NOMENCLATURE IN THERMAL ANALYSIS. PART II

R. C. MACKENZIE (Chairman), C. J. KEATTCH (Secretary)*,
D. DOLLIMORE, J. A. FORRESTER, A. A. HODGSON, and J. P. REDFERN
Nomenclature Committee of the International Confederation for Thermal Analysis
(Received March 7th, 1972)

The recommendations in the First Report of the Nomenclature Committee of the International Confederation for Thermal Analysis (ICTA)[1] have been generally well received and are at present being considered for adoption by both the International Union of Pure and Applied Chemistry and the International Standards Organization. Considerable interest has also been shown by individual scientists[2].

Since these proposals were promulgated, the Committee have drawn up a further report, the recommendations in which have been endorsed in Business Session at the Third International Conference on Thermal Analysis at Davos, Switzerland, in August, 1971. The Council of ICTA have therefore directed that this Second Report be also published as a definitive document of ICTA, with the recommendation that the conventions set out therein be adhered to in all publications in the English language. Background information on the reasons for adoption of certain conventions has already been published[3].

The Sub-Committees dealing with the German, Japanese and Russian languages have all been active and a nomenclature system in Japanese, based on the recommendations in the First Report, has now been published[4].

I. AMPLIFICATION OF FIRST REPORT

Because of the variety of opinions expressed on, and the different interpretations of, the term *pyrolysis*, the Committee consider the time inopportune to promulgate on *thermal decomposition* and related terms–see First Report, Section I (*f*).

Some confusion appears to have arisen over the term *isobaric weight-change determination* as defined in the First Report, Section IIIB, Sub-section 1. The Committee consider that this confusion could be obviated by the following statement:

> In the context of the report published in *Talanta*, 16 (1969) 1227–1230, Section IIIB, Sub-sections 1 and 2 headed, respectively, *Static* and *Dynamic*, these terms refer to environmental temperature. It should be noted that the same terms are also used with reference to environmental atmosphere.

---

*To whom enquires should be addressed: c/o Industrial and Laboratory Services, P.O. Box 9, Lyme Regis, Dorset, England.

II. DTA AND TG APPARATUS AND TECHNIQUE

In considering the terms available, certain arbitrary choices have had to be made (*e.g.* between *specimen* and *sample*) but the only term in fairly common use rejected is *inert material*.

A. DTA

The *sample* is the actual material investigated, whether diluted or undiluted.

The *reference material* is a known substance, usually inactive thermally over the temperature range of interest.

The *specimens* are the sample and reference material.

The *sample holder* is the container or support for the sample.

The *reference holder* is the container or support for the reference material.

The *specimen-holder assembly* is the complete assembly in which the specimens are housed. Where the heating or cooling source is incorporated in one unit with the containers or supports for the sample and reference material, this would be regarded as part of the specimen-holder assembly.

A *block* is a type of specimen-holder assembly in which a relatively large mass of material is in intimate contact with the specimens or specimen holders.

The *differential thermocouple** or *ΔT thermocouple** is the thermocouple* system used to measure temperature difference.

B. TG

A *thermobalance* is an apparatus for weighing a sample continuously while it is being heated or cooled.

The *sample* is the actual material investigated, whether diluted or undiluted**.

The *sample holder* is the container or support for the sample.

C. DTA and TG

The *temperature thermocouple** or *T thermocouple** is the thermocouple* system used to measure temperature; its position with respect to the sample should always be stated.

The *heating rate* is the rate of temperature increase, which is customarily quoted in degrees per minute (on the Celsius or Kelvin scales). Correspondingly, the cooling rate is the rate of temperature decrease. The heating or cooling rate is said to be *constant* when the temperature–time curve is linear.

In simultaneous DTA–TG definitions follow from those given for DTA and TG separately.

---

*Should another thermosensing device be used, its name should replace thermocouple.
**Samples used in TG are normally not diluted, but in simultaneous TG and DTA diluted samples might well be used.

III. DTA AND TG CURVES

The Committee, in reaffirming their decision to use the terms *differential thermal* or *DTA curve*, *thermogravimetric curve* or *TG curve* and *derivative thermogravimetric curve* or *DTG curve*, recommend disuse of the other terms which have appeared in the literature, such as thermogravimetric analysis curve, thermolysis curve, thermoweighing curve, thermogravigram, thermoponderogram, thermogram, differential thermogravimetric curve, differential thermogram, derivative thermogram, polytherm, etc.

Certain conventions and reporting procedures for DTA and TG curves have already been specified[1,5]. The following definitions are to be read in conjunction with these recommendations.

A. DTA

In DTA **it must be remembered** that although the ordinate is conventionally labelled ΔT, the output from the ΔT thermocouple will in most instances vary with temperature, and the measurement recorded is normally the e.m.f. output, E [*i.e.*, the conversion factor, b, in the equation $\Delta T = bE$ is not constant since $b = f(T)$]. A similar situation occurs with other sensor systems.
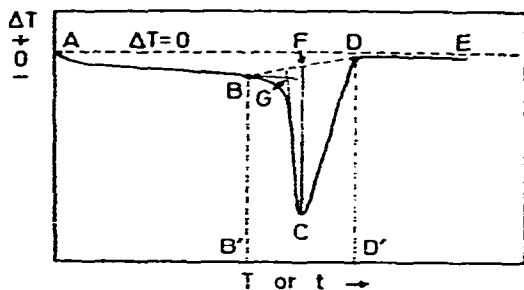

Fig. 1. Formalized DTA curve.

All definitions refer to a single peak such as that shown in Fig. 1: multiple peak systems, showing shoulders or more than one maximum or minimum, can be considered to result from superposition of single peaks.

The *base line* (Fig. 1, AB and DE) corresponds to the portion or portions of the DTA curve for which ΔT is approximately zero.

A *peak* (Fig. 1, BCD) is that portion of the DTA curve which departs from, and subsequently returns to, the base line.

An *endothermic peak* or *endotherm* is a peak where the temperature of the sample falls below that of the reference material (*i.e.*, ΔT is negative).

An *exothermic peak* or *exotherm* is a peak where the temperature of the sample rises above that of the reference material (*i.e.*, ΔT is positive).

74

Peak width (Fig. 1, B'D') is the time or temperature interval between the points of departure from and return to the base line*.

Peak height (Fig. 1, CF) is the distance, vertical to the time or temperature axis, between the interpolated base line* and the peak tip (Fig. 1, C).

Peak area (Fig. 1, BCDB) is the area enclosed between the peak and the interpolated base line*.

The *extrapolated onset* (Fig. 1, G) is the point of intersection of the tangent drawn at the point of greatest slope on the leading edge of the peak (Fig. 1, BC) with the extrapolated base line (Fig. 1, BG).
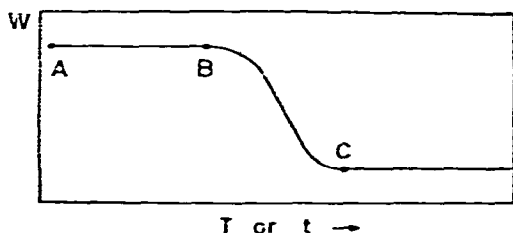

Fig. 2. Formalized TG curve.

B. TG

All definitions refer to a single-stage process such as that shown in Fig. 2; multistage processes can be considered as resulting from a series of single-stage processes.

A *plateau* (Fig. 2, AB) is that part of the TG curve where the weight is essentially constant.

The *initial temperature*, T_i, (Fig. 2, B) is that temperature (on the Celsius or Kelvin scales) at which the cumulative weight change reaches a magnitude that the thermobalance can detect.

The *final temperature*, T_f, (Fig. 2, C) is that temperature (on the Celsius or Kelvin scales) at which the cumulative weight change reaches a maximum.

The *reaction interval* is the temperature difference between T_f and T_i as defined above.

IV. ACKNOWLEDGMENTS

*There are several ways of interpolating the base line and that given in Fig. 1 is only an example. Location of points B and D (Fig. 1) depends on the method of interpolation of the base line.

REFERENCES

1 *Talanta*, 16 (1969) 1227.
2 *Chem. Ind.*, (1970) 272, 449, 515, 643; (1971) 57.
3 R. C. Mackenzie, *J. Therm. Anal.*, 4 (1972) 215.
4 *Calorim. Therm. Anal. Newslett.*, 2 (1971) 45.
5 *Anal. Chem.*, 39 (1967) 543.