OpenMOL Converter

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1 Introduction

OpenMOL is a python package that attempts to convert between popular molecular dynamics data file formats.

2 Features

- Convert AMBER PARM7 and Restart files into LAMMPS data file.
- Read and write MOL2 file.
- Save data files into portable *openmol* json format without losing any properties.
- Extensible.

3 Usage: Amber to LAMMPS

```
import sys
# add openmol to PYTHONPATH
sys.path.append("/path/to/openmol")

import openmol
import amber_parm7 as parm
import lammps_full as lammps

# read amber parm files
p = parm.read('oleylamine.prmtop', 'oleylamine.rst7')

# calculate necessary lammps items and write
p = lammps.build(p)
lmp = lammps.Writer(p, 'data.oleylamine')
lmp.write()

# save everything as openmol json file
openmol.write_json(p, 'oleylamine.json')
```

4 Current Implementations

Parser	Reader	Writer
Amber	Yes	x
LAMMPS	x	Yes
MOL2	Yes	Yes