

Structural and vibrational study of Zn(I0₃)₂ combining high-pressure experiments and density-functional theory

SUPPLEMENTARY MATERIAL

A. Liang¹, C. Popescu², F. J. Manjon³, P. Rodriguez-Hernandez⁴, A. Muñoz⁴, Z. Hebboul⁵, and D. Errandonea¹

1. *Departamento de Física Aplicada-ICMUV-MALTA Consolider Team, Universitat de València, c/Dr. Moliner 50, 46100 Burjassot (Valencia), Spain*
2. *CELLS-ALBA Synchrotron Light Facility, Cerdanyola del Vallès, 08290 Barcelona, Spain*
3. *Instituto de Diseño para la Fabricación y Producción Automatizada, MALTA Consolider Team, Universitat Politècnica de València, Camí de Vera s/n, 46022 València, Spain*
4. *Departamento de Física and Instituto de Materiales y Nanotecnología, MALTA Consolider Team, Universidad de La Laguna, 38206 La Laguna, Tenerife, Spain*
5. *Laboratoire Physico-Chimie des Matériaux (LPCM), University Amar Telidji of Laghouat, BP 37G, Ghardaïa Road, Laghouat 03000, Algeria*

Atom	Wyckoff position	x	y	z
Zn	2a	0.0000	0.2500	0.92165(9)
I ₁	2a	0.31386(9)	0.08034(9)	0.00743(9)
I ₂	2a	0.34883(9)	0.58960(9)	0.01114(9)
O ₁	2a	0.24208(9)	0.90521(9)	0.17200(9)
O ₂	2a	0.73877(9)	0.24060(9)	0.14379(9)
O ₃	2a	0.11494(9)	0.09319(9)	0.17200(9)
O ₄	2a	0.61677(9)	0.75785(9)	0.18891(9)
O ₅	2a	0.43218(9)	0.46389(9)	0.15811(9)
O ₆	2a	0.10050(9)	0.60654(9)	0.17200(9)

Table S1. Refined atomic positions for Zn(IO₃)₂ at ambient conditions.

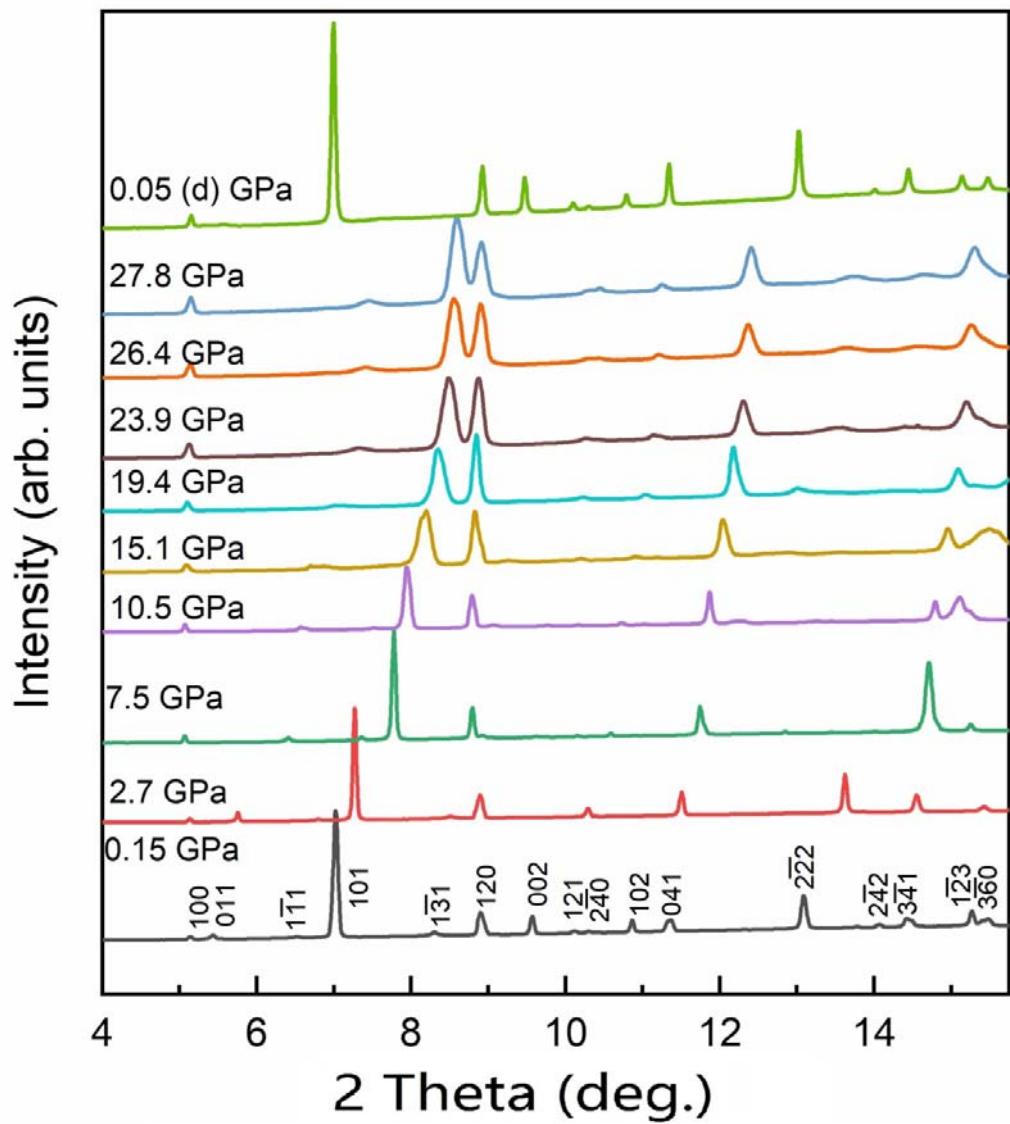


Fig. S1. XRD patterns measured at different pressures up to 27.8 GPa showing the gradual evolution of XRD with pressure.

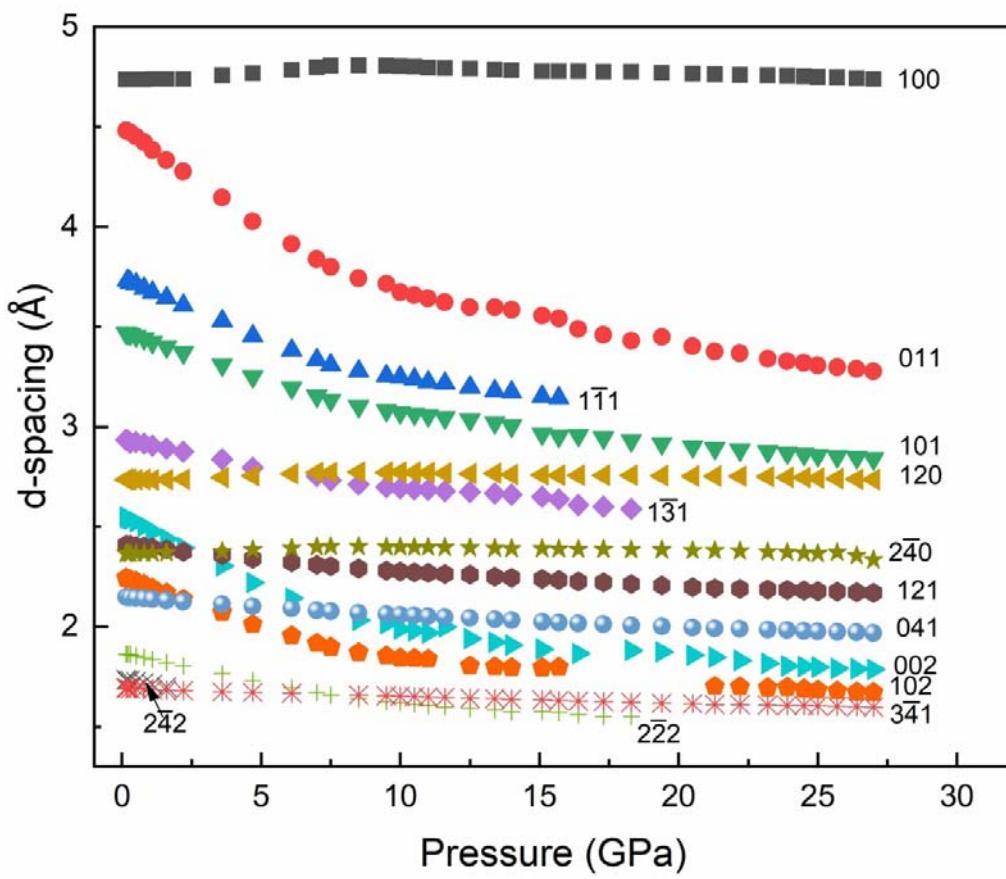


Fig. S2. Interplanar distance (d-spacing) evolution under pressure. The Miller indexes of the different planes are indicated.

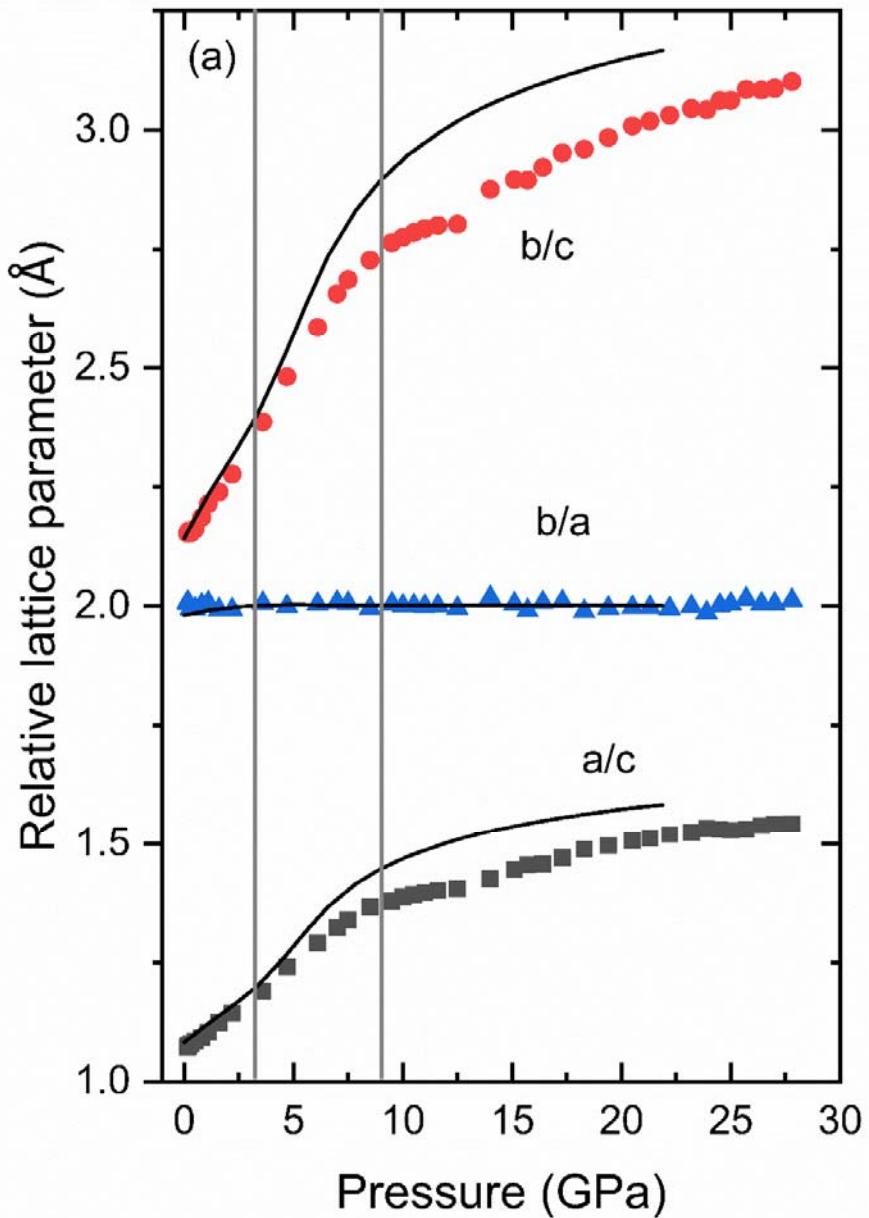


Fig. S3(a). Ratio of lattice parameters versus pressure. Dots are the experimental data while solid lines represent DFT calculated results. (b) Zoom for b/c. (c) Zoom for a/c.

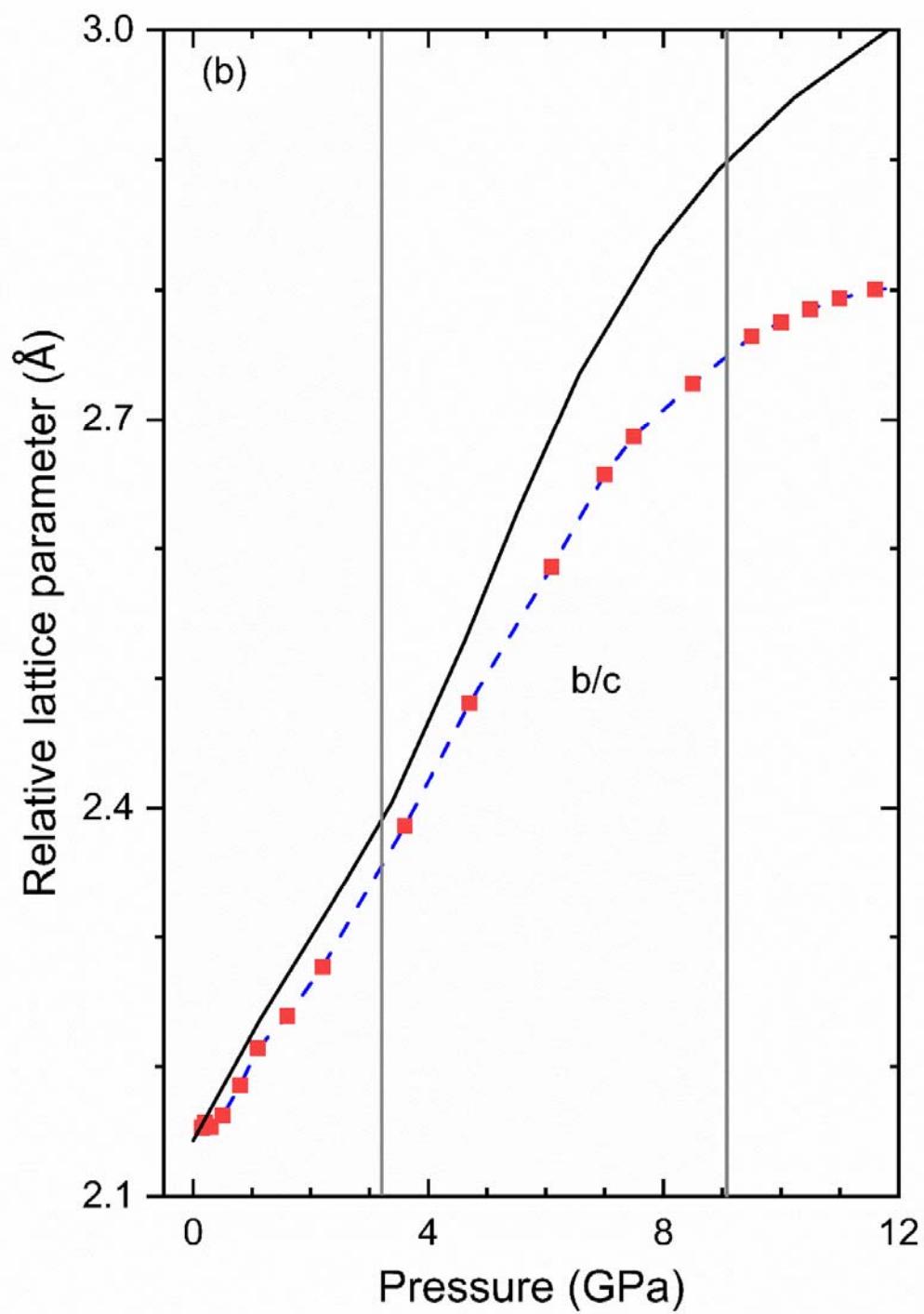


Fig. S3(b). Zoom for the b/c axial ratio versus pressure. Dots are the experimental data while solid lines represent DFT calculated results.

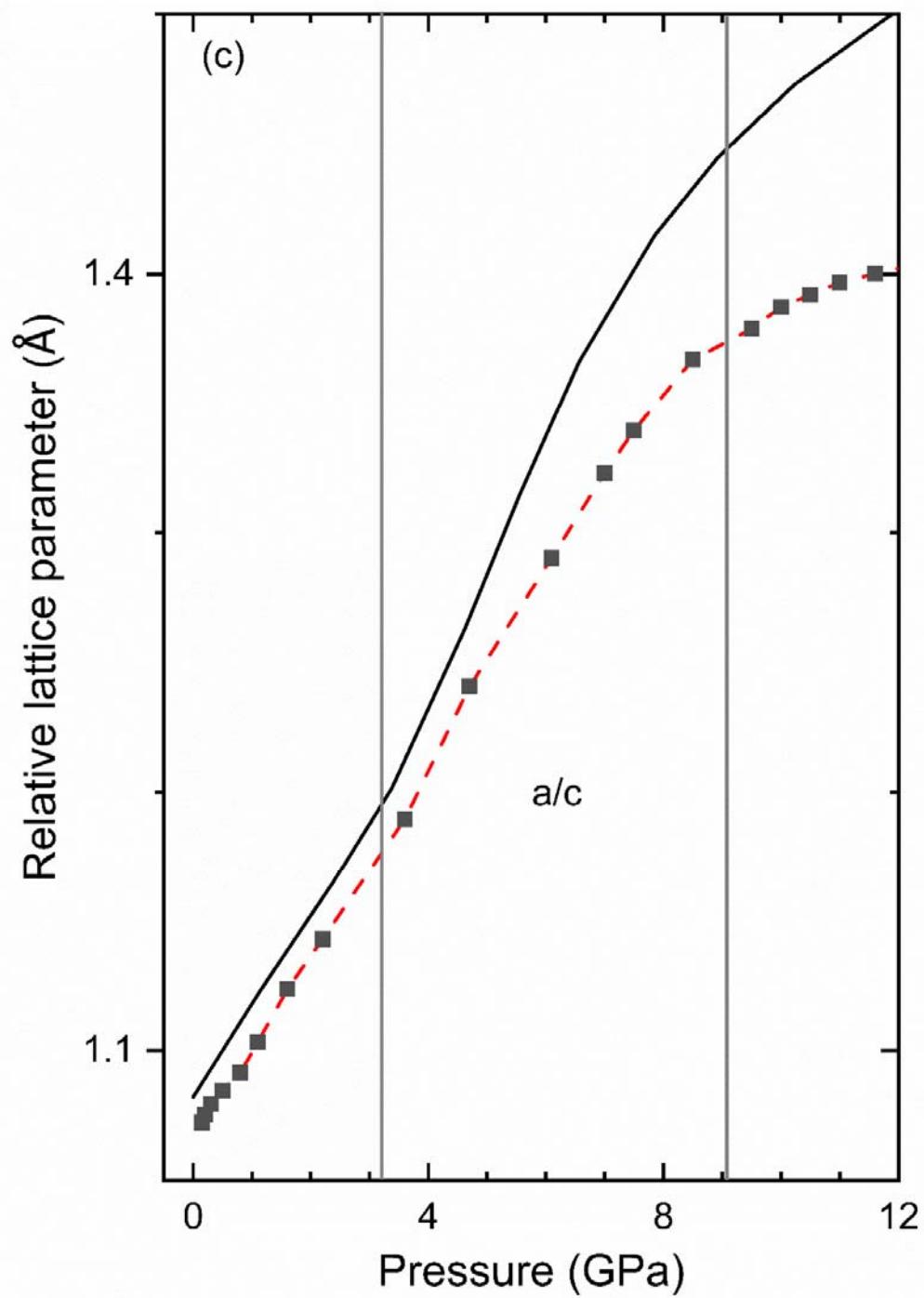


Fig. S3(c). Zoom of the a/c axial ratio versus pressure. Dots are the experimental data while solid lines represent DFT calculated results.

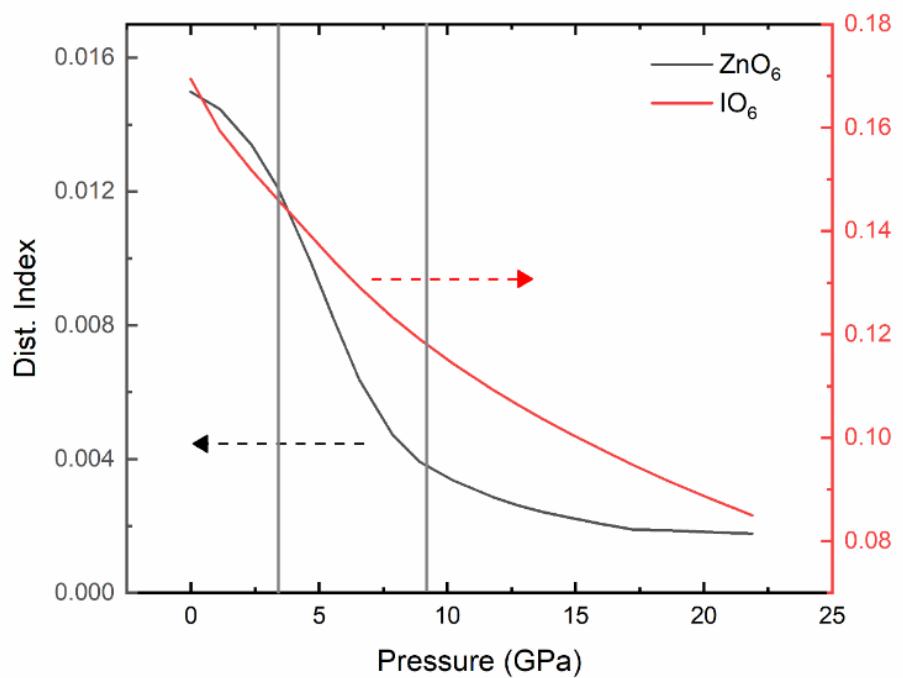


Fig. S4. Calculated pressure dependence of the distortion index of ZnO_6 and IO_6 octahedral units.

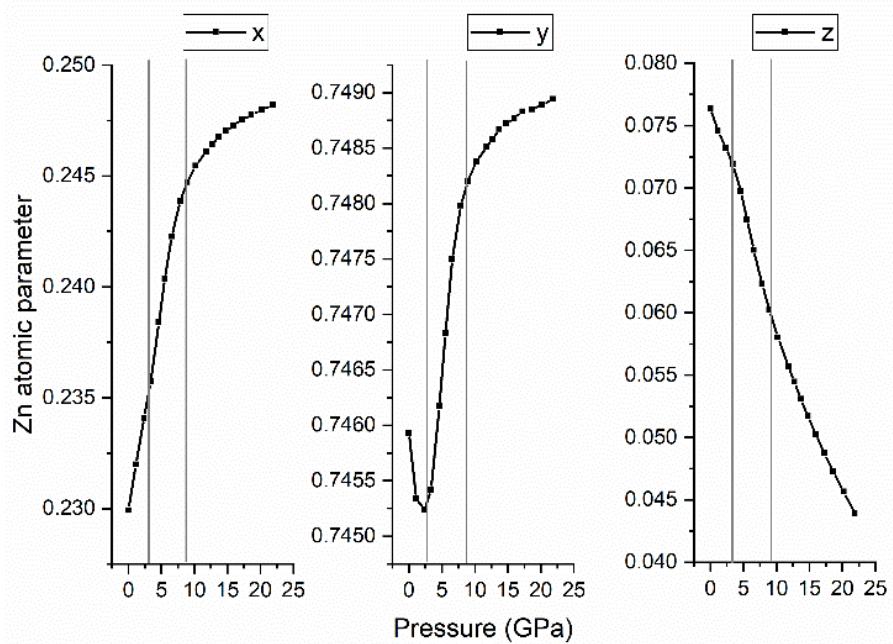


Fig. S5. Calculated pressure dependence of free atomic parameters of Zn atom in $\text{Zn}(\text{IO}_3)_2$. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

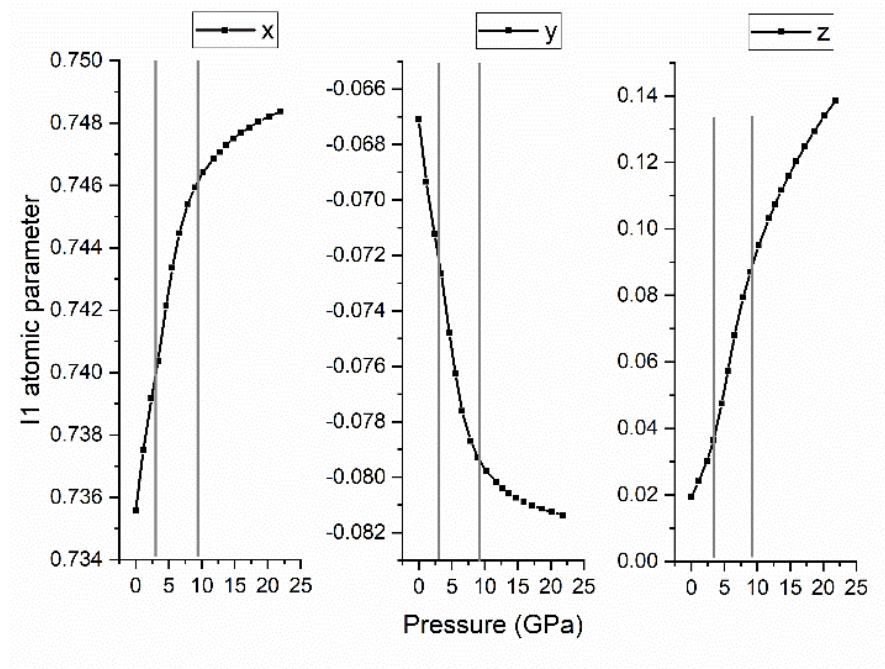


Fig. S6. Calculated pressure dependence of free atomic parameters of I_1 atom in $Zn(IO_3)_2$. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

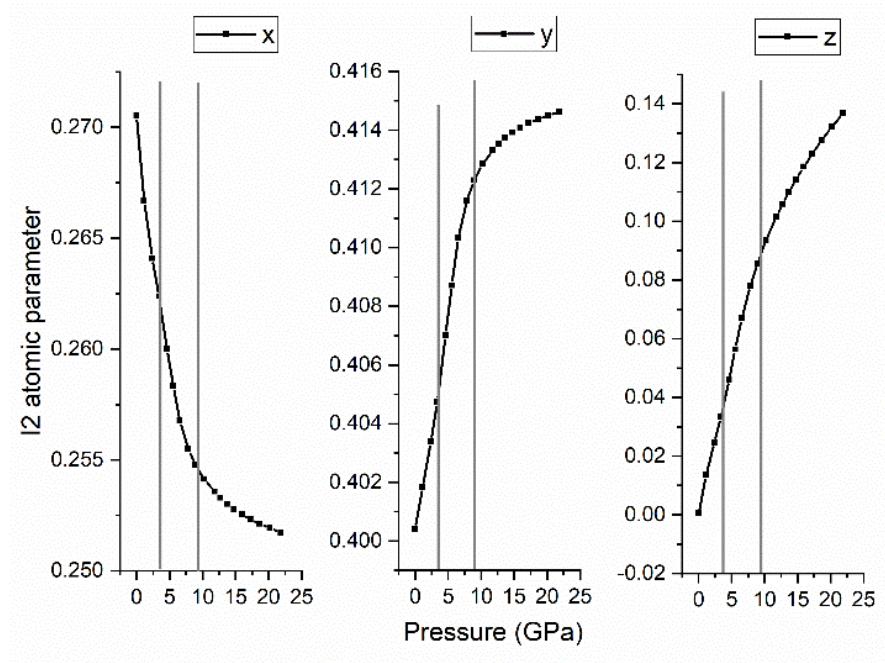


Fig. S7. Calculated pressure dependence of free atomic parameters of I_2 atom in $Zn(IO_3)_2$. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

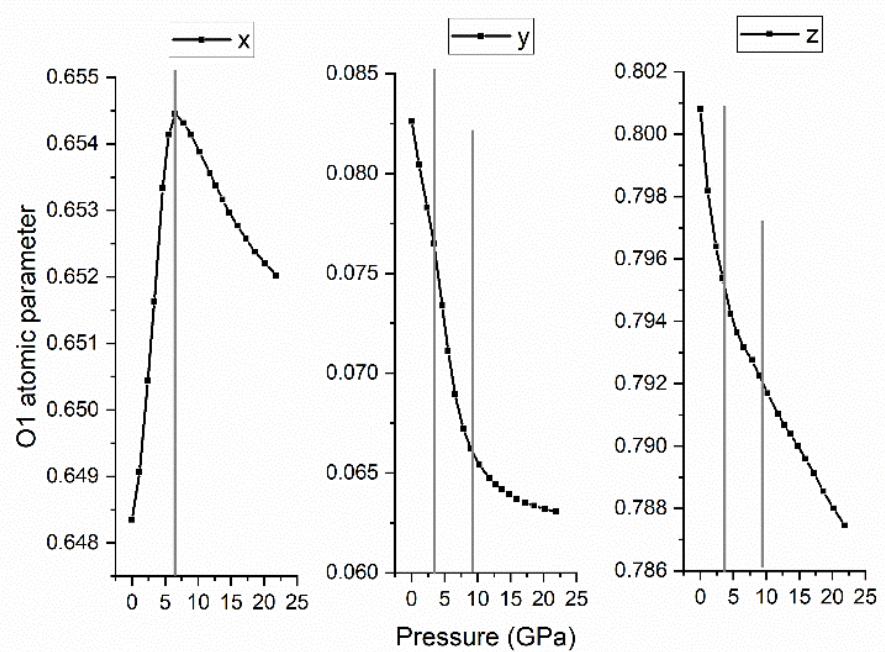


Fig. S8. Calculated pressure dependence of free atomic parameters of O₁ atom in Zn(IO₃)₂. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

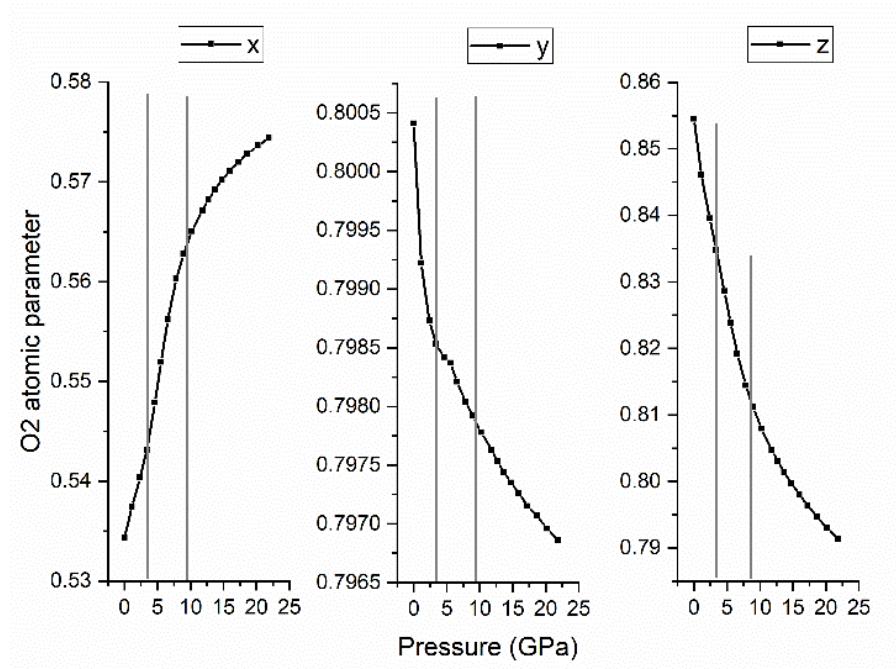


Fig. S9. Calculated pressure dependence of free atomic parameters of O₂ atom in Zn(IO₃)₂. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

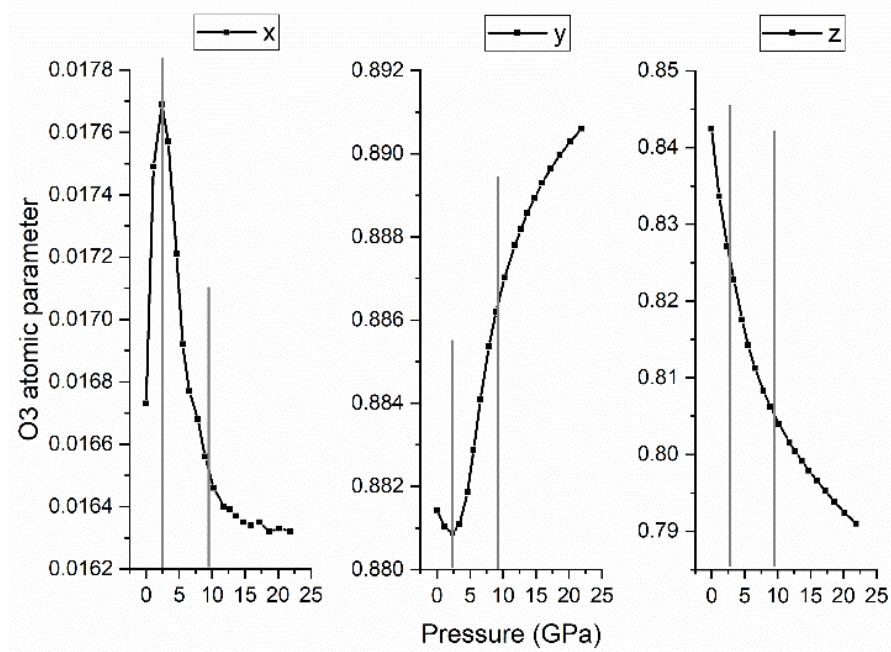


Fig. S10. Calculated pressure dependence of free atomic parameters of O_3 atom in $\text{Zn}(\text{IO}_3)_2$. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

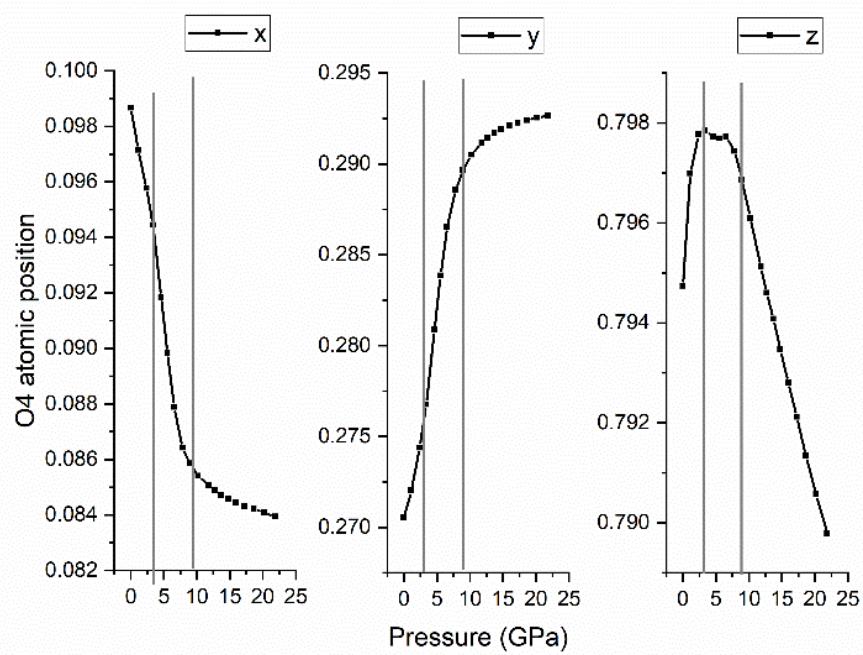


Fig. S11. Calculated pressure dependence of free atomic parameters of O_4 atom in $\text{Zn}(\text{IO}_3)_2$. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

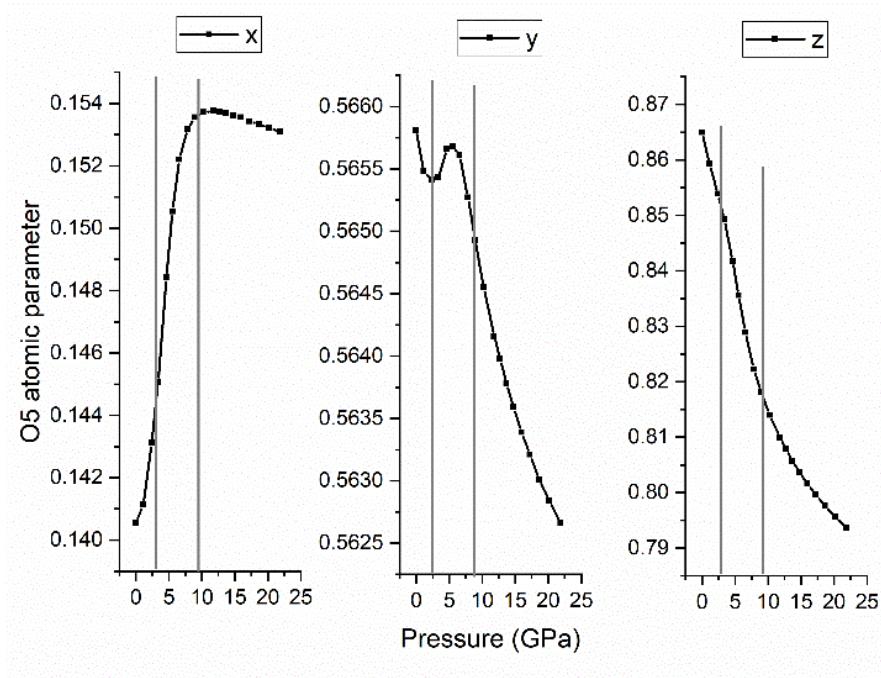


Fig. S12. Calculated pressure dependence of free atomic parameters of O₅ atom in Zn(IO₃)₂. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

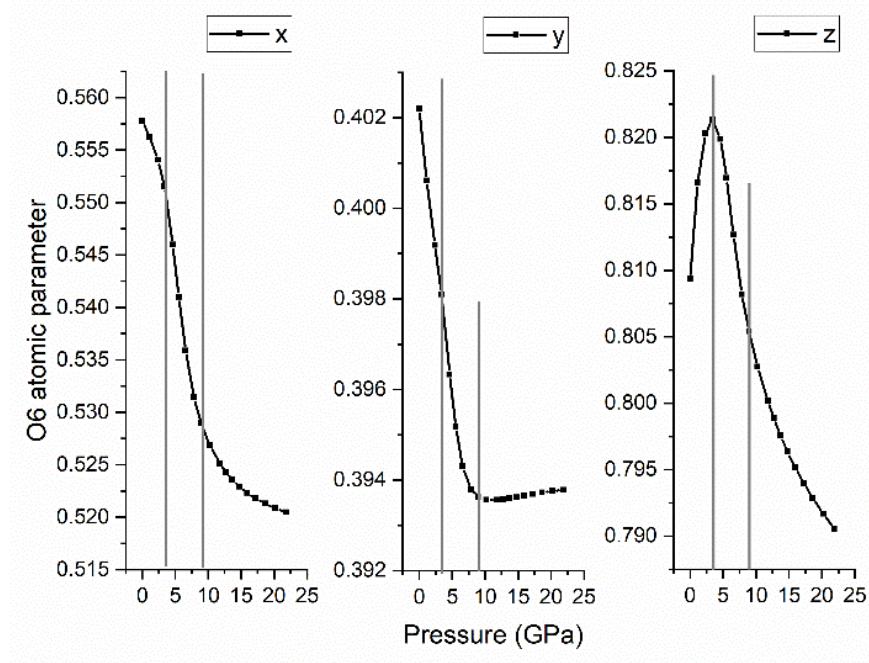


Fig. S13. Calculated pressure dependence of free atomic parameters of O_6 atom in $Zn(IO_3)_2$. Remarkable changes in the behavior happen at the pressures indicated by vertical lines.

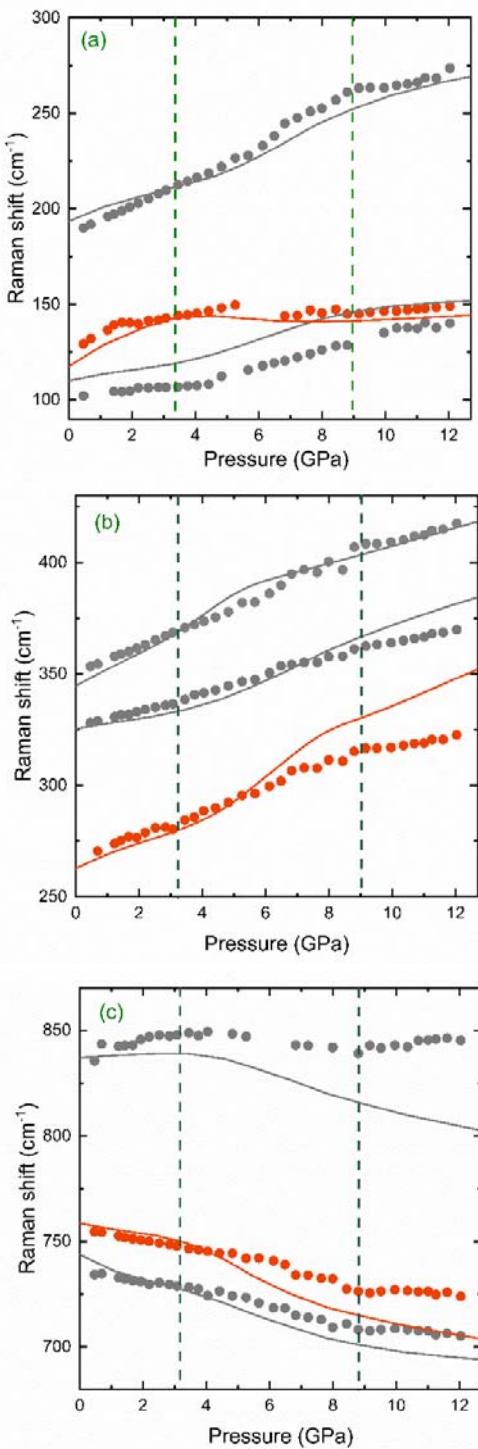


Fig. S14. Pressure dependence of selected Raman-active modes of $\text{Zn}(\text{IO}_3)_2$ to illustrate the non-linear behavior. Experiments are shown with symbols and calculations with lines. (a), (b), and (c) show different wavenumber regions. Red and gray colors are used for A and B modes, respectively. In (c), we shifted all calculated modes by $+70 \text{ cm}^{-1}$, in order to facilitate the comparison with experiments.

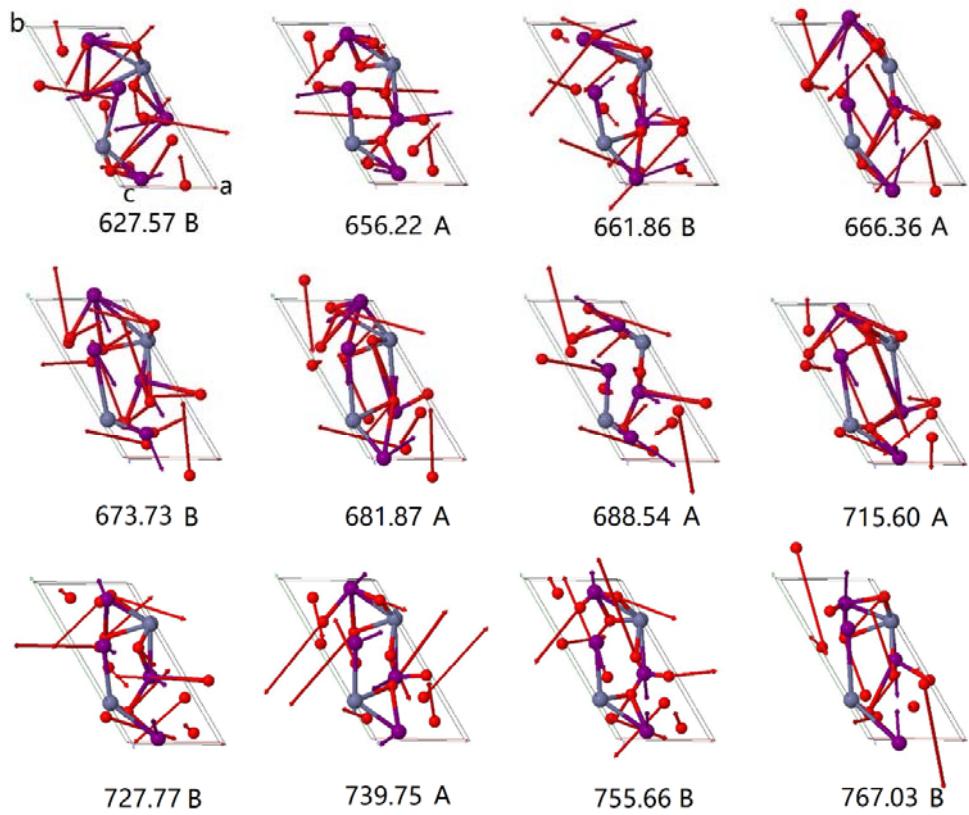


Fig. S15. Atomic movements of the soft modes of $\text{Zn}(\text{IO}_3)_2$. The three axes are marked in the first mode and the rest is the same. The red, pink, and gray balls represent oxygen, iodine, and zinc atoms, respectively. The calculated frequency (in cm^{-1}) and symmetry of each mode is shown at the bottom of each picture.