Moltemplate DREIDING Label Manual

Matthew Bone

Bristol Composites Institute, University of Bristol, UK

September 2020

1   Introduction

The replica of the DREIDING forcefield within Moltemplate is controlled by the user with a modular labelling system. It is inspired by the labelling system from the original DREIDING paper (Mayo *et al.*, J. Phys. Chem., 1990), but incorporates some additional "flags" to differentiate cases where properties cannot be inferred. This manual explains the logic behind these flags, lists all possible labels, and provides example molecules where these labels would be used. This implementation of DREIDING aims to be a full replica of the original DREIDING paper and all atoms included in that work are available here.

Labels are assigned as the atom type in the "Data Atoms" region of a Moltemplate input file, following the "@atom:" argument. The forcefield is added in the same manner as other force fields in Moltemplate with the following code:

```
import "dreiding.lt"

molecule inherits DREIDING {
    body
}
```

Where *molecule* is the name of the molecule in the file and *body* is the sections that make up the molecule.

2   Labels

The start of an atom label is adapted from the original DREIDING paper and uses almost the same logic. First, the elemental symbol is given followed by an underscore; this is the case for one and two letter elements e.g. C_ or Si_. The next character represents the hybridisation or geometry of the atom: 3 is sp^3, 2 is sp^2, 1 is sp^1 and R is an sp^2 atom involved in the resonance structure of an aromatic ring e.g. C_2 or Ga_3. There are some exceptions for hydrogen which uses H_HB to represent a hydrogen bonding hydrogen, and H_B for the bridging hydrogen of diborane. Carbon also includes united atom terms e.g. C_31 for carbon with one implicit hydrogen; all possible terms can be seen at the end of this manual. The rest of the original DREIDING labelling system is not used. Use of these labels are all that is required in the most simple cases of using this forcefield. The following sections detail how to add flags to label more complex atoms that exist in environments that cannot be inferred with simple labels. Note: all flags are preceded by an underscore.

2.1   Bonding - _b1 and _b2 flags

The DREIDING forcefield relies on bond order to calculate bond energies. In the cases of X_2-X_2, X_R-X_R and X_1-X_1, bond orders are assumed to be 2, 1.5 and 3 respectively. However, many atoms with these labels are found in bonding pairs joined by a single bond with a bond order of 1. To allow for this the "_b1" flag is attached directly after the initial label. The simplest example molecule of this system is 1,3-butadiene, labelled in Figure 1a. If both C_2 atoms are labelled with the _b1 flag the bond between them has a bond order of 1. The bond between C_2-C_2_b1 are correctly set as bond order 2. The inverse of the _b1 flag is the "_b2" flag, an example of which can be seen in cyclopentadienone (Figure 1b). When two bonded atoms have the _b2 flag the bond is set as bond order 2. All other bonding pairs to a _b2 labelled atom are bonded with single bonds. This is commonly used in cyclic systems of sp^2 atoms that are not aromatic.

Remember all _bX flags must be used in pairs. When multiple flags are used, the _bX flag is always first.
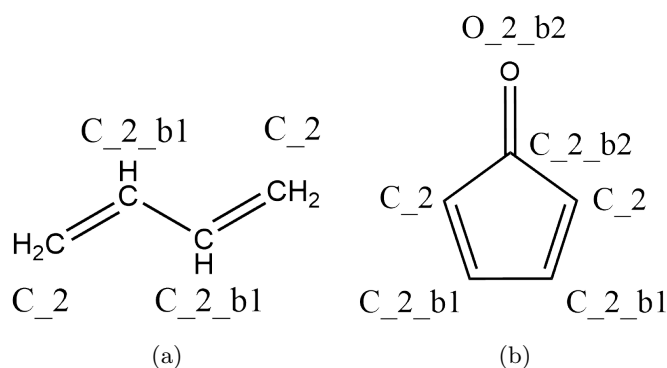
Figure 1: (a) 1,3-Butadiene, (b) Cyclopentadienone. Hydrogen atoms have been omitted.

2.2 Dihedrals - _d1 and _d2 flags

When calculating dihedral angles of an IJKL atom structure, the DREIDING forcefield uses the number of possible I and L atoms to determine the torsion energy. In most instances this can be inferred from the initial label. N_2 and N_R make use of the flags "_d1" and "_d2" as it is not obvious from the label how many I or L atoms are bonded to N_2 or N_R. The flag highlights how many I/L atoms are bonded to the nitrogen atom: this is limited to 1 or 2. Imidazole, amides, and imines (which can be seen in Figure 2) are clear examples of this flag in use. The "_ha" and "_hd" flags are explained in the next section. The _dX flag follows _bX flag if it has been used, and is always before the _hX flag if that is included. Other atoms besides nitrogen can have a _dX flag ranging from _d1 to _d5. These can be seen in Section 3 of this manual. It is believed that these labels cover the possible range of different _dX flags required. Please contact the author if you believe a _dX flag is missing for these atoms.
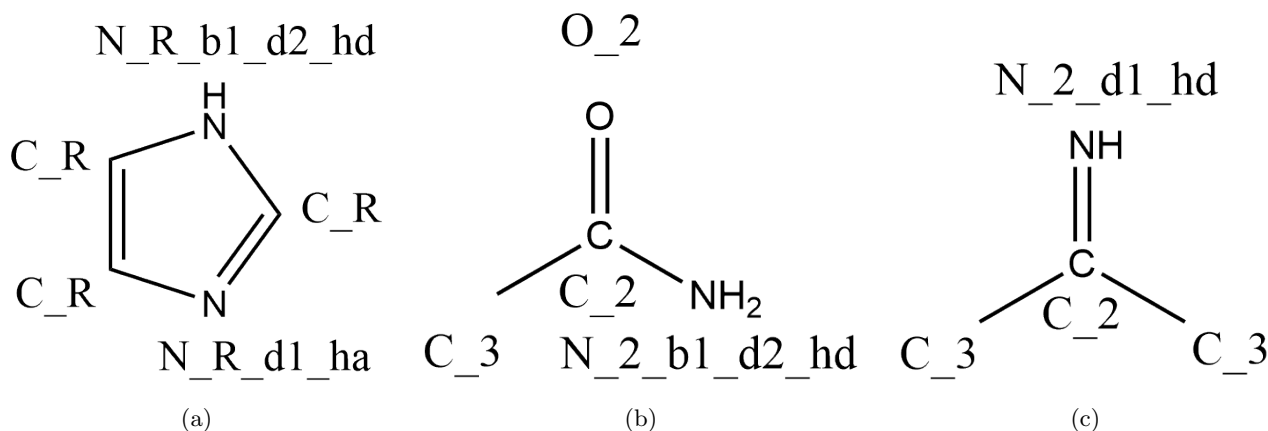

Figure 2: (a) Imidazole, (b) Amide, (c) Imine. Hydrogen atoms have been omitted.

2.3 Hydrogen Bonds - _hd and _ha flags

DREIDING uses a different LAMMPS pair_style to handle hydrogen bonding pairwise interactions. To signal to Moltemplate that this is needed, the flags "_hd" and "_ha" are added to the end of the existing label, see Figure 2a for an example. The _hd flag marks the atom as a hydrogen bond donor; the _ha flag is for hydrogen bond acceptors. The _ha flag is not essential in all systems: if a system has no hydrogen bond donors present then valid acceptor atoms do not need _ha flags. The _hX flag is always the last flag in labels that include multiple flags.

3 Possible Labels

This section contains all possible labels available in the Moltemplate replica of DREIDING. It is believed that these labels cover the full range of different possible atom environments. Please contact the author if you believe a label is missing.

- H
- H_HB
- C_3
- C_34
- C_33
- C_32
- C_31
- C_R
- C_R1
- C_R_b1
- C_R1_b1
- C_2
- C_2_b1
- C_2_b2
- C_1
- C_1_b1
- N_3
- N_3_ha
- N_3_hd
- N_R_d1
- N_R_d1_ha
- N_R_d2
- N_R_d2_ha
- N_R_d2_hd
- N_R_b1_d2
- N_R_b1_d2_ha
- N_R_b1_d2_hd
- N_2_d1
- N_2_d1_ha
- N_2_d1_hd
- N_2_b1_d1
- N_2_b1_d1_ha
- N_2_b2_d1
- N_2_b2_d1_ha
- N_2_d2
- N_2_d2_hd

- N_2_d2_ha
- N_2_b1_d2
- N_2_b1_d2_hd
- N_2_b1_d2_ha
- N_2_b2_d2
- N_2_b2_d2_hd
- N_2_b2_d2_ha
- N_1
- N_1_ha
- O_3
- O_3_hd
- O_3_ha
- O_R
- O_R_ha
- O_2
- O_2_ha
- O_2_b1
- O_2_b1_ha
- O_2_b1_hd
- O_2_b2
- O_2_b2_ha
- O_1
- O_1_ha
- H_B
- B_3
- B_2_d1
- B_2_d2
- B_2_b1_d1
- B_2_b1_d2
- B_2_b2_d1
- B_2_b2_d2
- F
- F_hd
- F_ha
- Cl
- Br

- I
- Al_3_d1
- Al_3_d2
- Si_3
- P_3_d2
- P_3_d3
- P_3_d4
- S_3
- Ga_3
- Ge_3_d1
- Ge_3_d2
- Ge_3_d3
- As_3_d1
- As_3_d2
- As_3_d3
- As_3_d4
- Se_3_d1
- Se_3_d2
- Se_3_d3
- Se_3_d5
- In_3_d1
- In_3_d2
- Sn_3_d2
- Sn_3_d3
- Sb_3_d2
- Sb_3_d3
- Sb_3_d4
- Te_3_d1
- Te_3_d2
- Te_3_d3
- Te_3_d5
- Na
- Ca
- Fe
- Zn