Supplementary Information (SI) for Dalton Transactions.
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Supplementary Material

High-Pressure Phase Transition and Amorphization of BaV_2O_6

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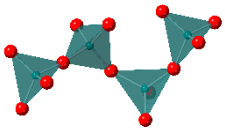
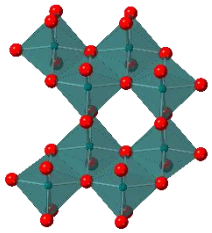
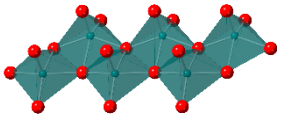
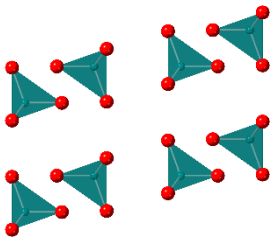
Table S1 Crystal structure of the *C*2 phase BaV_2O_6 at 4.2 GPa determined by Le Bail refinement and subsequently optimized by DFT calculation with the lattice parameters fixed at the experimental value.

Compound		BaV_2O_6	
Pressure		4.2 GPa	
Space group		*C*2	
a (Å)		11.8936	
b (Å)		8.3255	
c (Å)		7.6719	
β°		90.9302	
Z		6	
Ba1	0.8341	-0.0015	0.4992
Ba2	0	0.0016	0
V1	0.4315	0.8186	0.2658
V2	0.5681	0.1803	0.2633
V3	0.2482	0.7506	0.9264
O1	0.4994	-0.0017	0.7750
O2	0.9819	0.8330	0.3009
O3	0.0172	0.1646	0.3041
04	0.2386	0.9203	0.8152
O5	0.7587	0.0853	0.8087
06	0.1546	0.6722	0.4315
O7	0.8467	0.3283	0.4317
O8	0.1288	0.7411	0.0630
O9	0.8698	0.2579	0.0634

Table S2 Comparison of bulk modulus (B_0) of different MV_2O_6 (M = Ba, Mg, Zn, and Pb) compounds and $Ba_3V_2O_8$ compound.[1-5]

Compounds	B_0 / GPa	Range / GPa	B_0 / GPa	Range / GPa	B_0 / GPa	Range / GPa
BaV_2O_6	$50(1)_{Exp.}$ $57.2(2)_{Cal.}$	0-4	$50.4(8)_{Exp.}$ $58.6(5)_{Cal.}$	4-8		
MgV_2O_6	$53(5)_{Exp.}$	0-4	$188(5)_{Exp.}$	4-33	$255(9)_{Exp.}$	20-33
ZnV_2O_6	$147(2)_{Exp.}$ $146.74_{Cal.}$	0-15	$237(1)_{Exp.}$	15-25		
PbV_2O_6	$86.1(9)_{Exp.}$ $82.6(4)_{Cal.}$	0-20				
$Ba_3V_2O_8$	$136(4)_{Exp.}$	0-29				

Table S3 The type and connection of vanadium oxide polyhedra in MV_2O_6 (M = Ba, Mg, Zn, and Pb) compounds and $Ba_3V_2O_8$ compound.[6-10]

Compounds	Type and connection of vanadium oxide polyhedra
BaV_2O_6	
MgV_2O_6 and ZnV_2O_6	
PbV_2O_6	
$Ba_3V_2O_8$	

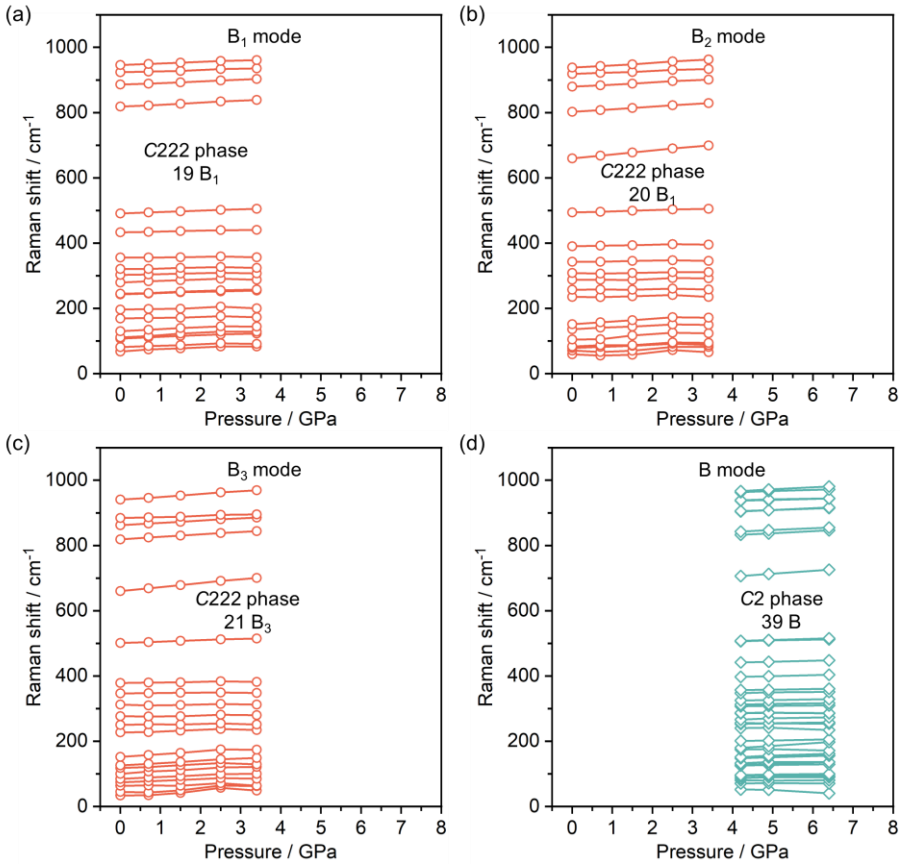


Figure S1 Pressure-dependence of Raman B_1, B_2 and B_3 modes of the *C*222 phase as well as Raman B modes of the *C*2 phase.

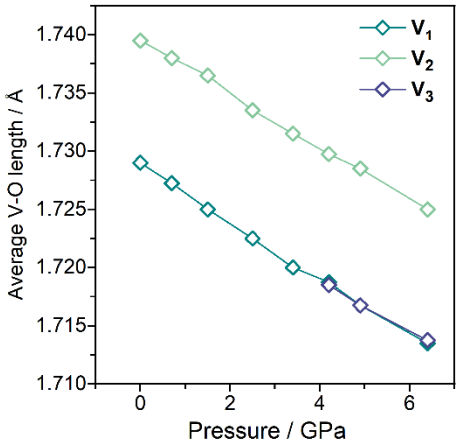


Figure S2 Pressure-dependence of the average V-O length in different [VO_4] tetrahedral units.

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