MOMA Mass Calibration

This page details how mass calibration is accomplished for MOMA's mass spectrometer. The mass calibration config file is currently being used by MOMA Data View, our python tools, and XINA Online.

Mass Cal Config File Format

All Versions

Conventions

- Any line that starts with '#' should be treated as a comment and ignored

Fields

- **version** - The version that this config file's format adheres to

Version 1

Fields

- **control_mode** - Defines the control mode that the data was calibrated with. The mapping is as follows:

```
0 = BIN
1 = RF_MON
2 = RF_DAC
```

- **entries** - Each entry defines a mass calibration. Entries are unique by their phase_cycle. A scan's phase cycle should be used to determine which mass calibration is applied.
- **constants** - The constants/coefficients for the mass transform polynomial. index 0 is the constant and so forth. Example:

`[1.0, 2.0, 3.0] --> m/z = 3x^2 + 2x + 1`

- **order** - The polynomials order
- **data_points** - The data points that were used to generate the curve fit. The control value is manually selected and mapped to a mass to achieve the necessary mass calibration.
- **rms** - The root mean square of the curve fit to the data_points
- **phase_cycle** - The phase cycle for this calibration entry. You should use a scan's phase cycle to determine which calibration is applied.

Example

```
{
  "control_mode":2,
  "entries":[
    {
      "constants":[
        0.0,
        1.0,
        0.0
      ],
      "data_points":[
      ],
      "order":0,
      "phase_cycle":-1,
      "rms":0.0
    },
    {
      "constants":[
        3.04691,
        0.568583,
        0.0
      ],
      "data_points":[
        {
          "amu":132.905,
          "control":228.389
        },
        {
          "amu":392.715,
          "control":685.332
        }
      ],
      "order":1,
      "phase_cycle":3,
      "rms":1.0
    },
    {
      "constants":[
        6.34889,
        0.992971,
        0.0
```

```
      ],
      "data_points":[
        {
          "amu":132.905,
          "control":127.214
        },
        {
          "amu":392.715,
          "control":389.253
        },
        {
          "amu":652.525,
          "control":651.162
        },
        {
          "amu":912.335,
          "control":912.074
        }
      ],
      "order":1,
      "phase_cycle":6,
      "rms":0.999999
    }
  ],
  "version":2
}
```


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