Autogamess_Water_example

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1 Import `autogamess` and set up input

```
[1]: import autogamess as ag
     maindir = './'
     csvfile = './input.csv'
     title   = 'Water\n'
     savedir = './'
     ag.input_builder(csvfile, savedir, proj_title=title)
```

2 Run the created input using GAMESS(US)

```
[2]: %%bash
     rungms AGv1-0-35_H2O_B3LYP_CCD_opt.inp &> AGv1-0-35_H2O_B3LYP_CCD_opt.log
```

```
[3]: %%bash
     cp ~/.gamess/AGv1-0-35_H2O_B3LYP_CCD_opt.dat .
```

3 Create the Hessian input and run

```
[4]: ag.opt2hes('AGv1-0-35_H2O_B3LYP_CCD_opt.inp','AGv1-0-35_H2O_B3LYP_CCD_opt.log')
```

```
[5]: %%bash
     rungms AGv1-0-35_H2O_B3LYP_CCD_hes.inp &> AGv1-0-35_H2O_B3LYP_CCD_hes.log
```

```
[6]: %%bash
     cp ~/.gamess/AGv1-0-35_H2O_B3LYP_CCD_hes.dat .
```

4 Create the Raman input and run

```
[7]: ag.hes2raman('AGv1-0-35_H2O_B3LYP_CCD_hes.inp','AGv1-0-35_H2O_B3LYP_CCD_hes.
     ↪dat')
```

```
[8]: %%bash
     rungms AGv1-0-35_H2O_B3LYP_CCD_raman.inp &> AGv1-0-35_H2O_B3LYP_CCD_raman.log
```

```
[9]: %%bash
     cp ~/.gamess/AGv1-0-35_H2O_B3LYP_CCD_raman.dat .
```

5 Create the project directory framework

```
[10]: title   = 'Water/'
     ag.new_project(maindir, csvfile, title=title)
     projdir = maindir + title
     logsdir = './'
```

6 Sort the log files into their respective directories

```
[11]: ag.sort_logs(projdir, logsdir)
```

7 Fill the spreadsheets with the parsed data

```
[12]: ag.fill_spreadsheets(projdir)
```

```
[13]: data = ag.get_data("Water/Logs/Pass/Optimization/H2O/
     ↪AGv1-0-35_H2O_B3LYP_CCD_opt.log")
```

```
[14]: data.bond_angles
```

```
[14]: {'H-O-2H Bond Angle': '1.7928203036195753',
      '2H-O-H Bond Angle': '1.7928203036195753',
      'O-H-2H Bond Angle': '0.674386174985109',
      '2H-H-O Bond Angle': '0.674386174985109',
      'O-2H-H Bond Angle': '0.674386174985109',
      'H-2H-O Bond Angle': '0.674386174985109'}
```

```
[15]: data.bond_lengths
```

```
[15]: {'O-H Bond Length': '0.9689095459293237',
      'O-2H Bond Length': '0.9689095459293237',
      'H-O Bond Length': '0.9689095459293237',
      'H-2H Bond Length': '1.513611854',
      '2H-O Bond Length': '0.9689095459293237',
      '2H-H Bond Length': '1.513611854'}
```

```
[16]: data = ag.get_data("Water/Logs/Pass/Hessian/H2O/AGv1-0-35_H2O_B3LYP_CCD_hes.
     ↪log")
```

```
[17]: data.vib_freq
```

```
[17]: {'A1': ['1658.02', '3748.43'], 'B2': ['3849.93']}
```

```
[18]: data.ir_inten
```

[18]: `{'A1': ['1.31682', '0.06709'], 'B2': ['0.46628']}`

[19]:
```
data = ag.get_data("Water/Logs/Pass/Raman/H2O/AGv1-0-35_H2O_B3LYP_CCD_raman.
 ↪log")
```

[20]:
```
data.raman
```

[20]: `{'A1': ['6.104', '75.736'], 'B2': ['33.331']}`