Energetic Study of Six Aminomethylbenzoic Acids

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Aminobenzoic acid derivatives are unnatural amino acids that are used as building blocks for peptide and peptidomimetic synthesis. The aim of this work is to study the energetics of some selected aminomethylbenzoic acids, centered on the study of the influence of the position of the groups in the relative stability in the gas phase. The amino group is an electron donor and the carboxylic acid group is an electron acceptor. The motivation to do this work arises from the unknown energetic effect of the insertion of a methyl group on the respective aminobenzoic acid.

Studied aminomethylbenzoic acid isomers:
2-amino-3-methylbenzoic acid;
2-amino-5-methylbenzoic acid;
2-amino-6-methylbenzoic acid;
3-amino-2-methylbenzoic acid;
3-amino-4-methylbenzoic acid;
4-amino-3-methylbenzoic acid;

The energies of combustion of the six aminomethylbenzoic acid isomers were measured at T=298.15 K by static bomb calorimetry. The standard molar enthalpies of formation in the gaseous state were derived using the molar enthalpies of sublimation published recently [1] for the same series of compounds.

The experimental results obtained in this series were compared with the relative stability obtained by *Ab-Initio*/DFT (B3LYP) calculations in terms of ring charge distribution, NICS values and aromatic stabilization energies.

[1] M.J.S. Monte, D.M. Hillesheim, *J. Chem. Thermodynamics* **33**, 745-754 (2001).