Installing and running GAMESS to Excel reader

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Fast tutorial:

- download Visual Studio code (look up, its popular)
 - go through typical "installing" process

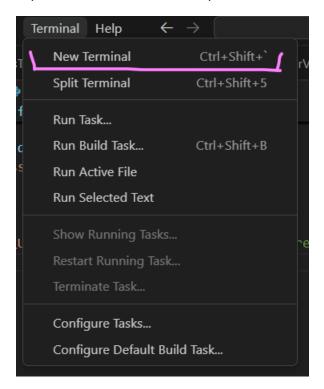
-add extension:



-search for "Python" and install



-open a terminal and install pandas:



While inside of terminal type:

pip install pandas

```
PS C:\Users\adenm\OneDrive\Documents\Python CH410 pip install pandas

Requirement already satisfied: pandas in c:\users\adenm\anaconda3\lib\site-packages (2.2.2)

Requirement already satisfied: numpy>=1.26.0 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (1.26.4)

Requirement already satisfied: python-dateutil>=2.8.2 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (2.9.0.post0)

Requirement already satisfied: pytbon-dateutil>=2.8.2 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (2024.1)

Requirement already satisfied: tzdata>=2022.7 in c:\users\adenm\anaconda3\lib\site-packages (from pandas) (2024.1)

Requirement already satisfied: six>=1.5 in c:\users\adenm\anaconda3\lib\site-packages (from python-dateutil>=2.8.2->pandas) (1.16.0)

PS C:\Users\adenm\oneDrive\Documents\Python CH410> \[ \]
```

-download attached "GAMEStoExcelReaderV2" from github

```
Code Blame 196 lines (89 loc) · 3.89 KB  Code 55% faster with GitHub Copilot

1 from pathlib import Path
2 import re
3 import pandas as pd

4
5 # === FUNCTIONS ===
6
7 × def extract_bond_length(text: str) -> float | None:
8 ""Extract the first bond length from the INTERNUCLEAR DISTANCES section.""
9 match = re.search(
10 r"INTERNUCLEAR DISTANCES \((ANGS\.\)).*?\n\s*\d+\s*[A-Z]+\s*([0-9]+\.\d+)\s*\*",
11 text,
12 re.DOTALL
```

-Change filepaths for input and output folders.

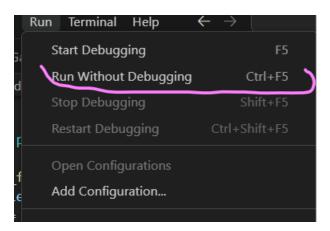
```
# === PATHS ===

input_path = Path(r'C:\Users\Public\gamess-64\outputs')
output_path = Path(r'C:\Users\Public\gamess-64\saved outputs\Python compiled csv')
output_path.mkdir(parents=True, exist_ok=True)
output_file = output_path / 'Gamess_summary.csv'

# === MAIN LOOP ===
```

These are the default directories, yours may be different. You can copy & paste your folder path by right clicking on the folder itself when in file explorer and "copy as path"

-run the code



-win

Output in Excel should look like this:

				_		_
molecule	force_field	basis	comp_met	bond_lengt	heat_of_fo	Total Energy (
C4H6	MMFF94	6-311ppG	Blyp	1.337955	NA	-155.931
C4H6	MMFF94	6-311ppG	RHF	1.337887	NA	-154.962
C6H8	MMFF94	6-311ppG	Blyp	1.445278	NA	-233.313
C6H8	MMFF94	6-311ppG	RHF	1.445278	NA	-231.874
HCl	Gaff	6311pp	AM1	1.099971	-11.3595	NA
HCl	Ghemical	6311pp	AM1	1.008097	10.5191	NA
HCl	MMFF94s	6311pp	AM1	1.305786	-24.4679	NA
HCl	MMFF94	6311pp	AM1	1.305889	-24.4666	NA
HCl	UFF	6311pp	AM1	1.375697	-22.4067	NA
He-neutra	MMFF94	6311ppG2	RHF	0	NA	-2.85998