

NOMENCLATURE IN THERMAL ANALYSIS, PART V: SYMBOLS

R. C. MACKENZIE

The Macaulay Institute for Soil Research, Craigiebuckler, Aberdeen, AB9 2QJ, UK.

(Received December 31, 1980)

The past few years have seen further evidence of the impact on international thinking of the reports [1–4] of the Nomenclature Committee of the International Confederation for Thermal Analysis (ICTA). For example, a combined version of the second and third reports has been published as definitive recommendations of IUPAC [5] (who are also publishing the fourth report as a provisional nomenclature document [6]), ASTM are revising their 1973 publication [7] in the light of more recent observations of the Committee and the second report has been quoted in a standard soil-science glossary [8]. The fourth report has now appeared in Japanese [9] and Chinese [10], whilst composite recommendations based on several reports have been framed in English [11], Portuguese [12], Slovak [13] and Russian [14]. Thus, of the major languages, only German and Spanish lack definitive publications.

Since the last report, a Working Group on Symbols, consisting of Dr. J. H. Sharp, UK (Chairman), Dr. J. H. Flynn, USA, and Dr. F. W. Wilburn, UK, have, after consultation with active thermal analysts in the USA (through ASTM) and the UK (through the Thermal Methods Group) drawn up a report that was accepted by the main Committee, Council of ICTA and the Business Session of the Sixth International Conference on Thermal Analysis, Bayreuth, Federal Republic of Germany, in July 1980. Council of ICTA have therefore directed that it be published as a definitive document of ICTA, with the request that the recommendations herein be adhered to in all publications in the English language. In doing so, the Committee also wish to draw attention to the recent IUPAC pronouncement on the use of abbreviations in the chemical literature [15].

Symbols in Thermal Analysis

The following recommendations relate to symbols employed in connection with TG, DTG, DTA and DSC – currently the most widely used techniques:

1. The international system of units (SI units) should be adhered to, except in rare instances where recommended symbols conflict with long-established practice.
2. The use of symbols with superscripts, such as \dot{T} , should be avoided.

3. The use of double subscripts, such as T_{sp} or T_{pd} , should be avoided. If such symbols are deemed necessary they must be clearly defined on first introduction in the publication.

4. Notwithstanding Recommendation 1 above, the symbol T should be used for temperature whether expressed in degrees Celsius ($^{\circ}\text{C}$) or in Kelvin (K). For temperature interval the symbol K or $^{\circ}\text{C}$ can be used in accordance with Resolution 3 of the 13th General Conference of Weights and Measures (CGPM) (see *Compt. rend. 13th CGPM*, 1967–68, p. 104).

5. The symbol t should be used for time, whether expressed in seconds (s), minutes (min) or hours (h).

6. The heating rate can be expressed either as dT/dt , when a true derivative is intended, or as β in K min^{-1} (see Recommendation 4 above). The heating rate so expressed need not be constant and can be positive or negative.

7. The symbols m for mass and W for weight* are recommended.

8. The symbol α is recommended for the fraction reacted.

9. The ordinate in DTA should be expressed in terms of ΔT , the difference in temperature between the sample and the reference material.

10. The ordinate in DSC should be expressed in terms of dQ/dT or dQ/dt rather than dH/dT or dH/dt , since Q represents quantity of heat or electricity whereas H represents enthalpy.

11. The following rules should be observed for subscripts:

(a) Where the subscript relates to an object, it should be a capital letter, e.g.

m_S represents the mass of the sample;

T_R represents the temperature of the reference material.

(b) Where the subscript relates to a phenomenon occurring, it should be in the lower case, e.g.

T_g represents the glass transition temperature;

T_c represents the temperature of crystallization;

T_m represents the temperature of melting;

T_{σ} represents the temperature of a solid-state transition.**

(c) Where the subscript relates to a specific point in time or to a point on the curve, it should be in lower case or in figures, e.g.

T_i represents the initial temperature;

m_f represents the final mass;

$t_{0.5}$ represents the time at which the fraction reacted is 0.5;

$T_{0.3}$ represents the temperature at which the fraction reacted is 0.3;

T_p represents the temperature of the peak;

T_e represents the temperature of the extrapolated onset (as defined in *Talanta*, 19 (1972), 1079–1081).

* A quantity of the same nature as a force — i.e. the product of mass and the acceleration due to gravity (see *Compt. rend. 3rd CGPM*, 1901, p. 70).

** The greek σ is recommended as subscript here since T_s could possibly be confused with T_s and double subscripts are to be avoided (see Recommendation 3).

Composition of Committee

During the period 1977–1980 the Committee was constituted as follows: *Chairman*: Dr. R. C. Mackenzie, UK; *Vice-Chairman*: Dr. T. Daniels, UK; *Secretary*: Dr. C. J. Keattch, UK; *Members*: Dr. D. Dollimore, UK, Dr. J. H. Sharp, UK, Dr. F. W. Wilburn, UK; *Ex-Officio Members*: The President and Secretary of ICTA (Dr. H. G. McAdie, Canada, and Dr. O. T. Sørensen, Denmark) and Chairmen of Standing Committees (Prof. P. D. Garn, USA, Dr. J. P. Redfern, UK, and Dr. C. B. Murphy, USA); *Corresponding Members*: Dr. J. H. Flynn, USA, Dr. B. O. Haglund, Sweden, Dr. J. O. Hill, Australia, Prof. H. Kambe, Japan, (the late) Dr. M. D. Karkhanavala, India, Dr. G. M. Kline, USA, Prof. G. Lombardi, Italy, Dr. J. Rouquerol, France, and Dr. J. Šesták, Czechoslovakia.

*

The Committee wish to express their thanks to the Working Group on Symbols for their efforts, to the Analytical Division of the Royal Society of Chemistry for providing accommodation for meetings and secretarial facilities, to the Thermal Methods Group of the Division for services rendered and to thermal analysts in many countries for providing valuable comments and suggestions.

References

1. *Talanta*, 16 (1969) 1227; *Pure appl. Chem.*, 37 (1974) 439.
2. *Talanta*, 19 (1972) 1079.
3. *J. Thermal Anal.*, 8 (1975) 197.
4. *Thermochim. Acta*, 28 (1979) 1.
5. *Pure appl. Chem.*, 52 (1980) 2385.
6. *Pure appl. Chem.*, (1981) 1597.
7. "Annual Book of ASTM Standards", ASTM, Philadelphia, USA, 1973, pt 41, E473-73.
8. "Glossary of Soil Science Terms", Soil Science Society of America, Madison, Wis., USA, 1978, 22.
9. *Netsusokutei*, 5 (1978) 167.
10. *Chemistry, Taiwan* (2), (1979) B1–B3.
11. G. Lombardi, "For Better Thermal Analysis", University of Rome and ICTA, 1977, 13; 2nd ed., 1980, 15.
12. *Cerâmica, Brasil*, 26 (1980) 17.
13. *Zborn. VIII Celoštát. Konf. term. Analýze, Vysoké Tatry, 1979* (M. Vaniš, ed.), SVST, Bratislava, 1979, 49.
14. "Termicheskii Analiz. Tezisy Dokladov VII Vsesoyuznogo Soveshchaniya" [Thermal Analysis, Summaries of papers presented at the VII All-Union Conference] (G. E. Domburg *et al.*, eds). *Zinatne, Riga*, 1979, 2, 139.
15. *Pure appl. Chem.*, 52 (1980) 2229.