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Thermochemical Data of Carboxylic acids, Esters and Iodo Compounds

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Abstract

Bond separation energy (BSE) group equivalents had been developed for aliphatic ethers. The developed equivalents were used in the calculations of the effective stabilization energy, SE_eff, values of aliphatic saturated carboxylic acids and esters. The strain energies of the compounds of both classes were also calculated by adding of the standard stabilization (resonance) energies of formic acid and methyl formate to the SE_eff value of the acid or the ester. The obtained strain energies correlate well with those obtained via the strain-free group equivalents. The developed equivalents were also used in the calculations of the SE_eff values of unsaturated and aromatic carboxylic acids and esters. The obtained results are consistent with known principles.

Iodine increment ("I" increment) had also been developed to calculate the zero point energy, ZPE, values of iodine-containing organic compounds. The reliability of the developed increment is tested by the calculation of the ZPE values of twenty-four compounds whose
experimental ZPE values are known. This test reveals that the developed increment is reliable in reproducing the ZPE values of iodine-containing organic compounds.