

Thermophysical Characterization of Anthraquinone Derivatives: A Comprehensive Study

V.L.S. Freitas^{1,*}, N.M.C.C. Mbelela¹, R. Castro^{2,3}, and M.D.M.C. Ribeiro da Silva¹

¹CIQUP-IMS, Department of Chemistry and Biochemistry, Faculty of Sciences,
University of Porto, Rua do Campo Alegre, P-4169-007 Porto, Portugal;

²CQC/IMS, Chemistry Department, University of Coimbra, Coimbra, Portugal

³Faculty of Pharmacy, University of Coimbra, Coimbra, Portugal

*vera.freitas@fc.up.pt

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Anthraquinones (AQs) have been considered for large-scale energy storage applications, garnering significant interest about the influence of different functional groups on their potential as anolytes in fully organic redox flow batteries [1]. Due to the scarcity of thermodynamic data for these compounds, our goal is to augment this knowledge by focusing on three specific AQs: leucoquinizarin, danthron, and 2-methylantraquinone (Figure 1). Analytical techniques such as thermal methods, infrared spectroscopy, and X-ray crystallography were employed to detect, study, and characterize the polymorphs present in these compounds.

A thermophysical study was conducted to determine the phase transition enthalpies of AQs. The differential scanning calorimetry (DSC) was used to determine the enthalpy of fusion of each AQ at the corresponding melting temperature. The enthalpies of sublimation of the AQs were determined using two techniques: i) Calvet microcalorimetry, considered a direct method for the determination of this parameter; and ii) the Knudsen effusion technique, regarded as an indirect method, as it measures vapor pressures as a function of temperature. For the latter technique, the Clausius-Clapeyron equation was employed to derive the enthalpy of sublimation.

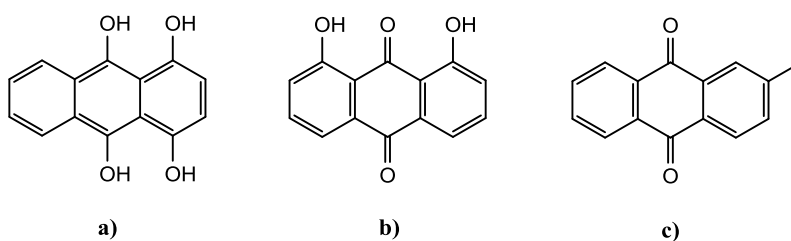


Figure 1. Structural formulae of anthraquinone derivatives: a) leucoquinizarin, b) danthron, c) 2-methylantraquinone..

[1] M.R. Gerhardt et al. (2017): **Anthraquinone derivatives in aqueous flow batteries**, *Adv. Energy Mater.* 8, 1601488.

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