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IUPAC Recommendations

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ICTAC nomenclature of thermal analysis (IUPAC Recommendations 2014)

Abstract: The widespread use of thermal analysis (TA) by scientists as a laboratory technique carries with it a working vocabulary. This document is intended to provide those working in the field with a consistent set of definitions to permit clear and precise communication as well as understanding. Included in the document are the definitions of 13 techniques, 54 terms within the glossary, as well as symbols and units.

Keywords: differential scanning calorimetry; differential thermal analysis; evolved gas analysis; International Confederation for Thermal Analysis and Calorimetry (ICTAC); IUPAC Physical and Biophysical Chemistry Division; sample-controlled thermal analysis; thermal properties; thermodilatometry; thermogravimetry.

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1 Scope

The scope of this document is to provide scientists working in the field of thermal analysis (TA) with a consistent "definitions of terms" that are commonly used within the field to allow precise communication and understanding. Since the scope of the International Confederation for Thermal Analysis and Calorimetry (ICTAC) also covers calorimetry, a further document dealing with this latter part of nomenclature is planned, once a satisfactory international consensus is reached on this matter.

In considering all the matters of nomenclature, the current ICTAC Nomenclature Committee has followed the advice of the late Robert Mackenzie in that

- terminology should be simple, and
- names based on particular instruments should be discouraged.

2 Intent

This document acknowledges that nomenclature develops without regulated definition as the field of thermal analysis develops. Some terms used by authors and scientists rapidly become accepted by the scientific community, even if the term is not consistent with past definitions or is not grammatically correct. However, if such a term is *widely* used and understood, it is reported here.

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3 Definition of the field of thermal analysis

Thermal analysis (TA) is the study of the relationship between a sample property and its temperature as the sample is heated or cooled in a controlled manner.

4 Techniques

A technique exists for each property or physical quantity that is measured versus temperature. A summary of some of these are presented below.

Property or physical quantity	Technique	Technique acronym	Notes
Heat	Scanning calorimetry		
Temperature	Thermometry		May also be described as heating or cooling curves.
Temperature difference	Differential thermal analysis	DTA	A technique where the temperature difference between a sample and a reference material is measured.
Heat flow rate difference	Differential scanning calorimetry	DSC	A technique where the difference between heat flow rates into a sample and a reference material is measured.
Mass	Thermogravimetry or Thermogravimetric analysis	TG TGA	In any work where a confusion may arise between TG and T_g (the glass transition temperature), the abbreviation TGA or the full term "thermogravimetry" should be used.
Dimensional and mechanical properties	Dynamic mechanical analysis	DMA	Moduli (storage/loss) are determined.
	Thermomechanical analysis	TMA	Deformations are measured.
	Thermodilatometry	TD	Dimensions are measured.
Electrical properties	Dielectric thermal analysis	DEA	Dielectric constant/dielectric loss is measured.
	Thermally stimulated current	TSC	Current is measured.
Magnetic properties	Thermomagnetometry		Often combined with TGA.
Gas flow	Evolved gas analysis	EGA	The nature and/or amount of gas/vapour are determined.
	Emanation thermal analysis	ETA	Trapped radioactive gas within the sample is released and measured.
Pressure	Thermomanometry		Evolution of gas is detected by pressure change.
	Thermobarometry		Pressure exerted by a dense sample on the walls of a constant volume cell is studied.
Optical properties	Thermoptometry		A family of techniques in which an optical characteristic or property of a sample is studied.
	Thermoluminescence	TL	Emitted light measured
Acoustic properties	Thermosonimetry or Thermoacoustimetry		Techniques where the sound emitted (sonimetry) or absorbed (acoustimetry) by the sample is studied.
Structure	Thermodiffractometry Thermospectrometry		Techniques where the compositional or chemical nature of the sample are studied.

5 Terminology and glossary

Note: For all the techniques listed here, the terminology defines the property that is measured, and each definition of a technique may be completed by adding... "as a function of temperature". For example: *dynamic mechanical analysis* (DMA), a technique where storage and loss viscoelastic moduli are determined with the help of a periodical stress as a function of temperature.

Note: Each entry listed below is followed by *n*. or *adj*. indicating if the term is either a noun or an adjective.

atmosphere, *n*.
Gaseous environment of the sample, which may be controlled by the instrumentation or generated by the sample.

combined, *adj*.
Application of two or more techniques to different samples at the same time. This can include thermal and nonthermal analytical techniques. Different from *simultaneous*.

controlled-rate thermal analysis (CRTA), *n*.
Sample-controlled method where the feedback used to control the heating is the rate of transformation.

controlled temperature program, *n*.
Temperature history imposed on the sample during the course of the thermal analysis experiment.

cooling curve, *n*.
Experimental result of measuring the temperature of the sample as a function of time during cooling. *Heating curves* are obtained for temperature-time experiments during heating.

derivative, *adj*.
Pertaining to the 1st derivative (mathematical) of any curve with respect to temperature or time.

dielectric thermal analysis (DEA), *n*.
Technique where dielectric properties are measured.

differential, *adj*.
Pertaining to a difference in measured or measurable quantities usually between a sample and a reference or standard material.

differential scanning calorimetry (heat-flow DSC), *n*.
Technique where the difference between the heat-flow rates into a sample and a reference material is measured.

differential scanning calorimetry (power compensation DSC), *n*.
Technique where the difference between the electrical powers into a sample and a reference material is measured.

differential thermal analysis (DTA), *n*.
Technique where the temperature difference between a sample and a reference material is measured.

dynamic, *adj*.
Indicates, especially in the mechanical analysis of materials, that a parameter changes continuously during the experiment; opposite of *static*.

dynamic mechanical analysis (DMA), *n*.
Technique where storage and loss viscoelastic moduli are determined with the help of a periodical stress.

emanation thermal analysis (ETA), *n*.
Special type of evolved gas analysis (EGA) where the emanation of previously trapped radioactive gas is measured.

evolved gas analysis (EGA), *n*.
Family of techniques where the nature and/or amount of gas or vapour evolved is determined. The term *evolved gas detection* (EGD) has also been used where the nature of gas is not determined.

gas flow, *n*.
Passage of gas from one part of the system to another. The gas may be either inert (carrier gas) or reactive, either introduced into the system or evolving from the sample.

isothermal, *adj*.
Applied to a technique to indicate that the temperature is maintained constant throughout the experiment

material, *n*.
The substance which is studied and from which the *sample* is taken.

micro-, *prefix*
Prefix used to denote that the technique measures small quantities, either with respect to the amount of sample studied, or with respect to the change in the properties measured. Mathematically, 1 micro = 1 μ = 10^{-6}.

Note 1: This prefix has been applied to many thermal methods, and the equipment associated with them, for example, *microbalance*, *microreactor*, *microcalorimeter* and also to the technique itself: *microthermal, microscopic*, and the property studied: *microstructural*.
Note 2: The opposite prefix, *macro*-, is also occasionally used.

modulated, *adj*.
Indicates that a parameter changes in a periodic manner during the experiment.

modulated temperature (MT...), *adj*.
Applied to the technique name to indicate that a temperature modulation has been applied to the temperature program.

Note 1: As an example, a DSC experiment carried out with a modulated temperature program would be *modulated temperature differential scanning calorimetry* (MT-DSC).
Note 2: Other modulated techniques are possible, such as *modulated force TMA*, *modulated rate SCTA*, etc.
Note 3: The prefix TM is occasionally used instead, but not recommended.

photo-, *prefix*
Indicates that the experiment involves the illumination of the sample or measures the amount of light emitted from a sample. Where possible, the wavelength range of the light should be specified.

sample, *n*.
The material under study during the entire experiment (starting material, intermediates, and final products) and its close atmosphere. This is equivalent to the thermodynamic system.

sample controlled, *adj*.
Applied to the technique to indicate that a property of the sample is used either continuously or discontinuously to control the sample heating. Without this term, it is assumed that the experiment is following a controlled-temperature program.

Note: The generic term for all TA techniques making use of such feedback is sample-controlled TA (SCTA), whereas specific names will be of the form sample-controlled TGA (SC-TGA), etc.

scan, *n*.
(*Discouraged*) A term used to describe the data produced from a thermal analysis experiment. More correct usage is a *thermal analysis curve*, or, for a specific technique *thermogravimetric curve*, etc.

scanning, *adj*.
Indicates that a specified experimental parameter, if not temperature, is changed in a controlled manner.

scanning calorimetry, *n*.
Techniques where heat is measured as a function of temperature.

simultaneous, *adj*.
Indicates the measurement of two or more properties of a single sample at the same time. Different from *combined*.

Note: A hyphen is used to separate the abbreviations of the techniques; for example, simultaneous measurement of mass and heat flow rate (thermogravimetric analysis and differential scanning calorimetry) would be TGA-DSC.

static, *adj*.
Indicates, especially in the mechanical analysis of materials, a constant parameter during the experiment. The opposite of *dynamic*.

stepwise, *adj*.
Indicates discrete, discontinuous changes in an experimental parameter, e.g., force, temperature, etc.

tan δ, *n*.
The dimensionless ratio of energy lost to energy returned during one cycle of a periodic process. For example, $\tan \delta = E''/E'$, in DMA.

temperature-programmed desorption (TPD), *n*.
EGA using an inert atmosphere or vacuum, in the absence of sample decomposition.

temperature-programmed oxidation (TPO), *n*.
Experiment using an oxidising atmosphere, usually oxygen. Oxidation is monitored by any appropriate technique (EGA, TGA, gas sorption, etc.).

temperature-programmed reduction (TPR), *n*.
Experiment using a reducing atmosphere, usually hydrogen. Reduction is monitored by any appropriate technique (EGA, TGA, gas sorption, etc.).

thermal curve, *n*.
(*Discouraged*) Any graph of any combination of property, time, temperature derived from a thermal analysis technique.

Note: Thermal curve is a loose abbreviation of the more correct term *thermoanalytical curve*.

thermally stimulated current (TSC), *n*.
Electrical current observed during heating and caused by the thermally initiated *relaxation* of the frozen-in electrical polarization of a sample.

Note 1: By extension, the same name and abbreviation (TSC) are given to the thermal analysis technique based on the measurement of this current.
Note 2: See also *thermally stimulated depolarization*.

thermally stimulated depolarization, *n*.
Relaxation of frozen-in electrical polarization caused by a temperature increase.
Note: The effect is measured through the *thermally stimulated current*.

thermo-, *prefix*
Indicating the use of changing temperature during the experiment, when in the name of a thermal analysis technique.

thermoacoustimetry, *n*.
A technique whereby the characteristics of sound waves passing through the sample are measured.

thermoanalytical, *adj*.
Of, or pertaining to, thermal analysis.

thermodiffractometry, *n*.
A technique where the X-ray diffraction of the sample is measured.

thermodilatometry (TD), *n*.
A technique where one or more dimensions of the sample are measured under negligible load.

thermogravimetric analysis (TGA), *n*.
A technique where the mass of the sample is measured, also known as thermogravimetry.

thermogravimetry (TG), *n*.
See *thermogravimetric analysis*.

thermoluminescence, *n*.
A technique where light emission from the sample is measured.

thermomagnetometry, *n*.
A technique where a magnetic property of the sample is measured.

thermomanometry, *n*.
A technique where the gas pressure is measured.

thermomechanical analysis (TMA), *n*.
A technique where the deformation of the sample is measured under constant load.

thermomicroscopy, *n*.
A technique where the optical properties of the sample are observed and measured through a microscope.

thermoptometry, *n*.
A technique where the optical properties of a sample are measured.

thermosonimetry, *n*.
A technique where the sound emitted by the sample is measured.

thermospectrometry, *n*.
A group of techniques where a spectrum of the sample is measured.

torsional braid analysis (TBA), *n*.
A dynamic mechanical analysis technique where the sample is supported on a braid.

6 Reporting experimental data

For the experimental conditions to be fulfilled and reported, the reader is referred to the specific guidelines given in the ICTAC publications [1, 2], which are reproduced and progressively updated and complemented on the ICTAC website [www.ictac.org].

For reporting uncertainties, it is recommended to follow the guidelines published by the Joint Committee for Guides in Metrology [3, 4].

For the conventions on quantities, units and symbols to be used when reporting any work in thermal analysis, the reader is referred to IUPAC recommendations, especially the "Green Book" *Quantities, Units and Symbols in Physical Chemistry* [5].

7 Symbols used in thermal analysis

Quantity	Symbol for quantity	Symbol (and name) for unit
length	l	m (metre)
mass	m	kg, g*, mg* (kilogram, gram, milligram)
time	t	s, min*, h* (second, minute, hour)
electric current	I	A (ampere)
thermodynamic temperature	T	K (kelvin)
Celsius temperature	θ	°C (degree Celsius)
heating rate	$\beta = (\mathrm{d}T/\mathrm{d}t)$	$K \cdot s^{-1}$ (kelvin per second)
fraction reacted	α	–
heat	q, Q	J (joule)
heat flow rate	$\Phi = (\mathrm{d}q/\mathrm{d}t)$	W (watt)
heat capacity at constant pressure	C_p	$J \cdot K^{-1} \cdot mol^{-1}$ (joule per kelvin and per mole)
heat capacity at constant volume	C_V	$J \cdot K^{-1} \cdot mol^{-1}$ (joule per kelvin and per mole)
pressure	p	Pa (pascal)
modulus of elasticity	E	Pa (pascal)

*Denotes a non-SI unit accepted for use with the SI.

7.1 Symbols describing specific events or materials

- In general, symbols for physical quantities should be in *italic* type, or, if vectors, in ***bold italic type.***
- The symbols for units do not take plural.
- Subscripts should generally be restricted to single letters.
- If the subscript relates to an object or property, it should be a CAPITAL letter:
  m_S = *mass* of sample S
  T_R = temperature of reference R
  T_C = Curie temperature

– If the subscript refers to a phenomenon, it should be lower case:
  T_{fus} = melting temperature
  T_g = glass transition temperature

– If the subscript refers to a specific event, time or point, it should be lower case or figures:
  T_i = *initial* temperature
  m_f = final mass
  T_p = peak temperature
  $t_{1/2}$ = half-life of the reaction

– Changes in extensive thermodynamic quantities X due to an event y should be represented by $\Delta_y X$:
  $\Delta_{vap}H$ = enthalpy of vaporization
  $\Delta_r G$ = Gibbs energy of reaction

– Symbols for the physical state of the material should be put in brackets after the formula symbol:
  $\Delta_{vap}H = H(g) - H(l)$

8 Overview and historical matters

This document is concerned with providing definitions of common terms that are used by thermal analysts to report, present, and explain their work.

The ICTAC Nomenclature Committee was initiated in 1965 under the guidance of Robert Mackenzie and with the secretarial expertise of Cyril Keattch. This document acknowledges the debt to previous members of the Committee under their succeeding Chairs, including John Sharp (1984–1988), Ed Gimzewski (1988–1992), and Wolfgang Hemminger (1992–2001), who continued the discussions and published their findings as listed in the references [6–16].

The task of the current committee has been to rationalise the work of all preceding committees and to deliver a document that covers current practice in thermal analysis that can be accepted internationally.

Thanks are due to recent members of the Nomenclature Committee listed for their contributions to the deliberations and to others for the advice received.

Recent members of the ICTAC Nomenclature Committee are as follows:

R. Blaine (2001–2006); D. Burlett (2001–2006); E. Charsley (2001–2006); V. Fernandez (2001–2006); P. C. Gravelle (1992–2001); B. O. Haglund (1992–2001); P. Haines (1997–2006, *Secretary*, 2003–2006); W. Hemminger (*Chair*, 1992–2001); G. Hakvoort (1992–2001); T. Lever (*Chair*, 2001–2006); M. Odlyha (1991–2001); T. Osawa (2001–2006); D. Price (2001–2006, *Secretary*, 2001–2003); M. Reading (1991–2007); S. Sarge (1992–2001, *Secretary*, 2000–2001); J. Simon (1992–2001); F. Wilburn (1992–2006, *Secretary*, 1991–2000).

9 Membership of sponsoring body

Membership of the IUPAC Physical and Biophysical Chemistry Division Committee for the period 2012–2013 was as follows:

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References

[1] (a) G. Lombardi. *For Better Thermal Analysis,* 1st ed., ICTA, Rome (1977); (b) G. Lombardi. *For Better Thermal Analysis,* 2nd ed., ICTA, Rome (1980).
[2] J. O. Hill. *For Better Thermal Analysis and Calorimetry*, 3rd ed., ICTAC (1991).
[3] BIPM. *International Vocabulary of Metrology – Basic and General Concepts and Associated Terms* (VIM), 3rd ed., Bureau International des Poids et Mesures, Geneva (2002); JCGM 200:2012 at http://www.bipm.org/en/publications/guides/vim.
[4] BIPM. *Guide for Expression of Uncertainty in Measurement* (GUM), Bureau International des Poids et Mesures, Sèvres (2008); JCGM 100:2008 at www.bipm.org/en/publications/guides/gum.html.
[5] IUPAC. *Quantities, Units and Symbols in Physical Chemistry*, 3rd ed. (the "Green Book"). Prepared for publication by E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. J. Thor, RSC Publishing, Cambridge, UK (2007).
[6] R. C. Mackenzie. *Talanta* **16**, 1227 (1969).
[7] R. C. Mackenzie, C. J. Keattch, D. Dollimore, J. A. Forrester, A. A. Hodgson, J. P. Redfern. *Talanta* **19**, 1079 (1972).
[8] H. W. Thompson. *Pure Appl. Chem*. **37**, 439 (1974).
[9] R. C. Mackenzie, C. J. Keattch, T. Daniels, D. Dollimore, J. A. Forrester, J. P. Redfern, J. H. Sharp. *Thermochim. Acta* **12**, 105 (1975).
[10] R. C. Mackenzie. *Thermochim. Acta* **28**, 1 (1979).
[11] G. G. Guilbault. *Pure Appl. Chem*. **52**, 2385 (1980).
[12] R. C. Mackenzie. *Thermochim Acta* **46**, 333 (1981).
[13] R. C. Mackenzie. *Pure Appl. Chem*. **57**, 1737 (1985).
[14] J. H. Sharp. *Thermochim. Acta* **104**, 395 (1986).
[15] R. C. Mackenzie. In *Treatise on Analytical Chemistry,* P. J. Elving (Ed.), Part 1, Vol. 12, p. 1, John Wiley, New York (1983).
[16] W. Hemminger, S. M. Sarge. *Handbook of Thermal Analysis and Calorimetry,* Vol. 1, M. E. Brown (Ed.), Chap. 1, Elsevier, Amsterdam (1998).

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