Calculating the Solvation energy of a charged sphere

Its is also output as the "corrected reaction field energy" by delphi. In this particular example the charge of the sphere is set as +1 eu and the radius is set as 3 Angstroms. Using the analytical expression (Born formula) the solvation energy is:

delG = (-K * q^2 / 2R) (1/e_int - 1/e_ext) = -92.33 kT

where q=1 is the charge of the sphere, R=3 is its radius, e_int=1 and e_ext=80 are the internal and external dielectric constant(s), and K=561 is the conversion factor to convert delG to kT units.

How to run:

Check that you have all the input files: born.pdb, born.crg, born.siz, param_charged_sphere.prm

To run it, type:

```
$DELPHI_EXE param_charged_sphere.prm > charged_sphere.log
```

Press enter key, and you should get the results.

*Note: $DELPHI_EXE is the full file-path of the delphi executable.

Details of the run:

This example is used to calculate the electrostatic component of solvation energy of the simplest system: a charged sphere.

born.pdb is the file which contains the coordinate information of a charged sphere. born.crg and born.siz files contain the charge and size information, respectively.

After the run, in log file you will see:

Energy > Corrected reaction field energy : -92.50 kT

Where “Corrected reaction field energy” is the electrostatic component of solvation energy for this charged sphere.

Note that Coulombic energy is zero since there is only one charge and no charge-charge interactions.

Applying Gaussian-based smooth dielectric function approach on the same problem, the charged sphere, results in different polar solvation energy. First, there is no analytical solution since the sphere

is no longer hard sphere, but rather a spherical object with smooth dielectric function having minimum value at the center of the sphere and smoothly reaching 80 in bulk solvent. DelPhi can be executed with this example as:

```
$DELPHI_EXE param_charged_sphere_gauss.prm > charged_sphere_gauss.log
```

The calculated polar solvation energy is in the log file:
Energy> Corrected reaction field energy : -211.20 kT
Note that that the computed energy depends on two parameters: sigma=0.9 and srfcut=20.0 and any change of these parameters will result in a different energy.