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Determination of Forces from a Potential in Molecular Dynamics (note)

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Abstract

In Molecular Dynamics (MD), the forces applied to atoms derive from potentials which describe the energy of bonds, valence angles, torsion angles, and Lennard-Jones interactions of which molecules are made. These definitions are classic; on the contrary, their implementation in a MD system which respects the local equilibrium of mechanical conditions is usually not described. The precise derivation of the forces from the potential and the proof that their application preserves energy is the object of this note. This work is part of the building of a multi-scale MD system, presently under development.

Keywords. Molecular Dynamics ; Force-Fields ; Potentials ; Forces.

1 Introduction

Numerical simulation at atomic scale predicts system states and properties from a limited number of physical principles, using a numerical resolution method implemented with computers. In Molecular Dynamics (MD) [2] systems are organic molecules, metallic atoms, or ions. We concentrate on organic molecules, but our approach could as well apply to other kinds of systems. The goal is to determine the temporal evolution of the geometry and energy of atoms.

At the basis of MD is the classical (newtonian) physics, with the fundamental equation:

$$\vec{F} = m \vec{a} \quad (1)$$

where \vec{F} is the force applied to a particle of mass m and \vec{a} is its acceleration (second derivative of the variation of the position, according to time).

A *force-field* is composed of several components, called *potentials* (of bonds, valence angles, dihedral angles, van der Waals contributions, electrostatic contributions, *etc.*) and is defined by the analytical form of each of these components, and by the parameters characterizing them. The basic components used to model molecules are the following:

- atoms, with 6 degrees of freedom (position and velocity);
- bonds, which link two atoms belonging to the same molecule; a bond between two atoms a, b tends to maintain constant the distance ab .
- valence angles, which are the angle formed by two adjacent bonds ba et bc in a same molecule; a valence angle tends to maintain constant the angle \widehat{abc} . A valence angle is thus concerned by the positions of three atoms.
- torsion angles (also called *dihedral angles*) are defined by four atoms a, b, c, d consecutively linked in the same molecule: a is linked to b , b to c , and c to d ; a torsion angle tends to privilege particular angles between the planes abc and bcd . These particular angles are the equilibrium positions of the torsion potential (minimal energies). In most cases, they are *Trans* (angle of 180°), *Gauche* (60°) or *Gauche'* (-60°).
- van der Waals interactions apply between two atoms which either belong to two different molecules, or are not linked by a chain of less than three (or sometimes, four) bonds, if they belong to the same molecule. They are pair potentials.

All these potentials depend on the nature of the concerned atoms and are parametrized differently in specific force-fields. Molecular models can also consider electrostatic interactions (Coulomb's law) which are pair potentials, as van der Waals potentials are; their implementation is close to van der Waals potentials, with a different dependence to distance.

Intra-molecular forces (bonds, valence angles, torsion angles) as well as inter-molecular forces (van der Waals) are conservative: the work between two points does not depend on the path followed by the force between these two points. Thus, forces can be defined as derivatives of scalar fields. From now on, we consider that potentials are scalar fields and we have:

$$\vec{F}(\mathbf{r}) = -\vec{\nabla}\mathcal{U}(\mathbf{r}) \quad (2)$$

where \mathbf{r} denotes the coordinates of the point on which the force $\vec{F}(\mathbf{r})$ applies, and \mathcal{U} is the potential from which the force derives.

The work presented here is part of a MD system presently under development[1]; the defined forces and their implementations have been tested with it.

Structure of the text

Bonds are considered in Section 2, valence angles in Section 3, torsion angles in Section 4, and finally Lennard-Jones potentials in Section 5. Section 6 summarises the force definitions, and Section 7 concludes the text. A summary of the notations used in the paper is given in the Annex.

2 Bonds

A bond models a sharing of electrons between two atoms which produces a force between them. This force is the derivative of the bond potential defined between the two atoms. Fig. 2.1 shows a (attractive) force produced between two linked atoms a and b .

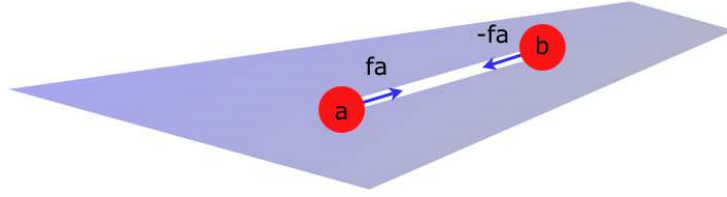


Figure 2.1: Attractive bond between two linked atoms

A *harmonic bond potential* is a scalar field \mathcal{U} which defines the potential energy of two atoms placed at distance r as:

$$\mathcal{U}(r) = k(r - r_0)^2 \quad (3)$$

where k is the strength of the bond and r_0 is the equilibrium distance (the distance at which the force between the two atoms is null). We thus have:

$$\frac{\partial \mathcal{U}(r)}{\partial r} = 2k(r - r_0) \quad (4)$$

The partial derivative of \mathcal{U} according to the position r_a of a is:

$$\frac{\partial \mathcal{U}(r)}{\partial r_a} = \frac{\partial \mathcal{U}(r)}{\partial r} \cdot \frac{\partial r}{\partial r_a}. \quad (5)$$

But:

$$\frac{\partial r}{\partial r_a} = 1 \quad (6)$$

We thus have:

$$\frac{\partial \mathcal{U}(r)}{\partial r_a} = 2k(r - r_0) \quad (7)$$

Let a and b be two atoms, and $\vec{u} = \text{norm}(\vec{ba})$ be the normalization of vector \vec{ba} . The force produced on atom a is:

$$\vec{f}_a = -\frac{\partial \mathcal{U}(r)}{\partial r_a} \cdot \vec{u} = -2k(r - r_0) \cdot \vec{u} \quad (8)$$

and the one on b is the opposite, according to the action/reaction principle:

$$\vec{f}_b = -\vec{f}_a \quad (9)$$

Therefore, if $r > r_0$, the force on a is a vector whose direction is opposite to \vec{u} and tends to bring a and b closer (attractive force), while it tends to bring them apart (repulsive force) when $r < r_0$.

According to the definition of \vec{f}_a and \vec{f}_b , the sum of the forces applied to a and b is null (i.e. equilibrium of forces):

$$\vec{f}_a + \vec{f}_b = 0 \quad (10)$$

Note that no torque is produced as the two forces are colinear.

3 Valence Angles

Valence angles tend to maintain at a fixed value the angle between three atoms a , b and c such that a is linked to b and b to c , as shown on Fig. 3.1.

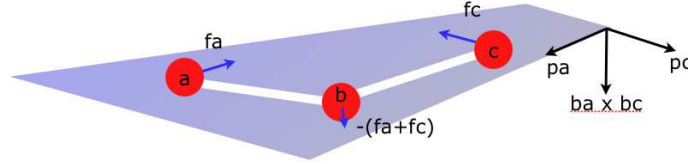


Figure 3.1: Valence angle

The forces applied to the three atoms all belong to the plane abc defined by the points a , b , c .

A *harmonic valence potential* is a scalar field \mathcal{U} which defines the potential energy of an atom configuration forming a valence angle θ by:

$$\mathcal{U}(\theta) = k(\theta - \theta_0)^2 \quad (11)$$

where k is the strength of the valence angle and θ_0 is the equilibrium angle (the one for which energy is null). The partial derivative of \mathcal{U} according to the angle θ is thus:

$$\frac{\partial \mathcal{U}(\theta)}{\partial \theta} = 2k(\theta - \theta_0) \quad (12)$$

The partial derivative of \mathcal{U} according to the position r_a of a is:

$$\frac{\partial \mathcal{U}(\theta)}{\partial r_a} = \frac{\partial \mathcal{U}(\theta)}{\partial \theta} \cdot \frac{\partial \theta}{\partial r_a} \quad (13)$$

that is:

$$\frac{\partial \mathcal{U}(\theta)}{\partial r_a} = 2k(\theta - \theta_0) \cdot \frac{\partial \theta}{\partial r_a} \quad (14)$$

As a describes a circle with radius $|ab|$, centered on b , we have¹:

$$\frac{\partial \theta}{\partial r_a} = \frac{1}{|ab|} \quad (15)$$

Let \vec{p}_a be the normalized vector in the plane abc , orthogonal to \vec{ba} :

$$\vec{p}_a = \text{norm}(\vec{ba} \times (\vec{ba} \times \vec{bc})) \quad (16)$$

The force applied on a is then:

$$\vec{f}_a = -\frac{\partial \mathcal{U}(\theta)}{\partial r_a} \cdot \vec{p}_a = -2k(\theta - \theta_0)/|ab| \cdot \vec{p}_a \quad (17)$$

In the same way, the force applied on c is:

$$\vec{f}_c = -2k(\theta - \theta_0)/|bc| \cdot \vec{p}_c \quad (18)$$

where \vec{p}_c is the normalized vector in plane abc , orthogonal to \vec{cb} :

$$\vec{p}_c = \text{norm}(\vec{cb} \times (\vec{ba} \times \vec{bc})) \quad (19)$$

The sum of the forces should be null:

$$\vec{f}_a + \vec{f}_b + \vec{f}_c = 0 \quad (20)$$

Thus, the force applied to b is:

$$\vec{f}_b = -\vec{f}_a - \vec{f}_c \quad (21)$$

3.1 Torques

Let us now consider torques (moment of forces). The torque exerted by \vec{f}_a on b is $\vec{ba} \times \vec{f}_a$ and the torque exerted by \vec{f}_c on b is $\vec{bc} \times \vec{f}_c$. As \vec{ba} and \vec{f}_a are orthogonal, one has²:

$$|\vec{ba} \times \vec{f}_a| = |\vec{ba}| |\vec{f}_a| = |ba| | -2k(\theta - \theta_0)/|ab| | = |2k(\theta - \theta_0)| \quad (22)$$

¹ The length of an arc of circle is equal to the product of the radius by the angle (in radians) corresponding to the arc of circle.

² If $u \perp v$ then $|u \times v| = |u||v|$.

For the same reasons:

$$|\vec{bc} \times \vec{f}_c| = |2k(\theta - \theta_0)| \quad (23)$$

Thus, the two vectors $\vec{ba} \times \vec{f}_a$ and $\vec{bc} \times \vec{f}_c$ have the same length. As they are by construction in opposite directions, the sum of the two torques on b is null:

$$\vec{ba} \times \vec{f}_a + \vec{bc} \times \vec{f}_c = 0 \quad (24)$$

As a consequence, no rotation around b can result from the application of the two forces \vec{f}_a and \vec{f}_c .

4 Torsion Angles

A torsion angle θ defined by four atoms a, b, c, d is shown on Fig. 4.1. In the OPLS [3] force-field, as in many other force-fields, potentials of torsion angles have a “triple-cosine” form. This means that the potential \mathcal{U} of a torsion angle θ is defined by³:

$$\mathcal{U}(\theta) = 0.5[A_1(1 + \cos(\theta)) + A_2(1 - \cos(2\theta)) + A_3(1 + \cos(3\theta)) + A_4] \quad (25)$$

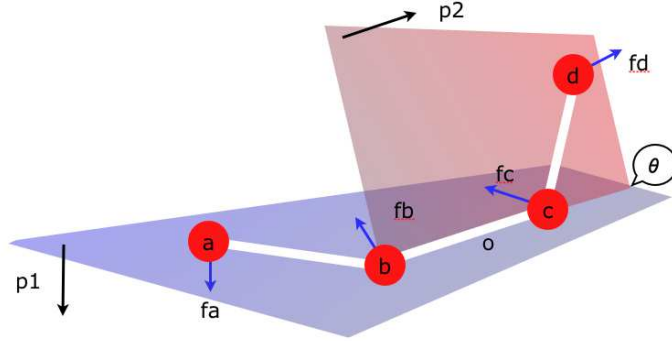


Figure 4.1: Torsion angle θ

The partial derivative of the torsion angle potential according to the position r_a of a is:

$$\frac{\partial \mathcal{U}(\theta)}{\partial r_a} = \frac{\partial \mathcal{U}(\theta)}{\partial \theta} \cdot \frac{\partial \theta}{\partial r_a} \quad (26)$$

The partial derivative of the potential according to the angle θ is:

$$\frac{\partial \mathcal{U}(\theta)}{\partial \theta} = 0.5(-A_1 \sin(\theta) + 2A_2 \sin(2\theta) - 3A_3 \sin(3\theta)) \quad (27)$$

$$= -0.5(A_1 \sin(\theta) - 2A_2 \sin(2\theta) + 3A_3 \sin(3\theta)) \quad (28)$$

³ In the following, we will always omit the last parameter A_4 .

4.1 Forces on a and d

Let us call θ_1 the angle \widehat{abc} . Atom a turns around direction bc , on a circle of radius $|ab|\sin(\theta_1)$. The partial derivative of θ according to the position of a is:

$$\frac{\partial \theta}{\partial r_a} = \frac{1}{|ab|\sin(\theta_1)} \quad (29)$$

We thus have:

$$\frac{\partial \mathcal{U}(\theta)}{\partial r_a} = \frac{-0.5}{|ab|\sin(\theta_1)} (A_1 \sin(\theta) - 2A_2 \sin(2\theta) + 3A_3 \sin(3\theta)) \quad (30)$$

Similarly, for atom d , noting θ_2 the angle \widehat{bcd} :

$$\frac{\partial \mathcal{U}(\theta)}{\partial r_d} = \frac{-0.5}{|cd|\sin(\theta_2)} (A_1 \sin(\theta) - 2A_2 \sin(2\theta) + 3A_3 \sin(3\theta)) \quad (31)$$

Let \vec{p}_1 the normalized vector orthogonal to the plane abc , and \vec{p}_2 the normalized vector orthogonal to the plane bcd (the angle between \vec{p}_1 and \vec{p}_2 is θ):

$$\vec{p}_1 = \text{norm}(\vec{ba} \times \vec{bc}) \quad (32)$$

$$\vec{p}_2 = \text{norm}(\vec{cd} \times \vec{cb}) \quad (33)$$

The force applied on a is:

$$\vec{f}_a = \frac{0.5}{|ab|\sin(\theta_1)} (A_1 \sin(\theta) - 2A_2 \sin(2\theta) + 3A_3 \sin(3\theta)) \cdot \vec{p}_1 \quad (34)$$

In the same way, the force applied on d is:

$$\vec{f}_d = \frac{0.5}{|cd|\sin(\theta_2)} (A_1 \sin(\theta) - 2A_2 \sin(2\theta) + 3A_3 \sin(3\theta)) \cdot \vec{p}_2 \quad (35)$$

4.2 Forces on b and c

We now have to determine the forces \vec{f}_b and \vec{f}_c to be applied on b and c . The equilibrium conditions imply two constraints: (A) the sum of the forces has to be null:

$$\vec{f}_a + \vec{f}_b + \vec{f}_c + \vec{f}_d = 0 \quad (36)$$

and (B) the sum of torques also has to be null⁴. Calling o the center of bond bc , this means:

$$\vec{oa} \times \vec{f}_a + \vec{od} \times \vec{f}_d + \vec{ob} \times \vec{f}_b + \vec{oc} \times \vec{f}_c = 0 \quad (37)$$

From (37) it results:

$$(\vec{ob} + \vec{ba}) \times \vec{f}_a + (\vec{oc} + \vec{cd}) \times \vec{f}_d + \vec{ob} \times \vec{f}_b + \vec{oc} \times \vec{f}_c = 0 \quad (38)$$

⁴ It is not possible to simply define $\vec{f}_b = -\vec{f}_a$ and $\vec{f}_c = -\vec{f}_d$, as the sum of torques would be non-null, thus leading to an increase of potential energy.

and:

$$(-\vec{oc} + \vec{ba}) \times \vec{f_a} + (\vec{oc} + \vec{cd}) \times \vec{f_d} - \vec{oc} \times \vec{f_b} + \vec{oc} \times \vec{f_c} = 0 \quad (39)$$

which implies:

$$\vec{oc} \times (-\vec{f_a} + \vec{f_d} - \vec{f_b} + \vec{f_c}) + \vec{ba} \times \vec{f_a} + \vec{cd} \times \vec{f_d} = 0 \quad (40)$$

From (36) it results:

$$-\vec{f_a} + \vec{f_d} - \vec{f_b} + \vec{f_c} = 2(\vec{f_d} + \vec{f_c}) \quad (41)$$

Substituting (41) in (40), one gets:

$$\vec{oc} \times (2(\vec{f_d} + \vec{f_c})) + \vec{ba} \times \vec{f_a} + \vec{cd} \times \vec{f_d} = 0 \quad (42)$$

thus:

$$2\vec{oc} \times \vec{f_d} + 2\vec{oc} \times \vec{f_c} + \vec{ba} \times \vec{f_a} + \vec{cd} \times \vec{f_d} = 0 \quad (43)$$

which implies:

$$2\vec{oc} \times \vec{f_c} = -2\vec{oc} \times \vec{f_d} - \vec{cd} \times \vec{f_d} - \vec{ba} \times \vec{f_a} \quad (44)$$

and we finally get the condition that the torque from $\vec{f_c}$ should verify in order (37) to be true:

$$\vec{oc} \times \vec{f_c} = -(\vec{oc} \times \vec{f_d} + 0.5\vec{cd} \times \vec{f_d} + 0.5\vec{ba} \times \vec{f_a}) \quad (45)$$

Let us state:

$$\vec{t_c} = -(\vec{oc} \times \vec{f_d} + 0.5\vec{cd} \times \vec{f_d} + 0.5\vec{ba} \times \vec{f_a}) \quad (46)$$

Equation $\vec{oc} \times \vec{x} = \vec{t_c}$ has an infinity of solutions in \vec{x} , all having the same component perpendicular to \vec{oc} . We thus simply choose as solution the force perpendicular to \vec{oc} defined by:

$$\vec{f_c} = (1/|oc|^2) \vec{t_c} \times \vec{oc} \quad (47)$$

Equation (45) is verified because:

$$\vec{oc} \times \vec{f_c} = (1/|oc|^2) \vec{oc} \times (\vec{t_c} \times \vec{oc}) \quad (48)$$

thus⁵ :

$$\vec{oc} \times \vec{f_c} = (1/|oc|^2) |oc|^2 \vec{t_c} = \vec{t_c} \quad (49)$$

The value of $\vec{f_b}$ is finally deduced from equation (36) stating the equilibrium of forces:

$$\vec{f_b} = -\vec{f_a} - \vec{f_c} - \vec{f_d} \quad (50)$$

We have thus determined four forces $\vec{f_a}, \vec{f_b}, \vec{f_c}, \vec{f_d}$ whose sum is null (36) and whose sum of torques is also null (37).

⁵ if $u \perp v$, then $u \times (v \times u) = |u|^2 v$.

5 Lennard-Jones Potentials

A Lennard-Jones (LJ) potential $\mathcal{U}(r)$ between two atoms placed at distance r is defined by⁶:

$$\mathcal{U}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (51)$$

In this definition, parameter σ is the distance at which the potential is null, and parameter ϵ is the minimum of the potential (corresponding to the maximum of the attractive energy).

Stating $A = \sigma^{12}$ and $B = \sigma^6$, Eq. (51) becomes:

$$\mathcal{U}(r) = 4\epsilon \left(\frac{A}{r^{12}} - \frac{B}{r^6} \right) \quad (52)$$

The partial derivative of \mathcal{U} according to distance is thus:

$$\frac{\partial \mathcal{U}(r)}{\partial r} = 4\epsilon \left(-12 \frac{A}{r^{13}} + 6 \frac{B}{r^7} \right) \quad (53)$$

$$= 24\epsilon \left(-2 \frac{A}{r^{13}} + \frac{B}{r^7} \right) \quad (54)$$

$$= \frac{24\epsilon}{r} \left(-2 \frac{A}{r^{12}} + \frac{B}{r^6} \right) \quad (55)$$

$$= -\frac{24\epsilon}{r} \left(2 \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right) \quad (56)$$

Let a and b be two atoms. The force on a is:

$$\vec{f}_a = \frac{24\epsilon}{r} \left(2 \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right) \cdot \vec{u} \quad (57)$$

where \vec{u} is the normalization of \vec{ba} . From the action/reaction principle, one deduces that the force on b should be the opposite of the force on a :

$$\vec{f}_b = -\vec{f}_a \quad (58)$$

According to the definition of \vec{f}_a and \vec{f}_b , the sum of the forces applied to a and b is null:

$$\vec{f}_a + \vec{f}_b = 0 \quad (59)$$

Note that, as for bonds, no torque is produced because the two forces are colinear.

6 Resume

The forces defined in the previous sections are summed up in the following table:

⁶ this is the 6-12 form; other forms of LJ potentials exist.

Bond ab	8	$\vec{f}_a = -2k(r - r_0) \cdot \vec{u}$
	9	$\vec{f}_b = -\vec{f}_a$
Valence abc	17	$\vec{f}_a = -2k(\theta - \theta_0)/ ab \cdot \vec{p}_a$
	21	$\vec{f}_b = -\vec{f}_a - \vec{f}_c$
	18	$\vec{f}_c = -2k(\theta - \theta_0)/ bc \cdot \vec{p}_c$
Torsion $abcd$	34	$\vec{f}_a = \frac{0.5}{ ab \sin(\theta_1)}(A_1\sin(\theta) - 2A_2\sin(2\theta) + 3A_3\sin(3\theta)) \cdot \vec{p}_1$
	50	$\vec{f}_b = -\vec{f}_a - \vec{f}_c - \vec{f}_d$
	47	$\vec{f}_c = (1/ oc ^2) \cdot \vec{t}_c \times \vec{oc}$
	35	$\vec{f}_d = \frac{0.5}{ cd \sin(\theta_2)}(A_1\sin(\theta) - 2A_2\sin(2\theta) + 3A_3\sin(3\theta)) \cdot \vec{p}_2$
LJ ab	57	$\vec{f}_a = \frac{24\epsilon}{r} \left(2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right) \cdot \vec{u}$
	58	$\vec{f}_b = -\vec{f}_a$

Bond In Eq. 8, k is the bond strength constant, r is the distance between atoms a and b , and r_0 is the equilibrium distance, for which energy is null. Vector \vec{u} is defined by $\vec{u} = \text{norm}(\vec{ba})$.

Valence In 17 and 18, k is the angle strength constant, θ is the angle \widehat{abc} , and θ_0 is the equilibrium angle, for which energy is null. In 17, \vec{p}_a is defined by $\vec{p}_a = \text{norm}(\vec{ba} \times (\vec{ba} \times \vec{bc}))$. In 18, \vec{p}_c is defined by $\vec{p}_c = \text{norm}(\vec{cb} \times (\vec{ba} \times \vec{bc}))$.

Torsion In 34 and 35, θ is the torsion angle, θ_1 is the angle \widehat{abc} , θ_2 is the angle \widehat{bcd} and A_1 , A_2 and A_3 are the parameters which define the “three-cosine” form of the torsion angle. Vector \vec{p}_1 is defined by $\vec{p}_1 = \text{norm}(\vec{ba} \times \vec{bc})$ and $\vec{p}_2 = \text{norm}(\vec{cd} \times \vec{cb})$. In 47, o is the middle of bc and \vec{t}_c is defined by $\vec{t}_c = -(\vec{oc} \times \vec{f}_d + 0.5\vec{cd} \times \vec{f}_d + 0.5\vec{ba} \times \vec{f}_a)$.

LJ In 57, σ is the distance at which the potential is null and ϵ is the depth of the potential (minimum of energy). As for bonds, one has $\vec{u} = \text{norm}(\vec{ba})$.

In each case (bond, valence, torsion, LJ interaction), the sum of the forces that are applied to atoms is always null (Eq. (10), (20), (36), (59)). Moreover, no torque is induced by application of these forces: no torque is produced by bonds and LJ interactions, as the produced forces are colinear; we have verified in Sec. 3.1 that no torque is produced by valence angles (24); for torsion angles, we have chosen the forces in such a way that the sum of the forces and the global sum of torques are always null (37). This means that no energy is ever added by the application of the forces during the simulation process.

7 Conclusion

We have precisely defined the forces that apply on atoms in MD simulations. The definitions are given in a purely vectorial formalism (no use of a specific

coordinate system). We have shown that the sum of the forces and the sum of the torques are always null, which means that the energy of molecular systems is preserved while the forces are applied.

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A Notations

- if a and b are two atoms, we note \overrightarrow{ab} the vector with origin a and end b ; the distance between the two atoms is noted $|ab|$.
- The null vector is noted 0.
- The length of vector \overrightarrow{u} is noted $|\overrightarrow{u}|$. One thus has: $|\overrightarrow{ab}| = |ab|$.
- Multiplication of \overrightarrow{u} by the scalar n is noted $n.\overrightarrow{u}$, or more simply $n\overrightarrow{u}$.
- The vectorial product of \overrightarrow{u} and \overrightarrow{v} is noted $\overrightarrow{u} \times \overrightarrow{v}$.
- The scalar product of \overrightarrow{u} and \overrightarrow{v} is noted $\overrightarrow{u} \bullet \overrightarrow{v}$.
- We write $\overrightarrow{u} \perp \overrightarrow{v}$ when \overrightarrow{u} and \overrightarrow{v} are orthogonal ($\overrightarrow{u} \bullet \overrightarrow{v} = 0$).
- We note $norm(\overrightarrow{u})$ the normalized vector from \overrightarrow{u} (same direction, but length equal to 1) defined by $norm(\overrightarrow{u}) = (1/|\overrightarrow{u}|).\overrightarrow{u}$.
- If a , b and c are atoms, we note \widehat{abc} the angle formed by a , b and c .