THE DETERMINATION OF CONSISTENT AND ACCURATE VALUES OF ?rHo(CaHbOd, a [?] 16) OF ATOMIZATION OF THE AROMATIC COMPOUNDS BY THE SIMULTANEOUS USE OF THE EMPIRICALLY CORRECTED RESULTS AND UNCERTAINTIES OF SEVERAL QUANTUM MECHANICAL APPROACHES.

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Abstract

The empirical linear scaling dependencies between the literature (?rHo(Xn,TAB)) and the calculated (?rHo((Xn)i,CALC)) values of atomization of 31 reference aromatic and related compounds (T=298.15K), as well as their standard errors ((SE4)i?(?4)i, Stand.Dev.), are determined for the different quantum mechanical (QMi) approaches. These dependencies are compared and used for the determination of the values of ?rHo((Xn)i,CORRE)±3(SE4)i of atomization reactions of considered not reference aromatic compounds, as well as for the determination of their values of ?fHo((Xn)i,CORRE)+-3(SE4)i. The values of ?fHo((Xn)i,CORRE)MEAN+-3SEYE ([?]99.4% confidence interval), determined using the intersections of the 3(SE4)i intervals, are consistent with all QMi approaches and their literature values. The M06-2X/6-311++G(d,p), M08HX/6-311++G(d,p) and wB97XD/6-311++G(d,p) approaches are recommended for the achievement of accuracy (SEYE)[?]3.8 kJ/mol of the calculated values of ?fHo((Xn)i,CORRE)MEAN. The effects of the number of O-H groups, size and multiplicity of compounds on values of error, also studied in this work, demonstrate the limitations of using of several scaled dependencies.

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