Lio

NaN

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Abstract

proyecto de manual de lio, hay q ponerle el formato adecuado

1 Restrains

Lio may add an extra potential term to Hamiltonian for penalty the distance between specified pairs of atoms.

1.1 Implemenation

The implementation is a simple harmonic potential over a generalized coordinate r.

$$U = \frac{1}{2}k[r - l_0]^2 \tag{1}$$

r may be defined as a weighted combination of distances between pairs of atoms.

$$r = \sum_i \sum_{j>i} w_{ij} |\vec{r_i} - \vec{r_j}| \tag{2}$$

In this formulation the force over an atom l is:

$$\vec{F_l} = -k[r - l_0] \sum_i \sum_{j>i} w_{ij} \frac{\vec{r_{ij}}}{r_{ij}} \eta_{ijl} \tag{3}$$

Where η_{ijl} is defines as:

$$\eta_{ijl} = \begin{cases} 1 & \text{if } l = i \\ -1 & \text{if } l = j \\ 0 & \text{in other case} \end{cases}$$

1.2 Using Restrain

The number of pairs of atoms that going to be added in potential(s) in lio is defined with the variable number_restr, and the list of distance restrains have to be added to in an extra lio.restrain file like in the following example:

ai	aj	index	k	wij	l0
1	2	0	0.1	1.0	7.86
3	4	0	0.1	-1.0	7.86
7	9	1	0.4	2.0	-2.3
13	1	1	0.4	1.0	-2.3
14	3	1	0.4	-3.0	-2.3
14	2	2	0.2	1.0	0.5
8	5	3	0.3	1.0	3.2

In columns ai and aj you find the atom numbers in de QM system to be restrained, index number determine which distances contribute to a same generalized reaction coordinate. Finally k, wij and l0 are the force constant, weight of that distance in the generalized coordinate and equilibrium position in atomic units.

1.3 Examples

1)In lio.in:

number_restr = 1

in lio.restrain:

ai	aj	index	k	wij	l0
1	2	0	0.1	1.0	7.86

Potential added to system:

$$U = \frac{1}{2}0.1\Big[1.0|\vec{r_1} - \vec{r_2}| - 7.86\Big]^2 \tag{4}$$

2)In lio.in:

number_restr = 2

in lio.restrain:

ai	aj	index	k	wij	l0
1	2	0	0.1	1.0	7.86
3	4	0	0.1	-1.0	7.86

Potential added to system:

$$U = \frac{1}{2}0.1\Big[1.0|\vec{r_1} - \vec{r_2}| - 1.0|\vec{r_3} - \vec{r_4}| - 7.86\Big]^2 \tag{5}$$

3)In lio.in:

number_restr = 4

in lio.restrain:

ai	aj	index	k	wij	l0
1	2	0	0.1	1.0	7.86
3	4	0	0.1	-1.0	7.86
1	3	1	0.3	3.5	-2.31
7	8	1	0.3	-2.2	-2.31

Potential added to system:

$$U = \frac{1}{2}0.1\Big[1.0|\vec{r_1} - \vec{r_2}| - 1.0|\vec{r_3} - \vec{r_4}| - 7.86\Big]^2 + \frac{1}{2}0.3\Big[3.5|\vec{r_1} - \vec{r_3}| - 2.2|\vec{r_7} - \vec{r_8}| + 2.31\Big]^2 \tag{6}$$