Nomenclature, Conventions and Standards for Reporting Mössbauer Data

by Professor R. H. Herber*

Text

The text of the paper reporting Mössbauer results should include: (a) Method of sample mounting, sample thickness control (if any), sample confinement; (b) Method of data reduction (visual, computer, XY recorder, etc.); (c) Absorber form (single crystal, polycrystalline powder, inert matrix if used, evaporated film, rolled foil, etc.); (d) Geometry of the experiment (transmission, scattering, etc.); (e) Critical absorbers if used; Detector used and comments about associated electronics (*i.e.*: single channel window, escape peak, solid state detector, etc.) if appropriate or unusual. (g) State isomer shift sign convention (commonly in a transmission experiment, when source approaches absorbers *i.e.*: when the gamma ray incident on the absorber increases in energy the shift is said to be positive) (Note 1), (Note 3); (h) Method of spectrometer calibration (Note 2).

Notes

1. Metallic iron has been recommended both as a velocity calibrator for constant acceleration spectrometers (See Note 2) and as an isomer shift standard for ^{57}Fe data. Thin foils (0.25 to 1.0 mil) of natural iron of at least 99.9% purity (preferably 99.99% and/or NBS Standard Reference Material), are adequate for isomer shift data. The centroid of the metallic iron absorption (or scattering) spectrum should be calculated from (at least) the resonance maximum positions for the four "inner" lines (*i.e.*: the $|{}^1\!/_2|\leftrightarrow|{}^1\!/_2|$ transitions). Sodium nitroprusside dihydrate [SNP, $Na_2[Fe(CN)_5NO]\cdot 2H_2O$] has been standardized by the National Bureau of Standards using an absolutely calibrated spectrometer. Samples of SNP and metallic iron are available from NBS as Standard Reference Materials. For interlaboratory comparison of data, isomer shifts for other standards (*e.g.* $K_4Fe(CN)_6$, stainless steels, iron oxides, etc.) should be determined experimentally using the spectrometer in question, rather than depending on literature values.

2. Constant acceleration spectrometers to be used for work in the mm/sec range should be calibrated with respect to velocity, using metallic iron of at least 99.99% purity. The ground state and excited state splittings reported in the literature [R. S. Preston, S. S. Hanna and J. Heberle, *Phys. Rev. 128,* 2207 (1962); J. G. Dash, R. D. Taylor, D. E. Nagle, P. P. Craig and M. Visscher, *Phys. Rev. 122,* 1116 (1961); S. S. Hanna *et al., Phys. Rev. Letters, 4,* 177 (1960); J. I. Budnick, L. J. Bruner, R. J. Blume and B. L. Boyd, *J. App. Phys. 32,* 1205 (1961); Fritz and Schulze, *Nuclear Inst. Methods, 62,* 317 (1968); H. Shechter, M. Ron, S. Niedzwiedz and R. H. Herber, *Nucl. Inst. Methods, 44,* 268 (1966)] are $g_0 = 3.924 \pm 0.004$ mm/sec, $g_1 = 2.244 \pm 0.003$ mm/sec at room temperature. The most recent values obtained with an 0.75 mil 99.99% pure iron foil absorber, using a laser interferometer calibrated constant velocity spectrometer are $g_0 = 3.9177$ and $g_1 = 2.2369$ mm/sec at 24.1 ± 0.5° C (J. J. Spijkerman, J. R. DeVoe and J. C. Travis, N.B.S. Special Publication 260-20, Standard Reference Materials: Standards for Mössbauer Spectroscopy, N.B.S., Washington, 1970). These can be considered the currently available most reliable values for these constants.

The quadrupole splitting in SNP, which has a value of 1.7048 ± 0.0025 mm/sec at 25° C (R. W. Grant, R. M. Hously, and U. Gonser, *Phys. Rev. 178,* 523 (1969), should not be used for velocity calibration.

3. There are at the present no generally accepted isomer shift standards for other nuclides. Stannic oxide (SnO_2) and barium stannate ($BaSnO_3$) (which give essentially identical isomer shifts) have been used in ^{119}Sn spectroscopy, as have various forms of metallic tin. K ^{129m}I has been used for ^{129}I spectroscopy. NpO_2 has been used in ^{237}Np spectroscopy. For metals, some possible standards are ^{40}K in K, ^{99}Ru in Ru, and ^{197}Au in Au. Whatever reference standard is employed, sufficient data should be reported to permit interconversion to other data.

Numerical (Tabular) Data

When numerical values of Mössbauer parameters (or parameters directly derived therefrom) are presented in tabular form, the following information should be indicated independent of the running text unless otherwise readily extracted from the presentation: (a) Chemical state of source and absorber; (b) Temperatures of source and absorber. Indicate constancy limits of these values; (c) Mössbauer parameters in mm/sec (or cm/sec, or other appropriate units) with estimated errors (Note 4); (d) Isomer Shift standard or data for

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reference absorber. (e) Line widths (full width at half maximum) observed if pertinent; (f) Line intensities observed, if pertinent.

Figures

(a) At least one spectrum (% transmission or counting rate *versus* Doppler velocity or isomer shift, or comparable data – not "channel number") should be shown to indicate the "quality" of the data (Note 4); (b) "Effect" or intensity (*i.e.* % transmission or counting rate) axis should be normalized to v = ∞ if possible; (c) Statistical counting error or limits should be indicated for at least one data point (Note 5); (d) Individual data points (rather than only a smoothed curve) should be shown.

Notes

4. It has become customary to display data obtained in transmission geometry with the resonance maximum "down" and scattering data with the resonance maximum "up". In either case, sufficient data should be shown far from the resonance peaks to establish the non-resonant base line.

5. In most instances (where the data are uncorrected counting results) the statistical counting error is given by $\pm N^{1}/_{2}$, where N is the total number of counts stored per channel or velocity point. For corrected data, the statistical counting error should be obtained by the usual statistical methods.

Symbols and Nomenclature

Name	Symbol	Units	Definition and Comments	Note
Isomer shift	δ	mm/sec	Displacement of center of resonance spectrum from reference point	6,7
Quadrupole splitting	Δ or ΔE_Q	mm/sec MC	Hyperfine interaction (line splitting) between the nuclear quadrupole moment and the electric field gradient	6, 8
Line width	Γ or Γ_{exp}	mm/sec	Full width at half maximum of the experimentally observed resonance line	
Natural line width	Γ_{nat}	mm/sec	Usually calculated from $\Gamma_{nat} = h/2\pi\tau$	
Extrapolated line width	Γ_o	mm/sec	The line width (Γ) extrapolated to zero thickness	
Resonance effect magnitude	ε	%	$100[I(\infty) - I(0)]/I(\infty)$	9
Recoil free fraction	f	%	The fraction of all gamma rays of the Mössbauer Transition which are emitted (f_s) or absorbed (f_a) without recoil	
Mössbauer thickness	T	–	The effective thickness of a source (T_s) or absorber (T_a) = $n\sigma_o af$	10
Resonance cross section	σ_o	cm^2	The cross section for resonant absorption, related to the nuclear spins of the resonant nuclide and the internal conversion coefficient	
Internal magnetic field	H_n	oersted	Magnitude of the magnetic field at the nucleus (from experiment)	
External magnetic field	H_e	oersted	Magnitude of the applied magnetic field	
Electric field gradient tensor	EFG		A tensor describing the electric field gradient which is specified by η and V_{zz} in addition to the Euler angles specifying the tensor orientation if required	11

Symbols and Nomenclature (Continued)

Name	Symbol	Units	Definition and Comments	Note
Asymmetry parameter	η		$= (V_{xx}-V_{yy})/V_{zz}$	
Principal component of EFG	V_{zz}	volts/cm^2	$= \partial V/\partial z^2 = eq$ (e is the proton charge)	
Nuclear quadrupole moment	Q	barn or cm^2	A parameter which describes the shape of the nuclear charge distribution	

Notes

6. Although mm/sec Doppler velocity units have become accepted usage in ^{57}Fe and ^{119}Sn spectroscopy, cm/sec units may be more appropriate for other nuclides, or where hyperfine interactions cause large Doppler velocities to be involved in the data.

7. The center of a Mössbauer spectrum is defined as the Doppler velocity at which the resonance maximum is observed when all hyperfine interactions are (or would be) absent. That is $\delta \equiv \lim (E-E_o)$, $H \rightarrow 0$, $V_{zz} \rightarrow 0$. The contribution of the second order Doppler shift should be indicated, if possible.

8. Quadrupole splittings are frequently reported in megacycles per second, especially when direct comparison with nmr or nqr data can be effected (*e.g.*: in the case of ^{129}I). If such units are used in conjunction with data derived from Doppler shift measurements, the conversion units should be stated.

9. I(0) is the counting rate (or transmission or scattering intensity) at the resonance maximum. I(∞) is the corresponding rate at a velocity at which the resonance effect is negligible. If corrections for non-resonant gamma or X rays, or other base line corrections have been made in evaluating I, these should be stated.

10. For an experiment involving element Z, n is the number of atoms of Z per cm^2, σ is the cross section for resonance absorption, a is the fractional abundance of the Z nuclide which show the Mössbauer effect being observed, f is the recoil-free fraction.

11. $V_{xx}+V_{yy}+V_{zz} = 0$ independent of the choice of axes. Principal axes are chosen so that the off diagonal matrix elements vanish, $V_{ij} = 0(i, j = x, y, z; i \neq j)$ and are relabeled such that $|V_{zz}| \geqq |V_{yy}| \geqq |V_{xx}|$ so that $0 \leqq \eta \leqq 1$.

$$\mathrm{EFG} = \frac{\partial^2 V}{\partial x_i \partial x_j} \qquad \begin{array}{l} i \rightarrow 1, 2, 3 \\ j = 1, 2, 3 \end{array}$$