

## Result

Task started: 14:52 30-06-2017  
Task ended: 14:52 30-06-2017  
Total time consumed: 0 min on 1 tasks

## Control

XC	pbe
Relativistic	atomic_zora
Charge	0
Max. number of iterations is	1000

**Relaxation was performed**

Other settings:

vdw\_correction\_hirshfeld  
sc\_accuracy\_rho 1E-3  
sc\_accuracy\_eev 1E-2  
sc\_accuracy\_etot 1E-5  
sc\_accuracy\_forces 5E-3

Figure 1: Atoms: H, O, C, N, Na, Ca

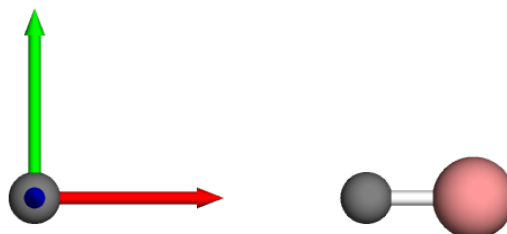


Figure 2: Energy convergence during geometry relaxation process.

