cclib

parsers and algorithms for computational chemistry

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Aims

- To provide a single interface to the results of all computational chemistry packages by parsing and normalising their output
- To allow computational chemists to implement algorithms without worrying about parsing multiple output files and new versions of packages
- To implement some common algorithms that are currently available only to users of particular packages
- To be interoperable with other Open Source chemistry libraries

cclib 0.5

- Parses the output of ADF, GAMESS (US), Gaussian and PC GAMESS
- Contains implementations of several molecular orbital-based population analysis methods: Mulliken, C^2, Mayer's bond orders
- Contains interfaces to Open Babel, PyQuante and Biopython
- Used by GaussSum and PyMOlyze to parse files

```
>>> from cclib.parser import guesstype
>>> t = guesstype("mylogfile.out")
>>> t.parse()
....
>>> print t.nbasis
60  # the number of basis functions
```

```
>>> from cclib.method import Mulliken
>>> m = Mulliken(t)
>>> m.calculate()
>>> print m.aoresults[0,45,0]
# prints the contribution of the 1st
# atomic orbital to the 46th M.O.
```

Technical Details

- Is a Python package that follows best practices (pylint, Cheesecake index)
- Uses Open Source (LGPL) development with Subversion, mailing lists and wiki
- Has unit tests for regression, functionality and agreement between parsers
- Uses the Numeric extension to Python for efficient matrix algebra

In Development

- Parsers for Jaguar and GAMESS-UK
- Methods to calculate the value of the electron density and a molecular orbital wavefunction at points in a volume
- Population analysis methods based on the electron density (e.g. Hirshfeld)
- Charge decomposition analysis (Frenking)

Project website

http://cclib.sf.net

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