1 Input tags

minimizer = {bfgs,var,ptn}
minimizer sets the optimization algorithm. We use the NLOpt library in MDFT. bfgs should be used for low-storage BFGS. See NLOpt documentation. bfgs is a good choice by default. var for Shifted limited-memory variable-metric. See NLOpt document for more information. ptn for Preconditioned truncated NEWTON. See the NLOpt documentation.

maximum_iteration_nb = N
where N should be an integer greater than 0. It is the maximum number of iterations the minimizer should be doing before reaching any convergence criteria. After that number, it stops.

epsg = N
where N is a real number. It is the convergence criteria in absolute value. Since we minimize the solvation free energy of the solute, the default value is 10^{-4} (implicitely kJ/mol) since this is better than chemical accuracy at 300 K.

translate_solute_to_center = {T,F}
This translates your solute to the center of the supercell: all solute coordinates are moved by {Lx/2., Ly/2., Lz/2.}, with {Lx,Ly,Lz} the length of the supercell.