Supporting materials

$[Ni(1,2\text{-}PDA)_3]_2(HOCH_2CH_2CH_2NH_3)_3(H_3O)_2[Ge_7O_{14}X_3]_3$ (X=F, OH): A new 1-D germanate with 12-ring hexagonal tubular channels

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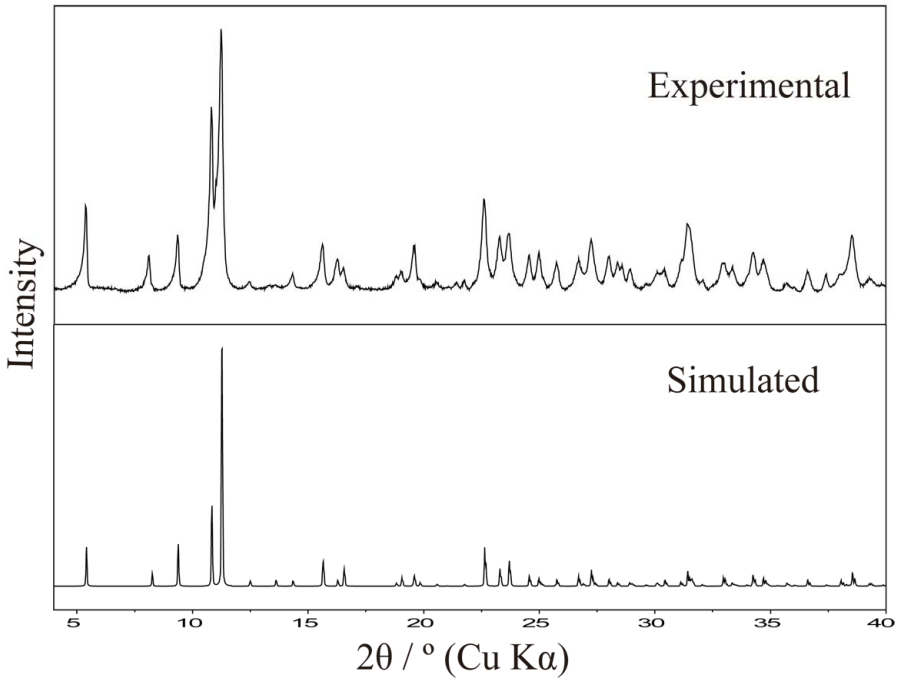
Experimental
Simulated
Intensity
5
10
15
20
25
30
35
40
2θ / º (Cu Kα)

Figure S1

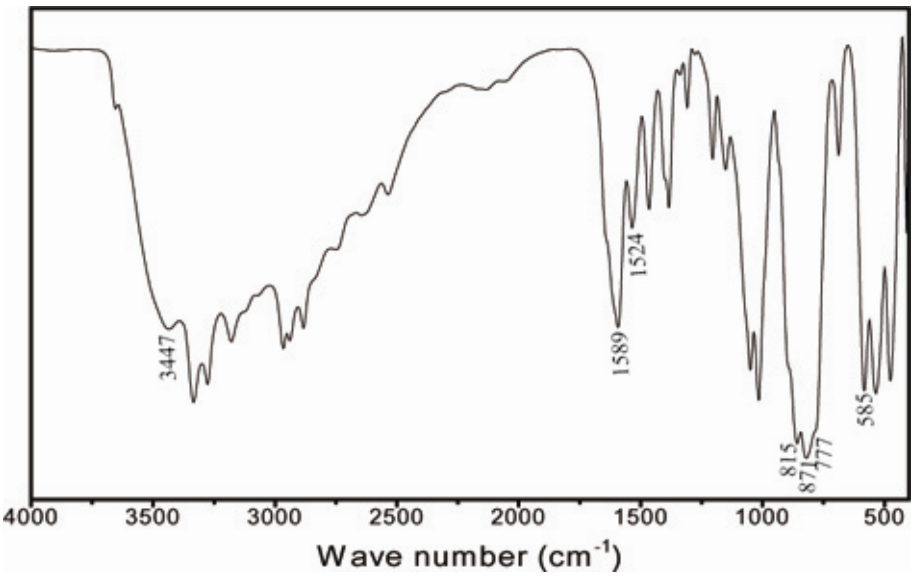
3447
1589
1524
815
871
777
585
4000
3500
3000
2500
2000
1500
1000
500
Wave number (cm-1)

Figure S2

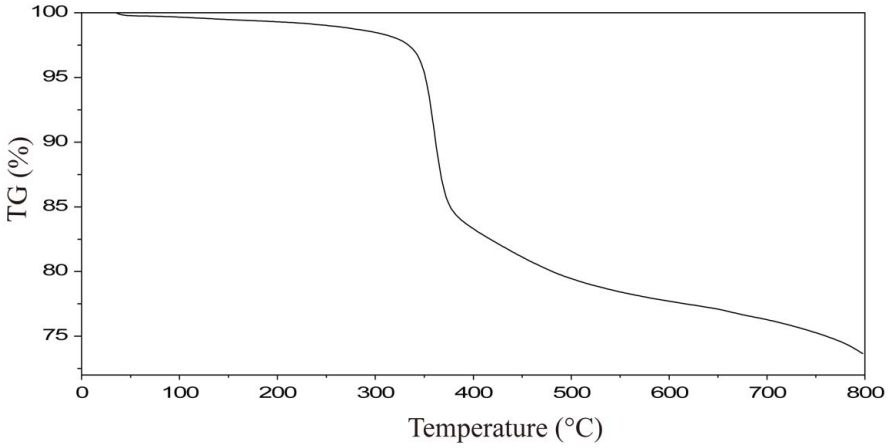
100
95
90
85
80
75
TG (%)
0
100
200
300
400
500
600
700
800
Temperature (°C)

Figure S3

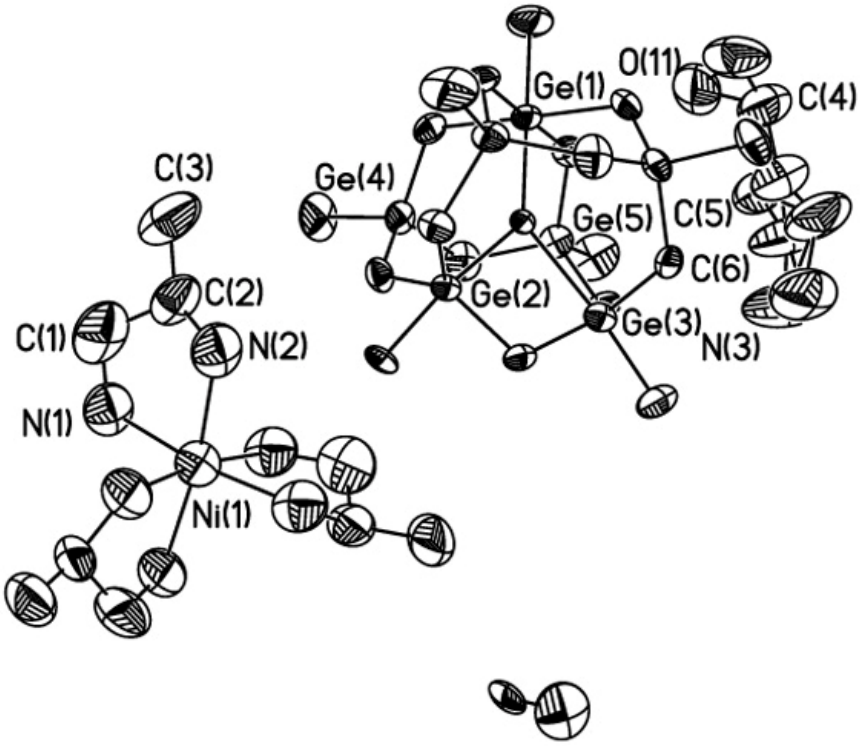

Figure S4

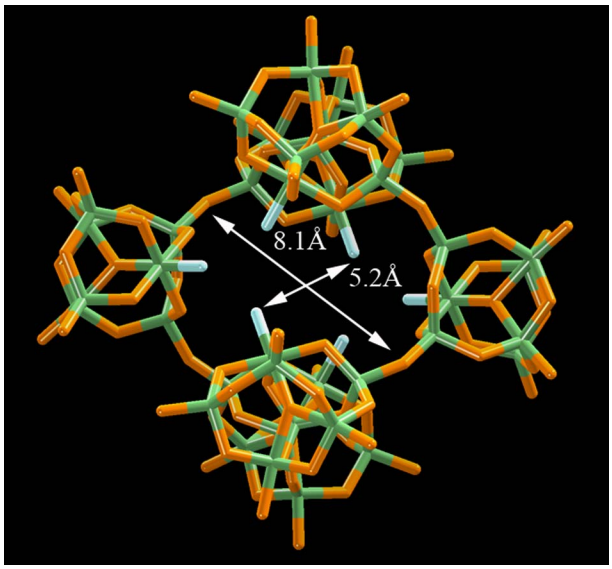

Figure S5

Table S1. Crystal data and structure refinement for compound **JLG-4.**

Empirical formula	C27H100.50F4.50Ge21N15Ni2O51.50
Formula weight	3187.03
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	hexagenal, $P6_3/m$
Unit cell dimensions	a = 18.800(3) Å α = 90 º
	b = 18.800(3) Å β = 90 º
	c = 14.147(3) Å γ = 120 º
Volume	4330.2(12) Å ^{3}
Z, Calculated density	2, 2.444 Mg/m^3
Absorption coefficient	7.699mm^{-1}
F(000)	3096
Crystal size(mm)	0.4 x 0.06 x 0.06 mm
Theta range for data collection	3.14 to 27.48 º
Limiting indices	-24≤h≤24, -24≤k≤24, -17≤l≤18
Reflections collected / unique	43665 / 3443 [R(int) = 0.0665]
Completeness to theta = 23.36	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3443 / 20 / 217
Goodness-of-fit on F^2	1.036
Final R indices [I>2σ(I)]	R_1 = 0.0459, wR_2 = 0.1167
R indices (all data)	R_1 = 0.0580, wR_2 = 0.1228
Largest diff. peak and hole	1.820 and -1.686 e. Å $^{-3}$

* $R_1=\sum(\Delta F/\sum(F_o))$; w$R_2=(\sum[w(F_o^2-F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$, $w=1/\sigma^2(F_o^2)$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **JLG-4.**

	x	y	z	U(eq)
Ge(1)	1970(1)	169(1)	2500	27(1)
Ge(2)	4177(1)	1139(1)	2500	24(1)
Ge(3)	3465(1)	-624(1)	2500	29(1)
Ge(4)	3135(1)	1144(1)	4153(1)	31(1)
Ge(5)	2320(1)	-714(1)	4134(1)	32(1)
Ni(1)	6667	3333	4767(1)	61(1)
F(1)	975(4)	98(4)	2500	50(2)
O(12)	975(4)	98(4)	2500	50(2)
O(1)	3035(3)	246(3)	2500	20(1)
O(2)	2326(2)	993(3)	3439(3)	35(1)
O(3)	1597(2)	-659(2)	3435(3)	34(1)
O(4)	4380(3)	319(4)	2500	30(1)
O(5)	5271(3)	1880(3)	2500	46(2)
F(2)	5271(3)	1880(3)	2500	46(2)
O(6)	4075(2)	1567(2)	3566(3)	33(1)
O(7)	3920(4)	-1262(4)	2500	58(3)
F(3)	3920(4)	-1262(4)	2500	58(3)
O(8)	2917(3)	-1042(3)	3557(3)	36(1)
O(9)	3343(4)	1860(4)	5028(4)	65(2)
O(10)	2924(3)	222(3)	4725(3)	42(1)
O(11)	176(8)	-2140(10)	3118(14)	114(6)
N(1)	6451(6)	4156(6)	5603(7)	83(2)
N(2)	5705(5)	3307(5)	3959(7)	83(2)
N(3)	1994(15)	-2930(17)	2768(17)	135(12)
C(1)	5902(9)	4350(8)	5083(10)	106(4)
C(2)	5279(6)	3630(6)	4562(10)	86(3)
C(3)	4705(8)	3811(8)	4018(12)	113(5)
C(4)	179(10)	-2697(11)	2500	92(5)
C(5)	958(12)	-2660(13)	2795(13)	81(6)
C(6)	1120(20)	-3260(20)	2970(20)	160(15)
O(1W)	9905(15)	919(18)	5770(20)	47(7)
O(1W')	9830(40)	510(30)	5140(30)	87(13)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S3. Selected bond lengths [Å] and angles [º] for compound **JLG-4**.

Ge(1)-F(1)	1.807(7)	Ge(1)-O(3)#1	1.890(4)
Ge(1)-O(3)	1.890(4)	Ge(1)-O(2)	1.891(4)
Ge(1)-O(2)#1	1.891(4)	Ge(1)-O(1)	1.933(5)
Ge(2)-O(6)	1.764(4)	Ge(2)-O(6)#1	1.764(4)
Ge(2)-O(4)	1.764(5)	Ge(2)-O(5)	1.817(5)
Ge(2)-O(1)	1.956(5)	Ge(3)-O(4)	1.746(6)
Ge(3)-O(8)	1.763(4)	Ge(3)-O(8)#1	1.763(4)
Ge(3)-O(7)	1.787(7)	Ge(3)-O(1)	2.157(5)
Ge(4)-O(9)	1.724(5)	Ge(4)-O(2)	1.727(4)
Ge(4)-O(6)	1.743(4)	Ge(4)-O(10)	1.769(5)
Ge(5)-O(3)	1.725(4)	Ge(5)-O(9)#2	1.729(5)
Ge(5)-O(8)	1.730(4)	Ge(5)-O(10)	1.758(5)
Ni(1)-N(2)#3	2.118(10)	Ni(1)-N(2)	2.118(10)
Ni(1)-N(2)#4	2.118(10)	Ni(1)-N(1)	2.141(9)
Ni(1)-N(1)#3	2.141(9)	Ni(1)-N(1)#4	2.141(9)
O(9)-Ge(5)#5	1.729(5)	O(11)-C(4)	1.367(19)
O(11)-O(11)#1	1.75(4)	N(1)-C(1)	1.456(16)
N(1)-H(1A)	0.9000	N(1)-H(1B)	0.9000
N(2)-C(2)	1.492(12)	N(2)-H(2A)	0.9000
N(2)-H(2B)	0.9000	N(3)-N(3)#1	0.76(5)
N(3)-C(6)	1.47(4)	N(3)-C(6)#1	1.78(4)
C(1)-C(2)	1.470(17)	C(1)-H(1C)	0.9700
C(1)-H(1D)	0.9700	C(2)-C(3)	1.497(17)
C(2)-H(2)	0.9800	C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600	C(3)-H(3C)	0.9600
C(4)-O(11)#1	1.367(19)	C(4)-C(5)	1.491(16)
C(4)-C(5)#1	1.491(16)	C(5)-C(5)#1	0.84(4)
C(5)-C(6)	1.327(18)	C(5)-C(6)#1	1.69(3)
C(6)-C(6)#1	1.33(7)	C(6)-C(5)#1	1.69(3)
C(6)-N(3)#1	1.78(4)	O(1W)-O(1W')	1.15(5)
O(1W')-O(1W')#6	1.21(4)	O(1W')-O(1W')#7	1.21(4)
F(1)-Ge(1)-O(3)#1	89.73(19)	F(1)-Ge(1)-O(3)	89.73(19)
O(3)#1-Ge(1)-O(3)	88.9(3)	F(1)-Ge(1)-O(2)	89.42(19)
O(3)#1-Ge(1)-O(2)	179.14(17)	O(3)-Ge(1)-O(2)	90.95(19)
F(1)-Ge(1)-O(2)#1	89.42(19)	O(3)#1-Ge(1)-O(2)#1	90.95(19)
O(3)-Ge(1)-O(2)#1	179.13(17)	O(2)-Ge(1)-O(2)#1	89.2(3)
F(1)-Ge(1)-O(1)	179.9(3)	O(3)#1-Ge(1)-O(1)	90.33(16)
O(3)-Ge(1)-O(1)	90.33(16)	O(2)-Ge(1)-O(1)	90.51(16)
O(2)#1-Ge(1)-O(1)	90.51(16)	O(6)-Ge(2)-O(6)#1	117.5(3)
O(6)-Ge(2)-O(4)	121.27(14)	O(6)#1-Ge(2)-O(4)	121.27(14)

O(6)-Ge(2)-O(5)	89.45(16)	O(6)#1-Ge(2)-O(5)	89.45(16)
O(4)-Ge(2)-O(5)	90.8(3)	O(6)-Ge(2)-O(1)	93.89(15)
O(6)#1-Ge(2)-O(1)	93.89(15)	O(4)-Ge(2)-O(1)	82.8(2)
O(5)-Ge(2)-O(1)	173.5(2)	O(4)-Ge(3)-O(8)	120.81(15)
O(4)-Ge(3)-O(8)#1	120.81(15)	O(8)-Ge(3)-O(8)#1	116.1(3)
O(4)-Ge(3)-O(7)	97.0(3)	O(8)-Ge(3)-O(7)	94.03(17)
O(8)#1-Ge(3)-O(7)	94.03(17)	O(4)-Ge(3)-O(1)	77.5(2)
O(8)-Ge(3)-O(1)	88.86(15)	O(8)#1-Ge(3)-O(1)	88.86(15)
O(7)-Ge(3)-O(1)	174.5(3)	O(9)-Ge(4)-O(2)	112.7(2)
O(9)-Ge(4)-O(6)	101.8(2)	O(2)-Ge(4)-O(6)	113.9(2)
O(9)-Ge(4)-O(10)	106.8(3)	O(2)-Ge(4)-O(10)	111.0(2)
O(6)-Ge(4)-O(10)	110.2(2)	O(3)-Ge(5)-O(9)#2	111.3(2)
O(3)-Ge(5)-O(8)	115.0(2)	O(9)#2-Ge(5)-O(8)	99.7(2)
O(3)-Ge(5)-O(10)	110.3(2)	O(9)#2-Ge(5)-O(10)	108.2(3)
O(8)-Ge(5)-O(10)	111.8(2)	N(2)#3-Ni(1)-N(2)	93.7(3)
N(2)#3-Ni(1)-N(2)#4	93.7(3)	N(2)-Ni(1)-N(2)#4	93.7(3)
N(2)#3-Ni(1)-N(1)	171.6(3)	N(2)-Ni(1)-N(1)	81.2(3)
N(2)#4-Ni(1)-N(1)	93.3(3)	N(2)#3-Ni(1)-N(1)#3	81.2(4)
N(2)-Ni(1)-N(1)#3	93.3(3)	N(2)#4-Ni(1)-N(1)#3	171.6(3)
N(1)-Ni(1)-N(1)#3	92.4(4)	N(2)#3-Ni(1)-N(1)#4	93.3(3)
N(2)-Ni(1)-N(1)#4	171.6(3)	N(2)#4-Ni(1)-N(1)#4	81.2(4)
N(1)-Ni(1)-N(1)#4	92.4(4)	N(1)#3-Ni(1)-N(1)#4	92.4(4)
Ge(1)-O(1)-Ge(2)	135.7(3)	Ge(1)-O(1)-Ge(3)	135.2(2)
Ge(2)-O(1)-Ge(3)	89.04(19)	Ge(4)-O(2)-Ge(1)	117.9(2)
Ge(5)-O(3)-Ge(1)	118.1(2)	Ge(3)-O(4)-Ge(2)	110.7(3)
Ge(4)-O(6)-Ge(2)	121.1(2)	Ge(5)-O(8)-Ge(3)	125.5(2)
Ge(4)-O(9)-Ge(5)#5	151.8(4)	Ge(5)-O(10)-Ge(4)	118.6(2)
C(4)-O(11)-O(11)#1	50.2(10)	C(1)-N(1)-Ni(1)	108.4(7)
C(1)-N(1)-H(1A)	110.0	Ni(1)-N(1)-H(1A)	110.0
C(1)-N(1)-H(1B)	110.0	Ni(1)-N(1)-H(1B)	110.0
H(1A)-N(1)-H(1B)	108.4	C(2)-N(2)-Ni(1)	108.0(7)
C(2)-N(2)-H(2A)	110.1	Ni(1)-N(2)-H(2A)	110.1
C(2)-N(2)-H(2B)	110.1	Ni(1)-N(2)-H(2B)	110.1
H(2A)-N(2)-H(2B)	108.4	N(3)#1-N(3)-C(6)	101.3(16)
N(3)#1-N(3)-C(6)#1	54.0(12)	C(6)-N(3)-C(6)#1	47(2)
N(1)-C(1)-C(2)	111.2(10)	N(1)-C(1)-H(1C)	109.4
C(2)-C(1)-H(1C)	109.4	N(1)-C(1)-H(1D)	109.4
C(2)-C(1)-H(1D)	109.4	H(1C)-C(1)-H(1D)	108.0
C(1)-C(2)-N(2)	108.6(8)	C(1)-C(2)-C(3)	112.5(10)
N(2)-C(2)-C(3)	113.2(11)	C(1)-C(2)-H(2)	107.5
N(2)-C(2)-H(2)	107.5	C(3)-C(2)-H(2)	107.5
C(2)-C(3)-H(3A)	109.5	C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5	C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5	H(3B)-C(3)-H(3C)	109.5

O(11)-C(4)-O(11)#1	80(2)	O(11)-C(4)-C(5)	99.6(13)
O(11)#1-C(4)-C(5)	121.6(15)	O(11)-C(4)-C(5)#1	121.6(15)
O(11)#1-C(4)-C(5)#1	99.6(13)	C(5)-C(4)-C(5)#1	32.5(14)
C(5)#1-C(5)-C(6)	100.8(17)	C(5)#1-C(5)-C(4)	73.7(7)
C(6)-C(5)-C(4)	131(2)	C(5)#1-C(5)-C(6)#1	50.3(11)
C(6)-C(5)-C(6)#1	51(3)	C(4)-C(5)-C(6)#1	106.7(16)
C(5)-C(6)-C(6)#1	79.2(17)	C(5)-C(6)-N(3)	107(3)
C(6)#1-C(6)-N(3)	78.7(16)	C(5)-C(6)-C(5)#1	28.9(13)
C(6)#1-C(6)-C(5)#1	50.3(11)	N(3)-C(6)-C(5)#1	98(2)
C(5)-C(6)-N(3)#1	99(2)	C(6)#1-C(6)-N(3)#1	54.0(12)
N(3)-C(6)-N(3)#1	24.8(16)	C(5)#1-C(6)-N(3)#1	80.5(18)
O(1W)-O(1W')-O(1W')#6	137(6)	O(1W)-O(1W')-O(1W')#7	109(7)
O(1W')#6-O(1W')-O(1W')#7	110(4)		

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2	#2 y,-x+y,-z+1	#3 -y+1,x-y,z
#4 -x+y+1,-x+1,z	#5 x-y,x,-z+1	#6 x-y,x-1,-z+1
#7 y+1,-x+y+1,-z+1		

Table S4. Selected hydrogen bonds for **JLG-4** [Å and º].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1B)...N(3)#1	0.90	2.27	2.76(2)	114.2
N(2)-H(2A)...O(5)#2	0.90	2.26	3.124(10)	161.1
N(2)-H(2B)...O(6)	0.90	2.37	3.222(10)	158.5
N(2)-H(2B)...O(5)	0.90	2.44	3.153(9)	136.2

Symmetry transformations used to generate equivalent atoms:

#1 y+1,-x+y+1,-z+1 #2 -x+y+1,-x+1,z