Recent Treatment of Data in Chemical Analysis

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Editorial

Not only in green chemistry but also in other fields of chemistry, there is a problem of analytical values spreading an error and noise in the case of arguing the data of substances or compounds thoroughly. Therefore, we have considered to establish a method of good assessed values based on a science of statistics for experimental data [1] taken from students' experiments of chemistry [2] including various types of analysis.

According to general discussion by Bayes's theorem, attracting attention recently, when a theoretical framework T is give, a product of probability $p(T \mid E) \propto p(T)p(E \mid T)$ can be assumed where $p(E \mid T)$ is probability after experiments, $p(T)$ is probability before experiments. Moreover, average, median, mode as the best estimated values will be within standard deviation (std) deviated from average in many cases. Thus, all the three values may be the best estimated values. Based on this theoretical background, we attempted to compare data of certain years by using two data groups (1) required amount of sodium hydroxide as before experiments (2) resulting concentration of oxalic acid as actual experimental results during neutralizing titrates (theoretical framework).

For example, neutralizing titrates of oxalic acid (weak acid) by sodium hydroxide (strong base) exhibited average required amount of sodium hydroxide was 11.3 mL (std 1.91) and pH 6.91 (std 0.42) in a certain year. Different results were obtained in another year (Table 1) or using different indicators, though theoretical framework (experiments of neutralizing titrates) was identical.

Table 1 Oxalic acid experimental results for 4 years.

Year	2010	2009	2008	2007
no. of data	32	32	36	32
average	0.049721	0.044708	0.045178	0.050472
std	0.004418	0.010489	0.010472	0.000583
median	0.0507	0.050131	0.050772	0.050477
frequency	0.06	0.06	0.06	0.06

References

1. Atsuo Yamazaki, Yosuke Mori, Maiko Ito, Takashiro Akitsu (2015) Poster presentation in 5th Chemistry Festa by the chemical society of Japan.

2. Department of Chemistry, Faculty of Science, Tokyo University of Science, Textbook of inorganic and analytical chemistry experiments 2015 edition, 2015.