Electronic Supplementary Material (ESI) for Dalton Transactions.

High pressure exploration in the Li – Ln – V – O system

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SUPPLEMENTARY INFORMATION

Table S1. Crystal parameters, data collection and structure refinement details for the crystal of β- $LiLa_5O_5(VO_4)_2$

Crystal data	
Formula	$LiLa_5O_5(VO_4)_2$
Formula weight (g/mol)	1011.3
Temperature (K)	293
Crystal system	triclinic
Space group	*P*-1
a (Å)	5.8167(15)
b (Å)	12.2954(28)
c (Å)	18.7221(69)
α (°)	102.03(2)
β (°)	98.76(2)
γ (°)	103.54(2)
V (Å^3)	1244.37(18)
Z	4
Data collection	
Diffractometer	X8 Bruker
Radiation; λ (Å)	Ag*Kα*; 0.56086
Absorption coefficient, *μ* (mm^{-1})	9.621
F (000)	1752
Data range θ (°); *h, k, l*	1.39 – 25.6; -8 < *h* < 8,
	-18 < *k* < 18, -28 < *l* < 28
No. of total reflections	9444
Total unique reflections	6539
Criterion for observed reflections	I >3σ(I)
R_{int} (%)	7.62
Refinement	
Refinement on	Full-matrix last squares on *F*
Weight scheme	$1/(\sigma^2 \|F\| + 0.0004 F^2)$
R_{gt}, R_{all}	7.59, 11.26
wR_{gt}, wR_{ref},	10.31, 11.25
GOF_{gt}, GOF_{ref}	2.10, 2.32
Max. /min. residual *e* density, (*e*Å^{-3})	10.84 / -8.89

Table S2. Atomic parameters β- $LiLa_5O_5(VO_4)_2$

Atom	X	Y	Z	U_{eq}
La1	0.75802(17)	0.87839(8)	0.13743(5)	0.0082(3)
La2	0.25481(17)	0.61367(8)	0.38578(5)	0.0069(3)
La3	0.80795(17)	0.10021(9)	0.01963(5)	0.0089(3)
La4	0.86837(19)	0.84533(8)	0.43356(6)	0.0103(3)
La5	0.68837(17)	0.61847(8)	0.25351(5)	0.0077(3)
La6	0.38684(17)	0.09521(8)	0.18105(5)	0.0084(3)
La7	0.96482(18)	0.11704(9)	0.31787(6)	0.0112(3)
La8	0.58736(18)	0.37294(8)	0.34621(6)	0.0102(3)
La9	0.32247(17)	0.86472(8)	0.29150(6)	0.0090(3)
La10	0.0193(2)	0.35818(9)	0.21394(6)	0.0159(3)
V1	0.5072(6)	0.9061(2)	0.56732(16)	0.0136(9)
V2	0.1489(6)	0.6722(3)	0.12267(18)	0.016(010)
V3	0.5510(6)	0.6722(3)	0.92121(19)	0.0184(10)
V4	0.1096(7)	0.3683(3)	0.47882(19)	0.0210(12)
O1	0.432(2)	0.8224(12)	0.4803(8)	0.019(3)
O2	0.529(3)	0.8244(13)	0.6287(8)	0.024(4)
O3	0.034(2)	0.7461(9)	0.3436(6)	0.007(2)
O4	0.609(2)	0.9797(10)	0.2354(7)	0.013(2)
O5	0.969(2)	0.7196(11)	0.1780(7)	0.017(3)
O6	0.574(5)	0.6667(16)	0.0098(10)	0.041(4)
O7	0.891(2)	0.4926(12)	0.2967(8)	0.019(3)
O8	0.222(2)	0.2378(11)	0.2578(7)	0.015(3)
O9	0.539(2)	0.9878(10)	0.0782(7)	0.012(2)
O10	0.028(2)	0.9892(10)	0.0790(7)	0.011(2)
O11	0.809(2)	0.9947(11)	0.5853(7)	0.018(3)
O12	0.231(3)	0.4139(14)	0.4121(9)	0.031(3)
O13	0.140(4)	0.7324(18)	0.0505(11)	0.050(5)
O14	0.434(2)	0.7215(11)	0.1761(7)	0.015(2)
O15	0.823(4)	0.7330(17)	0.9009(11)□	0.049(5)
O16	0.328(2)	0.9950(11)	0.5931(8)	0.019(3)
O17	0.357(3)	0.7538(16)	0.8989(11)	0.045(5)
O18	0.748(2)	0.2398(11)	0.2643(7)	0.014(2)
O19	0.828(3□)	0.3939(13)	0.4803(8)	0.027(3)
O20	0.047(3)	0.2220(13)	0.4520(9)	0.029(4)
O21	0.064(6)	0.532(3)	0.0927(18)	0.103(10)
O22	0.543(2)	0.7438(10)	0.3384(6)	0.010(2)
O23	0.281(3)	0.3972(13)	0.5662(8)	0.026(3)
O24	0.099(2)	0.9802(10)	0.2380(6)	0.010(2)
O25	0.376(2)	0.4931(11)	0.2891(7)	0.010(2)
O26	0.433(4)	0.536(2)	0.8710(14)	0.073(7)
Li1	0.2651	0.4929	0.9965	0.010(7)
Li2	0.5	0.5	0.5	0.01
Li3	0	0	0.5	0.01

Table S3. Anisotropic atomic displacement parameters of β- $LiLa_5O_5(VO_4)_2$

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0066(4)	0.0083(4)	0.0094(4)	0.0018(3)	0.0014(3)	0.0021(3)
La2	0.0067(4)	0.0060(4)	0.0078(4)	0.0001(3)	0.0024(3)	0.0024(3)
La3	0.0077(4)	0.0132(4)	0.0061(4)	0.0033(3)	0.0025(3)	0.0020(3)
La4	0.0135(4)	0.0078(4)	0.0081(4)	0.0009(3)	0.0018(3)	0.0014(3)
La5	0.0071(4)	0.0058(4)	0.0101(4)	0.0001(3)	0.0032(3)	0.0030(3)
La6	0.0085(4)	0.0079(4)	0.0083(4)	0.0020(3)	0.0011(3)	0.0017(3)
La7	0.0103(4)	0.0123(4)	0.0090(4)	0.0038(3)	0.0004(3)	-0.0014(3)
La8	0.0118(4)	0.0096(4)	0.0102(4)	0.0024(3)	0.0026(3)	0.0050(3)
La9	0.0078(4)	0.0087(4)	0.0118(4)	0.0026(3)	0.0012(3)	0.0057(3)
La10	0.0133(5)	0.0133(5)	0.0168(5)	0.0015(4)	0.0020(4)	-0.0022(4)
V1	0.0267(15)	0.0060(12)	0.0054(11)	0.0045(10)	0.0013(10)	-0.0025(10)
V2	0.0137(15)	0.0184(15)	0.0123(14)	0.0042(12)	0.0003(11)	-0.0036(12)
V3	0.0113(15)	0.0188(16)	0.0190(16)	-0.0009(12)	-0.0003(12)	0.0001(13)
V4	0.0275(16)	0.0258(18)	0.0134(14)	0.0126(15)	0.0036(12)	0.0073(13)

Table S4. Selected interatomic distances for β- $LiLa_5O_5(VO_4)_2$

Atom1	Atom2	d, Å
O1	La2	2.6668(14)
	La4	2.7680(18)
O2	La8	2.5324(22)
	La7	2.8548(22)
O3	La4	2.3304(13)
	La5	2.4035(10)
	La9	2.4253(13)
	La2	2.4642(14)
O4	La1	2.3952(16)
	La6	2.4017(17)
	La7	2.4086(13)
	La9	2.4345(16)
O5	La5	2.5885(18)
	La1	2.6955(19)
	La9	2.7071(14)
O7	La5	2.3553(18)
	La10	2.3754(17)
	La8	2.4078(17)
	La2	2.4415(13)
O8	La10	2.3104(19)
	La7	2.4259(18)
	La8	2.4588(14)
	La6	2.4837(18)
O9	La3	2.3690(10)
	La3	2.3792(13)
	La1	2.3885(14)
	La6	2.5072(13)
O10	La3	2.3795(17)
	La3	2.3888(18)
	La1	2.3941(17)
	La6	2.4877(13)
O11	La4	2.5098(18)
	La7	2.8455(20)
	La9	2.8881(19)
O12	La2	2.5989(22)
	La8	2.6410(24)
O13	La3	2.6644(39)
O14	La5	2.6224(18)
	La1	2.6522(16)
	La9	2.7408(16)
O15	La3	2.5908(22)
	La10	2.6280(30)
O16	La4	2.5840(18)
	La9	2.6808(14)
	La7	2.8864(18)
O17	La3	2.5868(29)
	La10	2.6625(24)
	La6	2.8952(30)
O18	La10	2.3615(17)
	La7	2.4288(18)
	La8	2.4373(17)
	La6	2.4743(13)
O19	La8	2.6181(19)
	La2	2.6228(22)
O20	La4	2.4411(24)
	La7	2.5089(21)
O22	La4	2.2987(10)
	La9	2.3721(14)
	La5	2.3888(13)
	La2	2.4361(13)
O23	La2	2.7953(18)
	La8	2.8087(17)
	La4	2.9180(20)
O24	La7	2.3649(13)
	La1	2.3968(10)
	La9	2.4127(14)
	La6	2.4398(13)
O25	La5	2.3552(14)
	La10	2.3573(10)
	La2	2.4141(14)
	La8	2.4324(16)
O26	La5	2.5770(25)
V1	O2	1.6754(23)
	O1	1.6759(15)
	O16	1.7430(19)
	O11	1.7592(16)
V2	O13	1.6432(37)
	O21	1.6764(46)
	O5	1.6983(19)
	O14	1.7163(15)
V3	O6	1.646(31)
	O26	1.6890(22)
	O15	1.6931(30)
	O17	1.6969(30)
V4	O12	1.6595(23)
	O23	1.6847(18)
	O20	1.7138(22)
	O19	1.7412(20)
	O19	2.7812(20)
Li1	O21	2.2083(58)
	O21	2.2983(65)
	O6	2.3504(41)
	O6	2.4264(34)
	O26	2.8163(43)
	O26	2.9606(40)
	O13	2.9766(36)
Li2	O12	1.9904(18)
	O12	1.9909(18)
	O23	2.2693(20)
	O23	2.2701(20)
	O19	2.5708(20)
	O19	2.5709(20)
Li3	O11	2.0905(20)
	O11	2.0912(20)
	O16	2.4080(17)
	O16	2.4086(17)
	O20	2.9865(24)
	O20	2.9871(24)

Table S5. BVS calculation for β- $LiLa_5O_5(VO_4)_2$

Atom	La1	La2	La3	La4	La5	La6	La7	La8	La9	La10	V1	V2	V3	V4	Li1	Li2	Li3	∑a
O1		0.26		0.04+0.04							1.37							1.70
O2						0.03	0.15+0.04	0.37			1.38							1.98
O3		0.45		0.65	0.54				0.50									2.15
O4	0.55					0.54	0.53		0.49									2.10
O5	0.24				0.32				0.23			1.30						2.09
O6	0.09												1.48		0.17+0.15			1.89
O7		0.48			0.61			0.53		0.58								2.20
O8						0.43	0.50	0.46		0.69								2.08
O9	0.56		0.59+0.57			0.40												2.12
O10	0.55		0.57+0.56			0.42												2.10
O11				0.40+0.06			0.16		0.14		1.11						0.20+0.20	2.27
O12		0.31						0.28						1.43		0.24+0.24		2.49
O13			0.26									1.50			0.04+0.04			1.83
O14	0.27				0.29				0.21			1.24						2.01
O15			0.32			0.05				0.29			1.31					1.97
O16				0.32			0.14		0.25		1.16						0.12+0.12	2.11
O17			0.32			0.14				0.26			1.30					2.02
O18						0.44	0.50	0.49		0.60								2.03
O19		0.29						0.29						1.16		0.10+0.10		1.93
O20				0.48			0.40							1.25			0.05+0.05	2.23
O21										0.04		1.37			0.13+0.11			1.65
O22		0.49		0.72	0.56				0.59									2.35
O23		0.18+0.04		0.13	0.03			0.17						1.35		0.15+0.15		2.21
O24	0.55					0.48	0.60		0.52									2.15
O25		0.52			0.61			0.49		0.61								2.23
O26					0.33								1.33		0.08+0.06			1.80
∑c	2.79	3.02	3.19	2.84	3.29	2.93	3.01	3.09	2.92	3.06	5.01	5.41	5.43	5.18	0.77	0.97	0.75	

(R, b) [(1)] parameters being for La-O (2.179; 0.359), V-O (1.799; 0.388), Li-O (1.062; 0.642).

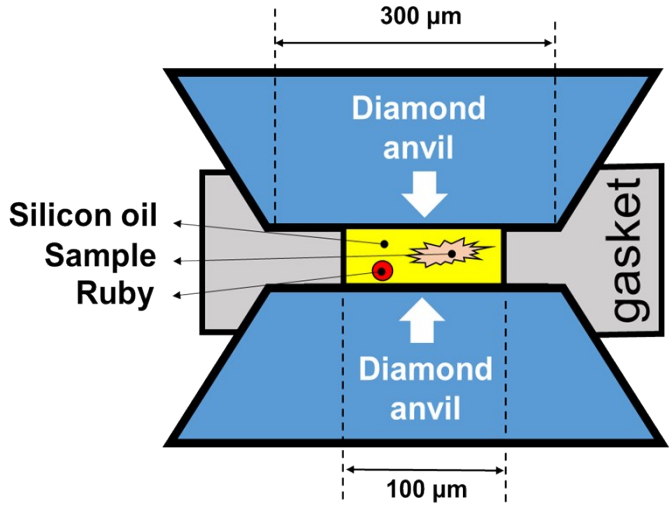

Figure S1. Organization scheme of the Diamond Anvil Cell used for in situ Raman spectroscopy.

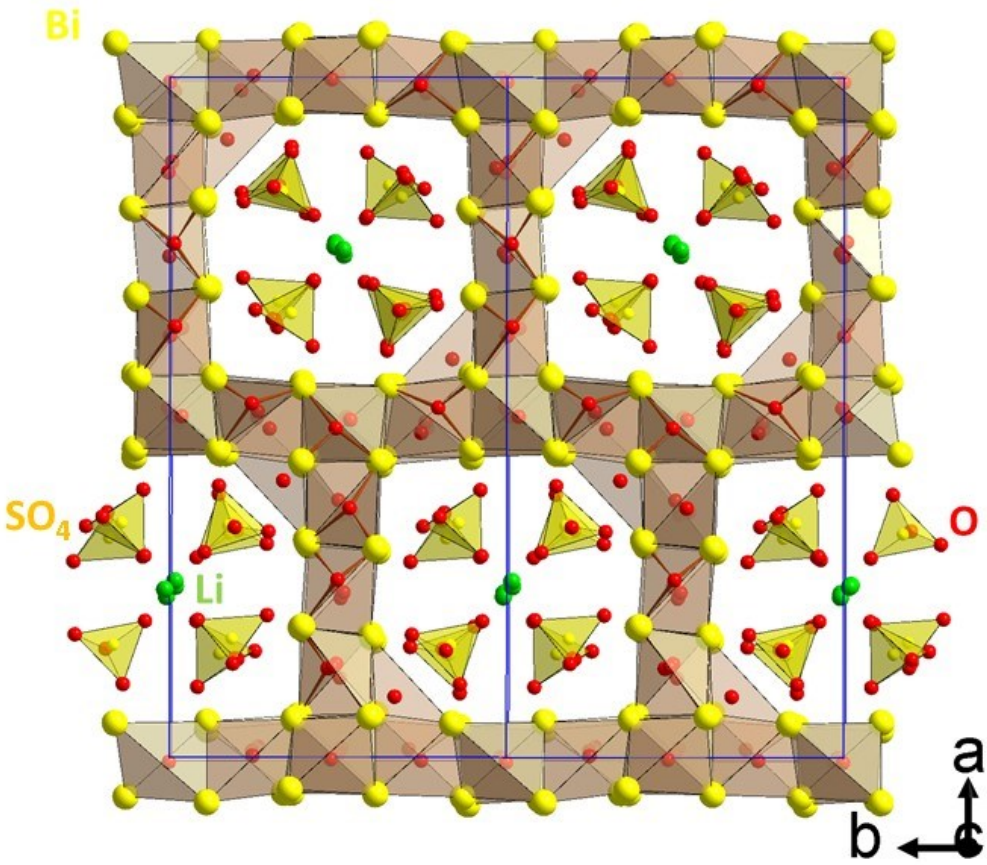

Figure S2. Reminder of the crystal structure of $[Bi_{12}O_{15}]Li_2(SO_4)_4]$ (ref Lü et al., Inorg Chem, 2014, 53, 12058). The multi-dimensional framework is evidenced (3D porous cationic framework with 1D channels hosting sulfates and Li^+ cations.

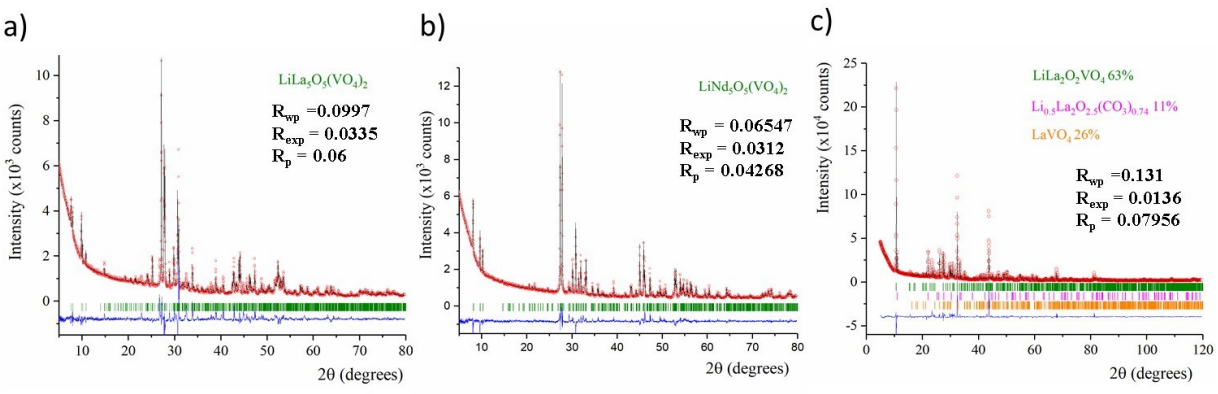

Figure S3: Rietveld refinement of a) HP $LiLa_5O_5(VO_4)_2$, b) $LiNd_5O_5(VO_4)_2$ and c) $LiLa_2O_2(VO_4)$. The refinements were performed using TOPAS software. Note that the small amount of sample drastically damaged the quality of the data and also of the refinement but at least it undoubtedly confirmed the purity of the samples for a) and b) and the presence of impurities for c).

Table S6. Crystal parameters, data collection and structure refinement details for the crystal of β-$LiLa_2O_2VO_4$

Crystal data	
Formula	$LiLa_2O_2VO_4$
Formula weight (g/mol)	431.7
Temperature (K)	293
Crystal system	triclinic
Space group	*P* -1
a (Å)	5.8144(7)
b (Å)	5.8167(7)
c (Å)	8.527(1)
α (°)	98.184(7)
β (°)	100.662(7)
γ (°)	92.579(7)
V (Å^3)	279.7(2)
Z	2
Data collection	
Diffractometer	SMART APEX DUO
Radiation; λ (Å)	Mo$K\alpha$; 0.71073
Absorption coefficient, μ (mm^{-1})	16.583
F (000)	376
Data range θ (°); *h, k, l*	2.46 – 23.42; -6 < *h* < 6,
	-6 < *k* < 6, -9 < *l* < 9
No. of measured reflections	2980
Total reflections (N_2)/unique (N_1)	917 / 667
Criterion for observed reflections	I >3σ(I)
R_{int} (%)	2.07
Refinement	
Refinement on	Full-matrix last squares on *F*
Weight scheme	$1/(\sigma^2 \lvert F\rvert + 0.0001 F^2)$
R_{gt}, R_{all}	0.0494, 0.0564
wR_{gt}, wR_{ref},	0.0646, 0.0651
GOF_{gt}, GOF_{ref}	3.84, 3.47
Max. /min. residual *e* density, (*e*Å^{-3})	6.44 / -1.95

Table S7. Atomic parameters for β-$LiLa_2O_2VO_4$

Atom	X	Y	Z	U_{eq}
La1	0.79396(16)	0.53683(15)	0.64942(10)	0.0036(4)
La2	0.29049(16)	0.02787(15)	0.6488(1)	0.0036(4)
V1	0.7888(6)	0.1786(6)	0.9378(4)	0.0155(11)
O1	0.827(3)	0.238(3)	0.1319(16)	0.059(7)
O2	0.9974(18)	0.7476(18)	0.4964(12)	0.003(4)
O3	0.5069(18)	0.2472(19)	0.4996(12)	0.005(4)
O4	0.574(2)	0.356(2)	0.8627(15)	0.023(5)
O5	0.030(2)	0.263(2)	0.8566(14)	0.023(5)
O6	0.668(2)	0.896(2)	0.8561(14)	0.024(5)
Li1	0.660(6)	0.660(5)	0.000(4)	0.022(12)

Table S8. Anisotropic atomic displacement parameters for β-$LiLa_2O_2VO_4$

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0042(6)	0.0037(6)	0.0029(6)	-0.0006(4)	0.0007(4)	0.0006(4)
La2	0.0039(6)	0.0036(6)	0.0029(6)	-0.0009(4)	0.0001(4)	0.0005(4)
V1	0.0140(18)	0.0142(18)	0.0187(18)	0.0011(14)	0.0023(14)	0.0052(14)
O1	0.092(13)	0.050(11)	0.028(9)	-0.082(10)	0.065(9)	-0.057(8)
O2	0.000(6)	0.005(6)	0.001(6)	0.002(5)	-0.009(5)	0.001(5)
O3	0.004(6)	0.013(7)	-0.004(6)	-0.002(5)	-0.005(5)	0.008(5)
O4	0.023(8)	0.024(8)	0.023(8)	-0.007(6)	0.012(6)	0.005(6)
O5	0.018(7)	0.030(8)	0.021(8)	0.004(6)	0.001(6)	0.009(6)
O6	0.032(9)	0.020(8)	0.019(8)	-0.003(6)	0.006(7)	-0.001(6)
Li1	0.025(19)	0.017(18)	0.03(2)	0.010(15)	0.009(16)	0.004(15)

Table S9. Selected interatomic distances (Å)

Atom 1	Atom2	d, Å
O1	La2	2.7490(17)
	La1	2.7523(15)
O2	La1	2.3455(11)
	La2	2.3619(93)
	La1	2.4306(11)
	La2	2.4351(11)
O3	La1	2.3664(95)
	La2	2.3866(11)
	La2	2.3958(12)
	La1	2.4663(11)
O4	La2	2.7018(11)
	La1	2.7082(14)
O5	La1	2.7645(12)
	La2	2.7917(12)
O6	La1	2.7523(12)
	La2	2.7630(11)
V1	O1	1.6132(14)
	O4	1.7446(12)
	O6	1.7522(11)
	O5	1.7552(13)
Li1	O4	1.9596(40)
	O4	1.9652(30)
	O6	1.9716(36)
	O5	1.9749(33)

Table S10. Bond-valence analysis (v.u.) for the crystal structure of β-$LiLa_2O_2VO_4$

Atom	La1	La2	V1	Li1	$\sum_v a$
O1	0.20	0.20	1.61		2.02
O2	0.50+0.63	0.50+0.49			2.22
O3	0.59+0.45	0.56+0.55			2.15
O4	0.23	0.23	1.15	0.25+0.24	2.10
O5	0.20	0.18	1.12	0.24	1.74
O6	0.20	0.20	1.13	0.24	1.77
$\sum_v c$	3.00	3.01	5.01	0.98	

$\sum$va and $\sum$vc are the bond valence sums for anions and cations, respectively.

(R, b) [1] parameters being for La-O (2.179; 0.359), V-O (1.799; 0.388), Li-O (1.062; 0.642).

Table S11. Crystal parameters, data collection and structure refinement details for the crystal of *$LiNd_5O_5(VO_4)_2$*

Crystal data	
Formula	*$LiNd_5O_5(VO_4)_2$*
Formula weight (g/mol)	1038
Temperature (K)	293
Crystal system	monoclinic
Space group	*C*2/*m*
a (Å)	19.4507(2)
b (Å)	5.7848(5)
c (Å)	12.2593(1)
β (°)	117.847(5)°
V (Å^3)	1219.7(2)
Z	4
Data collection	
Diffractometer	X8 Bruker
Radiation; λ (Å)	Ag*Kα*; 0.56086
Absorption coefficient, μ (mm^{-1})	5.649
F (000)	1812
Data range θ (º); *h, k, l*	1.48– 25.38; -29 < *h* < 29,
	-8 < *k* < 8, -18 < *l* < 18
No. of measured reflections	11412
Total reflections (N_2)/unique (N_1)	2474 / 1496
Criterion for observed reflections	I >3σ(I)
R_{int} (%)	8.15
Refinement	
Refinement on	Full-matrix last squares on *F*
Weight scheme	1/(σ^2 |F| + 0.0001 F^2)
$R_{Ft,}$ R_{all}	3.80, 8.14
$wR_{gt,}$ $wR_{ref,}$	3.78, 6.31
GOF_{gt}, GOF_{ref}	1.19, 1.53
Max. /min. residual *e* density, (*e*Å^{-3})	3.80 / -3.99

Table S12. Atomic parameters for *$LiNd_5O_5(VO_4)_2$*

Atom	X	Y	Z	Ueq
Nd1	0.89074(5)	0	0.44057(9)	0.0057(3)
Nd2	0.76267(5)	0.5	0.25519(9)	0.0067(3)
Nd3	0.19110(5)	0.5	0.41550(9)	0.0070(4)
Nd4	0.83240(5)	0	0.10994(9)	0.0088(4)
Nd5	0.96954(5)	0.5	0.33388(10)	0.0081(3)
V1	0.14892(18)	0.5	0.0552(3)	0.0110(12)
V2	0.05691(17)	0	0.2462(3)	0.0082(11)
O1	1	0.256(2)	0.5	0.007(2)
O2	0.1165(7)	0	0.1824(13)	0.021(3)
O3	0.9655(8)	0	0.1292(14)	0.028(4)
O4	0.0741(5)	0.2359(19)	0.3397(9)	0.018(2)
O5	0.8633(4)	0.7509(84)	0.2669(7)	0.0065(17)
O6	0.9304(10)	0.5	0.0820(18)	0.051(6)
O7	0.2080(5)	0.7343(83)	0.0672(8)	0.0107(18)
O8	0.7840(5)	0.7467(85)	0.4169(8)	0.0087(16)
O9	0.1233(10)	0.5	0.1666(19)	0.054(6)
Li1	1	0.257(16)	0	0.10(2)

Table S13. Anisotropic atomic displacement parameters for *$LiNd_5O_5(VO_4)_2$*

Atom	U^{11}	U^{22}	U^{33}	U^{13}
Nd1	0.0042(4)	0.0058(5)	0.0066(5)	0.0021(3)
Nd2	0.0061(4)	0.0068(5)	0.0066(4)	0.0025(3)
Nd3	0.0069(4)	0.0047(5)	0.0112(5)	0.0059(4)
Nd4	0.0104(5)	0.0090(5)	0.0057(4)	0.0028(4)
Nd5	0.0064(4)	0.0057(4)	0.0107(4)	0.0028(3)
V1	0.0114(15)	0.0070(16)	0.0164(16)	0.0080(12)
V2	0.0070(13)	0.0091(16)	0.0095(15)	0.0048(11)

Table S14. Selected interatomic distances (Å) in *$LiNd_5O_5(VO_4)_2$*

Atom 1	Atom 2	d, Å
O1	Nd5	2.3157(71)
	Nd5	2.3163(71)
	Nd1	2.4070(72)
	Nd1	2.4071(72)
O2	Nd2	2.5515(13)
O3	Nd4	2.4877(17)
O4	Nd5	2.5178(11)
	Nd3	2.5301(97)
	Nd1	2.8048(11)
O5	Nd4	2.2489(87)
	Nd5	2.3387(81)
	Nd2	2.3864(88)
	Nd1	2.4147(88)
O6	Nd5	2.8138(22)
O7	Nd4	2.4698(95)
	Nd2	2.5518(92)
	Nd4	2.6046(99)
O8	Nd2	2.3180(96)
	Nd3	2.3199(10)
	Nd3	2.3588(95)
	Nd1	2.4450(97)
O9	Nd3	2.7005(21)
V1	O9	1.6585(27)
	O6	1.6689(16)
	O7	1.7385(10)
	O7	1.7386(10)
V2	O2	1.6748(18)
	O3	1.6834(12)
	O4	1.7118(11)
	O4	1.7120(11)
Li1	O6	2.4671(57)
	O6	2.4676(57)
	O3	2.4821(58)
	O3	2.4826(58)
	O9	2.7060(50)
	O9	2.7062(50)
	O2	2.7588(51)
	O2	2.7590(51)

Table S15. Bond-valence analysis (v.u.) for the crystal structure of *$LiNd_5O_5(VO_4)_2$*

	Nd1	**Nd2**	**Nd3**	**Nd4**	**Nd5**	**V1**	**V2**	**Li1**	∑va
O1	0.44 x2				0.56 x2				2.01
O2		0.30					1.38	0.07 x2	1.82
O3				0.35			1.34	0.11 x2	1.92
O4	0.15 x2		0.32 x2		0.33 x2		1.25 x2		4.09
O5	0.43 x2	0.47 x2		0.67 x2	0.53 x2				4.20
O6					0.15	1.40		0.11 x2	1.77
O7		0.30 x2		0.37 x2 + 0.26 x2		1.17 x2			4.19
O8	0.40 x2	0.56 x2	0.56 x2 + 0.50 x2						4.03
O9			0.20			1.44		0.08 x2	1.79
∑vc	2.85	2.95	2.95	2.96	2.99	5.17	5.23	0.74	

∑va and ∑vc are the bond valence sums for anions and cations, respectively.

(R, b) [1] parameters being for Nd-O (2.103; 0.371), V-O (1.799; 0.388), Li-O (1.062; 0.642).

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