Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry


# Supplementary Material

# Investigation of solute-solvent interactions in phenol compounds: accurate *ab initio* calculations of solvent effects on $^1$H NMR chemical shifts

Michael G. Siskos*[,a], Vassiliki G. Kontogianni[a], Constantinos G. Tsiafoulis[b], Andreas G. Tzakos[a] and Ioannis P. Gerothanassis*[,a]

*Corresponding authors. E-mail: igeroth@uoi.gr, msiskos@cc.uoi.gr

[a]Section of Organic Chemistry and Biochemistry, Department of Chemistry, University of Ioannina, Ioannina GR 45110, Greece

[b]NMR Center, University of Ioannina, Ioannina GR 45110, Greece

*Corresponding authors. E-mail: igeroth@uoi.gr, msiskos@cc.uoi.gr

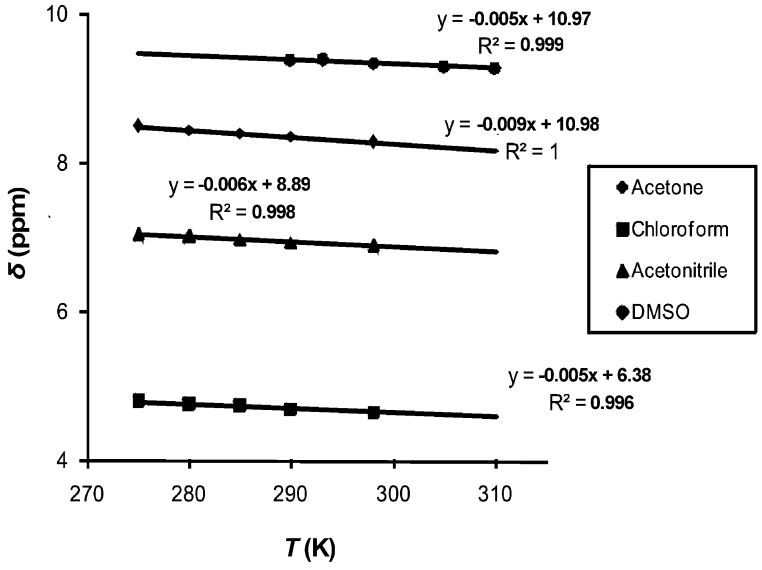


**Figure S1**. Temperature dependencies of the –OH proton of phenol (**1**) in DMSO-$d_6$, acetone-$d_6$, acetonitrile-$d_3$ and chloroform-$d_1$.

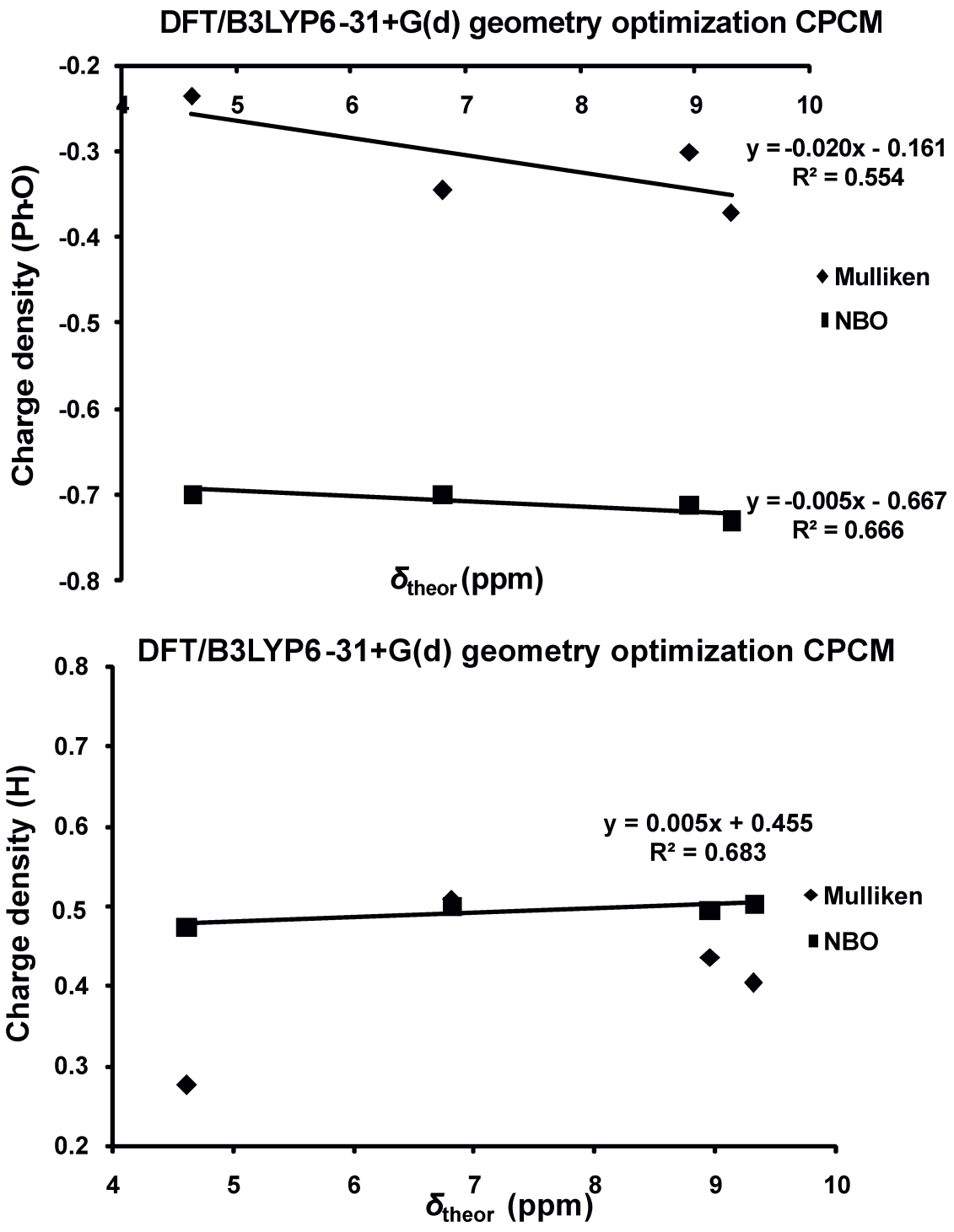


**Figure S2.** Charge density (calculated by the Mulliken and natural bond orbital (NBO) at the DFT/B3LYP/6-31+G(d) level of theory) of Ph-O and –H of the intermolecular hydrogen bond of 1:1 phenol (**1**)+solvent complexes as a function of $\delta_{theor}$.

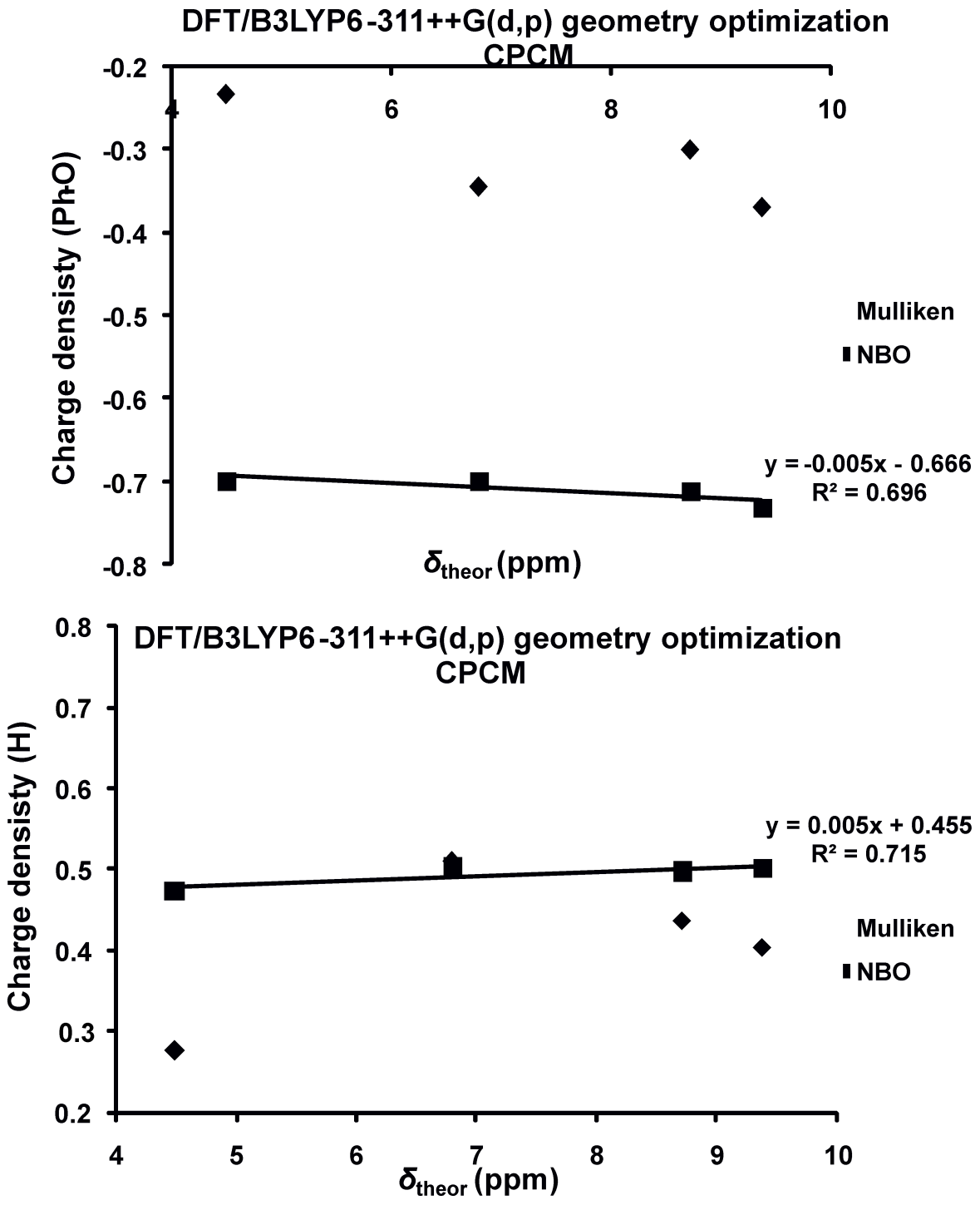


**Figure S3.** Charge density (calculated by the Mulliken and natural bond orbital (NBO) at the DFT/B3LYP/6-311++G(d,p) level of theory) of Ph-O and –H of the intermolecular hydrogen bond of 1:1 phenol (**1**)+solvent complexes as a function of $\delta_{theor}$.