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REVISED RECOMMENDATIONS ON NOMENCLATURE AND CONVENTIONS FOR REPORTING MÖSSBAUER DATA

Prepared by the Mössbauer Nomenclature Review Group appointed by the Commission for the International Conference on the Applications of the Mössbauer Effect.

The Group, composed of F. Berry, U. Gonser, J.G. Stevens and H. de Waard (secretary), has based the present document in large measure on the Information Bulletin published in August 1973 by the International Union of Pure and Applied Chemistry (Nr. 33 of "Appendices on Tentative Nomenclature, Symbols, Units, and Standards), which in turn has taken into account various earlier documents, mentioned in that Bulletin.

Introduction

A long time has elapsed since the publication of the previous recommendations, referred to on the title page. This document was drawn up by Commission I.1 (on Physico-Chemical Symbols, Terminology and Units) and Commission I.5 (on Molecular Structure and Spectroscopy) of the Physical Chemistry Division of IUPAC.

Since then, the extent to which Mössbauer Spectroscopy is used in physics and chemistry has stabilized. Along with this, the customs for presenting Mössbauer data have become more standardized, along with the materials used for standard single line sources and for calibration absorbers. There is not much purpose in tabulating these here, because their precise data are listed in the industrial specifications. For isomer shift standards, reference is made to the tables published in the Mössbauer Effect Data Index[1]. Therefore, the list of materials presented in the previous compilation has been omitted here. On the other hand, proper conventions for reporting results remain very useful for the purpose of this Bulletin, so they have been kept and when relevant, amended. We recommend their use in any publication involving results of Mössbauer spectroscopy.

A. Nomenclature and conventions for reporting Mössbauer spectroscopic data

I. Text

The text should contain at least the following information:

a) approximate current source strength and composition,

b) the method of absorber mounting: thickness and confinement; precise composition if not standard,

c) the physical form of the absorber: single crystal, polycrystalline powder, inert filler if used, evaporated film, rolled foil, isotopic enrichment, texture (see note A1), etc.,

d) the detector and data acquisition equipment, associated electronics and method of detection, if unusual,

e) the type of experiment (emission, absorption, transmission, scattering, in-beam, angular dependent, etc.),

f) use of critical absorbers or other filters,

g) method of data reduction (visual, by computer, etc.) and curve fitting procedure (see note A2),

h) the isomer shift convention used and the isomer shift relative to a standard reference absorber (or source) (see also note B1).

II. Numerical and tabulated data

a) Source and absorber temperatures

b) Values of the parameters used to characterize the relevant features of the Mössbauer spectra (in mm/s or other appropriate units) with estimated errors, in particular:

- isomer shift reference point
- line widths, defined as the full-width at half maximum peakheight (may be abbreviated to "half width")
- line intensities defined as fractions of background intensity (see note A3)
- estimates of systematic and statistical errors of the parameters derived from the spectra.

III. Figures illustrating spectra

Communications in which Mössbauer effect measurements constitute a primary source of information should include an illustration by at least one spectrum (i.e. a plot of transmission or of number of counts per channel *vs* velocity). Such figures should include the following information:

a) velocity units along the horizontal scale,

b) percentage or fractional transmission along the vertical scale (see note A4),

c) statistical error of the number of counts for at least one channel,

d) individual data points and, whenever possible, a computer fit, given as a continuous line clearly distinguishable from the experimental points plus the subspectra if these can not be easily discerned from the overall fit.

B. Terminology, symbols and units for Mössbauer spectroscopy

(if non SI units are used they should be explicitly defined in the text)

Name	symbol	SI unit	suggested unit	definition and comment
isomer shift	δ	m/s	mm/s	Note B1.
nuclear quadrupole moment (spectroscopic)	Q	m^2	b(arn) ($10^{-28}m^2$)	Note B2.
electric field gradient(EFG) tensor		V/m^2	V/cm^2	Note B2.
principal component of EFG	V_{zz}	V/m^2	V/cm^2	Note B2.
quadrupole coupling constant	e^2qQ/h	Hz	MHz	Note B2.
quadrupole splitting	Δ	m/s	mm/s	Note B2, B3.
asymmetry parameter	η			$(V_{xx}-V_{yy})/V_{zz}$
line width	Γ_{exp}	m/s	mm/s	full width at half maximum of the observed resonance line
natural line width	Γ_{nat}	m/s	mm/s	usually derived from lifetime
resonance effect				difference in transmitted or scattered intensity at resonance and off resonance divided by intensity off resonance
recoilless fraction	f			fraction of gamma-rays emitted (f_{s}) or absorbed (f_{a}) without energy change
effective thickness	t			Note B4.
resonance cross-section	σ_0	m^2	b(arn) ($10^{-28}m^2$)	
magnetic field	B	$T(Wb/m^2)$		Note B5.

Notes

A1 The concept of texture implies a non-random orientation of crystal axes, spins etc. in an polycrystalline sample.

A2 In the analysis of complex spectra, constraints should be specified (e.g. fixed line widths, intensity ratio's).

A3 Line intensities may also be expressed as percentages (percentage=100×fraction). Since these numbers depend on detector quality etc., it is often advisable to give relative intensities. Line areas and relative line areas are sometimes prefered (but they should never be equalled to relative fractions of atoms in different sites, since the effect of differences of recoilless fractions is then disregarded).

A4 It is customary to display data obtained in transmission geometry with the resonance maximum down and scattering data with the maximum up. In both cases sufficient data should be shown far enough from the resonance peaks to firmly establish the non-resonant base line.

B1 In an absorber experiment, where absorber quantities are determined, the isomer shift is the energy difference between the absorber and source transition energies (E_a–E_s), usually given in terms of the Doppler velocity shift $S{=}c(E_a{-}E_s)/E_\gamma$, where E_γ is the Mössbauer gamma energy and c is the speed of light in vacuum. Here, the isomer shift of the absorber relative to the source is positive if $E_a > E_s$; i.e. if the source must be moving towards the absorber (or the absorber towards the source) to achieve resonance. In this case, the velocity shift and the isomer shift are equal.

In an emission experiment, where the isomer shift of the source relative to the absorber is considered, the velocity shift of the source relative to the absorber needed to achieve resonance is the <u>opposite</u> of the source isomer shift. Since absorber experiments are much more common than source experiments a statement to this effect should be made in the text.

To avoid confusion, it is advisable to always label the horizontal scale in a Mössbauer spectrum “velocity scale”.

The isomer shift defined as above includes a term corresponding to a relativistic effect known as the “second order Doppler shift”. The term that only depends on the change of the electron density at the nucleus is sometimes specified as the “chemical isomer shift”. When this designation is used other effects should have been corrected for or stated to be negligeable.

B2 The nuclear quadrupole moment describes the effective deviation of the shape of the nuclear charge distribution from spherical; e is the positive elementary charge; a prolate nucleus has $Q{>}0$, an oblate one $Q{<}0$.

In its interaction with a field gradient, the quadrupole moment of a general charge distribution has tensor character. By using a transformation of the coordinate axes, this interaction can be reduced to one with only two components: the z-component of the field gradient, $V_{zz}{=}eq$ and the asymmetry parameter, η.

B3 To facilitate a direct comparison with NMR and NQR data, quadrupole splittings are frequently reported in MHz. If this unit is used, the conversion factor to Doppler shift values should be stated.

B4 The reduced thickness is usually calculated for a thin absorber from the relation $t = n\sigma_0 f$, in which n is the number of Mössbauer active nuclei per unit area in the path of the gamma rays, σ_0 is the cross section for recoilless scattering and f is the recoilless fraction.

B5 1 T = 10^4 Gauss.

Reference [1] W.L. Gettys and J.C. Stevens, Isomer Shift Reference Scales (Mossbauer Effect Data Center, University of North Caroline, Asheville, N.C. 28804) 1979.