

ESTIMATION OF FUNDAMENTAL PROPERTIES OF NITROGEN-CONTAINING
ORGANIC COMPOUNDS

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The observed data of fundamental, or non-spectral, physical properties of organic compounds, such as thermodynamic properties, critical constants, et al., are unexpectedly scarce because of the difficulty in measurements and in obtaining specimens with high purity necessitated, as compared with those of spectral information. Thus various methods for estimating the former have been developed.¹⁾ A new contribution method, the ABWY method, for estimating the following ones was developed by us:²⁾ vapor pressure; thermodynamic functions, including molar heat, of the ideal gas, liquid as well as solid; critical properties; heat of evaporation; normal boiling point. A computer program package EROICA²⁾ on a TSS will estimate above mentioned properties along with the others derived from the former (e.g., heat of combustion), and also retrieve the observed data from a database prepared by us, storing 7500 compounds; this system permits a rational formula, CHEMO input,⁴⁾ as an input for estimation and retrieval.

Estimation methods can be classified as depend on either structural model or functional model. On the other hand physical properties are usually estimated hierarchically; a property may be better estimated by using already estimated properties, guided by a route-map for estimation. The ABWY method employs mainly the structural model with a sophisticated group contribution method, and also utilize the functional model only when the former is not applicable as in the case of molar heat of liquid.

In the present version,²⁾ properties of compounds having even some of 28 nitrogen-containing functional groups can be processed. The accuracy of estimated values is fair; e.g., 0.5-1 kcal mol⁻¹ for enthalpies.

1) R.C. Reid, J.M. Prausnitz and T.K. Sherwood, "The Properties of Gases and Liquids," 3rd ed, McGraw-Hill Book Co., New York (1977).

2) Y. Yoneda, Bull. Chem. Soc. Jpn., 52, 1297(1979).

3) Y. Yoneda, "Information Chemistry. Computer Assisted Chemical Research Design," ed by S. Fujiwara and H.B. Mark, Jr., University of Tokyo Press, Tokyo (1975), p. 239.

4) Y. Yoneda, "Kemoguramu (CHEMOGRAM)," Maruzen, Tokyo (1972), Vol. 1. Also, see ref. 3).