ap-rdf

requirements

Originally, it was planned to provide as input **cif** structures. However, cif format is complicated and for that the `obabel` package should be used instead to transforn the cif file to a **pdb** file.

```
obabel LiFePO4.cif --fillUC -OLiFePO4.pdb
```

or

```
obabel -icif LiFePO4.cif --fillUC -opdb -OLiFePO4.pdb
```

ap-rdf usage

```
./ap-rdf.x -i filename.pdb
```

On the output the code provides the distribution of electronegativity, polarizability and vdw volume. See the JPCC paper below for details.

The following optional/required arguments can be provided:

-i string [required] filename of the pdb input file

-rmax float [optional] default: 20

-rmin float [optional] default: 2.d0

-repcell char: F/T [optional] default T. if T (true) then it replicates the unit cell so each one of its linear dimensions is larger that 2*rmax

-bfac float [optional] default: 1. It is the **B** exponent in the exponential.

-ngrid integer [optional] default: 100.

-of filename [optional] default: out_grid.dat

Example :

Convert first the cif file to pdb. Use:

```
obabel MIL-47.cif --fillUC -OMIL-47.pdb
```

After run the code and save the results in the mil-47.aprdf.

```
./ap-rdf.x -i MIL-47.pdb -bfac 1.0 -rmin 3.0 -rmax 50.0 -ngrid 50 -of mil-47.aprdf
```

to be clarified

- I am not sure that the code works correctly. I **can not** reproduce exactly the results for the *IRMOF-1* and *MIL-47* which can be found in dx.doi.org/10.1021/jp404287t | J. Phys. Chem. C 2013, 117, 14095−14105.
- I dont know if **repcell** should be True or False. In my opinion should be True, but I see that the results are closer to the published ones, if repcell is False.