Determination of quadrupole moment and isomeric shift for ^{119}Sn. Comparison of different methods based on DFT calculations

H.K. Narro[1], C.G. Brusasco[1,2], L.A. Errico[1,2,3], A.V. Gil Rebaza[1,2]

1 Instituto de Física La Plata IFLP - CONICET, CCT La Plata, 1900 La Plata, Argentina.

2 Departamento de Física, Facultad de Ciencias Exactas de la Universidad Nacional de La Plata UNLP, 1900 La Plata, Argentina.

3 Universidad del Noroeste de la Provincia de Buenos Aires UNNOBA, Buenos Aires, Argentina.

The isomer shift (IS) is defined as the transition energy γ that occur between the source and absorbed nuclei, and is determined as:

$$IS = \frac{4\pi c}{5E_\gamma} ZR^2 \left(\frac{\Delta R}{R}\right) (\rho_a(0) - \rho_s(0)) \quad (1)$$

where, c is the light speed, Z the atomic number, E_γ is the energy of the γ *quantum*, ΔR the variation of the nuclear radius, $\rho_a(0)$ and $\rho_s(0)$ are the electronic charge densities in the absorbing and source nuclei, respectively.

Considering the properties of the source as constants, we can express 1 as:

$$IS = \alpha\,(\rho_a(0) - \rho_s(0)) = \alpha\Delta\rho(0), \quad (2)$$

where $\alpha = \frac{4\pi c}{5E_\gamma} ZR^2 \left(\frac{\Delta R}{R}\right)$, known as the isomeric calibration constant.

The quadrupolar splitting (QS) is a "fingerprint" of the charge symmetry around the probe nucleus. For I=*3/2* to I=*1/2* transition of ^{119}Sn, QS is determined by:

$$QS = \frac{1}{2} e|Q_N V_{zz}| \left(1 + \frac{1}{3}\eta^2\right)^{1/2} \quad (3)$$

where e is the elementary charge, Q_N is the quadrupole magnetic moment, V_{zz} is the principal component electric field gradient (EFG) tensor, and η is the asymmetry parameter, defined as $\eta = \frac{V_{xx} - V_{yy}}{V_{zz}}$ [1].

Computational Details

- The Sn-based compounds considered for the study are: $\alpha - Sn$, $\beta - Sn$, $SnCl_2$, SnO, SnO_2, SnS, $SnSe$, $SnSe_2$, $SnSb$, $SnTe$, SnS_2, $SnBr_2$, SnP, $SnAs$, $BaSnO_3$, $CsSnI_3$, Cs_2SnI_6, Cs_2SnCl_6, Cs_2SnBr_6, $SnNa$, SnI_2, SnI_4, $SnBr_4$, $SnCl_4$, αSnF_2, Sn_2O_3.
- FP-LAPW method (WIEN2k [2]): $R_{MT}(Sn) = 2.00\ a_0$, XC: PBE-GGA [3], core-valence energy $= -8.0\ Ry$, $G_{max} = 15$, $R_{mt}^{min} \times K_{max} = 8.0$ and k-points= 5000.
- PP-PW/GIPAW method (Quantum Espresso [4]): $E_{cut} = 80Ry$, $E_{rho} = 800Ry$, XC: PBE-GGA, GIPAW-type Pseudopotentials [5], k-points= 5000.
- FPLO method [6]: XC: PBE-GGA, k-points= 5000, finite-size nuclear model, both *scalar* (SR) and *full* (FR) *relativistic* cases were considered.

Results

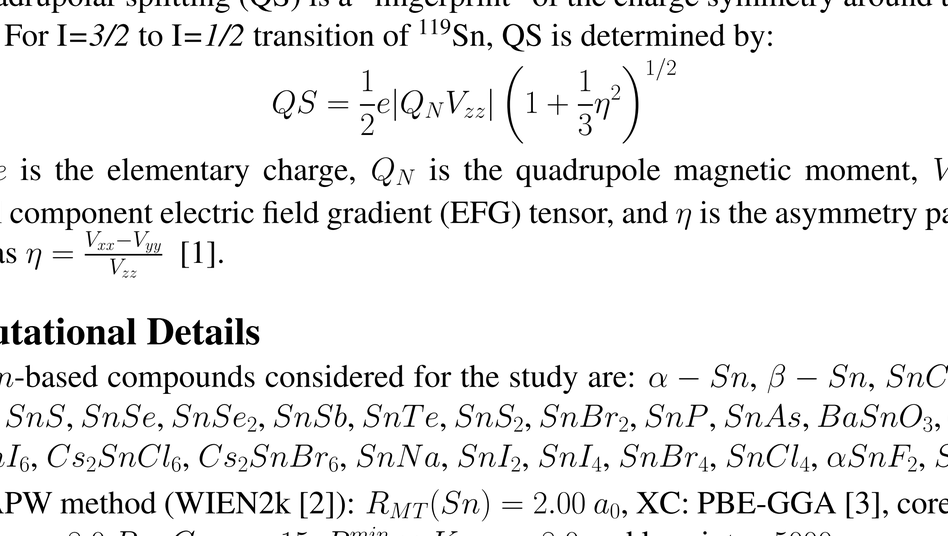

Figure 1: Variation of the electronic contact density for Sn atoms at different R_0 determined by the FP-LAPW method. Values were referenced respect to Sn of SnO_2 rutile.

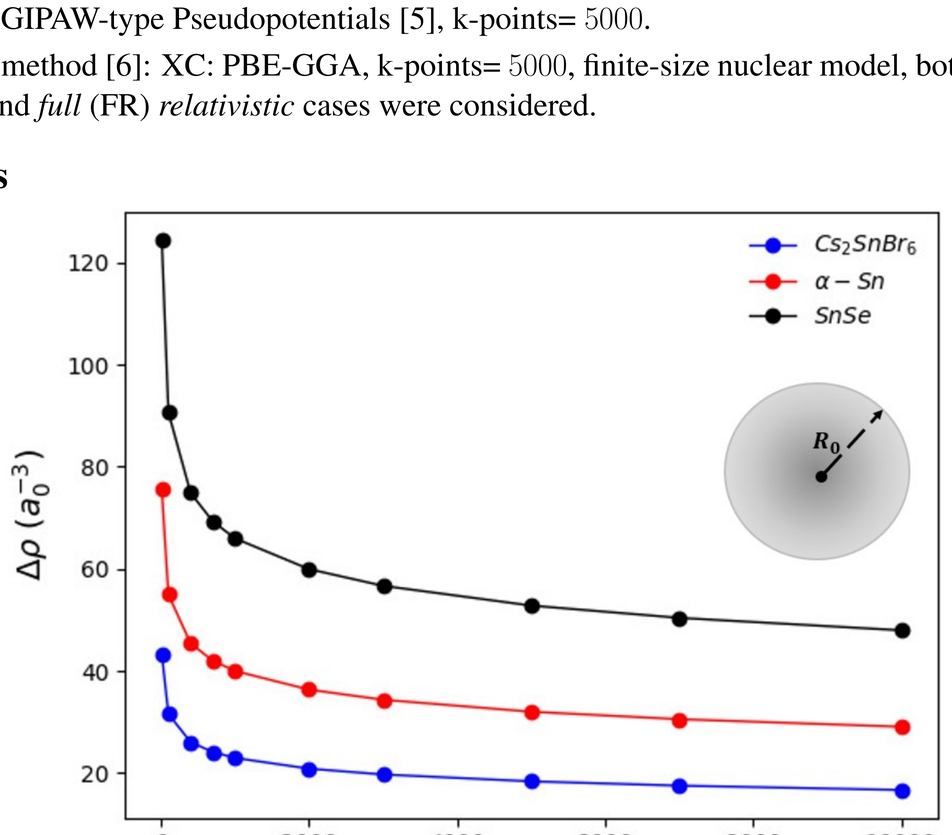

Figure 2: Experimental values of the IS of ^{119}Sn compared to calculated values $\Delta\rho = \rho_a(0) - \rho_s(0)$ for several Sn-based compounds. Values of α= 0.0226, 0.0427 and 0.0587 $a_0^{-3}mm/s$ for R_0=10, 1000 and 10000 $\times 10^{-9}a_0$, respectively.

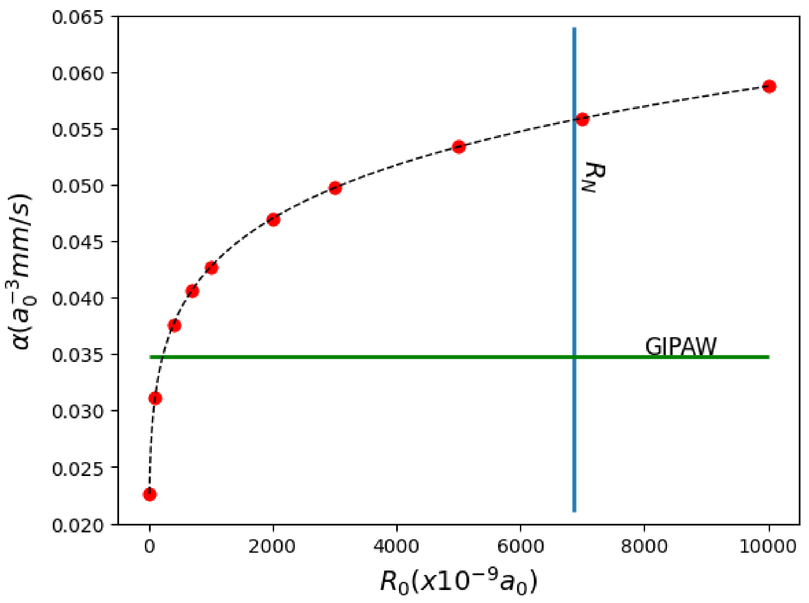

Figure 3: Variation of α with R_0. $R_N = 6864.5 \times 10^{-9}a_0$.

The value of R_N was obtained using the expression of the semi-empirical method:

$$R_N = \left(A_0 + \frac{A_1}{A^{2/3}} + \frac{A_2}{A^{4/3}}\right) A^{1/3} \quad (4)$$

where $A_0 = 0.9071fm$, $A_1 = 1.105fm$, and $A_2 = -0.548fm$. A is the atomic mass number [7].

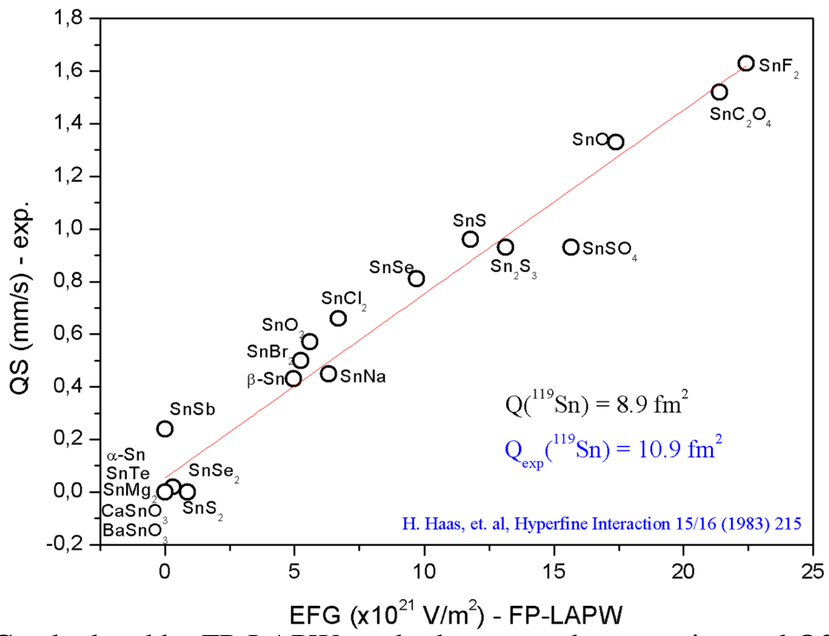

Figure 4: EFG calculated by FP-LAPW method compared to experimental QS for ^{119}Sn.

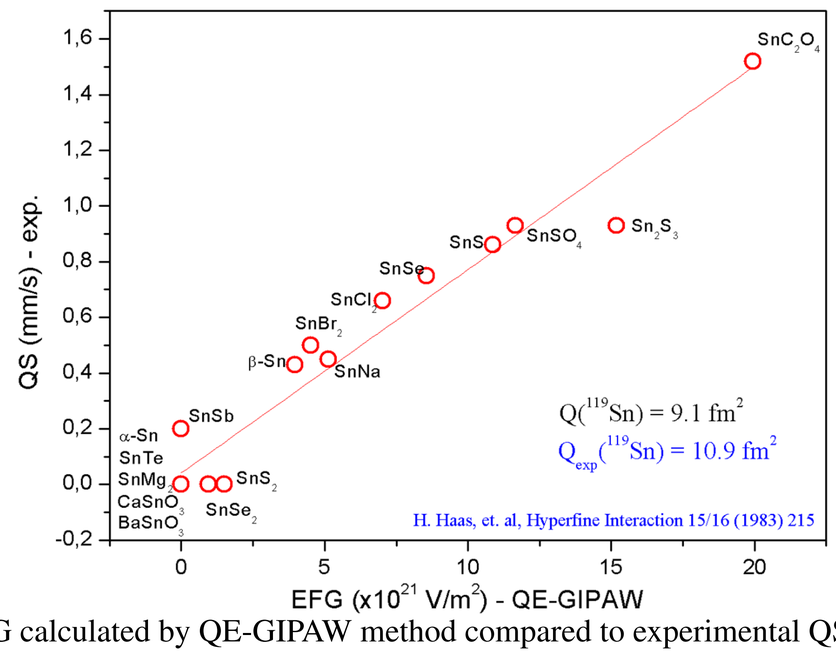

Figure 5: EFG calculated by QE-GIPAW method compared to experimental QS for ^{119}Sn.

Comments

- Reported values of α for ^{119}Sn are : 0.092 [8], 0.084 [9], 0.086 [10], 0.081 [11], 0.091 [11], 0.092 [11], 0.037 [12], 0.082 [13], 0.086 [14], 0.071 [15], 0.084 [16], and 0.085 [17] $a_0^{-3}mm/s$. Similarly, the reported values for Q_N are: 15.2 [18], 10.9 (exp) [19], 12.8 [8], 11.9 [20], 13.2 [21], 8.0 [22], 6.15 [10], 6.0 [23], 6.50 [24], and 6.15 [14] fm^2.
- The GIPAW method determines a value of $\alpha = 0.03474\ a_0^{-3}mm/s$, corresponding to $R_0 = 221 \times 10^{-9}\,a_0$ in the FP-LAPW method.
- The FPLO method determines a value of $\alpha = 0.1055\ a_0^{-3}mm/s$ and $0.1062\,a_0^{-3}mm/s$ for SR and FR, respectively. Does not obey the relation proposed by Filotov [25]. According to these α value, corresponding to $R_0 = 700 \times 10^{-9}\,a_0$ in the FP-LAPW method.
- Svane [8] using $R_N = 1.2 \times A^{1/3}$, report a $\alpha = 0.092a_0^{-3}mm/s$.
- The Q_N value determined by both methods are in excellent agreement with experimental value reported. Validating the accuracy of the GIPAW method to determinate EFG and QS parameters.

QR references

QR on-line version