

CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

DEBUGGING

ERROR MESSAGES

- ▶ The purpose of an error message is to alert the user of a problem in their code
- ▶ These are different from *warnings* in that errors will cause the code to **stop** running
- ▶ Python error messages are typically quite helpful and instructive
- ▶ This is not the case for all programming languages

ERROR TRACEBACK

- ▶ An *error traceback* traces through the program from the written code to where the error is *thrown* in the underlying code
- ▶ These tracebacks are important, but often we can debug from just understanding the *final* line of the traceback
- ▶ This will contain the error type and some additional instructive information

ERROR MESSAGES



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SOME ERROR TYPES

Error Type	Context
<code>IndexError</code>	Trying to access an invalid index
<code>ModuleNotFoundError</code>	Trying to import a non-existent module or library
<code>TypeError</code>	Performing an action on an inappropriate type
<code>ValueError</code>	Function argument is an inappropriate type
<code>NameError</code>	Object with given variable name could not be found
<code>ZeroDivisionError</code>	Trying to divide something by zero

SOME ERROR TYPES



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LEVERAGING THE INTERNET

- ▶ Sometimes the error message is not very clear
- ▶ However, one of the great things about the Python language is the popularity
- ▶ This means that, typically, you are not the first to encounter a particular error

LEVERAGING THE INTERNET



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DON'T BE SCARED

- ▶ Some libraries contain a **very** modular structure
- ▶ This means that error tracebacks can on occasion be **very** long
- ▶ But don't be scared of these, just remember *read from the bottom*

DON'T BE SCARED



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RAISING YOUR OWN ERRORS

- ▶ Errors can be added to your own functions
- ▶ This is achieved using the `raise` command
- ▶ You **should** include a string of text explaining why the error has occurred

RAISING YOUR OWN ERRORS



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PROBLEM

- ▶ You will be working to rotate a water molecule on a surface
- ▶ There is a module on Moodle to help with visualisation
- ▶ Create a function within a module to rotate the water molecule on a surface
- ▶ The handout details the following relationships

$$x' = x \cos \beta - y \sin \beta,$$

$$y' = y \cos \beta - x \sin \beta.$$

PROBLEM



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