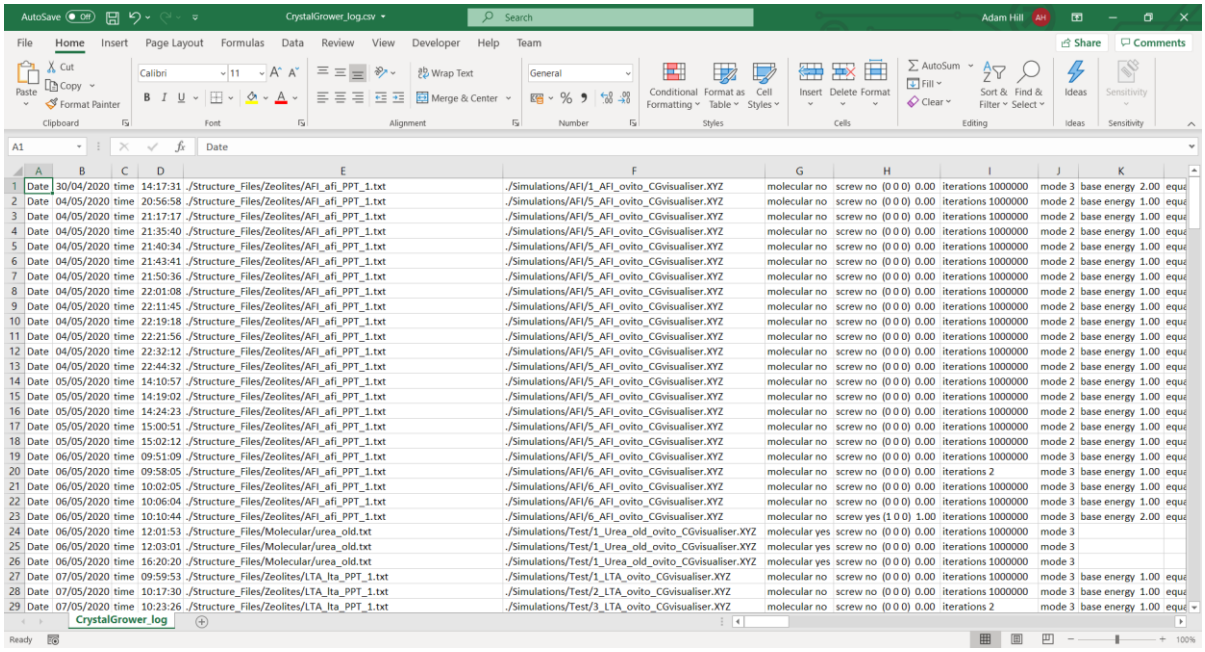
CrystalGrower Log

CrystalGrower_log.csv: this is a continuous log of all simulations performed.

Each line in this log file is a record for each time a simulation is run. Every time the user runs a simulation, a new line is appended to this file. This file will contain information such as the date and time the simulation was run, along with the version of the code used and values for several important parameters used in the simulation. The *CrystalGrower* log file will always be generated in the same directory as the *CrystalGrower* executable and be titled "CrystalGrower_log.csv". The "csv." extension allows the file to be immediately opened in Excel or another spreadsheet program. Columns can then be resized to show the data in a more readable format. The format of the appended line can vary slightly based on the options chosen in *CrystalGrower* but will generally follow one of the two below formats.



	A	B	C	D	E	F	G	H	I	J	K
1	Date	30/04/2020	time	14:17:31	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/1_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 3	base energy 2.00
2	Date	04/05/2020	time	20:56:58	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
3	Date	04/05/2020	time	21:17:17	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
4	Date	04/05/2020	time	21:35:40	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
5	Date	04/05/2020	time	21:40:34	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
6	Date	04/05/2020	time	21:43:41	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
7	Date	04/05/2020	time	21:50:36	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
8	Date	04/05/2020	time	22:01:08	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
9	Date	04/05/2020	time	22:11:45	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
10	Date	04/05/2020	time	22:19:18	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
11	Date	04/05/2020	time	22:21:56	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
12	Date	04/05/2020	time	22:32:12	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
13	Date	04/05/2020	time	22:44:32	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
14	Date	05/05/2020	time	14:10:57	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
15	Date	05/05/2020	time	14:19:02	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
16	Date	05/05/2020	time	14:24:23	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
17	Date	05/05/2020	time	15:00:51	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
18	Date	05/05/2020	time	15:02:12	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 2	base energy 1.00
19	Date	06/05/2020	time	09:51:09	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/5_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 3	base energy 1.00
20	Date	06/05/2020	time	09:58:05	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/6_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 2	mode 3	base energy 1.00
21	Date	06/05/2020	time	10:02:05	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/6_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 3	base energy 1.00
22	Date	06/05/2020	time	10:06:04	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/6_AFI_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 3	base energy 1.00
23	Date	06/05/2020	time	10:10:44	./Structure_Files/Zeolites/AFI_afi_PPT_1.txt	./Simulations/AFI/6_AFI_ovito_CGvisualiser.XYZ	molecular no	screw yes (1 0 0) 1.00	iterations 1000000	mode 3	base energy 2.00
24	Date	06/05/2020	time	12:01:53	./Structure_Files/Molecular/urea_old.txt	./Simulations/Test/1_Urea_old_ovito_CGvisualiser.XYZ	molecular yes	screw no (0 0 0) 0.00	iterations 1000000	mode 3	
25	Date	06/05/2020	time	12:03:01	./Structure_Files/Molecular/urea_old.txt	./Simulations/Test/1_Urea_old_ovito_CGvisualiser.XYZ	molecular yes	screw no (0 0 0) 0.00	iterations 1000000	mode 3	
26	Date	06/05/2020	time	16:20:20	./Structure_Files/Molecular/urea_old.txt	./Simulations/Test/1_Urea_old_ovito_CGvisualiser.XYZ	molecular yes	screw no (0 0 0) 0.00	iterations 1000000	mode 3	
27	Date	07/05/2020	time	09:59:53	./Structure_Files/Zeolites/LTA_lta_PPT_1.txt	./Simulations/Test/1_LTA_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 3	base energy 1.00
28	Date	07/05/2020	time	10:17:30	./Structure_Files/Zeolites/LTA_lta_PPT_1.txt	./Simulations/Test/2_LTA_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 1000000	mode 3	base energy 1.00
29	Date	07/05/2020	time	10:23:26	./Structure_Files/Zeolites/LTA_lta_PPT_1.txt	./Simulations/Test/3_LTA_ovito_CGvisualiser.XYZ	molecular no	screw no (0 0 0) 0.00	iterations 2	mode 3	base energy 1.00

Natural Tiles Log Entry

Example

Date,02/06/2020,time,10:47:34,./Structure_Files/Zeolites/AFI_afi_PPT_1.txt,./Simulations/AFI/13_AFI_ovito_CGvisualiser.XYZ,molecular no ,screw no (0 0 0).00,iterations 1000000,mode 2,base energy 2.00, equal energies yes,1.00 1.00 1.00 1.00 , equal Q-scaling yes, final supersaturation 5.00, Checkpoint yes, ./Simulations/AFI/3_AFI_checkpoint.txt, CrystalGrower_v9_debug6.f90, supersat. excess 1 to 1000000, .00 .00 .00 .00

General Example

Date, DD/MM/YY, time, HH:MM:SS, Structure File Path, Visualisation Output Path, molecular Molecular Answer yes/no,screw Screw Answer yes/no (Screw X Screw Y Screw Z) Burgers Vector, iterations Number of Iterations, mode Delta Mu Mode, base energy Baseline Scaling Applied To Tile Vertices, equal energies Answer To Question About Keeping Tile Energy Scaling The Same Across All Tiles (yes/no), Energy Scaling For Tile 1 -Repeat For All Tiles In Unit Cell-, equal Q-scaling Answer To Question About Keeping Q Scaling Energy The Same For All Tiles (yes/no), Energy Scaling For Q2 -Repeat For All Q Numbers In Tiles-, final supersaturation Supersaturation at the end of the simulation, Checkpoint Checkpoint Answer yes/no, Checkpoint File Path, CrystalGrower Code Version, supersat. excess Excess Start to Excess End, Excess For Species 1
-Repeat For All Species In System-, -Repeat for all supersaturation excess periods-

Molecular Log Entry

Example

Date,02/06/2020,time,12:17:33,./Structure_Files/Molecular/MOF-5_Mike.txt,./Simulations/Test/12_MOF-5_ovito_CGvisualiser.XYZ,molecular yes,screw no (0 0 0).00,iterations 1000000,mode 3,,,,,final supersaturation 1.22,Checkpoint no ,N/A ,CrystalGrower_v9_debug7.f90,supersat. excess 1 to 100000,-1.00 2.40 2.60 ,supersat. excess 100001 to 1000000,-1.00 2.10 2.30

General Example

Date, DD/MM/YY, time, HH:MM:SS, Structure File Path, Visualisation Output Path, molecular Molecular Answer yes/no,screw Screw Answer yes/no (Screw X Screw Y Screw Z) Burgers Vector, iterations Number of Iterations, mode Delta Mu Mode,,,,,final supersaturation Supersaturation at the end of the simulation, Checkpoint Checkpoint Answer yes/no, Checkpoint File Path, CrystalGrower Code Version, supersat. excess Excess Start to Excess End, Excess For Species 1 -Repeat For All Species In System-, -Repeat for all supersaturation excess periods-