In [3]:
```
from pymatgen.symmetry.analyzer import SpacegroupAnalyzer
from pymatgen.core.structure import Structure
```

In [4]:
```
pip show -v pymatgen
```

```
Name: pymatgen
Version: 2023.9.2
Summary: Python Materials Genomics is a robust materials analysis code that defines core object representations for structures and molecules with support for many
electronic structure codes. It is currently the core analysis code powering the Materials Project (https://materialsproject.org).
Home-page: https://pymatgen.org
Author: Pymatgen Development Team
Author-email: ongsp@ucsd.edu
License: MIT
Location: /Users/kavanase/miniconda3/lib/python3.10/site-packages
Requires: joblib, matplotlib, monty, mp-api, networkx, numpy, palettable, pandas, plotly, pybtex, pydantic, requests, ruamel.yaml, scipy, spglib, sympy, tabulate,
tqdm, uncertainties
Required-by: bsym, doped, emmet-core, matools, mp-api, mp-pyrho, mpcontribs-client, nonrad, pdyna, polyhedral-analysis, py-sc-fermi, pymatgen-analysis-defects, pyt
aser, shakenbreak, sumo, vasppy
Metadata-Version: 2.1
Installer: pip
Classifiers:
  Development Status :: 4 - Beta
  Intended Audience :: Science/Research
  License :: OSI Approved :: MIT License
  Operating System :: OS Independent
  Programming Language :: Python :: 3.9
  Programming Language :: Python :: 3.10
  Programming Language :: Python :: 3.11
  Programming Language :: Python :: 3
  Topic :: Scientific/Engineering :: Chemistry
  Topic :: Scientific/Engineering :: Information Analysis
  Topic :: Scientific/Engineering :: Physics
  Topic :: Software Development :: Libraries :: Python Modules
Entry-points:
  [console_scripts]
  feff_plot_cross_section = pymatgen.cli.feff_plot_cross_section:main
  feff_plot_dos = pymatgen.cli.feff_plot_dos:main
  get_environment = pymatgen.cli.get_environment:main
  pmg = pymatgen.cli.pmg:main
Project-URLs:
  Docs, https://pymatgen.org
  Package, https://pypi.org/project/pymatgen
  Repo, https://github.com/materialsproject/pymatgen
Note: you may need to restart the kernel to use updated packages.
```

In [13]:
```
SbSiTe_prim = Structure.from_file("Sb2Si2Te6_prim_POSCAR")
SbSiTe_supercell = Structure.from_file("Sb2Si2Te6_supercell_POSCAR")
```

In [14]:
```
SbSiTe_prim
```

Out[14]:
```
Structure Summary
Lattice
    abc : 8.042144031949908 8.042144031949908 8.042144031949908
 angles : 52.21741644896751 52.21741644896751 52.21741644896751
 volume : 300.5368925047317
      A : 7.22152928660791 -3.539151790089226 0.0
      B : 7.22152928660791 3.539151790089226 0.0
      C : 5.487049663777871 0.0 5.879486934917253
    pbc : True True True
PeriodicSite: Si (8.869, 2.315e-16, 2.617) [0.445, 0.445, 0.445]
PeriodicSite: Si (11.06, -3.082e-16, 3.263) [0.555, 0.555, 0.555]
PeriodicSite: Sb (3.313, 1.762e-17, 0.9772) [0.1662, 0.1662, 0.1662]
PeriodicSite: Sb (16.62, 6.101e-16, 4.902) [0.8338, 0.8338, 0.8338]
PeriodicSite: Te (7.526, 1.195, 4.358) [0.07057, 0.4083, 0.7413]
PeriodicSite: Te (12.4, -1.195, 1.521) [0.9294, 0.5917, 0.2587]
PeriodicSite: Te (8.689, 1.178, 0.4149) [0.4083, 0.7413, 0.07057]
PeriodicSite: Te (11.24, -1.178, 5.465) [0.5917, 0.2587, 0.9294]
PeriodicSite: Te (8.103, -2.374, 2.401) [0.7413, 0.07057, 0.4083]
PeriodicSite: Te (11.83, 2.374, 3.479) [0.2587, 0.9294, 0.5917]
```

In [15]:
```
sga = SpacegroupAnalyzer(SbSiTe_prim)
sga.get_symmetrized_structure()
```

Out[15]:
```
SymmetrizedStructure
Full Formula (Si2 Sb2 Te6)
Reduced Formula: SiSbTe3
Spacegroup: R-3 (148)
abc   :   8.042144   8.042144   8.042144
angles:  52.217416  52.217416  52.217416
Sites (10)
  #  SP          a         b         c  Wyckoff
---  ----  --------  --------  --------  ---------
  0  Si    0.445025  0.445025  0.445025  2c
  1  Sb    0.166212  0.166212  0.166212  2c
  2  Te    0.070568  0.408338  0.741259  6f
```

In [16]:
```
SbSiTe_supercell
```

Out[16]:
```
Structure Summary
Lattice
    abc : 14.44306 14.156608 12.259981770552354
 angles : 90.0 106.43634013821695 90.0
 volume : 2404.295546766097
      A : 14.44306 0.0 0.0
      B : 0.0 14.156608 0.0
      C : -3.468959999999999 0.0 11.758974
    pbc : True True True
PeriodicSite: Si (9.326, 10.62, 9.142) [0.8325, 0.75, 0.7775]
PeriodicSite: Si (9.326, 3.539, 9.142) [0.8325, 0.25, 0.7775]
PeriodicSite: Si (11.06, 7.078, 3.263) [0.8325, 0.5, 0.2775]
PeriodicSite: Si (2.105, 7.078, 9.142) [0.3325, 0.5, 0.7775]
PeriodicSite: Si (3.839, 10.62, 3.263) [0.3325, 0.75, 0.2775]
PeriodicSite: Si (11.06, 14.16, 3.263) [0.8325, 1.0, 0.2775]
PeriodicSite: Si (2.105, 14.16, 9.142) [0.3325, 1.0, 0.7775]
PeriodicSite: Si (3.839, 3.539, 3.263) [0.3325, 0.25, 0.2775]
PeriodicSite: Si (7.135, 10.62, 8.496) [0.6675, 0.75, 0.7225]
PeriodicSite: Si (7.135, 3.539, 8.496) [0.6675, 0.25, 0.7225]
PeriodicSite: Si (8.869, 7.078, 2.617) [0.6675, 0.5, 0.2225]
PeriodicSite: Si (-0.08661, 7.078, 8.496) [0.1675, 0.5, 0.7225]
PeriodicSite: Si (1.648, 10.62, 2.617) [0.1675, 0.75, 0.2225]
PeriodicSite: Si (8.869, 0.0, 2.617) [0.6675, 0.0, 0.2225]
PeriodicSite: Si (-0.08661, 0.0, 8.496) [0.1675, 0.0, 0.7225]
PeriodicSite: Si (1.648, 3.539, 2.617) [0.1675, 0.25, 0.2225]
PeriodicSite: Sb (0.4399, 10.62, 10.78) [0.2507, 0.75, 0.9169]
PeriodicSite: Sb (0.4399, 3.539, 10.78) [0.2507, 0.25, 0.9169]
PeriodicSite: Sb (2.174, 7.078, 4.902) [0.2507, 0.5, 0.4169]
PeriodicSite: Sb (7.661, 7.078, 10.78) [0.7507, 0.5, 0.9169]
PeriodicSite: Sb (9.396, 10.62, 4.902) [0.7507, 0.75, 0.4169]
PeriodicSite: Sb (2.174, 0.0, 4.902) [0.2507, 0.0, 0.4169]
PeriodicSite: Sb (7.661, 0.0, 10.78) [0.7507, 0.0, 0.9169]
PeriodicSite: Sb (9.396, 3.539, 4.902) [0.7507, 0.25, 0.4169]
PeriodicSite: Sb (1.578, 10.62, 6.857) [0.2493, 0.75, 0.5831]
PeriodicSite: Sb (1.578, 3.539, 6.857) [0.2493, 0.25, 0.5831]
PeriodicSite: Sb (3.313, 7.078, 0.9772) [0.2493, 0.5, 0.08311]
PeriodicSite: Sb (8.8, 7.078, 6.857) [0.7493, 0.5, 0.5831]
PeriodicSite: Sb (10.53, 10.62, 0.9772) [0.7493, 0.75, 0.08311]
PeriodicSite: Sb (3.313, 0.0, 0.9772) [0.2493, 0.0, 0.08311]
PeriodicSite: Sb (8.8, 0.0, 6.857) [0.7493, 0.0, 0.5831]
PeriodicSite: Sb (10.53, 3.539, 0.9772) [0.7493, 0.25, 0.08311]
PeriodicSite: Te (9.507, 9.439, 11.34) [0.8899, 0.6668, 0.9647]
PeriodicSite: Te (9.507, 2.361, 11.34) [0.8899, 0.1668, 0.9647]
PeriodicSite: Te (11.24, 5.9, 5.465) [0.8899, 0.4168, 0.4647]
PeriodicSite: Te (2.285, 5.9, 11.34) [0.3899, 0.4168, 0.9647]
PeriodicSite: Te (4.02, 9.439, 5.465) [0.3899, 0.6668, 0.4647]
PeriodicSite: Te (11.24, 12.98, 5.465) [0.8899, 0.9168, 0.4647]
PeriodicSite: Te (2.285, 12.98, 11.34) [0.3899, 0.9168, 0.9647]
PeriodicSite: Te (4.02, 2.361, 5.465) [0.3899, 0.1668, 0.4647]
PeriodicSite: Te (6.955, 11.8, 6.294) [0.6101, 0.8332, 0.5353]
PeriodicSite: Te (6.955, 4.717, 6.294) [0.6101, 0.3332, 0.5353]
PeriodicSite: Te (8.689, 8.257, 0.4149) [0.6101, 0.5832, 0.03528]
PeriodicSite: Te (-0.2669, 8.257, 6.294) [0.1101, 0.5832, 0.5353]
PeriodicSite: Te (1.468, 11.8, 0.4149) [0.1101, 0.8332, 0.03528]
PeriodicSite: Te (8.689, 1.178, 0.4149) [0.6101, 0.08323, 0.03528]
PeriodicSite: Te (-0.2669, 1.178, 6.294) [0.1101, 0.08323, 0.5353]
PeriodicSite: Te (1.468, 4.717, 0.4149) [0.1101, 0.3332, 0.03528]
PeriodicSite: Te (10.09, 12.99, 9.358) [0.8899, 0.9177, 0.7958]
PeriodicSite: Te (10.09, 5.913, 9.358) [0.8899, 0.4177, 0.7958]
PeriodicSite: Te (11.83, 9.452, 3.479) [0.8899, 0.6677, 0.2958]
PeriodicSite: Te (2.871, 9.452, 9.358) [0.3899, 0.6677, 0.7958]
PeriodicSite: Te (4.605, 12.99, 3.479) [0.3899, 0.9177, 0.2958]
PeriodicSite: Te (11.83, 2.374, 3.479) [0.8899, 0.1677, 0.2958]
PeriodicSite: Te (2.871, 2.374, 9.358) [0.3899, 0.1677, 0.7958]
PeriodicSite: Te (4.605, 5.913, 3.479) [0.3899, 0.4177, 0.2958]
PeriodicSite: Te (6.369, 8.244, 8.28) [0.6101, 0.5823, 0.7042]
PeriodicSite: Te (6.369, 1.165, 8.28) [0.6101, 0.08233, 0.7042]
PeriodicSite: Te (8.103, 4.705, 2.401) [0.6101, 0.3323, 0.2042]
PeriodicSite: Te (-0.8528, 4.705, 8.28) [0.1101, 0.3323, 0.7042]
PeriodicSite: Te (0.8817, 8.244, 2.401) [0.1101, 0.5823, 0.2042]
PeriodicSite: Te (8.103, 11.78, 2.401) [0.6101, 0.8323, 0.2042]
PeriodicSite: Te (-0.8528, 11.78, 8.28) [0.1101, 0.8323, 0.7042]
PeriodicSite: Te (0.8817, 1.165, 2.401) [0.1101, 0.08233, 0.2042]
PeriodicSite: Te (10.67, 9.422, 7.401) [0.8899, 0.6656, 0.6294]
PeriodicSite: Te (10.67, 2.344, 7.401) [0.8899, 0.1656, 0.6294]
PeriodicSite: Te (12.4, 5.883, 1.521) [0.8899, 0.4156, 0.1294]
PeriodicSite: Te (3.448, 5.883, 7.401) [0.3899, 0.4156, 0.6294]
PeriodicSite: Te (5.183, 9.422, 1.521) [0.3899, 0.6656, 0.1294]
PeriodicSite: Te (12.4, 12.96, 1.521) [0.8899, 0.9156, 0.1294]
PeriodicSite: Te (3.448, 12.96, 7.401) [0.3899, 0.9156, 0.6294]
PeriodicSite: Te (5.183, 2.344, 1.521) [0.3899, 0.1656, 0.1294]
PeriodicSite: Te (5.791, 11.81, 10.24) [0.6101, 0.8344, 0.8706]
PeriodicSite: Te (5.791, 4.735, 10.24) [0.6101, 0.3344, 0.8706]
PeriodicSite: Te (7.526, 8.274, 4.358) [0.6101, 0.5844, 0.3706]
PeriodicSite: Te (-1.43, 8.274, 10.24) [0.1101, 0.5844, 0.8706]
PeriodicSite: Te (0.3042, 11.81, 4.358) [0.1101, 0.8344, 0.3706]
PeriodicSite: Te (7.526, 1.195, 4.358) [0.6101, 0.08444, 0.3706]
PeriodicSite: Te (-1.43, 1.195, 10.24) [0.1101, 0.08444, 0.8706]
PeriodicSite: Te (0.3042, 4.735, 4.358) [0.1101, 0.3344, 0.3706]
```

Corresponds to:

```
[[ 1  1  0]
 [-2  2  0]
 [-1 -1  2]]
```

supercell matrix expansion of the primitive.

In [17]:
```
sga = SpacegroupAnalyzer(SbSiTe_supercell)
sga.get_symmetrized_structure()
```

Out[17]:
```
SymmetrizedStructure
Full Formula (Si16 Sb16 Te48)
Reduced Formula: SiSbTe3
Spacegroup: R-3 (148)
abc   :  14.443060  14.156608  12.259982
angles:  90.000000 106.436340  90.000000
Sites (80)
  #  SP          a         b         c  Wyckoff
---  ----  --------  --------  --------  ---------
  0  Si    0.832462  0.75      0.777487  16c
  1  Sb    0.250682  0.75      0.916894  16c
  2  Te    0.889917  0.66677   0.964716  16f
  3  Te    0.889917  0.917673  0.795831  16f
  4  Te    0.889917  0.665558  0.62937   16f
```

Detects the same space group, but now with three different Te inequivalent sites?

Converting to `SpacegroupAnalyzer` primitive and then getting the `symmetrized_structure`, gives the original result:

In [19]:
```
sga = SpacegroupAnalyzer(SbSiTe_supercell)
sga = SpacegroupAnalyzer(sga.get_primitive_standard_structure())
sga.get_symmetrized_structure()
```

Out[19]:
```
SymmetrizedStructure
Full Formula (Si2 Sb2 Te6)
Reduced Formula: SiSbTe3
Spacegroup: R-3 (148)
abc   :   8.042145   8.042145   8.042145
angles:  52.217415  52.217415  52.217415
Sites (10)
  #  SP          a         b         c  Wyckoff
---  ----  --------  --------  --------  ---------
  0  Si    0.554975  0.554975  0.554975  2c
  1  Sb    0.833788  0.833788  0.833788  2c
  2  Te    0.25874   0.591662  0.929432  6f
```

Not sure if this is the desired behavior, but I would've guessed `get_symmetrized_structure()` should return the same result for both.

In [ ]: