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

Unveiling Peculiar Hydrogen Bonding Behavior of Solvated N-Heterocyclic Carbenes.

Supporting Information

Oldamur Hollóczki[a,b*]

[a]Mulliken Center for Theoretical Chemistry, University of Bonn, Beringstr. 4+6, D-53115 Bonn, Germany

[b]Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Szt. Gellért tér 4, 1111 Budapest, Hungary

holloczki@gmail.com

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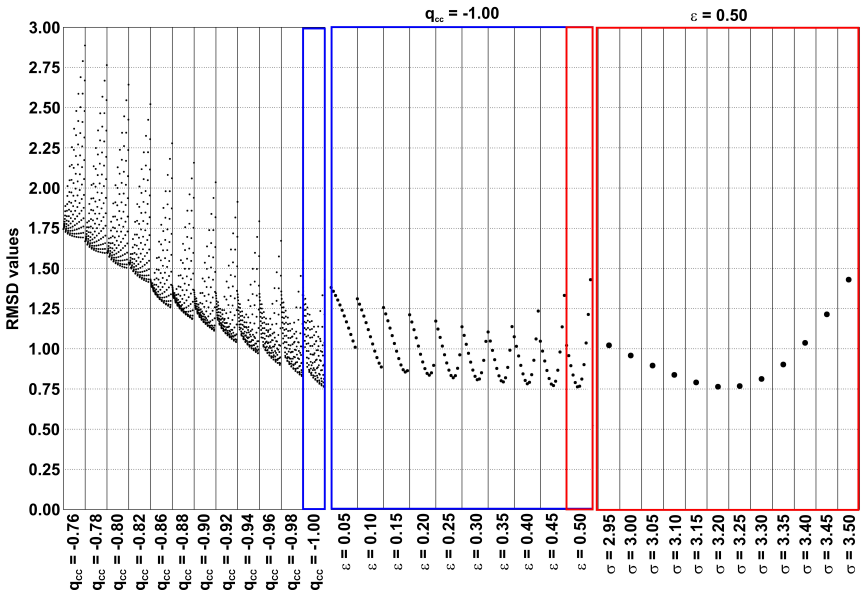

Figure 1: RMSD values calculated for the "in-plane" potential curve by changing the charge at the CC atom, the σ and ϵ values. The left panel contains all values that are obtained, and it is divided according to the different charge models. The panel in the middle highlights the last section of the previous one, namely the charge model with a $q_{CC} = -1.0e$, and it is divided according to the different ϵ values. The right panel highlights the last section of the middle one, with an $\epsilon = 0.50$ kcal mol^{-1}, and it is divided according to the σ values. The increased negative charge at the CC atom was compensated by increased positive charges at the NA atoms. RMSD and ϵ_{ii} values are shown in kcal mol^{-1}, σ_{ii} in Å, and the charges in atomic units.

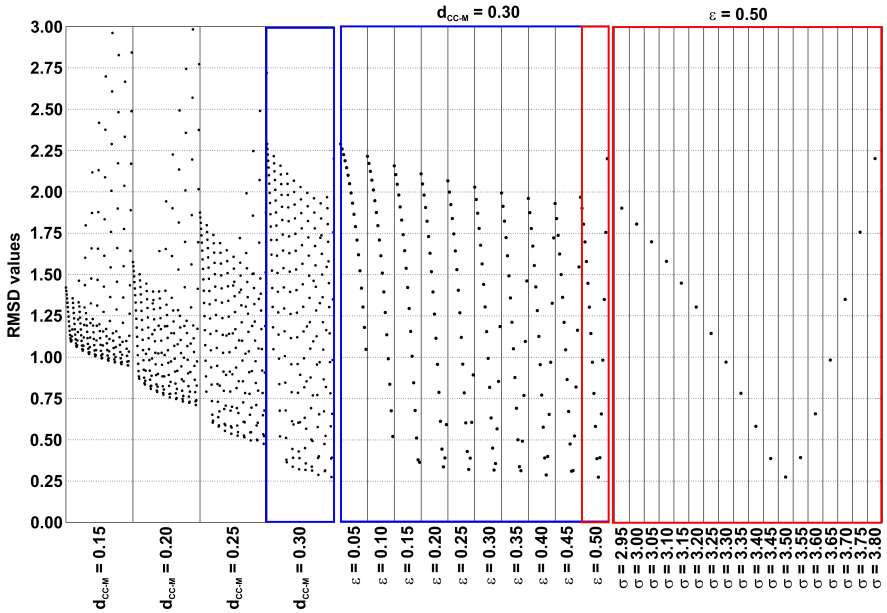

Figure 2: RMSD values calculated for the "in-plane" potential curve, by shifting off the charge of the CC atom into the massless charged point L, and changing the σ and ϵ values. The left panel contains all values that are obtained, and it is divided according to the different CC-L distances. The panel in the middle highlights the last section of the previous one, namely the CC-L distance of 0.30 Å, and it is divided according to the different ϵ values. The right panel highlights the last section of the middle one, with an $\epsilon = 0.50$ kcal mol^{-1}, and it is divided according to the σ values. RMSD and ϵ values are shown in kcal mol^{-1}, while the d_{CC-L} and σ data in Å.

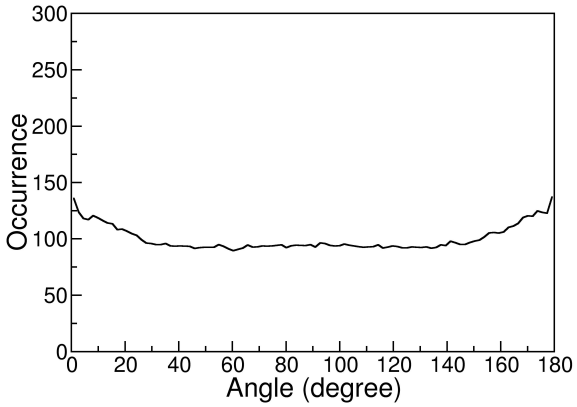

Figure 3: Distribution of the angles between the ring normal vectors of the neighboring carbene and toluene molecules.

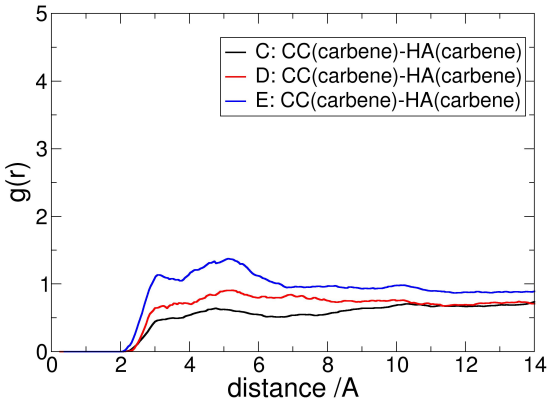

Figure 4: RDFs for the HA-CC hydrogen bond in systems C-E.