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

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

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

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

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

# Generation

**Notes:**

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

In [4]:

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

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

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


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

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

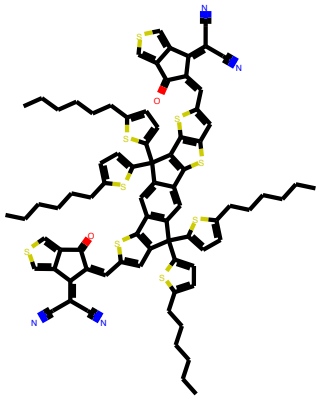
                sub_mol = Chem.MolFromSmiles(step_f['partial-graph'])
                print('Attaching fragment {} of config {}'.format(frag[0], fr
                print('Latest partial graph: {}'.format(step_f['partial-graph
                print('Lastest graph (left) vs graph in last step (right)')
              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

In [10]:

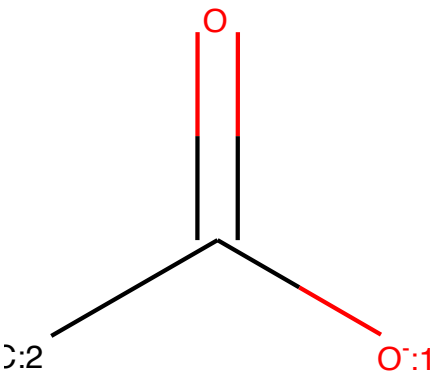
```
view(w_te_data, 12, original)
```

```
Original: CCCCCCC1=CC=C(S1)C2(C(S3)=CC=C3CCCCCC)C(C(SC(/C=C(C4=O)/C(C5=CSC=C45
```

)=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

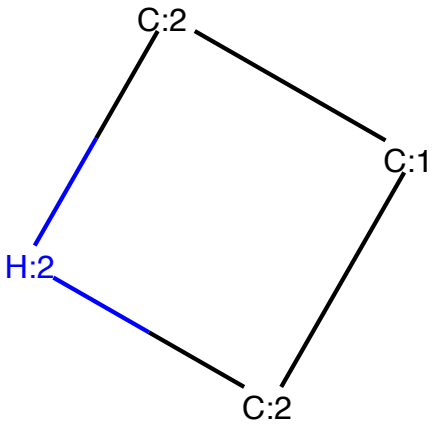


**********Sample 12th**********
-----Step-0-----
Root motif: CC(=O)[O-]
Top 5 root motif configs: ('O=C([O-:1])[CH3:2]', tensor(13.9317))
('O=C([O-])[CH3:1]', tensor(-12.5431))
('CC(=O)[O-:1]', tensor(-16.1744))
('[O:1]=[CH2:2]', tensor(-980.1329))
('C(#C[CH3:2])[CH3:1]', tensor(-980.1487))
Displaying partial graph (aka molecule): CC(=O)[O-]

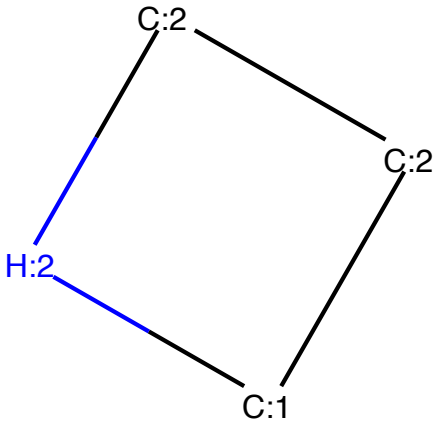



---
-----Step-1-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.0707383155822754

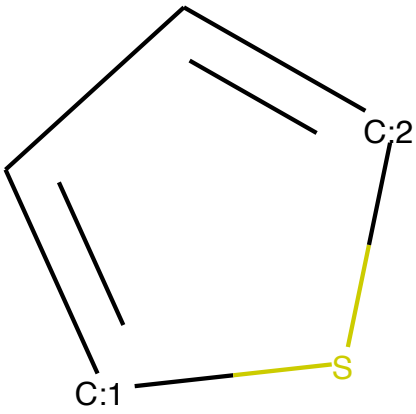
---
Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][NH:2][CH2:2]1 w/ p=-1.16451895236969




---
Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][CH2:2][NH:2]1 w/ p=-1.808347225189209

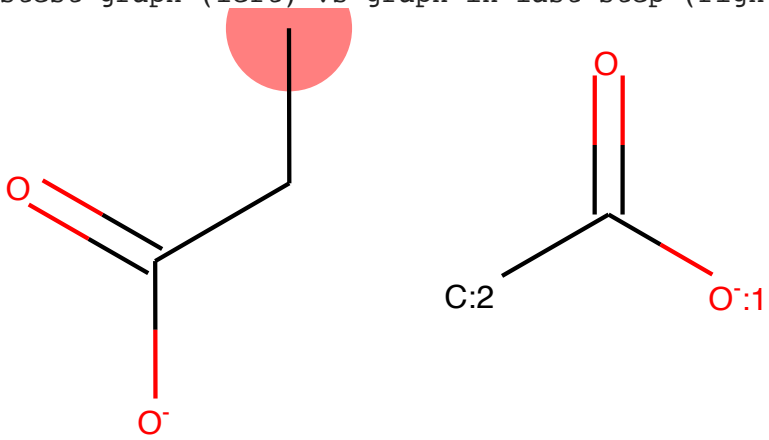



---
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-2.6687560081481934

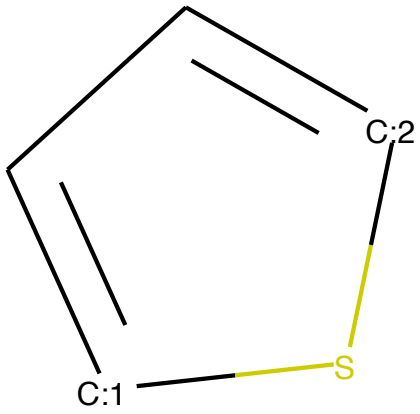



---
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-3.1203184127807617

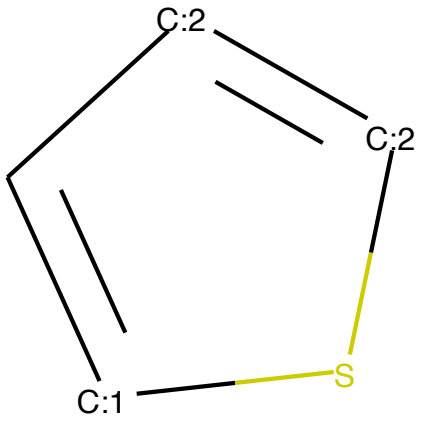
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: CCC(=O)[O-]
Lastest graph (left) vs graph in last step (right)
```



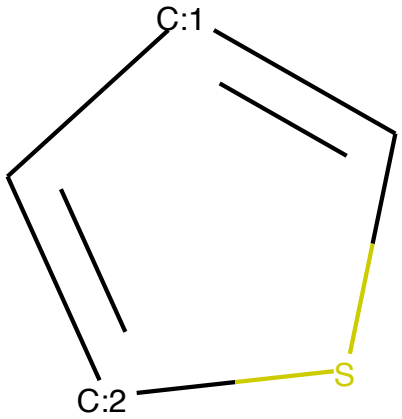

```
------------------------------------------------------------
-----Step-2-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.0152112
70190775394
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-4.91
3881301879883
```

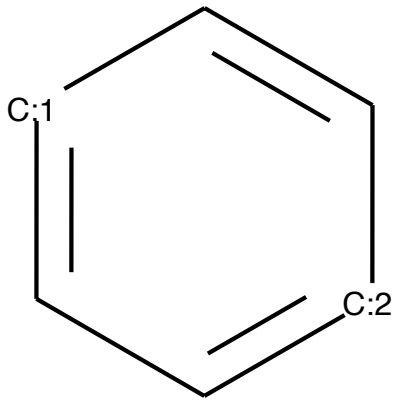



```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]C=[CH:2]S1 w/ p=-5.4744892
12036133
```

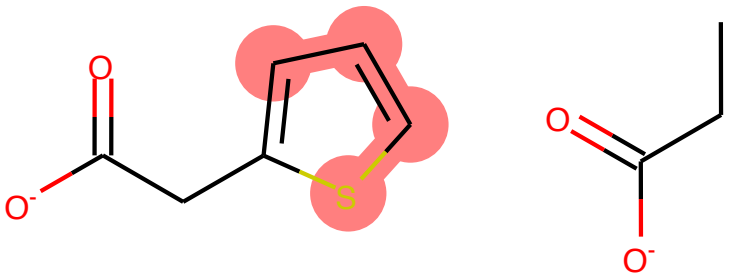



```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-5.725157260894775
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-8.778
680801391602
```

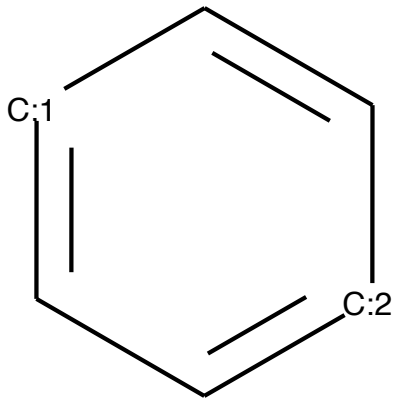



```
------------------------------------------------------------
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: O=C([O-])Cc1cccs1
Lastest graph (left) vs graph in last step (right)
```



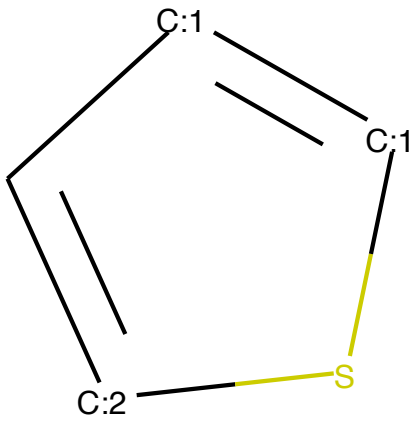

```
------------------------------------------------------------
-----Step-3-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-1.811964830267243e-05
```

```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-11.43
4046745300293
```

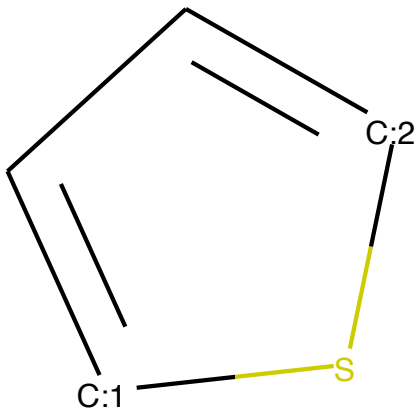



```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-11.994294166564941
```

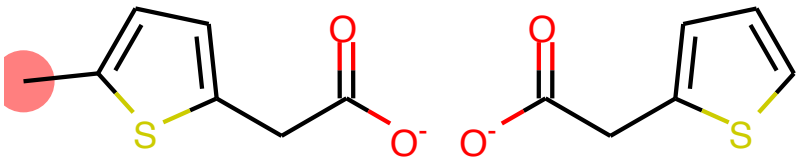
```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-13.7
05684661865234
```



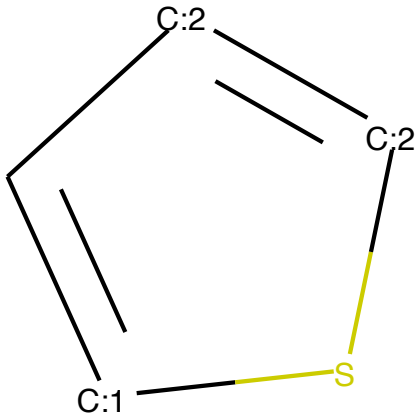

```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-17.187797
54638672
```



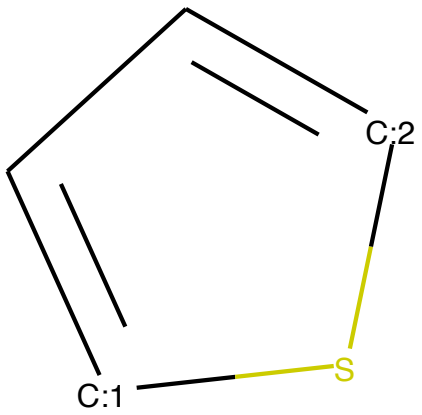

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(CC(=O)[O-])s1
Lastest graph (left) vs graph in last step (right)
```




```
------------------------------------------------------------
-----Step-4-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-0.00
9146904572844505
```

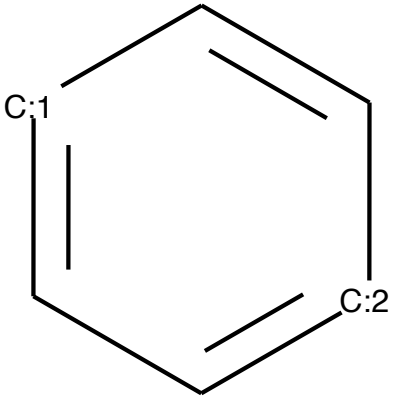



```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-4.7870278
35845947
```

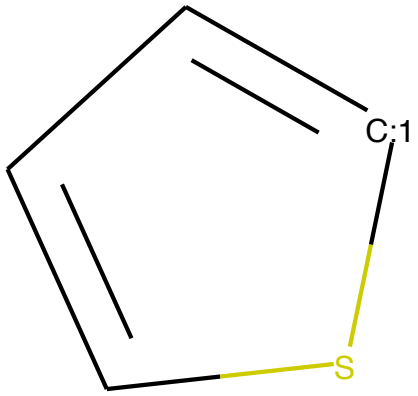



---
Molecule C and its specific config C w/ p=-7.912520408630371

---
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-8.354876518249512



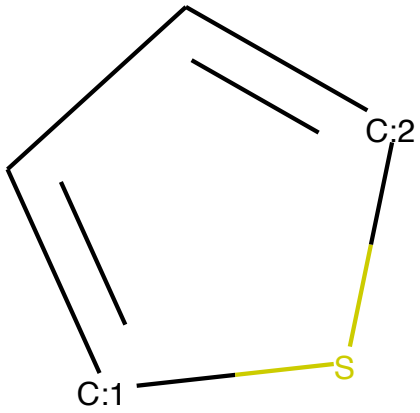

---
Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ p=-8.974496841430664




---
Attaching fragment C1=[CH:1]S[CH:2]=[CH:2]1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: O=C([O-])Cc1ccc(-c2cccs2)s1
Lastest graph (left) vs graph in last step (right)

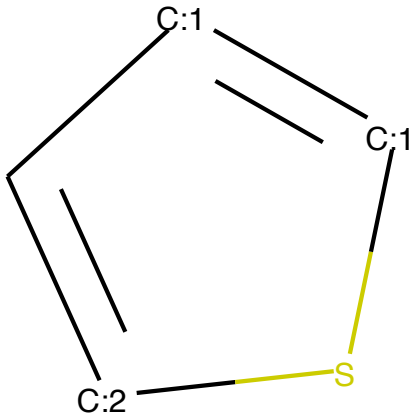

---
-----Step-5-----
Generate next fragment p = 0.9997887015342712
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.5695070624351501

---
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-1.1753448247909546



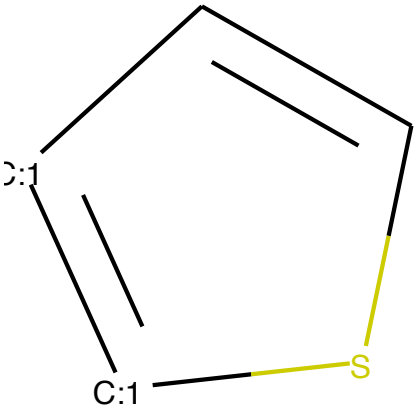

---

Molecule C1=CSC=C1 and its specific config C1=[CH:2]S[CH:1]=[CH:1]1 w/ p=-2.70
43516635894775




---

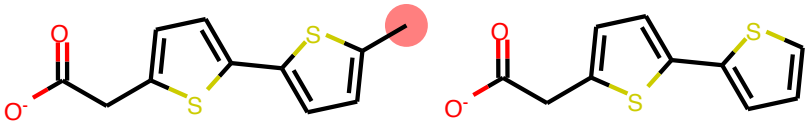
Molecule C1=CSC=C1 and its specific config C1=C[CH:1]=[CH:1]S1 w/ p=-3.2616009
71221924



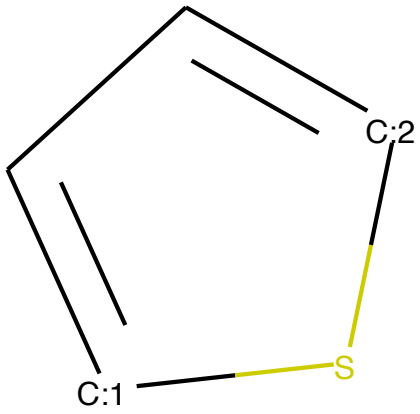

---

Molecule C[SiH3] and its specific config [CH3:1][SiH3:2] w/ p=-4.3368959426879
88

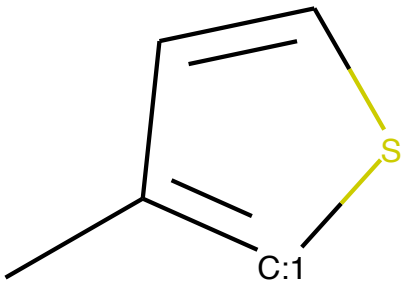
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(-c2ccc(CC(=O)[O-])s2)s1
Lastest graph (left) vs graph in last step (right)
```



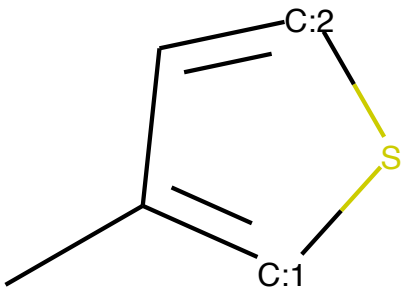

```
------------------------------------------------------------
-----Step-6-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.0103656
60302340984
```



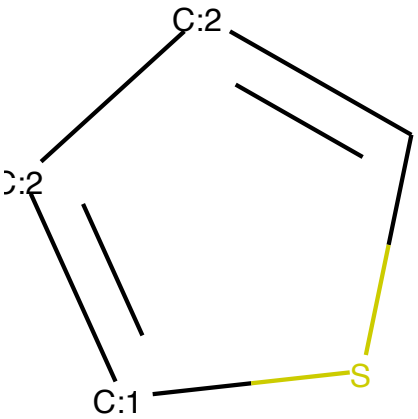

```
------------------------------------------------------------
Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]SC=C1 w/ p=-4.7038173675
53711
```




---
Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ p=-6.87516
5939331055

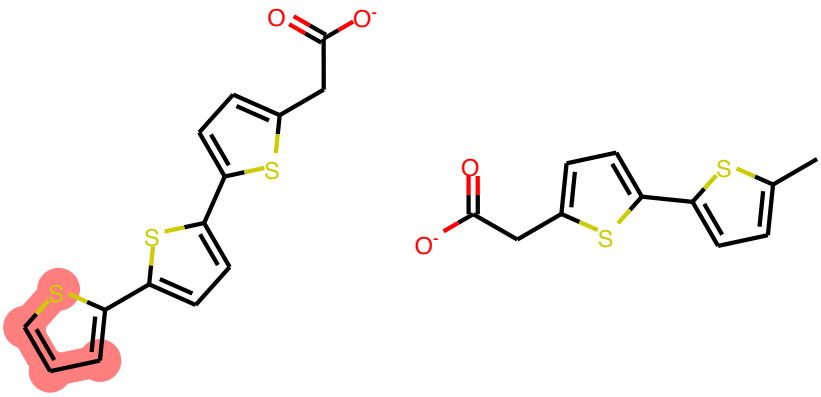



---
Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:2]=[CH:1]S1 w/ p=-9.22
6217269897461




---
Molecule C and its specific config C w/ p=-9.870923042297363

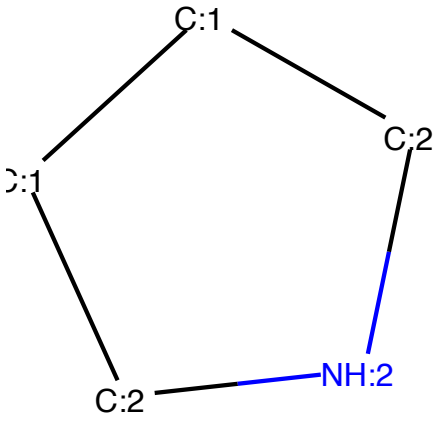
```
------------------------------------------------------------
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3cccs3)s2)s1
Lastest graph (left) vs graph in last step (right)
```



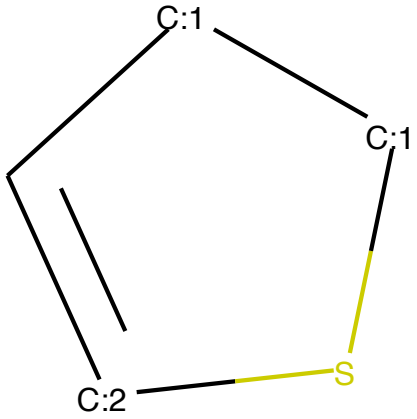

```
------------------------------------------------------------
-----Step-7-----
Generate next fragment p = 0.9998983144760132
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0063044242560863495
```

```
------------------------------------------------------------
Molecule CC and its specific config C[CH3:1] w/ p=-5.355673313140869
```

```
------------------------------------------------------------
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][CH2:2][NH:2][CH2:2]1
w/ p=-7.019346714019775
```

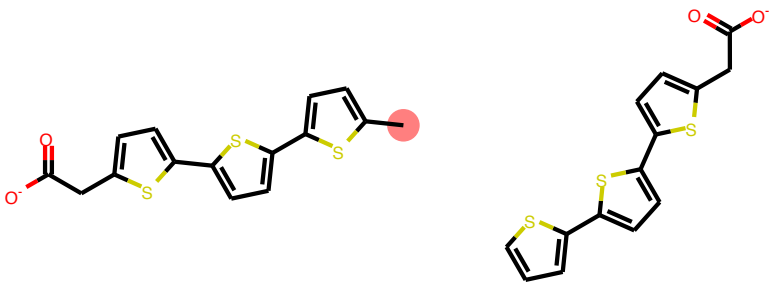



```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-7.96
6949939727783
```

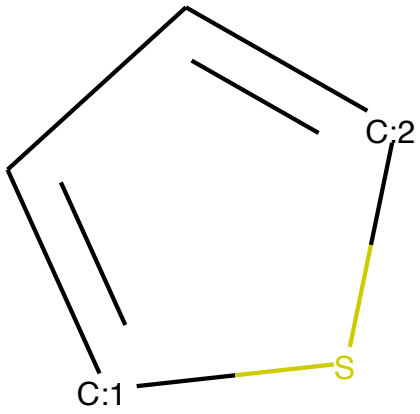



```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-9.378978729248047
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(CC(=O)[O-])s3)s2)s1
Lastest graph (left) vs graph in last step (right)
```

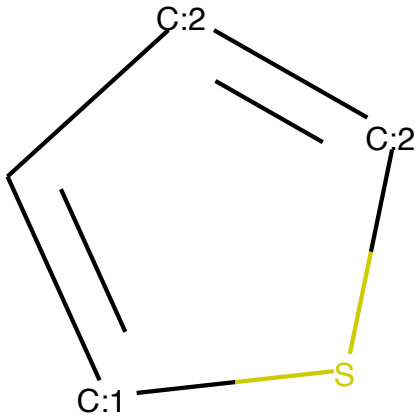



```
------------------------------------------------------------
-----Step-8-----
Generate next fragment p = 0.9967923760414124
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.1238685
6973171234
```

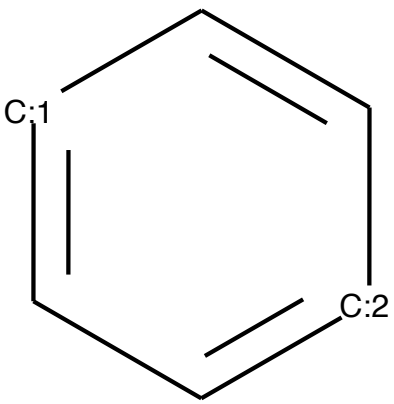



```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-2.2312333583831787
```

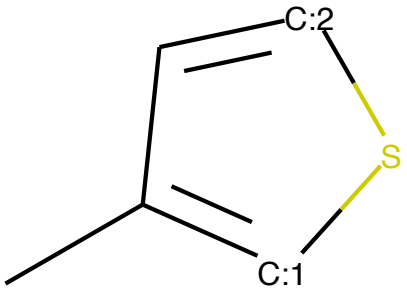
---
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=[CH:2]1 w/ p=-5.37
5985622406006




---
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-6.157
557010650635



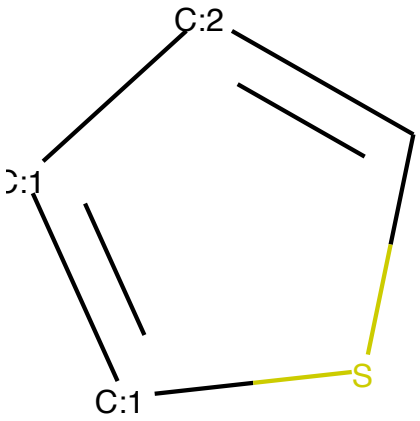

---
Molecule CC1=CSC=C1 and its specific config CC1=[CH:1]S[CH:2]=C1 w/ p=-6.57070
3983306885




```
------------------------------------------------------------
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4cccs4)s3)s2)s1
Lastest graph (left) vs graph in last step (right)
```

```
------------------------------------------------------------
-----Step-9-----
Generate next fragment p = 0.9993383288383484
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0006313720368780196

------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:1]=[CH:1]S1 w/ p=-7.51
4693737030029
```

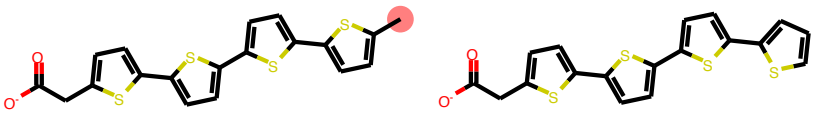



```
------------------------------------------------------------
Molecule CS and its specific config [CH3:1][SH:2] w/ p=-11.040324211120605
```

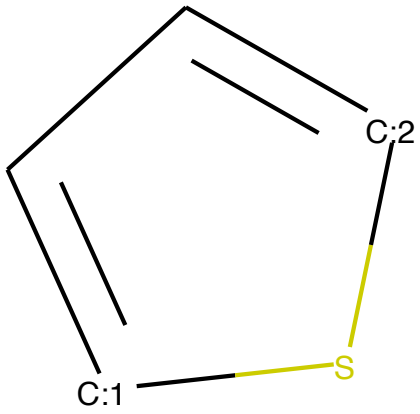
```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-11.106101036071777
```

```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-11.327986717224121
```

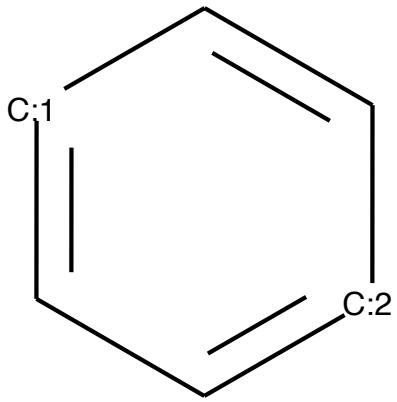
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(-c4ccc(CC(=O)[O-])s4)s3)s2)s1
Lastest graph (left) vs graph in last step (right)
```



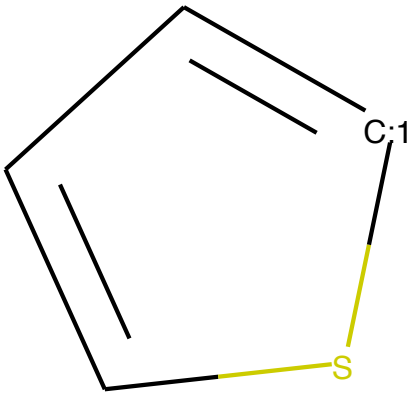
```
------------------------------------------------------------
-----Step-10-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.0962555
2594661713
```




```
------------------------------------------------------------
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-2.943
636894226074
```



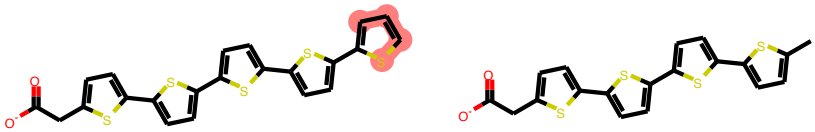

---
Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ p=-3.416629076004
0283




---
Molecule C and its specific config C w/ p=-5.316184997558594

---
Molecule [SiH4] and its specific config [SiH4] w/ p=-6.750178337097168

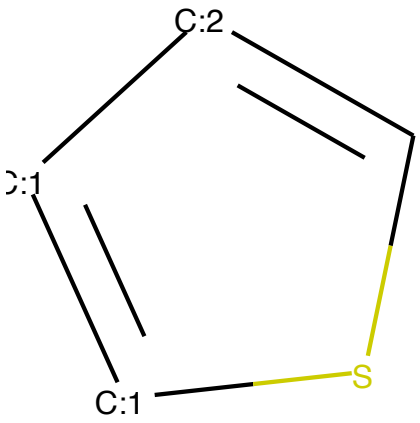
```
------------------------------------------------------------
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5cccs5)s4)s3)s2)s
1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-11-----
Generate next fragment p = 0.8303309679031372
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.041510120034217834
```

```
------------------------------------------------------------
Molecule CS and its specific config [CH3:1][SH:2] w/ p=-3.2143540382385254
```

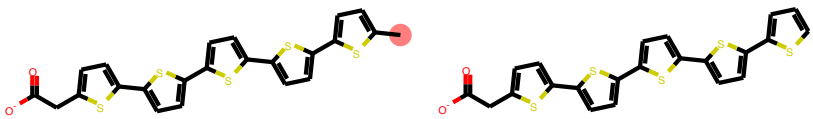
```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=[CH:2][CH:1]=[CH:1]S1 w/ p=-7.84
6226692199707
```



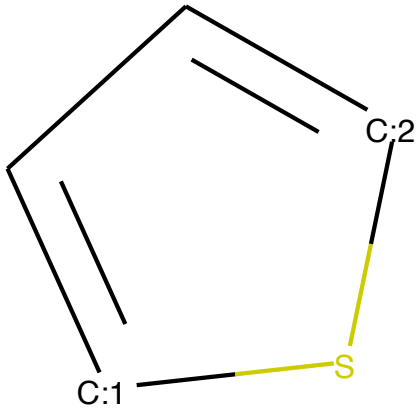

```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-10.278705596923828
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-10.48699951171875
```

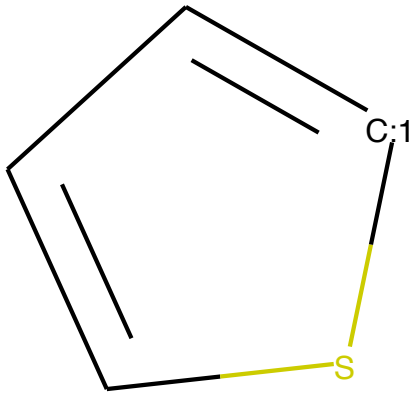
```
------------------------------------------------------------
Attaching fragment [CH3:1][CH3:2] of config ['C[CH3:1]']
Latest partial graph: Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)s
2)s1
Lastest graph (left) vs graph in last step (right)
```



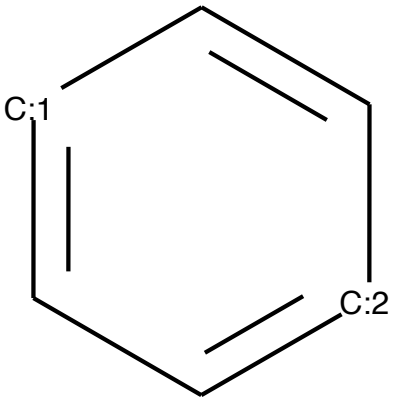
```
------------------------------------------------------------
-----Step-12-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-0.5011690
258979797
```




```
------------------------------------------------------------
Molecule C1=CSC=C1 and its specific config C1=CS[CH:1]=C1 w/ p=-1.384701490402
2217
```



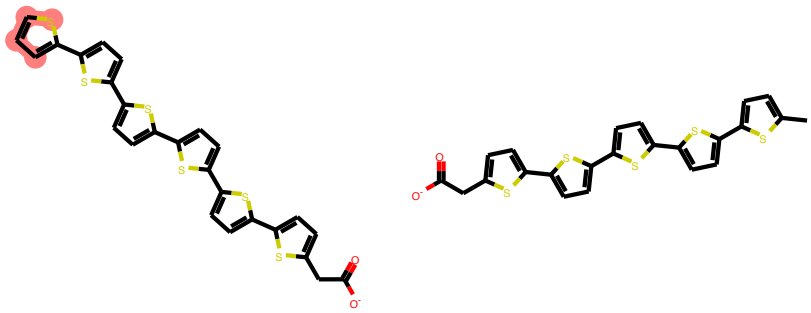

---
Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ p=-2.001
3294219970703




---
Molecule C and its specific config C w/ p=-4.850032329559326

---
Molecule C#N and its specific config N#[CH:1] w/ p=-7.40615701675415

```
------------------------------------------------------------
Attaching fragment C1=[CH:1]S[CH:2]=C1 of config ['C1:C:S:[CH:1]:C:1']
Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4ccc(-c5ccc(-c6cccs6)s5)
s4)s3)s2)s1
Lastest graph (left) vs graph in last step (right)
```

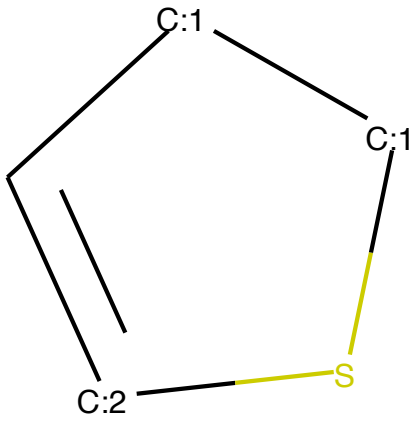


```
------------------------------------------------------------
-----Step-13-----
Generate next fragment p = 0.31631457805633545
-----Step-14-----
Generate next fragment p = 2.1378728306289908e-15
-----Step-15-----
Generate next fragment p = 6.014240057083953e-07
-----Step-16-----
Generate next fragment p = 1.5512888011919718e-13
-----Step-17-----
Generate next fragment p = 0.9976533055305481
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0001510267611593008
```

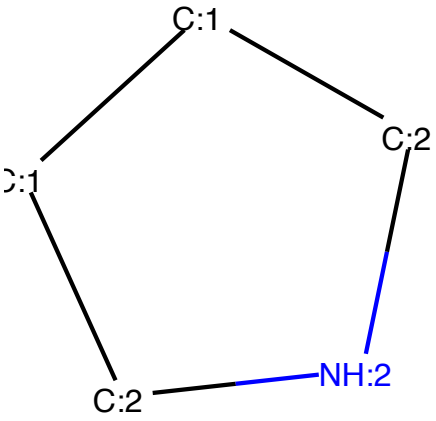
```
------------------------------------------------------------
Molecule C=N and its specific config [CH2:1]=[NH:2] w/ p=-9.659462928771973
```

```
------------------------------------------------------------
Molecule S and its specific config S w/ p=-9.775293350219727
```

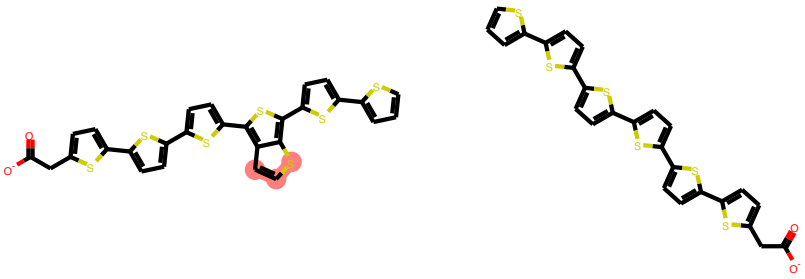
```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-10.8
77622604370117
```




```
------------------------------------------------------------
Molecule C1CCNC1 and its specific config [CH2:1]1[CH2:1][CH2:2][NH:2][CH2:2]1
w/ p=-11.646870613098145
```




```
------------------------------------------------------------
Attaching fragment C1=[CH:2]S[CH2:1][CH2:1]1 of config ['C1=CS[CH2:1]C1', 'C1=
C[CH2:1]CS1']
Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)c
5sccc45)s3)s2)s1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-18-----
Generate next fragment p = 0.98321932554245
Top 5 next motifs to attach:
Molecule CS and its specific config [CH3:1][SH:2] w/ p=-3.814624506048858e-05
```

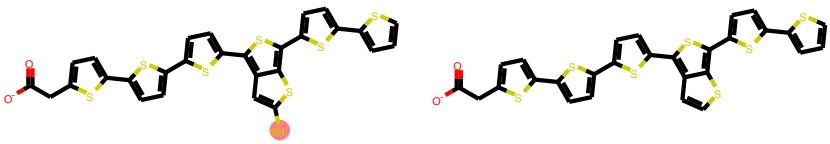
```
------------------------------------------------------------
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-10.231485366821289
```

```
------------------------------------------------------------
Molecule [SiH4] and its specific config [SiH4] w/ p=-14.029769897460938
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-14.399831771850586
```

```
------------------------------------------------------------
Molecule [CH2-]C and its specific config [CH3:1][CH2-:2] w/ p=-14.918670654296
875
```

```
------------------------------------------------------------
Attaching fragment [CH3:1][SH:2] of config ['S[CH3:1]']
Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)c
5sc(S)cc45)s3)s2)s1
Lastest graph (left) vs graph in last step (right)
```

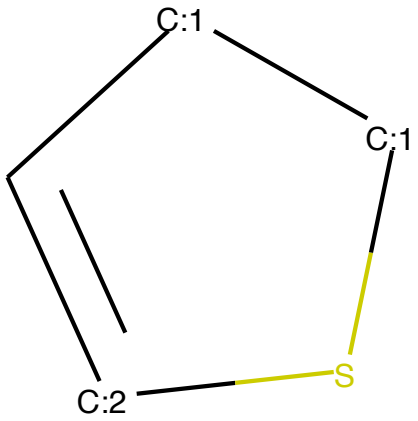


```
------------------------------------------------------------
-----Step-19-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule S and its specific config S w/ p=-0.9460978507995605
```

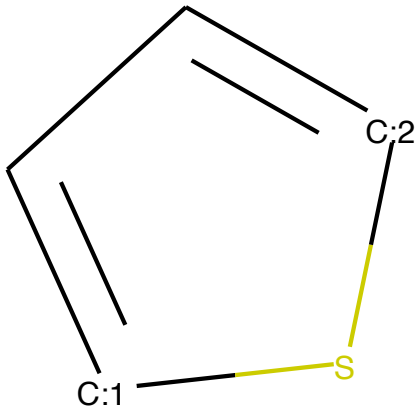
```
------------------------------------------------------------
Molecule CS and its specific config C[SH:1] w/ p=-1.0368585586547852
```

```
------------------------------------------------------------
Molecule C and its specific config C w/ p=-1.455458164215088
```

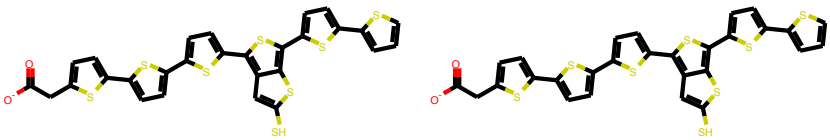
```
------------------------------------------------------------
Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ p=-3.82
0958375930786
```




---
Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ p=-6.7731676
10168457




---
Attaching fragment S of config ['[SH2:1]']
Latest partial graph: O=C([O-])Cc1ccc(-c2ccc(-c3ccc(-c4sc(-c5ccc(-c6cccs6)s5)c
5sc(S)cc45)s3)s2)s1
Lastest graph (left) vs graph in last step (right)



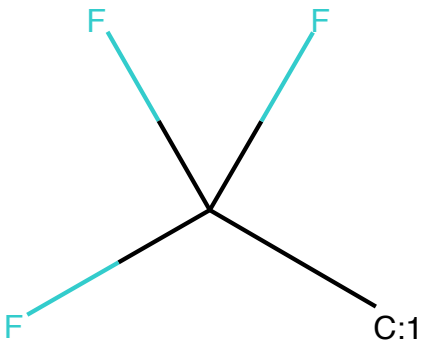
---
-----Step-20-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule CS and its specific config C[SH:1] w/ p=-2.7656173188006505e-05

```
------------------------------------------------------------
Molecule C[SiH3] and its specific config C[SiH3:1] w/ p=-10.856226921081543
```

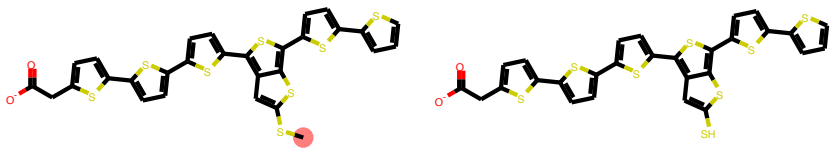
```
------------------------------------------------------------
Molecule CC#N and its specific config N#C[CH3:1] w/ p=-11.877511024475098
```

```
------------------------------------------------------------
Molecule O=S and its specific config O=[S:1] w/ p=-14.073086738586426
```

```
------------------------------------------------------------
Molecule CC(F)(F)F and its specific config FC(F)(F)[CH3:1] w/ p=-14.8952589035
03418
```




```
------------------------------------------------------------
Attaching fragment C[SH:1] of config ['C[SH:1]']
Latest partial graph: CSc1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)sc(-c3
ccc(-c4cccs4)s3)c2s1
Lastest graph (left) vs graph in last step (right)
```



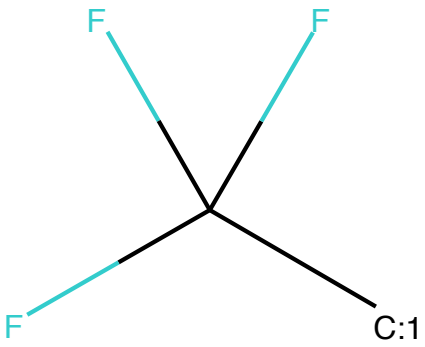
```
------------------------------------------------------------
-----Step-21-----
Generate next fragment p = 7.399842871791407e-08
-----Step-22-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule O=S and its specific config O=[S:1] w/ p=-4.2199197196168825e-05
```

```
------------------------------------------------------------
Molecule CS and its specific config C[SH:1] w/ p=-10.079389572143555
```

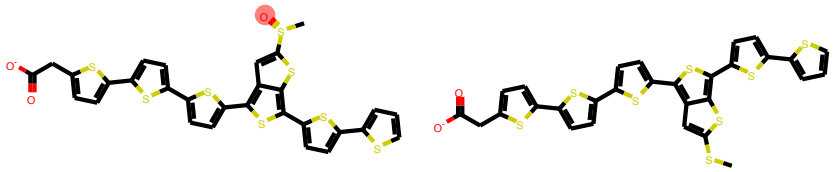
```
------------------------------------------------------------
Molecule C[SiH3] and its specific config C[SiH3:1] w/ p=-15.358508110046387
```

```
------------------------------------------------------------
Molecule [SiH4] and its specific config [SiH4] w/ p=-17.474271774291992
```

```
------------------------------------------------------------
Molecule CC(F)(F)F and its specific config FC(F)(F)[CH3:1] w/ p=-19.0468444824
21875
```




```
------------------------------------------------------------
Attaching fragment O=[S:1] of config ['O=[S:1]']
Latest partial graph: CS(=O)c1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s3)sc
(-c3ccc(-c4cccs4)s3)c2s1
Lastest graph (left) vs graph in last step (right)
```



```
------------------------------------------------------------
-----Step-23-----
Generate next fragment p = 0.0
-----Step-24-----
Generate next fragment p = 1.0
Top 5 next motifs to attach:
Molecule O=S and its specific config O=[S:1] w/ p=0.0
```

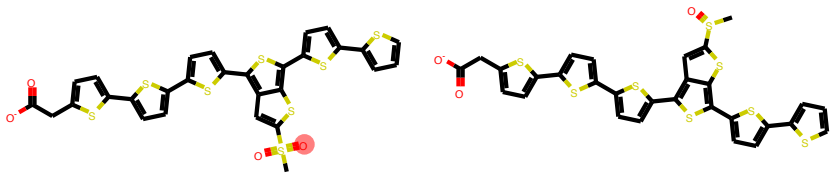
```
------------------------------------------------------------
Molecule CC#N and its specific config N#C[CH3:1] w/ p=-19.532554626464844
```

```
------------------------------------------------------------
Molecule CS and its specific config C[SH:1] w/ p=-20.424989700317383
```

```
------------------------------------------------------------
Molecule C[SiH3] and its specific config C[SiH3:1] w/ p=-21.05328941345215
```

```
------------------------------------------------------------
Molecule CN and its specific config N[CH3:1] w/ p=-22.404373168945312
```

```
------------------------------------------------------------
Attaching fragment O=[S:1] of config ['O=[S:1]']
Latest partial graph: CS(=O)(=O)c1cc2c(-c3ccc(-c4ccc(-c5ccc(CC(=O)[O-])s5)s4)s
3)sc(-c3ccc(-c4cccs4)s3)c2s1
Lastest graph (left) vs graph in last step (right)
```



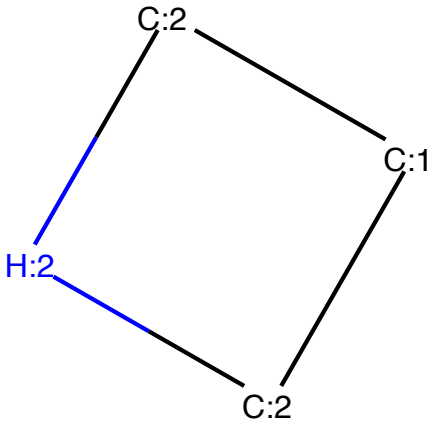
```
------------------------------------------------------------
-----Step-25-----
Generate next fragment p = 1.737397008713094e-36
-----Step-26-----
Generate next fragment p = 5.188417517842936e-08
-----Step-27-----
Generate next fragment p = 1.4229140250709093e-15
-----Step-28-----
Generate next fragment p = 4.507595943096902e-15
-----Step-29-----
Generate next fragment p = 2.1907074678612082e-13
-----Step-30-----
Generate next fragment p = 2.852038053189957e-24
-----Step-31-----
Generate next fragment p = 2.4798725917207776e-06
-----Step-32-----
Generate next fragment p = 1.7128844150028954e-20
-----Step-33-----
Generate next fragment p = 0.24527804553508759
-----Step-34-----
Generate next fragment p = 3.1638699495767303e-27
-----Step-35-----
Generate next fragment p = 9.040126514037183e-08
-----Step-36-----
Generate next fragment p = 6.324027771182904e-23
-----Step-37-----
Generate next fragment p = 0.9880258440971375
Top 5 next motifs to attach:
Molecule CC and its specific config [CH3:1][CH3:2] w/ p=-0.0001016803507809527
2
```

```
------------------------------------------------------------
Molecule CN and its specific config [NH2:1][CH3:2] w/ p=-9.30424690246582
```

```
------------------------------------------------------------
Molecule CN and its specific config [CH3:1][NH2:2] w/ p=-11.479131698608398
```

```
------------------------------------------------------------
Molecule C=O and its specific config O=[CH2:1] w/ p=-15.407944679260254
```

```
------------------------------------------------------------
Molecule C1CNC1 and its specific config [CH2:1]1[CH2:2][NH:2][CH2:2]1 w/ p=-17
.559106826782227
```




```
------------------------------------------------------------
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
-----Step-38-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-39-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-40-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-41-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-42-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-43-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-44-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-45-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-46-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-47-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-48-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-49-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-50-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-51-----
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Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-52-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-53-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-54-----
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vious fragment.
-----Step-55-----
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vious fragment.
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vious fragment.
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vious fragment.
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vious fragment.
-----Step-59-----
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vious fragment.
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vious fragment.
-----Step-61-----
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vious fragment.
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vious fragment.
-----Step-63-----
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vious fragment.
-----Step-64-----
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vious fragment.
-----Step-65-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-66-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-67-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-68-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-69-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-70-----
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```
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-71-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-72-----
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vious fragment.
-----Step-73-----
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vious fragment.
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vious fragment.
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vious fragment.
-----Step-76-----
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vious fragment.
-----Step-77-----
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vious fragment.
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vious fragment.
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vious fragment.
-----Step-80-----
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vious fragment.
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vious fragment.
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vious fragment.
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vious fragment.
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vious fragment.
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vious fragment.
-----Step-86-----
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vious fragment.
-----Step-87-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-88-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-89-----
```

```
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-90-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-91-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-92-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-93-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-94-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-95-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-96-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-97-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-98-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-99-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
-----Step-100-----
Skip, current fragment has no next fragment to be attached. Go back to the pre
vious fragment.
```

In [ ]: