Supp 1. Experimental electrostatic potentials for TGG, ASPA2, ENK and LAP water molecules. Contour intervals are 0.02 eÅ⁻¹; negative contours are dashed and zero contour is in heavy line.
Supp 2. Up to hexadecapole level electric moments generated electrostatic potential for TGG, ASPA2, ENK and LAP water molecules. Contour intervals are 0.02 eÅ⁻¹; negative contours are dashed and zero contour is in heavy line.
**Supp 3.** Difference between experimental (Fig. 1) and up to hexadecapole level electric moments generated electrostatic potentials (Fig. 4) for ASPA1 and NAT water molecules. Contour intervals are 0.02 eÅ⁻¹; negative contours are dashed and zero contour is in heavy line.
Supp 4. List of hexadecapole electric moments obtained for the six water molecules.

<table>
<thead>
<tr>
<th>hexadecapoles ($10^{-20}$ Cm$^4$)</th>
<th>TGG</th>
<th>ENK</th>
<th>ASPA1</th>
<th>ASPA2</th>
<th>LAP</th>
<th>NAT</th>
<th>Averaged moments (rmsd)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Phi_{xxx}$</td>
<td>-1.647</td>
<td>-6.908</td>
<td>-3.145</td>
<td>-1.892</td>
<td>-1.934</td>
<td>-0.195</td>
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<tr>
<td>$\Phi_{yyy}$</td>
<td>7.600</td>
<td>9.467</td>
<td>8.998</td>
<td>10.057</td>
<td>7.155</td>
<td>6.168</td>
<td>8.2(1.5)</td>
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<tr>
<td>$\Phi_{zzz}$</td>
<td>-6.997</td>
<td>-10.733</td>
<td>-8.975</td>
<td>-9.381</td>
<td>-6.764</td>
<td>-5.031</td>
<td>-8.0(2.0)</td>
</tr>
<tr>
<td>$\Phi_{xxxy}$</td>
<td>0.001</td>
<td>0.026</td>
<td>0.174</td>
<td>-0.018</td>
<td>0.00</td>
<td>0.942</td>
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<tr>
<td>$\Phi_{yyxy}$</td>
<td>-0.002</td>
<td>0.029</td>
<td>0.136</td>
<td>0.005</td>
<td>0.072</td>
<td>-1.243</td>
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<tr>
<td>$\Phi_{zzxz}$</td>
<td>0.091</td>
<td>0.118</td>
<td>-0.044</td>
<td>-0.080</td>
<td>1.597</td>
<td>-2.357</td>
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<tr>
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<td>-0.153</td>
<td>0.122</td>
<td>0.024</td>
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<td>0.629</td>
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<tr>
<td>$\Phi_{yyxz}$</td>
<td>-0.003</td>
<td>0.099</td>
<td>0.064</td>
<td>0.167</td>
<td>0.271</td>
<td>0.504</td>
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<tr>
<td>$\Phi_{zzxz}$</td>
<td>0.001</td>
<td>-0.162</td>
<td>0.123</td>
<td>-0.269</td>
<td>0.886</td>
<td>1.128</td>
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<tr>
<td>$\Phi_{xxyy}$</td>
<td>-0.014</td>
<td>0.035</td>
<td>-0.078</td>
<td>0.056</td>
<td>-1.320</td>
<td>1.728</td>
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<tr>
<td>$\Phi_{yyxy}$</td>
<td>0.002</td>
<td>0.063</td>
<td>-0.187</td>
<td>0.102</td>
<td>-1.157</td>
<td>-1.631</td>
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<tr>
<td>$\Phi_{zzxz}$</td>
<td>0.001</td>
<td>-0.055</td>
<td>-0.310</td>
<td>0.013</td>
<td>-0.072</td>
<td>0.300</td>
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</tr>
<tr>
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<td>10.560</td>
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<td>-1.284</td>
<td>-1.162</td>
<td>-0.666</td>
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</table>