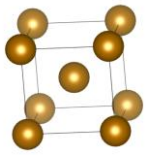
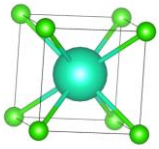
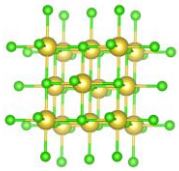
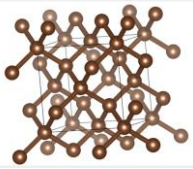
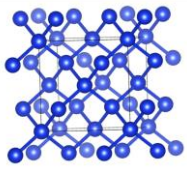
1. Table 1: Lattice parameters of Fe, CsCl, NaCl, diamond, and Si

Name	a (Å)	b (Å)	c (Å)	Alpha	Beta	Gamma	Crystal
Fe	2.8664	2.8664	2.8664	90.0000	90.0000	90.0000	
CsCl	4.1230	4.1230	4.1230	90.0000	90.0000	90.0000	
NaCl	5.6200	5.6200	5.6200	90.0000	90.0000	90.0000	
Diamond	3.5560	3.5560	3.5560	90.0000	90.0000	90.0000	
Si	5.4300	5.4300	5.4300	90.0000	90.0000	90.0000	

2. C6H6 molecule (Benzene)
    a. Code (Python)

```
#Generate Benzene.xyz file

import math
from math import cos
from math import sin

theta = range(0, 360, 60)
r_CC = 1.39000
r_H = r_CC + 1.09000

print("12")
print("Benzene")

for x in theta:
    C_x = r_CC * cos(math.radians(x))
    C_y = r_CC * sin(math.radians(x))
    C_z = 0.00000

    H_x = r_H * cos(math.radians(x))
    H_y = r_H * sin(math.radians(x))
    H_z = 0.00000

    C = [C_x, C_y, C_z]
    H = [H_x, H_y, H_z]

    print("C", str((C[0])), str(C[1]), str(C[2]))
    print("H", str(H[0]), str(H[1]), str(H[2]))
```

b. .xyz file

```
12
Benzene
C 1.39 0.0 0.0
H 2.48 0.0 0.0
C 0.6950000000000001 1.2037753112603695 0.0
H 1.2400000000000002 2.1477430013854075 0.0
C -0.6949999999999996 1.2037753112603697 0.0
H -1.2399999999999995 2.147743001385408 0.0
C -1.39 1.702259050814821e-16 0.0
H -2.48 3.037124061885436e-16 0.0
C -0.6950000000000006 -1.2037753112603695 0.0
H -1.240000000000001 -2.1477430013854075 0.0
C 0.6950000000000001 -1.2037753112603695 0.0
H 1.2400000000000002 -2.1477430013854075 0.0
```

c. .vasp file

```
Benzene
1.0
        6.1999998093         0.0000000000
0.0000000000
        0.0000000000         6.1999998093
0.0000000000
        0.0000000000         0.0000000000
6.1999998093
    C     H
```

```
    6    6
Cartesian
     4.490000014        3.099999905        3.099999905
     3.794999960        4.303775142        3.099999905
     2.404999850        4.303775142        3.099999905
     1.709999795        3.099999905        3.099999905
     2.404999850        1.896224667        3.099999905
     3.794999960        1.896224667        3.099999905
     5.579999681        3.099999905        3.099999905
     4.339999793        5.247742801        3.099999905
     1.860000017        5.247742801        3.099999905
     0.619999944        3.099999905        3.099999905
     1.860000017        0.952257008        3.099999905
     4.339999793        0.952257008        3.099999905
```

d. Visualized molecule structure