

**Supporting Material**

Table 1. Coordinates of the three water cluster used for EFP basis set superposition error analysis.

<b>Atom</b>	<b>Atomic Number</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
O	8	-0.915052382	1.310233088	0.133644674
H	1	-1.598119457	1.570018025	0.755115152
H	1	-0.95576261	0.35188736	0.119134807
O	8	1.877686568	0.754168074	0.190624133
H	1	1.093478596	1.3023899	0.25965372
H	1	2.468512113	1.094492491	0.865456601
O	8	0.00650246	-1.381570885	0.156015834
H	1	0.066227551	-2.001730194	-0.573456402
H	1	0.861508697	-0.946824178	0.17195411