# mol2crystal.py: Processing Flow and Subroutine Overview

## Overview

mol2crystal.py is a Python script that takes a molecular structure file (precursor.mol) as input and automatically generates and evaluates candidate molecular crystal structures by leveraging space group symmetry. The entire process is automated, including initial structure generation, application of space groups, atomic overlap detection, structure saving, and density evaluation.

## Processing Flow

1. 1. Read and center the molecular structure
2. 2. Obtain symmetry via point group analysis (using pymsym)
3. 3. Extract candidate space groups (group-theoretical and physical expansion)
4. 4. Rotate the molecule and define the unit cell
5. 5. Generate crystal structures by applying space groups
6. 6. Check for atomic overlaps
7. 7. Convert to primitive unit cell (using spglib)
8. 8. Save structure (VASP format) and evaluate density
9. 9. Record results (structure\_vs\_energy.txt)

## Detailed Explanation of Key Subroutines

### rotate\_molecule(positions, theta, phi)

Rotates the molecule around the Z and Y axes to ensure structural diversity.  
- theta: Rotation angle around the Z-axis (horizontal rotation)  
- phi: Rotation angle around the Y-axis (vertical rotation)  
Constructs a rotation matrix and applies it to the atomic positions.

### has\_overlap\_neighborlist(atoms, covalent\_radii, scale)

Uses NeighborList to efficiently detect atomic overlaps.  
- Determines overlap if the interatomic distance is less than scale × (r1 + r2).  
Employs ASE's NeighborList for efficient checking.

### adjust\_cellpar\_by\_spacegroup(sg, cellpar)

Adjusts unit cell parameters according to the space group to construct a lattice suitable for symmetry.  
- Applies lattice constraints (orthogonality, angles, axis ratios) corresponding to space group sg.  
- Modifies cellpar (a, b, c, α, β, γ).

### get\_primitive\_cell(atoms)

Converts the structure to a primitive unit cell using spglib.  
- Extracts the primitive cell from the given structure.  
- Reconstructs lattice vectors and atomic positions.

### density\_calc(fname)

Calculates density from the structure file and records it in the log.  
- Computes density from the total atomic mass and unit cell volume.  
- Records the result in a log file.

### get\_all\_subgroups(group, relation\_dict)

Recursively retrieves strict subgroups of the specified point group.  
- Refers to the group-theoretical relation dictionary relation\_dict.  
- Recursively explores subgroups.

### expand\_physical\_supergroups(base\_dict, max\_depth)

Expands physically similar supergroups to a specified depth to broaden space group candidates.  
- Expands neighboring relationships of point groups based on base\_dict.  
- Limits the depth of exploration using max\_depth.