

**Please read the following instructions for the input and output of the function.**

**Input:**

1. **vectors:** A list containing three lists that each has three float numbers, representing the three unit cell vectors a, b and c ( $[[a_x, a_y, a_z], [b_x, b_y, b_z], [c_x, c_y, c_z]]$ ) in angstrom.  
e.g.,  $[[9.8, 0.0, 0.0], [0.0, 5.4, 1.3], [2.2, 0.9, 7.5]]$
2. **atomic\_nums:** A list containing the atomic numbers for each atom in the unit cell. The format should be integer number.  
e.g.,  $[6, 6, 6, \dots, 8, 8, \dots, 1, \dots]$
3. **coordinates:** A list containing sublists that has three float numbers, representing the XYZ coordinates of an atom in angstrom. The number of sublists equals to the number of atoms. The order of atoms in **coordinates** list should be the same as **atomic\_nums** list, meaning the first entry of both lists are describing the same atom, etc.  
e.g.  $[[5.91, 4.18, 6.33], [4.74, 1.19, 0.99], \dots]$

**Output:**

**atom\_types:** A list containing number of strings that equals to the number of atoms. Each string represents the atom type assigned to that atom. The order of atoms in **atom\_types** list is the same as **atomic\_nums** list.

e.g.  $['6[1-(0),6-(1,6),7-(6,27)]', \dots, '8[6-(6,8),27-(7,7,8,8,8)]', \dots, '1[6-(6,7)]', \dots]$