Supporting Information (PART III)

Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions

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Functional Forms for Atomic Surface Tensions Used by SMD

The atomic surface tensions given by eq 7 in the article are decribed here in more detail.

For Z_k = H:

$$\sigma_k = \tilde{\sigma}_{\mathrm{H}} + \tilde{\sigma}_{\mathrm{HC}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{C}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{HC}}, \Delta r_{\mathrm{HC}}) + \tilde{\sigma}_{\mathrm{HO}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{O}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{HO}}, \Delta r_{\mathrm{HO}})$$

For Z_k = C:

$$\sigma_k = \tilde{\sigma}_{\mathrm{C}} + \tilde{\sigma}_{\mathrm{CC}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{C} \\ k' \neq k}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{CC}}, \Delta r_{\mathrm{CC}}) + \tilde{\sigma}_{\mathrm{CN}} \left[\sum_{\substack{k' \\ Z_{k'}=\mathrm{N}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{CN}}, \Delta r_{\mathrm{CN}}) \right]^2$$

For Z_k = N:

$$\sigma_k = \tilde{\sigma}_{\mathrm{N}} + \tilde{\sigma}_{\mathrm{NC}} \left\{ \sum_{\substack{k' \\ Z_{k'}=\mathrm{C}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{NC}}, \Delta r_{\mathrm{NC}}) \left[\sum_{\substack{k'' \\ k'' \neq k' \\ k'' \neq k}}^{\text{atoms}} T(R_{k'k''}, r_{\mathrm{C}Z_{k''}}, \Delta r_{\mathrm{C}Z_{k''}}) \right]^2 \right\}^{1.3} +$$

$$\tilde{\sigma}_{\mathrm{NC(3)}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{C}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{NC(3)}}, \Delta r_{\mathrm{NC(3)}})$$

For Z_k = O:

$$\sigma_k = \tilde{\sigma}_{\mathrm{O}} + \tilde{\sigma}_{\mathrm{OC}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{C}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{OC}}, \Delta r_{\mathrm{OC}}) + \tilde{\sigma}_{\mathrm{ON}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{N}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{ON}}, \Delta r_{\mathrm{ON}}) +$$

$$\tilde{\sigma}_{\mathrm{OO}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{O} \\ k' \neq k}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{OO}}, \Delta r_{\mathrm{OO}}) + \tilde{\sigma}_{\mathrm{OP}} \sum_{\substack{k' \\ Z_{k'}=\mathrm{P}}}^{\text{atoms}} T(R_{kk'}, r_{\mathrm{OP}}, \Delta r_{\mathrm{OP}})$$

For Z_k = F, Si, S, Cl, and Br:

$$\sigma_k = \tilde{\sigma}_{Z_k}$$

For $Z_k \neq$ H, C, N, O, F, Si, S, Cl, or Br:

$$\sigma_k = 0$$

In the equations above, k runs over all atoms in a molecule, Z_k is the atomic symbol of atom k, σ_k is the atomic surface tension of atom k, $\tilde{\sigma}_{Z_k}$ is an atomic-number-specific parameter, $\tilde{\sigma}_{Z_k Z_{k'}}$ is a parameter that depends on the atomic numbers of atoms k and k', $T(R_{k\,k'}, r_{Z_k Z_{k'}}, \Delta r_{Z_k Z_{k'}})$ is a geometry-dependent switching function called a cutoff tanh. This function is described as follows

$$T(R_{kk'}, r_{Z_k Z_{k'}}, \Delta r_{Z_k Z_{k'}}) = \begin{cases} \exp\left(\dfrac{\Delta r_{Z_k Z_{k'}}}{R_{k\,k'} - \Delta r_{Z_k Z_{k'}} - r_{Z_k Z_{k'}}} \right) & \text{if } R_{kk'} < r_{Z_k Z_{k'}} + \Delta r_{Z_k Z_{k'}} \\ 0 & \text{otherwise} \end{cases}$$

where $R_{kk'}$ is the interatomic distance between atoms k and k' and $r_{Z_k Z_{k'}}$ and $\Delta r_{Z_k Z_{k'}}$ are atomic-number-specific parameters described in Table.

Table. Values of $r_{ZZ'}$ and $\Delta r_{ZZ'}$ (Å) [a]

Z, Z′	$r_{ZZ'}$	$\Delta r_{ZZ'}$
H, C	1.55	0.3
H, O	1.55	0.3
C, H	1.55	0.3
C, C	1.84	0.3
C, N	1.84	0.3
C, O	1.84	0.3
C, F	1.84	0.3
C, P	2.2	0.3
C, S	2.2	0.3
C, Cl	2.1	0.3
C, Br	2.3	0.3
C, I	2.6	0.3
N, C	1.84	0.3
N, C(3)	1.225	0.065
O, C	1.33	0.1
O, N	1.5	0.3
O, O	1.8	0.3
O, P	2.1	0.3

[a] Any possible $r_{ZZ'}$ or $\Delta r_{ZZ'}$ that is not in the table is set equal to zero in the SMD model.