D1CH9116 - MMCO

Molecular Modelling applied to organic chemistry

Practical 3: Potential energy surfaces

A/ 1D Potental Energy Surfaces

1/ Use the *Reaction Path* tool of AGUI to visualize the evolution of the total energy (heat of formation) of the CH_3-CH_2-CH_2–CH_3 molecule as a function of the torsional angle. Evaluate the magnitude of the rotational barrier and compare to experimental data.

2/ Visualize the evolution of the total energy as a function and the formation of the co-ordinate (dative covalent) bond between ammonia and boron trifluoride:

$$NH_3 + BH_3 \rightarrow H_3N\text{–}BH_3$$

The *Reaction Path* tool of AGUI should be used here by specifying the B-N distance as the reaction coordinate.

Other examples of co-ordinate bond formations:

Reaction between ammonia and hydrogen chloride: $NH_3 + HCl \rightarrow NH_4Cl$

Dissolving hydrogen chloride in water to make hydrochloric acid: $H_2O + HCl \rightarrow H_3O^+ + Cl^-$

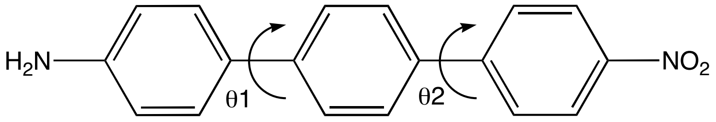
3/ Energy profile of the hydroxycarbene–formaldehyde conversion.

a. Visualize the evolution of the total energy along the hydrogen migration in the intramolecular hydroxycarbene–formaldehyde conversion. The *Reaction Path* tool of AGUI should be used here by specifying the ONH angle as the reaction coordinate.

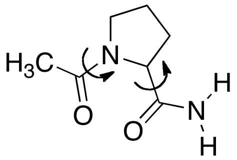
b. Copy/paste the geometry of the transition structure in a new window, and compute the vibrational frequencies (*job=opt+freq with gradient minimization*). Confirm that the structure corresponds to a first-order saddle point of the PES, by checking the presence of a single imaginary wavenumber arising from a negative force constant. Use the graphical interface to check that this vibrational mode actually corresponds to the reactive process under study.

B/ 2D Potental Energy Surfaces

1/ Use the *Reaction Grid* tool of AGUI to visualize the evolution of the total energy of the molecule below as a function of the two torsional angles θ1 and θ2.



2/ Build the potential energy surface of the N-Acetyl Proline Amide molecule as a function of the orientation of the two substituents.


H3C
N
O
O
N
H
H