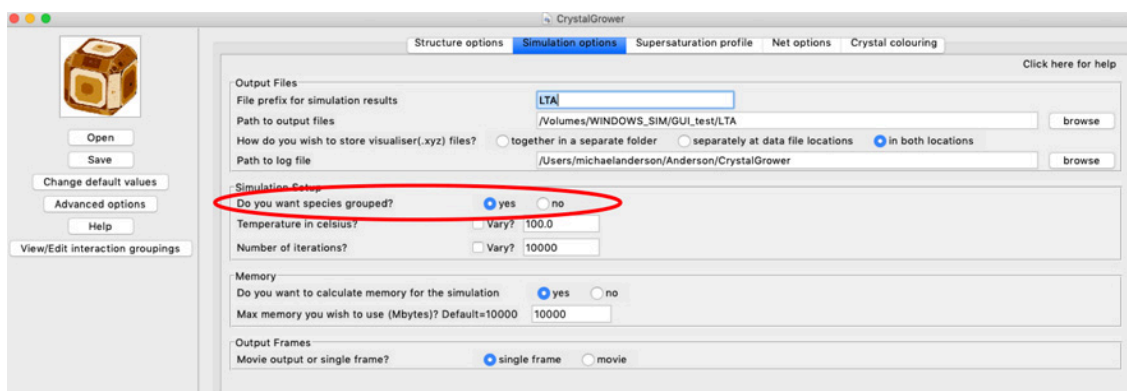


Grouping

Do you want species grouped: this option will only appear for net type simulations. In the structure file each molecule is given both a name and a number. If "yes" is checked the molecules will be treated the same if they have the same name. If "no" is checked then all molecules will be treated differently according to both name and number. Grouping molecules improves efficiency of the calculation and decreases other information required.

This question is only asked if you are performing a net type simulation as grouping is performed automatically for a tile type simulation. The purpose of grouping is to make the simulation more efficient both in terms of speed of calculation and memory used during the calculation. Grouping allows molecules within the primitive unit cell that are the same in terms of connectivity to be considered together as a group.



For example, in the case of L-cystine for which the structure file is shown below, there are 6 molecules in the primitive unit cell. However, these molecules are all equivalent and so can be treated as a group. Setting this to grouped is recommended, however, in some instances the grouping may not be desired in which case it can be switched off. A number of parameters are checked to ensure equivalence and this works in the vast majority of situations. If the grouping does not appear to be correct for your system then it should be switched off.

50:Hexagonal L-cystine

6

C6H12N2O4S2 1 (10,0) 8

1(-1,0,0) 1(0,1,0) 1(1,0,0) 1(0,-1,0) 1(-1,-1,0) 1(1,1,0) 3(0,1,0) 6

H 0[1] 6[1]
H 0[1] 1(0,1,0)[1]
H 0[1] 1(1,1,0)[1]
O 0[2] 1(0,-1,0)[1] 6[1]
O 0[1] 1(-1,-1,0)[1]
H 0[1] 3(0,1,0)[1]
H 0[1] 1(0,-1,0)[1]
H 0[1] 1(1,0,0)[1]
O 0[2] 1(0,1,0)[1] 3(0,1,0)[1]
O 0[1] 1(-1,0,0)[1]

C6H12N2O4S2 2 (10,0) 8

2(0,-1,0) 2(-1,-1,0) 2(0,1,0) 2(1,1,0) 2(1,0,0) 2(-1,0,0) 6(-1,0,0) 4(0,1,1)

H 0[1] 4(0,1,1)[1]
H 0[1] 2(-1,-1,0)[1]
H 0[1] 2(-1,0,0)[1]
O 0[2] 2(1,1,0)[1] 4(0,1,1)[1]
O 0[1] 2(1,0,0)[1]
H 0[1] 6(-1,0,0)[1]
H 0[1] 2(1,1,0)[1]
H 0[1] 2(0,1,0)[1]
O 0[2] 2(-1,-1,0)[1] 6(-1,0,0)[1]
O 0[1] 2(0,-1,0)[1]

C6H12N2O4S2 3 (10,0) 8

3(0,1,0) 3(1,1,0) 3(0,-1,0) 3(-1,-1,0) 3(-1,0,0) 3(1,0,0) 5(1,0,0) 1(0,-1,0)

H 0[1] 1(0,-1,0)[1]
H 0[1] 3(1,1,0)[1]
H 0[1] 3(1,0,0)[1]
O 0[2] 3(-1,-1,0)[1] 1(0,-1,0)[1]
O 0[1] 3(-1,0,0)[1]
H 0[1] 5(1,0,0)[1]
H 0[1] 3(-1,-1,0)[1]
H 0[1] 3(0,-1,0)[1]
O 0[2] 3(1,1,0)[1] 5(1,0,0)[1]
O 0[1] 3(0,1,0)[1]

C6H12N2O4S2 4 (10,0) 8

4(1,0,0) 4(0,-1,0) 4(-1,0,0) 4(0,1,0) 4(1,1,0) 4(-1,-1,0) 2(0,-1,-1) 5

H 0[1] 5[1]
H 0[1] 4(0,-1,0)[1]
H 0[1] 4(-1,-1,0)[1]
O 0[2] 4(0,1,0)[1] 5[1]
O 0[1] 4(1,1,0)[1]
H 0[1] 2(0,-1,-1)[1]
H 0[1] 4(0,1,0)[1]
H 0[1] 4(-1,0,0)[1]
O 0[2] 4(0,-1,0)[1] 2(0,-1,-1)[1]
O 0[1] 4(1,0,0)[1]

C6H12N2O4S2 5 (10,0) 8

5(1,1,0) 5(1,0,0) 5(-1,-1,0) 5(-1,0,0) 5(0,1,0) 5(0,-1,0) 4 3(-1,0,0)

H 0[1] 3(-1,0,0)[1]
H 0[1] 5(1,0,0)[1]
H 0[1] 5(0,-1,0)[1]
O 0[2] 5(-1,0,0)[1] 3(-1,0,0)[1]
O 0[1] 5(0,1,0)[1]
H 0[1] 4[1]
H 0[1] 5(-1,0,0)[1]
H 0[1] 5(-1,-1,0)[1]
O 0[2] 5(1,0,0)[1] 4[1]
O 0[1] 5(1,1,0)[1]

C6H12N2O4S2 6 (10,0) 8

6(-1,-1,0) 6(-1,0,0) 6(1,1,0) 6(1,0,0) 6(0,-1,0) 6(0,1,0) 1 2(1,0,0)

H 0[1] 2(1,0,0)[1]
H 0[1] 6(-1,0,0)[1]
H 0[1] 6(0,1,0)[1]
O 0[2] 6(1,0,0)[1] 2(1,0,0)[1]
O 0[1] 6(0,-1,0)[1]
H 0[1] 1[1]
H 0[1] 6(1,0,0)[1]
H 0[1] 6(1,1,0)[1]
O 0[2] 6(-1,0,0)[1] 1[1]
O 0[1] 6(-1,-1,0)[1]