SUPPORTING INFORMATION

Journal of Physical Chemistry A

Jiří Šebek, Bela Gyurcsik, Jaroslav Šebestík, Zdeněk Kejík, Lucie Bednárová, and Petr Bouř:

Interpretation of Synchrotron Radiation Circular Dichroism Spectra of Anionic, Cationic and Zwitterionic Dialanine Forms

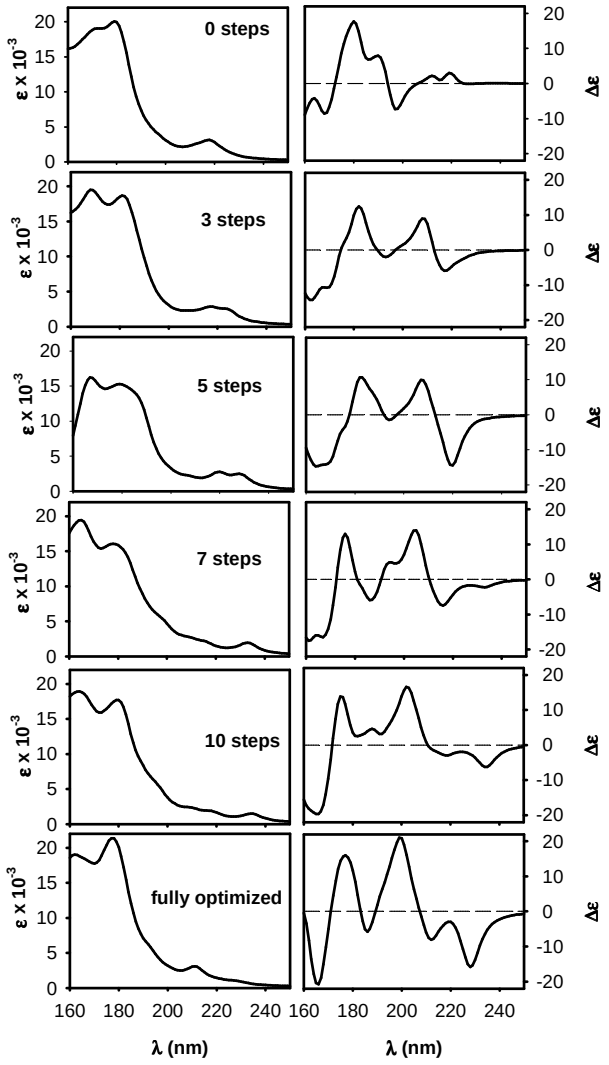

Figure 1s. Dependence of the absorption and CD spectra of a AA^-/water MD cluster on the number of Gaussian preoptimization steps (B3LYP/6-311++G**(6-31G)/CPCM calculation). The most significant geometry changes occur quickly within 1-3 step (high-frequency vibrational mode relaxation), then the spectra are relatively stabilized until slower redistribution of the solvent molecules and solute conformation start to change more.

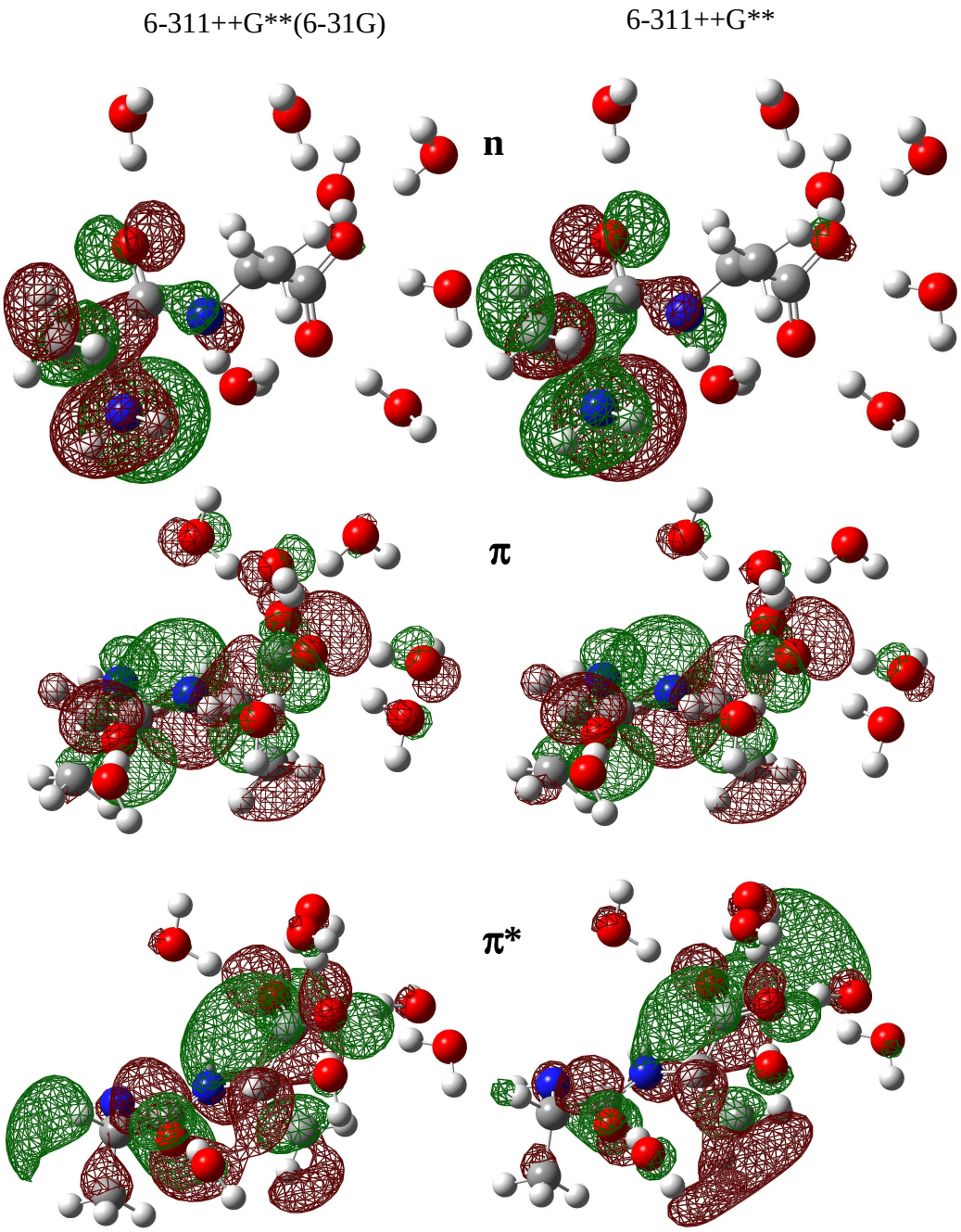

Figure 2s. Comparison of the n, π and π* orbitals (isosurfaces at 0.02 a.u.) calculated for a randomly selected anion (AA^-) cluster with the smaller mixed (left) and full 6-311+G** (right) basis set.

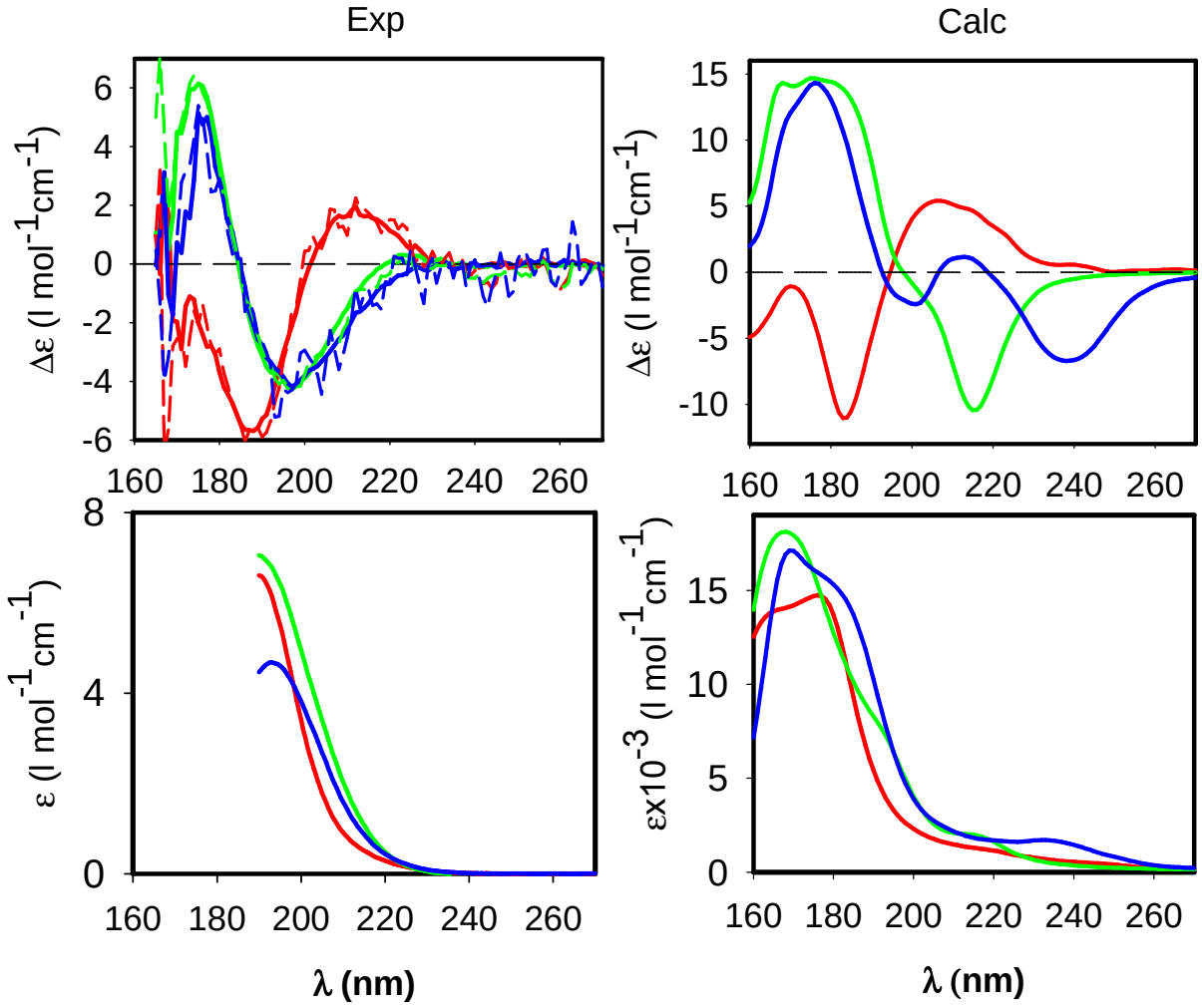

Figure 3s An alternative comparison plot of the experimental and computed AA spectra (to Fig. 9).

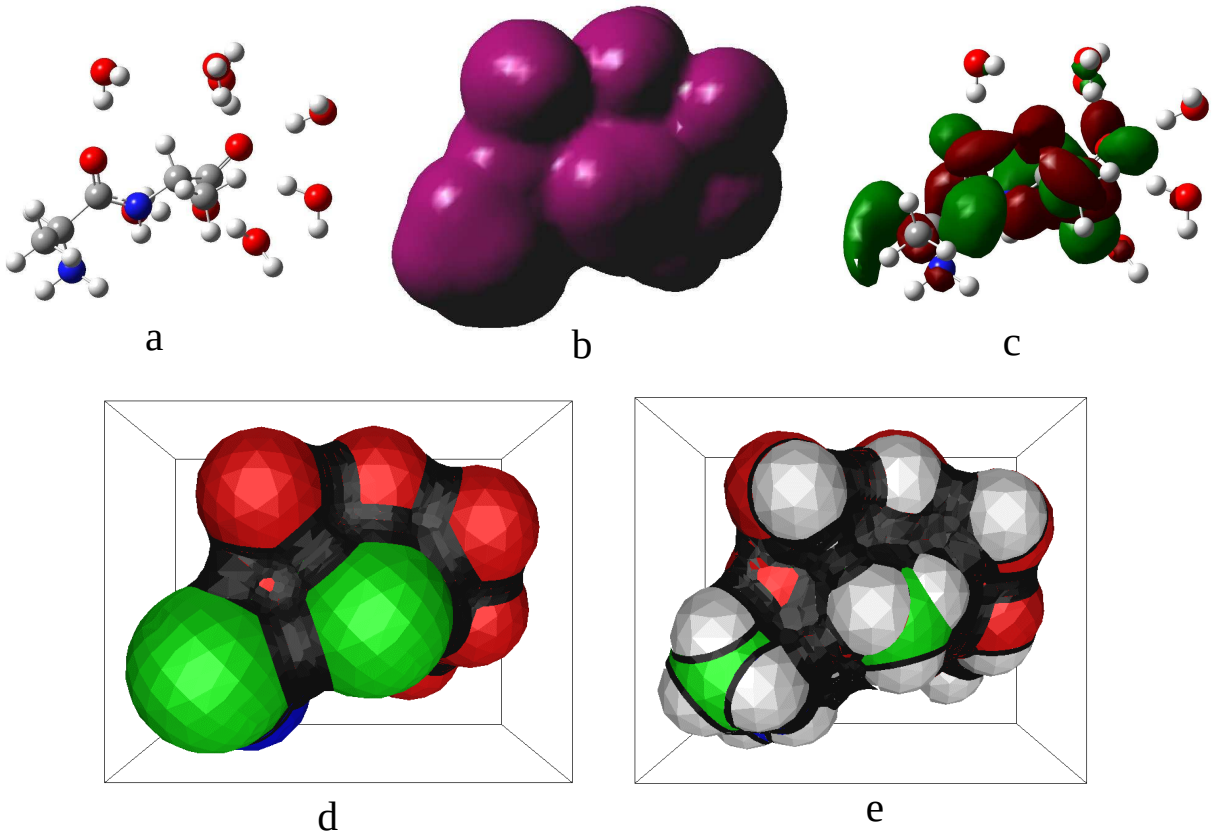

Figure 4s. Comparison of the cavity size and electron extent for a randomly selected AA$^-$/water cluster. Top: (a) the geometry, (b) total electronic density (isodensity surface at 0.0004 a.u.) and the LUMO orbital (c, isodensity at ±0.02 a.u.). Bottom: solvent cavities with (d) the united atom topological model and (e) explicit hydrogen spheres of the UFF radii.

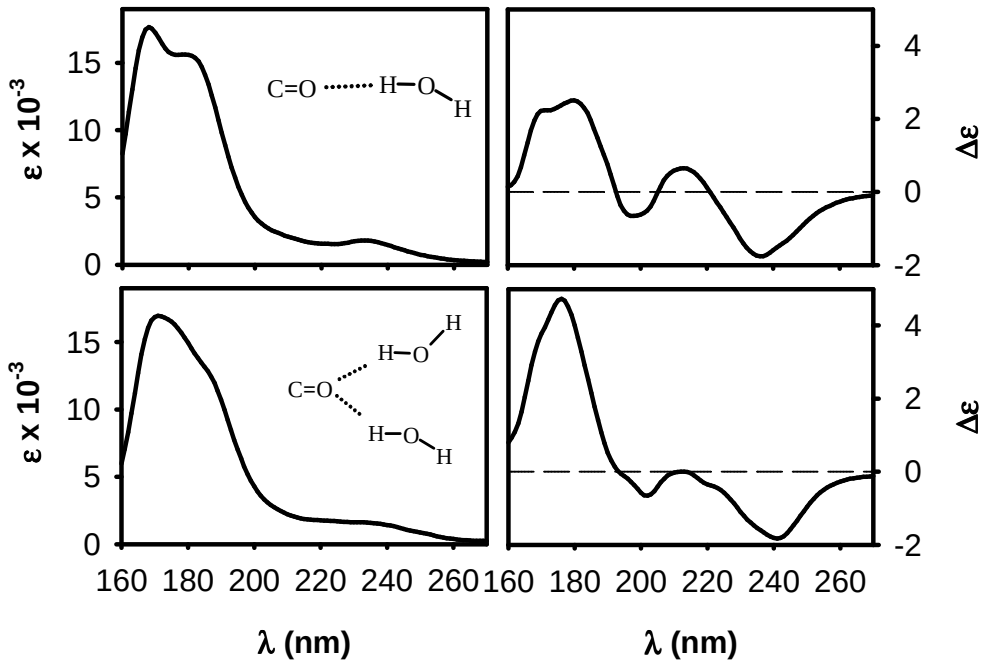

Figure 5s. B3LYP/6-311++G**(6-31G)/CPCM AA^-/water cluster calculation. Average absorption (left) and CD (right) spectra of (top) 49 clusters with one hydrogen bond and (bottom) 49 clusters with two hydrogen bonds on the carbonyl oxygen.

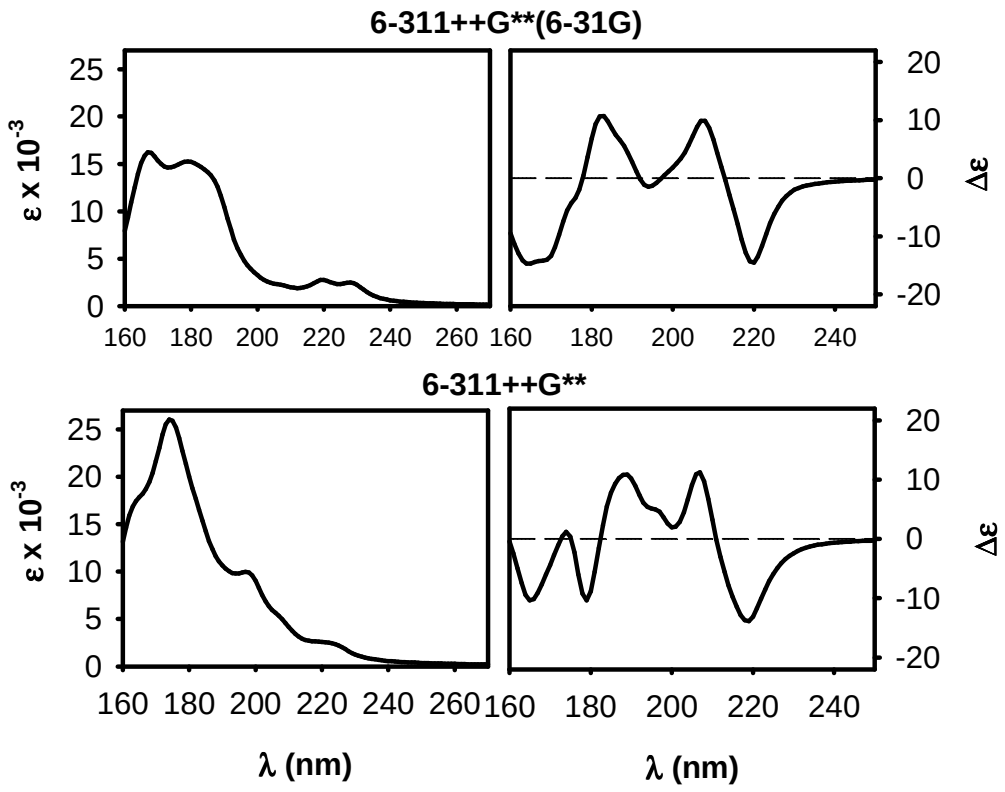

Figure 6s. Calculated (B3LYP/CPCM) absorption (left) and CD (right) spectra for an arbitrarily selected AA^-/water cluster with the (top) combined and (bottom) bigger basis set.