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Investigation on molar heat capacity, standard molar enthalpy of combustion for guaiacol and acetyl guaiacol ester

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Abstract: The molar heat capacities (C_p) of guaiacol(CAS 90-50-1) and acetyl guaiacol ester (AGE, CAS 613-70-7) were determinated from 290 K to 350 K by differential scanning calorimetry (DSC), and expressed as a function of temperature. Two kinds of group contribution models were used to estimate the molar heat capacities of both guaiacol and AGE, the average relative deviation is less than 10%. The standard molar enthalpies of combustion of guaiacol and AGE were -3590.0 kJ·mol^{-1} and -4522.1 kJ·mol^{-1} by a precise thermal isolation oxygen bomb calorimeter. The standard molar enthalpies of formation of guaiacol and AGE in a liquid state at 298.15 K were calculated to be -307.95 kJ·mol^{-1}and -448.72 kJ·mol^{-1}, respectively, based on the standard molar enthalpies of combustion. The thermodynamic properties are useful for exploiting the new synthesis method, engineering design and industry production of AGE using guaiacol as a raw material.

Key words: Guaiacol; Acetyl guaiacol ester (AGE); Molar heat capacity; Standard molar enthalpy of combustion

List of symbols

ε	The heat capacity of calorimeter, J·K^{-1}
C	The molar heat capacity of sample, J·K^{-1}·mol^{-1}
D	The signal value of DSC for sample, mW
H	Enthalpy, kJ·mol^{-1}
m	Mass of the tested sample, mg
Q	Quantity of heat, J·mol^{-1} or kJ·mol^{-1}