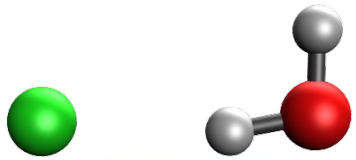
ALMO-EDA-II practice

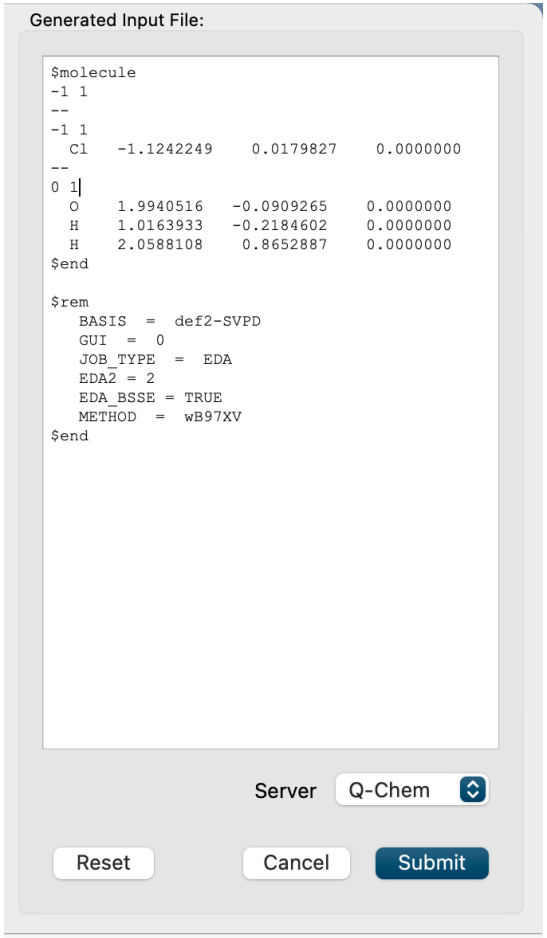
- ALMO-EDA-II for water···Cl^- at equilibrium structure:
  - At the ωB97X-V/def2-SVPD level of theory
  - Because of the use of a relatively small basis set, we choose `EDA2 = 2` (ALMO polarization + decomposition of the frozen interaction)
  - Counterpoise correction for BSSE will be performed (`EDA_BSSE = TRUE`)
  - Perform the EDA calculation (i) in vacuum and (ii) in solvent water described by the SMD model. Report the results for the ELEC, PAULI, DISP, POL, CT terms (focusing on the results of "quasiclassical" decomposition) as well as the total interaction energies

	ELEC	PAULI	DISP	POL	CT	Total
vacuum						
SMD water						



ALMO-EDA-II practice

- **Note:** IQmol doesn't provide a full support for ALMO-EDA-II jobs yet so the input file needs to be manually edited
- **Procedure for job setup:**
  - Open the XYZ file "water_cl.xyz" using IQmol
  - Change the charge to "−1" (the multiplicity should then automatically update to "1"). Under the dropdown menu of "`Calculate`" select "`Energy Decompose`", and set "`Method`" to "`Omega-B97X-V`"
  - We then need to manually edit the generated input file on the right of job setup panel: (i) set "`BASIS = def2-SVPD`" and "`GUI = 0`" (since we are not doing any visualization here); (ii) add the following two lines under "`JOB_TYPE = EDA`": `EDA2 = 2`, and `EDA_BSSE = TRUE`
  - As the last step, we need to edit the `$molecule` section to specify the fragments: frag 1: −1 1; frag 2: 0 1
  - The generated input is shown on the right. It's ready to submit!



ALMO-EDA-II practice

- After the job is finished, copy it back to your computer. Then under "Files" (in the "Model View" column on the left), double-click the output file; scroll down to find the section as shown on the right

```
================================
        Results of EDA2
================================
Basic EDA Quantities
--------------------
Fragment Energies (Ha):
1 -460.0529423442
2  -76.3470870124
--------------------
  E_prp (kJ/mol) = 0.0000
  E_frz (kJ/mol) = -32.9000
  E_pol (kJ/mol) = -15.0941
  E_vct (kJ/mol) = -16.6774 (CP-corrected)
  E_int (kJ/mol) = -64.6715 (CP-corrected)
--------------------


Decomposition of frozen interaction energy
--------------------
  --------------------
  Orthogonal Frozen Decomposition:
  --------------------
     E_elec   (ELEC)    (kJ/mol) = -119.8483
     E_pauli  (PAULI)   (kJ/mol) = 99.4947
     E_disp   (DISP)    (kJ/mol) = -12.5464
  --------------------
  Classical Frozen Decomposition:
  --------------------
     E_cls_elec  (CLS ELEC)   (kJ/mol) = -81.5197
     E_mod_pauli (MOD PAULI)  (kJ/mol) = 61.1661
     E_disp      (DISP)       (kJ/mol) = -12.5464
  --------------------
--------------------
```

- Starting from the output file we go ahead to set up a second EDA2 calculation with SMD water: click "Calculation → Q-Chem setup", make sure that the generated input is the same as the previous job (you may need to set "`GUI = 0`" again); then click "Advanced → Solvent Model" and choose "SMD" and the solvent model and set solvent to "water". Make sure that "`SOLVENT_METHOD = SMD`" appears in the `$rem` section and a new `$smx` section also appears:

```
$smx
   SOLVENT  WATER
$end
```

Submit the calculation and collect the EDA results from the output file.

ALMO-EDA-II practice

EDA results in solvation environment: check out how each term differs from the results in vacuum

```
================================
        Results of EDA2
================================
Basic EDA Quantities
--------------------
Fragment Energies (Ha):
1 -460.1558667113
2  -76.3591018936
--------------------
  E_prp (kJ/mol) = 0.0000
  E_sol (kJ/mol) = 43.6322
  E_frz (kJ/mol) = -45.6542 (unscreened)
[E_frz(solv) = -2.0220 kJ/mol (unscreened FRZ + SOL)]
  E_pol (kJ/mol) = -4.0923
  E_vct (kJ/mol) = -15.3228 (CP-corrected)
  E_int (kJ/mol) = -21.4370 (CP-corrected)
--------------------


Decomposition of frozen interaction energy
--------------------
  ------------------------------
  Classical Frozen Decomposition (unscreened):
  ------------------------------
     E_cls_elec  (CLS ELEC)   (kJ/mol) = -92.0390
     E_mod_pauli (MOD PAULI)  (kJ/mol) = 57.9297 (FRZ - CLS ELEC - DISP)
     E_disp      (DISP)       (kJ/mol) = -11.5449
  ------------------------------
  Classical Decomposition Terms with Solvent Contributions:
  ------------------------------
     E_sol_elec               (kJ/mol) = 46.0173
     E_cls_elec(solv)         (kJ/mol) = -46.0217 (CLS ELEC + SOL ELEC)
     E_sol_nonelec            (kJ/mol) = -2.3851
     E_mod_pauli(solv)        (kJ/mol) = 55.5446 (MOD PAULI + SOL non-ELEC)
  --------------------
```

Collection of EDA results (in kJ/mol):

	ELEC	PAULI	DISP	POL	CT	Total
Vacuum	-81.5	61.2	-12.5	-15.1	-16.7	-64.7
SMD water	-46.0	55.5	-11.5	-4.1	-15.3	-21.4