PREADER

John Kendrick
School of Chemistry, University of Leeds, Leeds, LS2 9JT United Kingdom.
j.kendrick@leeds.ac.uk

Andrew Burnett
School of Chemistry, University of Leeds, Leeds, LS2 9JT United Kingdom
a.d.burnett@leeds.ac.uk

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1. INTRODUCTION

preader is a 'helper' program which uses the underlying modules of PDielec to read output files and summarise the results of various MM/QM packages. The program can be used to perform some straightforward calculations. For instance projection of any remaining centre of mass motion of the crystal can be performed to make sure that there are three zero frequencies. Also the masses used in the calculation of the dynamical matrix can be altered.

2. MM/QM PACKAGES

The MM / QM packages supported are summarised below. Unlike PDielec it is not necessary to have performed a full calculation of the dynamical matrix. In the majority of cases preader will read geometry optimisation runs.

VASP (-program vasp OUTCAR)
The name provided on the command line is an OUTCAR file. The OUTCAR is read by preader to determine the unit cell, atomic masses, frequencies, normal modes, Born charge tensors and optical permittivity.

CASTEP (-program castep seedname)

The name provided on the command line is the seedname for the calculation. The corresponding seedname.castep file in the current directory is read and processed to determine the unit cell, atomic masses, optical permittivity and born charge tensors. The normal modes and their frequencies are determined from the seedname.phonon file.

- CRYSTAL (-program crystal outputfilename) The name on the command line is a file ending in .out, containing the output of a CRYSTAL14 run. The contents of this file alone are sufficient to provide the unit cell, atomic masses, frequencies, normal modes and Born charge tensors. However, the number of significant figures for the normal modes is not sufficient for an accurate calculation and it is therefore recommended that the HESSFREQ.DAT and BORN.DAT files are also made available. If they are present in the directory where preader is run from , it uses these files to calculate the Born charge tensors, frequencies and normal modes. By default CRYSTAL projects out the pure translational modes of the system before calculating the frequencies, this can also done by the preader package. Small differences in the calculated frequencies between the CRYSTAL program and preader have been observed. These have been found to be due to a slightly different method for symmetrising the 2^{nd} derivative matrix, because of this an optional directive "-hessian crystal" can be used to indicate that preader should use the same symmetrisation as CRYSTAL14.

- **ABINIT (-program abinit outputfilename)**

  The output file should come from a run containing three datasets. One to calculate the wavefunction at the optimized geometry, one to calculate the field perturbations and one to calculate the second derivatives. Examples of input files and output files are available with the distribution.

- **QE (-program qe outputfilename)**

  The output file is the dynamical matrix file, specified by "filedyn" in a run of the quantum espresso phonon package. Examples of input and output files are given in the preader distribution

*GULP (-program gulp outputfilename) : The name on the command line is a file ending in .gout, containing the output of a GULP run. The contents of this file alone are sufficient to provide the unit cell, atomic masses, frequencies, normal modes, Born charge tensors and optical permittivity. Because GULP only writes out the Born charge matrices for the asymmetric unit, it is necessary to run a frequency calculation using P1 symmetry and a complete unit cell. The key words; nosymm, phonon, intensity, eigen and cart are recommended for the

GULP calculation. In the case that no shells are used in the calculation the optical permittivity is not available in the output and it is necessary to provide it on the command line (see -optical and -optical_tensor options below).

3. COMMAND OPTIONS

Examples of data sets for these packages are included with the distribution and can be found in the Examples/'Package'/preader directory. The program is run from the command line. There are several command options and these are summarized below. Those options which may be repeated are indicated by a .

-program program
Program can be "abinit", "castep", "crystal", "gulp", "qe", "experiment" or "vasp" and specifies the program which generated the results to be analysed

-neutral
Impose neutrality on the Born charge matrices

-nocalculation
No calculations are performed. This results in a single line of output with just information from the program. If -eckart, -mass, -masses, -neutral or -crystal have -hessian crystal have been specified they will be ignored

-eckart
Translational modes are projected out of the hessian before diagonalisation

-hessian symm
The hessian can be symmetrised in one of two ways; either "crystal" or "symm". In the case of "crystal" the hessian is symmetrised using the same algorithm as Crystal14.

-masses average
The element mass_definition can be either "program", "average" or "isotopic", meaning that the masses used in the calculation of the frequencies are either taken from the QM program or are the average of the isotope abundances or are the most abundant isotope mass.

-mass element mass
The atomic mass of the element is set to mass. This can be used to explore the effect of isotope substitution on the calculated frequencies

4. EXAMPLES

```
preader -program vasp 'find . -name OUTCAR' > results.csv
```

This reads all the VASP OUTCAR files in the current and any of its subdirectories and summarises the results to results.csv.

```
preader -program castep -eckart 'find . -name \*.castep' > results.csv
```

This reads all the castep output files in the current and any of its subdirectories and summarises the results to results.csv. For each file the centre of mass motion

of the crystal is projected. The results file contains both the unprojected and the projected results.

There are examples of preader being used in the Examples/'Package'/preader subdirectories of the distribution of PDielec.