Supplementary Information

A DFT study of the hydrogen bonded structures of pyruvic acid-water complexes

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Figure S 1. (**A**) Variation of the electron density (ρ_{BCP} in a. u., rectangle symbol) and its Laplacian, ($\nabla^2\rho_{BCP}$ in a. u., triangle symbol) of the hydrogen bonds formed in the PA-$(H_2O)_2$ versus their H···O lengths, $d_{H\cdots O}$ in Å. (**B**) The Hamiltonian kinetic energy (H_{BCP} in a. u., circle symbol), the kinetic energy density (G_{BCP} in a. u., rectangle symbol), and the potential energy density (V_{BCP} in a. u., triangle symbol) at bond critical points in the PA-$(H_2O)_2$ as function of the hydrogen bond lengths, $d_{H\cdots O}$ in Å.

Figure S 2. (**A**) Variation of the electron density (ρ_{BCP} in a. u., rectangle symbol) and its Laplacian, ($\nabla^2\rho_{BCP}$ in a. u., triangle symbol) of the hydrogen bonds formed in the PA-$(H_2O)_3$ versus their H···O lengths, $d_{H\cdots O}$ in Å. (**B**) The Hamiltonian kinetic energy (H_{BCP} in a. u., circle symbol), the kinetic energy density (G_{BCP} in a. u., rectangle symbol), and the potential energy density (V_{BCP} in a. u., triangle symbol) at bond critical points in the PA-$(H_2O)_3$ as function of the hydrogen bond lengths, $d_{H\cdots O}$ in Å.

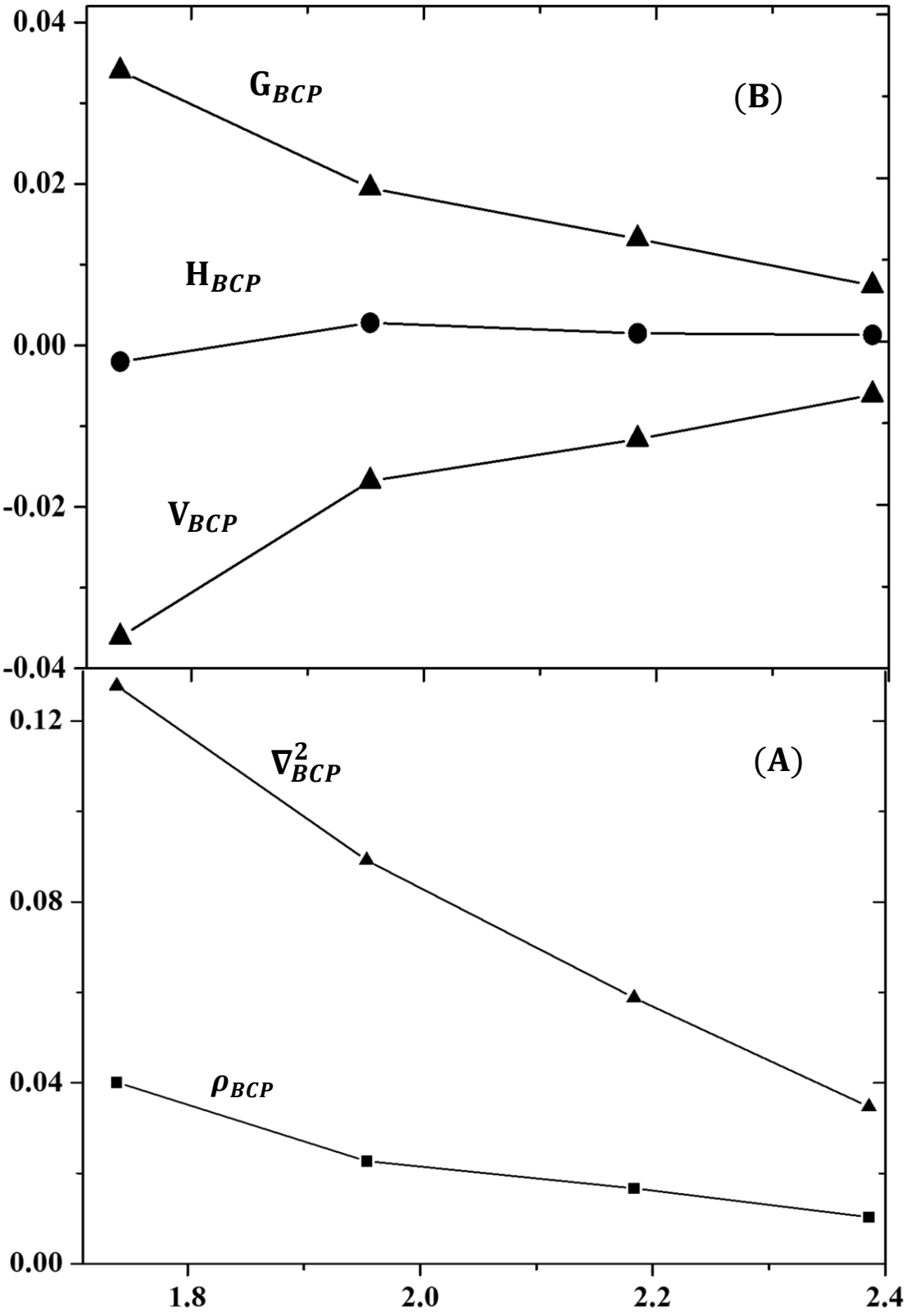
0.04
0.02
0.00
-0.02
-0.04
G_{BCP}
(B)
H_{BCP}
V_{BCP}
0.12
0.08
0.04
0.00
∇^2_{BCP}
(A)
ρ_{BCP}
1.8
2.0
2.2
2.4

Figure S 1.

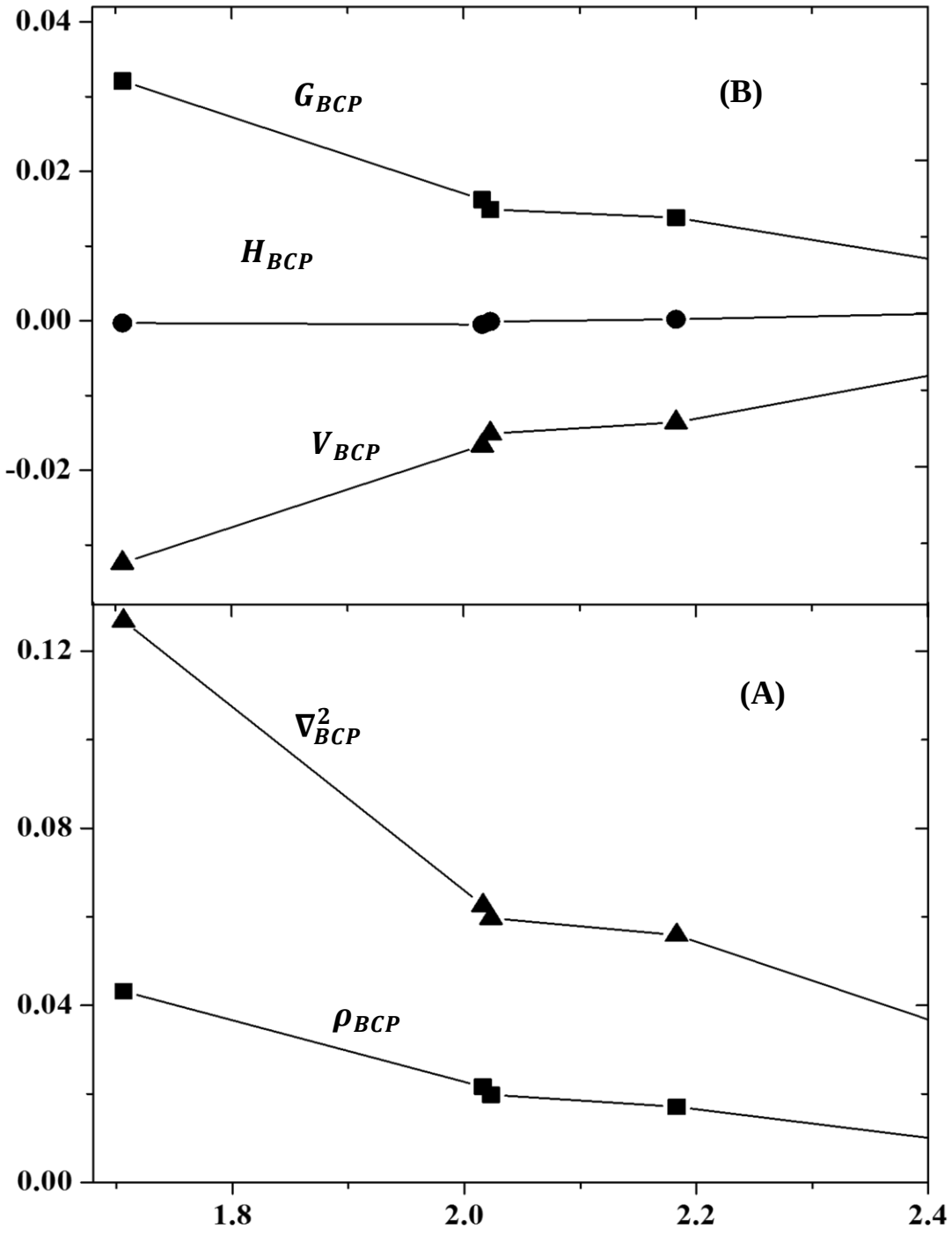
0.04
0.02
0.00
-0.02
G_{BCP}
(B)
H_{BCP}
V_{BCP}
0.12
0.08
0.04
0.00
(A)
∇^2_{BCP}
ρ_{BCP}
1.8
2.0
2.2
2.4

Figure S 2.