In [1]:
```
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 [2]:
```
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
```

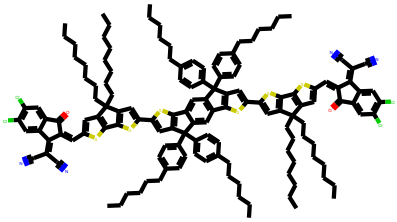
In [3]:
```
def mol_with_atom_index(mol, indices=[]):
    new_idx = []
    for atom in mol.GetAtoms():
        #print(atom.GetIdx(), indices)
        idx = atom.GetIdx()
        if idx in indices:
            atom.SetAtomMapNum(idx)
        new_idx.append(idx)
    return mol, new_idx
```

Generation

In [18]:

```
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
    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
        else:
            print('Skip, current fragment has not next fragment to be attache
        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('------------------------------------------------------
        else:
            print("Skip, the best next fragment to be attached to the current
```

```
'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'
```

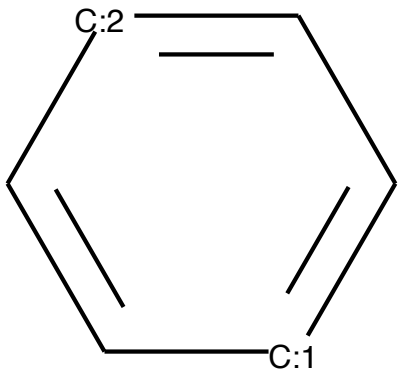


```
'***************Sample 7th***************'
'-----Step-0-----'
{'Top 5 super-root-idxs (aka blank roots that wont exist in the root fragments
)': tensor([ 10, 610,   1, 653, 663]),
 'super-root-idx': tensor(10),
 'top-5-root-fragment-cands': [('[N:1]#[CH:2]', tensor(19.6517)),
  ('N#[CH:1]', tensor(-19.0220)),
  ('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'
```

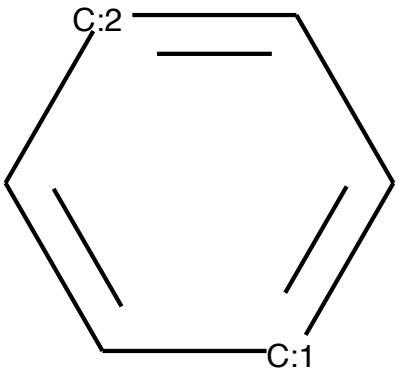



```
'------------------------------------------------------------'

'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'
```

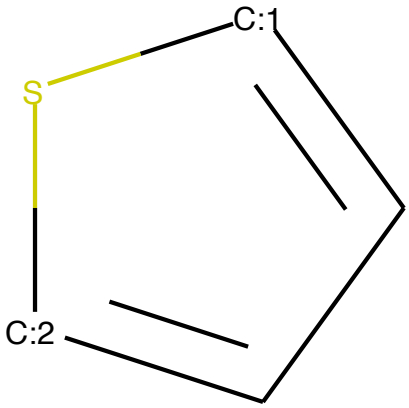
```
'------------------------------------------------------------'

'-----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'
```

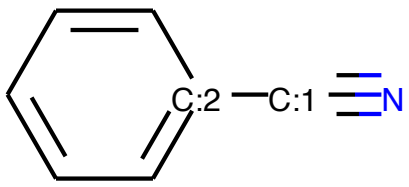


'--'

'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'



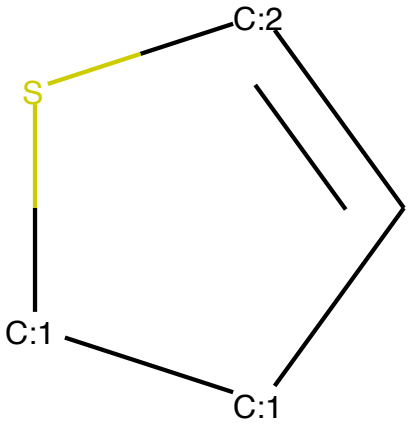
'--'

'-----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'
```

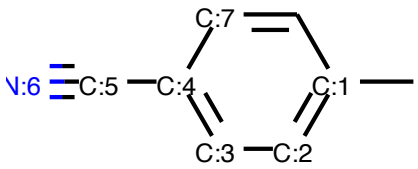
```
'------------------------------------------------------------'

'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'
```

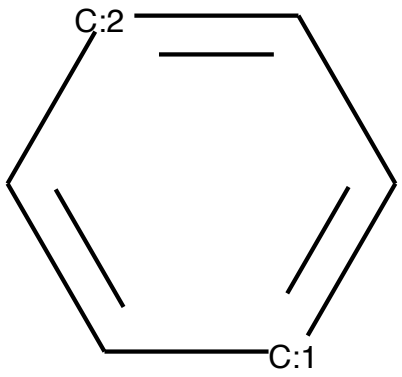
```
'------------------------------------------------------------'

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



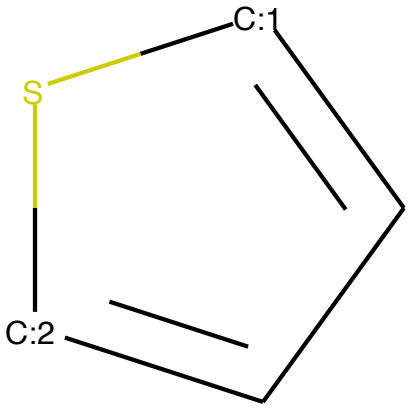

```
'------------------------------------------------------------'

'-----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'
```

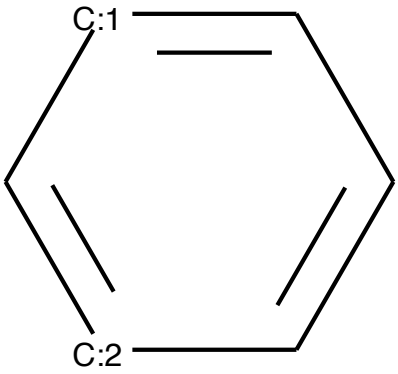



```
'------------------------------------------------------------'

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



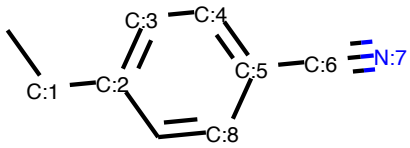
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=C[CH:2]=C[CH:1]=C1 w/ probabi
lity -9.907465934753418'



'--'

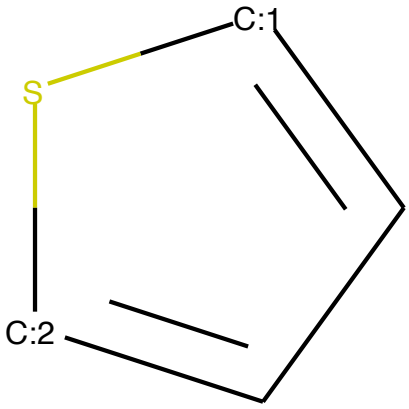
'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: CCc1ccc(C#N)cc1'



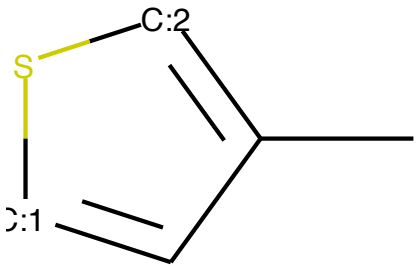
'--'

'-----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'

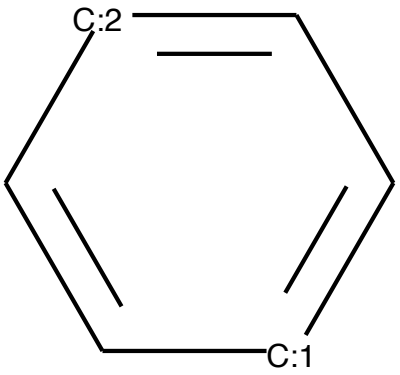
```
'------------------------------------------------------------'

'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'
```

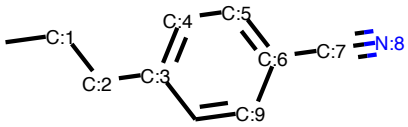


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -6.933335
781097412'

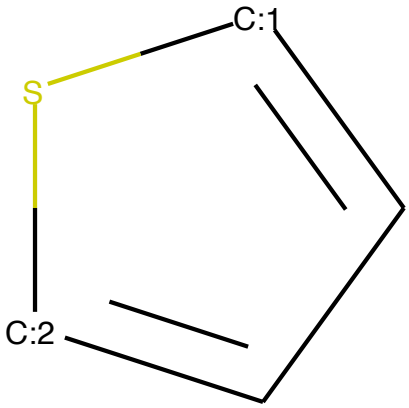
'--'

'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'

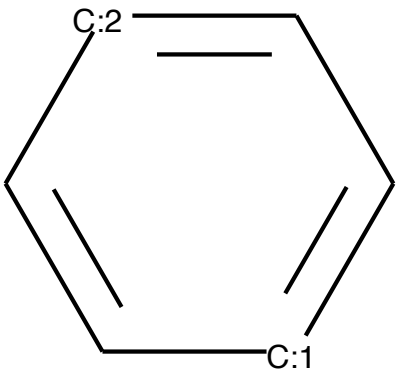


'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -3.92018461
227417'

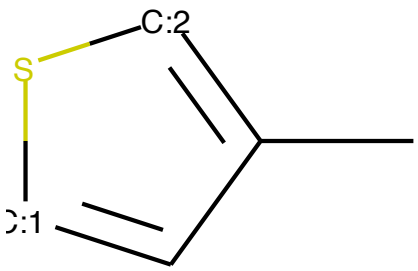
'--'

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



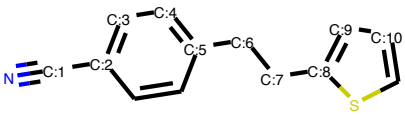
'--'

'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'
```

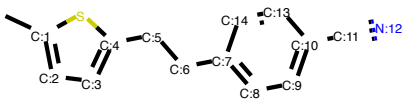
```
'------------------------------------------------------------'

'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'
```

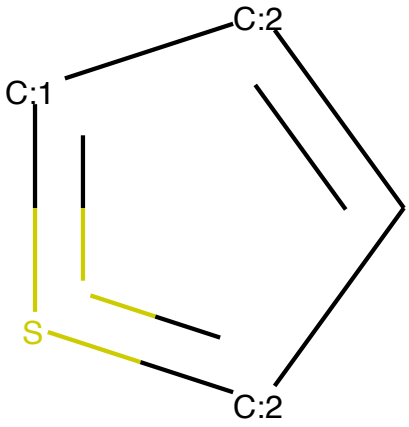
```
'------------------------------------------------------------'

'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'
```

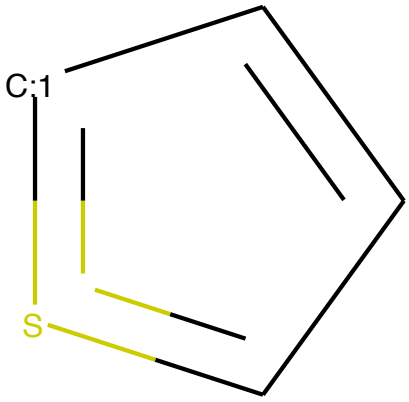



```
'------------------------------------------------------------'

'-----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'
```



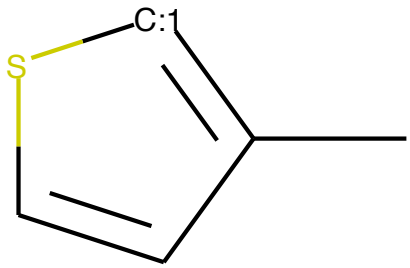
'--'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ probability -3
.591478109359741'



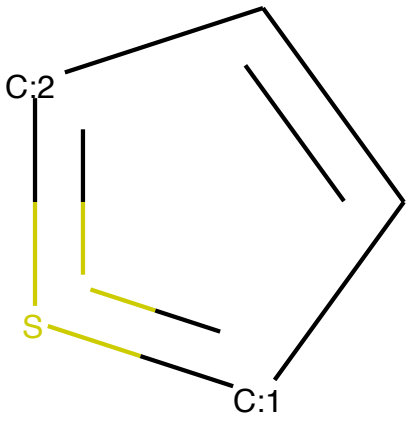
'--'

'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'

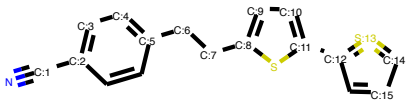


'--'

'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'

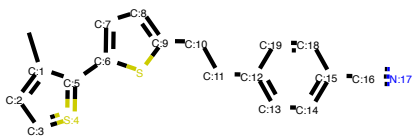
```
'------------------------------------------------------------'

'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'
```

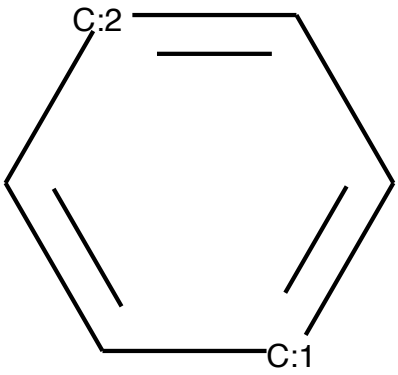
```
'------------------------------------------------------------'

'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'
```

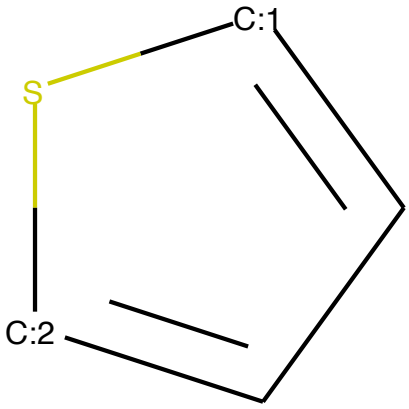



```
'------------------------------------------------------------'

'-----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'
```



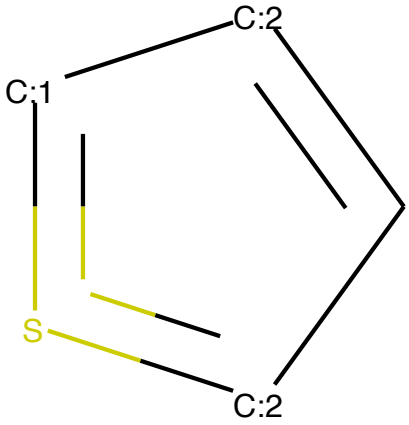
'--'

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



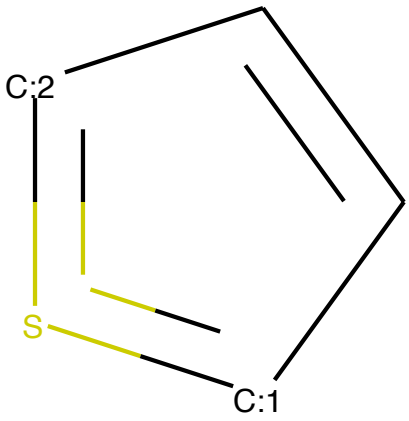
'--'

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



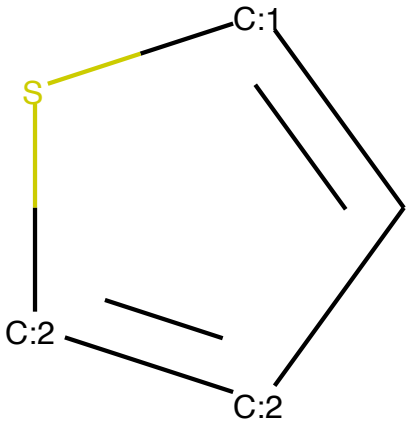
'--'

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



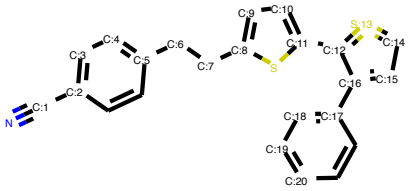
'--'

'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'



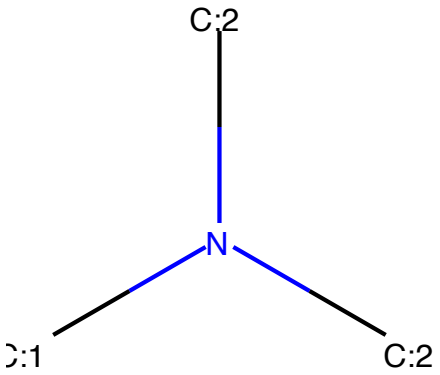
'--'

'-----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'
```

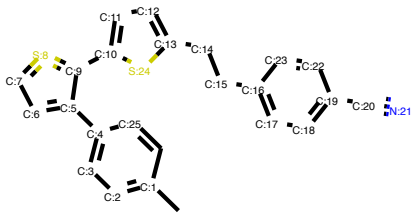


'--'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -4.87333488
4643555'

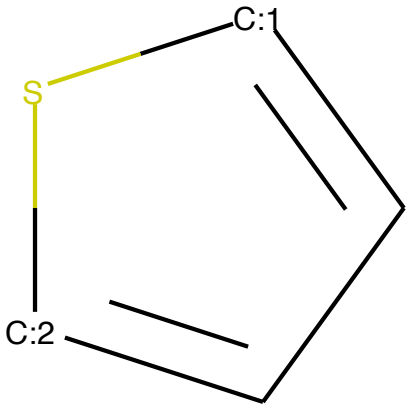
'--'

'Attaching fragment [CH3:1][CH3:2]'
'Latest partial graph: Cc1ccc(C2=CC=S=C2c2ccc(CCc3ccc(C#N)cc3)s2)cc1'



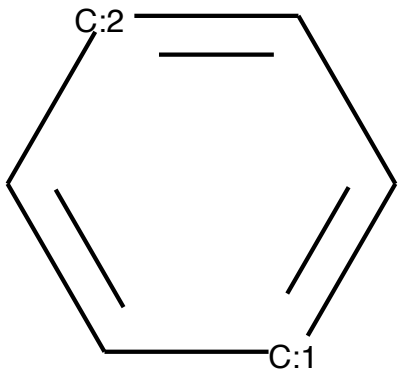
'--'

'-----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'

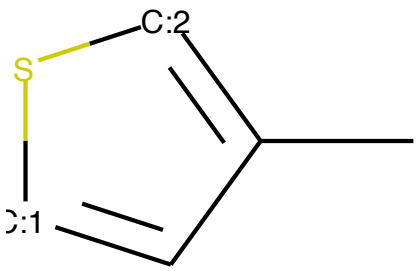


'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -10.78921
3180541992'

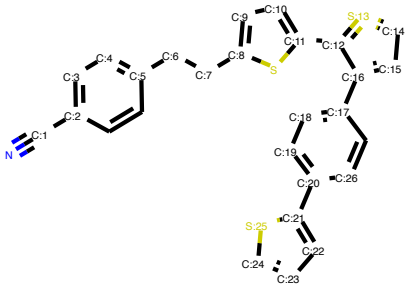
'--'

'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'
```

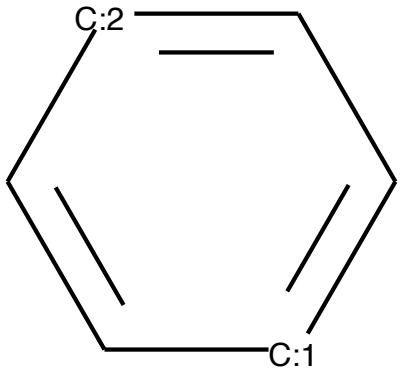
```
'------------------------------------------------------------'

'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'
```

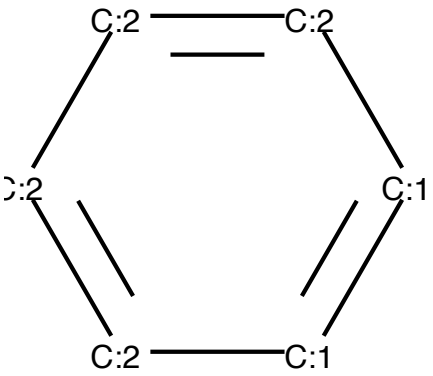
```
'------------------------------------------------------------'

'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'
```

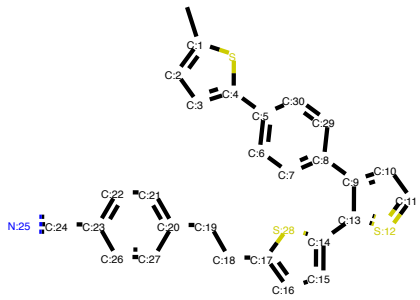



```
'------------------------------------------------------------'

'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'
```



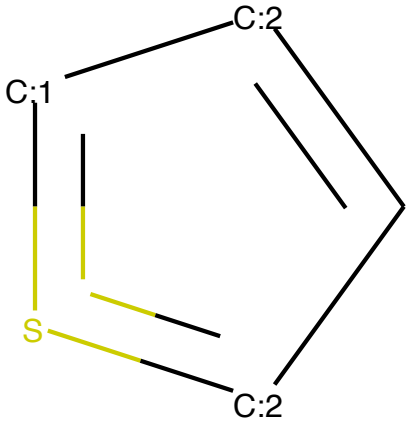

```
'------------------------------------------------------------'

'Attaching fragment C[CH3:1]'
'Latest partial graph: Cc1ccc(-c2ccc(C3=CC=S=C3c3ccc(CCc4ccc(C#N)cc4)s3)cc2)s1
'
```



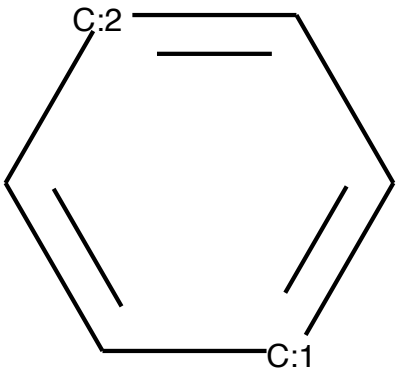

```
'------------------------------------------------------------'

'-----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'
```

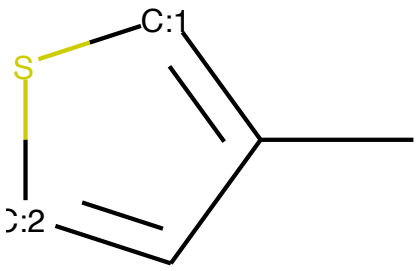



```
'------------------------------------------------------------'

'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'



'--'

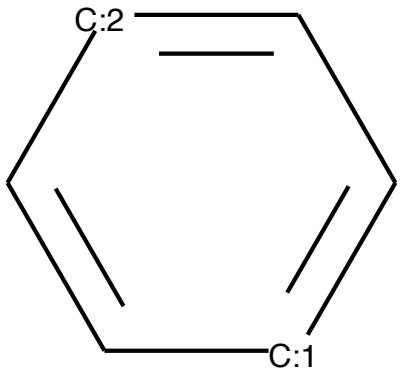
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-15-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config C[CH3:1] w/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

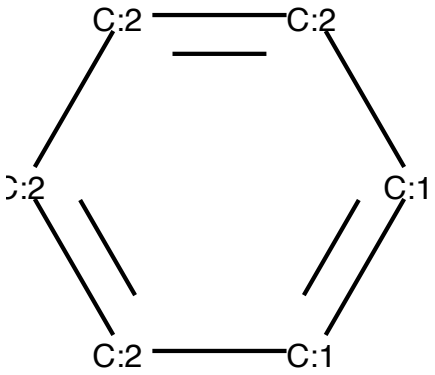


'--'

'Molecule CF and its specific config F[CH3:1] w/ probability -15.8360939025878
9'

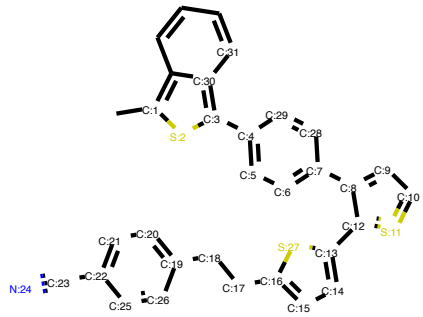
'--'

'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'

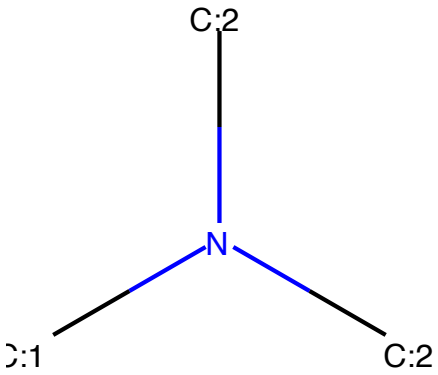


'--'

'-----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'

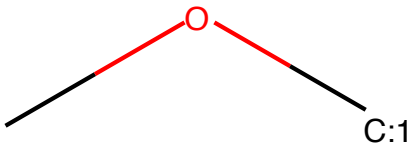
'--'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -16.55008316040039'



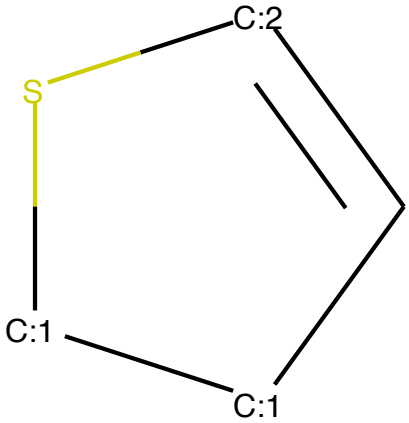
'--'

'Molecule COC and its specific config CO[CH3:1] w/ probability -18.54360198974
6094'



'--'

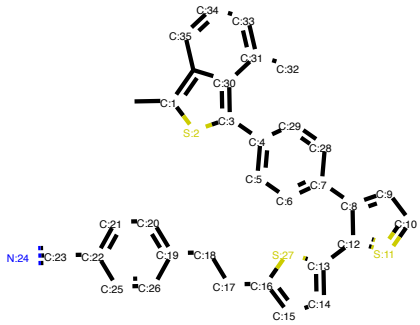
'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -20.33526039123535'



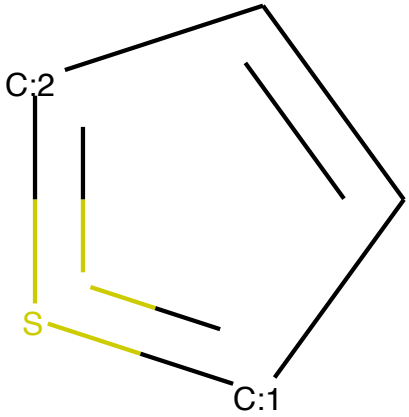
'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -21.7356300354003
9'

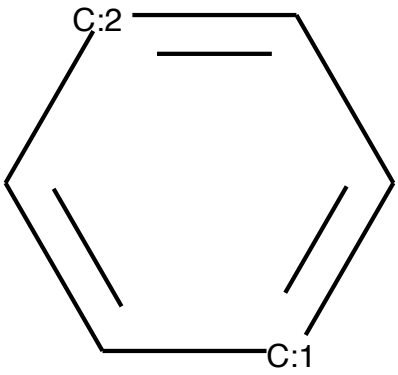
```
'------------------------------------------------------------'

'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'
```

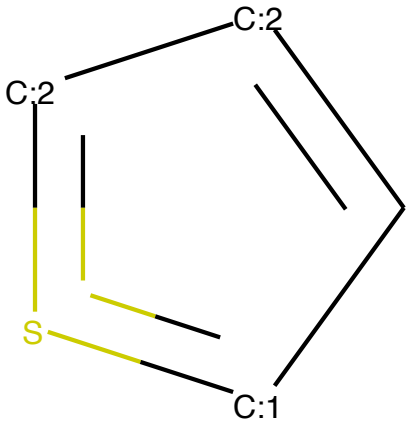



```
'------------------------------------------------------------'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.6073691844940186'
```



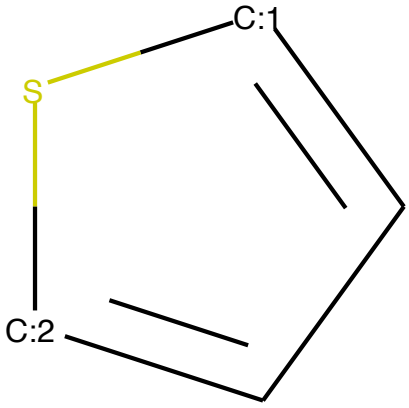
'--'

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



'--'

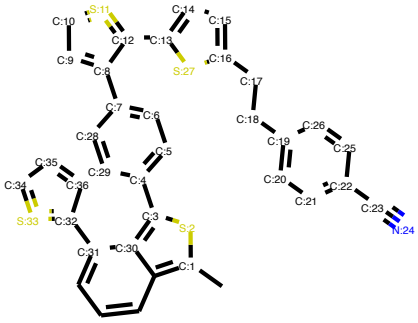
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability -5.211851119995117'



'--'

'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'
```

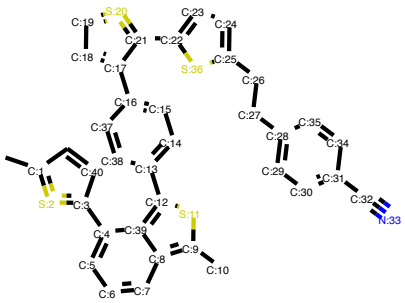
```
'------------------------------------------------------------'

'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'
```

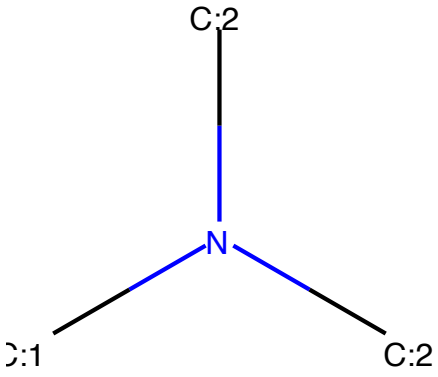
```
'------------------------------------------------------------'

'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'
```



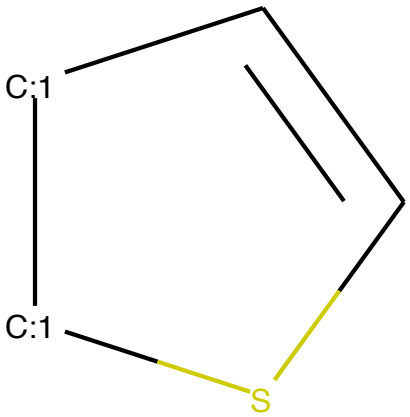

```
'------------------------------------------------------------'

'-----Step-19-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-20-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-21-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'
```

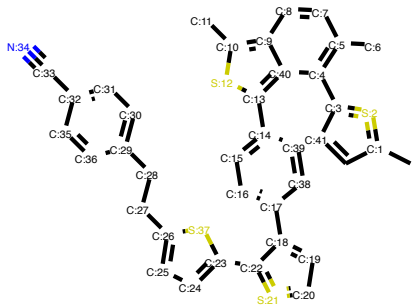


'--'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -19.9521503
44848633'

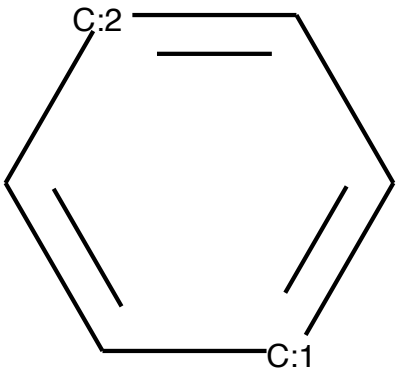
'--'

'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'



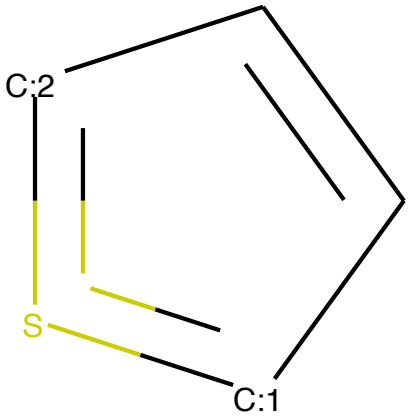
'--'

'-----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'



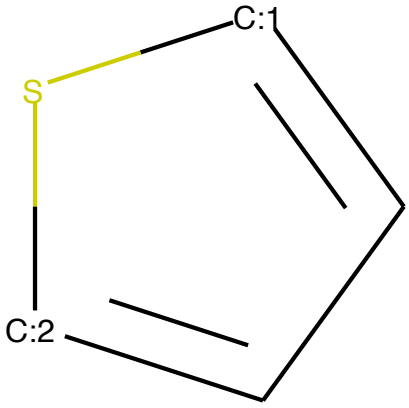
'--'

'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'

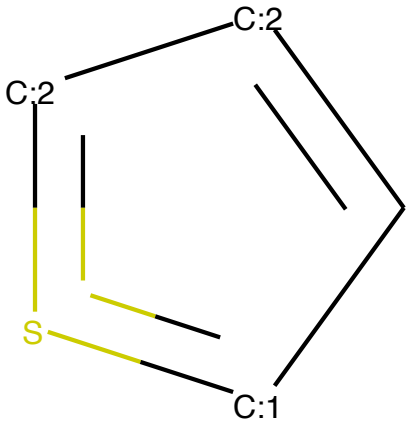


'--'

'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -5.70397138
59558105'

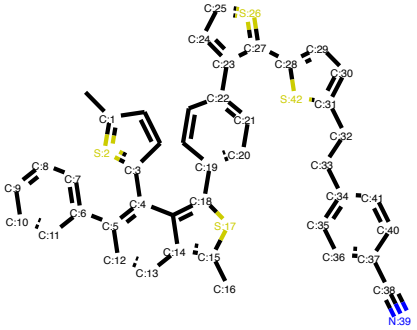
'--'

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

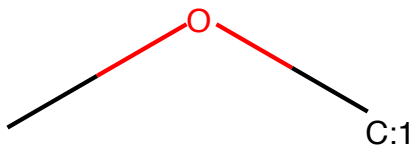


'--'

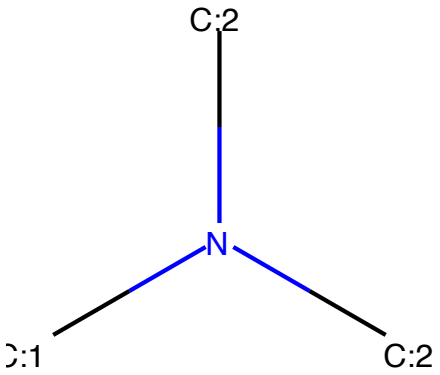
'-----Step-24-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.25249555
706977844'

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

'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'
```

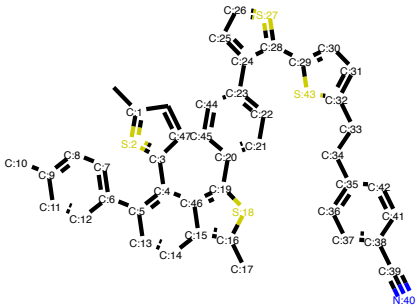


'--'

'Molecule CN and its specific config [CH3:1][NH2:2] w/ probability -19.6560955
04760742'

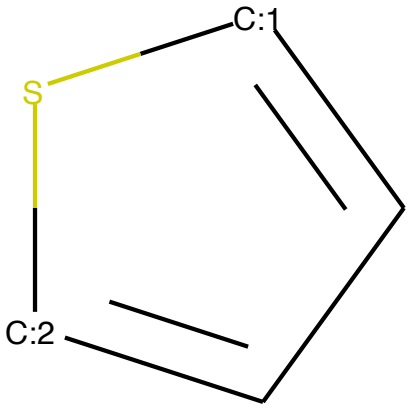
'--'

'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'



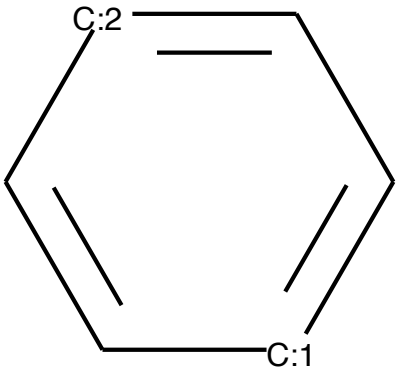
'--'

'-----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'



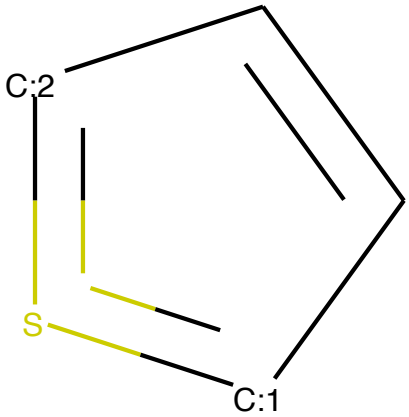
'--'

'Molecule C1=CC=CC=C1 and its specific config C1=[CH:1]C=C[CH:2]=C1 w/ probabi
lity -2.83522891998291'



'--'

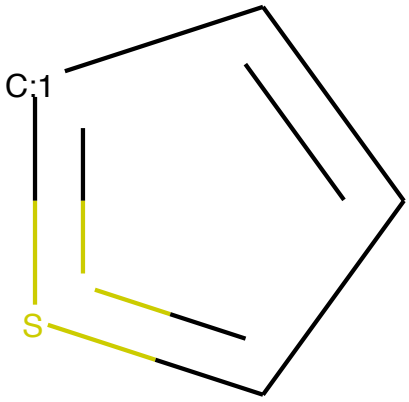
'Molecule C1=CC=S=C1 and its specific config C1=C[CH:2]=S=[CH:1]1 w/ probabili
ty -7.261528968811035'



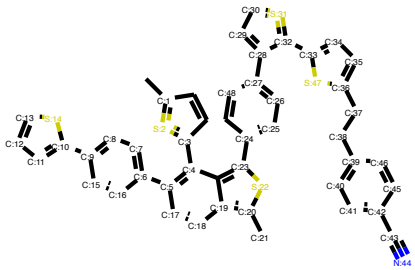
'--'

'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'
```



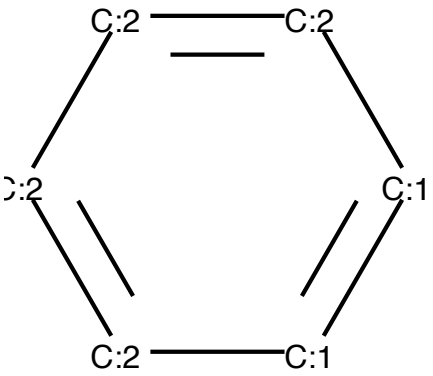
```
'------------------------------------------------------------'

'-----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'
```

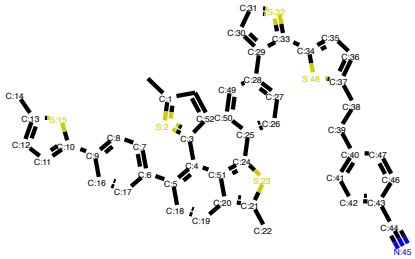
```
'------------------------------------------------------------'

'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'
```



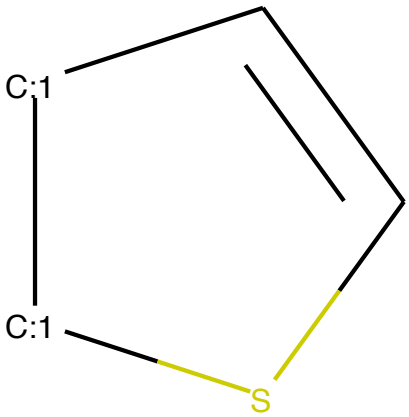

```
'------------------------------------------------------------'

'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-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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.
```

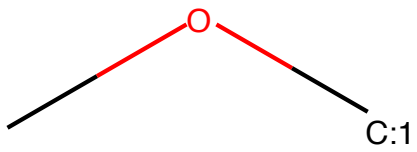
```
'-----Step-28-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-29-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'
```

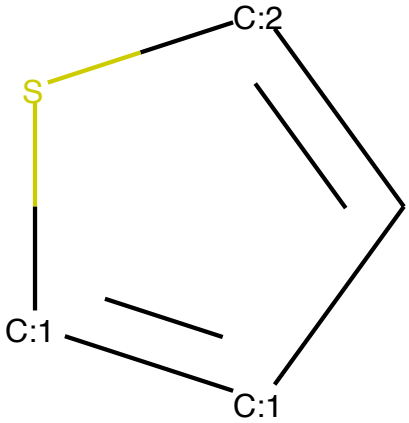



```
'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -3.87171745300292
97'
```

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

'Molecule COC and its specific config CO[CH3:1] w/ probability -4.779026508331
299'
```



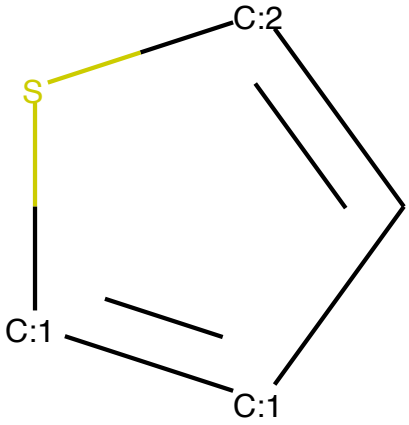

```
'------------------------------------------------------------'

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

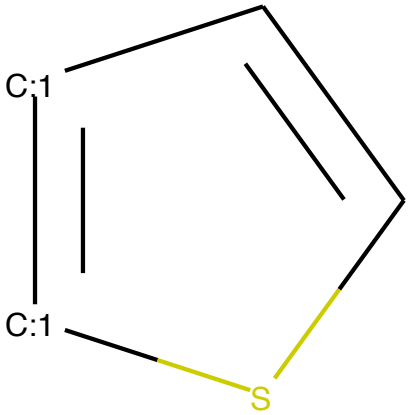
```
'------------------------------------------------------------'

'-----Step-31-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'
```

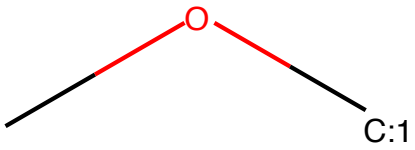


```
'------------------------------------------------------------'

'Molecule CC and its specific config C[CH3:1] w/ probability -13.0446128845214
84'
```

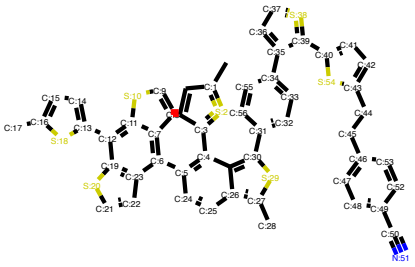
```
'------------------------------------------------------------'

'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'
```



'--'

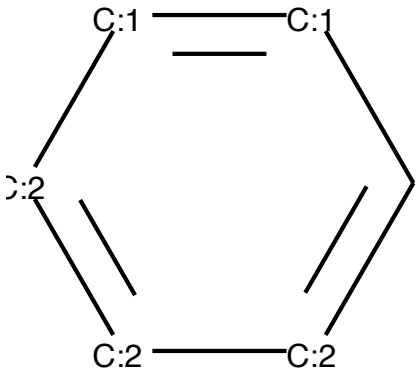
'-----Step-33-----'
'Generate next fragment: 0.9991055130958557'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.10141272
097826004'

'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -2.33883476257324
2'

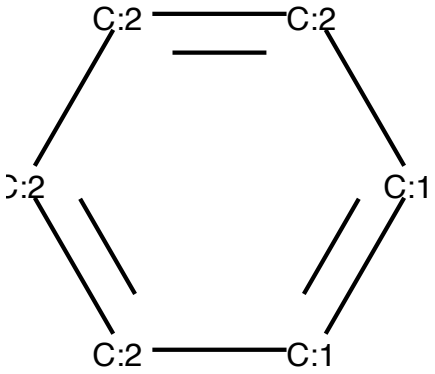
'--'

'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'

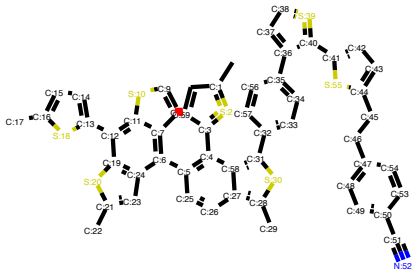


'--'

'Molecule CF and its specific config F[CH3:1] w/ probability -24.9132843017578
12'

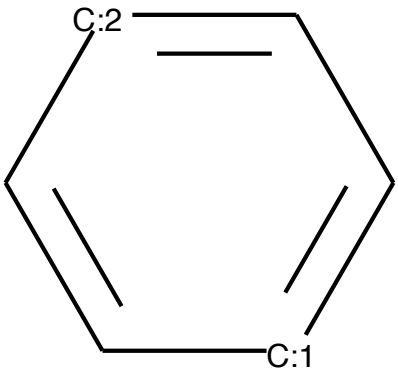
'--'

'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'



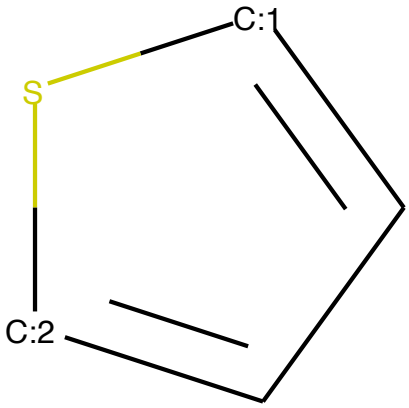
'--'

'-----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'



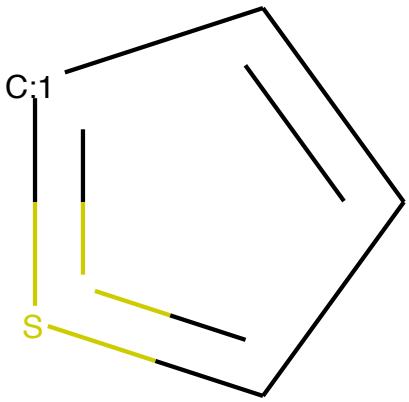
'--'

'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-1.0630781650543213'



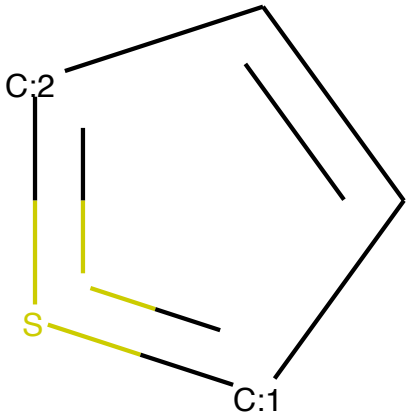
'--'

'Molecule C1=CC=S=C1 and its specific config C1=C[CH:1]=S=C1 w/ probability -4
.04391622543335'

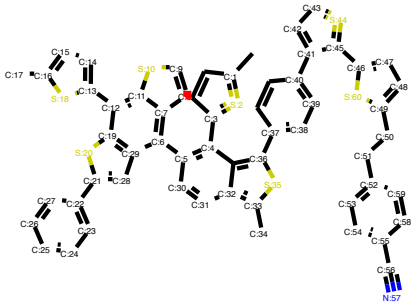



```
'------------------------------------------------------------'

'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'
```



'--'

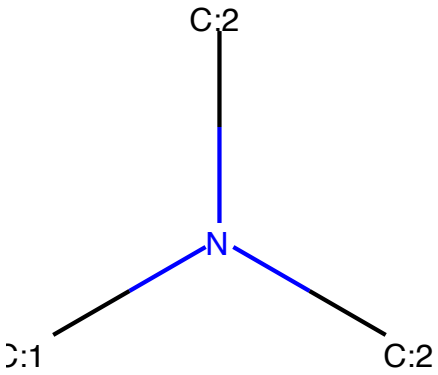
'-----Step-35-----'
'Generate next fragment: 1.0'
'Top 5 next fragments to attach (current and potential graph)'
'Molecule CC and its specific config [CH3:1][CH3:2] w/ probability -0.00494720
46084702015'

'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -5.31625699996948
2'

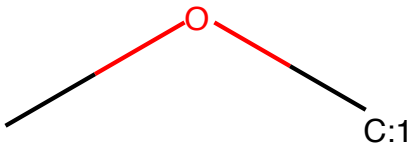
'--'

'Molecule CN(C)C and its specific config N([CH3:1])([CH3:2])[CH3:2] w/ probabi
lity -10.642192840576172'



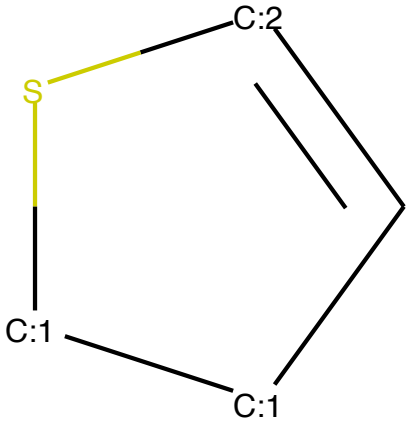
'--'

'Molecule COC and its specific config CO[CH3:1] w/ probability -19.70873260498
047'



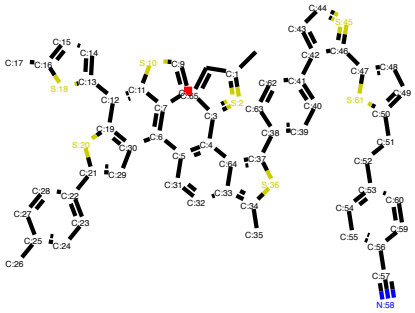
'--'

'Molecule C1=CSCC1 and its specific config C1=[CH:2]S[CH2:1][CH2:1]1 w/ probab
ility -22.31403923034668'



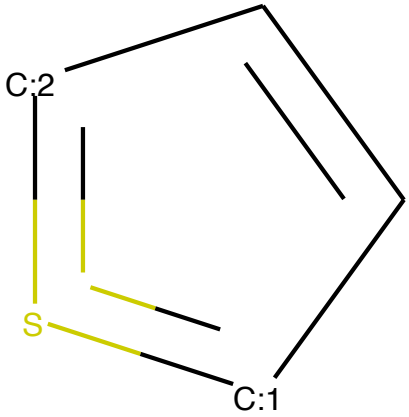
'--'

'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'



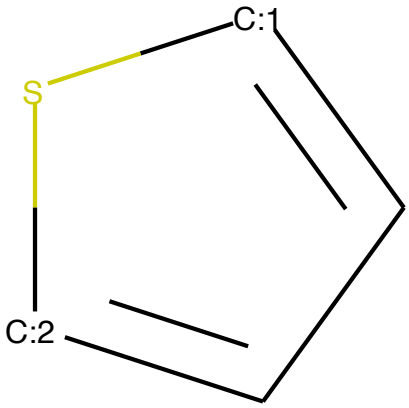
'--'

'-----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'



'--'

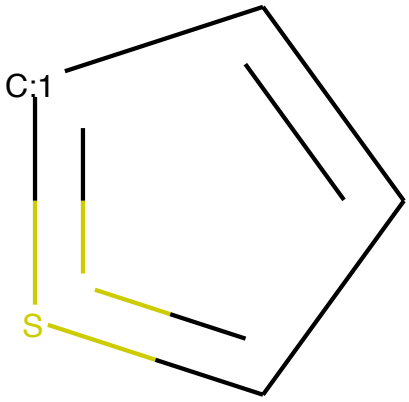
'Molecule C1=CSC=C1 and its specific config C1=[CH:1]S[CH:2]=C1 w/ probability
-1.1682732105255127'



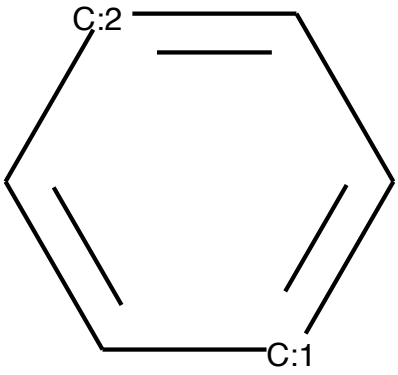
'--'

'Molecule C=C and its specific config [CH2:1]=[CH2:2] w/ probability -1.210477
590560913'

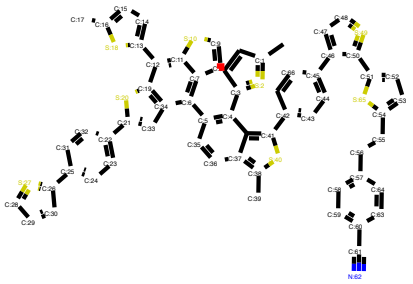
```
'------------------------------------------------------------'

'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'

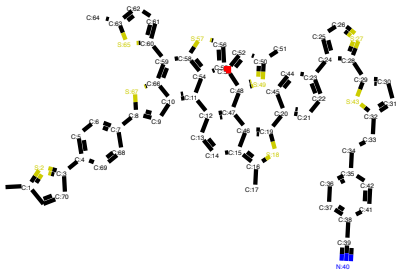
'--'

'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'
```

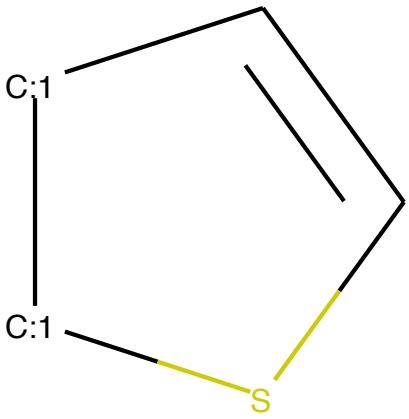


```
'------------------------------------------------------------'

'-----Step-38-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-39-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-40-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-41-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-42-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-43-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-44-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-45-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-46-----'
```

```
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-47-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-48-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'
```

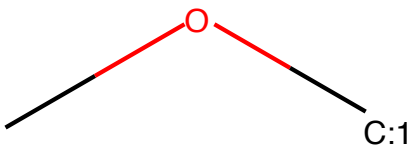
```
'------------------------------------------------------------'

'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'
```

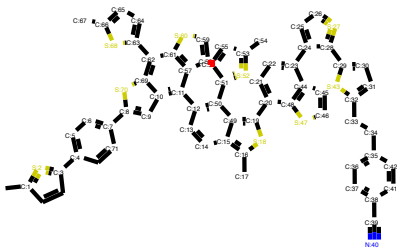



```
'------------------------------------------------------------'

'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'
```



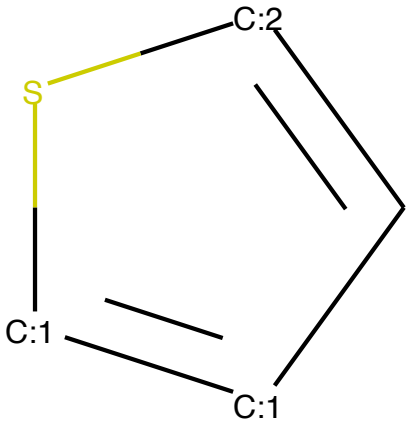
'--'

'-----Step-50-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'

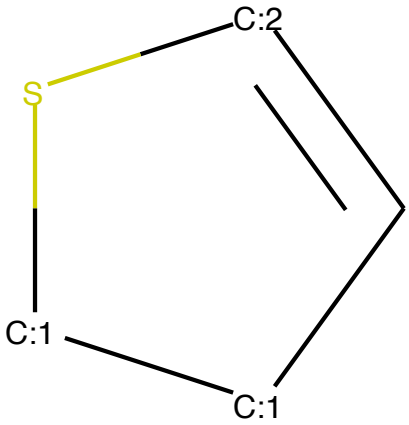
'--'

'Molecule CC and its specific config C[CH3:1] w/ probability -8.18435764312744
1'

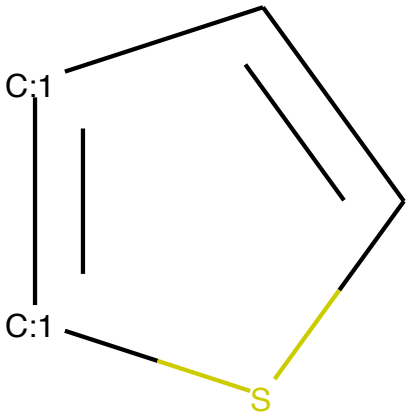
```
'------------------------------------------------------------'

'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'
```

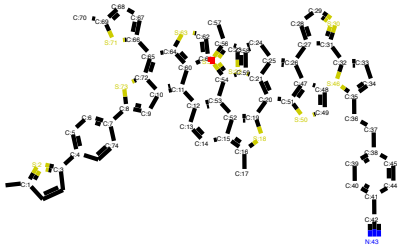



```
'------------------------------------------------------------'

'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'

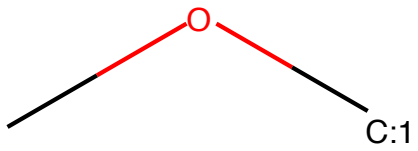


'--'

'-----Step-52-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-53-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-54-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'

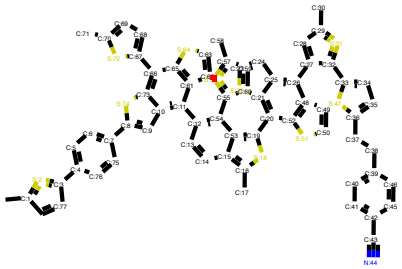



```
'------------------------------------------------------------'

'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'
```

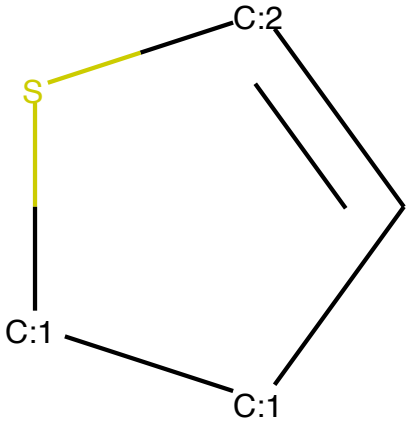
```
'------------------------------------------------------------'

'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'
```



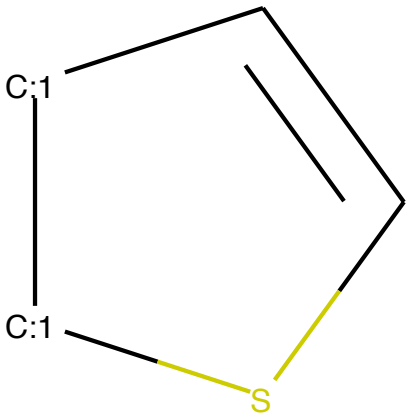
```
'------------------------------------------------------------'

'-----Step-56-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-57-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-58-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-59-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-60-----'
```

```
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-61-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-62-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'
```

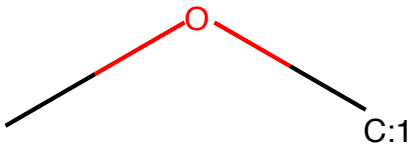



```
'------------------------------------------------------------'

'Molecule C1=CSCC1 and its specific config C1=C[CH2:1][CH2:1]S1 w/ probability
-9.53537368774414'
```



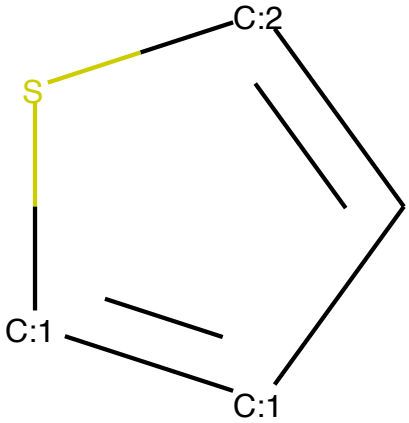
'--'

'Molecule COC and its specific config CO[CH3:1] w/ probability -9.582482337951
66'



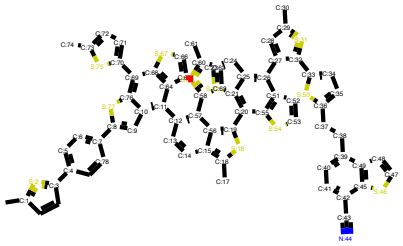
'--'

'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'



'--'

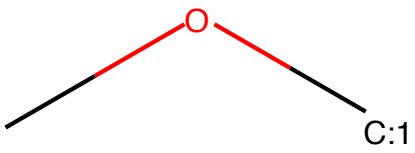
'-----Step-64-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-65-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-66-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-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'
```

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

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-68-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-69-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-70-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-71-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-72-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-73-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-74-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-75-----'
```

```
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-76-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-77-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-78-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-79-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-80-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-81-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-82-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-83-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-84-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-85-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-86-----'
```

```
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-87-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-88-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-89-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-90-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-91-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-92-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
Skip, the best next fragment to be attached to the current fragment does not y
ield a valid sub-molecule . Go back to the previous fragment.
'-----Step-93-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-94-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-95-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-96-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-97-----'
```

```
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-98-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-99-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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-100-----'
Skip, current fragment has not next fragment to be attached. Go back to the pr
evious fragment.
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.
```

In [ ]: