

Step	Error or Issue	Possible Reason	Resolution
12	Various “Traceback...” errors when attempting to execute the python script.	The python script and the “.sdf” file are not located in the same directory.	Review Steps 7 and 9 to ensure that these files are properly stored in the same directory.
12	<p>The following syntax error is displayed after executing the Python script:</p> <pre data-bbox="229 381 523 542">"File "write-g09- inputs-sdf.py", line 53 print(gaussian_ input(..."</pre>	<p>A version of Python was executed that is not compatible with the executed Python script. For this error, the Python scripts written for Version 3 were executed on a computer that has Python Version 2 installed.</p>	<p>Only execute the Python script that corresponds with the version of Python that is installed on the user’s hard drive. For this error, download the Python scripts from the Python-Version-2 directory within Supplementary Data 1.</p>
12	<p>The following syntax error is displayed after executing the Python script:</p> <pre data-bbox="229 743 579 940">"File "write-g09- inputs-sdf.py", line 182 """ % (str(sys.argv[1]), TITLE_OF_STRUCTURE)"</pre>	<p>A version of Python was executed that is not compatible with the executed Python script. For this error, the Python scripts written for Version 2 were executed on a computer that has Python Version 3 installed.</p>	<p>Only execute the Python script that corresponds with the version of Python that is installed on the user’s hard drive. For this error, download the Python scripts from Supplementary Data 1.</p>