Supporting information for

On the Interfragment Exchange in the X-Pol Method

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Computed total electronic energies and interaction energy components using the unpolarized (gas-phase), $\psi_1^0\psi_2^0\psi_3^0$, and polarized (cluster), $\psi_1\psi_2\psi_3$, monomer wave functions for two water trimer complexes, one at the cyclic, minimum energy configuration (**c-W$_3$**) and another that includes a symmetrically placed, repulsive pair (**s-W$_3$**). The 6-31+G(d) basis set were used in all calculations and energies are give in hartrees.

Table S1. Computed total energies and energy components (in hartrees) for the cyclic water trimer minimum structure (**c-W$_3$**) and for a symmetric trimer geometry (**s-W$_3$**). All calculations were performed using HF/6-31+G(d).

Method	**c-W$_3$**	**s-W$_3$**
$E(\psi_a^0) + E(\psi_b^0) + E(\psi_c^0)$	-228.05297	-228.05318
$E_{\text{Coulomb}}(\psi_1^0\psi_2^0\psi_3^0)$	-228.09376	-228.07863
$E_{\text{BLW}}(\hat{A}\psi_1^0\psi_2^0\psi_3^0\})$	-228.06774	-228.06150
$E(\psi_1) + E(\psi_2) + E(\psi_3)$	-228.04723	-228.05067
$E_{\text{Coulomb}}(\psi_1\psi_2\psi_3)$	-228.09790	-228.07990
$E_{\text{BLW}}(\hat{A}\psi_1\psi_2\psi_3\})$	-228.07286	-228.06382
$E_{\text{HF}}(\psi_{123})$	-228.07775	-228.06724