

Count File

name_count.txt: this contains the number of all the different site types along with the coordination of each site type. Further it contains counts of internal sites if layer colouring is engaged. This file is useful for determining which sites to target with growth modifier.

Count files contain information about the population of all possible site types at the end of the simulation. The format differs slightly for crystals constructed with natural tiles and molecules.

Count – Natural Tile CrystalsExample

Total count t-apf					404913
Total count t-afi					829987
Total count t-kah					2512982
Total count t-lov					1271675
Total Q2 count t-apf					175
Total Q2 count t-afi					363
Total Q2 count t-kah					7233
Total Q2 count t-lov					849
Total surface count t-apf					39983
Total surface count t-afi					45886
Total surface count t-kah					245998
Total surface count t-lov					66650
t-apf					
empty site number	1	312	72.00	0	Q4, 12 Q3, 12 Q2
empty site number	2	0	70.00	1	Q4, 11 Q3, 12 Q2
bulk empty site	248	0	0.00		
t-apf					
grown site number	399	0	72.00	0	Q4, 12 Q3, 12 Q2

grown site number	400	0	70.00	1	Q4,	11	Q3,	12	Q2
bulk grown site	646	364930	0.00						

Total internal count t-apf	39983
Total internal count t-afi	45886
Total internal count t-kah	245998
Total internal count t-lov	66650

t-apf	Internal count							
grown site number	399	0	0	Q4,	12	Q3,	12	Q2
grown site number	400	0	1	Q4,	11	Q3,	12	Q2
bulk grown site	646	0						

General Example

Total count tile type 1 Population
 -Repeat for all tile types in unit cell-

Total Q2 count tile type 1 Population
 -Repeat for all tile types in unit cell-

Total surface count tile type 1 Population
 -Repeat for all tile types in unit cell-

(EMPTY SITES ARE SITES THAT HAVE NOT YET GROWN, I.E. POTENTIAL GROWTH SITES)

Tile type

empty site number	Site number	Population	Site	type
energy (kcal/mol)	Number of Q4 sites	Q4	Number of Q3 sites	
Q3	Number of Q2 Sites	Q2		

-Repeat for all non-bulk sites-

bulk empty site	Site number	Population	Site	type
energy (kcal/mol)				

-Repeat for all tiles in unit cell-

(GROWN SITES ARE SITES THAT HAVE GROWN, I.E. POTENTIAL DISSOLUTION SITES. THESE ARE THE SITES SHOWN WHEN VISUALISING, EXCLUDING BULK)

Tile type

grown site number	Site number	Population	Site	type
energy (kcal/mol)	Number of Q4 sites	Q4	Number of Q3 sites	
Q3	Number of Q2 Sites	Q2		

-Repeat for all non-bulk sites-

bulk grown site	Site number	Population	Site	type
energy (kcal/mol)				

-Repeat for all tiles in unit cell-

(INTERNAL SITES ARE SITES THAT HAVE GROWN AND ARE BELOW THE NUMBER OF LAYERS DETECTED WITH THE FACET FINDING ROUTINE IN CG I.E. GROWN BUT NON-BULK SITES INSIDE THE CRYSTAL, BELOW THE SURFACE. THE POPULATIONS OF THESE SITES WILL BE EMPTY IF THE FACET COLOURING ROUTINE IS NOT USED)

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Total internal count	tile type 1	Population
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-Repeat for all tile types in unit cell-

Tile type Internal Count

grown site number	Site number	Population	Site	type
energy (kcal/mol)	Number of Q4 sites	Q4	Number of Q3 sites	
Q3	Number of Q2 Sites	Q2		

-Repeat for all non-bulk sites-

bulk grown site	Site number	Population	Site	type
energy (kcal/mol)				

-Repeat for all tiles in unit cell-

-REPEAT ALL DATA ABOVE FOR EVERY FRAME IN SIMULATION-

Count – Molecular CrystalsExample

C03	1				
empty site number	1	0	-10.44	6(1)	
empty site number	2	2	-6.96	5(1)	
bulk empty site	32	0	-10.44		

C03	1				
grown site number	33	0	-10.44	6(1)	
grown site number	34	6807	-6.96	5(1)	
bulk grown site	56	141114	-10.44		

General Example

(EMPTY SITES ARE SITES THAT HAVE NOT YET GROWN, I.E. POTENTIAL GROWTH SITES)

Molecule / Group type

empty site number	Site number	Population	Site	type
energy (kcal/mol)	Number of interactions of type connected to species (Interaction type) -Repeat for number of interaction types-			
-Repeat for all non-bulk sites-				

bulk empty site	Site number	Population	Site	type
energy (kcal/mol)				
-Repeat for all molecules / groups in unit cell-				

(GROWN SITES ARE SITES THAT HAVE GROWN, I.E. POTENTIAL DISSOLUTION SITES. THESE ARE THE SITES SHOWN WHEN VISUALISING, EXCLUDING BULK)

Molecule / Group type

grown site number Site number Population Site type
 energy (kcal/mol) Number of interactions of type connected
 (Interaction type) -Repeat for number of interaction types-

-Repeat for all non-bulk sites-

 bulk grown site Site number Population Site
 type energy (kcal/mol)

-Repeat for all molecules in unit cell-

-REPEAT ALL DATA ABOVE FOR EVERY FRAME IN SIMULATION-

-IF BOND WEIGHTING IS ENABLED, FORMAT DIFFERS SLIGHTLY. EACH SITE
 ENTRY (EXCLUDING BULK BECOMES):

grown site number Site number Population Site type
 energy (kcal/mol) Energy contribution from interaction type
 (Interaction type after split by weighting) -Repeat for number of

interaction types-

-Repeat for all non-bulk sites-