

In [15]:

```
from pymatgen.ext.matproj import MPRester
from pymatgen.symmetry.analyzer import SpacegroupAnalyzer
from pymatgen.symmetry.analyzer import PointGroupAnalyzer
from pymatgen.core.operations import SymmOp
from pprint import pprint
with MPRester("UTLDwneEpLqJ3EtR") as m:
    structure = m.get_structure_by_material_id("mp-757100")

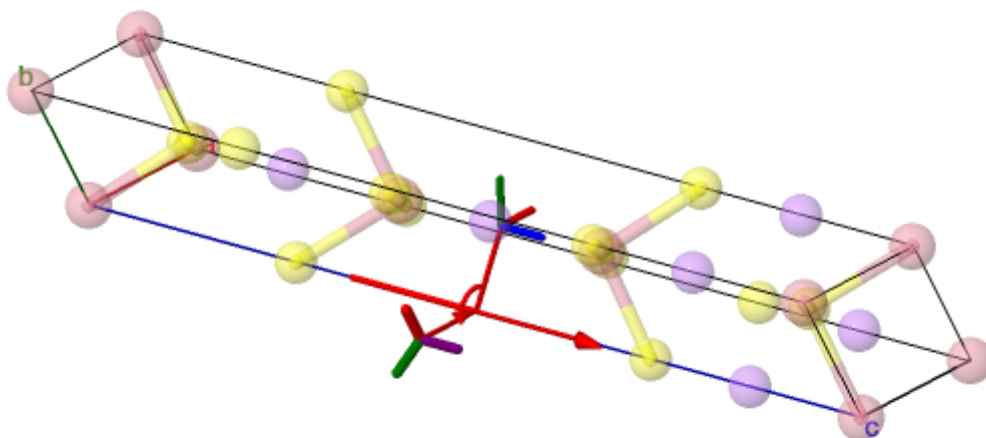
sga = SpacegroupAnalyzer (structure)

Sym1=SymmOp.from_xyz_string("-x, x-y, z")
print("-- \n SYM 1 : along C2 axis (-x, x-y, z)")
print(Sym1)
print("-- \n Applied on (1/2,1/2,1/2) :")
```

```
--
SYM 1 : along C2 axis (-x, x-y, z)--
Rot:
[[-1.  0.  0.]
 [ 1. -1.  0.]
 [ 0.  0.  1.]]
tau
[0. 0. 0.]
--
Applied on (1/2,1/2,1/2) :
```

HM:R3m #160
a=3.418Å
b=3.418Å
c=18.627Å
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=120.000^\circ$

2: -y,x-y,z
C3 axis



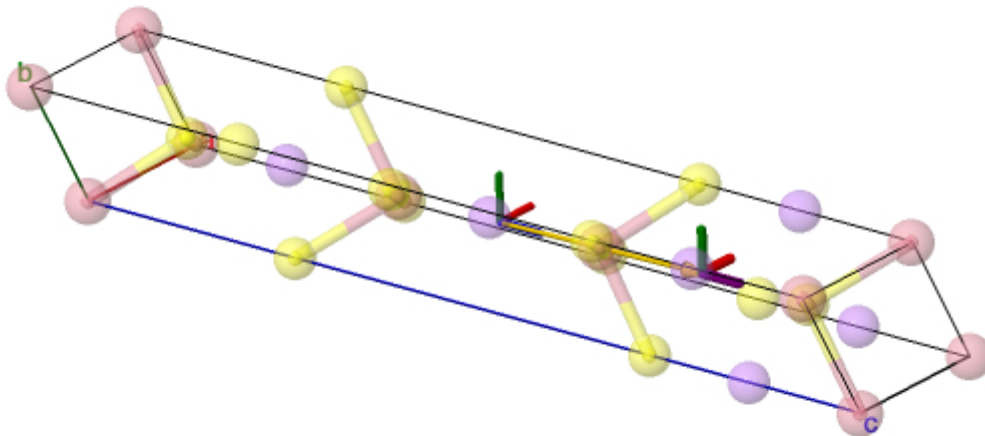
In [14]:

```
Sym2=SymmOp.from_xyz_string("x-1/3,y+1/3,z+1/3")
print("-- \n SYM 2 : translation (x-1/3,y+1/3,z+1/3)")
print(Sym2)
print("-- \n Applied on (1/2,1/2,1/2) :")
```

```
--
SYM 2 : translation (x-1/3,y+1/3,z+1/3)--
Rot:
[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]
tau
[-0.33333333  0.33333333  0.33333333]
--
Applied on (1/2,1/2,1/2) :
```

```
HM:R3m #160
a=3.418Å
b=3.418Å
c=18.627Å
α=90.000°
β=90.000°
γ=120.000°
```

7: $x-1/3, y+1/3, z+1/3$
translation: $-1/3 \ 1/3 \ 1/3$



In [16]:

```
Sym3=SymmOp.from_xyz_string("x-1/3,y+1/3,z+1/3")
print("-- \n SYM 3 : 3-fold screw axis (-y-1/3,x-y+1/3,z+1/3)")
print(Sym3)
print("-- \n Applied on (1/2,1/2,1/2) :")
```

```
--
SYM 3 : 3-fold screw axis (-y-1/3,x-y+1/3,z+1/3)
```

Rot:

```
[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]
```

tau

```
[-0.33333333  0.33333333  0.33333333]
```

```
--
```

Applied on (1/2,1/2,1/2) :

```
HM:R3m #160
a=3.418Å
b=3.418Å
c=18.627Å
α=90.000°
β=90.000°
γ=120.000°
```

8: $-y-1/3, x-y+1/3, z+1/3$
 3-fold screw axis
 translation: $0\ 0\ 1/3$

