Tuning the reactivity of a dissociative force field: proton transfer properties of aqueous H_3O^+ and their dependence on the three–body interaction – Supplementary Information.

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Supplementary Information

In the Results section of our article the influence of the second derivative of the screening function with respect to the pair distance $\mathbf{r}_{ij}$ is discussed. Equations S1 to S3 show the screening function f_{scr} and its first and second derivatives.

$$f_{scr} = e^{\frac{\gamma_{ij}}{\|\mathbf{r}_{ij}\| - r_{ij}^0}} \tag{S1}$$

$$\frac{\partial f_{scr}}{\partial \mathbf{r}_i} = -\frac{\gamma_{ij}}{(\|\mathbf{r}_{ij}\| - r_{ij}^0)^2} e^{\frac{\gamma_{ij}}{\|\mathbf{r}_{ij}\| - r_{ij}^0}} \tag{S2}$$

$$\frac{\partial^2 f_{scr}}{\partial \mathbf{r}_i^2} = \frac{\gamma_{ij}}{(\|\mathbf{r}_{ij}\| - r_{ij}^0)^3} \left(2 + \frac{\gamma_{ij}}{\|\mathbf{r}_{ij}\| - r_{ij}^0}\right) e^{\frac{\gamma_{ij}}{\|\mathbf{r}_{ij}\| - r_{ij}^0}} \tag{S3}$$

Figure S1 depicts the screening function and the second derivative as a function of the pair distance $\mathbf{r}_{ij}$. The slightly lowered curvature of set A (red) compared to the original parameter set C (black) is clearly visible.

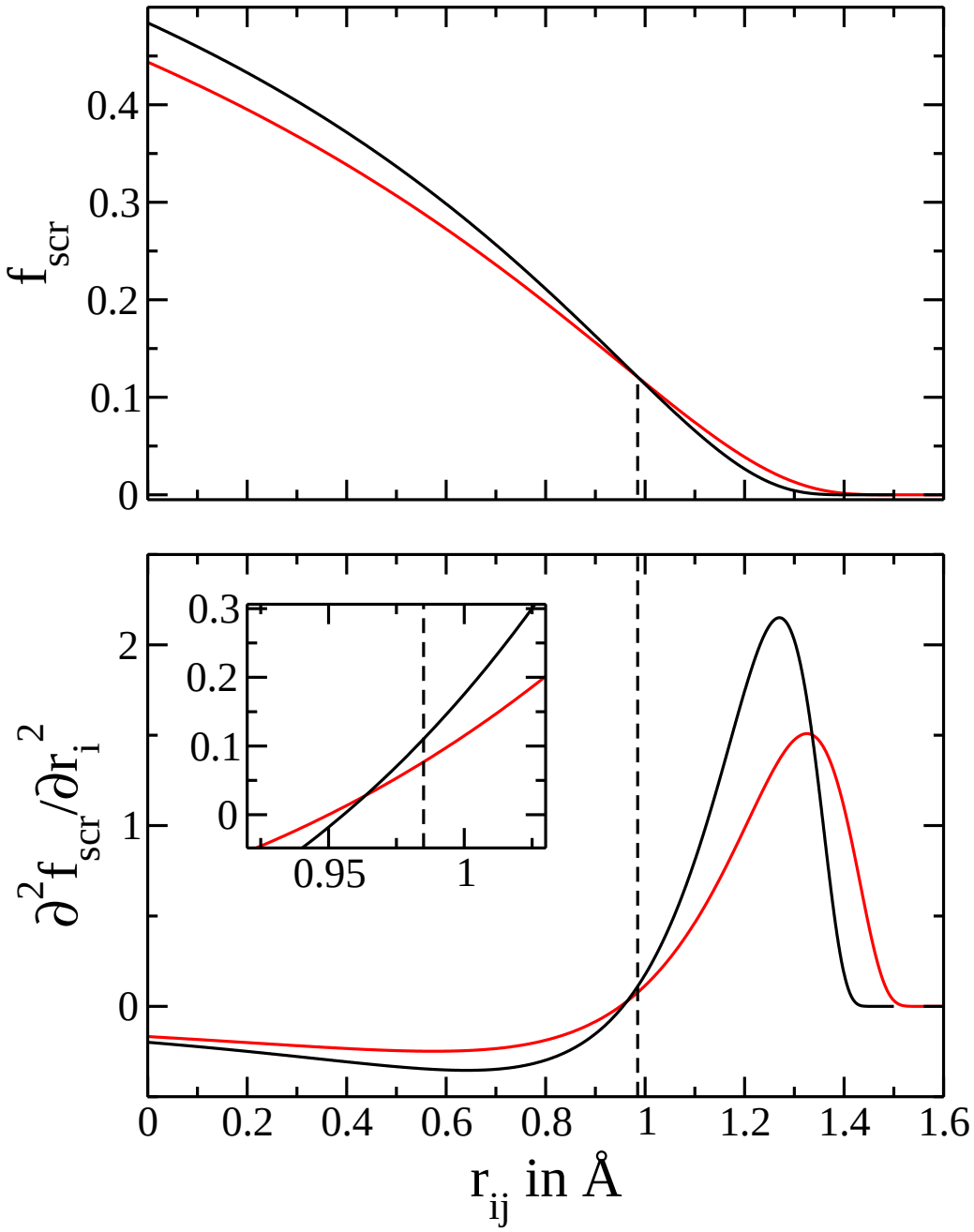

Figure S1: Screening function f_{scr} (top) and its second derivative (bottom) as a function of the pair distance $\mathbf{r}_{ij}$. The curvature obtained for the newly developed parameter set A (red) is smaller compared to the original parametrization of the model set C (black) at the average value of the OH distance being 0.985Å.