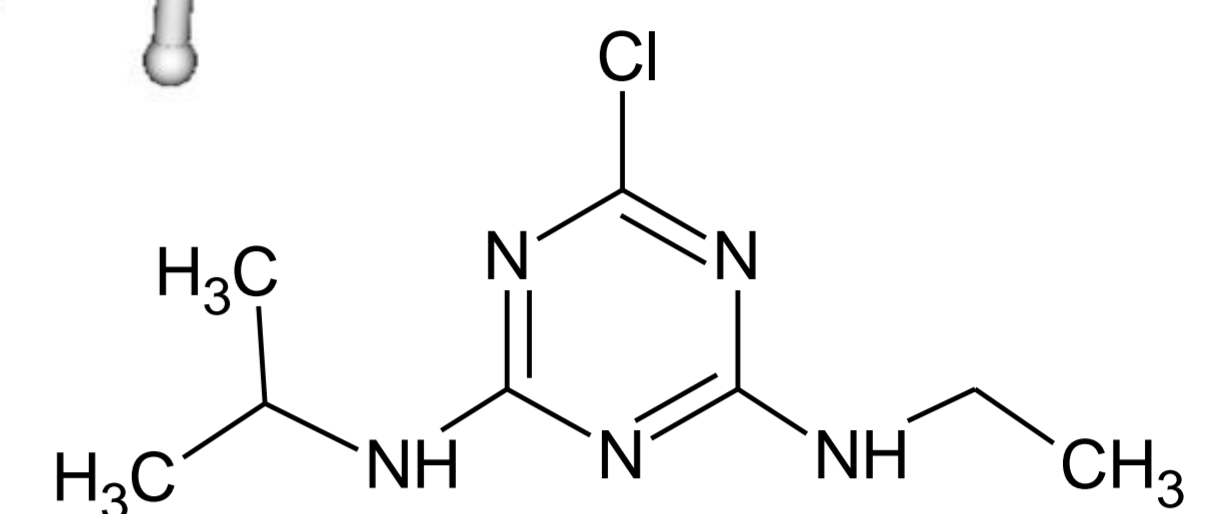
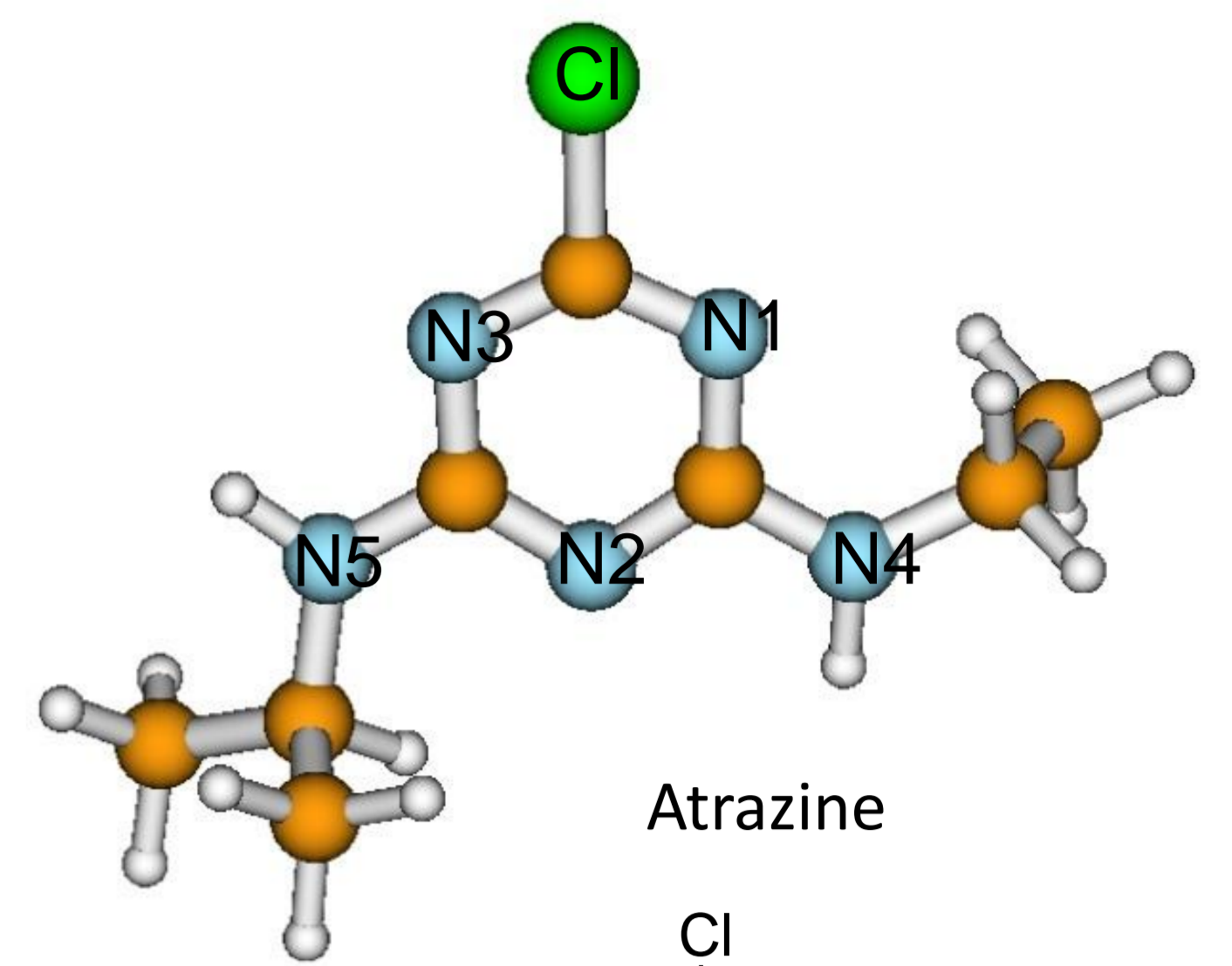


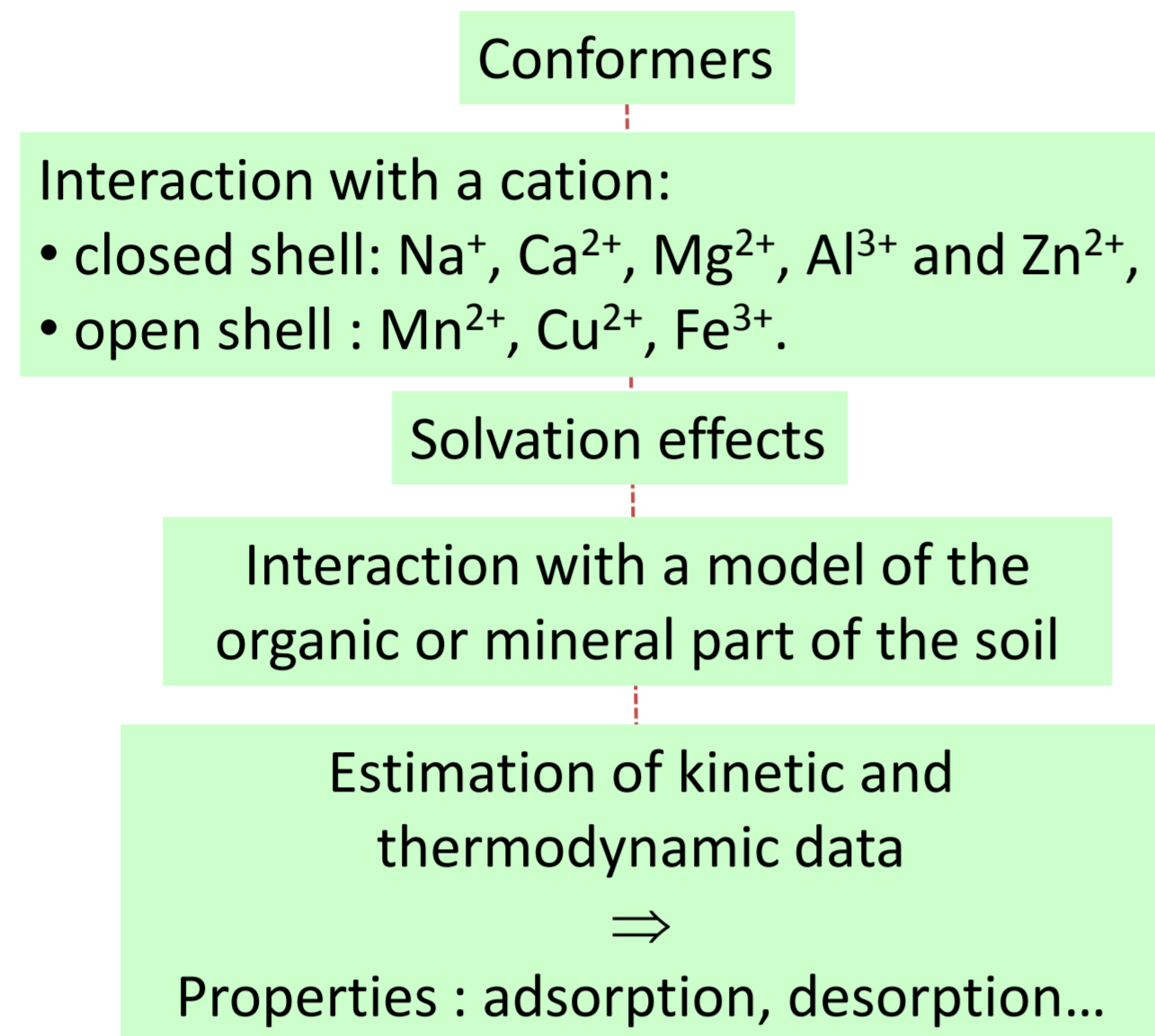
**Pesticides** glyphosate and atrazine (herbicides)

**Goal** predicting their interactions with the soil organic and/or mineral matter accessing to physical and chemical properties of pesticides

**Task force** collaborations between an **experimental** group in soil science and a group in **theoretical chemistry**



Duties



Methods

Geometry optimisations & Energy calculations

HF/6-31G\*  
HF/6-31G\*//B3LYP/6-31G\*  
B3LYP/6-31G\*  
B3LYP/6-31G\*//B3LYP/6-311+G(2d,2p)  
B3LYP/6-311+G(2d,2p)  
MP2/6-311+G(2d,2p)

Accuracy ↗

## Interaction & relative energies

Na <sup>+</sup>			
34,8 kcal/mol	29,9	25,0	E <sub>int</sub>
0,0 kcal/mol	4,9	9,7	Relative energy
atraModNa1	atraModNa2	atraModNa3	

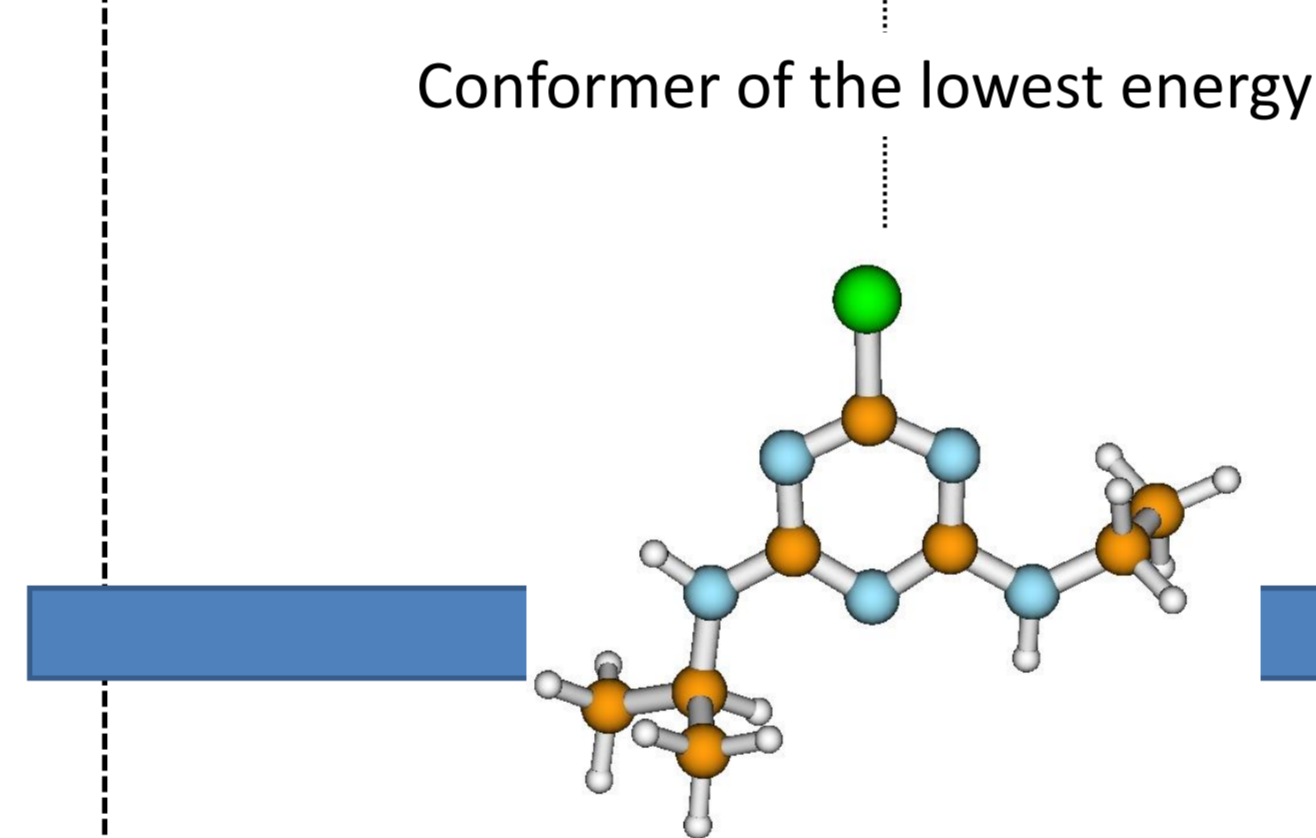
  

Ca <sup>2+</sup>			
104,3	105,6 kcal/mol	93,6	E <sub>int</sub>
1,3	0,0 kcal/mol	12,0	Relative energy
atraModCa1	atraModCa2	atraModCa3	

The three lowest conformers of the atrazine model in interaction with Na<sup>+</sup> and Ca<sup>2+</sup>. The energetic order of these conformers is different for both cations.

B3LYP/6-311+G(2d,2p)

Model → **First results ATRAZINE** → Complete molecule



## Complete molecule

E <sub>int</sub> = 38,9 kcal/mol	E <sub>int</sub> = 122,7 kcal/mol
Na <sup>+</sup>	Ca <sup>2+</sup>

The energetically lowest conformers of the real atrazine in interaction with Na<sup>+</sup> and Ca<sup>2+</sup>.

➤ The model is adapted to replace the complete molecule.

B3LYP/6-31G\*//B3LYP/6-311+G(2d,2p)

## First results Analysis & Solvation ATRAZINE model

### Solvation

Solvent: water modelled with PCM (polarisable continuum model)

Solvation has a great influence on energies and geometries.

**atraModNaSolv1** and **atraModCaSolv1** are of similar type and are both the lowest laying conformers with solvation effects modelled by PCM.

Na <sup>+</sup>			
0,0 kcal/mol	0,3	1,2	= order
atraModNaSolv1	atraModNaSolv2	atraModNaSolv3	

Ca <sup>2+</sup>			
0,0 kcal/mol	6,5	1,6	≠ order
atraModCaSolv1	atraModCaSolv2	atraModCaSolv3	

B3LYP/6-311+G(2d,2p)

### Interaction energy

### Energy decomposition

E<sub>int</sub>: interaction energy  
E<sub>prep</sub>: preparation energy  
E<sub>elect</sub>: electrostatic energy  
E<sub>exch</sub>: exchange repulsion energy  
E<sub>pol</sub>: polarisation energy  
E<sub>CT</sub>: charge transfer energy

kcal/mol	Na <sup>+</sup>			Ca <sup>2+</sup>		
	atraModNa1	atraModNa2	atraModNa3	atraModCa1	atraModCa2	atraModCa3
E <sub>int</sub>	35,3	40,8	35,6	91,2	113,6	99,9
E <sub>prep</sub>	1,87	10,0	9,6	8,0	23,5	22,6
E <sub>elect</sub>	30,9	35,1	30,1	66,5	90,8	77,8
E <sub>exch</sub>	11,3	10,5	10,5	30,7	33,0	32,9
E <sub>pol</sub>	12,0	12,5	12,2	43,9	46,5	45,5
E <sub>CT</sub>	2,5	2,0	2,0	9,8	6,9	7,2

- E<sub>elect</sub> is the greatest contribution to E<sub>int</sub>.
- Dipole moments and electrostatic energies are coherent.
- **atraModNa1**: E<sub>int</sub> is low but the preparation energy is very low.
- **atraModCa2**: E<sub>int</sub> is the highest of the three conformers even if the preparation energy is high.

### Dipole moment

Dipole moments are not sufficient to explain the position of the cations.

Na <sup>+</sup>			
4,7 D	4,7	3,1	
atraModNa1	atraModNa2	atraModNa3	

Ca <sup>2+</sup>			
5,4	5,6 D	2,3	
atraModCa1	atraModCa2	atraModCa3	

HF/6-31G\*//B3LYP/6-31G\*

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