Supporting Information

New and Modified MM3 Force Field parameters for triple proton transfer in the cyclic water trimer.

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atom          6      O       "C-O-H, C-O-C, O-O"       8       15.995       2
atom         21      H       "-OH ALCOHOL"             1       1.008        1
atom        210      H       "transferring hydrogen"   1       1.008        1
bond          6     21            8.6300       0.9760
bond          6    210            8.0300       0.9760
angle        21     6    210      0.630      104.520       0.000       0.000
dipole        6     21           -2.0700       0.500
dipole        6    210           -2.0700       0.500
vdw          21                  1.600        0.016       0.923
vdw         210                  1.600        0.016       0.923
vdwpr         6     21            3.110        1.000
vdwpr         6    210            1.900        0.100
vdwpr         6      6            3.100        1.000
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A new atom type 210 was defined for the transferring hydrogen, and its parameters were taken to be the same as those of atom type 21. The stretching force constant and equilibrium bond distance for the stretches between the O atom and the H atoms were chosen to be 8.63 mdyn/Å and 0.9760 Å for O6-H21 bond, and 8.03 mdyn/Å and 0.9760 Å for O6-H210 bond, respectively. In order to reproduce the geometries from the quantum mechanics calculations, the van der Waals pair parameters were modified to values as described above.