Results of all simulations since all mols set up

# August 2nd

**PAA Ion hydration energy**

print energy 1 (ion\_solv) - 2 (ion\_ref) end

Local net energy (PE 0) = -1.411714919080E+04 kJ/mol

Global net ELEC energy = -1.411714919080E+04 kJ/mol

**PAA hydration energy**

print energy 3 (undissc\_solv) - 4 (undissc\_ref) end

Local net energy (PE 0) = -8.026121400968E+04 kJ/mol

Global net ELEC energy = -8.026121400968E+04 kJ/mol

**Ionisation + Solvation**

print energy 1 (ion\_solv) - 4 (undissc\_ref) end

Local net energy (PE 0) = -8.070843553663E+04 kJ/mol

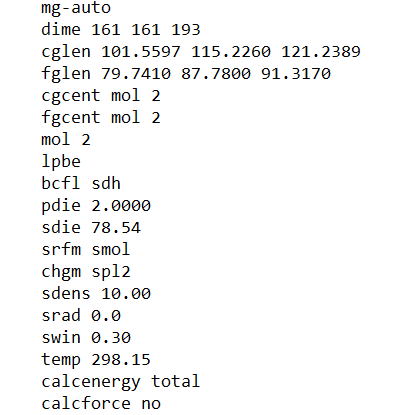
Global net ELEC energy = -8.070843553663E+04 kJ/mol

**Only the polar component of solvation**

print energy 1 (ion\_solv) - 2 (ion\_ref) - 3 (undissc\_solv) + 4 (undissc\_ref) end

Local net energy (PE 0) = 6.614406481887E+04 kJ/mol

Global net ELEC energy = 6.614406481887E+04 kJ/mol

**Params**