See discussions, stats, and author profiles for this publication at: https://www.researchgate.net/publication/263982234

Comment on "Measurement of Low Air-Water Partition Coefficients of Organic Acids by Evaporation from a Water Surface"

ARTICLE in JOURNAL OF CHEMICAL & ENGINEERING DATA · MAY 2013

Impact Factor: 2.04 · DOI: 10.1021/je400209b

READS

6

1 AUTHOR:



Sierra Rayne Chemologica Research

270 PUBLICATIONS 2,291 CITATIONS

SEE PROFILE



Comment on "Measurement of Low Air—Water Partition Coefficients of Organic Acids by Evaporation from a Water Surface"

Sierra Rayne*

Chemologica Research, PO Box 74, 318 Rose Street, Mortlach, Saskatchewan SOH 3EO, Canada

In their article, Li et al. 1 report on experimental determinations of the air—water partitioning coefficient $(K_{\rm AW})$ for n-perfluorooctanoic acid (n-PFOA). The authors use an aqueous phase pH of 0.6 to determine the $K_{\rm AW}$ for n-PFOA and state "that the pH of 0.6 used to necessitate complete protonation of PFOA in solution may have an impact on the measured $K_{\rm AW}$. Further work is being conducted at higher pHs where partial ionization occurs and allowance of this effect must be included." The monomeric aqueous p $K_{\rm a}$ of n-PFOA is now established at about zero. 2-4 Thus, Li et al. 1 determined the $K_{\rm AW}$ of this compound at a pH value (0.6) for which a significant portion of n-PFOA would apparently have been dissociated (in contrast to the authors' claims of achieving "complete protonation of PFOA in solution"). This calls into question the accuracy of the experimental data for n-PFOA reported in Li et al. 1 as the authors do not appear to have accounted for analyte dissociation in their calculations.

AUTHOR INFORMATION

Corresponding Author

*E-mail: sierra.rayne@live.co.uk. Tel.: + 1 306 690 0573. Fax: + 1 306 690 0573.

Notes

The authors declare no competing financial interest.

■ REFERENCES

- (1) Li, H.; Ellis, D.; Mackay, D. Measurement of low air—water partition coefficients of organic acids by evaporation from a water surface. *J. Chem. Eng. Data* **2007**, *52*, 1580–1584.
- (2) Goss, K. U. The pK_a values of PFOA and other highly fluorinated carboxylic acids. *Environ. Sci. Technol.* **2008**, 42, 456–458.
- (3) Cheng, J.; Psillakis, E.; Hoffmann, M. R.; Colussi, A. J. Acid dissociation versus molecular association of perfluoroalkyl oxoacids: Environmental implications. *J. Phys. Chem. A* **2009**, *113*, 8152–8156.
- (4) Rayne, S.; Forest, K. Theoretical studies on the pK_a values of perfluoroalkyl carboxylic acids. *J. Mol. Struc. THEOCHEM* **2010**, 949, 60–69.

Received: March 2, 2013 Accepted: April 10, 2013 Published: May 2, 2013

