Electronic Supplementary Information for Dalton Transactions

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Supplementary Information

Synthesis and Characterization of the Primary Amido Tin (II) Dimer $Sn_2\{N(H)Dipp\}_4$ (Dipp = C_6H_3-2,6-Pr^i_2) and the First Sesqui-amido Hemi-chloride Derivative $Sn_2\{N(H)Dipp\}_3Cl$ and a New Route to Tin (II) Imides by Facile Conversion of a Primary Amide to the Imide $(SnNDipp)_4$

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Mössbauer Spectroscopy

For **1** the temperature-dependence of the log of the recoil-free fraction (1n *f*), which for an optically "thin" absorber scales with the temperature dependence of the log of the area under the resonance curve {ln[A(T)/A(R)], where A(T) is at the experimental temperature and A(R) is at a reference temperature}, is well fitted by a linear regression as shown in Fig. S1. In this context it should be noted that $f=\exp(-k^2\langle x^2\rangle)$, where k is the wave vector Fig.S1 of the 23.87 keV ^{119m}Sn gamma ray, and $\langle x^2\rangle$ is the expectation value of the mean-square-amplitude-of-vibration (msav) of the tin atom. Assuming that the high-temperature ln *f* data extrapolate to zero in the low temperature limit permits a calculation of the msav of the metal atom at all temperatures in the high temperature limit. These values, in turn, can be compared to the msav values calculated from the U_{ij} values extracted from a single crystal X-ray structure determination. While no U_{ij} values have been reported for **1**, a comparison for compound **3** will be discussed below. For the moment it is worth noting the $k^2\langle x^2\rangle$ for **1** extracted from the Mössbauer data at 130 K is 1.988.

For **3 t**he temperature dependence of ln[A(T)/A(90)] is well fitted by a linear correlation with a slope of -15.49±0.19K^{-1} (correlation coefficient = 0.997 for 8 data points) and the comparable

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data for **1** and **3** are summarized in Fig. S2. In the case **3**, single crystal X-ray diffraction data have been reported, and the value of $k^2\langle x^2\rangle$ extracted from such data at 130K is 1.982±0.023. The corresponding value at 130 K extracted from the Mössbauer data is 2.023±0.023 in excellent agreement within the quoted experimental errors. As noted above, the corresponding U_{ij} values for **1** have not been reported, but from the close correspondence of the ln{A(T)/A(90)] data for **1** and **3** it may be inferred that the msav of the tin atom, averaged over all Sn atoms in each structure, is nearly identical in the two cases.

The Mössbauer spectra of **3** show a small, but significant temperature-dependent intensity ratio (R) of the two components of the doublet. This deviation from equal intensity may have two major origins: (a) a "texture" effect arising out of preferential orientation of the crystallites with respect to the optical axis of the experiment, or (b) anisotropy in the metal atom motion with respect to the major symmetry axis involving the Mössbauer active atom. The former is temperature independent, whereas the latter is a function of T. From the value of R and *f* at given temperature it is possible to calculate the value of $k^2\langle x^2\rangle$ for motion both parallel and perpendicular to the symmetry axis, and the results of this calculation are summarized graphically in Fig. S2. In the absence of a reliable value for M_{eff} (due to the small variation of the IS parameter with T) experimental data have been compared to the values calculated for M_{eff} = 119 daltons and Θ_M , the Mössbauer lattice temperature is 109 K as indicated by the full line in Fig. S2.

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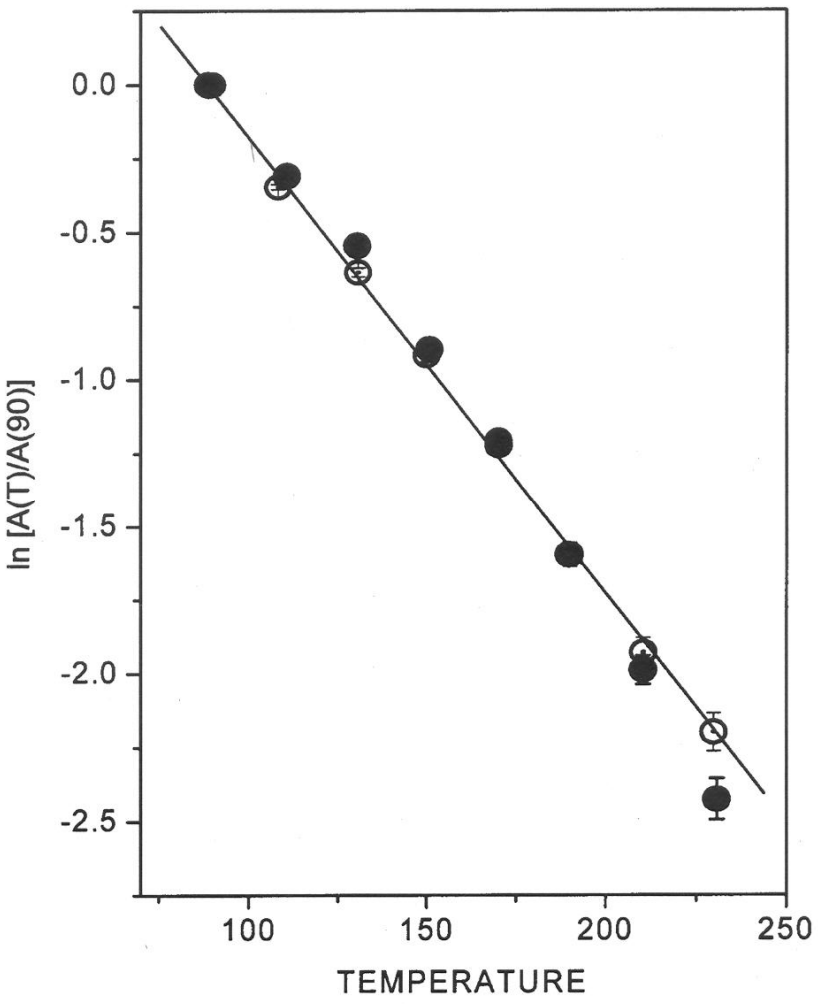

Fig S1. In [A(T)/A(90)] for compounds **1** (open circles) and **3** (closed circles) as described in the text.

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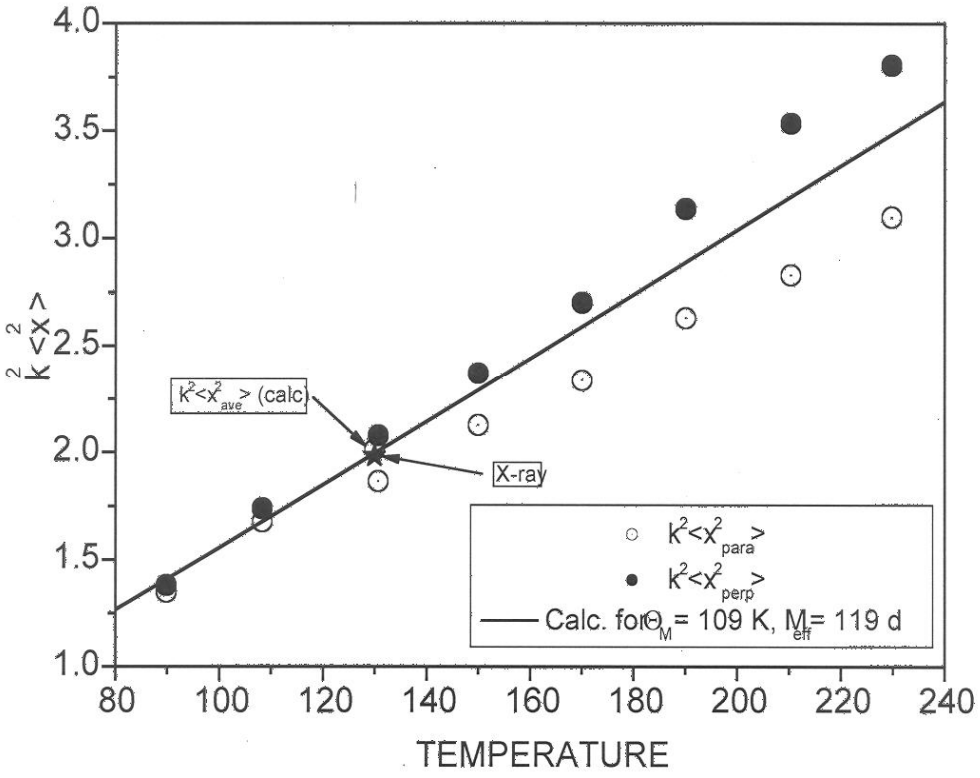

Fig. S2. The $k^2\langle x^2\rangle$ parameters for **3** as a function of temperature. The values calculated from the X-ray diffraction data (star) and the average Mössbauer data (open circle) are indicated. The full line reflects the assumption that M_{eff} is the "bare" Sn atom mass and that the Mössbauer lattice temperature is 109 K.