Supplementary Material

PbV₂O₆ under compression: Near zero-linear compressibility and pressure-induced change in vanadium coordination

Josu Sánchez Martín,*[a] Julio Pellicer-Porres,[a] Robin Turnbull,[a] Daniel Díaz-Anichtchenko,[a] Simone Anzellini,[a] Akun Liang,[a,b] Catalin Popescu,[c] Marco Bettinelli,[d] Plácida Rodríguez-Hernández,[e] Alfonso Muñoz [e] and Daniel Errandonea [a]

a. Departamento de Física Aplicada-ICMUV, Universidad de Valencia, Dr. Moliner 50, Burjassot, 46100 Valencia, Spain. *E-mail: Josu.Sanchez@uv.es

b. Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, EH9 3FD Edinburgh, United Kingdom

c. CELLS-ALBA Synchrotron Light Facility, Cerdanyola del Vallès, 08290 Barcelona, Spain

d. Laboratorio Materiali Luminescenti, Dipartimento di Biotecnologie, Università di Verona, and INSTM, UdR Verona, Strada Le Grazie 15, 37134 Verona, Italy

e. Departamento de Física, MALTA-Consolider Team, Instituto de Materiales y Nanotecnología, Universidad de La Laguna, San Cristóbal de La Laguna, E-38200 Tenerife, Spain

Table S1. Raman modes, wavenumbers and pressure coefficients corresponding to the active Raman modes at ambient conditions for PbV_2O_6. ω_0 is expressed in cm^{-1}, and P in GPa. Pressure coefficients in italics mark the assignation of this value from another close mode. The DFT-calculated ω_0 has a related uncertainty of ±5%.

Mode	Experimental		DFT	
	ω_0	$\partial\omega/\partial P$	ω_0	$\partial\omega/\partial P$
B_{3g}^1	33(2)	3.0(3)	36	3.3(1)
B_{1g}^1	38(2)	1.8(3)	37	3.6(1)
A_g^1	44(2)	1.3(1)	42	1.4(1)
A_g^2	49(3)	2.7(1)	45	4.1(1)
B_{2g}^1	47(3)	1.8(1)	58	1.9(1)
B_{2g}^2	59(4)	3.1(4)	65	6.7(2)
A_g^3	78(2)	15.2(3)	75	10.6(1)
B_{1g}^2	94(4)	-	94	6.4(1)
A_g^4	103(2)	10.5(5)	98	8.6(2)
B_{3g}^2	113(3)	5.0(1)	100	5.5(1)
B_{2g}^3	108(4)	3.3(1)	108	2.7(1)
B_{2g}^4	129(3)	4.1(2)	119	5.6(1)
A_g^5	142(4)	7.6(2)	131	6.0(1)
B_{2g}^5	146(3)	3.3(1)	132	4.0(1)
B_{3g}^3	173(3)	2.7(1)	163	2.3(1)
B_{1g}^3	177(2)	2.8(1)	166	2.7(1)
B_{2g}^6	183(4)	3.1(2)	176	5.3(1)
A_g^6	186(3)	3.5(1)	183	5.0(1)
A_g^7	222(2)	3.5(1)	212	3.9(1)
B_{2g}^7	232(4)	-	229	3.5(1)
B_{1g}^4	248(2)	1.2(6)	232	3.7(2)
B_{3g}^4	260(3)	0.8(4)	242	0.6(2)
B_{3g}^5	253(4)	2.7(2)	249	2.4(1)
A_g^8	270(2)	2.5(1)	258	6.7(1)
B_{1g}^5	253(4)	*2.7(2)*	258	2.3(1)
B_{2g}^8	238(3)	-	261	5.0(1)
B_{1g}^6	280(3)	3.5(4)	270	3.2(1)
B_{3g}^6	287(3)	3.6(1)	273	3.5(1)
B_{3g}^7	298(3)	6.1(1)	277	4.7(1)
B_{1g}^7	300(4)	6.7(2)	279	4.7(1)
A_g^9	323(2)	2.8(2)	300	4.9(1)
B_{2g}^9	334(4)	2.3(7)	307	7.8(3)
A_g^{10}	340(2)	1.6(2)	320	1.5(2)

B_{2g}^{10}	351(3)	1.9(5)	322	1.6(1)
B_{2g}^{11}	370(3)	7.6(2)	372	3.8(1)
A_{g}^{11}	397(2)	3.0(3)	382	3.0(1)
A_{g}^{12}	435(4)	5.5(3)	430	3.4(1)
B_{2g}^{12}	440(3)	4.2(5)	431	3.5(1)
B_{1g}^{8}	485(2)	10.0(1)	456	10.7(1)
B_{3g}^{8}	485(2)	*10.0(1)*	457	10.6(1)
A_{g}^{13}	447(2)	2.1(1)	476	1.3(1)
B_{2g}^{13}	452(3)	1.9(3)	477	1.2(1)
A_{g}^{14}	483(5)	1.3(5)	511	1.3(1)
B_{2g}^{14}	523(3)	1.5(6)	526	1.3(1)
B_{3g}^{9}	678(2)	8.0(1)	668	5.7(1)
B_{1g}^{9}	678(2)	*8.0(1)*	668	5.7(1)
A_{g}^{15}	758(3)	8.3(1)	777	5.6(1)
B_{2g}^{15}	797(2)	3.2(3)	780	5.9(1)
A_{g}^{16}	817(3)	3.2(5)	816	2.9(1)
B_{2g}^{16}	855(2)	5.2(1)	873	2.4(1)
A_{g}^{17}	877(3)	3.0(3)	906	1.0(1)
B_{2g}^{17}	890(2)	1.5(1)	917	0.9(2)
A_{g}^{18}	956(2)	0.6(4)	984	0.6(4)
B_{2g}^{18}	992(2)	1.5(2)	1030	-0.2(1)

Table S2. Infrared modes, wavenumbers and pressure coefficients corresponding to the DFT calculated active IR modes at ambient conditions for PbV_2O_6. ω_0 is expressed in cm^{-1} (uncertainty of ±5%) and P in GPa.

| Mode	ω_0	$\partial\omega/\partial P$	Mode	ω_0	$\partial\omega/\partial P$
B_{1u}^2	49	2.6(1)	B_{3u}^9	292	2.2(4)
B_{3u}^2	50	6.9(1)	B_{3u}^{10}	339	2.1(1)
B_{2u}^2	51	5.0(1)	B_{1u}^{10}	350	4.0(1)
B_{1u}^3	63	10.4(1)	B_{1u}^{11}	367	2.9(1)
B_{3u}^3	73	1.7(1)	B_{3u}^{11}	376	4.4(1)
B_{1u}^4	79	3.6(1)	B_{1u}^{12}	414	2.2(1)
B_{3u}^4	93	2.3(1)	B_{3u}^{12}	421	1.9(1)
B_{3u}^5	118	10.3(1)	B_{2u}^8	450	7.1(1)
B_{1u}^5	140	4.6(1)	B_{3u}^{13}	485	1.9(1)
B_{1u}^6	152	6.7(1)	B_{1u}^{13}	486	1.8(1)
B_{2u}^3	167	2.4(1)	B_{3u}^{14}	515	1.0(2)
B_{3u}^6	210	4.6(1)	B_{1u}^{14}	525	0.8(3)
B_{2u}^4	219	1.8(1)	B_{2u}^9	661	3.9(1)
B_{3u}^7	220	1.9(1)	B_{1u}^{15}	754	4.7(1)
B_{1u}^7	228	1.5(1)	B_{3u}^{15}	766	2.7(1)
B_{2u}^5	238	0.9(2)	B_{3u}^{16}	833	2.8(1)
B_{1u}^8	260	2.4(1)	B_{1u}^{16}	869	1.7(1)
B_{3u}^8	262	2.2(3)	B_{3u}^{17}	886	1.0(1)
B_{2u}^6	263	2.5(1)	B_{1u}^{17}	902	0.9(1)
B_{2u}^7	278	3.2(1)	B_{1u}^{18}	984	1.2(1)
B_{1u}^9	290	1.4(1)	B_{3u}^{18}	1000	0.7(1)
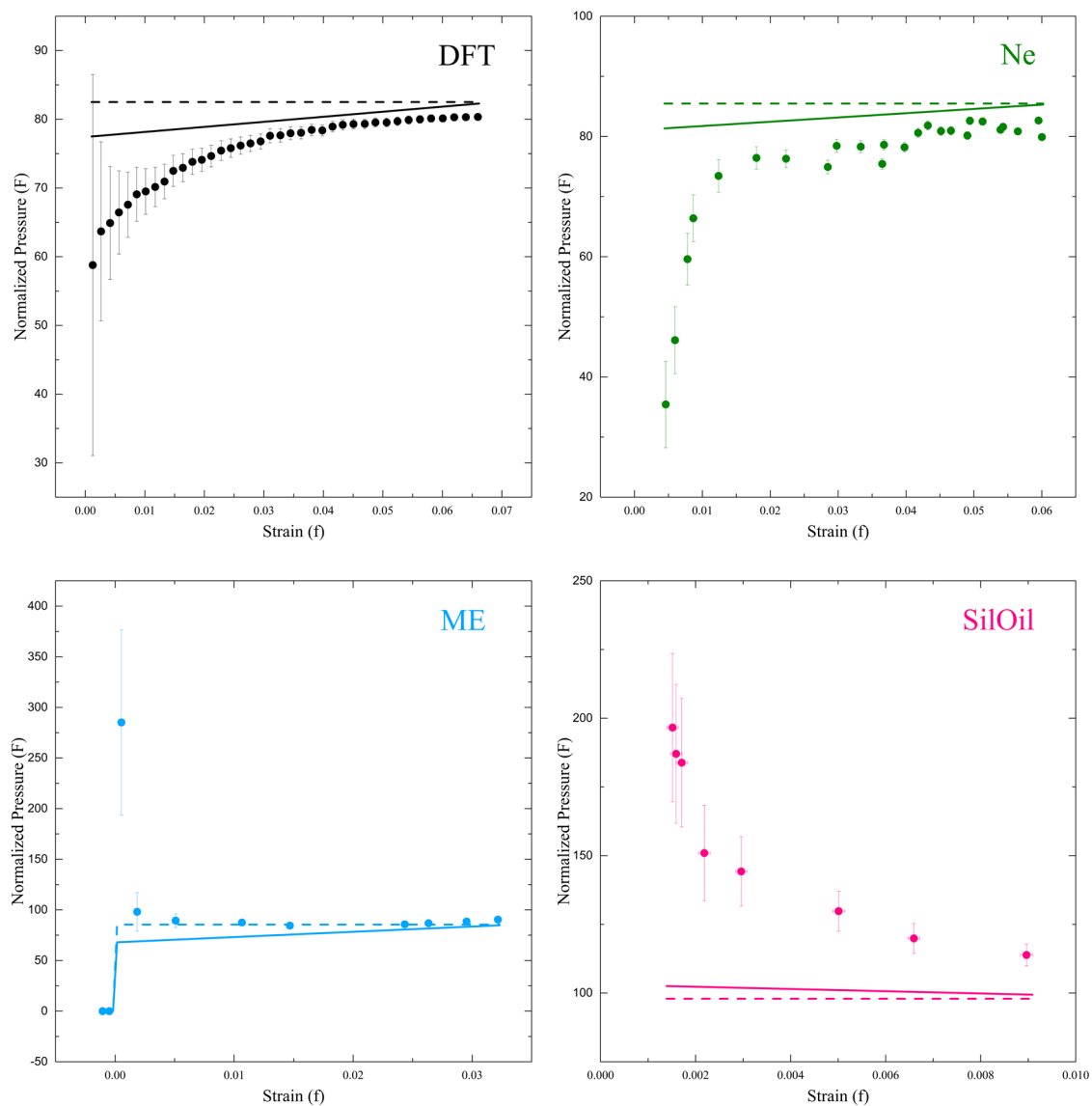
Figure S1. Normalized pressure (F) vs the Euler strain (f) for all data (dots) used to fit the EOS in Table 1. The Birch-Murnaghan fits are represented with solid lines for 3rd order and dashed lines for 2nd order.
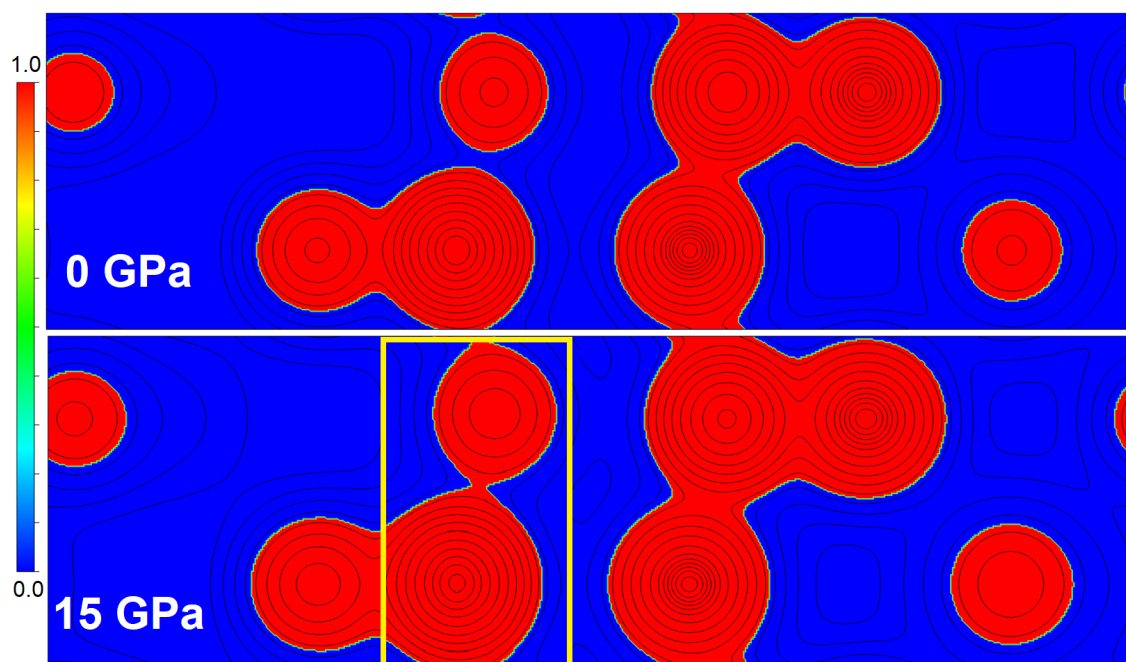
Figure S2. Contour plot of the calculated electron-localization function of PbV_2O_6 at 0 and 15 GPa. The region highlighted with a yellow framework shows the formation of an additional V-O bond.