Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Recognition of Naphthalene Diimide Ligands by Telomeric Quadruplex-DNA: The Importance of the Protonation State and Mediated Hydrogen Bonds

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Supporting Information

The total energy values obtained from the conformational searches on the isolated ligands are reported in Table S1. The terminal protonation states are always the most stable isomers.

Table S1: Calculated MM total energy for the isolated ligands (implicit water model, global minimum conformation, in kJ/mol)

	1	**2**	**3**	**4**
intra	-136.48	0.72	-45.33	-15.86
ter	-264.27	-103.91	-181.14	-149.43

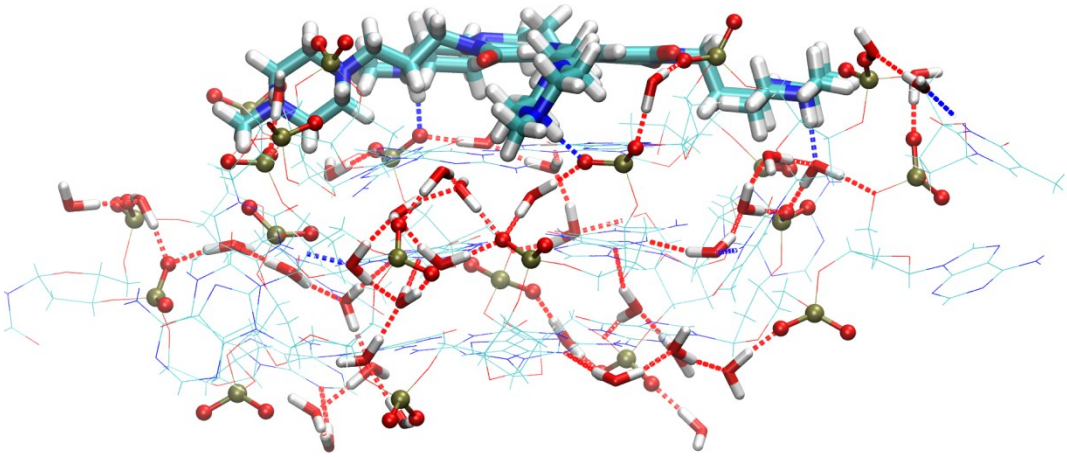

Figure S1: Network of hydrogen bonds mediated by water in ligand **2** complex.

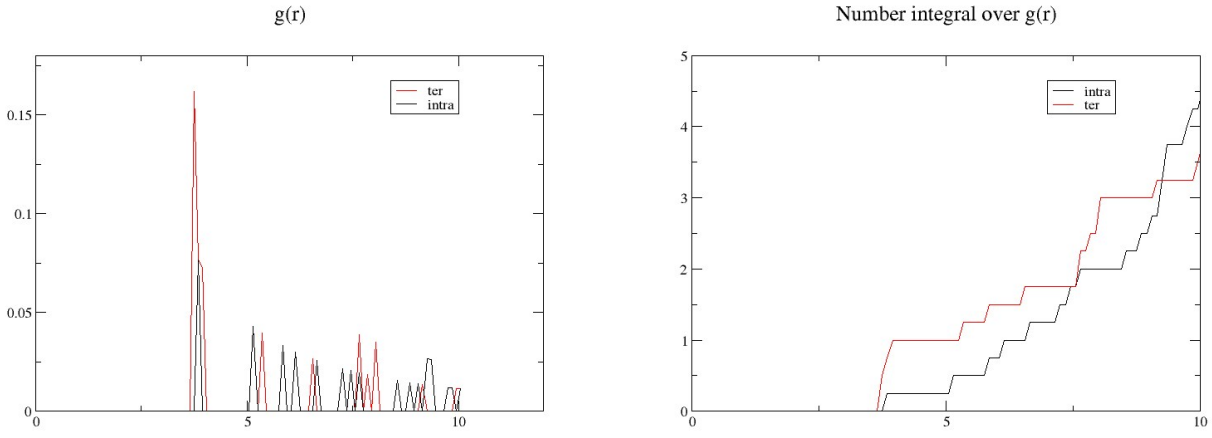

Figure S2: Radial distribution functions (left) and related integrals (right) of the charged nitrogens and phosphorous atoms for ligands ND **1.**