Quantum Calculations to Estimate the Heat of Hydrogenation Theoretically

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Abstract

Standard enthalpies of hydrogenation of 29 unsaturated hydrocarbon compounds were calculated in the gas phase by CCSD(T) theory with complete basis set cc-pVXZ, where X = DZ, TZ, as well as by complete basis set limit extrapolation. Geometries of reactants and products were optimized at the M06-2X/6-31g(d) level. These M06-2X geometries were used in the CCSD(T)/cc-pVXZ//M06-2X/6-31g(d) and cc-PV(DT)Z extrapolation calculations. (MAD) the mean absolute deviations of the enthalpies of hydrogenation between the calculated and experimental results range from 8.8 to 3.4 kJ mol-1 based on the Comparison between the calculation at CCSD(T) and experimental results. The MAD value has improved and decreased to 1.5 kJ mol-1 after using a complete basis set limit extrapolation. The deviations of the experimental values are located inside the "chemical accuracy" (±1 kcal mol-1 [?] +-4.2 kJ mol-1) as some results showed. Very good linear correlations between experimental and calculated enthalpies of hydrogenation have been obtained at CCSD(T)/cc-pVTZ//M06-2X/6-31g(d) level and CCSD(T)/cc-PV(DT)Z extrapolation levels (SD =2.11 and 2.12 kJ mol-1, respectively).

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References

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