Electronic Supplementary Information (ESI)

Flux Synthesis, Crystal Structures, and Physical Properties of New Lanthanum Vanadium Oxyselenides

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Table S1 Crystallographic data of $LaVSe_2O$.

Formula weight/g mol^{-1}	363.8
Space group, Z	$C2/m$, 4
a, b, c/pm	1171.1(1), 388.6(1), 843.6(1)
β/°	90.19(1)
V/Å^3, $\rho_{\text{X-ray}}$/g cm^{-3}	383.9(1), 6.29
Crystal size/mm^3	0.04 × 0.02 × 0.02
Diffractometer	Bruker D8 QUEST
Radiation λ/pm	71.073
Absorption coeff. μ/mm^{-1}	32.1
2θ range/°	4.82–70.14
Index range (hkl)	$h \pm 18$, $-5 \leq k \leq 6$, $l \pm 13$
No. reflections collected	5307
No. unique data, R_{int}, R_σ	943, 0.03, 0.02
No. data with $I > 3\sigma(I)$	866
No. parameters	34
R_1(obs/all)	0.018/0.020
wR_2(obs/all)	0.046/0.054
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$/eÅ^{-3}	1.86/−2.38

Atomic and displacement parameters

	Site	x, y, z	U_{11}	U_{22}	U_{33}	U_{13}
La1	$4i$	0.2303(2), 0, 0.1979(1)	0.0058(1)	0.0050(1)	0.0047(1)	0.0009(1)
Se1	$4i$	0.9531(1), 0, 0.1994(1)	0.0063(2)	0.0065(2)	0.0043(2)	0.0001(1)
Se2	$4i$	0.1407(1), $\frac{1}{2}$, 0.4648(1)	0.0061(2)	0.0067(2)	0.0060(2)	0.0008(1)
V1	$2b$	0, $\frac{1}{2}$, 0	0.0037(4)	0.0069(4)	0.0050(4)	−0.0002(3)
V2	$2c$	0, 0, $\frac{1}{2}$	0.0059(4)	0.0082(4)	0.0052(4)	0.0009(3)
O1	$4i$	0.1629(1), $\frac{1}{2}$, 0.0582(1)	0.0052(11)	0.0082(12)	0.0052(11)	0.0006(9)

Table S2 Crystallographic data of $La_5V_3Se_6O_7$.

Formula weight/g mol^{-1}	1433.1
Space group, Z	$Pmmn$, 2
a, b, c/pm	1817.4(1), 391.1(1), 1046.7(1)
V/Å^3, $\rho_{\text{X-ray}}$/g cm^{-3}	774.0(3), 6.40
Crystal size/mm^3	0.05 × 0.01 × 0.005
Diffractometer	Bruker D8 QUEST
Radiation λ/pm	71.073
Absorption coeff. μ/mm^{-1}	30.5
2θ range/°	5.94–70.00
Index range (hkl)	$-28 \le h \le 29$, $-6 \le k \le 5$, $l \pm 16$
No. reflections collected	20542
No. unique data, R_{int}, R_σ	1514, 0.06, 0.04
No. data with $I > 3\sigma(I)$	1233
No. parameters	69
R_1(obs/all)	0.023/0.036
wR_2(obs/all)	0.047/0.050
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$/eÅ^{-3}	2.44/−2.96

Atomic and displacement parameters

	Site	x, y, z	U_{11}	U_{22}	U_{33}	U_{13}
La1	4f	0.3851(2), $\frac{1}{2}$, 0.0207(1)	0.0063(2)	0.0039(2)	0.0078(2)	0.0006(1)
La2	2b	$\frac{1}{2}$, 0, 0.7740(1)	0.0052(2)	0.0041(2)	0.0063(2)	0
La3	4f	0.1654(2), $\frac{1}{2}$, 0.5898(1)	0.0073(2)	0.0054(2)	0.0067(2)	−0.0015(1)
Se1	2b	$\frac{1}{2}$, 0, 0.1386(1)	0.0078(4)	0.0058(4)	0.0051(4)	0
Se2	2b	0, $\frac{1}{2}$, 0.5341(1)	0.0070(4)	0.0063(4)	0.0049(4)	0
Se3	4f	0.1179(1), 0, 0.3578(1)	0.0066(3)	0.0052(3)	0.0058(3)	−0.0005(2)
Se4	4f	0.2345(3), $\frac{1}{2}$, 0.8571(1)	0.0065(3)	0.0062(3)	0.0056(3)	0.0004(2)
V1	2a	0, 0, 0.6896(1)	0.0051(6)	0.0083(7)	0.0075(7)	0
V2	4f	0.3065(1), 0, 0.7500(1)	0.0060(5)	0.0075(5)	0.0046(4)	−0.0014(4)
O1	4f	0.2480(1), 0, 0.6042(1)	0.0054(19)	0.007(2)	0.011(2)	0.0019(16)
O2	2a	$\frac{1}{2}$, $\frac{1}{2}$, 0.9003(1)	0.008(3)	0.008(3)	0.003(3)	0
O3	4f	0.3782(1), 0, 0.8847(1)	0.0087(19)	0.006(2)	0.008(2)	0.0016(16)
O4	4f	0.0993(1), 0, 0.7090(1)	0.007(2)	0.010(2)	0.013(2)	−0.0003(17)

Table S3 Crystallographic data of $La_5V_3Se_7O_5$.

Formula weight/g mol^{-1}	1480.1
Space group, Z	*Pnma*, 4
a, b, c/pm	1650.4(1), 390.1(1), 2475.7(1)
V/Å^3, $\rho_{\text{X-ray}}$/g cm^{-3}	1594.0(3), 6.17
Crystal size/mm^3	0.07 × 0.01 × 0.01
Diffractometer	Bruker D8 QUEST
Radiation λ/pm	71.073
Absorption coeff. μ/mm^{-1}	30.7
2θ range/°	4.94–70.16
Index range (hkl)	$h \pm 26$, $-6 \leq k \leq 5$, $l \pm 39$
No. reflections collected	41381
No. unique data, R_{int}, R_σ	3959, 0.06, 0.04
No. data with $I > 3\sigma(I)$	2958
No. parameters	121
R_1(obs/all)	0.024/0.045
wR_2(obs/all)	0.042/0.047
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$/eÅ^{-3}	2.88/−2.84

Atomic and displacement parameters

	Site	x, y, z	U_{11}	U_{22}	U_{33}	U_{13}
La1	4c	0.0340(2), $\frac{3}{4}$, 0.0880(1)	0.0073(1)	0.0045(1)	0.0058(1)	0.0004(1)
La2	4c	0.1802(2), $\frac{1}{4}$, 0.1778(1)	0.0083(1)	0.0046(1)	0.0061(1)	−0.0001(1)
La3	4c	0.0021(2), $\frac{3}{4}$, 0.2474(1)	0.0094(1)	0.0042(1)	0.0054(1)	0.0000(1)
La4	4c	0.1993(2), $\frac{1}{4}$, 0.8867(1)	0.0064(1)	0.0045(1)	0.0060(1)	−0.0006(1)
La5	4c	0.3621(2), $\frac{3}{4}$, 0.9650(1)	0.0071(1)	0.0043(1)	0.0063(1)	−0.0009(1)
Se1	4c	0.5711(1), $\frac{3}{4}$, 0.1329(2)	0.0066(2)	0.0061(2)	0.0069(2)	−0.0001(2)
Se2	4c	0.8887(1), $\frac{1}{4}$, 0.0243(2)	0.0092(2)	0.0092(3)	0.0062(2)	0.0006(2)
Se3	4c	0.4481(1), $\frac{1}{4}$, 0.0467(2)	0.0079(2)	0.0067(2)	0.0069(2)	−0.0008(2)
Se4	4c	0.2663(1), $\frac{3}{4}$, 0.0816(1)	0.0065(2)	0.0061(2)	0.0083(2)	−0.0009(2)
Se5	4c	0.2610(1), $\frac{1}{4}$, 0.7730(2)	0.0097(2)	0.0067(2)	0.0062(2)	0.0007(2)
Se6	4c	0.9302(1), $\frac{1}{4}$, 0.1620(2)	0.0079(2)	0.0063(2)	0.0068(2)	−0.0015(2)
Se7	4c	0.3844(1), $\frac{1}{4}$, 0.1810(2)	0.0099(2)	0.0074(2)	0.0076(2)	−0.0005(2)
V1	4c	0.1964(1), $\frac{1}{4}$, 0.0297(1)	0.0064(4)	0.0082(4)	0.0059(3)	0.0019(3)
V2	4c	0.1529(1), $\frac{1}{4}$, 0.3183(1)	0.0074(4)	0.0076(4)	0.0047(3)	−0.0016(3)
V3	4c	0.4160(1), $\frac{3}{4}$, 0.1136(1)	0.0070(4)	0.0091(4)	0.0076(3)	−0.0010(3)
O1	4c	0.2779(1), $\frac{3}{4}$, 0.8830(1)	0.0031(15)	0.0065(16)	0.0050(14)	0.0007(12)
O2	4c	0.0821(1), $\frac{1}{4}$, 0.2567(1)	0.0046(16)	0.0078(17)	0.0073(15)	−0.0008(12)
O3	4c	0.1119(1), $\frac{1}{4}$, 0.0843(1)	0.0052(16)	0.0063(17)	0.0044(14)	0.0024(12)
O4	4c	0.1012(1), $\frac{3}{4}$, 0.1712(1)	0.0070(17)	0.0042(16)	0.0070(15)	0.0002(12)
O5	4c	0.2753(1), $\frac{1}{4}$, 0.9712(1)	0.0068(17)	0.0056(17)	0.0054(15)	0.0002(12)

Table S4 Crystallographic data of $La_7VSe_5O_7$.

Formula weight/g mol^{-1}	1530.1
Space group, Z	$Cmcm$, 4
a, b, c/pm	398.6(1), 1286.3(1), 3229.0(1)
V/Å^3, $\rho_{\text{X-ray}}$/g cm^{-3}	1655.5(1), 6.14
Crystal size/mm^3	0.04 × 0.005 × 0.005
Diffractometer	Bruker D8 Venture
Radiation λ/pm	71.073
Absorption coeff. μ/mm^{-1}	29.2
2θ range/°	6.47–49.99
Index range (hkl)	$h \pm 4$, $k \pm 14$, $l \pm 38$
No. reflections collected	6698
No. unique data, R_{int}, R_σ	854, 0.05, 0.03
No. data with $I > 2\sigma(I)$	769
No. parameters	54
R_1(obs/all)	0.032/0.037
wR_2(obs/all)	0.074/0.079
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$/eÅ^{-3}	1.77/−1.97

Atomic and displacement parameters

	Site	x, y, z	U_{11}	U_{22}	U_{33}	U_{23}
La1	4c	0, 0.0580(1), $\frac{1}{4}$	0.0075(6)	0.0092(6)	0.0046(6)	0
La2	8f	$\frac{1}{2}$, 0.8655(1), 0.3131(1)	0.0084(5)	0.0101(5)	0.0033(4)	0.0001(3)
La3	8f	0, 0.0359(1), 0.3862(1)	0.0083(5)	0.0097(5)	0.0048(4)	0.0001(3)
La4	8f	$\frac{1}{2}$, 0.8205(1), 0.4372(1)	0.0087(5)	0.0103(5)	0.0045(4)	0.0006(3)
Se1	8f	0, 0.7241(1), 0.3680(1),	0.0118(8)	0.0111(8)	0.0081(7)	0.0016(6)
Se2	4c	$\frac{1}{2}$, 0.2468(2), $\frac{1}{4}$	0.0112(11)	0.0110(11)	0.0072(10)	0
Se3	8f	$\frac{1}{2}$, 0.8787(1), 0.5302(1)	0.0138(8)	0.0128(8)	0.0044(7)	0.0004(6)
V1	4a	0, 0, $\frac{1}{2}$	0.0103(19)	0.0139(19)	0.0020(16)	−0.0036(14)
				U_{iso}		
O1	4c	$\frac{1}{2}$, 0.9654(10), $\frac{1}{4}$		0.003(3)		
O2	8f	0, 0.0824(8), 0.5511(3)		0.006(2)		
O3	8f	$\frac{1}{2}$, 0.9394(8), 0.3823(3)		0.008(2)		
O4	8f	0, 0.9763(8), 0.3172(3)		0.009(2)		

Table S5 Crystallographic data of $La_{13}V_7Se_{16}O_{15}$.

Formula weight/g mol^{-1}	3665.7
Space group, Z	$Cmc2_1$, 4
a, b, c/pm	393.8(1), 5400.9(1), 1834.9(1)
V/Å^3, $\rho_{\text{X-ray}}$/g cm^{-3}	3902.9(1), 6.24
Crystal size/mm^3	0.03 × 0.02 × 0.005
Diffractometer	Bruker D8 QUEST
Radiation λ/pm	71.073
Absorption coeff. μ/mm^{-1}	30.4
2θ range/°	4.68–70.02
Index range (hkl)	$-5 \le h \le 6$, $-83 \le k \le 86$, $l \pm 29$
No. reflections collected	73357
No. unique data, R_{int}, R_σ	6370, 0.05, 0.04
No. data with $I > 2\sigma(I)$	5694
No. parameters	263
R_1(obs/all)	0.017/0.023
wR_2(obs/all)	0.036/0.038
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$/eÅ^{-3}	0.81/−1.12

Atomic and displacement parameters

	Site	x, y, z	U_{11}	U_{22}	U_{33}	U_{23}
La1	4a	0, 0.1582(1), 0.0370(1)	0.0039(3)	0.0079(3)	0.0061(3)	0.0010(3)
La2	4a	0, 0.1586(1), 0.2709(1)	0.0045(3)	0.0075(3)	0.0063(3)	−0.0020(2)
La3	4a	0, 0.3509(1), 0.2632(1)	0.0053(3)	0.0066(3)	0.0067(3)	−0.0004(2)
La4	4a	$\frac{1}{2}$, 0.1139(1), 0.1546(1)	0.0043(1)	0.0058(2)	0.0045(1)	0.0000(3)
La5	4a	$\frac{1}{2}$, 0.0399(1), 0.2835(1)	0.0047(3)	0.0056(3)	0.0068(3)	−0.0001(2)
La6	4a	0, 0.4724(1), 0.1566(1)	0.0056(1)	0.0070(2)	0.0090(2)	−0.0008(3)
La7	4a	0, 0.0630(1), 0.4493(1)	0.0044(3)	0.0076(3)	0.0063(3)	−0.0010(2)
La8	4a	0, 0.2670(1), 0.8183(1)	0.0066(3)	0.0066(3)	0.0079(3)	−0.0019(2)
La9	4a	$\frac{1}{2}$, 0.2319(1), 0.9875(1)	0.0062(3)	0.0072(3)	0.0078(3)	−0.0015(2)
La10	4a	0, 0.9367(1), 0.3567(1)	0.0047(3)	0.0066(3)	0.0094(3)	−0.0023(2)
La11	4a	$\frac{1}{2}$, 0.9597(1), 0.5251(1)	0.0047(3)	0.0055(3)	0.0063(3)	−0.0006(2)
La12	4a	$\frac{1}{2}$, 0.3021(1), 0.1531(1)	0.0041(1)	0.0058(2)	0.0058(1)	−0.0003(3)
La13	4a	0, 0.3493(1), 0.0396(1)	0.0046(3)	0.0084(3)	0.0061(3)	0.0006(2)
Se1	4a	$\frac{1}{2}$, 0.0163(1), 0.4899(1)	0.0083(6)	0.0065(5)	0.0061(5)	−0.0001(4)
Se2	4a	0, 0.1210(1), 0.4226(1)	0.0077(6)	0.0067(5)	0.0092(5)	−0.0018(4)
Se3	4a	$\frac{1}{2}$, 0.1811(1), 0.3890(1)	0.0066(6)	0.0066(5)	0.0060(5)	−0.0008(4)
Se4	4a	0, 0.3199(1), 0.4161(1)	0.0065(6)	0.0063(5)	0.0066(5)	−0.0010(4)
Se5	4a	0, 0.2767(1), 0.0338(1)	0.0059(6)	0.0066(5)	0.0057(5)	0.0011(4)
Se6	4a	$\frac{1}{2}$, 0.2433(1), 0.1524(1)	0.0070(2)	0.0054(3)	0.0070(3)	0.0011(5)
Se7	4a	$\frac{1}{2}$, 0.1808(1), 0.1539(1)	0.0050(2)	0.0059(3)	0.0082(3)	0.0002(6)
Se8	4a	0, 0.0843(2), 0.0537(1)	0.0063(6)	0.0063(5)	0.0082(5)	−0.0025(4)
Se9	4a	0, 0.0199(1), 0.1550(1)	0.0082(3)	0.0093(3)	0.0088(3)	0.0003(6)
Se10	4a	0, 0.2775(1), 0.2717(1)	0.0062(6)	0.0056(5)	0.0073(5)	0.0012(4)

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Atomic and displacement parameters

	Site	x, y, z	U_{11}	U_{22}	U_{33}	U_{23}
Se11	$4a$	$\frac{1}{2}$, 0.3719(1), 0.1484(1)	0.0070(3)	0.0050(3)	0.0096(4)	−0.0008(4)
Se12	$4a$	0, 0.0844(2), 0.2571(1)	0.0065(6)	0.0069(5)	0.0078(5)	0.0009(4)
Se13	$4a$	0, 0.8784(1), 0.3896(1)	0.0061(6)	0.0089(6)	0.0072(5)	−0.0007(4)
Se14	$4a$	0, 0.4114(2), 0.2525(1)	0.0059(4)	0.0111(4)	0.0070(4)	−0.0025(3)
Se15	$4a$	0, 0.4215(2), 0.0700(1)	0.0072(4)	0.0140(4)	0.0069(4)	0.0030(3)
Se16	$4a$	$\frac{1}{2}$, 0.9833(1), 0.3216(1)	0.0073(6)	0.0056(5)	0.0074(5)	−0.0005(4)
V1	$4a$	$\frac{1}{2}$, 0.2989(1), 0.3459(1)	0.0089(1)	0.0055(8)	0.0042(8)	0.0019(6)
V2	$4a$	$\frac{1}{2}$, 0.2975(1), 0.9600(1)	0.0067(1)	0.0040(8)	0.0075(9)	−0.0006(7)
V3	$4a$	0, 0.2133(2), 0.1537(1)	0.0079(4)	0.0063(5)	0.0044(4)	0.0008(9)
V4	$4a$	$\frac{1}{2}$, 0.1048(1), 0.3429(1)	0.0070(1)	0.0053(9)	0.0060(9)	0.0017(7)
V5	$4a$	0, 0.9997(1), 0.4048(1)	0.0080(4)	0.0047(4)	0.0068(4)	0.0018(3)
V6	$4a$	$\frac{1}{2}$, 0.8954(1), 0.4664(1)	0.0111(1)	0.0037(9)	0.0063(9)	0.0003(7)
V7	$4a$	$\frac{1}{2}$, 0.4181(1), 0.1623(1)	0.0064(5)	0.0051(5)	0.0101(8)	−0.0004(6)
				U_{iso}		
O1	$4a$	$\frac{1}{2}$, 0.1323(1), 0.2769(1)		0.0072(2)		
O2	$4a$	$\frac{1}{2}$, 0.3248(1), 0.2746(1)		0.0078(2)		
O3	$4a$	0, 0.9687(15), 0.4553(1)		0.0102(2)		
O4	$4a$	$\frac{1}{2}$, 0.0708(1), 0.3831(1)		0.0055(2)		
O5	$4a$	$\frac{1}{2}$, 0.9287(1), 0.4250(1)		0.0059(2)		
O6	$4a$	0, 0.0314(1), 0.3527(1)		0.0042(2)		
O7	$4a$	0, 0.1373(1), 0.1548(1)		0.0065(1)		
O8	$4a$	0, 0.3257(1), 0.1501(1)		0.0056(1)		
O9	$4a$	$\frac{1}{2}$, 0.2700(1), 0.8992(1)		0.0059(2)		
O10	$4a$	0, 0.2097(1), 0.0535(1)		0.0089(2)		
O11	$4a$	$\frac{1}{2}$, 0.3232(1), 0.0308(1)		0.0076(2)		
O12	$4a$	$\frac{1}{2}$, 0.8674(1), 0.5328(1)		0.0055(1)		
O13	$4a$	$\frac{1}{2}$, 0.4534(1), 0.1832(1)		0.0143(2)		
O14	$4a$	$\frac{1}{2}$, 0.2708(1), 0.4037(1)		0.0095(2)		
O15	$4a$	0 0.2096(1), 0.2506(1)		0.0088(2)		

Note: Values of unlisted U_{xy} are equal zero.

Table S6: Calculations of the bond valence sum of vanadium by the bond valence method.

	V(*n*)	element	number of neighbours	distance /Å		valence sum
LaVSe2O	V(1)	Se	4	2,6294	1,7809	3,02
		O	2	1,9684	1,2349	
	V(2)	Se	6	2,5744	3,0994	3,10
La5V3Se6O7	V(2)	Se	4	2,6248	1,8034	3,34
		O	2	1,8885	1,5328	
	V(1)	Se	4	2,6006	1,9253	3,79
		O	2	1,8161	1,8638	
La5V3Se7O5	V(1)	Se	4	2,6777	1,5631	2,88
		O	2	1,9451	1,3153	
	V(2)	Se	4	2,6620	1,6307	2,95
		O	2	1,9445	1,3173	
	V(3)	Se	6	2,6108	2,8090	2,81
La7VSe5O7	V(1)	Se	4	2,7123	1,4234	2,69
		O	2	1,9584	1,2687	
La13V7Se16O15	V(1)	Se	4	2,6348	1,7551	3,35
		O	2	1,8729	1,5985	
	V(2)	Se	4	2,6353	1,7527	3,28
		O	2	1,8891	1,5301	
	V(3)	Se	4	2,5952	1,9533	3,80

		O	2	1,8187	1,8507	
	V(4)	Se	4	2,6779	1,5621	2,83
		O	2	1,9573	1,2725	
	V(5)	Se	4	2,6553	1,6605	3,01
		O	2	1,9352	1,3508	
	V(6)	Se	4	2,6777	1,5629	2,88
		O	2	1,9445	1,3173	
	V(7)	Se	4	2,5822	2,0232	3,36
		O	2	1,9404	1,3320	