

ELECTRONIC SUPPLEMENTARY INFORMATION

High-pressure phase transition of AB₃-type compounds: case of tellurium trioxide

Dominik Kurzydłowski,¹ Mikhail A. Kuzovnikov,² Marek Tkacz³

¹ Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University, Warsaw 01-038, Poland;

² Institute of Solid State Physics RAS, 142432 Chernogolovka, Moscow District, Russian Federation;

³ Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw 01-224, Poland.

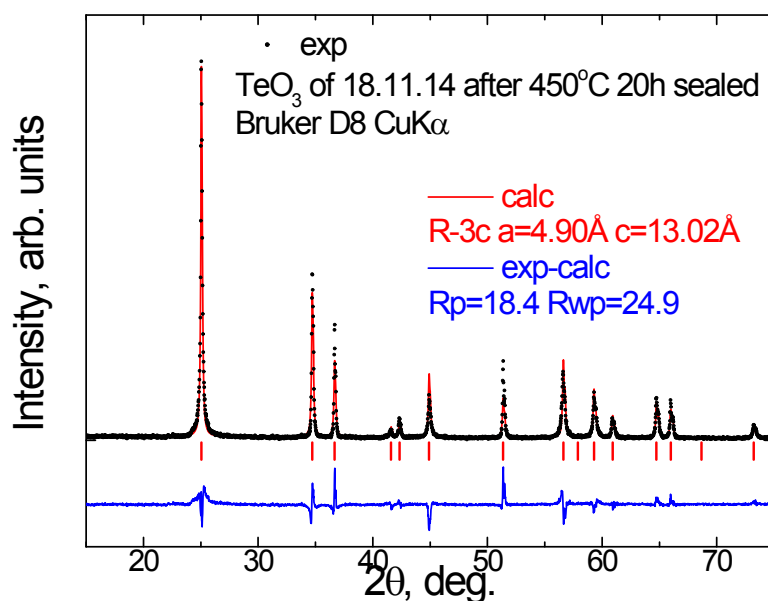


Figure S 1 Powder X-ray diffraction pattern of freshly synthesized TeO₃ (black points) obtained using Bruker D8 diffractometer and CuK α radiation. The Rietveld fit assuming the R $\bar{3}$ c structure is shown with a red curve. Blue curve represents the difference between the fit and experimental points.

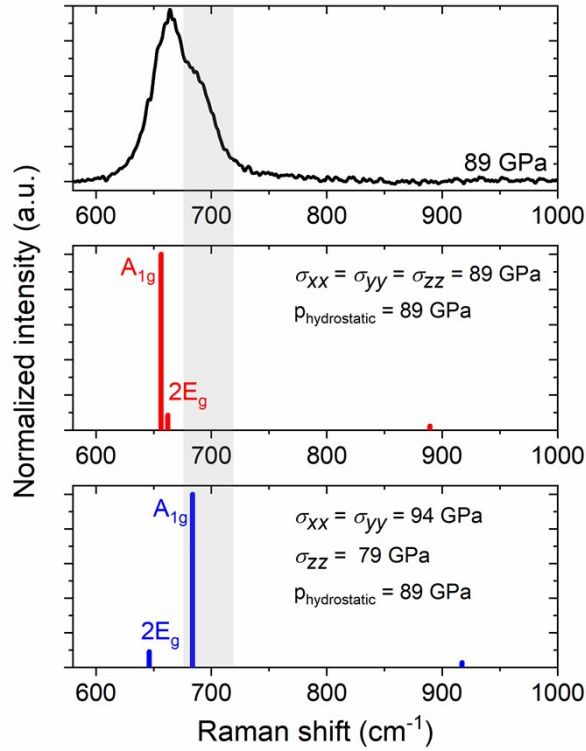


Figure S 2 Raman spectrum (black curve) of TeO_3 at 89 GPa compared with the Raman band intensities simulated with LDA for the $R\bar{3}c$ structure at a hydrostatic pressure of 89 GPa (red bars), and at non-hydrostatic conditions (blue bars). Diagonal elements of the stress tensor (σ_{xx} , σ_{yy} , σ_{zz}), under which the geometry optimization of the $R\bar{3}c$ structure were conducted are also specified. These values were selected as reasonable parameters for non-hydrostatic conditions inside the DAC (deviatoric stress of 5 GPa). We note that the shift of the A_{1g} mode to higher frequencies (with respect to hydrostatic conditions) requires the stress component along the x and y directions to be larger than that along the z direction

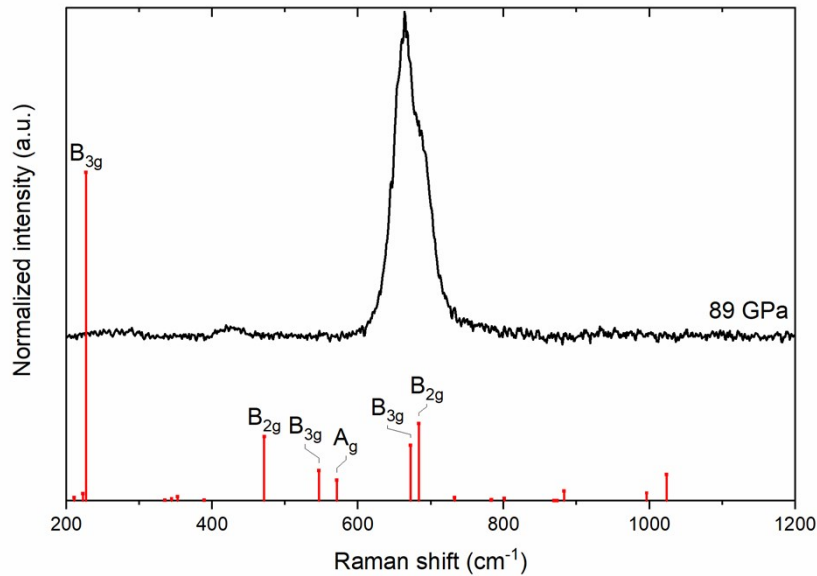


Figure S 3 Comparison of the Raman spectrum of TeO_3 at 89 GPa (black curves) with the Raman intensities simulated at that pressure for the YF_3 -type ($Pnma$ symmetry) structure (red bars).

Table S 1 Comparison of the experimental geometry (from this work and ref. ¹) and the frequencies of the Raman-active vibrational modes (this work and ref. ²) of the ambient pressure polymorph of TeO₃ (space group $R\bar{3}c$) with data obtained from calculations utilizing the SCAN and LDA functionals. Cell vectors and the Te-O bond length are given in Å, volume in Å³, while frequencies in cm⁻¹. Percentage differences between our experimental data and calculations are given in parenthesis.

	Exp.	Exp. (this work)	SCAN (this work)	LDA (this work)
a	4.901	4.900	4.933 (+0.7 %)	4.959 (+1.2 %)
c	13.030	13.020	13.074 (+0.4 %)	13.314 (+2.3 %)
V/Z	45.17	45.12	45.91 (+1.8 %)	47.25 (+4.7 %)
R_{Te-O}	1.911	1.910	1.917 (+0.4 %)	1.975 (+3.4 %)
1E_g	258	255	255 (-0.0 %)	251 (-1.6 %)
A_g	336	334	333 (-0.3 %)	360 (+7.8 %)
2E_g	485	484	476 (-1.7 %)	457 (-5.6 %)
3E_g	666	677	655 (-3.2 %)	624 (-7.8 %)

Table S 2 Comparison of the calculated phase transition pressure (in GPa) between the VF₃-type structure ($R\bar{3}c$ symmetry) and the YF₃-type structure ($Pnma$ symmetry).

LDA	PBE	SCAN	HSE06
46	55	66	71

Table S 3 Computed (SCAN calculations) structural parameters of the high-pressure polymorphs of TeO₃.

	a	b	c	α	β	γ	V	Fractional coordinates
VF₃ ($R\bar{3}c$) p = 60 GPa	4.412	4.412	12.561	90	90	120	211.78	O1 18e (0.685 0.0 0.25) Te1 6b (0.0 0.0 0.0)
HP-WO₃ ($P2_1/c$) p = 110 GPa	4.809	4.343	5.857	90	96.15	90	121.61	O1 4e (0.052 0.663 0.846) O2 4e (0.615 0.0146 0.347) O3 4e (0.724 0.509 0.455) Te1 4e (0.743 0.683 0.161)
YF₃ ($Pnma$) p = 100 GPa	4.888	5.960	4.074	90	90	90	118.69	O1 8d 0.670 0.065 0.153) O2 4c (0.525 0.25 0.623) Te1 4c (0.871 0.250.465)
$R\bar{3}$ p = 100 GPa	5.851	5.851	17.358	90	90	120	514.77	O1 18f(0.352 0.376 0.303) O2 18f(0.745 -0.027 0.186) O3 6c (0.0 0.0 0.715) O4 6c (0.0 0.0 0.437) O5 6c (0.0 0.0 -0.074) Te1 18f(0.003 0.326 0.251)

References

- 1 M. Dušek and J. Loub, *Powder Diffr.*, 1988, **3**, 175–176.
- 2 J. Loub, *Collect. Czechoslov. Chem. Commun.*, 1977, **42**, 960–966.