Electronic Supplementary Information

Simulation Details

Aqueous solutions of **1** and **2** were modelled through molecular dynamics simulations at 300 K. These involved solvation of a single molecule of **1** or **2** in a water sphere of radius 25 Å containing 2165 TIP3P[1] water molecules. This assembly was partitioned into a 23 Å/25 Å reaction region/buffer region for stochastic boundary molecular dynamics. The solvent was first minimized and subjected to an equilibration period of 22.5 ps at 300 K, during which the solute was restrained. A 10 ps unrestrained equilibration was then performed followed by a 500 ps unrestrained production simulation at 300 K. The molecular dynamics calculations were performed using the CHARMM[2] program with the CHARMM22[3] force field and the SHAKE[4] algorithm to constrain bonds to hydrogen, allowing a time step of 1 fs, and a deformable boundary potential with a Langevin frictional coefficient of 62 ps^{-1}, applied to the water oxygen atoms.[5]

All ab initio calculations were performed using the Gaussian98 program.[6]

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