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Euroopa Sotsiaalfond**



Eesti tuleviku heaks

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Revision of the Gas-Phase Acidity Scale below 300 kcal mol⁻¹

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The gas-phase acidity (*GA*) scale from (CF₃CO)₂NH to (C₂F₅SO₂)₂NH – ca 24 kcal mol⁻¹ range of gas-phase acidities – was re-examined using the FT-ICR equilibrium measurement approach [1]. Some additions and modifications to the standard methodology of *GA* measurements were introduced (estimation of partial pressures from mass spectra of the compounds, instead of the pressure gauge readings and use of long reaction times) to achieve higher reliability.

Gas-phase acidities of 18 compounds were determined for the first time. The results reveal a contraction of the previously published values in this part of the scale. In particular, the *GA* values of (CF₃SO₂)₂NH and (C₂F₅SO₂)₂NH (important components of lithium ion battery electrolytes and ionic liquids) were revised towards stronger acidities from 291.8 kcal mol⁻¹ to 286.5 kcal mol⁻¹ and from 289.4 kcal mol⁻¹ to 283.7 kcal mol⁻¹ (i.e. by 5.3 and 5.7 kcal mol⁻¹) respectively.

References

1. Leito, I.; Raamat, E.; Kütt, A.; Saame, J.; Kipper, K.; Koppel, I.A.; Koppel, I.; Zhang, M.; Mishima, M.; Yagupolskii, L. M.; Garlyauskayte, R. Yu.; Filatov, A. A. Submitted to *J. Phys. Chem. A*, **2009**, *113* (29), pp 8421–8424.