

Thermodynamic Properties of Green Solvents

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Green chemistry involves reducing waste from an industrial chemical process to a minimum. Volatile organic solvents are the normal media for the industrial synthesis of organics. However, many organic solvents evaporate into the atmosphere with detrimental effects on both the environment and human health. But some high boiling liquids (alkylcarbonates or polyethers), as well as room-temperature ionic liquids, with very low vapor pressures, can be used as environmentally benign media for a range of industrially important chemical processes. We have launched the systematic study of the thermodynamic properties of prospective “green solvents”.

In this work, we have measured the vapor pressures, enthalpies of vaporization, enthalpies of sublimation, and enthalpies of combustion of ethylenecarbonate and propylenecarbonate. From these data, the enthalpies of formation in the gaseous states have been obtained.

For the sake of comparison, the high-level ab initio calculations of the same nine molecules have been performed using the GAUSSIAN-03 program package. Absolute electronic energy values of the molecules have been obtained at the G3(MP2) level of theory. Gaseous enthalpies of formation data have been calculated from atomization and isodesmic reactions, and have been found to be in good agreement with the data obtained from the thermochemical measurements.

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