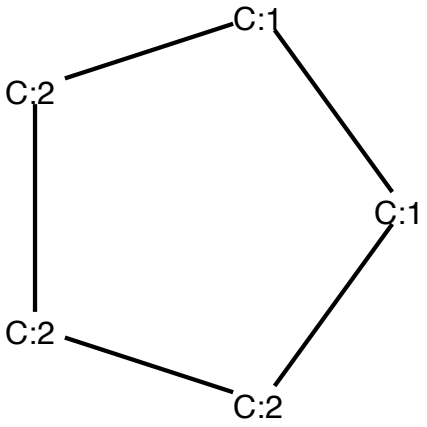

```
'-------------------------------------------------------------'

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



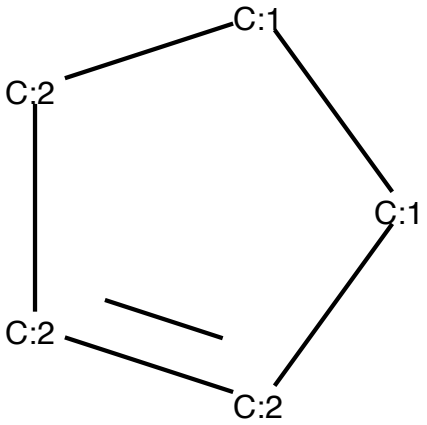

```
'-------------------------------------------------------------'

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



'--'

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

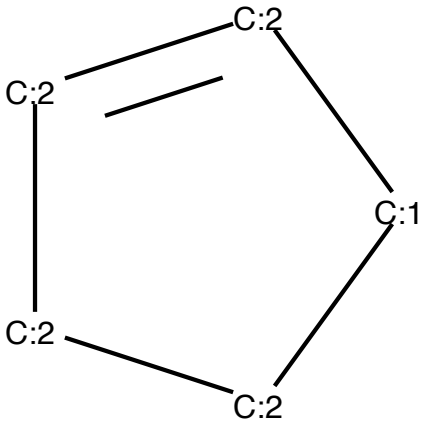


'--'

'-----Step-125-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -7.39094866
7307384e-06'

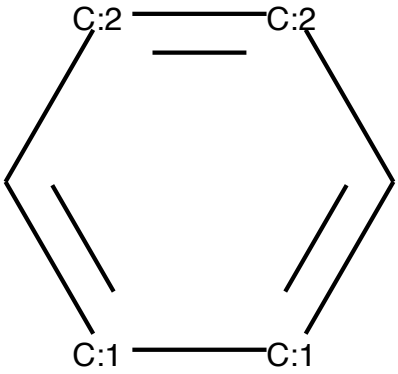
'--'

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



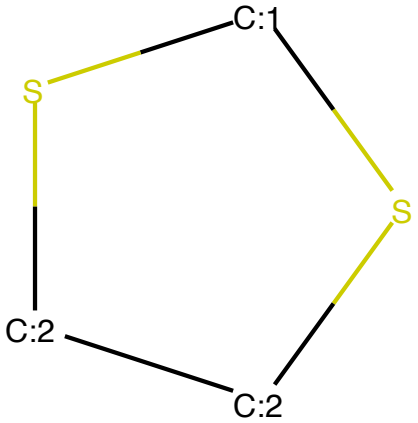
'--'

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



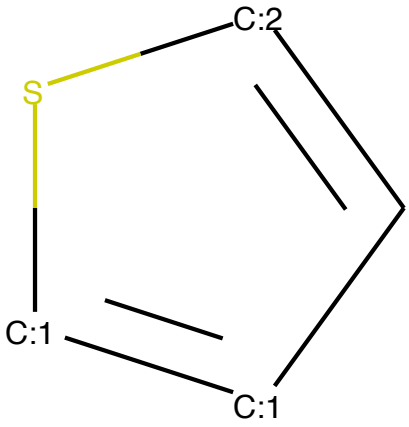
'--'

'Molecule C1CSCS1 and its specific config S1[CH2:1]S[CH2:2][CH2:2]1 w/ probability -13.665506362915039'



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probability -14.96162223815918'



'--'

'-----Step-126-----'

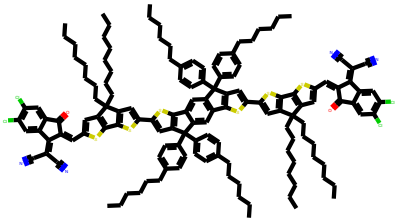
In [86]:

```
for i, sample in enumerate(wo_te_data):
    if i > 7:
        break
    elif i < 7:
        continue
    display('Original: {}'.format(original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(original[i])]))

    # step 0
    step_f0 = sample[0]
    display('***************Sample {}th***************'.format(i))
    display('-----Step-0-----')
    display(step_f0)
    mol = Chem.MolFromSmiles(step_f0['partial-graph'])
    display('Displaying partial graph (aka molecule): {}'.format(step_f0['par
            Draw.MolsToGridImage([mol]))
    display('------------------------------------------------------------', HTML

    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        display('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            display('Generate next fragment: {}'.format(step_f['Generate frag
        if 'top-5-inter-cands' in step_f:
            display('Top 5 next fragments to attach (current and potential gr
            for fragment in step_f['top-5-inter-cands']:
                display('Molecule {} and its specific config {} w/ probabilit
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                display('------------------------------------------------------
        if 'Attaching Fragment' in step_f:
            frag = step_f['Attaching Fragment'][0]
            num_atom = len(list(Chem.MolFromSmiles(step_f['top-5-inter-cands'
            mol, indices = mol_with_atom_index(Chem.MolFromSmiles(step_f['par
                                               list(range(num_atom)))
            display('Attaching fragment {}'.format(frag))
            display('Latest partial graph: {}'.format(step_f['partial-graph']
                    Draw.MolsToGridImage([mol]))
            display('------------------------------------------------------
```

```
'Original: CCCCCCC1=CC=C(C2(C3=CC=C(CCCCCC)C=C3)C4=CC(C(SC(C5=CC(C6(CCCCCCCC)C
CCCCCCC)=C(C7=C6C=C(/C=C(C8=O)/C(C9=CC(Cl)=C(Cl)C=C89)=C(C#N)/C#N)S7)S5)=C%10)
=C%10C%11(C%12=CC=C(CCCCCC)C=C%12)C%13=CC=C(CCCCCC)C=C%13)=C%11C=C4C%14=C2C=C(
C%15=CC(C%16(CCCCCCCC)CCCCCCCC)=C(C%17=C%16C=C(/C=C(C%18=O)/C(C%19=CC(Cl)=C(Cl
)C=C%18%19)=C(C#N)\\C#N)S%17)S%15)S%14)C=C1'
```



```
'***************Sample 7th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([653,  10, 575, 506, 620]),
 'super-root-idx': tensor(653),
 'top-5-root-fragment-cands': [('[NH2:1][CH3:2]', tensor(4.3962)),
  ('[CH3:1][NH2:2]', tensor(-3.9628)),
  ('C[NH2:1]', tensor(-15.1147)),
  ('N[CH3:1]', tensor(-19.5112)),
  ('C([OH:1])[CH3:2]', tensor(-975.5828))],
 'Attaching Fragment': '[NH2:1][CH3:2]',
 'partial-graph': 'CN'}
'Displaying partial graph (aka molecule): CN'
```

```
'------------------------------------------------------------'

'-----Step-1-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.01824887
6556754112'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config [O:1]=[CH2:2] w/ probability -4.56167793
2739258'
```

```
'------------------------------------------------------------'

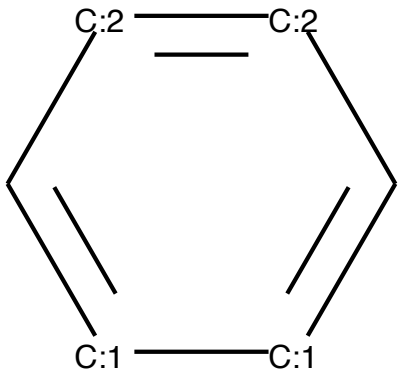
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -5.438595
294952393'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -5.834055900573
7305'
```

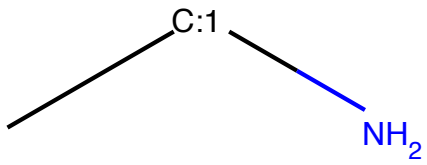
```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=[CH:2]1
w/ probability -8.586238861083984'
```



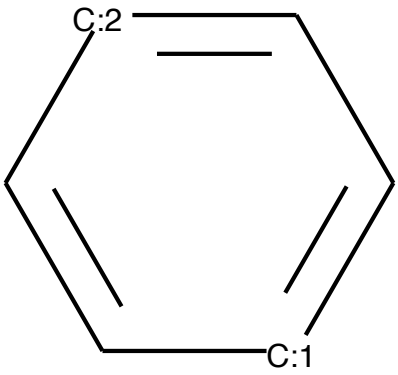

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CCN'
```




```
'------------------------------------------------------------'

'-----Step-2-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.5155307054519653'
```

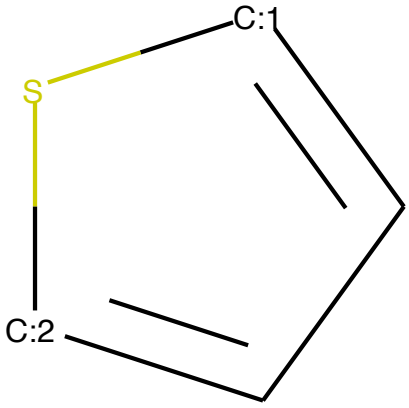


'--'

'Molecule C#N and its specific config N#[CH:1] w/ probability -1.1474868059158325'

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -2.9674770832061768'

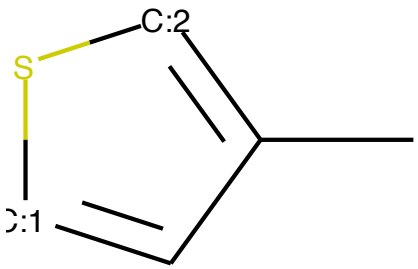


'--'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -3.7076351642608643'

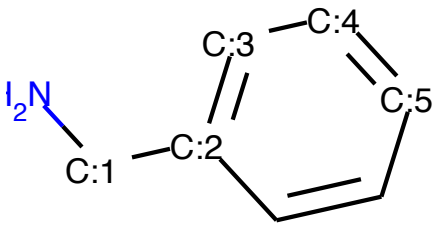
```
'------------------------------------------------------------'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ probabili
ty -5.489928245544434'
```




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: NCc1ccccc1'
```

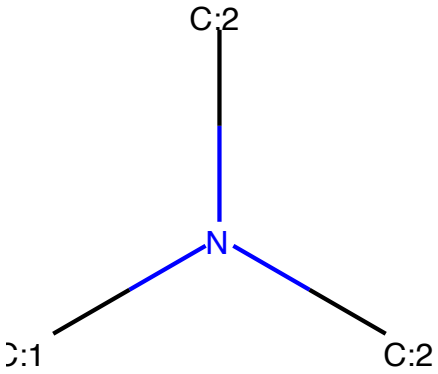



```
'------------------------------------------------------------'

'-----Step-3-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.78668922
18589783'
```

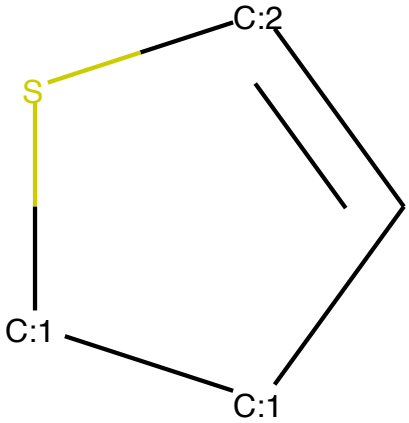
```
'------------------------------------------------------------'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -1.0030741691589355'
```



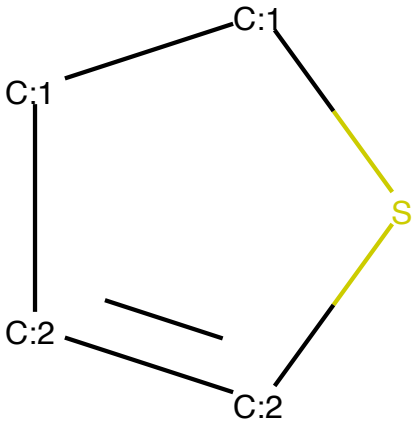

```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -2.7415366172790527'
```



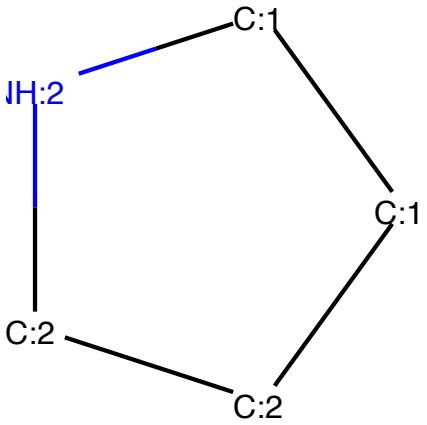

```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config S1[CH2:1][CH2:1][CH:2]=[CH:2]1 w/ p
robability -2.939915180206299'
```



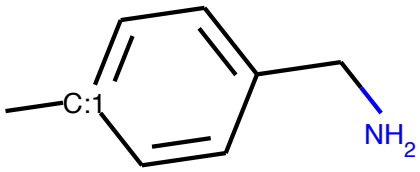
'--'

'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][NH:2][CH2:2][CH2:2]1 w/ probability -3.278656482696533'



'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(CN)cc1'

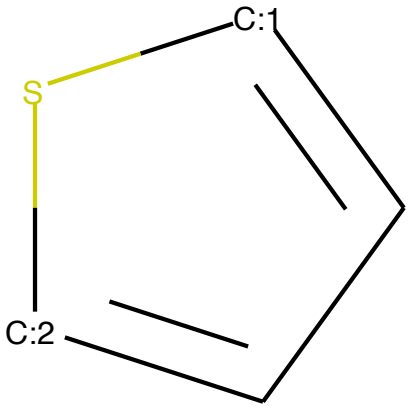


'--'

'-----Step-4-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -0.5388051867485046'

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-1.7531983852386475'
```

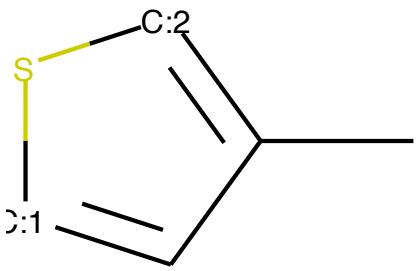



```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -2.007772922515869'
```

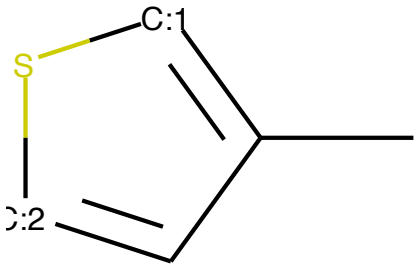
```
'------------------------------------------------------------'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ probabili
ty -2.707206964492798'
```



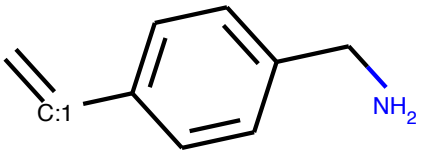

```
'------------------------------------------------------------'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -3.8809521198272705'
```




```
'------------------------------------------------------------'

'Attaching fragment [CH2:1]=[CH2:2]'
'Latest partial graph: C=Cc1ccc(CN)cc1'
```




```
'------------------------------------------------------------'

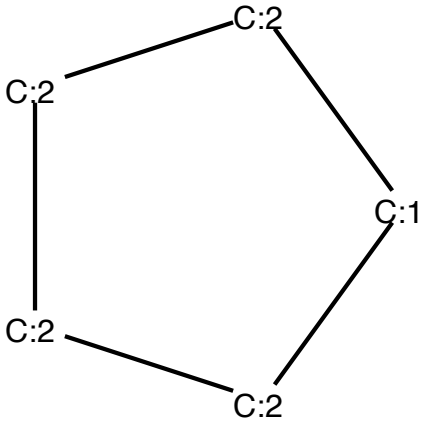
'-----Step-5-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.023258958011865616'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -3.81381678
5812378'
```

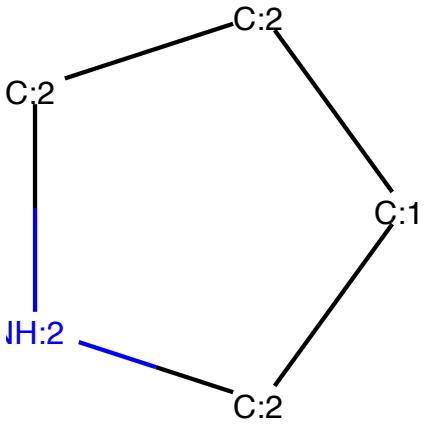
```
'------------------------------------------------------------'

'Molecule C1CCCC1 and its specific config [CH2:1]1[CH2:2][CH2:2][CH2:2][CH2:2]
1 w/ probability -7.317326545715332'
```




```
'------------------------------------------------------------'

'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2][CH2:2]1
w/ probability -8.82868766784668'
```

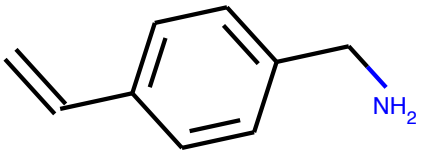



```
'------------------------------------------------------------'

'Molecule [CH3-] and its specific config [CH3-] w/ probability -9.969855308532
715'
```

```
'------------------------------------------------------------'

'Attaching fragment C'
'Latest partial graph: C=Cc1ccc(CN)cc1'
```




```
'------------------------------------------------------------'

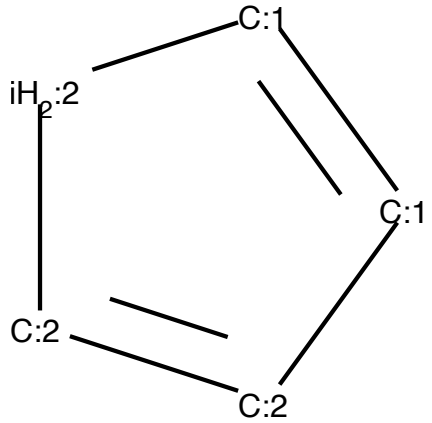
'-----Step-6-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -6.07965512
2448457e-06'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -12.47726345062
2559'
```

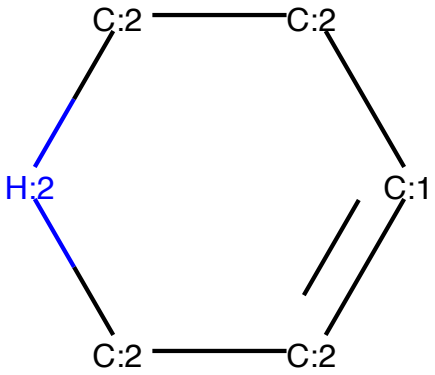
```
'------------------------------------------------------------'

'Molecule C1=C[SiH2]C=C1 and its specific config [CH:1]1=[CH:1][SiH2:2][CH:2]=
[CH:2]1 w/ probability -13.782573699951172'
```




```
'------------------------------------------------------------'

'Molecule C1=CCNCC1 and its specific config [CH:1]1=[CH:2][CH2:2][NH:2][CH2:2]
[CH2:2]1 w/ probability -14.539703369140625'
```

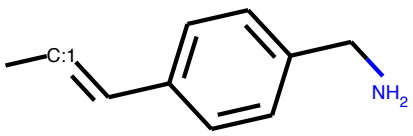


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -14.90920
639038086'

'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC=Cc1ccc(CN)cc1'

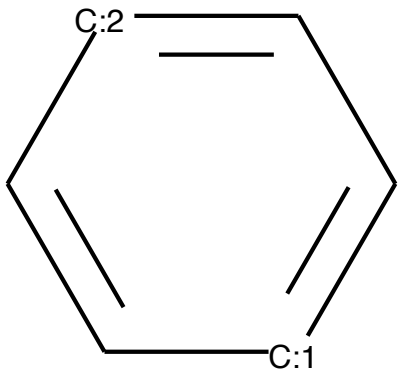


'--'

'-----Step-7-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C#N and its specific config N#[CH:1] w/ probability -0.0003427871561
1435473'

```
'------------------------------------------------------------'
```

```
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -8.029106140136719'
```




```
'------------------------------------------------------------'
```

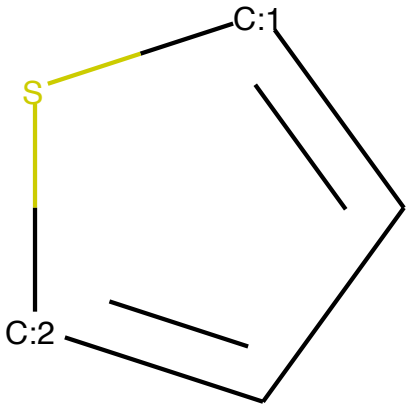
```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -11.65356349945
0684'
```

```
'------------------------------------------------------------'
```

```
'Molecule C and its specific config C w/ probability -11.745807647705078'
```

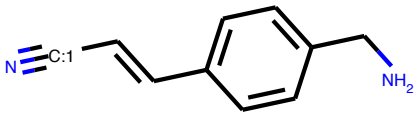
```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-15.35542106628418'
```




```
'------------------------------------------------------------'

'Attaching fragment N#[CH:1]'
'Latest partial graph: N#CC=Cc1ccc(CN)cc1'
```




```
'------------------------------------------------------------'

'-----Step-8-----'
'-----Step-9-----'
'-----Step-10-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00130127
60318815708'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -6.718320
369720459'
```

```
'------------------------------------------------------------'
```

```
'Molecule C=O and its specific config O=[CH2:1] w/ probability -9.343752861022
95'
```

```
'------------------------------------------------------------'
```

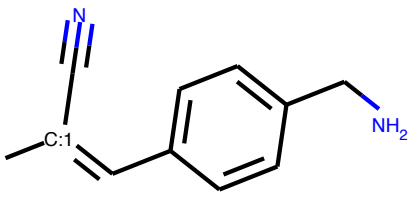
```
'Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ probability -12.6
15152359008789'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -14.4693117
14172363'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC(C#N)=Cc1ccc(CN)cc1'
```

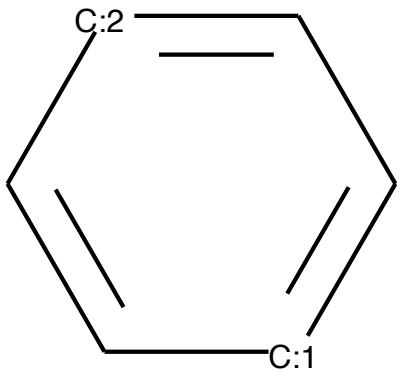



```
'------------------------------------------------------------'

'-----Step-11-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C and its specific config C w/ probability -0.360306978225708'
```

'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -1.3809020519256592'

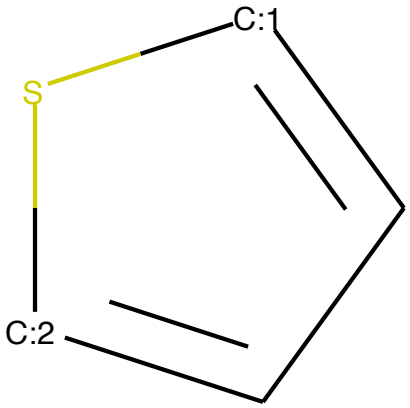


'--'

'Molecule C#N and its specific config N#[CH:1] w/ probability -2.9761645793914
795'

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-9.291977882385254'

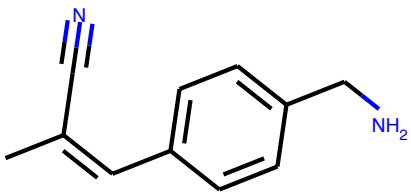



```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -9.369268417358
398'
```

```
'------------------------------------------------------------'

'Attaching fragment C'
'Latest partial graph: CC(C#N)=Cc1ccc(CN)cc1'
```




```
'------------------------------------------------------------'

'-----Step-12-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=O and its specific config O=[CH2:1] w/ probability -8.344646857949
556e-07'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config N[CH3:1] w/ probability -14.1970643997192
38'
```

```
'------------------------------------------------------------'

'Molecule C=[NH2+] and its specific config [NH2+]=[CH2:1] w/ probability -16.5
51809310913086'
```

```
'------------------------------------------------------------'

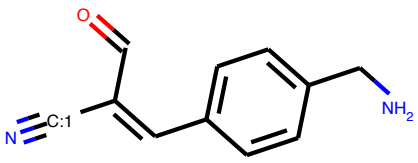
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -17.0043087
00561523'
```

```
'------------------------------------------------------------'

'Molecule CF and its specific config F[CH3:1] w/ probability -17.0630321502685
55'
```

```
'------------------------------------------------------------'

'Attaching fragment O=[CH2:1]'
'Latest partial graph: N#CC(C=O)=Cc1ccc(CN)cc1'
```




```
'------------------------------------------------------------'

'-----Step-13-----'
'-----Step-14-----'
'Generate next fragment: 0.9999996423721313'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CO and its specific config O[CH3:1] w/ probability -0.05614574998617
172'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config N[CH3:1] w/ probability -3.57013297080993
65'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -3.91674113
2736206'
```

```
'------------------------------------------------------------'

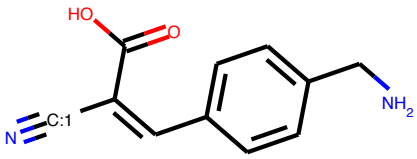
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.13302564
6209717'
```

```
'------------------------------------------------------------'

'Molecule CF and its specific config F[CH3:1] w/ probability -7.98659944534301
8'
```

```
'------------------------------------------------------------'

'Attaching fragment O[CH3:1]'
'Latest partial graph: N#CC(=Cc1ccc(CN)cc1)C(=O)O'
```

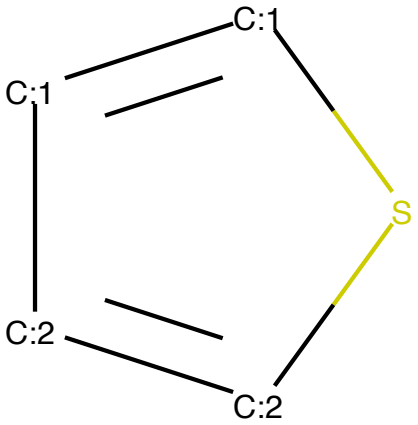



```
'------------------------------------------------------------'

'-----Step-15-----'
'-----Step-16-----'
'-----Step-17-----'
'-----Step-18-----'
'-----Step-19-----'
'-----Step-20-----'
```

```
'-----Step-21-----'
'-----Step-22-----'
'-----Step-23-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.01930461
0788822174'
```

```
'------------------------------------------------------------'
'Molecule C1=CSC=C1 and its specific config S1[CH:1]=[CH:1][CH:2]=[CH:2]1 w/ p
robability -5.553902626037598'
```




```
'------------------------------------------------------------'
'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -5.95
3650951385498'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -6.00821304
3212891'
```

```
'------------------------------------------------------------'
```

```
'Molecule CS and its specific config [CH3:1][SH:2] w/ probability -6.018149852
7526855'
```

```
'------------------------------------------------------------'
```

```
'-----Step-24-----'
'-----Step-25-----'
'-----Step-26-----'
'-----Step-27-----'
'-----Step-28-----'
'-----Step-29-----'
'-----Step-30-----'
'-----Step-31-----'
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'-----Step-43-----'
'-----Step-44-----'
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```
'-----Step-45-----'
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'-----Step-98-----'
'-----Step-99-----'
'-----Step-100-----'
'-----Step-101-----'
```

```
'-----Step-102-----'
'-----Step-103-----'
'-----Step-104-----'
'-----Step-105-----'
'-----Step-106-----'
'-----Step-107-----'
'-----Step-108-----'
'-----Step-109-----'
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'-----Step-118-----'
'-----Step-119-----'
'-----Step-120-----'
'-----Step-121-----'
'-----Step-122-----'
'-----Step-123-----'
'-----Step-124-----'
'-----Step-125-----'
'-----Step-126-----'
```

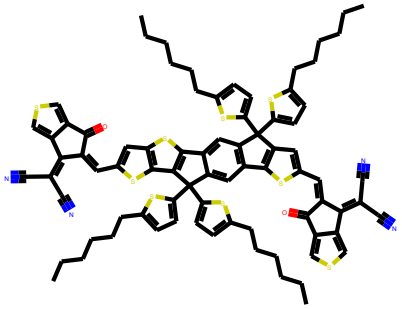
In [87]:

```
for i, sample in enumerate(wo_te_data):
    if i > 12:
        break
    elif i < 12:
        continue
    display('Original: {}'.format(original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(original[i])]))

    # step 0
    step_f0 = sample[0]
    display('***************Sample {}th***************'.format(i))
    display('-----Step-0-----')
    display(step_f0)
    mol = Chem.MolFromSmiles(step_f0['partial-graph'])
    display('Displaying partial graph (aka molecule): {}'.format(step_f0['par
            Draw.MolsToGridImage([mol]))
    display('------------------------------------------------------------', HTML

    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        display('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            display('Generate next fragment: {}'.format(step_f['Generate frag
        if 'top-5-inter-cands' in step_f:
            display('Top 5 next fragments to attach (current and potential gr
            for fragment in step_f['top-5-inter-cands']:
                display('Molecule {} and its specific config {} w/ probabilit
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                display('------------------------------------------------------
        if 'Attaching Fragment' in step_f:
            frag = step_f['Attaching Fragment'][0]
            num_atom = len(list(Chem.MolFromSmiles(step_f['top-5-inter-cands'
            mol, indices = mol_with_atom_index(Chem.MolFromSmiles(step_f['par
                                               list(range(num_atom)))
            display('Attaching fragment {}'.format(frag))
            display('Latest partial graph: {}'.format(step_f['partial-graph']
                    Draw.MolsToGridImage([mol]))
            display('------------------------------------------------------
```

```
'Original: CCCCCCC1=CC=C(S1)C2(C(S3)=CC=C3CCCCCC)C(C(SC(/C=C(C4=O)/C(C5=CSC=C4
5)=C(C#N)\\C#N)=C6)=C6S7)=C7C8=CC9=C(C(SC(/C=C(C%10=O)/C(C%11=CSC=C%10%11)=C(C
#N)\\C#N)=C%12)=C%12C9(C(S%13)=CC=C%13CCCCCC)C(S%14)=CC=C%14CCCCCC)C=C28'
```



```
'***************Sample 12th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([653,  10, 575, 506, 620]),
 'super-root-idx': tensor(653),
 'top-5-root-fragment-cands': [('[NH2:1][CH3:2]', tensor(3.4918)),
  ('[CH3:1][NH2:2]', tensor(-2.9572)),
  ('C[NH2:1]', tensor(-13.9794)),
  ('N[CH3:1]', tensor(-18.6545)),
  ('C([OH:1])[CH3:2]', tensor(-977.5619))],
 'Attaching Fragment': '[NH2:1][CH3:2]',
 'partial-graph': 'CN'}
'Displaying partial graph (aka molecule): CN'
```

```
'------------------------------------------------------------'

'-----Step-1-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.01869018
7484025955'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config [O:1]=[CH2:2] w/ probability -4.19925642
0135498'
```

```
'------------------------------------------------------------'

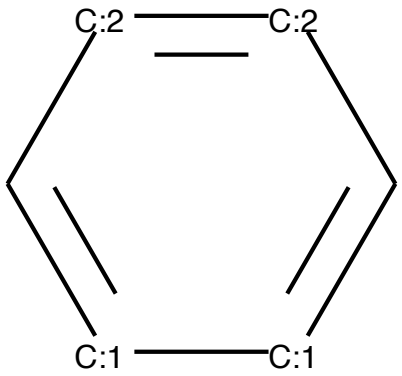
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -6.180079
460144043'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -6.762899398803
711'
```

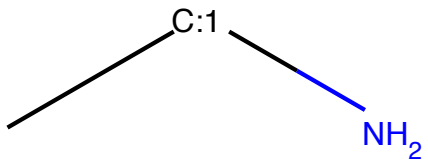
```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1][CH:1]=C[CH:2]=[CH:2]1
w/ probability -9.228087425231934'
```




```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CCN'
```

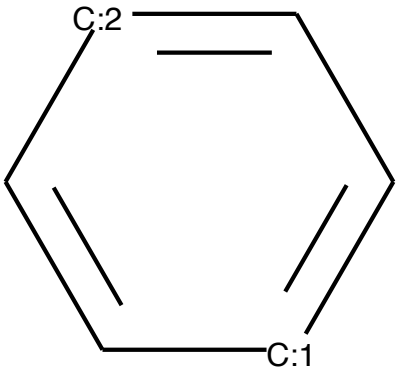



```
'------------------------------------------------------------'

'-----Step-2-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C#N and its specific config N#[CH:1] w/ probability -0.3776191174983
978'
```

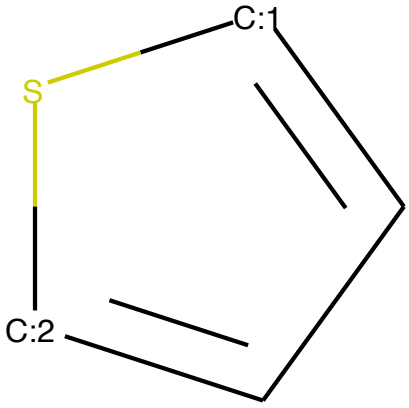
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -1.6490508317947388'



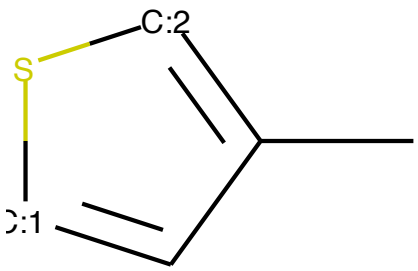
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-2.462209939956665'



'--'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ probabili
ty -3.976339101791382'

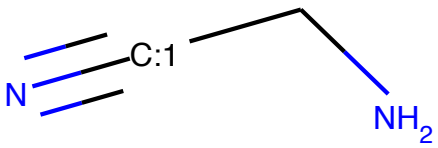



```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -4.291350841522
217'
```

```
'------------------------------------------------------------'

'Attaching fragment N#[CH:1]'
'Latest partial graph: N#CCN'
```




```
'------------------------------------------------------------'

'-----Step-3-----'
'-----Step-4-----'
'-----Step-5-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
```

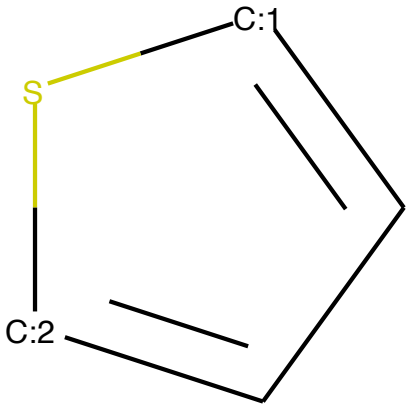
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -0.322565
31715393066'

'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.29867482
18536377'

'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-6.360332489013672'

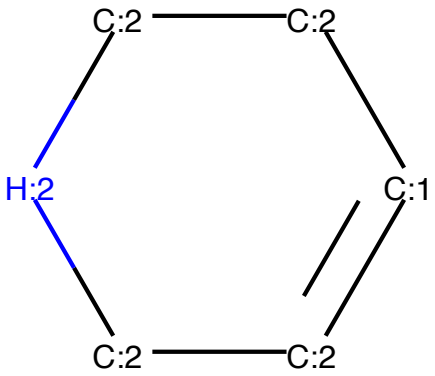


'--'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -7.436509132385
254'

```
'------------------------------------------------------------'

'Molecule C1=CCNCC1 and its specific config [CH:1]1=[CH:2][CH2:2][NH:2][CH2:2]
[CH2:2]1 w/ probability -9.168729782104492'
```




```
'------------------------------------------------------------'

'-----Step-6-----'
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'-----Step-123-----'
'-----Step-124-----'
'-----Step-125-----'
'-----Step-126-----'
```

Generation by w-tie-embedding-motif-only

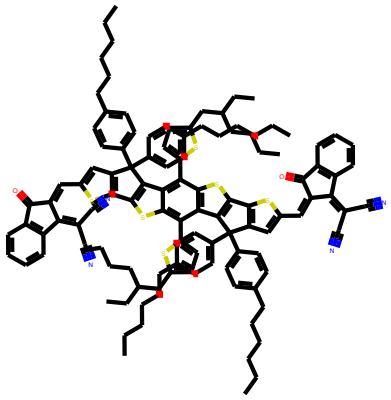
In [88]:

```
for i, sample in enumerate(w_te_data):
    if i > 11:
        break
    elif i < 11:
        continue
    display('Original: {}'.format(original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(original[i])]))

    # step 0
    step_f0 = sample[0]
    display('***************Sample {}th***************'.format(i))
    display('-----Step-0-----')
    display(step_f0)
    mol = Chem.MolFromSmiles(step_f0['partial-graph'])
    display('Displaying partial graph (aka molecule): {}'.format(step_f0['par
            Draw.MolsToGridImage([mol]))
    display('------------------------------------------------------------', HTML

    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        display('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            display('Generate next fragment: {}'.format(step_f['Generate frag
        if 'top-5-inter-cands' in step_f:
            display('Top 5 next fragments to attach (current and potential gr
            for fragment in step_f['top-5-inter-cands']:
                display('Molecule {} and its specific config {} w/ probabilit
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                display('------------------------------------------------------
        if 'Attaching Fragment' in step_f:
            frag = step_f['Attaching Fragment'][0]
            num_atom = len(list(Chem.MolFromSmiles(step_f['top-5-inter-cands'
            mol, indices = mol_with_atom_index(Chem.MolFromSmiles(step_f['par
                                               list(range(num_atom)))
            display('Attaching fragment {}'.format(frag))
            display('Latest partial graph: {}'.format(step_f['partial-graph']
                    Draw.MolsToGridImage([mol]))
            display('------------------------------------------------------
```

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



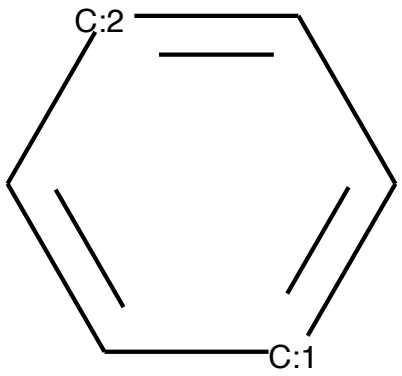
```
'***************Sample 11th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([653, 575,   0, 663, 579]),
 'super-root-idx': tensor(653),
 'top-5-root-fragment-cands': [('[CH3:1][NH2:2]', tensor(10.6275)),
  ('[NH2:1][CH3:2]', tensor(-14.2601)),
  ('N[CH3:1]', tensor(-24.1133)),
  ('C[NH2:1]', tensor(-37.7583)),
  ('CC([CH3:1])[CH3:2]', tensor(-953.2549))],
 'Attaching Fragment': '[CH3:1][NH2:2]',
 'partial-graph': 'CN'}
'Displaying partial graph (aka molecule): CN'
```

```
'------------------------------------------------------------'

'-----Step-1-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.30765676
498413086'
```

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -1.4975374937057495'
```

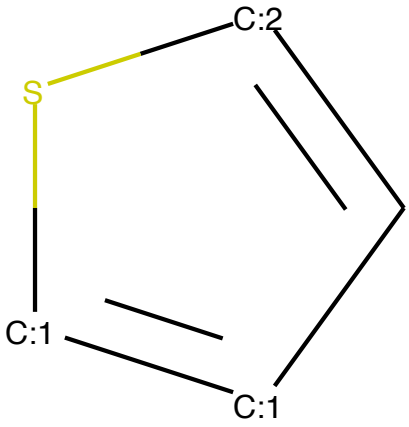



```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -3.778448
5816955566'

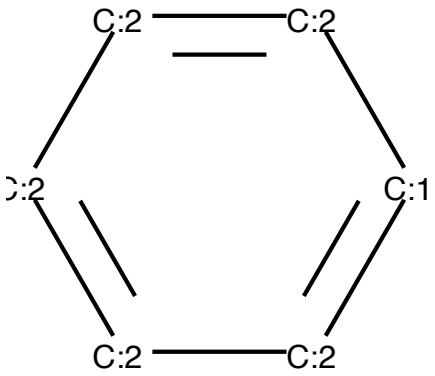
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -4.451709747314453'
```



'--'

'Molecule C1=CC=CC=C1 and its specific config [CH:1]1=[CH:2][CH:2]=[CH:2][CH:2
]=[CH:2]1 w/ probability -5.410152435302734'



'--'

'-----Step-2-----'
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'-----Step-83-----'
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'-----Step-96-----'
'-----Step-97-----'
'-----Step-98-----'
'-----Step-99-----'
'-----Step-100-----'
```

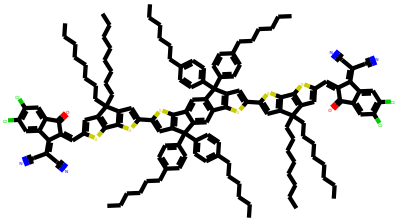
In [89]:

```
for i, sample in enumerate(w_te_data):
    if i > 7:
        break
    elif i < 7:
        continue
    display('Original: {}'.format(original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(original[i])]))

    # step 0
    step_f0 = sample[0]
    display('***************Sample {}th***************'.format(i))
    display('-----Step-0-----')
    display(step_f0)
    mol = Chem.MolFromSmiles(step_f0['partial-graph'])
    display('Displaying partial graph (aka molecule): {}'.format(step_f0['par
            Draw.MolsToGridImage([mol]))
    display('------------------------------------------------------------', HTML

    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        display('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            display('Generate next fragment: {}'.format(step_f['Generate frag
        if 'top-5-inter-cands' in step_f:
            display('Top 5 next fragments to attach (current and potential gr
            for fragment in step_f['top-5-inter-cands']:
                display('Molecule {} and its specific config {} w/ probabilit
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                display('------------------------------------------------------
        if 'Attaching Fragment' in step_f:
            frag = step_f['Attaching Fragment'][0]
            num_atom = len(list(Chem.MolFromSmiles(step_f['top-5-inter-cands'
            mol, indices = mol_with_atom_index(Chem.MolFromSmiles(step_f['par
                                               list(range(num_atom)))
            display('Attaching fragment {}'.format(frag))
            display('Latest partial graph: {}'.format(step_f['partial-graph']
                    Draw.MolsToGridImage([mol]))
            display('------------------------------------------------------
```

```
'Original: CCCCCCC1=CC=C(C2(C3=CC=C(CCCCCC)C=C3)C4=CC(C(SC(C5=CC(C6(CCCCCCCC)C
CCCCCCC)=C(C7=C6C=C(/C=C(C8=O)/C(C9=CC(Cl)=C(Cl)C=C89)=C(C#N)/C#N)S7)S5)=C%10)
=C%10C%11(C%12=CC=C(CCCCCC)C=C%12)C%13=CC=C(CCCCCC)C=C%13)=C%11C=C4C%14=C2C=C(
C%15=CC(C%16(CCCCCCCC)CCCCCCCC)=C(C%17=C%16C=C(/C=C(C%18=O)/C(C%19=CC(Cl)=C(Cl
)C=C%18%19)=C(C#N)\\C#N)S%17)S%15)S%14)C=C1'
```



```
'***************Sample 7th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([ 10, 610,   1, 653, 663]),
 'super-root-idx': tensor(10),
 'top-5-root-fragment-cands': [('[N:1]#[CH:2]', tensor(19.6517)),
  ('N#[CH:1]', tensor(-19.0220)),
  ('C#[N:1]', tensor(-25.1142)),
  ('C(N=[CH2:2])[CH3:1]', tensor(-972.3458)),
  ('C(#C[CH3:2])[CH3:1]', tensor(-973.3757))],
 'Attaching Fragment': '[N:1]#[CH:2]',
 'partial-graph': 'C#N'}
'Displaying partial graph (aka molecule): C#N'
```

```
'------------------------------------------------------------'

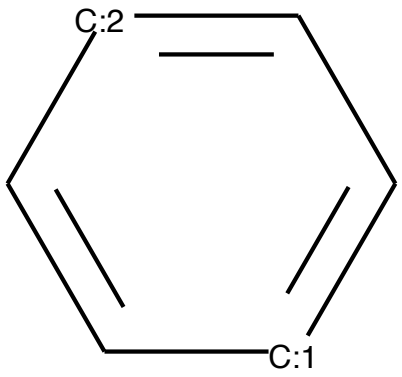
'-----Step-1-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.96046277
2236497e-07'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -14.3672351
8371582'
```

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -17.007352828979492'
```




```
'------------------------------------------------------------'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -17.7662086
4868164'
```

```
'------------------------------------------------------------'

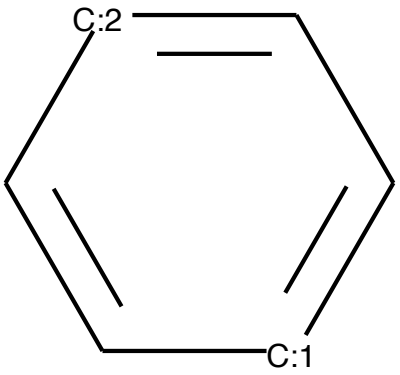
'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -21.821922
302246094'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC#N'
```

```
'------------------------------------------------------------'

'-----Step-2-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.6716226935386658'
```




```
'------------------------------------------------------------'

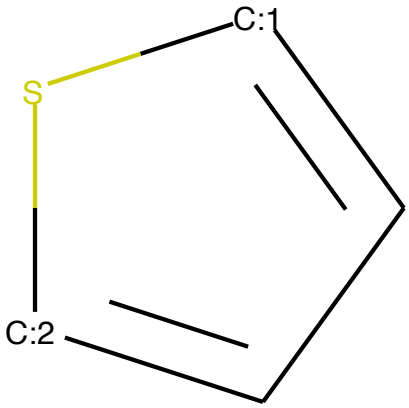
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.73742669
82078552'
```

```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -4.924198
150634766'
```

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-5.664557456970215'
```

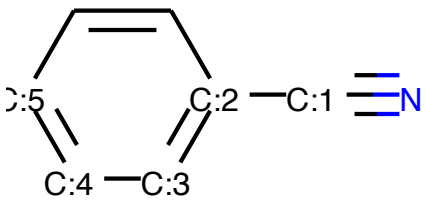



```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -11.33038330078125'
```

```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: N#Cc1ccccc1'
```




```
'------------------------------------------------------------'

'-----Step-3-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00211551
3663738966'
```

```
'------------------------------------------------------------'

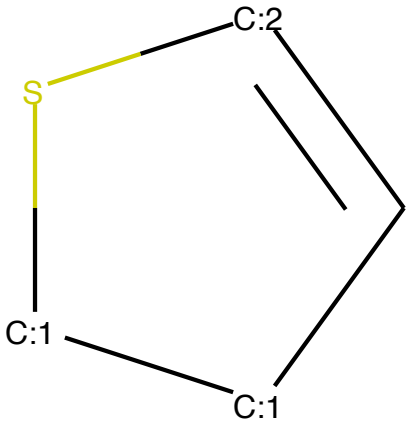
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -6.18443107
6049805'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -10.4975051
87988281'
```

```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -10.819089889526367'
```

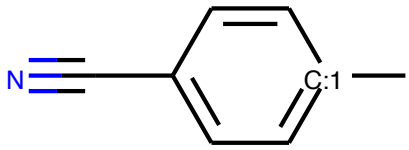



```
'------------------------------------------------------------'

'Molecule C[NH3+] and its specific config [NH3+:1][CH3:2] w/ probability -13.2
59058952331543'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(C#N)cc1'
```




```
'------------------------------------------------------------'

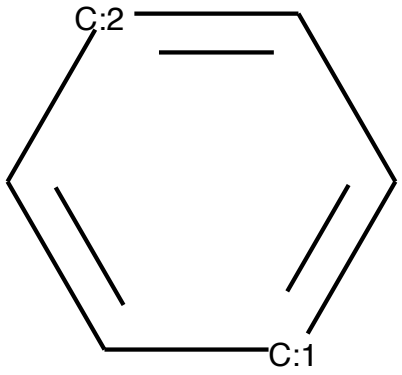
'-----Step-4-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.13669045
269489288'
```

```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -2.097678
1845092773'
```

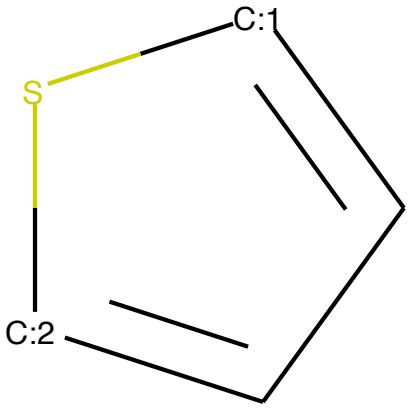
```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -5.903273582458496'
```



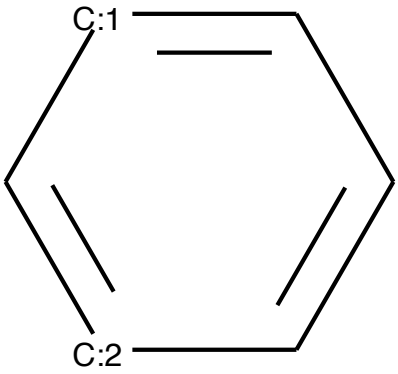

```
'------------------------------------------------------------'

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



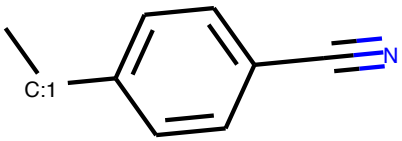
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=C[CH:2]=C[CH:1]=C1 w/ probabi
lity -9.907465934753418'



'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CCc1ccc(C#N)cc1'

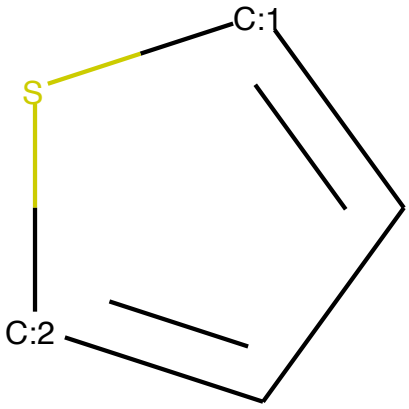


'--'

'-----Step-5-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.64209955
93070984'

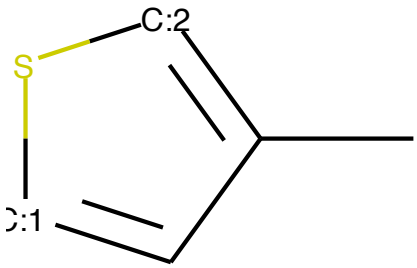
```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.8148662447929382'
```



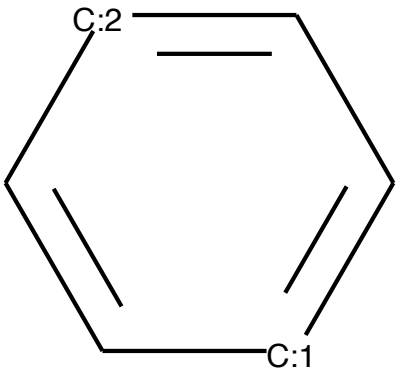

```
'------------------------------------------------------------'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:2]S[CH:1]=C1 w/ probabili
ty -3.8200552463531494'
```




```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -4.8768839836120605'
```

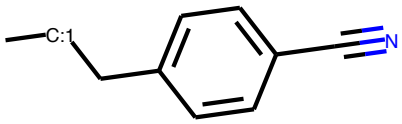


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -6.933335
781097412'

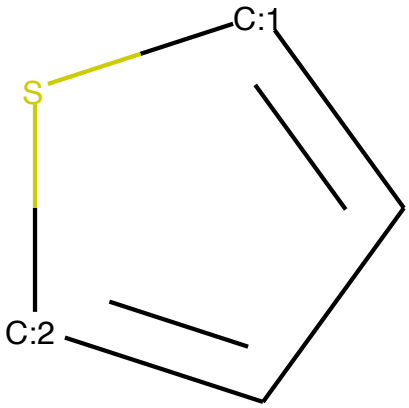
'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CCCc1ccc(C#N)cc1'



'--'

'-----Step-6-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.02030952088534832'

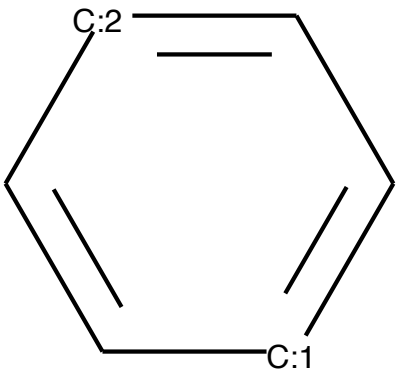


'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -3.92018461
227417'

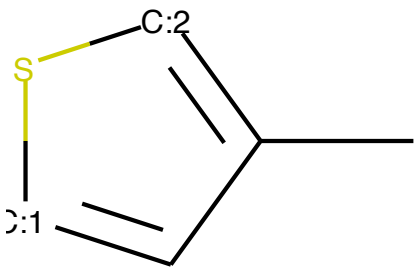
'--'

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



'--'

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

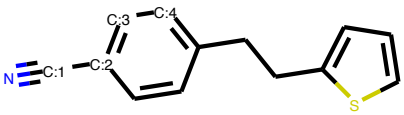



```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -11.24948
9784240723'
```

```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: N#Cc1ccc(CCc2cccs2)cc1'
```




```
'------------------------------------------------------------'

'-----Step-7-----'
'Generate next fragment: 0.9999597072601318'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability 0.0'
```

```
'------------------------------------------------------------'

'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -16.710937
5'
```

```
'------------------------------------------------------------'

'Molecule C=N and its specific config N=[CH2:1] w/ probability -21.72887611389
16'
```

```
'------------------------------------------------------------'

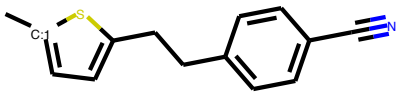
'Molecule CC and its specific config C[CH3:1] w/ probability -22.0816459655761
72'
```

```
'------------------------------------------------------------'

'Molecule C=N and its specific config [NH:1]=[CH2:2] w/ probability -22.576707
83996582'
```

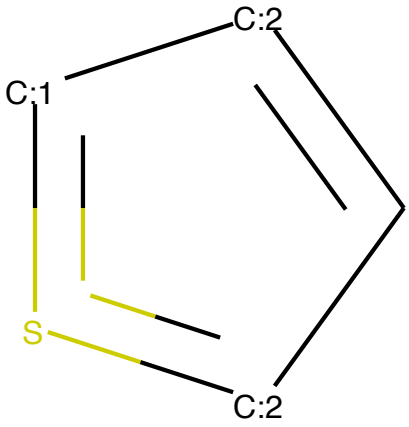
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(CCc2ccc(C#N)cc2)s1'
```



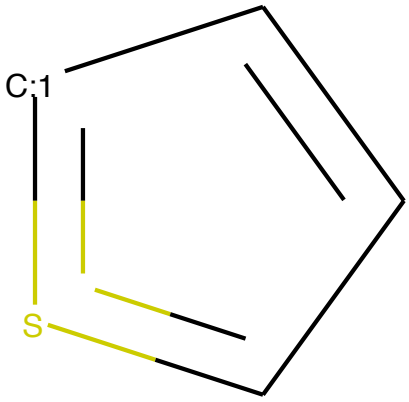

```
'------------------------------------------------------------'

'-----Step-8-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:1]=S=[CH:2]1 w/ prob
ability -0.07804661989212036'
```



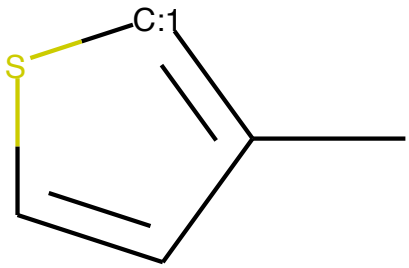
'--'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ probability -3
.591478109359741'



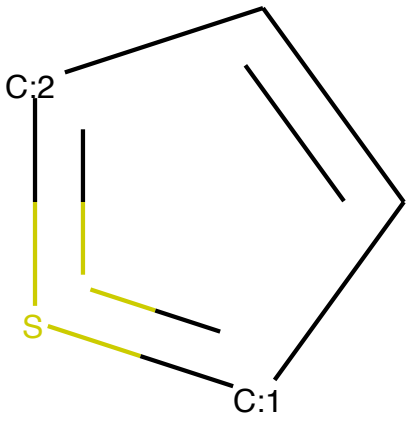
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]SC=C1 w/ probability -4
.145951747894287'



'--'

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

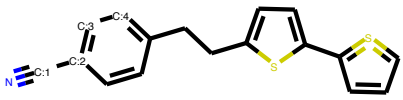


'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -4.62260150
9094238'

'--'

'Attaching fragment C1=[CH:2][CH:1]=S=[CH:2]1'
'Latest partial graph: N#Cc1ccc(CCc2ccc(C3=S=CC=C3)s2)cc1'



'--'

'-----Step-9-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00053999
14807640016'

```
'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -7.52424049377441
4'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -26.3571147
91870117'
```

```
'------------------------------------------------------------'

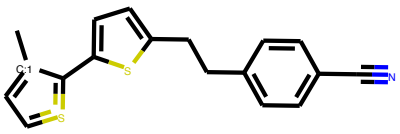
'Molecule CO and its specific config O[CH3:1] w/ probability -30.4642486572265
62'
```

```
'------------------------------------------------------------'

'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -32.347686
767578125'
```

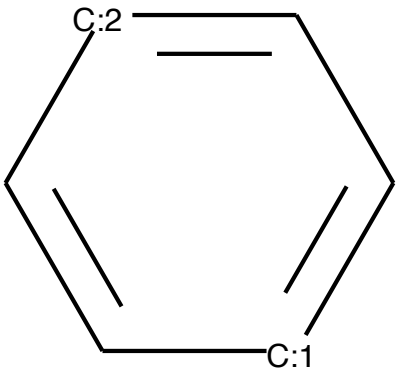
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC1=CC=S=C1c1ccc(CCc2ccc(C#N)cc2)s1'
```



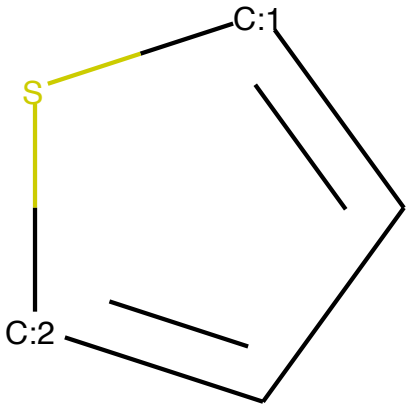

```
'------------------------------------------------------------'

'-----Step-10-----'
'Generate next fragment: 0.9998513460159302'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.5373675227165222'
```



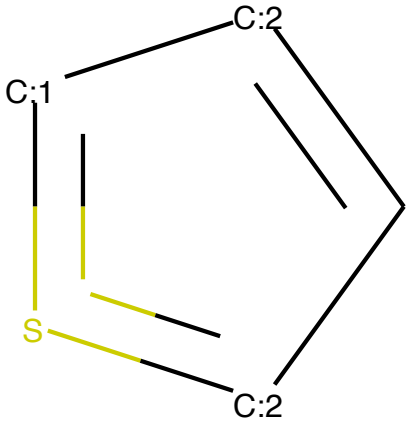
'--'

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



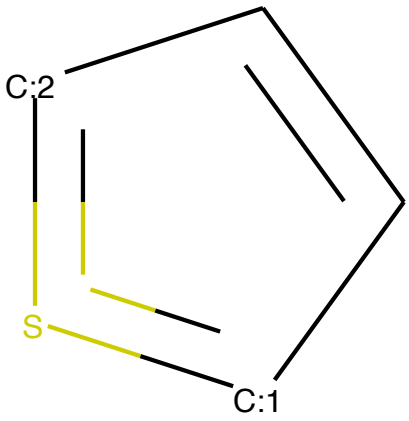
'--'

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



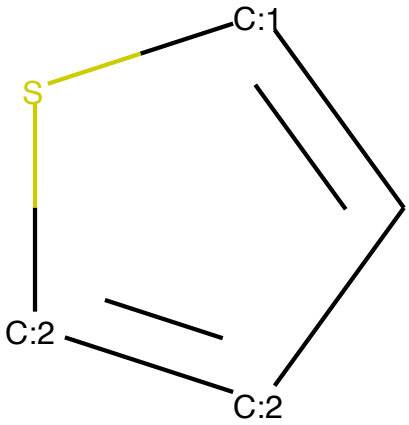
'--'

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



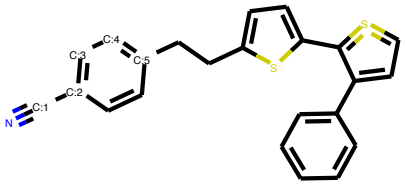
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -3.5445308685302734'



'--'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: N#Cc1ccc(CCc2ccc(C3=S=CC=C3c3ccccc3)s2)cc1'



'--'

'-----Step-11-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.72624355
55458069'

```
'------------------------------------------------------------'

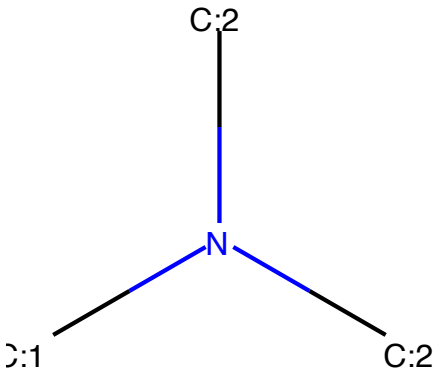
'Molecule CC and its specific config C[CH3:1] w/ probability -0.81903463602066
04'
```

```
'------------------------------------------------------------'

'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -3.20
60482501983643'
```

```
'------------------------------------------------------------'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -3.8265373706817627'
```

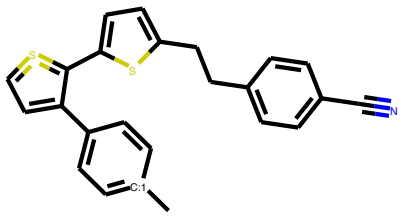



```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -4.87333488
4643555'
```

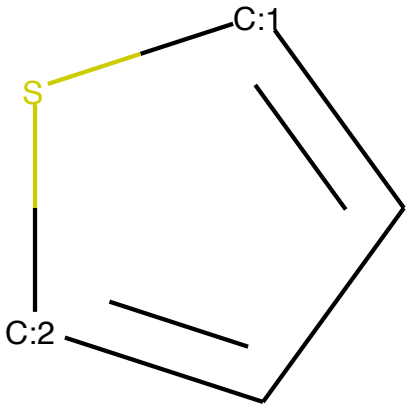
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(C2=CC=S=C2c2ccc(CCc3ccc(C#N)cc3)s2)cc1'
```



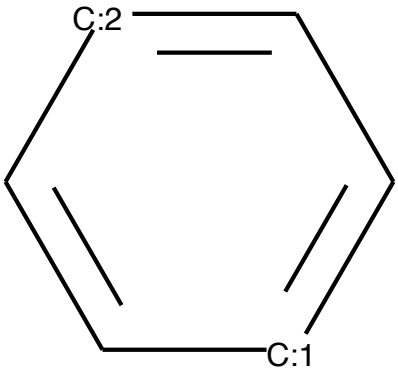

```
'------------------------------------------------------------'

'-----Step-12-----'
'Generate next fragment: 0.9999996423721313'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.00392892025411129'
```



'--'

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

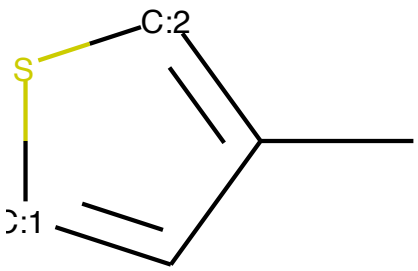


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -10.78921
3180541992'

'--'

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

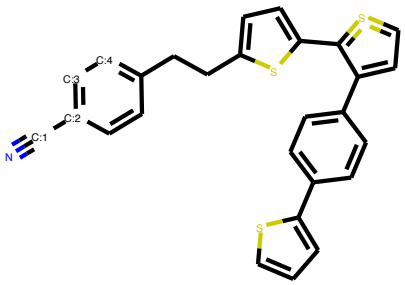


'--'

'Molecule C#N and its specific config N#[CH:1] w/ probability -11.757345199584
961'

'--'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: N#Cc1ccc(CCc2ccc(C3=S=CC=C3c3ccc(-c4cccs4)cc3)s2)cc1'



'--'

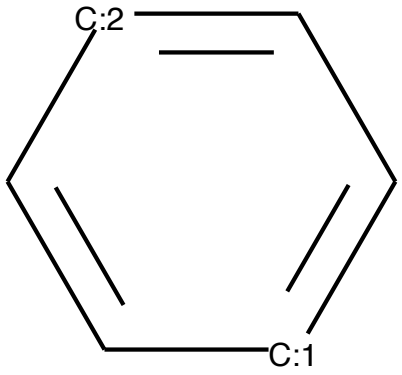
'-----Step-13-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config C[CH3:1] w/ probability -0.32609090209007
263'

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.27920889
85443115'
```

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -12.744547843933105'
```

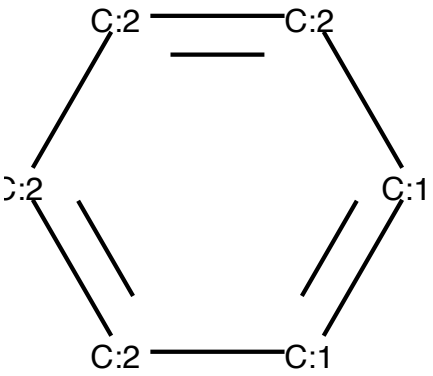



```
'------------------------------------------------------------'

'Molecule CF and its specific config F[CH3:1] w/ probability -15.8360939025878
9'
```

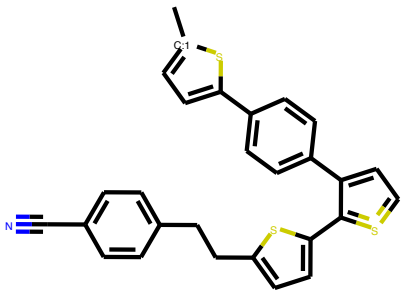
```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

'Attaching fragment C[CH3:1]'
'Latest partial graph: Cc1ccc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)s1
'
```




```
'------------------------------------------------------------'

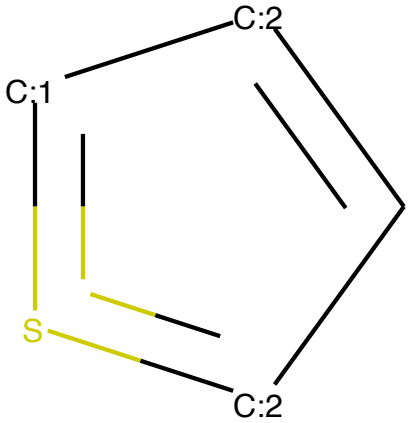
'-----Step-14-----'
'Generate next fragment: 0.9981449842453003'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -0.007015
240378677845'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.22525024
4140625'
```

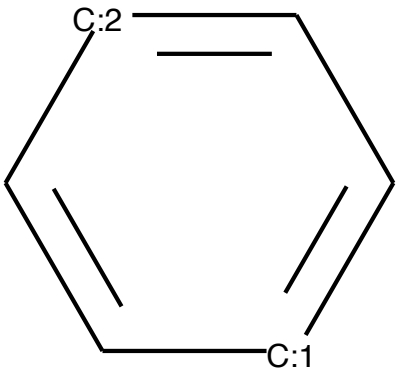
```
'------------------------------------------------------------'

'Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:1]=S=[CH:2]1 w/ prob
ability -7.219426155090332'
```



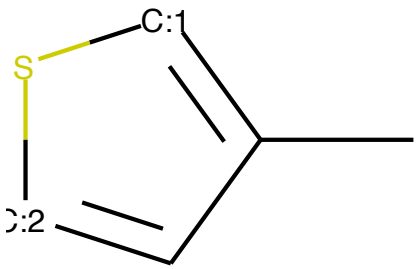

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -7.761297225952148'
```




```
'------------------------------------------------------------'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -7.8881096839904785'
```




```
'------------------------------------------------------------'

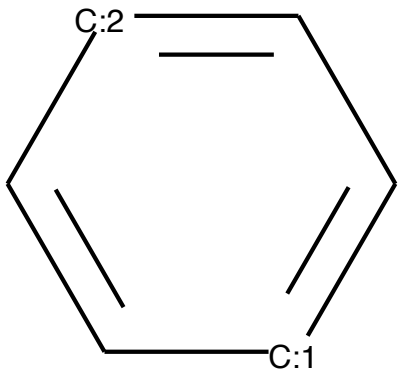
'-----Step-15-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config C[CH3:1] w/ probability -0.32609090209007
263'

'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.27920889
85443115'
```

'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -12.744547843933105'

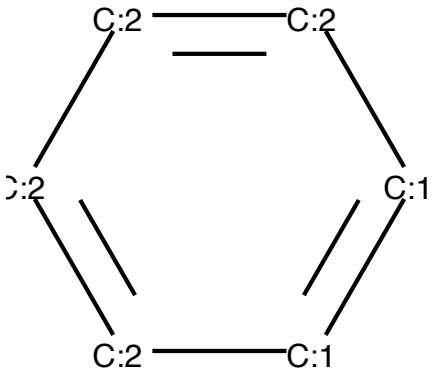


'--'

'Molecule CF and its specific config F[CH3:1] w/ probability -15.8360939025878
9'

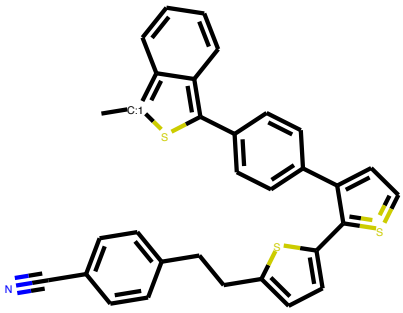
'--'

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



'--'

'Attaching fragment [CH:1]1=[CH:1][CH:2]=[CH:2][CH:2]=[CH:2]1'
'Latest partial graph: Cc1sc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)c2c
cccc12'

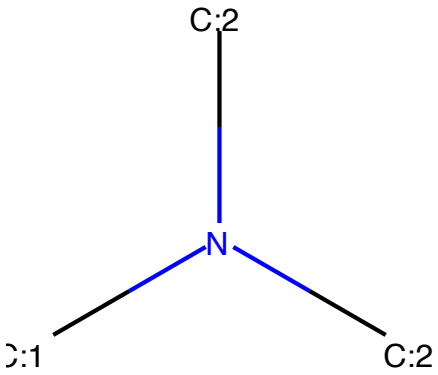


'--'

'-----Step-16-----'
'Generate next fragment: 0.9999998807907104'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.19209282
44535389e-07'

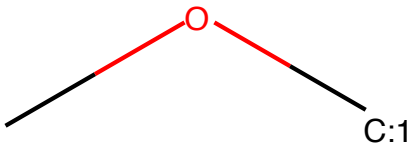
'--'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -16.55008316040039'



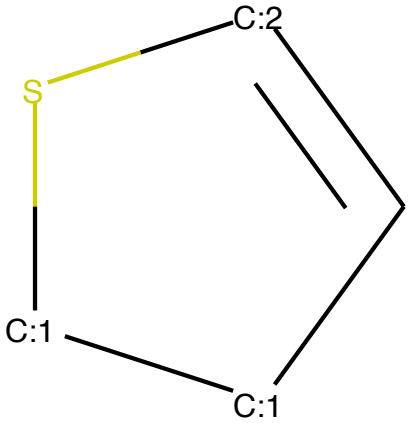
'--'

'Molecule COC and its specific config CO[CH3:1] w/ probability -18.54360198974
6094'



'--'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -20.33526039123535'

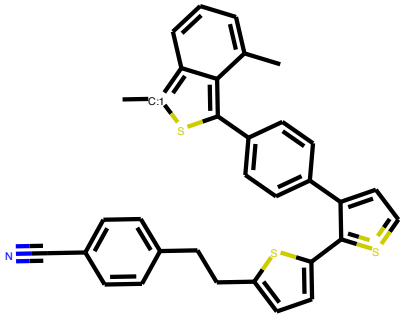


'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -21.7356300354003
9'

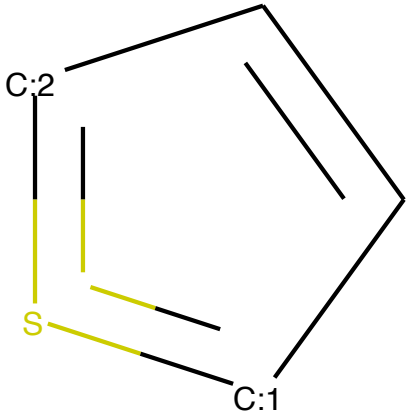
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1sc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)c2c
(C)cccc12'
```



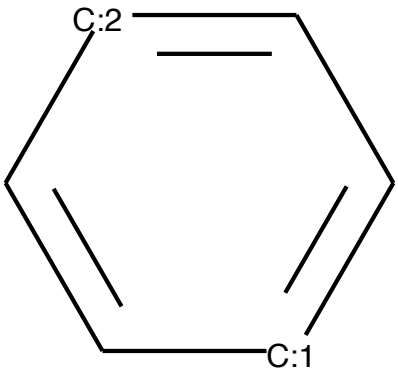

```
'------------------------------------------------------------'

'-----Step-17-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ probabili
ty -0.1079174280166626'
```



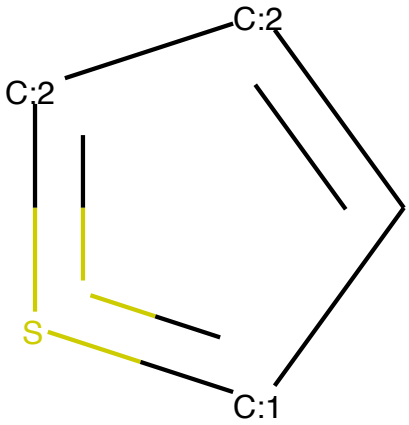

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.6073691844940186'
```



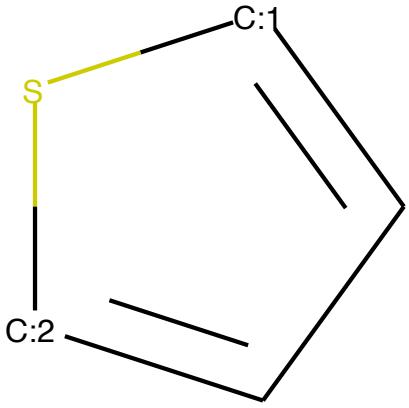
'--'

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



'--'

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

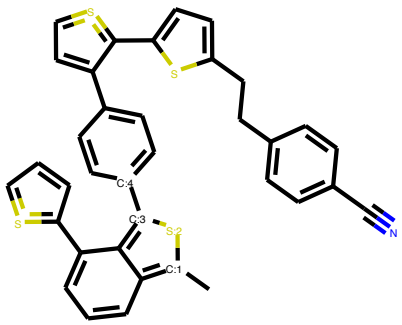


'--'

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

```
'------------------------------------------------------------'

'Attaching fragment C1=C[CH:2]=S=[CH:1]1'
'Latest partial graph: Cc1sc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)c2c
(C3=S=CC=C3)cccc12'
```




```
'------------------------------------------------------------'

'-----Step-18-----'
'Generate next fragment: 0.9999998807907104'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config C[CH3:1] w/ probability -2.10998223337810
5e-05'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -10.7668075
56152344'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -31.4693832
39746094'
```

```
'------------------------------------------------------------'

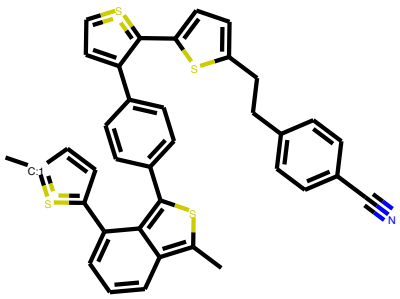
'Molecule CF and its specific config F[CH3:1] w/ probability -34.2855072021484
4'
```

```
'------------------------------------------------------------'

'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -34.701736
45019531'
```

```
'------------------------------------------------------------'

'Attaching fragment C[CH3:1]'
'Latest partial graph: CC1=S=C(c2cccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#
N)cc6)s5)cc4)c23)C=C1'
```




```
'------------------------------------------------------------'

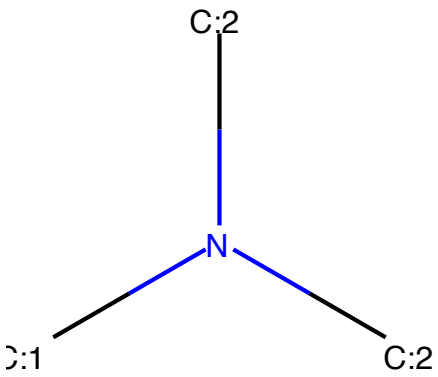
'-----Step-19-----'
'-----Step-20-----'
'-----Step-21-----'
'-----Step-22-----'
'Generate next fragment: 0.9575585126876831'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -8.34464685
7949556e-07'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config C[CH3:1] w/ probability -13.9809322357177
73'
```

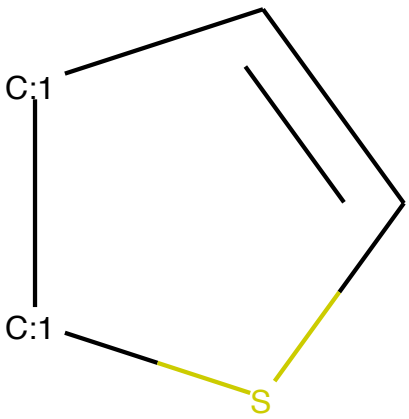
```
'------------------------------------------------------------'
```

```
'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -16.989187240600586'
```




```
'------------------------------------------------------------'
```

```
'Molecule C1=CSCC1 and its specific config C1=C[CH2:1][CH2:1]S1 w/ probability
-17.516544342041016'
```

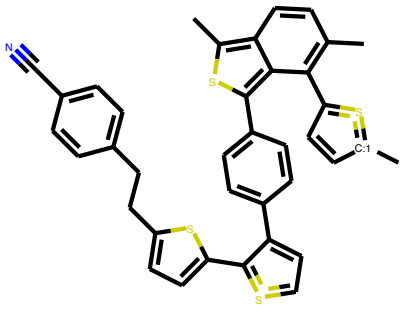



```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -19.9521503
44848633'
```

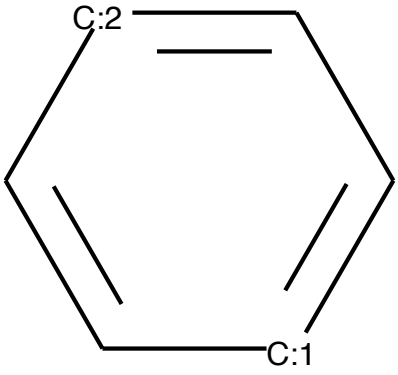
'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC1=S=C(c2c(C)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc
(C#N)cc6)s5)cc4)c23)C=C1'



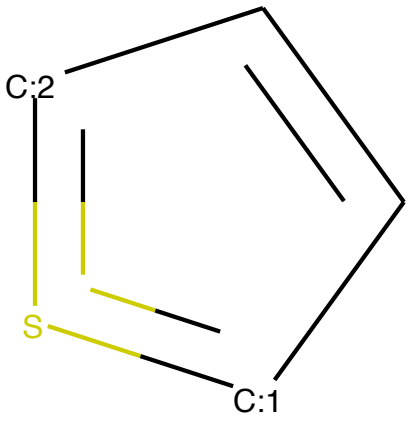
'--'

'-----Step-23-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.027290765196084976'



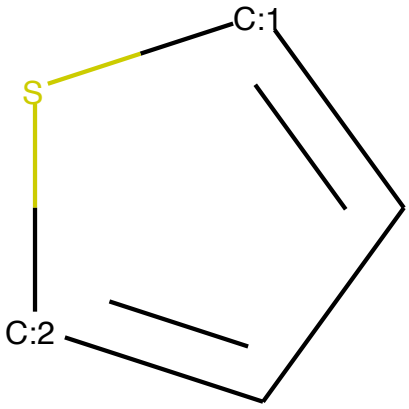
'--'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ probabili
ty -4.422307968139648'



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -4.530383586883545'

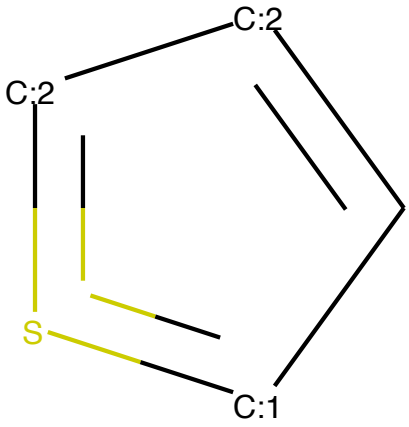


'--'

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

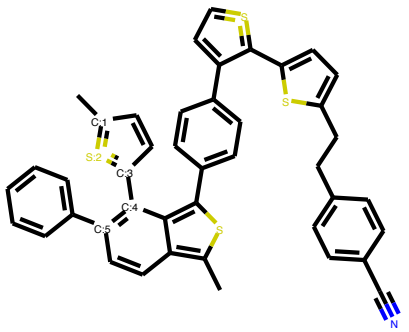
'--'

'Molecule C1=CC=S=C1 and its specific config C1=[CH:2][CH:2]=S=[CH:1]1 w/ probability -7.235950469970703'



'--'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: CC1=S=C(c2c(-c3ccccc3)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc
(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1'



'--'

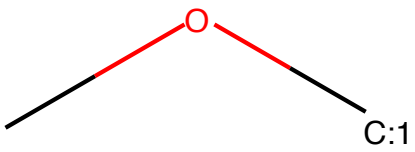
'-----Step-24-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.25249555
706977844'

'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -1.49995529651641
85'

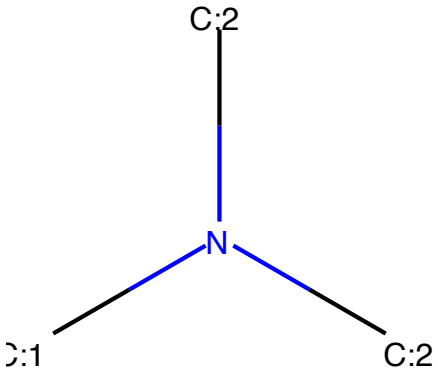
```
'------------------------------------------------------------'

'Molecule COC and its specific config CO[CH3:1] w/ probability -15.37720489501
9531'
```




```
'------------------------------------------------------------'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -18.22846221923828'
```

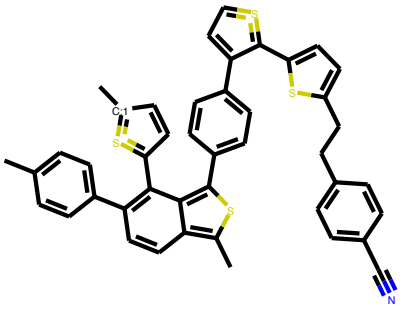



```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -19.6560955
04760742'
```

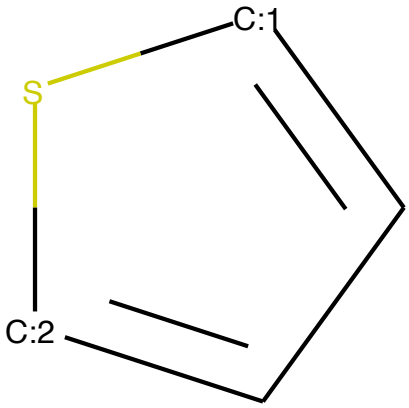
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC1=S=C(c2c(-c3ccc(C)cc3)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5
ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1'
```



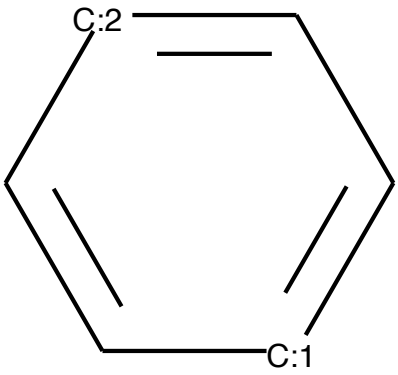

```
'------------------------------------------------------------'

'-----Step-25-----'
'Generate next fragment: 0.9999969005584717'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.06222383305430412'
```



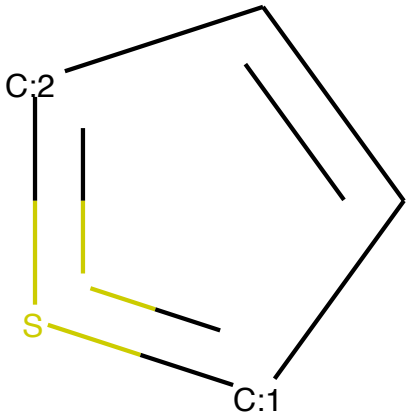

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.83522891998291'
```




```
'------------------------------------------------------------'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ probabili
ty -7.261528968811035'
```

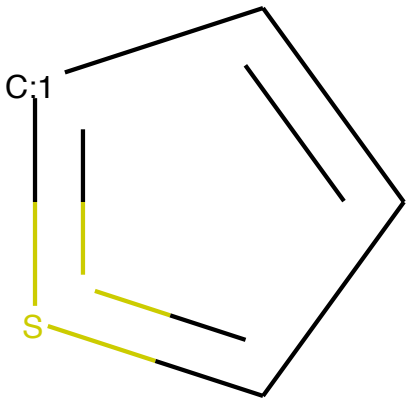



```
'------------------------------------------------------------'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -7.476279
7355651855'

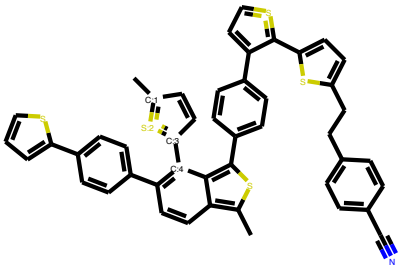
'------------------------------------------------------------'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ probability -8
.11657428741455'
```



'--'

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



'--'

'-----Step-26-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config C[CH3:1] w/ probability -0.00247517623938
6201'

'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -6.00269031
5246582'

```
'------------------------------------------------------------'

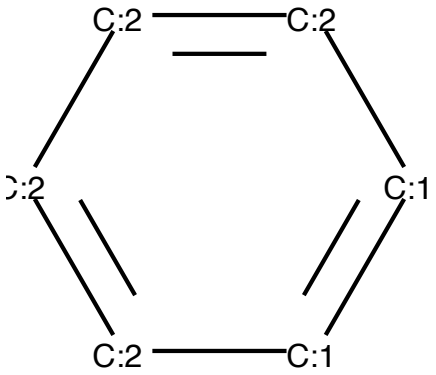
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -22.8222007
75146484'
```

```
'------------------------------------------------------------'

'Molecule CF and its specific config F[CH3:1] w/ probability -23.8284397125244
14'
```

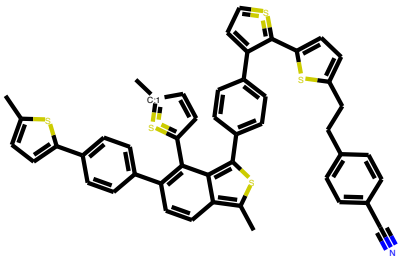
```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

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

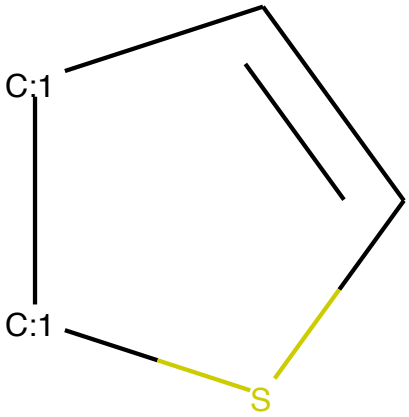


```
'------------------------------------------------------------'

'-----Step-27-----'
'-----Step-28-----'
'-----Step-29-----'
'-----Step-30-----'
'Generate next fragment: 0.9999982118606567'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.09698729
21705246'
```

```
'------------------------------------------------------------'
```

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

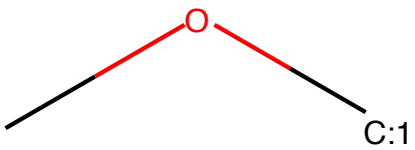


'--'

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

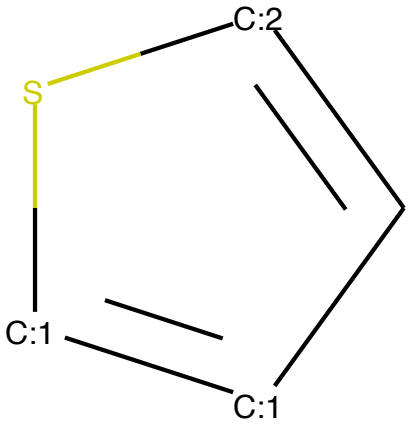
'--'

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



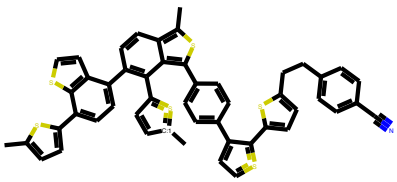
'--'

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




```
'------------------------------------------------------------'

'Attaching fragment C1=C[CH2:1][CH2:1]S1'
'Latest partial graph: CC1=S=C(c2c(-c3ccc(-c4ccc(C)s4)c4sccc34)ccc3c(C)sc(-c4c
cc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1'
```

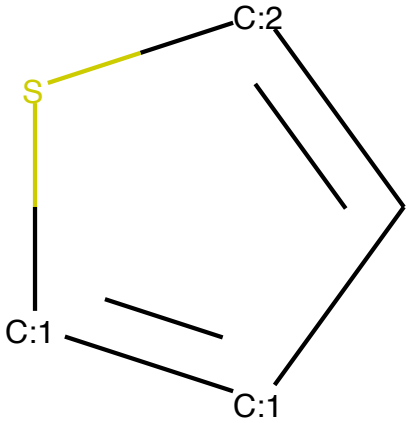


```
'------------------------------------------------------------'

'-----Step-31-----'
'-----Step-32-----'
'Generate next fragment: 0.9999061822891235'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -6.10334172
9613021e-05'
```

```
'------------------------------------------------------------'
```

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -9.753477096557617'

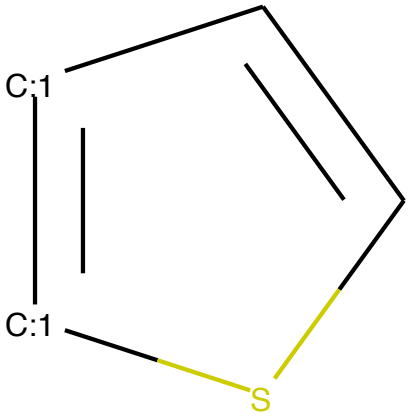


'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -13.0446128845214
84'

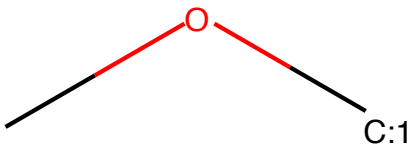
'--'

'Molecule C1=CSC=C1 and its specific config C1=C[CH:1]=[CH:1]S1 w/ probability
-14.950750350952148'



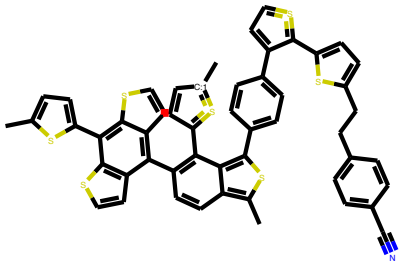
'--'

'Molecule COC and its specific config CO[CH3:1] w/ probability -15.15875434875
4883'




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:2]S[CH:1]=[CH:1]1'
'Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sccc34)ccc3c(C)sc
(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1'
```



```
'------------------------------------------------------------'

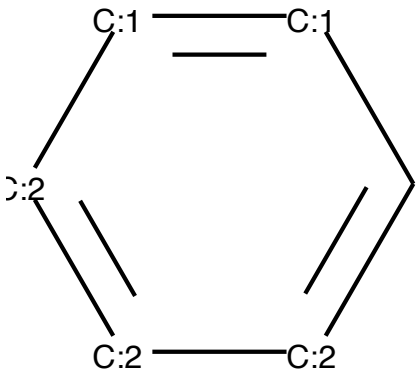
'-----Step-33-----'
'Generate next fragment: 0.9991055130958557'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.10141272
097826004'

'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -2.33883476257324
2'
```

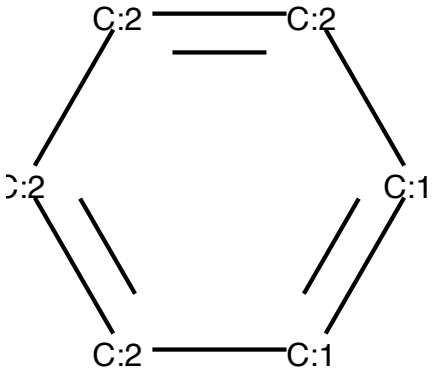
```
'------------------------------------------------------------'

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




```
'------------------------------------------------------------'

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

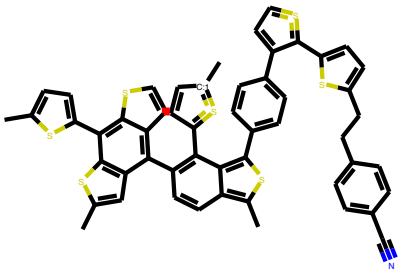



```
'------------------------------------------------------------'

'Molecule CF and its specific config F[CH3:1] w/ probability -24.9132843017578
12'
```

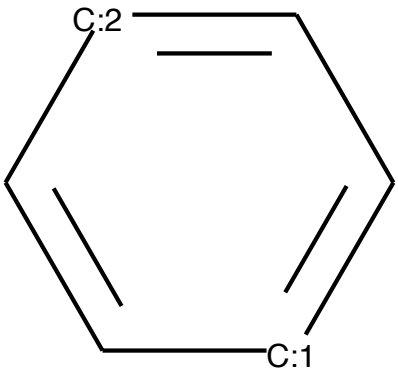
```
'------------------------------------------------------------'

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



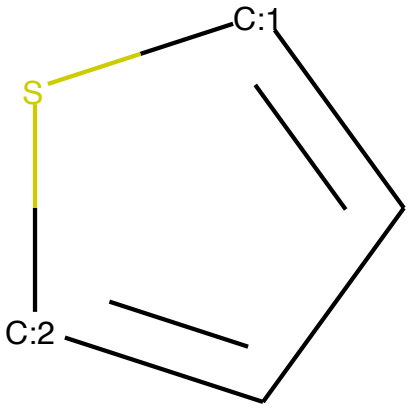
```
'------------------------------------------------------------'

'-----Step-34-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -0.4778480529785156'
```



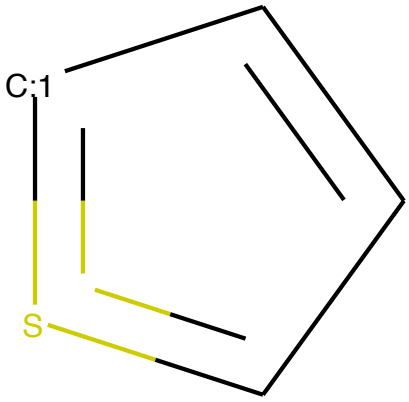

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-1.0630781650543213'
```



'--'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ probability -4
.04391622543335'

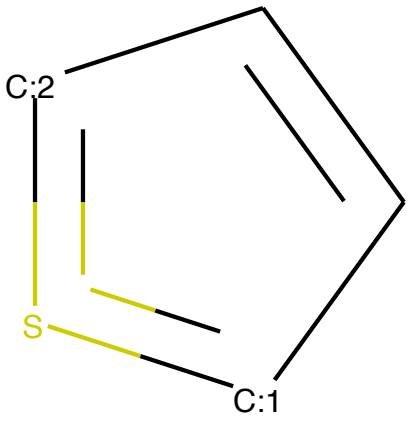


'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -4.75646018
9819336'

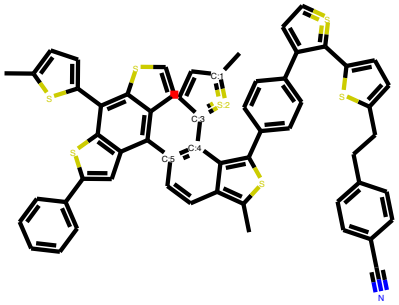
'--'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ probabili
ty -4.956562042236328'




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]C=C[CH:2]=C1'
'Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sc(-c5ccccc5)cc34
)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1'
```



```
'------------------------------------------------------------'

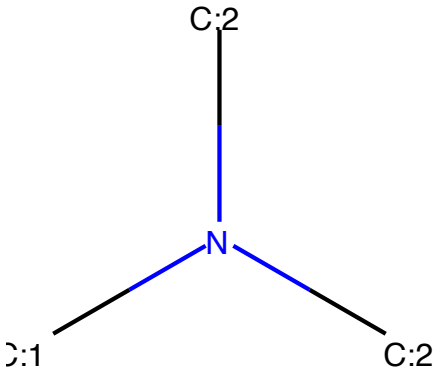
'-----Step-35-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00494720
46084702015'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -5.31625699996948
2'
```

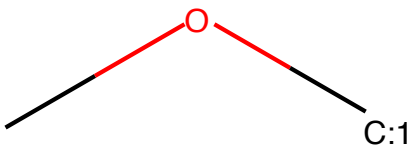
```
'------------------------------------------------------------'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -10.642192840576172'
```



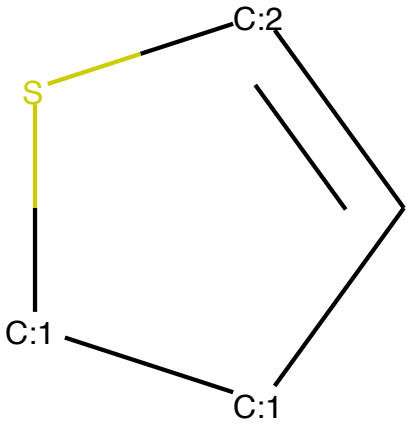

```
'------------------------------------------------------------'

'Molecule COC and its specific config CO[CH3:1] w/ probability -19.70873260498
047'
```



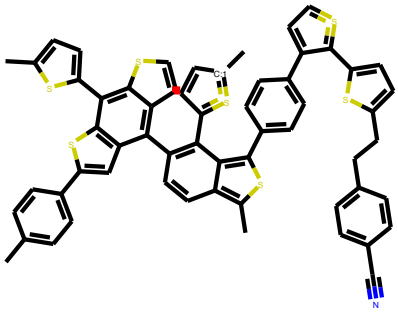

```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -22.31403923034668'
```



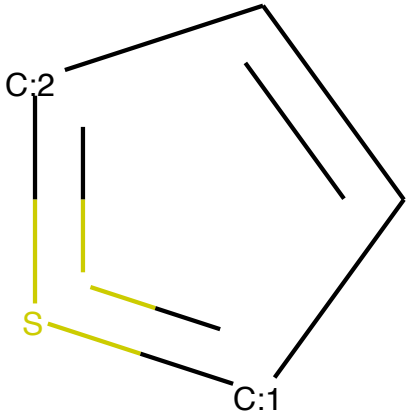
'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CC1=S=C(c2c(-c3c4ccsc4c(-c4ccc(C)s4)c4sc(-c5ccc(C)cc5)c
c34)ccc3c(C)sc(-c4ccc(C5=CC=S=C5c5ccc(CCc6ccc(C#N)cc6)s5)cc4)c23)C=C1'



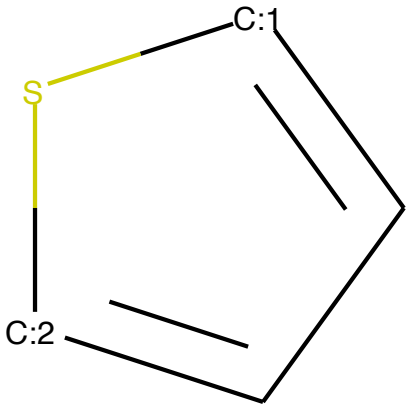
'--'

'-----Step-36-----'
'Generate next fragment: 0.9999997615814209'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ probabili
ty -0.9870807528495789'



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-1.1682732105255127'

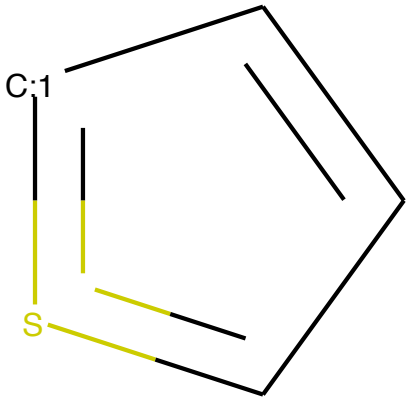


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -1.210477
590560913'

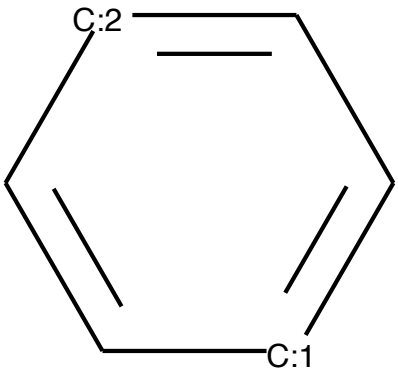
'--'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ probability -4
.201565742492676'



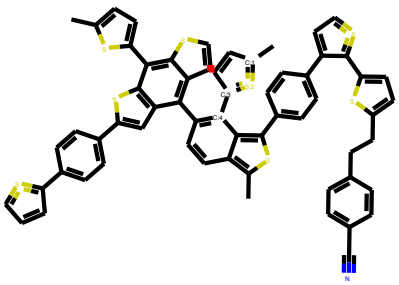
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -6.060859203338623'




```
'------------------------------------------------------------'

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



```
'------------------------------------------------------------'

'-----Step-37-----'
'Generate next fragment: 0.9999994039535522'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config C[CH3:1] w/ probability -0.07598993927240
372'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -2.61490917
20581055'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -32.0628700
25634766'
```

```
'------------------------------------------------------------'
```

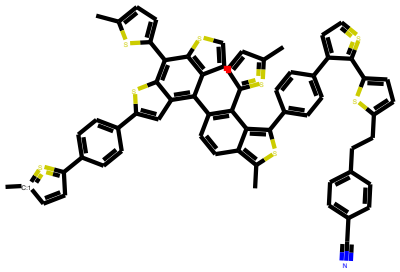
```
'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -40.745975
494384766'
```

```
'------------------------------------------------------------'
```

```
'Molecule CF and its specific config F[CH3:1] w/ probability -41.1009063720703
1'
```

```
'------------------------------------------------------------'

'Attaching fragment C[CH3:1]'
'Latest partial graph: CC1=S=C(c2ccc(-c3cc4c(-c5ccc6c(C)sc(-c7ccc(C8=CC=S=C8c8
ccc(CCc9ccc(C#N)cc9)s8)cc7)c6c5C5=S=C(C)C=C5)c5ccsc5c(-c5ccc(C)s5)c4s3)cc2)C=C
1'
```



```
'------------------------------------------------------------'

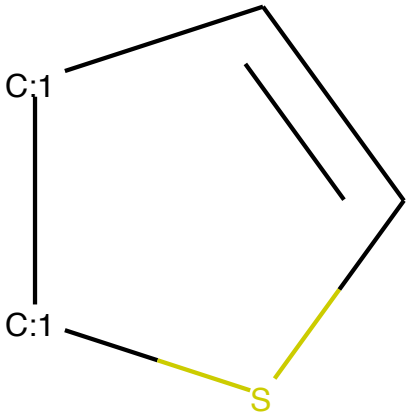
'-----Step-38-----'
'-----Step-39-----'
'-----Step-40-----'
'-----Step-41-----'
'-----Step-42-----'
'-----Step-43-----'
'-----Step-44-----'
'-----Step-45-----'
'-----Step-46-----'
'-----Step-47-----'
'-----Step-48-----'
'-----Step-49-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.33375895
02334595'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -1.40422677993774
41'
```

```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=C[CH2:1][CH2:1]S1 w/ probability
-3.840881824493408'
```

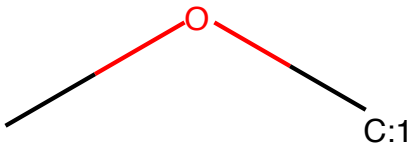



```
'------------------------------------------------------------'

'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -4.18
5676574707031'
```

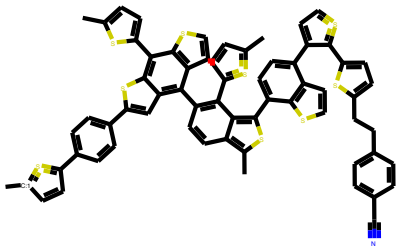
```
'------------------------------------------------------------'

'Molecule COC and its specific config CO[CH3:1] w/ probability -7.125823020935
059'
```




```
'------------------------------------------------------------'

'Attaching fragment C1=C[CH2:1][CH2:1]S1'
'Latest partial graph: CC1=S=C(c2ccc(-c3cc4c(-c5ccc6c(C)sc(-c7ccc(C8=CC=S=C8c8
ccc(CCc9ccc(C#N)cc9)s8)c8ccsc78)c6c5C5=S=C(C)C=C5)c5ccsc5c(-c5ccc(C)s5)c4s3)cc
2)C=C1'
```



```
'------------------------------------------------------------'

'-----Step-50-----'
'-----Step-51-----'
'Generate next fragment: 0.9866913557052612'
'Top 5 next fragments to attach (current and potential graph)'
```

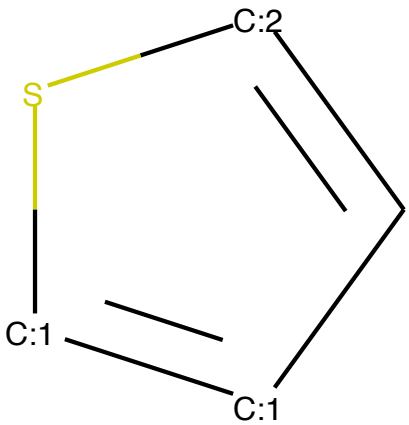
```
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00036414
1829777509'
```

```
'------------------------------------------------------------'
```

```
'Molecule CC and its specific config C[CH3:1] w/ probability -8.18435764312744
1'
```

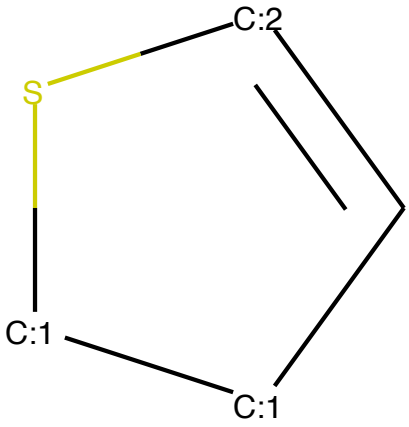
```
'------------------------------------------------------------'
```

```
'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -9.875532150268555'
```



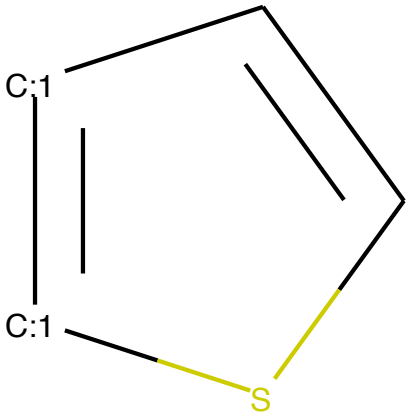

```
'------------------------------------------------------------'
```

```
'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -11.466437339782715'
```



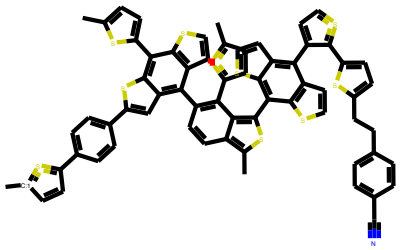

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=C[CH:1]=[CH:1]S1 w/ probability
-11.515392303466797'
```




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:2]S[CH:1]=[CH:1]1'
'Latest partial graph: CC1=S=C(c2ccc(-c3cc4c(-c5ccc6c(C)sc(-c7c8sccc8c(C8=CC=S
=C8c8ccc(CCc9ccc(C#N)cc9)s8)c8ccsc78)c6c5C5=S=C(C)C=C5)c5ccsc5c(-c5ccc(C)s5)c4
s3)cc2)C=C1'
```

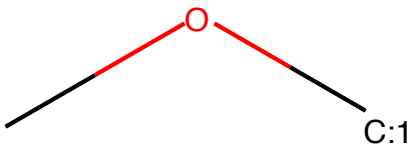


```
'------------------------------------------------------------'

'-----Step-52-----'
'-----Step-53-----'
'-----Step-54-----'
'-----Step-55-----'
```

```
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config C[CH3:1] w/ probability 0.0'
```

```
'------------------------------------------------------------'
'Molecule COC and its specific config CO[CH3:1] w/ probability -27.92363357543
9453'
```




```
'------------------------------------------------------------'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -28.6232357
0251465'
```

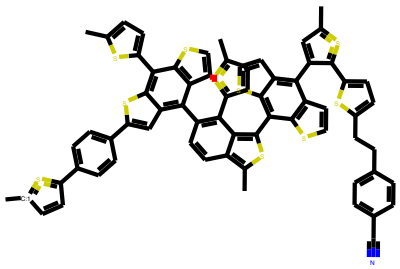
```
'------------------------------------------------------------'
'Molecule C=N and its specific config N=[CH2:1] w/ probability -29.23524093627
9297'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config N[CH3:1] w/ probability -30.8571548461914
06'
```

```
'------------------------------------------------------------'

'Attaching fragment C[CH3:1]'
'Latest partial graph: CC1=S=C(c2ccc(-c3cc4c(-c5ccc6c(C)sc(-c7c8sccc8c(C8=CC(C
)=S=C8c8ccc(CCc9ccc(C#N)cc9)s8)c8ccsc78)c6c5C5=S=C(C)C=C5)c5ccsc5c(-c5ccc(C)s5
)c4s3)cc2)C=C1'
```



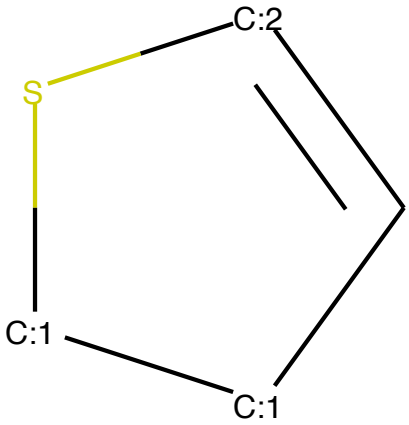
```
'------------------------------------------------------------'

'-----Step-56-----'
'-----Step-57-----'
'-----Step-58-----'
'-----Step-59-----'
```

```
'-----Step-60-----'
'-----Step-61-----'
'-----Step-62-----'
'-----Step-63-----'
'Generate next fragment: 0.5920002460479736'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00485183
1588894129'
```

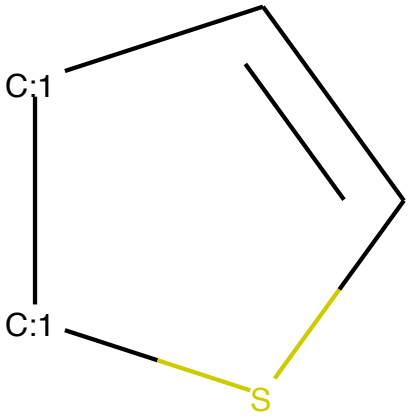
```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -5.367512226104736'
```



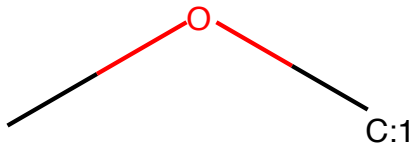

```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=C[CH2:1][CH2:1]S1 w/ probability
-9.53537368774414'
```



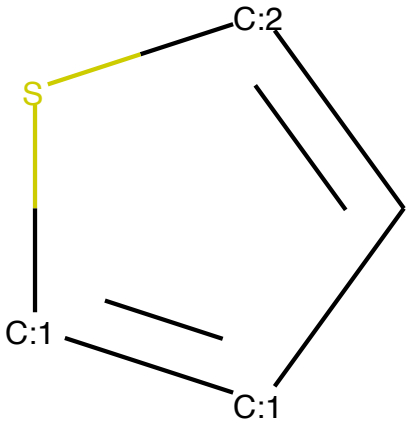
'--'

'Molecule COC and its specific config CO[CH3:1] w/ probability -9.582482337951
66'



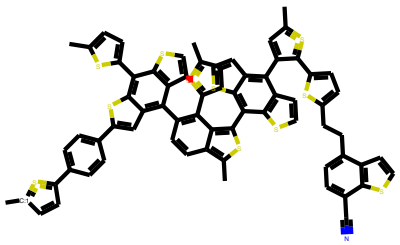
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -10.683775901794434'



'--'

'Attaching fragment C1=[CH:2]S[CH2:1][CH2:1]1'
'Latest partial graph: CC1=S=C(c2ccc(-c3cc4c(-c5ccc6c(C)sc(-c7c8sccc8c(C8=CC(C
)=S=C8c8ccc(CCc9ccc(C#N)c%10sccc9%10)s8)c8ccsc78)c6c5C5=S=C(C)C=C5)c5ccsc5c(-c
5ccc(C)s5)c4s3)cc2)C=C1'



'--'

'-----Step-64-----'

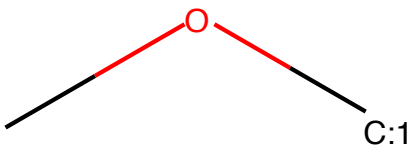
```
'-----Step-65-----'
'-----Step-66-----'
'-----Step-67-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00045610
9904916957'
```

```
'------------------------------------------------------------'
'Molecule CC and its specific config C[CH3:1] w/ probability -7.69293689727783
2'
```

```
'------------------------------------------------------------'
'Molecule C[NH3+] and its specific config [CH3:1][NH3+:2] w/ probability -17.5
26927947998047'
```

```
'------------------------------------------------------------'
```

'Molecule COC and its specific config CO[CH3:1] w/ probability -19.24920082092
285'



'--'

'Molecule C[NH3+] and its specific config [NH3+:1][CH3:2] w/ probability -20.9
7563934326172'

'--'

'-----Step-68-----'
'-----Step-69-----'
'-----Step-70-----'
'-----Step-71-----'
'-----Step-72-----'
'-----Step-73-----'
'-----Step-74-----'
'-----Step-75-----'
'-----Step-76-----'
'-----Step-77-----'
'-----Step-78-----'
'-----Step-79-----'
'-----Step-80-----'
'-----Step-81-----'
'-----Step-82-----'
'-----Step-83-----'
'-----Step-84-----'
'-----Step-85-----'
'-----Step-86-----'
'-----Step-87-----'
'-----Step-88-----'

```
'-----Step-89-----'
'-----Step-90-----'
'-----Step-91-----'
'-----Step-92-----'
'-----Step-93-----'
'-----Step-94-----'
'-----Step-95-----'
'-----Step-96-----'
'-----Step-97-----'
'-----Step-98-----'
'-----Step-99-----'
'-----Step-100-----'
```

In [90]:

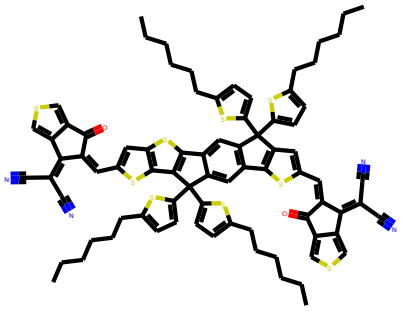
```
for i, sample in enumerate(w_te_data):
    if i > 12:
        break
    elif i < 12:
        continue
    display('Original: {}'.format(original[i]))
    display(Draw.MolsToGridImage([Chem.MolFromSmiles(original[i])]))

    # step 0
    step_f0 = sample[0]
    display('***************Sample {}th***************'.format(i))
    display('-----Step-0-----')
    display(step_f0)
    mol = Chem.MolFromSmiles(step_f0['partial-graph'])
    display('Displaying partial graph (aka molecule): {}'.format(step_f0['par
            Draw.MolsToGridImage([mol]))
    display('------------------------------------------------------------', HTML

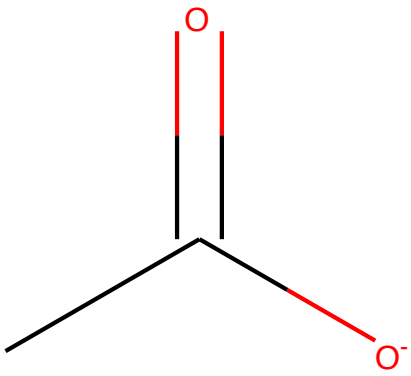
    # the remaing steps
    for i, step_f in enumerate(sample[1:]):
        display('-----Step-{}-----' .format(i + 1))
        if 'Generate fragment' in step_f:
            display('Generate next fragment: {}'.format(step_f['Generate frag
        if 'top-5-inter-cands' in step_f:
            display('Top 5 next fragments to attach (current and potential gr
            for fragment in step_f['top-5-inter-cands']:
                display('Molecule {} and its specific config {} w/ probabilit
                display(Draw.MolsToGridImage([Chem.MolFromSmiles(fragment[1])
                display('------------------------------------------------------
        if 'Attaching Fragment' in step_f:
            frag = step_f['Attaching Fragment'][0]
            num_atom = len(list(Chem.MolFromSmiles(step_f['top-5-inter-cands'
            mol, indices = mol_with_atom_index(Chem.MolFromSmiles(step_f['par
                                               list(range(num_atom)))
            display('Attaching fragment {}'.format(frag))
            display('Latest partial graph: {}'.format(step_f['partial-graph']
                    Draw.MolsToGridImage([mol]))
            display('------------------------------------------------------
```

```
'Original: CCCCCCC1=CC=C(S1)C2(C(S3)=CC=C3CCCCCC)C(C(SC(/C=C(C4=O)/C(C5=CSC=C4
```

```
5)=C(C#N)\\C#N)=C6)=C6S7)=C7C8=CC9=C(C(SC(/C=C(C%10=O)/C(C%11=CSC=C%10%11)=C(C
#N)\\C#N)=C%12)=C%12C9(C(S%13)=CC=C%13CCCCCC)C(S%14)=CC=C%14CCCCCC)C=C28'
```



```
'***************Sample 12th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([590, 670, 653, 675, 663]),
 'super-root-idx': tensor(590),
 'top-5-root-fragment-cands': [('O=C([O-:1])[CH3:2]', tensor(13.9317)),
  ('O=C([O-])[CH3:1]', tensor(-12.5431)),
  ('CC(=O)[O-:1]', tensor(-16.1744)),
  ('[O:1]=[CH2:2]', tensor(-980.1329)),
  ('C(#C[CH3:2])[CH3:1]', tensor(-980.1487))],
 'Attaching Fragment': 'O=C([O-:1])[CH3:2]',
 'partial-graph': 'CC(=O)[O-]'}
'Displaying partial graph (aka molecule): CC(=O)[O-]'
```

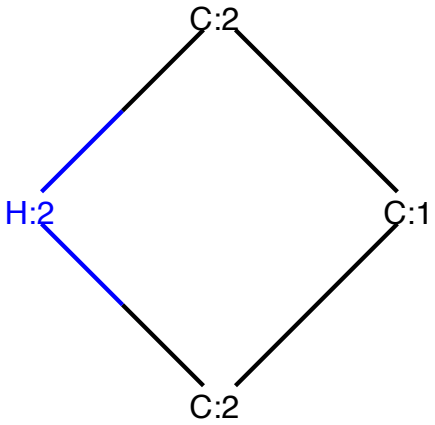



```
'------------------------------------------------------------'

'-----Step-1-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.07073831
55822754'
```

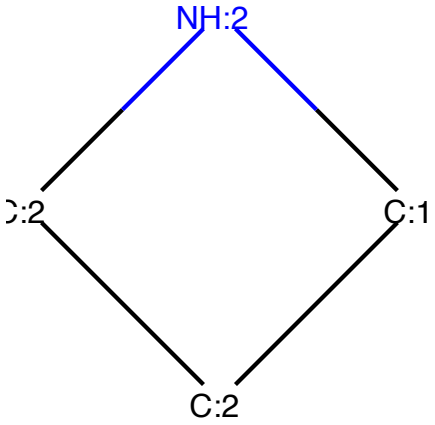
```
'------------------------------------------------------------'

'Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][NH:2][CH2:2]1 w/ prob
ability -1.16451895236969'
```



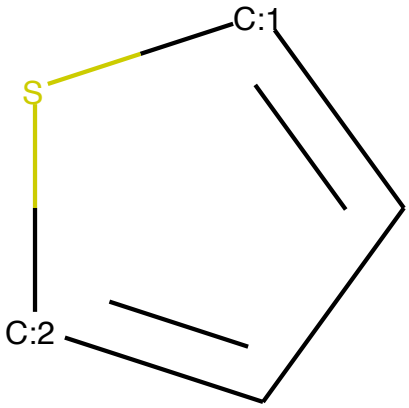

```
'------------------------------------------------------------'

'Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2]1 w/ prob
ability -1.808347225189209'
```




```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-2.6687560081481934'
```

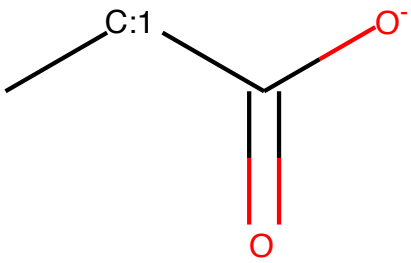



```
'------------------------------------------------------------'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -3.12031841
27807617'
```

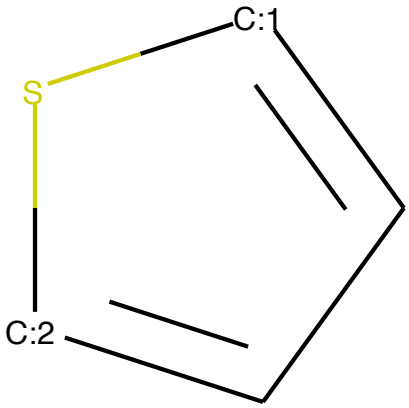
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CCC(=O)[O-]'
```



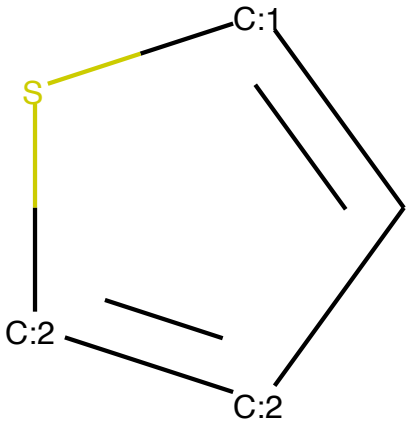

```
'------------------------------------------------------------'

'-----Step-2-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.015211270190775394'
```



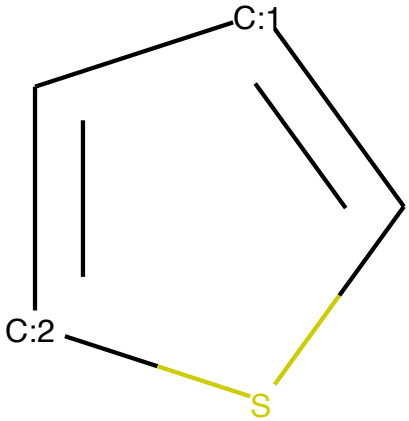
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -4.913881301879883'



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]C=[CH:2]S1 w/ probability
-5.474489212036133'

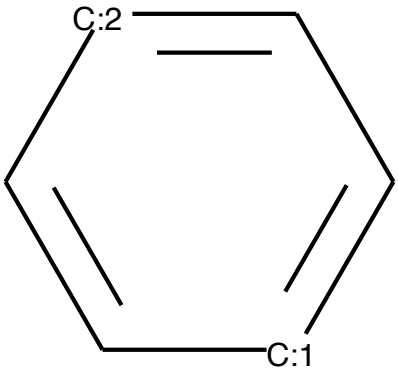


'--'

'Molecule C and its specific config C w/ probability -5.725157260894775'

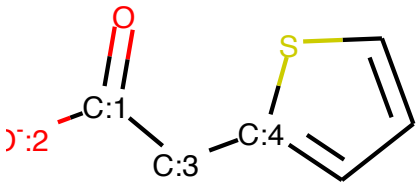
```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -8.778680801391602'
```




```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1cccs1'
```

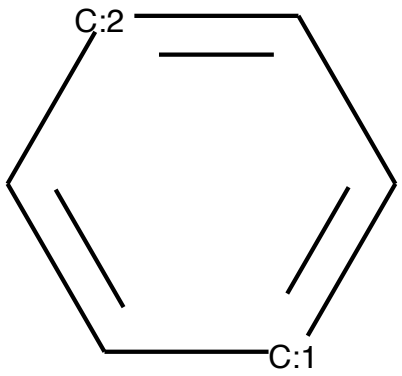



```
'------------------------------------------------------------'

'-----Step-3-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -1.81196483
0267243e-05'
```

```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -11.434046745300293'
```

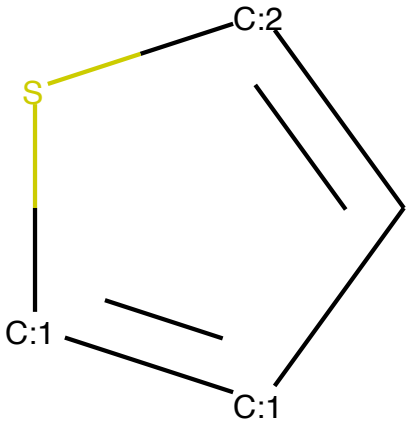



```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -11.994294166564941'

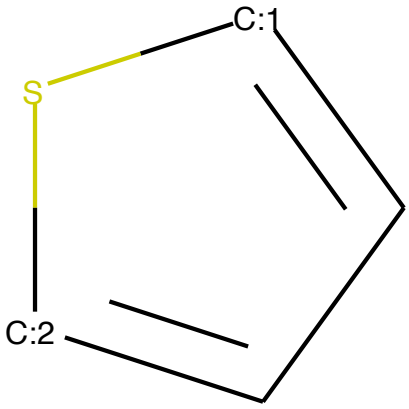
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -13.705684661865234'
```



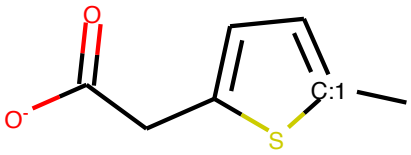
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -17.18779754638672'



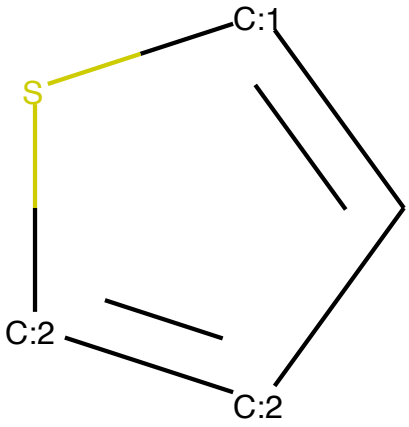
'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(CC(=O)[O-])s1'



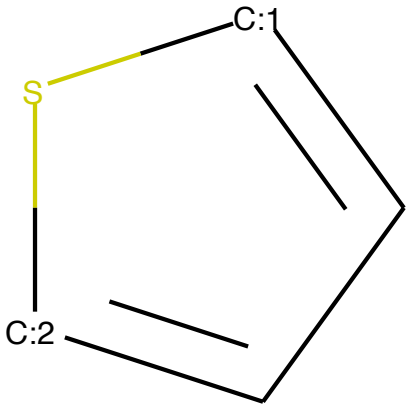
'--'

'-----Step-4-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probability -0.009146904572844505'



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -4.787027835845947'

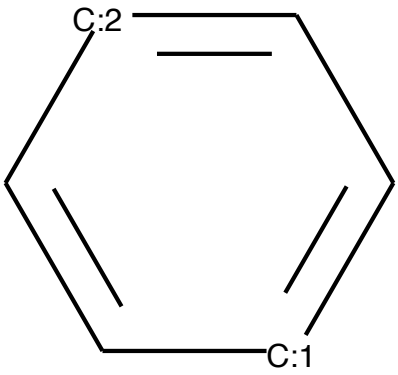


'--'

'Molecule C and its specific config C w/ probability -7.912520408630371'

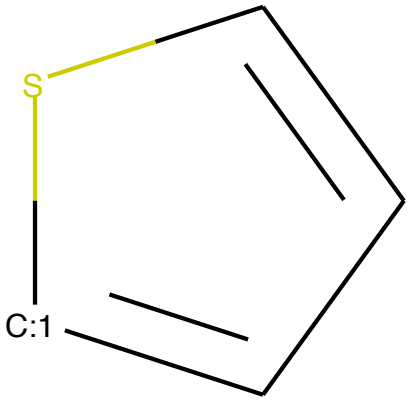
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probability -8.354876518249512'



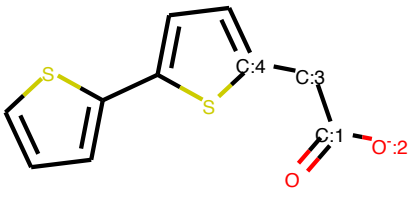
'--'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -8.9
74496841430664'



'--'

'Attaching fragment C1=[CH:1]S[CH:2]=[CH:2]1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2cccs2)s1'

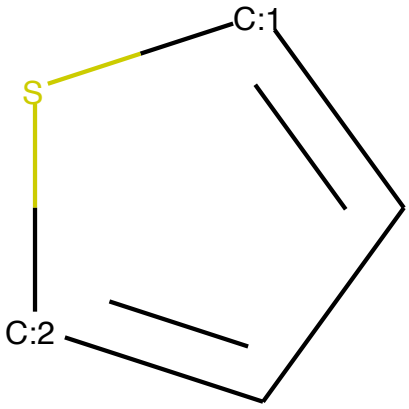


'--'

'-----Step-5-----'
'Generate next fragment: 0.9997887015342712'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.56950706
24351501'

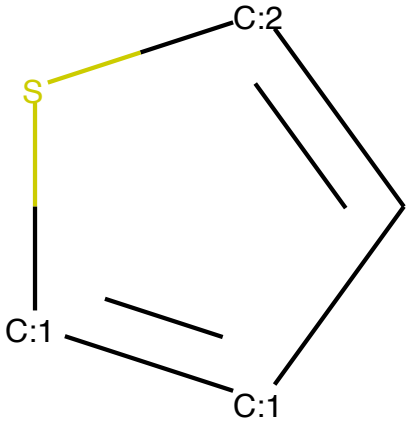
```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-1.1753448247909546'
```



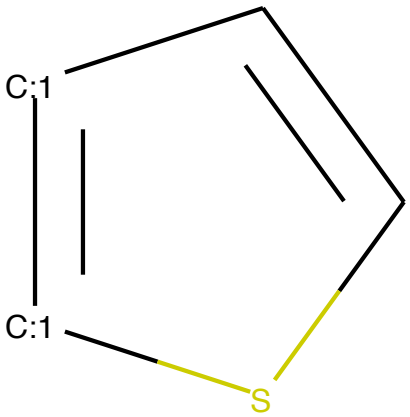

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ probab
ility -2.7043516635894775'
```




```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=C[CH:1]=[CH:1]S1 w/ probability
-3.261600971221924'
```

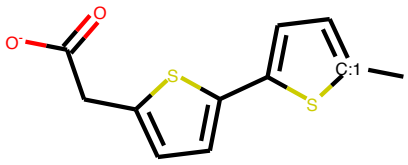



```
'------------------------------------------------------------'

'Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ probability -4.33
6895942687988'
```

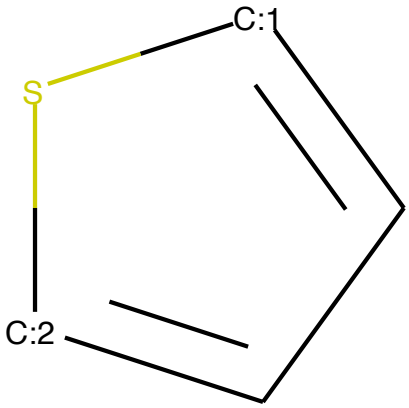
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(-c2ccc(CC(=O)[O-])s2)s1'
```



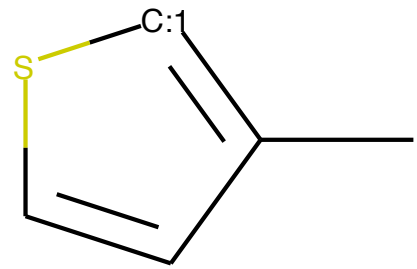

```
'------------------------------------------------------------'

'-----Step-6-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.010365660302340984'
```



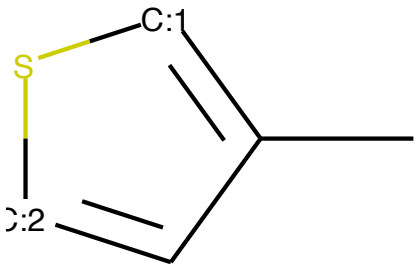
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]SC=C1 w/ probability -4
.703817367553711'



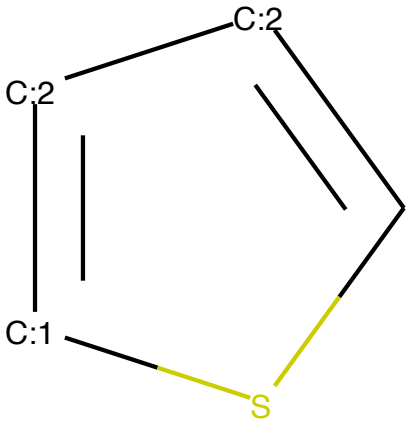
'--'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -6.875165939331055'



'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:2]=[CH:1]S1 w/ probab
ility -9.226217269897461'

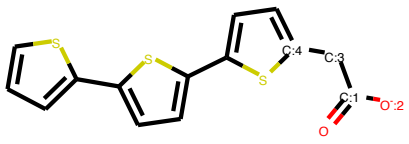


'--'

'Molecule C and its specific config C w/ probability -9.870923042297363'

'--'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3cccs3)s2)s1'



'--'

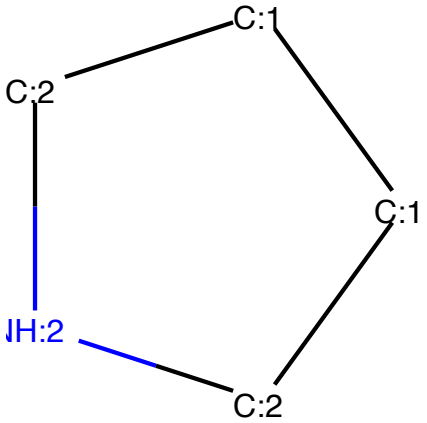
'-----Step-7-----'
'Generate next fragment: 0.9998983144760132'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00630442
42560863495'

```
'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -5.35567331314086
9'
```

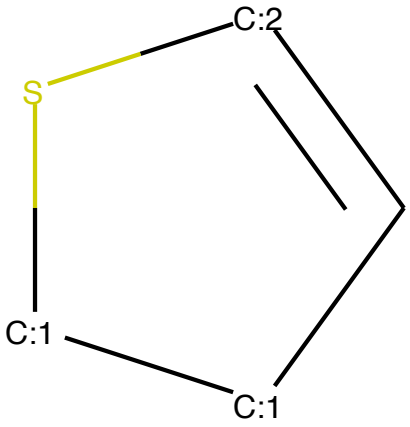
```
'------------------------------------------------------------'

'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][CH2:2][NH:2][CH2:2]1
w/ probability -7.019346714019775'
```




```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -7.966949939727783'
```

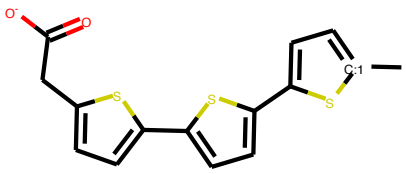



```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -9.378978729248
047'
```

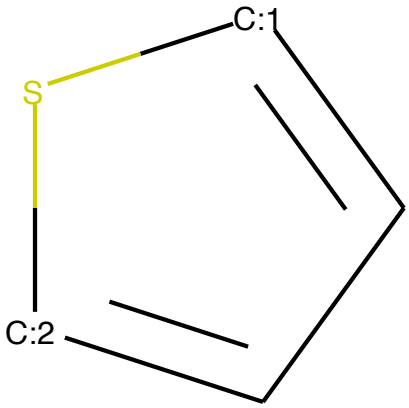
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(CC(=O)[O-])s3)s2)s1'
```




```
'------------------------------------------------------------'

'-----Step-8-----'
'Generate next fragment: 0.9967923760414124'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.12386856973171234'
```

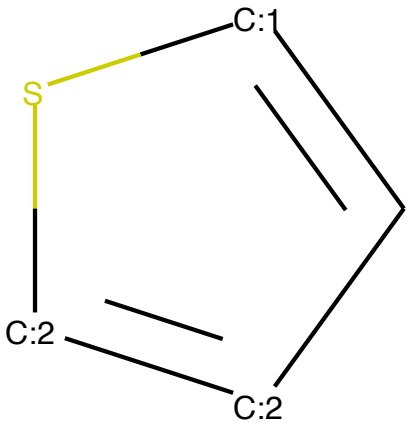


'--'

'Molecule C and its specific config C w/ probability -2.2312333583831787'

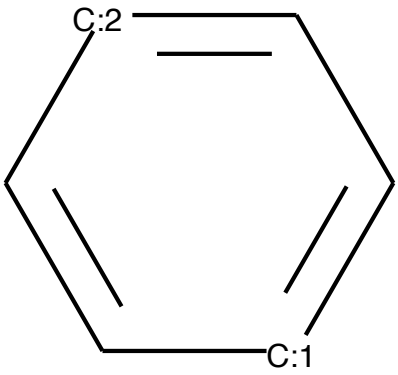
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ probab
ility -5.375985622406006'



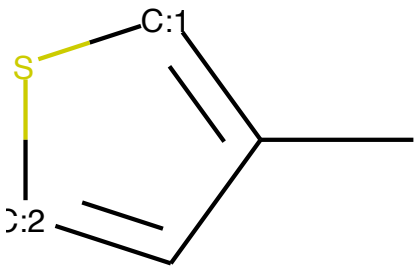
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -6.157557010650635'



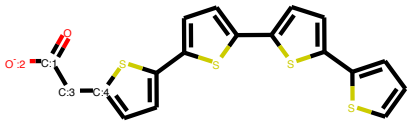

```
'-------------------------------------------------------------'

'Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ probabili
ty -6.570703983306885'
```




```
'-------------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4cccs4)s3)s2)s1'
```

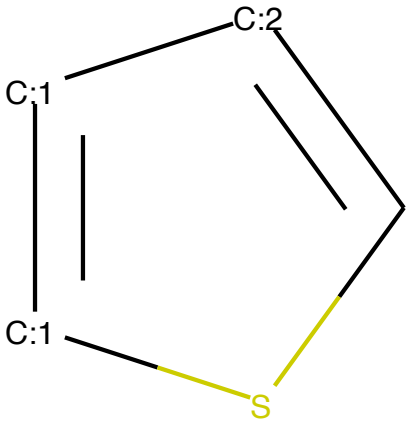



```
'-------------------------------------------------------------'

'-----Step-9-----'
'Generate next fragment: 0.9993383288383484'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00063137
20368780196'
```

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:1]=[CH:1]S1 w/ probab
ility -7.514693737030029'
```




```
'------------------------------------------------------------'

'Molecule CS and its specific config [CH3:1][SH:2] w/ probability -11.04032421
1120605'

'------------------------------------------------------------'

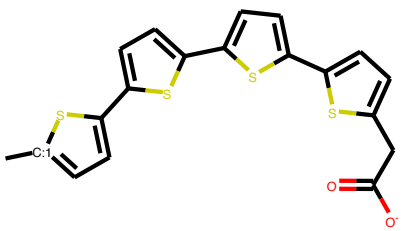
'Molecule C=O and its specific config O=[CH2:1] w/ probability -11.10610103607
1777'
```

```
'------------------------------------------------------------'

'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -11.327986
717224121'
```

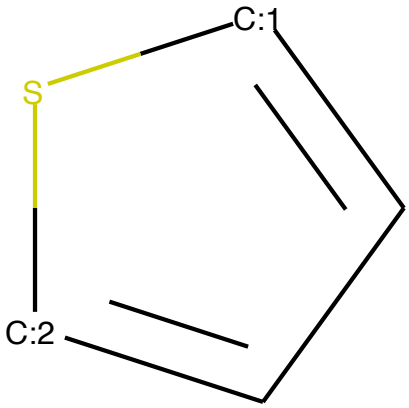
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(-c4ccc(CC(=O)[O-])s4)s3)s2)s1'
```



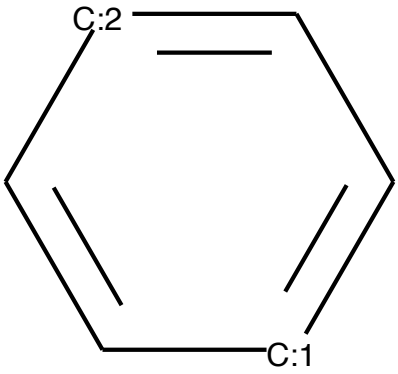

```
'------------------------------------------------------------'

'-----Step-10-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.09625552594661713'
```



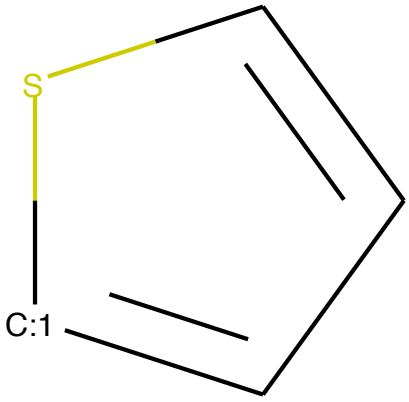
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.943636894226074'



'--'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -3.4
166290760040283'



'--'

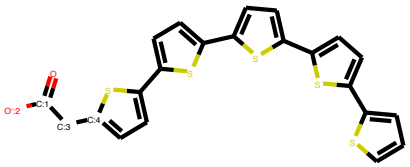
'Molecule C and its specific config C w/ probability -5.316184997558594'

```
'------------------------------------------------------------'

'Molecule [SiH4] and its specific config [SiH4] w/ probability -6.750178337097
168'
```

```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5cccs5)s4)s3)s2)
s1'
```




```
'------------------------------------------------------------'

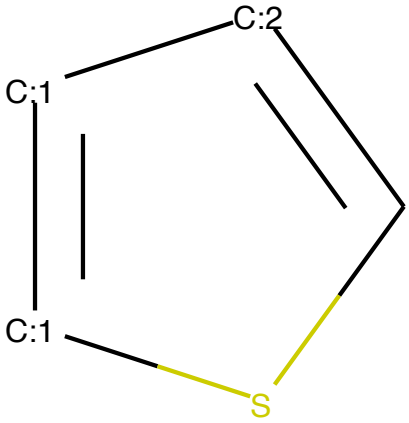
'-----Step-11-----'
'Generate next fragment: 0.8303309679031372'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.04151012
0034217834'
```

```
'------------------------------------------------------------'

'Molecule CS and its specific config [CH3:1][SH:2] w/ probability -3.214354038
2385254'
```

```
'------------------------------------------------------------'

'Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:1]=[CH:1]S1 w/ probab
ility -7.846226692199707'
```




```
'------------------------------------------------------------'

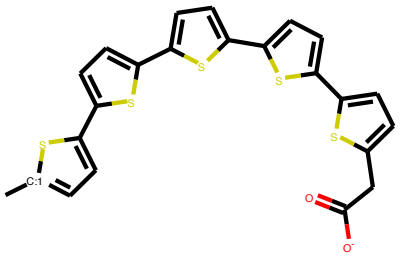
'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -10.278705
596923828'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -10.48699951171
875'
```

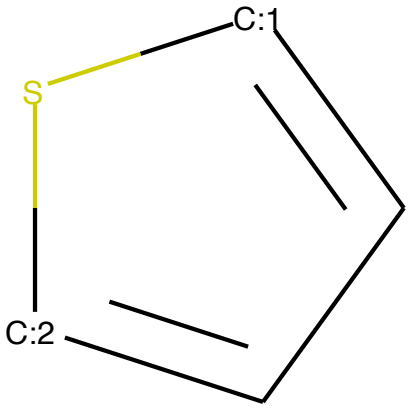
```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)
s2)s1'
```



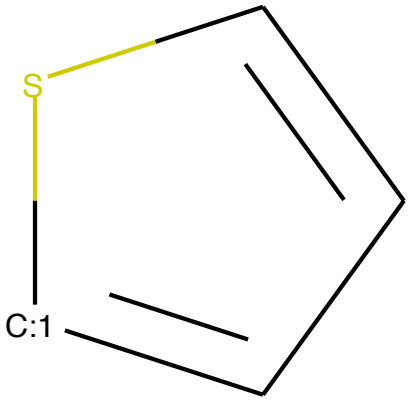

```
'------------------------------------------------------------'

'-----Step-12-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-0.5011690258979797'
```



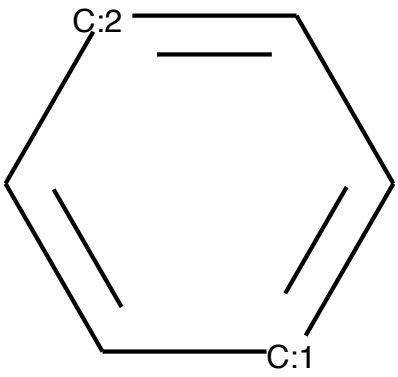
'--'

'Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ probability -1.3
847014904022217'



'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.0013294219970703'



'--'

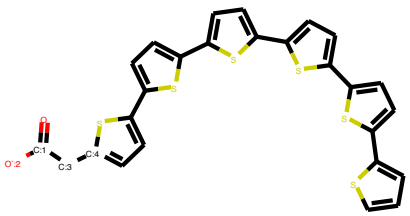
'Molecule C and its specific config C w/ probability -4.850032329559326'

```
'------------------------------------------------------------'

'Molecule C#N and its specific config N#[CH:1] w/ probability -7.4061570167541
5'
```

```
'------------------------------------------------------------'

'Attaching fragment C1=[CH:1]S[CH:2]=C1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccc(-c6cccs6)s5
)s4)s3)s2)s1'
```




```
'------------------------------------------------------------'

'-----Step-13-----'
'-----Step-14-----'
'-----Step-15-----'
'-----Step-16-----'
'-----Step-17-----'
```

```
'Generate next fragment: 0.9976533055305481'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00015102
67611593008'
```

```
'-----------------------------------------------------------'
```

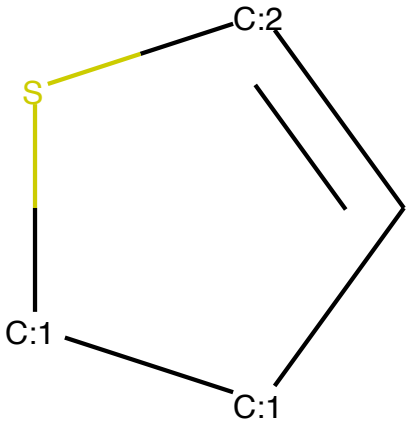
```
'Molecule C=N and its specific config [CH2:1]=[NH:2] w/ probability -9.6594629
28771973'
```

```
'-----------------------------------------------------------'
```

```
'Molecule S and its specific config S w/ probability -9.775293350219727'
```

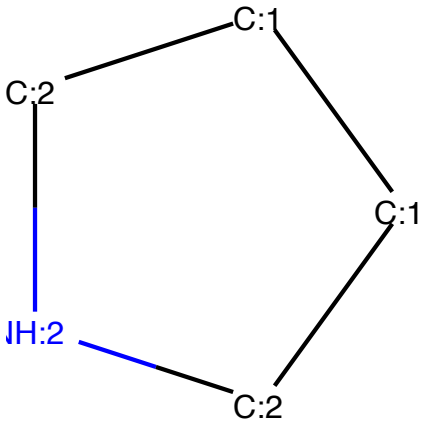
```
'-----------------------------------------------------------'
```

```
'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -10.877622604370117'
```



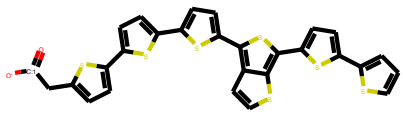

```
'-------------------------------------------------------------'

'Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][CH2:2][NH:2][CH2:2]1
w/ probability -11.646870613098145'
```




```
'-------------------------------------------------------------'

'Attaching fragment C1=[CH:2]S[CH2:1][CH2:1]1'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)
c5sccc45)s3)s2)s1'
```



```
'-------------------------------------------------------------'

'-----Step-18-----'
'Generate next fragment: 0.98321932554245'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CS and its specific config [CH3:1][SH:2] w/ probability -3.814624506
048858e-05'
```

```
'------------------------------------------------------------'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -10.2314853
66821289'
```

```
'------------------------------------------------------------'

'Molecule [SiH4] and its specific config [SiH4] w/ probability -14.02976989746
0938'
```

```
'------------------------------------------------------------'

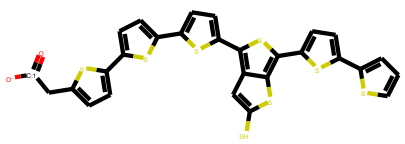
'Molecule C=O and its specific config O=[CH2:1] w/ probability -14.39983177185
0586'
```

```
'------------------------------------------------------------'

'Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ probability -14.9
18670654296875'
```

```
'------------------------------------------------------------'

'Attaching fragment [CH3:1][SH:2]'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)
c5sc(S)cc45)s3)s2)s1'
```



```
'------------------------------------------------------------'

'-----Step-19-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule S and its specific config S w/ probability -0.9460978507995605'
```

```
'------------------------------------------------------------'

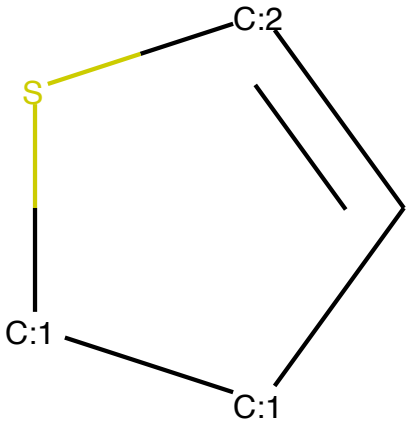
'Molecule CS and its specific config C[SH:1] w/ probability -1.036858558654785
2'
```

```
'------------------------------------------------------------'

'Molecule C and its specific config C w/ probability -1.455458164215088'
```

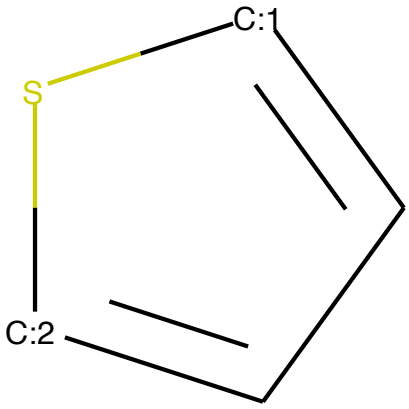
```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -3.820958375930786'
```



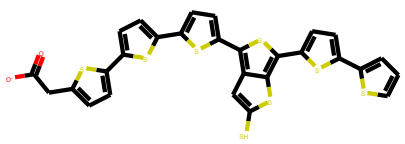
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -6.773167610168457'



'--'

'Attaching fragment S'
'Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)c5sc(S)cc45)s3)s2)s1'



'--'

'-----Step-20-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CS and its specific config C[SH:1] w/ probability -2.7656173188006505e-05'

```
'------------------------------------------------------------'

'Molecule C[SiH3] and its specific config C[SiH3:1] w/ probability -10.8562269
21081543'
```

```
'------------------------------------------------------------'

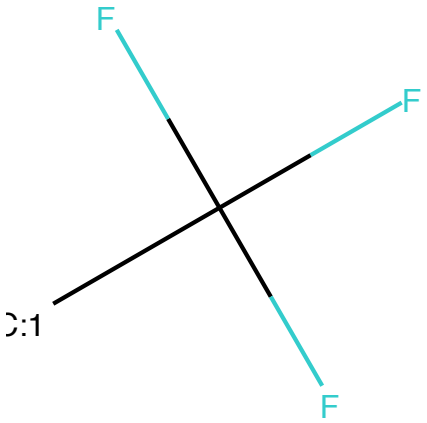
'Molecule CC#N and its specific config N#C[CH3:1] w/ probability -11.877511024
475098'
```

```
'------------------------------------------------------------'

'Molecule O=S and its specific config O=[S:1] w/ probability -14.0730867385864
26'
```

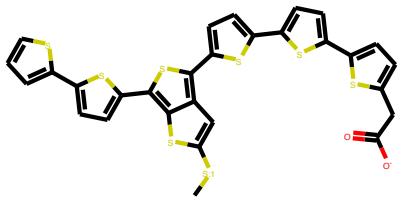
```
'------------------------------------------------------------'

'Molecule CC(F)(F)F and its specific config FC(F)(F)[CH3:1] w/ probability -14
.895258903503418'
```




```
'------------------------------------------------------------'

'Attaching fragment C[SH:1]'
'Latest partial graph: CSc1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)sc(-c
3ccc(-c4cccs4)s3)c2s1'
```



```
'------------------------------------------------------------'

'-----Step-21-----'
'-----Step-22-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
```

```
'Molecule O=S and its specific config O=[S:1] w/ probability -4.21991971961688
25e-05'
```

```
'------------------------------------------------------------'
```

```
'Molecule CS and its specific config C[SH:1] w/ probability -10.07938957214355
5'
```

```
'------------------------------------------------------------'
```

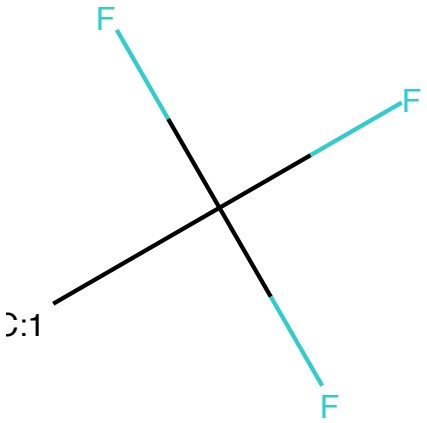
```
'Molecule C[SiH3] and its specific config C[SiH3:1] w/ probability -15.3585081
10046387'
```

```
'------------------------------------------------------------'
```

```
'Molecule [SiH4] and its specific config [SiH4] w/ probability -17.47427177429
1992'
```

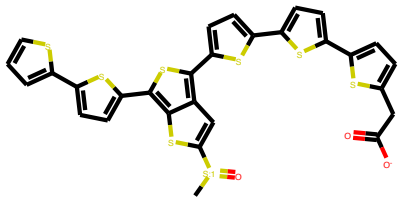
```
'------------------------------------------------------------'

'Molecule CC(F)(F)F and its specific config FC(F)(F)[CH3:1] w/ probability -19
.046844482421875'
```




```
'------------------------------------------------------------'

'Attaching fragment O=[S:1]'
'Latest partial graph: CS(=O)c1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)s
c(-c3ccc(-c4cccs4)s3)c2s1'
```



```
'------------------------------------------------------------'

'-----Step-23-----'
'-----Step-24-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule O=S and its specific config O=[S:1] w/ probability 0.0'
```

```
'------------------------------------------------------------'

'Molecule CC#N and its specific config N#C[CH3:1] w/ probability -19.532554626
464844'
```

```
'------------------------------------------------------------'

'Molecule CS and its specific config C[SH:1] w/ probability -20.42498970031738
3'
```

```
'------------------------------------------------------------'

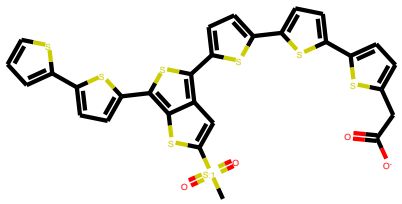
'Molecule C[SiH3] and its specific config C[SiH3:1] w/ probability -21.0532894
1345215'
```

```
'------------------------------------------------------------'

'Molecule CN and its specific config N[CH3:1] w/ probability -22.4043731689453
12'
```

```
'------------------------------------------------------------'

'Attaching fragment O=[S:1]'
'Latest partial graph: CS(=O)(=O)c1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)
s3)sc(-c3ccc(-c4cccs4)s3)c2s1'
```



```
'------------------------------------------------------------'

'-----Step-25-----'
'-----Step-26-----'
'-----Step-27-----'
'-----Step-28-----'
'-----Step-29-----'
```

```
'-----Step-30-----'
'-----Step-31-----'
'-----Step-32-----'
'-----Step-33-----'
'-----Step-34-----'
'-----Step-35-----'
'-----Step-36-----'
'-----Step-37-----'
'Generate next fragment: 0.9880258440971375'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00010168
035078095272'
```

```
'------------------------------------------------------------'
```

```
'Molecule CN and its specific config [NH2:1][CH3:2] w/ probability -9.30424690
246582'
```

```
'------------------------------------------------------------'
```

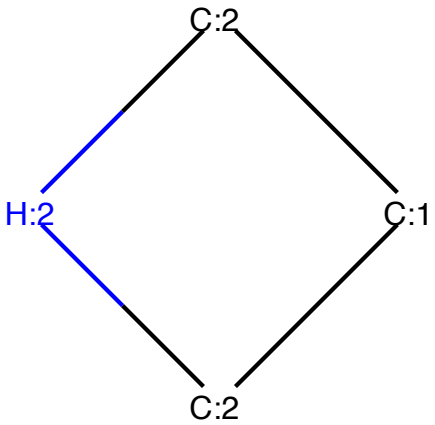
```
'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -11.4791316
98608398'
```

```
'------------------------------------------------------------'

'Molecule C=O and its specific config O=[CH2:1] w/ probability -15.40794467926
0254'
```

```
'------------------------------------------------------------'

'Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][NH:2][CH2:2]1 w/ prob
ability -17.559106826782227'
```




```
'------------------------------------------------------------'

'-----Step-38-----'
'-----Step-39-----'
'-----Step-40-----'
'-----Step-41-----'
'-----Step-42-----'
'-----Step-43-----'
```

```
'-----Step-44-----'
'-----Step-45-----'
'-----Step-46-----'
'-----Step-47-----'
'-----Step-48-----'
'-----Step-49-----'
'-----Step-50-----'
'-----Step-51-----'
'-----Step-52-----'
'-----Step-53-----'
'-----Step-54-----'
'-----Step-55-----'
'-----Step-56-----'
'-----Step-57-----'
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