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CORRIGENDUM TO: STRUCTURAL AND THERMODYNAMIC PROPERTIES OF Cu_2ZnSnS_4 MATERIAL: THEORETICAL PREDICTION

(AWUTP, 65 (2023) 160-170, DOI: 10.2478/awutp-2023-0012**)**

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Article Info	Abstract
Received: 02.06.2024 *Accepted: 19.09.2024* **Keywords:** Cu_2ZnSnS_4 material, Thermodynamic properties, DFT, Quantum Espresso.	We would like to correct some inaccuracies in our previous paper "STRUCTURAL AND THERMODYNAMIC PROPERTIES OF Cu_2ZnSnS_4 MATERIAL: THEORETICAL PREDICTION", Annals of West University of Timisoara-Physics, 65 (2023) 160-170. https://doi.org/10.2478/awutp-2023-0012 During the analysis of the data we forget to divide by N (N = 2 is the number of formula units per cell) to transform the unities from Ry/cell/K to $J.mol^{-1}.K^{-1}$, and from Ry/cell to kJ/mol, respectively. So with consequence, we found that some of our data of the thermodynamic properties are muliplied by 2. In addition, we rectified the unity from kJ $N^{-1}mol^{-1}$ to kJ/mol.

In the present corrigendum, we would like to correct some small mistakes contained in the original version of our previous paper [1] on the thermodynamic properties of CZTS material.

The corrected results on the variations of the vibrational energy U_{ph}, the vibrational free energy $F_{vib,}$ the vibrational entropy S and the constant volume heat capacity Cv of CZTS material are plotted in figures 1, 2, 3 and 4, respectively.

The following paragraph: "At zero-temperature the Debye's vibrational energy U_{ph} was found to be 49.31 kJ $N^{-1}mol^{-1}$, while at 298 K it is found to be at around 126.24 kJ $N^{-1}mol^{-1}$" must be rectified by: " At zero-temperature the Debye's vibrational energy U_{ph} was found to be

24.66 kJ/mol, while at 298 K it is found to be at around 63.12 kJ/mol ".

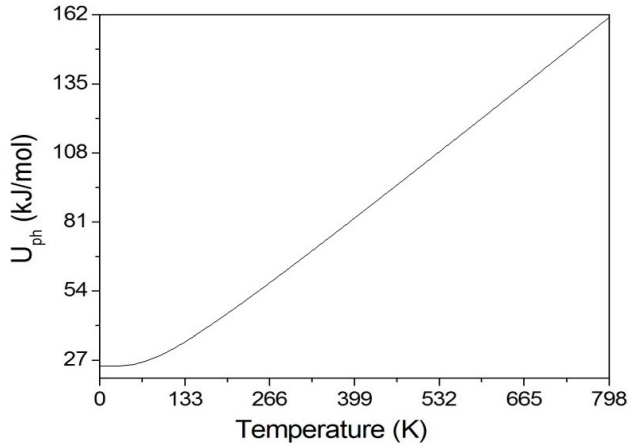

Figure 1. Variations of the vibrational energy U_{ph} of CZTS material as a function of temperature T

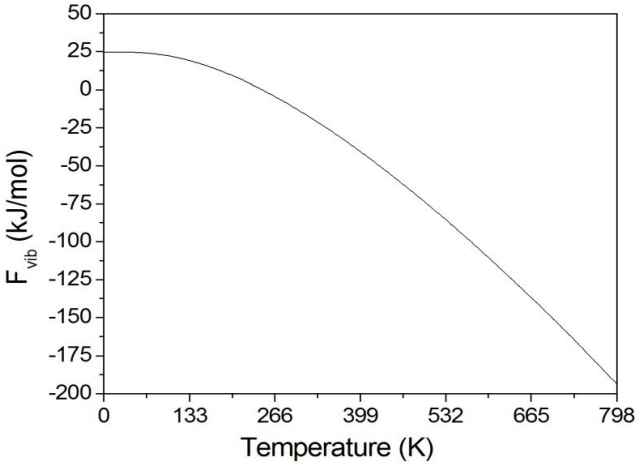

Figure 2. Variations of the vibrational free energy F_{vib} of CZTS as a function of temperature T

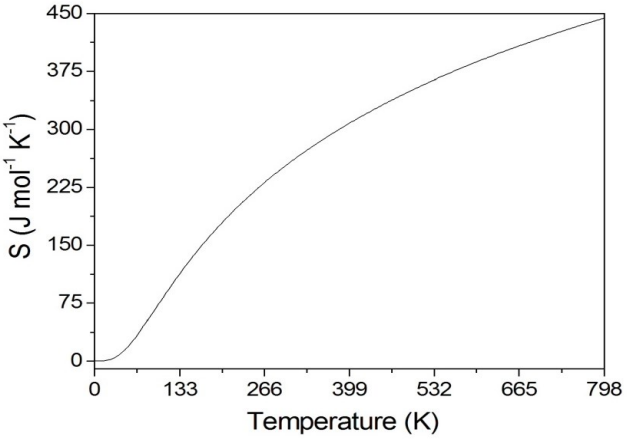

Figure 3. Entropy S of Cu_2ZnSnS_4 material versus temperature T

The following paragraph: "At zero-temperature the F_{vib} was found to be 49.3 kJ.N^{-1}.mol^{-1}, while at 298 K it is found to be at around -24.2 kj.N^{-1}.mol^{-1}" must be rectified by: "At zero-

temperature the vibrational free energy F_{vib} was found to be 24.65 kJ/mol, while at 298 K it was found to be at around -12.1 kJ/mol", while the following paragraph: " The correlation between F_{vib} (expressed in $kJN^{-1}mol^{-1}$) and T (expressed in K) is given by the following expression: $F_{vib}= 50.42 + 0.036T - 0.11 \times 10^{-2}T^2 + 0.45 \times 10^{-6}T^3$ " must be rectified by: " The correlation between F_{vib} (expressed in kJ/mol) and T (expressed in K) is given by the following expression: $F_{vib}= 25.21 + 1.81 \times 10^{-2}T - 5.45 \times 10^{-4}T^2 + 2.27 \times 10^{-7}T^3$ ".

The following paragraph: "At 298 K, the vibrational entropy S is found to be 504.76 $J.mol^{-1}.K^{-1}$" must be rectified by: "At 298 K, the vibrational entropy S was found to be 252.38 $J.mol^{-1}.K^{-1}$".

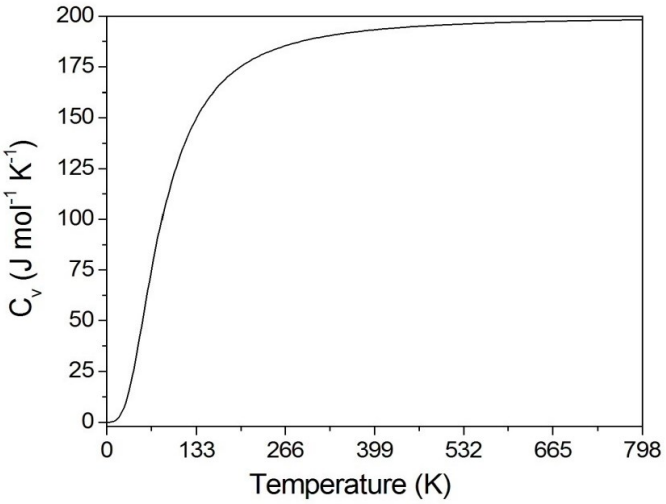

Figure 4. Constant volume heat capacity C_V of Cu_2ZnSnS_4 versus temperature T

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The following paragraph: "At 298 K, the constant volume heat capacity C_V was found to be at around 376.44 $J.mol^{-1}K^{-1}$" must be rectified by: "At 298 K, the constant volume heat capacity C_V was found to be around 188.22 $J.mol^{-1}K^{-1}$".

The authors would like to apologize for any inconvenience caused.

REFERENCES

[1] L. Boutahar, A. Benamrani, Z. Rouabah, S. Daoud, Structural and thermodynamic properties of Cu_2ZnSnS_4 material: Theoretical prediction**,** Annals of West University of Timisoara Physics, 65 (2023) 160-170. https://doi.org/10.2478/awutp-2023-0012