

Erratum: High-temperature magnetism and crystallography of a YCrO₃ single crystal [Phys. Rev. B **101**, 014114 (2020)]

Yinghao Zhu, Si Wu, Bao Tu, Shangjian Jin, Ashfia Huq, Jörg Persson, Haoshi Gao, Defang Ouyang, Zhubing He,
Dao-Xin Yao, Zikang Tang, and Hai-Feng Li

(Received 17 June 2020; published 1 July 2020)

DOI: [10.1103/PhysRevB.102.019901](https://doi.org/10.1103/PhysRevB.102.019901)

An error has been found in the published paper. This was mentioned to the authors by Professor Y. Xiao (Peking University, Shenzhen Graduate School) to whom we are grateful.

In Fig. 10 of the original version of this paper, while calculating the distortion parameter Δ of Y, Cr, O1, and O2 ions of the single-crystal YCrO₃ compound, we estimated the error bars using the root-mean-square deviations. This was incorrect and led to irrational errors for the distortion parameter of Y, Cr, O1, and O2 ions. Especially for the Cr ions, taking into account the deviations, the distortion parameter Δ may get negative values, which makes physical non-sense.

When one uses the software FULLPROF SUITE [1] to analyze diffraction data for extracting the crystallographic information, the software does not give the uncertainty of the distortion parameter Δ [2,3]. That is why we took the root-mean square as the deviation, which is an improper way for estimating the error bars.

We performed the correction as follows. We first extracted the respective bond lengths of Y-O1 ($\times 2$) and Y-O2 ($\times 4$) (for the calculation of ΔY), Cr-O1 ($\times 2$) and Cr-O2 ($\times 4$) (for the calculation of ΔCr), O1-Y ($\times 2$) and O1-Cr ($\times 2$) (for the calculation of $\Delta O1$), and O2-Y ($\times 2$) and O2-Cr ($\times 2$) (for the calculation of $\Delta O2$), as well as the estimated standard deviations based on the structure refinements using the software FULLPROF SUITE [1]. Then, we estimated the error bars based on the propagation law of errors as listed in Table E1 [4,5], supposing that the bond lengths are not correlated.

Correspondingly, Fig. 10 should be updated to the current version as shown in Fig. E1.

To evaluate the validity of the conclusions of the paper, we compared the original version of Fig. 10 with the present latest one as shown in Fig. E2. The difference is only in the figures with the size of the error bars. We can see that the new calculated error bars are, indeed, much smaller than the original ones estimated with root-mean-square deviations. The size of the distortion parameter Δ keeps the same value.

To check the effect of the observed dielectric anomaly of the YCrO₃ compound at ~ 473 K [6] on the distortion parameter Δ of Y, Cr, O1, and O2 ions, we constrained the temperature range of the corrected Fig. 10 (i.e., Fig. E1) into 400–550 K as shown in Fig. E3. Indeed, the distortion parameter Δ has no response to the observed anomaly in agreement with our results obtained in the original version of the published paper.

As the foregoing discussion, the error does not affect the results and conclusions of this article.

TABLE E1. For two uncorrelated variables x and y , δ_x and δ_y are their standard deviations, respectively. Here, we list the simple combined functions (V) of variables x and y as well as the corresponding propagated stand deviations (δ_V), where m , n , and k are constants.

Combined function	Propagation of errors
$V = mx + ny$	$\delta_V = \sqrt{(m\delta_x)^2 + (n\delta_y)^2}$
$V = mx - ny$	$\delta_V = \sqrt{(m\delta_x)^2 + (n\delta_y)^2}$
$V = mxy$	$\delta_V = V\sqrt{\left(\frac{\delta_x}{x}\right)^2 + \left(\frac{\delta_y}{y}\right)^2}$
$V = m\frac{x}{y}$	$\delta_V = V\sqrt{\left(\frac{\delta_x}{x}\right)^2 + \left(\frac{\delta_y}{y}\right)^2}$
$V = mx^n y^k$	$\delta_V = V\sqrt{n^2\left(\frac{\delta_x}{x}\right)^2 + k^2\left(\frac{\delta_y}{y}\right)^2}$

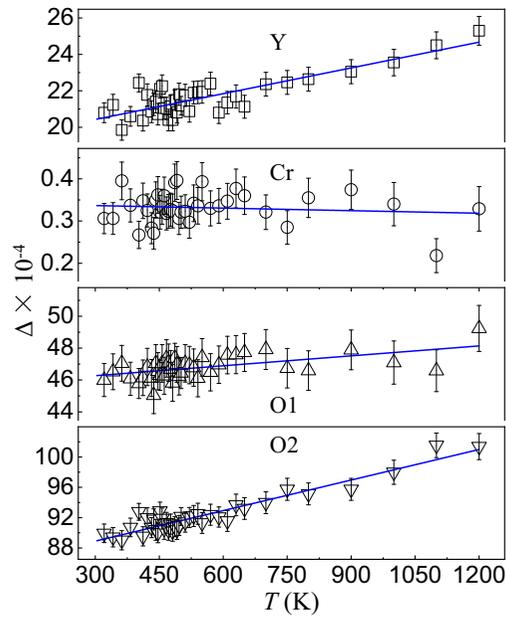


FIG. E1. Corrected Fig. 10. Temperature variation of the distortion parameter Δ of Y, Cr, O1, and O2 ions of the single-crystal YCrO_3 compound (void symbols), calculated by Eq. (6) from the refined structural parameters between 321 and 1200 K. The error bar was estimated based on the propagation law of errors. The solid lines are tentative linear fits.

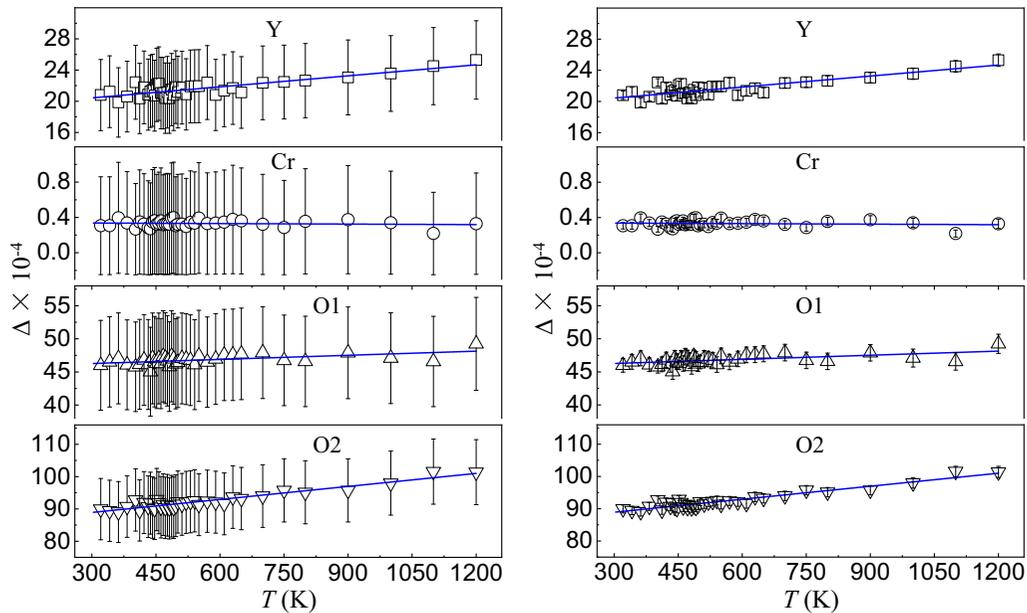


FIG. E2. (Left) Original Fig. 10. (Right) Corrected Fig. 10. For a clear comparison, we made them into the same vertical and horizontal coordinates.

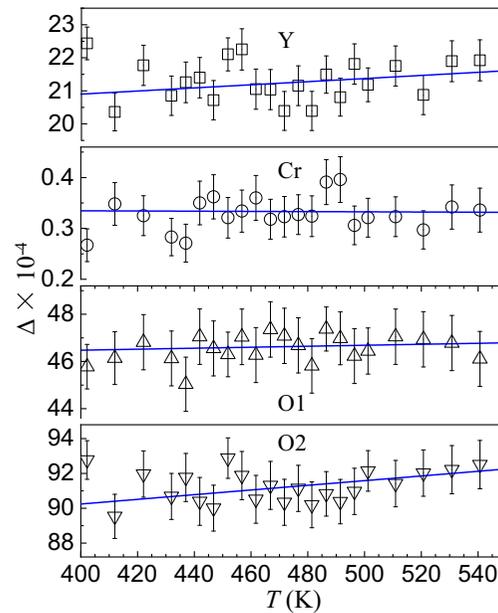


FIG. E3. Corrected Fig. 10 that is constrained within a temperature range of 400–550 K.

This project was funded by the Science and Technology Development Fund, Macao SAR (Files No. 028/2017/A1 and No. 0051/2019/AFJ).

-
- [1] J. Rodríguez-Carvajal, *Physica B* **192**, 55 (1993).
 - [2] A. Dönni, V. Y. Pomjakushin, L. Zhang, K. Yamaura, and A. A. Belik, *Phys. Rev. B* **101**, 054442 (2020).
 - [3] F. L. M. Bernal, J. Sottmann, D. S. Wragg, H. Fjellvåg, Ø. S. Fjellvåg, C. Drathen, and W. A. Sławiński, *Phys. Rev. Mater.* **4**, 054412 (2020).
 - [4] H. H. Ku, *J. Res. Natl. Bur. Stand.* **70C**, 263 (1966).
 - [5] https://en.wikipedia.org/wiki/Propagation_of_uncertainty.
 - [6] C. R. Serrao, A. K. Kundu, S. B. Krupanidhi, U. V. Waghmare, and C. N. R. Rao, *Phys. Rev. B* **72**, 220101(R) (2005).