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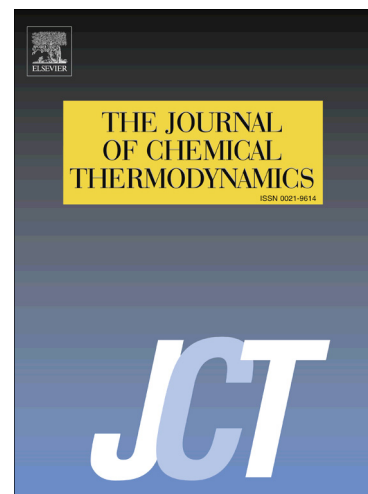
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Thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of three sulfur imidazole derivatives

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Thermochemical properties of sulfur derivatives of Imidazole were determined.

Gaussian G-n (3, 4) composite method was used to calculate formation enthalpies in gas phase

The enthalpies of sublimation were determined by Calvet-drop microcalorimetry

Experimental and theoretical results of formation enthalpies are in good agreement

Abstract

In the present work, we report the standard combustion energies of 2-mercapto-1-methylimidazole, 2-mercapto-5-aminobenzimidazole and 2-mercapto-5-methoxybenzimidazole, obtained experimentally from measurements with a rotatory-bomb combustion calorimeter. With these data, for each one of the three aforementioned compounds, the corresponding standard molar combustion enthalpies and the standard molar enthalpies of formation, in the crystalline phase, are calculated. The enthalpies of sublimation of each compound, obtained experimentally using a Calvet Setaram HT 1000 microcalorimeter, are also reported. Using the values of the enthalpies of formation in the crystalline phase and the enthalpies of sublimation, both at 298.15 K, for each compound, the corresponding standard molar enthalpies of formation in gas phase were calculated. Complementary, the enthalpies of formation in the gaseous phase were derived from theoretical calculations made with Gaussian-n composite methodology with $n = 3$ and 4. The experimental and computational studies suggest that in gaseous phase, the form more stable of each compound is the thione form.

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