Investigating the corrosion inhibition of copper using DFT theoretical study with three organic molecules

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Optimized molecular structures of the three organic inhibitors at B3LYP/6-31G(d) level of theory.

ATTC molecule

```
0 1
 C                  1.68709100   -1.26733000   -0.57558800
 C                  0.86454400   -0.30763700    0.03717400
 C                  1.48222100    0.79836600    0.64293000
 C                  2.86867800    0.93213000    0.63496200
 C                  3.69081800   -0.02481800    0.02675200
 C                  3.07229000   -1.12903300   -0.57429900
 H                  1.23216700   -2.11858000   -1.07464800
 H                  0.88000700    1.55306100    1.13840400
 H                  3.31997800    1.79683200    1.11622700
 H                  3.68379100   -1.88707500   -1.05895800
 C                 -1.57900600    0.58106700   -0.07514200
 C                 -2.89288700    0.13597400   -0.01465200
 C                  5.19122600    0.14458600   -0.00819700
 H                  5.70418400   -0.82257900   -0.04143100
 H                  5.50662900    0.71047400   -0.89516000
 H                  5.55354700    0.69071400    0.86932200
 N                 -4.03358900    0.87908000   -0.20482500
 H                 -4.86740300    0.57642100    0.28159800
H                 -3.89434700    1.88334700   -0.17621000
 C                 -1.31534700    1.96123400   -0.27406600
 N                 -1.18940900    3.11120000   -0.42526100
 S                 -2.95881900   -1.59331100    0.20124000
 C                 -0.60269300   -0.48758300    0.05978000
 C                 -1.21222100   -1.69816200    0.22392900
 H                 -0.74476200   -2.65435700    0.41012000
```

AMTC molecule

```
0 1
 C                  1.82035300    0.32066100   -0.36119500
 C                  0.99551300   -0.74530700    0.06866500
 C                  1.60418900   -1.86498200    0.64806000
 C                  2.98737000   -1.94063400    0.81695300
 C                  3.78219500   -0.87316600    0.40728900
 C                  3.20569700    0.25579900   -0.17900700
 H                  0.96892500   -2.67559200    0.99388500
 H                  3.43313500   -2.81701600    1.27786200
 H                  3.83928700    1.07388600   -0.50153500
 C                 -1.33919200    0.38078700    0.34344400
 C                 -2.68445100    0.13168800    0.11981800
 N                 -3.74485600    0.97590900    0.36518900
 H                 -4.62162400    0.53933900    0.62075100
 H                 -3.51528800    1.76998500    0.95381300
 C                 -0.94070100    1.56883000    1.01022700
 N                 -0.70490700    2.55957100    1.57884300
 S                 -2.91778800   -1.41859900   -0.64696300
 C                 -0.47535400   -0.70148700   -0.09668100
 C                 -1.19474000   -1.72945400   -0.63100900
```

H	-0.81832200	-2.65153400	-1.05041100
H	4.86007100	-0.90886300	0.54141100
O	1.18114700	1.35978700	-0.96670500
C	1.90790600	2.55265100	-1.22432400
H	2.69170400	2.39092900	-1.97590000
H	1.17825400	3.26568900	-1.61060000
H	2.35492100	2.95179300	-0.30588400

ABTC molecule

0 1

C	0.60421800	-1.31197600	-0.57842700
C	-0.20058000	-0.33517000	0.03224300
C	0.43162800	0.76801800	0.62918700
C	1.81972200	0.89102800	0.62287800
C	2.59045700	-0.09847700	0.01699800
C	1.99255100	-1.20349300	-0.58614100
H	0.13567400	-2.15635800	-1.07548800
H	-0.15857600	1.53728100	1.11569600
H	2.29664600	1.74641100	1.08843300
H	2.60255900	-1.96117100	-1.06591000
C	-2.63031900	0.58999200	-0.07589100
C	-3.95030400	0.16267400	-0.01161500
N	-5.07966200	0.92065400	-0.19786700
H	-5.92293400	0.62380700	0.27520300
H	-4.93143500	1.92350300	-0.17111200
C	-2.34559300	1.96556400	-0.27596900
N	-2.19634900	3.11282000	-0.42611600
S	-4.03920500	-1.56561600	0.20735100
C	-1.67026600	-0.49288100	0.05671300
C	-2.29527600	-1.69529600	0.22339900
H	-1.84096200	-2.65779600	0.40997200
Br	4.49431300	0.06628500	0.00437800