Erratum: First-principles study of phonons and related ground-state properties and spectra in Zn-IV-N₂ compounds [Phys. Rev. B **78, 115204 (2008)]**

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The first part of Table IX for the a_1 modes, which contained typographical errors, should be replaced by the present Table I. Several errors occurred in the figures. Figures 3–6 used a line-shape function for each mode n of the form

$$\frac{\gamma_n \omega}{(\omega^2 - \omega_n^2)^2 + \gamma_n^2 \omega^2},$$

which, for $\omega \rightarrow \omega_n$, becomes $1/(\gamma_n \omega_n)$ and is, thus, not properly normalized. The factor $1/\omega_n$ was already included in Eq. (26) of Veithen *et al.*,¹ which was supposed to be used with a normalized line-shape function, such as a Lorentzian. Additional errors occurred in the original Fig. 3 for ZnSiN₂. The corrected figures are given below in Figs. 1–4.

For completeness, we add Table II, providing the phonon frequencies of ZnSiN₂ used in Figs. 1–6 of the original paper, obtained in the local density approximation (LDA). These are slightly different from the ones given in Ref. 2 obtained in the generalized gradient approximation.

In Table V, the values of the eighth a_{1T} and a_{1L} modes were interchanged. They should be 477 and 527 cm⁻¹, respectively. Finally, the frequencies used for the infrared spectra in Fig. 1 for ZnSnN₂ did not exactly correspond to the ones given in Table V. A corrected Fig. 1 is given in Fig. 5.

 TABLE I. Raman tensor components for the a_1 modes.

Modes	ZnSiN ₂			ZnGeN ₂			ZnSnN ₂		
	xx	yy	zz	xx	yy	zz	xx	yy	zz
a_1	-1.22×10^{-5}	1.13×10^{-4}	7.53×10^{-5}	5.92×10^{-5}	-2.06×10^{-4}	-7.70×10^{-6}	3.05×10^{-4}	-3.86×10^{-4}	-3.79×10^{-5}
	3.13×10^{-4}	-1.04×10^{-4}	6.92×10^{-6}	8.32×10^{-5}	-5.15×10^{-4}	3.72×10^{-5}	-4.65×10^{-5}	1.13×10^{-5}	4.38×10^{-5}
	7.09×10^{-4}	6.01×10^{-4}	-1.46×10^{-3}	-2.19×10^{-4}	1.14×10^{-3}	5.63×10^{-4}	2.49×10^{-4}	7.23×10^{-5}	-1.22×10^{-5}
	-7.15×10^{-4}	9.40×10^{-4}	1.10×10^{-5}	3.97×10^{-4}	5.30×10^{-4}	-4.42×10^{-4}	2.93×10^{-4}	1.22×10^{-4}	5.54×10^{-4}
	1.70×10^{-4}	-3.51×10^{-4}	7.85×10^{-4}	3.27×10^{-4}	2.21×10^{-4}	5.47×10^{-4}	3.80×10^{-4}	1.39×10^{-4}	7.13×10^{-4}
	-9.72×10^{-4}	-3.24×10^{-4}	2.87×10^{-5}	-5.74×10^{-5}	1.34×10^{-3}	5.39×10^{-3}	-3.11×10^{-4}	-7.23×10^{-4}	-3.27×10^{-4}
	1.88×10^{-4}	-6.01×10^{-4}	1.04×10^{-3}	-4.39×10^{-5}	-8.77×10^{-4}	1.60×10^{-8}	-5.15×10^{-4}	1.82×10^{-3}	1.21×10^{-3}
	-1.48×10^{-3}	2.24×10^{-4}	1.32×10^{-3}	-5.96×10^{-5}	4.67×10^{-4}	-9.72×10^{-4}	1.23×10^{-3}	2.83×10^{-3}	-1.60×10^{-4}
	-6.03×10^{-5}	-6.21×10^{-4}	8.91×10^{-4}	-6.33×10^{-3}	-3.75×10^{-3}	-3.72×10^{-3}	-6.97×10^{-3}	-6.77×10^{-3}	-6.72×10^{-3}
	1.16×10^{-3}	1.21×10^{-3}	7.64×10^{-5}	-1.88×10^{-3}	-2.18×10^{-4}	9.40×10^{-4}	4.71×10^{-3}	-2.11×10^{-4}	-3.07×10^{-4}
	-1.59×10^{-3}	-5.13×10^{-4}	-1.72×10^{-3}	1.91×10^{-3}	4.72×10^{-4}	-1.09×10^{-4}	-2.94×10^{-4}	-1.34×10^{-3}	-1.13×10^{-3}

FIG. 1. (Color online) Calculated Raman spectra for modes of a_{1T} symmetry for the Zn-IV-N₂ compounds. Note that the peak intensities depend on the Raman tensor component as selected by the scattering geometry: xx is measured in $y(x\bar{x})\bar{y}$, yy in $x(yy)\bar{x}$, and zz in $\perp(zz)\perp$ with $\perp$ as any wave vector in the c plane.

FIG. 2. Calculated Raman spectra for modes of b_{1T} symmetry for the Zn-IV-N₂ compounds. This component is measured in $y(zx)\bar{y}$ geometry.

FIG. 3. Calculated Raman spectra for modes of b_{2T} symmetry for the Zn-IV-N₂ compounds. This component is measured in $x(zy)\bar{x}$ geometry.

FIG. 4. Calculated Raman spectra for modes of a_2 symmetry for the Zn-IV-N₂ compounds. This component is measured in $z(xy)\bar{z}$ geometry.

TABLE II. Phonon frequencies of ZnSnN₂ at the Γ point obtained in the LDA.

a_2	b_{1T}	b_{1L}	b_{2T}	b_{2L}	a_{1T}	a_{1L}
147	180	181	152	152	146	146
171	200	200	184	185	181	181
197	298	309	255	265	277	291
314	442	449	391	391	299	300
380	517	524	468	469	482	482
467	553	560	507	516	495	496
554	625	626	583	638	542	573
584	707	718	676	705	652	652
643	731	796	777	777	693	772
752	875	892	873	922	864	864
897	904	989	940	1014	917	1016
921

FIG. 5. (Color online) Infrared absorption spectra related to the modes at Γ for Zn-IV-N₂ compounds. The solid black lines give the $\text{Im}[\epsilon(\omega)]$, the dashed red lines give the loss function $\text{Im}[-\epsilon^{-1}(\omega)]$. The three panels in each plot are for the group IV elements Si, Ge, Sn from top to bottom. The different plots correspond to the different infrared active symmetries. The arrows at the top of each panel give the individual modes: shorter and longer arrows represent transverse and longitudinal phonon modes, respectively. Note that only 11 phonons modes are shown visible as the lowest one is the zero-frequency acoustic phonon mode. The spectra are calculated using Eq. (2) with a damping factor Γ chosen between 5 and 30 cm^{-1} with increasing width for higher-frequency modes as suggested by the experimental data for ZnSnN₂.²

¹M. Veithen, X. Gonze, and P. Ghosez, *Phys. Rev. B* **71**, 125107 (2005).

²T. R. Paudel and W. R. L. Lambrecht, *Phys. Rev. B* **76**, 115205 (2007).