Erratum: Theoretical study of the structure of calcium in phases IV and V via ab initio metadynamics simulation [Phys. Rev. B 77, 020101(R) (2008)]

著者	Ishikawa Takahiro, Ichikawa Ayako, Nagara Hitose, Geshi Masaaki, Kusakabe Kouichi, Suzuki Naoshi
journal or publication title	PHYSICAL REVIEW B
volume	78
number	2
page range	29901-29901
year	2008-07-10
権利	(C) 2008 The American Physical Society
URL	http://hdl.handle.net/10112/2551

doi: 10.1103/PhysRevB.78.029901

Erratum: Theoretical study of the structure of calcium in phases IV and V via *ab initio* metadynamics simulation
[Phys. Rev. B **77, 020101(R) (2008)]**

Takahiro Ishikawa, Ayako Ichikawa, Hitose Nagara, Masaaki Geshi, Koichi Kusakabe, and Naoshi Suzuki
 (Received 19 May 2008; published 10 July 2008)

DOI: [10.1103/PhysRevB.78.029901](https://doi.org/10.1103/PhysRevB.78.029901) PACS number(s): 61.50.Ah, 61.50.Ks, 62.50.-p, 64.70.K-, 99.10.Cd

In page 020101-4 of our paper, we mentioned the space group of our structure Ca-IV and wrote that the space group of the structure of Ca-IV is identified to be $P4_3$ (No.78: C_4^4). But the space group of the structure of Ca-IV can also be identified to be $P4_32_12$ (No.96: D_4^8) whose positions are (8b) sites. The parameters of the sites at 120 GPa are $x=0.32$, $y=0.01$, and $z=-0.345$ with lattice parameters $a=3.14$ Å, and $c=9.11$ Å. Since the space group $P4_32_12$ has more symmetry operations than the $P4_3$, the space group $P4_32_12$ should rather be assigned to the structure of Ca-IV. We confirmed our structure to be of space group $P4_32_12$ after receiving the space group name $P4_32_12$ and its experimental structure data from Dr. Hiroshi Fujihisa, Dr. Yuki Nakamoto, and Dr. Katsuya Shimizu. We appreciate their courtesy in disclosing their experimental data¹ prior to their publication. This correction does not affect the other parts of the paper.

¹Hiroshi Fujihisa, Yuki Nakamoto, Katsuya Shimizu, Takahiro Yabuuchi, and Yoshito Gotoh (unpublished).