# Commentary

# Why Not Replace pH and pOH by Just One Real Acidity Grade, AG?

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At several stages of the educational process students encounter pH. Depending on the curriculum involved, this term may be introduced without a formal definition. With the introduction of pH several problems arise. A significant number of these could be eliminated if instead of pH and pOH a new quantity, the acidity grade AG, were introduced:

$$AG = \log [H^+]/[OH^-]$$

This article discusses the pros and cons regarding an introduction of AG.

# Historical and Linguistic Background

Most likely, the term "acid" was used for the first time in the "Rasarnava" manuscript by Indian scientists (1200 B.C.E.) (1). It would take some thirty centuries before the three famous acids nitric acid, sulfuric acid, and hydrochloric acid were described. Around 1800, both Davy and Dulong recognized hydrogen as the essential element of acids. Yet in some languages, such as German and Dutch, the word for oxygen literally means "acid substance". In 1889 Walter Nernst, a German scientist, expressed the electric potential as a function of [logarithms of] concentrations, and in 1909 Sörensen, a Danish scientist, introduced pH with the formula

$$pH = -log [H^+]$$

According to some sources, Sörensen was studying indicators (2); other sources, however, mention that he was investigating problems concerning the brewing of... beer (3). In fact, our present pH meter is based on a combination of the thoughts of Nernst and Sörensen.

In various languages pH is referred to "acidity" or "acidity grade". This term is all but universal. For instance the corresponding terms in German (Säuregrad = Azidität) are frequently used for [H<sup>+</sup>] itself. In some German books, however, the term pH (Latin: potentia hydrogenii) is translated literally: "Wirksamkeit des Wasserstoffes" (activity of hydrogen) (4). Strangely enough, in Anglo-American textbooks there seems to be some restraint in using an expressive paraphrase for pH. During my research I ran into rather sloppy translations such as "hydrogen-ion exponent" (5). With the introduction of pH, however, you get rid of the very small and therefore inconvenient figures representing [H<sup>+</sup>].

# Disadvantages of pH and pOH

The definition of pH results in some striking disadvantages, especially at the beginning of a chemistry course. Without some knowledge of water equilibrium ( $K_w$ ) and logarithms, it is impossible for students to understand that pH = 7.0 refers to a *neutral* solution. A solution, by the way, with a rather

unusual high temperature: 25 °C (6). But it gets even worse: the *more* acidic the solution is, the *lower* the pH. In a later stage, calculating the pH of a solution of extreme acidity, a *negative* pH appears!<sup>1</sup>

After the introduction of water equilibrium and the corresponding  $K_{\rm w}$ , students will face a new surprise: even in solutions of extremely high acidity there are always some hydroxide ions present. Nonaqueous solvents offer yet more new surprises. The equivalent of pH in pure liquid ammonia equals 16.5.

# AG, a Real Acidity Grade

A lot of the disadvantages of pH mentioned above automatically disappear by defining the acidity grade AG as

$$AG = \log [H^+]/[OH^-]$$

Of course one has got to get used to this AG, especially its numerical values.<sup>2</sup> Let us compare some pH values with their AG equivalents, the latter at three different temperatures:

[H <sup>+</sup> ]/mol L <sup>-1</sup>	рН	AG		
		20 °C	25 °C	62 °C
1	0.0	14.2	14.0	13.0
0.1	1.0	12.2	12.0	11.0
0.01	2.0	10.2	10.0	9.0
1 × 10 <sup>-6</sup>	6.0	2.2	2.0	1.0
$3 \times 10^{-7}$ $(1 \times 10^{-6.5})$	6.5	1.2	1.0	0.0
$1 \times 10^{-7}$	7.0	0.2	0.0	-1.0
$8 \times 10^{-8}$ $(1 \times 10^{-7.1})$	7.1	0.0	-0.2	-1.2
1 × 10 <sup>-8</sup>	8.0	-1.8	-2.0	-1.2
1 × 10 <sup>-12</sup>	12.0	-9.8	-10.0	-11.0
1 × 10 <sup>-13</sup>	13.0	-11.8	-12.0	-13.0
1 × 10 <sup>-14</sup>	14.0	-13.8	-14.0	-15.0

Note: At the three recorded temperatures, the  $pK_w$  values are 14.2, 14.0, and 13.0, respectively.

### A Closer Look at AG versus pH

The minus in the definition of pH has been eliminated, along with the whole concept of pOH! Acidic solutions always show positive AG values. Alkaline solutions, of course being nonacidic, show negative AG values. The stronger the acidic solution, the higher the acidity grade. Unlike the pH of a neutral solution, which varies with temperature, the AG of neutral solutions always equals zero. The same holds good

for nonaqueous solutions. These AG values look more logical than the corresponding pH values, especially for the beginning student who might have no knowledge of logarithms. To the more advanced student looking at the formula of AG, it is quite clear that even the most acidic solution contains some hydroxide ions. This might increase the understanding of the chemistry of solutions. Nevertheless, at the same time the use of AG complicates simpler pH calculations: the pH of a  $0.1 \, \mathrm{M}$  HCl solution is  $-\log 0.1 = 1.0$ , that is all.

In order to calculate  $\overline{AG}$  one has to know the magnitude of  $[H^+]$  as well as  $[OH^-]$ . So the student must have some knowledge of chemical equilibrium—in particular, the heterolytic dissociation of water. On the other hand, the very same knowledge is required if one calculates the pH of alkaline solutions!

From a formal mathematical point of view, AG offers another rather unexpected advantage over pH. It is impossible to take the logarithm of a number that has a dimension, such as  $[H^+]$ . Of course, we as advanced scientists know we are dealing with relative activities instead of concentrations here, but did we ever tell this to our students? Since  $[H^+]/[OH^-]$  has no dimension we have got rid of this unwanted situation too.

Direct measurement of AG with a slightly recalibrated pH meter looks quite possible to me, since one can easily derive  $AG = pK_w - 2pH$ . Keep in mind that the present pH meter is provided with a dial to adjust for temperature.

Finally, another, though minor, advantage of AG: The *x*-axis in titration diagrams (AG versus the volume of added reagent) distinguishes the acidic area from the alkaline area.

#### Conclusion

The replacement of pH as well as pOH with acidity grade (AG, defined as AG =  $log [H^+]/[OH^-]$ ) has several advantages. Acceptance of AG after using pH and pOH for almost a century appears to be worth considering. Doing so and taking everything into account, the replacement of pH and pOH with AG faces one inevitable objection: it requires breaking with a long and therefore strong tradition...

#### **Notes**

- 1. In reality pH will never reach a negative value since such high concentrations require the use of activity constants.
- 2. Probably "acidity-base-grade" ( $\dot{A}BG$ ) is an even better, though slightly inconvenient, term.

#### **Literature Cited**

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- Vogel, A. I. A Textbook of Quantitative Inorganic Analysis; Longmans: London, 1971.
- 6. Hawkes, S. J. *J. Chem. Educ.* **1995**, *72*, 799.  $pK_w$  is almost never 14.0. This article gives some very interesting data. Most striking:  $K_w$  and so pH of pure water varies enormously under different circumstances. Under extreme geological conditions, for instance, the pH of pure water equals—1.5!