Fe Isomer Shifts and the Problem of Calibration

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The $^{57}$Fe isomer shift calibration problem is discussed, and critical comments concerning the paper "$^{57}$Fe Isomer Shift Calibration Experiment" by Daniel et al. (1985) are given. We consider $\langle \Delta r^2 \rangle = (20 \pm 3) \cdot 10^{-3}$ fm$^2$ at the moment as the most reliable estimate for the change of nuclear radius during gamma absorption; this value has been derived by measuring changes in isomer shift and calculating corresponding changes in electron contact density $g(0)$ according to $\Delta \delta = C \langle \Delta r^2 \rangle \cdot g(0)$.

A reliable calibration of the isomer shift $\delta$ is the prerequisite for deriving contact densities $g(0)$ from Mössbauer spectra. It is therefore important to design experiments with the aim to measure directly the change of nuclear radius $\langle \Delta r^2 \rangle$ during gamma resonance absorption. Such experiments have been performed for $^{57}$Fe on the basis of life time variations in the electron capture decay of $^{52}$Fe [1] or on the basis of conversion electron spectroscopy with $^{57}$Co($^{57}$Fe) sources [2]. However, the results, which have been obtained with these two methods, $\langle \Delta r^2 \rangle = (33 \pm 3) \cdot 10^{-3}$ fm$^2$ [1] and $\langle \Delta r^2 \rangle < 9 \cdot 10^{-3}$ fm$^2$ [2], respectively, do not agree at all. Other authors, including ourselves, strived for this goal by measuring changes in $\delta$ and calculating corresponding changes in $g(0)$.

$$\Delta \delta = C \langle \Delta r^2 \rangle \cdot g(0). \quad (1)$$

If $\delta$ is given in mm s$^{-1}$, $\langle \Delta r^2 \rangle$ in $10^{-3}$ fm$^2$, and $g(0)$ in $\alpha_0^{-3}$, the constant $C$ takes the value 0.011 for $^{57}$Fe.

From the combined experimental ($\Delta \delta$) and calculational ($\langle \Delta r^2 \rangle$) procedure we have derived $\langle \Delta r^2 \rangle$ for a large variety of iron-containing compounds, i.e. $\langle \Delta r^2 \rangle = (20 \pm 3) \cdot 10^{-3}$ fm$^2$ [4–6].

Due to its importance it is desirable to have a widely accepted isomer shift calibration. In our view there are serious drawbacks which cause us to question the value $\langle \Delta r^2 \rangle < 9 \cdot 10^{-3}$ fm$^2$ (at 80% confidence) [2], due to the following reasons:

(i) The absolute value of the Fe 4s contact density $g_4s(0)$ was obtained in [2] from the experimental ratio $x_4s/x_{3s}$ and the calculated relativistic Fe 3s value $g_{3s}(0) \sim 180 \alpha_0^{-3}$, i.e.

$$x_4s/x_{3s} = 0.061 \pm 0.005 \text{ the value } g_{4s}(0) = (10.98 \pm 0.90) \alpha_0^{-3} \text{ for } ^{57}\text{Fe/Au.} \quad (2a)$$

and

$$x_4s/x_{3s} = 0.17 \pm 0.10 \text{ the value } g_{4s}(0) = (30.6 \pm 18.0) \alpha_0^{-3} \text{ for } ^{57}\text{Fe/graphite.} \quad (2b)$$

With the experimental isomer shifts 0.65 mm s$^{-1}$ for $^{57}$Fe/Au and 0.25 mm s$^{-1}$ for $^{57}$Fe/graphite and the values (2a, b) we derive from (1)

$$\langle \Delta r^2 \rangle = 1.85 \cdot 10^{-3} \text{ fm}^2.$$
reported in [2] as conclusive, and because the value 
-\(\langle 4r^2 \rangle = (33 \pm 3) \cdot 10^{-3} \text{ fm}^2\) given by Meykens et al. [1] seems to be overestimated by about 30 per cent due to reasons described in [2].
