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Remarkable Conformational Flexibility of Aqueous 18-Crown-6 and its Strontium(II) Complex - Ab initio Molecular Dynamics Simulations: Supporting Information

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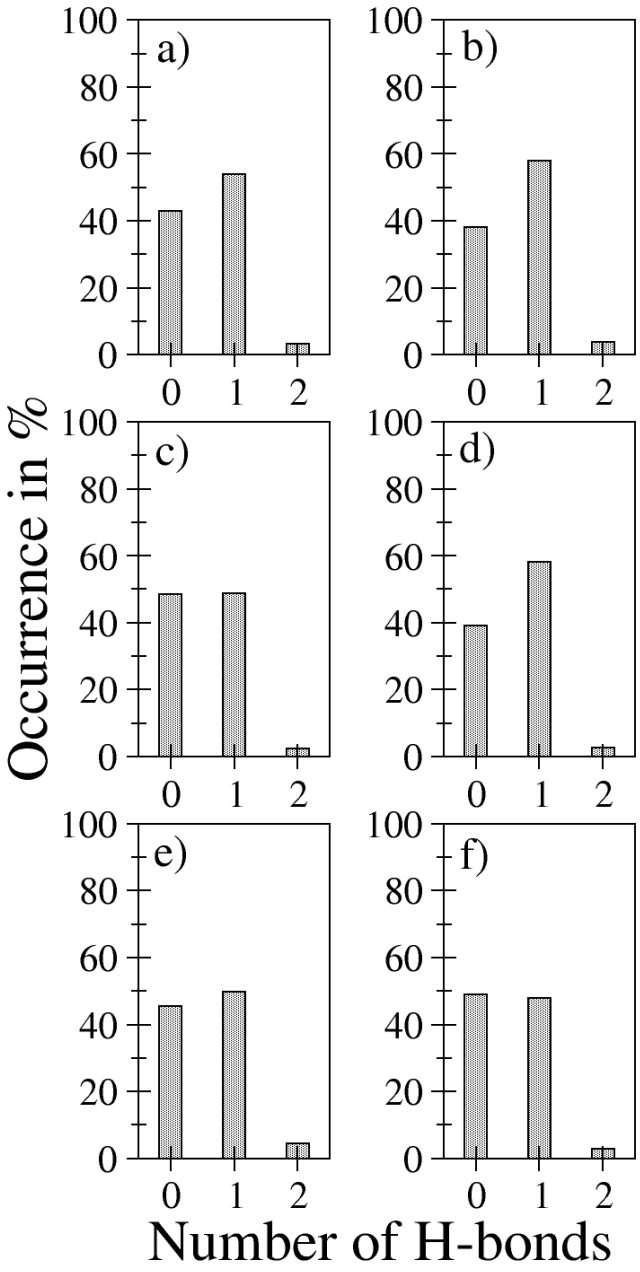

Figure S.1: Distribution of the number of H-bonds formed between each of the six O_{crown} atoms and bulk water molecules obtained from the QMCF-MD simulation of 18C6.

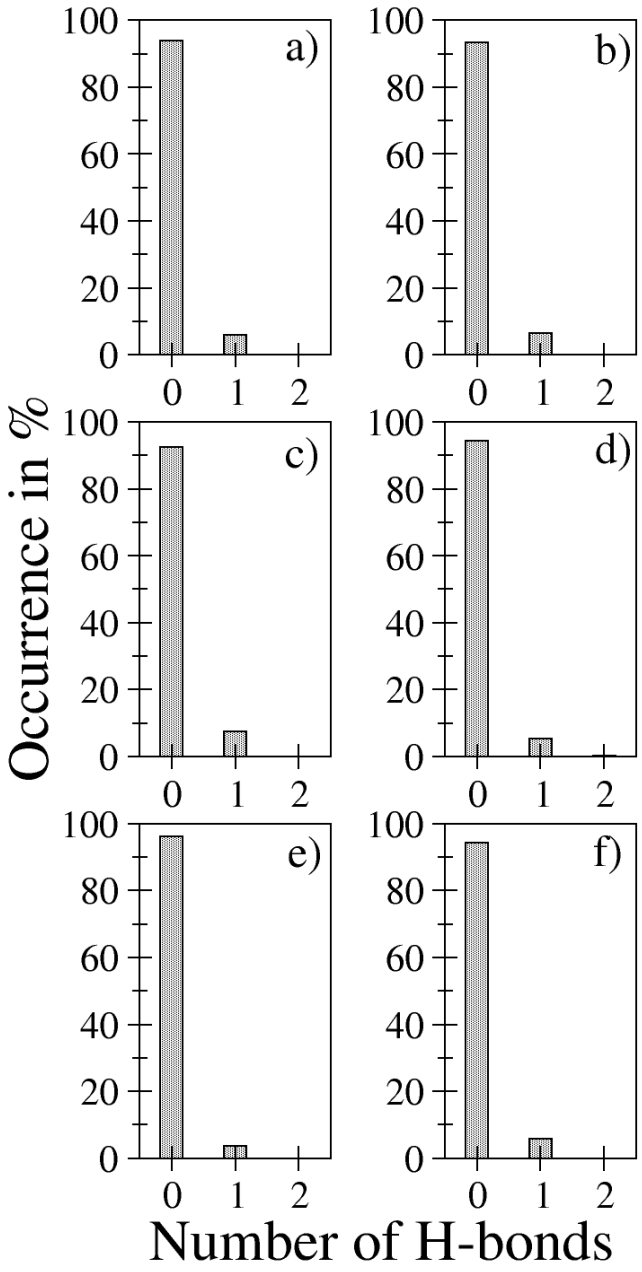

Figure S.2: Distribution of the number of H-bonds formed between each of the six O_{crown} atoms and bulk water molecules obtained from the QMCF-MD simulation of 18C6-Sr.