CHEMISTRY OF MOLECULAR SYSTEMS

Thermodynamic properties of some furan derivatives in different aggregate states

A.Yu. Arlovich, Y.N. Yurkshtovich, A.A. Aleinikava,
A.V. Blokhin, M.B. Charapennikau
Belarusian State University, Minsk, Belarus,
e-mail: *arlovicha@mail.ru*

Furan derivatives are promising heterocyclic compounds, which can exhibit unique cytotoxic, antitumor, antispamidic or anti-feeding activities [1]. Ethyl-2-cyano-3-(furan-2-yl)-prop-2-enoate (ECFP) and its phenyl derivative (PhECFP) are prepared via the Knoevenagel condensation reaction. The standard thermodynamic functions of ECFP and PhECFP in the ideal gas state were calculated using statistical thermodynamics approach in the temperature range (0 – 1500) K. The optimized geometry, harmonic vibrational frequencies, potential energy surface scans have been investigated by density functional theory (DFT) on B3LYP method with 6-311++G(d, p) level of theory. An excellent agreement between the optimized geometry in gaseous state and the molecular structure in solid state obtained through X-ray study of ECFP [2] was noticed. The molar heat capacities at 298.15 K were (201.4 ± 0.8) $J \cdot mol^{-1} \cdot K^{-1}$ and (279.2 ± 1.1) $J \cdot mol^{-1} \cdot K^{-1}$ for ECFP and PhECFP respectively. These values were compared with the results of Joback's additive scheme. The standard thermodynamic functions of ECFP and PhECFP in the crystalline state were obtained using the temperature dependence of the heat capacity in the range of (80 – 340) K for ECFP and (80 – 370) K for PhECFP.

The standard enthalpies of formation in gaseous state for ECFP and PhECFP were determined using isodesmic reaction scheme and the composite quantum chemical method Gaussian-4. The obtained results were –(232.2 ± 1.3) kJ mol^{-1} for ECFP and –(111.2 ± 12.6) kJ mol^{-1} for PhECFP. The calculated enthalpies of formation in gaseous state are in good accordance with the experimental values [3]: –(230.0 ± 8.5) kJ mol^{-1} for ECFP and –(113.4 ± 7.5) kJ mol^{-1} for PhECFP. Applying of Joback's additive scheme for prediction standard enthalpies of formation in gaseous state for furan derivatives was considered. The way of modifying this scheme was offered.

The additive scheme for prediction standard enthalpy of sublimation based on isodesmic reactions was proposed. The results obtained were (106.5 ± 1.2), (104.3 ± 0.5) and (111.2 ± 0.2) kJ mol^{-1}, for 2-furanacrylic acid, 3-furanacrylic acid and ECFP, respectively.

References

[1] H. Ghalla et al. J. Molecular Structure (2014) 1059
[2] R.G. Kalkhambkar et al. Acta Crystallographica. Section E (2012) 68:5
[3] R. Kos et al. Modern Organic Chem. Res.(2017) 2:2