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Note

RESONANCE ENERGY OF HEXAETHYLBENZENE AND HEXAMETHYLBENZENE

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In the recent literature a number of articles have appeared concerning methods of calculation of resonance energies of aromatic and pseudo-aromatic systems [1–3]. These procedures have involved combinations of theoretically estimated and experimentally determined thermochemical data. In this paper the experimental measurement of heats of atomization and resonance energy of two hexa-substituted benzene systems were derived by combustion and differential scanning calorimetry.

EXPERIMENTAL

High purity grades of commercial samples of hexaethylbenzene (HEB) and hexamethylbenzene (HMB) were obtained from Aldrich Chemical Company. All compounds were purified by zone refining and the purity was checked by C and H analysis and by high performance liquid chromatography as previously described [4]. A Perkin-Elmer DSC-1B was used for analysis of heats of sublimation at a heating rate of 8 K min^{-1} as previously described [5]. The combustion apparatus was an oxygen bomb calorimeter with a 500 ml internal volume oxygen bomb from Parr Instrument Company and its use and the equations for calculation of molecular energetics have been recently defined elsewhere [3].

RESULTS AND DISCUSSION

Table 1 contains the values for the heat of combustion (ΔH_c^0) and sublimation (ΔH_{sub}^0) as determined by these thermochemical techniques. Intrasample variation for the ΔH_c^0 and ΔH_{sub}^0 for each compound tested ($n = 10$) was $< 1.0\%$ (C.V.) and intersample variation ($n = 10$) was $< 1.4\%$ (C.V.). Resonance energy (RE) may be determined from the difference between the heat of atomization ($\Delta H_{f,a}^0$) in the gas phase and the sum of the

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TABLE 1

Heats of combustion, sublimation and formation, bond and resonance energies (kcal mol^{-1})

Compound	ΔH_c^0	ΔH_{sub}^0	$\Delta H_{f,a}^0$	$\Sigma \bar{E}_b$	RE
HMB	1700.10 ± 1.25	17.90 ± 0.15	3014.08	2973.90	40.18
HEB	2635.42 ± 1.33	9.88 ± 0.22	4711.60	4666.50	45.10

bond energies ($\Sigma \bar{E}_b$) of a fixed bond structure for a resonating molecule. The respective values for the two compounds are listed in Table 1. It should be noted that the RE of these two substituted benzene systems are within the range of agreement of the RE of some *ortho*-substituted benzoic acids that have been previously determined by this experimental method [3]. Also, the use of these instrumental techniques have provided rapid and accurate analysis of some previously unknown thermochemical data for the compounds in question.

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