



Excess Molar Volume of Aqueous 1-Propanol and Apparent Molar Volume of 2-Naphthol in Water, 1-Propanol and Their Binary Mixtures at Various Temperatures with DFT Study

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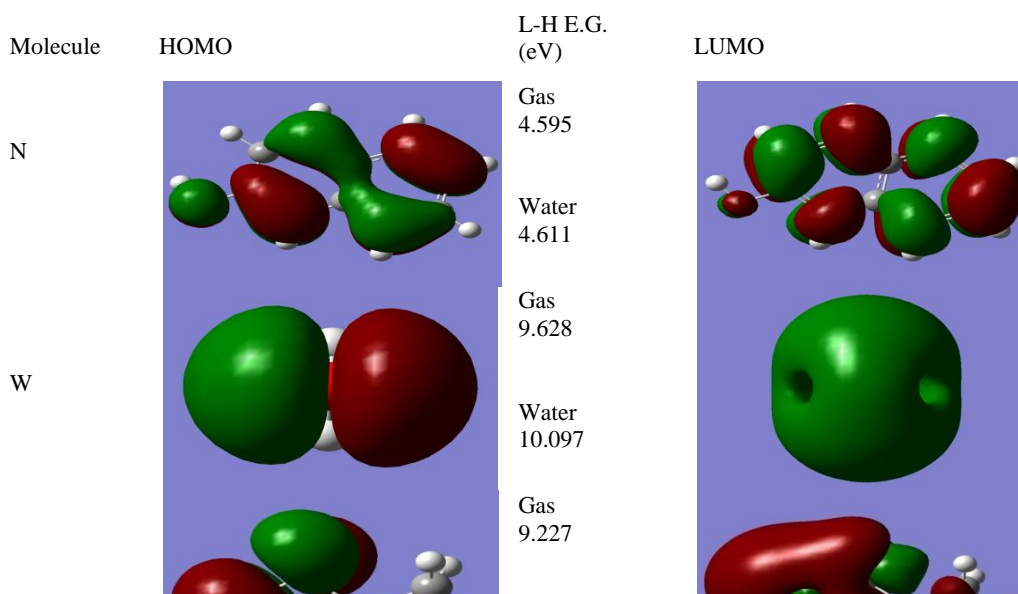
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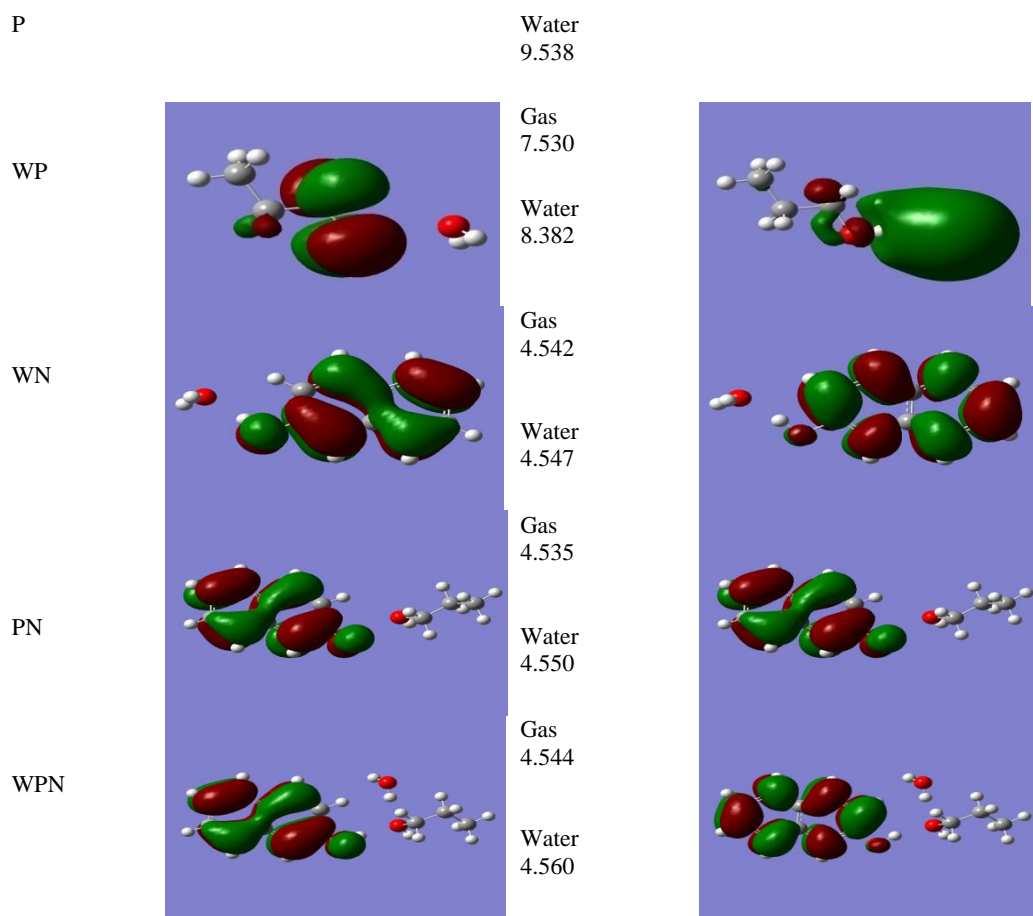
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ABSTRACT

Density of water, 1-propanol and water+1-propanol binary solvent in pure form were experimentally measured. In these same solvents 2-naphthol was added to make saturated solutions of 2-naphthol at equilibrium. These saturated supernatant solutions were used to measured densities and molalities of 2-naphthol at (293.15 to 313.15) K and experimental data used to calculate the excess molar volumes (V^E), apparent molar volume (V_ϕ). Redlich–Kister Equation was used to calculate excess molar volumes (V^E) to correlate with the experimental excess molar volumes (V^E) of binary solvent mixture. Regressed Parameters A_i obtained from Redlich–Kister Equation were used for calculation of partial excess molar volumes at infinite dilution ($\bar{V}_i^{E,\infty}$). Molecular interaction was explained by using Gaussian 09W software, DFT method, B3LYP 6-31(G)d as basis set.

Graphical Abstract:





HOMO, LUMO structures with LUMO-HOMO Energy Gap

Keywords: 2-Naphthol, Excess Molar Volumes (V^E), Apparent Molar Volume (V_ϕ), DFT.