User Manual

Contents

License

1. Introduction

This user manual contains information pertaining to the use of the *MAGELLAN* program. It does not, however, contain an explanation of the theory behind the code – this information can be found in the following publication:

N. F. Chilton, D. Collison, E. J. L. McInnes, R. E. P. Winpenny and A. Soncini, *Nat. Commun.*, 2013, 4:2551, doi: 10.1038/ncomms3551

The construction of the input files and operation of the code is not onerous; the only difficult task is determining the partial charges associated with the ligands in a compound. In many cases this is very easy, however in cases with highly conjugated or delocalized ligands, the nature of the partial charges may be more elusive.

2. User Guide

2.1 Input files and syntax

Input files are simple text files, very similar to common Cartesian xyz files. In general, the input can be prepared in any text editor and can have any extension, however Windows users should use 'WordPad' and ***not*** 'Notepad' to prepare their input files. For Macintosh users, DOS or UNIX formatting should be used and files can be converted using the free utility flip, found here: https://ccrma.stanford.edu/~craig/utility/flip/

The first line must begin with an exclamation mark '!', indicating the command line. The possible command keywords are given in Table 1.1. The most important command is the 'sites' command, which specifies the number and location of the dysprosium(III) sites to be evaluated. There is no limit to the number of dysprosium(III) sites.

Table 2.1.1 – Command keywords

Command keyword	Effect	Comments
sites *n a b c d* …	Selection of the Dy^{III} sites to evaluate	*n* is the number of sites followed by their locations in the input coordinates *a, b, c, d* … etc. Default = sites 1 1
spherical	Produce a spherical plot in Cartesian space	Default = Off
zcwN	Change the plot gridding type to ZCW	N specifies the ZCW level and must be >= 0. Default = On, N = 10
stepN	Change the plot gridding type to STEP	N specifies the number of steps. Default = Off, N = 60
vec *x y z*	Specify a vector direction for the anisotropy axis as opposed to an optimization	*x*, *y*, and *z* are the Cartesian coordinates of the vector, in the reference frame of the input coordinates. Default = Off
expert	Ignore checking selected sites for 'Dy' label and charge of 3	Default = Off

Following the command line, all subsequent lines contain the input coordinates and partial charges. These must be in the following notation: 'Label x y z charge'. There is no limit to the number of atoms in this file and charges may take any value.

An example input file is given on the following page, where there are five dysprosium(III) sites to be evaluated, in the $[Dy_5(O)(^{i}PrO)_{13}]$ structure – see: R. J. Blagg, C. A. Muryn, E. J. L. McInnes, F. Tuna, and R. E. P. Winpenny, *Angew. Chem. Int. Ed.*, 2011, **50**, 6530–6533

```
!sites 5 1 41 42 57 58
Dy1   0     0     0     3
C1    -1.3123     -3.2062     -3.28593    0
C2    -2.62568    0.23775     2.45581     0
C3    -2.15769    0.17084     -5.405      0
C4    0.6955      -3.25848    -1.67224    0
C5    -5.44868    -2.04567    -2.91066    0
C6    1.6897      3.03558     -4.76203    0
C7    3.99727     0.10811     -2.14009    0
C8    3.55732     -0.26828    0.14911     0
C9    -1.04919    6.02369     -0.1336     0
C10   -0.71923    -2.80263    -1.95495    0
C11   -3.22521    -0.17627    1.16986     0
C12   -4.73053    4.16893     -2.13008    0
C13   -4.66367    2.70938     -2.33773    0
C14   -3.40853    -1.63164    1.05478     0
C15   0.60924     2.8662      2.09304     0
C16   -3.58752    0.46359     -5.57012    0
C17   -1.377      0.77725     -6.4883     0
C18   -5.61689    1.92732     -1.53464    0
C19   3.12816     -0.37283    -1.2094     0
C20   -5.45731    3.97655     1.86788     0
C21   -0.74727    5.58666     -1.43206    0
C22   -5.27615    -2.84027    -4.11154    0
C23   -1.11389    6.35408     -2.5604     0
C24   -5.92313    -2.77754    -1.75981    0
C25   -4.09001    4.29021     2.04301     0
C26   1.7544      3.34924     1.29245     0
C27   -3.57243    4.29021     3.36899     0
C28   -1.97654    5.54484     -6.71347    0
C29   -4.19785    4.45749     -6.2131     0
C30   1.10742     1.8855      3.04375     0
C31   -2.81761    4.68751     -5.96291    0
C32   0.82706     -2.27569    2.36825     0
C33   1.21525     -1.7111     3.66921     0
C34   0.15851     -3.57214    2.39327     0
C35   2.12102     4.10202     -4.21162    0
C36   2.05632     2.80556     -5.96291    0
C37   2.05632     -1.83657    -5.51258    0
C38   1.45247     -2.48479    -6.38823    0
C39   3.19933     -1.54382    -5.96291    0
Dy2   -2.70655    -0.06858    -2.1586     3
Dy3   0.55619     0.16436     -3.29119    3
O1    -0.85726    1.36065     -1.76481    -2
O2    1.78243     0.07884     -1.39704    -1
O3    -3.30717    2.1657      -2.11757    -1
O4    -1.19369    4.21284     -1.67224    -1
O5    -1.73068    0.51586     -4.16909    -1
O6    -2.42296    0.2733      0.10157     -1
O7    -0.77531    -1.33262    -1.8849     -1
O8    -0.15204    2.07788     0.9572      -1
O9    0.66531     2.29117     -4.0565     -1
O10   -4.3294     -1.24271    -2.58041    -1
O11   0.39358     -1.4079     1.42005     -1
O12   1.48051     -1.04824    -4.65945    -1
O13   -3.26835    3.60016     1.0898      -1
O14   -2.20082    3.97655     -5.0022     -1
Dy4   -1.98387    2.68637     -0.17939    3
Dy5   -1.39619    2.85512     -3.46882    3
```

2.2 Program execution

The program can be run on Linux, Windows or MaxOS and is executed *via* the command line as: 'magellan <input-file>', where '<input-file>' is the name of the input file. Alternatively, the program can be run in a 'drag-and-drop' style, by dropping the input file onto the executable.

Linux and MacOS users may have to run 'chmod +x magellan' and/or 'chown *user* magellan' before running the program, if permission errors are obtained.

2.3 Output files and interpretation

MAGELLAN produces three types of output files. The first output file, named '<input-file>_magellan.out' contains the electrostatic energies, curvatures of the potential surface and minimal reorientation energies. The second output file, named '<input-file>_magellan.xyz' is a standard Cartesian xyz file, containing the input coordinates as well as the orientations of the ground state magnetic anisotropy for each Dy^{III} ion, expressed as two 'Be' atoms at 5 Å radius. The remaining output files, named '<input-file>_*a*_magellan.plot' where *a* is the index of the site from the input file, contain the 3D electrostatic potential surface data for the site in question.

Unless the command keyword 'vec *x y z*' is used, the output contained in '<input-file>_magellan.out' and '<input-file>_magellan.xyz' pertain to the electrostatically optimized orientation for each site. If the command keyword 'vec *x y z*' is used, then the output corresponds to the chosen orientation.

3. Bugs and Feedback

The authors are keen to hear from users who have bug reports, feature requests, comments, suggestions or queries about the code. Please address correspondence to nfchilton@gmail.com and asoncini@unimelb.edu.au.