

# pH measurement and acidity scale development of acid solutions in 1,2-dichloroethane

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Measuring pH in aqueous media is typically straightforward, however it becomes a challenge when dealing with pure organic solvents or solvent mixtures. The difficulty lies on the incomparability of conventional pH values between different solvents, which means that each solvent has its own pH scale.<sup>1,2</sup> The introduction of the unified pH ( $\text{pH}_{\text{abs}}$ ) concept allows the measurement of absolute  $\text{pH}_{\text{abs}}$  values from different solvents and align their specific scales with the conventional aqueous pH scale.<sup>3,4</sup> The measurements of  $\text{pH}_{\text{abs}}$  had already been performed in aqueous-organic mixtures (ethanol, methanol and acetonitrile).<sup>1,3,5,6</sup> In this work, the focus was on a low polarity organic solvent, 1,2-dichloroethane (1,2-DCE). Despite its low conductivity, 1,2-DCE exhibits very low basicity and sufficient polarity, making it suitable for studying acids and superacids.<sup>7</sup>

19 different acid solutions (0.001 M) at half-equivalence point ( $\text{pH} \approx \text{p}K_{\text{a}}$ ) were prepared in 1,2-DCE and potential measurements were taken using the method called differential potentiometry. The setup included a symmetric cell with two glass (half-cell) electrodes and an ionic liquid, triethylammonium bis(trifluoromethylsulfonyl)imide  $[\text{N}_{2225}][\text{NTf}_2]$ , as the salt bridge electrolyte to measure the potential difference between two solutions.<sup>3,8,9</sup> A  $\text{pH}_{\text{abs}}^{\text{DCE}}$  scale in 1,2-DCE, where the  $\text{pH}_{\text{abs}}$  scale is shifted to align to the previously reported UV-Vis spectrophotometric/computational 1,2-DCE pH scale,<sup>7</sup> was constructed using the “ $\text{pH}_{\text{abs}}$  ladder” method and is presented in this work. The  $\text{pH}_{\text{abs}}^{\text{DCE}}$  values of the studied solutions were also compared to the previously reported  $\text{p}K_{\text{a}}$  values<sup>7</sup> using UV-vis spectrophotometric titration method.

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## References

- 1 L. Deleebeeck, A. Snedden, D. Nagy, Z. Szilágyi Nagyné, M. Roziková, M. Vičarová, A. Heering, F. Bastkowski, I. Leito, R. Quendera, V. Cabral and D. Stoica, *Sensors*, 2021, **21**, 3935.
- 2 D. Himmel, S. K. Goll, I. Leito and I. Krossing, *Angewandte Chemie International Edition*, 2010, **49**, 6885–6888.
- 3 A. Suu, L. Jalukse, J. Liigand, A. Kruve, D. Himmel, I. Krossing, M. Rosés and I. Leito, *Anal. Chem.*, 2015, **87**, 2623–2630.
- 4 V. Radtke, D. Stoica, I. Leito, F. Camões, I. Krossing, B. Anes, M. Roziková, L. Deleebeeck, S. Veltzé, T. Näykki, F. Bastkowski, A. Heering, N. Dániel, R. Quendera, L. Liv, E. Uysal and N. Lawrence, *Pure and Applied Chemistry*, 2021, **93**, 1049–1060.
- 5 F. Bastkowski, A. Heering, E. Uysal, L. Liv, I. Leito, R. Quendera, L. Ribeiro, L. Deleebeeck, A. Snedden, D. Nagy, Z. N. Szilágyi, F. Camões, B. Anes, M. Roziková and D. Stoica, *Anal Bioanal Chem*, 2024, **416**, 461–465.
- 6 A. Heering, M. Lahe, M. Vilbaste, J. Saame, J. P. Samin and I. Leito, *Analyst*, 2024, **149**, 1481–1488.
- 7 E. Paenurk, K. Kaupmees, D. Himmel, A. Kütt, I. Kaljurand, I. A. Koppel, I. Krossing and I. Leito, *Chem. Sci.*, 2017, **8**, 6964–6973.
- 8 A. Heering, D. Stoica, F. Camões, B. Anes, D. Nagy, Z. Nagyné Szilágyi, R. Quendera, L. Ribeiro, F. Bastkowski, R. Born, J. Nerut, J. Saame, S. Lainela, L. Liv, E. Uysal, M. Roziková, M. Vičarová, A. Snedden, L. Deleebeeck, V. Radtke, I. Krossing and I. Leito, *Symmetry*, 2020, **12**, 1150.
- 9 A. Heering, F. Bastkowski and S. Seitz, *J. Sens. Sens. Syst.*, 2020, **9**, 383–389.