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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Compilation of Henry's law constants, version 3.99" *by* R. Sander

Anonymous Referee #2

Received and published: 28 December 2014

Henry's law values are of great importance for the calculation of partitioning of species between the aqueous phase and gas phase. It is especially useful for modeling aqueous aerosol and cloud chemistry. Sander (2014) ACPD is an ambitious and useful compilation of Henry's law constants for a variety of compounds. I find the section on the different ways that Henry's law constants are calculated to be particularly thorough. I found some other sections to be too concise. Overall, I have minor comments and recommend publication after minor revisions.

General Comments

1. I don't like the use of k_H for the Henry volatility symbol. I understand that the author is endeavoring to be consistent with IUPAC terminology, but in chemistry k is reserved for rate constants, while K is used for equilibrium constants. This work has the potential to set standards for notation and I can envision this value being used in

equations also involving rate constants where the use of k_H could be confusing since it is an equilibrium constant. Unless there are conflicts with fields outside of chemistry with using K_H, I would recommend K_H over k_H for the volatility symbol.

2. Table 6: Can the author explain why all values have two significant figures, especially for when the original measurements may have had the precision to merit additional significant figures? This might be best addressed in the supplemental information unless the explanation is short.

Specific Comments

3. Line 20, page 29619: Can the author provide a brief (1-2 sentence) overview of Ostwald coefficients?

4. Line 10, page 29622: Does the author have a reference for K_{AW}?

5. Line 2, page 29625: The section on Setschenow constants is extremely brief. Can the author provide examples of how Setschenow parameters are defined, and explain why molality is preferred?

6. Line 15, page 29625 and following paragraph: Upon reading the conclusion, it became clear that this paper is to be the peer-reviewed reference for the online database henrys-law.org. However, out of that context this paragraph is confusing. I recommend an explanation in this paragraph of the online database. Even in the context of understanding the database and that this is the reference, several points are unclear. Why was it necessary to recalculate values and how were they recalculated? I am unfamiliar with the term "grey literature". I suggest addressing this and the comment on Table 6 (comment 2 above) about significant digits with a detailed explanation in the supplemental information.

7. Line 22, page 29625 and following paragraph: The description of the sorting order requires elaboration. It is currently unclear where to locate compounds containing multiple elements – e.g. does NO_2 appear in the N section or the O section?

8. Line 3, page 29630 and following paragraph: This section seems too brief since it has the potential to be quite useful to people making Henry's law measurements. If the review articles have a theme (e.g. inorganic gas solubility in sea water), could the author indicate that in the review list?

9. Line 6, page 29630: Is there any practical guidance from Smith and Harvey (2007) that is worth repeating here?

10. Line 10, page 20630: If these papers contain one way of measuring (or calculating) Henry's law values, can that briefly be listed next to the citation?

11. Section 3.2.4: The author is missing several references, including the original reference to Setschenow constants:

Setschenow, J. Über die Konstitution der Salzlösungen auf Grund ihres Verhaltens zu Kohlensäure. Z. Phys. Chem. 1889, Vierter Band (1), 117−125.

Additional references on salting constants (in addition to those mentioned by Reviewer 1) include:

McDevit and Long (1952) JACS, The Activity Coefficient of Benzene in Aqueous Salt Solutions

Gordon and Thorne (1967) JPC, Salt Effects on the Activity Coefficient of Naphthalene in Mixed Aqueous Electrolyte Solutions I Mixtures of Two Salts

Gordon and Thorne (1967) Geochimica et Cosmochimica Acta, Salt effects on non-electrolyte activity coefficients in mixed aqueous electrolyte solutions - II Artificial and natural sea waters

Almeida et al (1983) Can J Chem, Setchenow coefficients for naphthols by distribution method

Sanemasa et al (1984) Bull Chem Soc Jpn, The Effects of Salts on the Solubilities of Benzene, Toluene, Ethylbenzene, and Propylbenzene in Water

Endo et al (2012) EST, Salting-Out Effect in Aqueous NaCl Solutions - Trends with Size and Polarity of Solute Molecules

Yu and Yu (2013) Industrial Engineering Chemistry Research, Setschenow Constant Prediction Based on the IEF-PCM Calculations

Wang et al (2014) EST, Measuring and Modeling the Salting-out Effect in Ammonium Sulfate Solutions

Environmental Organic Chemistry by Rene P. Schwartzenbach (2002) Wiley-Interscience also has a nice section on salting constants and Henry's law constants.

Technical Corrections

12. Line 6, page 29624: change "ways" to "methods"

13. Line 11, page 29625: change "(about 20...25C and 1 atm)" to "(between 20 and 25C and 1 atm)"

14. Line 23, page 29625: The term "organic" typically refer to those that contain C and H (and heteroatoms if applicable). I suggest changing "organic substances" to "carbon-containing compounds".

15. Line 22, page 29626: I think that CO and CO_2 are likely to be species of very high interest and would thus merit their own listings in this section.

16. Line 23, page 29629: You could say this more concisely as "The table in the online version of this document has been hyperlinked to the appropriate notes, and to NIST Chemistry WebBook from the CAS numbers.

17. It should be Setschenow constants, rather than Setschenov constants.

Interactive comment on Atmos. Chem. Phys. Discuss., 14, 29615, 2014.