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Thermodynamic Properties of 1,4-Benzoquinones in Gaseous and Condensed Phases: Experimental and Theoretical Studies

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Abstract

© 2017 American Chemical Society. A complete study of thermodynamic properties of 1,4-benzoquinones in the condensed and gaseous phases was carried out using experimental techniques and theoretical approaches. Enthalpies of combustion and formation of 2-methyl-1-4-benzoquinone were evaluated using combustion calorimetry. The transpiration method was utilized to determine the temperature dependence of the vapor pressures of 1,4-benzoquinone and 2-methyl-1,4-benzoquinone for the sublimation and vaporization enthalpies calculation. The group additivity scheme was used independently for verification of sublimation enthalpy of 2-methyl-1,4-benzoquinone. For this procedure the enthalpy of solution of 2-methyl-1-4-benzoquinone in benzene was measured at 298.15 K. The experimental values obtained were combined with published data and organized to obtain a reliable set of the experimental enthalpies of formation and enthalpies of phase transition of compounds. The methods of quantum chemistry and statistical physics based on the "rigid rotator-anharmonic oscillator" model were used to calculate thermodynamic functions of 1,4-benzoquinones in the ideal gas state in the temperature range 273.15-150 0 K. The strain enthalpy and the enthalpy of π-conjugation were also estimated.

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