

1 Introduction

Mtzdump is a CCP4 “jiffy” program for extracting MTZ header information into a human readable form. This class is designed to provide this functionality at the Python interface level.

2 Use Cases

2.1 Simple: Display the Contents

This will need to be able to:

- Display the contents of an MTZ file.
- Raise appropriate errors if the input file is not MTZ.
- Ascertain the “kind” of mtz file.

Mtzdump has output like:

```
* Title:
.

* Base dataset:
      0 HKL_base
      HKL_base
      HKL_base

* Number of Datasets = 1

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:
      1 Unspecified
      12287_1_E1
      Unspecified
      51.6515   51.6515  157.6742   90.0000   90.0000   90.0000
      0.97966

* Number of Columns = 18

* Number of Reflections = 6199

* Missing value set to NaN in input mtz file

* Number of Batches = 10

* HISTORY for current MTZ file :
From MOSFLM run on  5/ 6/06

* Column Labels :
H K L M/ISYM BATCH I SIGI IPR SIGIPR FRACTIONCALC XDET YDET ROT WIDTH LP MPART FLAG BGPKRATIOS

* Column Types :
H H H Y B J Q J Q R R R R R R I I R

* Associated datasets :
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)
51.6515  51.6515  157.6742   90.0000   90.0000   90.0000

* Resolution Range :
```

```

0.00036  0.11111  (  52.559 -  3.000 A )
* Sort Order :
      0  0  0  0  0
* Space group = 'P43212' (number  96)

Batch number:
  1
Batch number:
  2
.... etc ....

```

then a small amount of “overall” information from the whole of the reflection file. This is run as “mtzdump hklin foo.mtz”.

3 API

3.1 Output Dictionary

The output dictionary will contain:

- column_labels - the column labels.
- column_types - the (single character) column types.
- spacegroup - the spacegroup.
- datasets - a list of pname/xname/dname tokens.
- dataset_info - a dictionary of unit cell and wavelengths associated with different datasets.

So far the output dictionary looks like:

```

{'dataset_info': {'Unspecified/12287_1_E1/Unspecified':
{'cell': [51.651499999999999, 51.651499999999999, 157.67420000000001,
90.0, 90.0, 90.0],
'wavelength': 0.97965999999999998}},
'column_labels': ['H', 'K', 'L', 'M/ISYM', 'BATCH', 'I', 'SIGI', 'IPR',
'SIGIPR', 'FRACTIONCALC', 'XDET', 'YDET', 'ROT', 'WIDTH',
'LP', 'MPART', 'FLAG', 'BGPKRATIOS'],
'datasets': ['Unspecified/12287_1_E1/Unspecified'],
'column_types': ['H', 'H', 'H', 'Y', 'B', 'J', 'Q', 'J',
'Q', 'R', 'R', 'R', 'R', 'R', 'R', 'I', 'I', 'R'],
'spacegroup': 'P43212'}

```