

Electronic Properties and High-Pressure Behavior of Wolframite-Type CoWO_4

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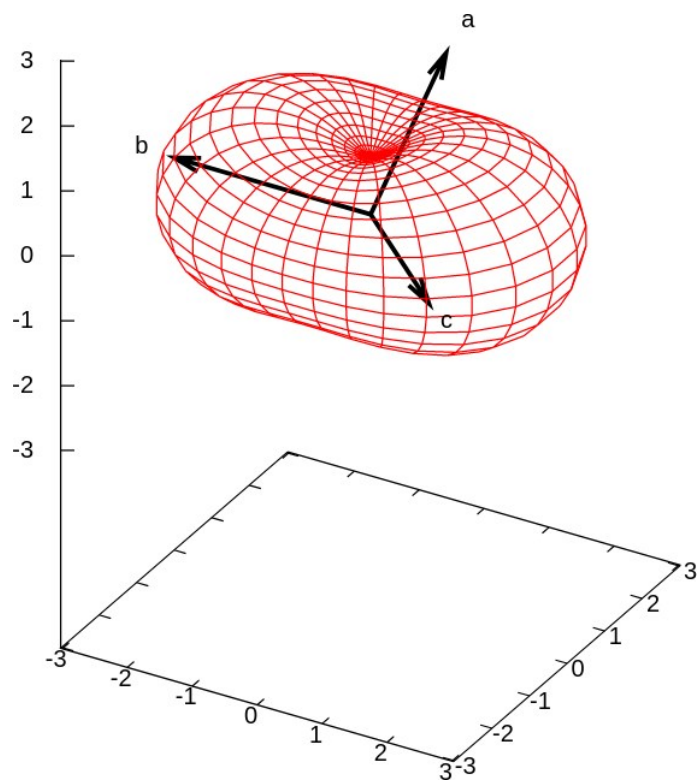


Figure S1. Compressibility indicatrix of CoWO_4 . Red regions indicate positive linear compressibility.

	Experiment	Calculations	Literature ^a
a (Å)	4.670(5)	4.61176	4.6698(9)
b (Å)	5.687(6)	5.67847	5.6873(23)
c (Å)	4.951(5)	4.93178	4.9515(17)
β (deg)	90.08(9)	90.3215	90.00
V (Å ³)	131.5(2)	129.15	131.50

Table S1. Unit-cell parameters a , b and c and cell volume V for CoWO_4 at ambient pressure, as obtained from our experiments and calculations *ab initio* simulations, and comparison with Literature.

^aH. Weitzel, *Zeitschrift für Krist. - New Cryst. Struct.*, 1976, **144**, 238–258.

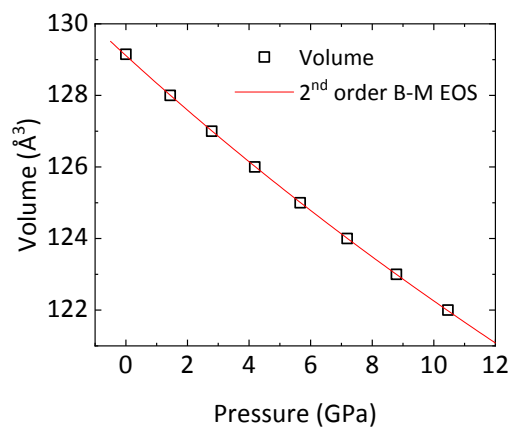


Figure S2. Pressure-Volume data for CoWO₄ (squares) as obtained from *ab initio* simulations. In red, the fitting of the data to a 2nd order Birch-Murnaghan EOS.

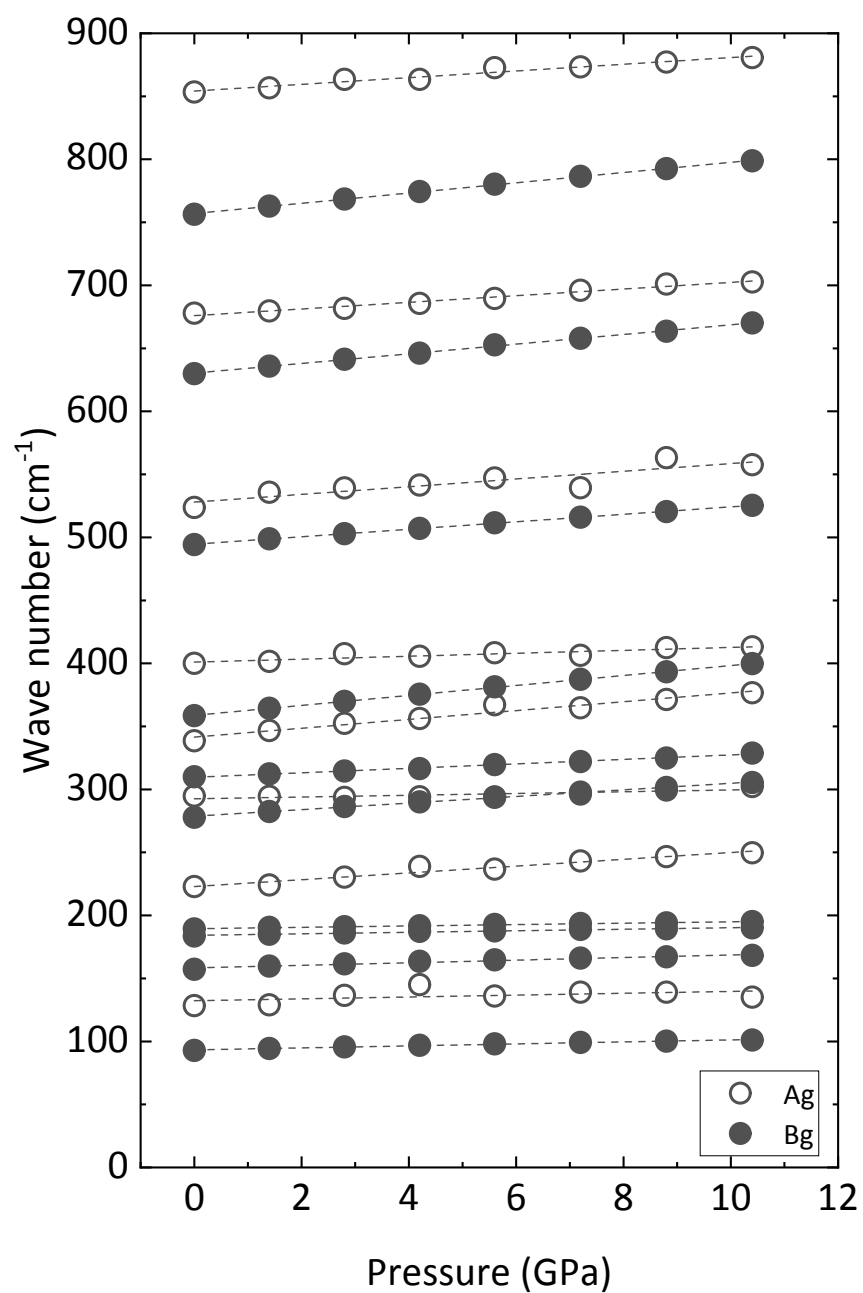


Figure S3. Frequency of Raman modes vs. pressure for wolframite-type CoWO_4 (circles), as calculated by ab initio simulations. Dashed lines are the linear fits used for the calculation of the pressure coefficients and Grüneisen parameters reported in the main manuscript.

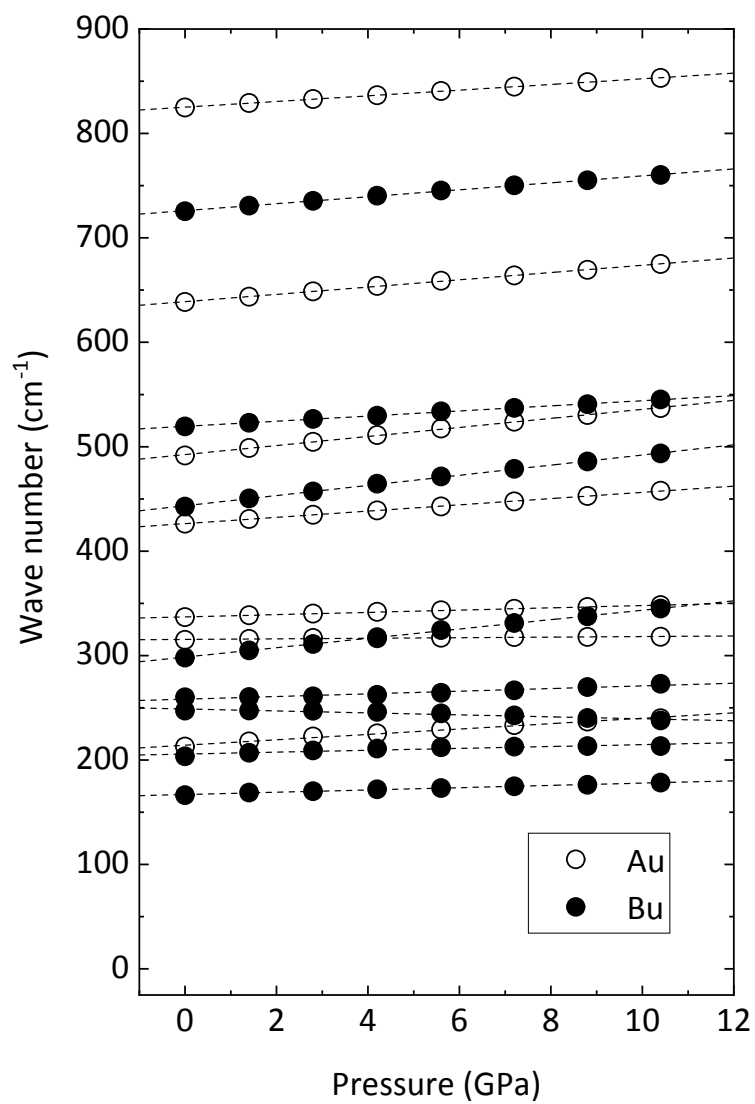


Figure S4. Evolution of IR modes vs. pressure for wolframite-type CoWO_4 (circles), as calculated by ab initio simulations. Dashed lines are the linear fits used for the calculation of the pressure coefficients.

Mode	ω_0^c (cm ⁻¹)	Linear fit	
		ω_0 (cm ⁻¹)	$\partial\omega/\partial P$ (cm ⁻¹ GPa ⁻¹)
B _u	166.38	167.0(2)	1.09(4)
B _u	203.54	206(1)	0.90(15)
A _u	212.75	214.2(6)	2.6(1)
B _u	247.20	249.0(7)	-0.94(12)
B _u	260.08	258.3(8)	1.27(13)
B _u	298.07	298.6(3)	4.48(5)
A _u	314.98	315.5(2)	0.27(4)
A _u	336.77	337.05(12)	1.09(2)
A _u	426.39	426.40(15)	2.99(3)
B _u	442.64	443.5(4)	4.86(7)
A _u	491.64	492.5(3)	4.33(6)
B _u	519.43	519.6(2)	2.45(4)
A _u	638.58	639.0(2)	3.48(3)
B _u	725.47	726.1(3)	3.33(5)
A _u	824.84	825.18(13)	2.71(2)

Table S2. Ab-initio calculated IR modes for CoWO₄, ω_0^c , and parameters of the linear fits of their evolution with pressure, ω_0 and $\partial\omega/\partial P$ (intercept and pressure coefficient, respectively). The symmetry of each phonon is also shown.

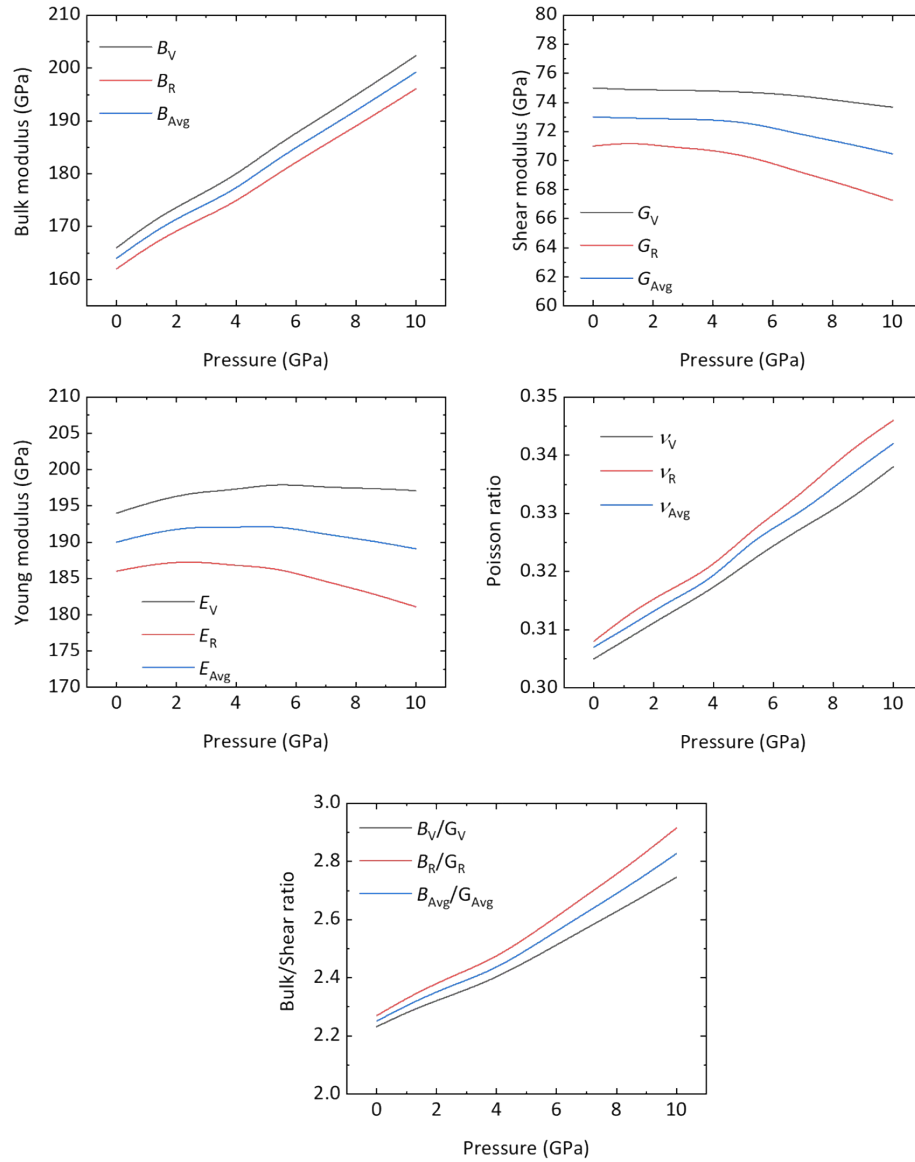


Figure S5: Elastic moduli of wolframite-type CoWO_4 as a function of pressure; a) Bulk modulus, b) Shear modulus, c) Young modulus, d) Poisson ratio, and e) bulk/shear ratio. “V”, “R” and “Avg” subscripts indicate Voigt and Reuss approximation and their average, respectively.