

Result

Task started: 15:52 06-06-2017
Task ended: 16:18 06-06-2017
Total time consumed: 26 min on 1 tasks

Control

XC	pbe
Relativistic	atomic_zora
Charge	1
Max. number of iterations is	10000
Relaxation was performed	

Other settings:

vdw_correction_hirshfeld
sc_accuracy_rho 1E-4
sc_accuracy_eev 1E-3
sc_accuracy_etot 1E-6
sc_accuracy_forces 5E-4

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

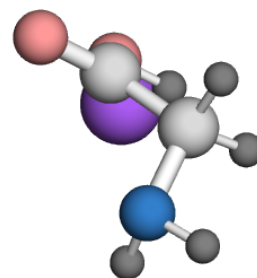


Figure 2: Energy convergence during geometry relaxation process.

