

Result

Task started: 20:59 02-07-2017
Task ended: 21:01 02-07-2017
Total time consumed: 2 min on 64 tasks

Control

XC	pbe
Relativistic	atomic_zora
Charge	1
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
check_cpu_consistency .false.
cpu_consistency_threshold 5E-3

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

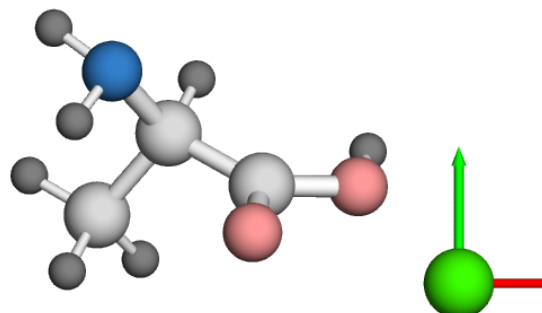


Figure 2: Energy convergence during geometry relaxation process.

