

Supporting information:

A crystalline germanate with mesoporous 30-ring channels

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Table S1 Crystal data and structure refinement for JLG-12.

Figure S1 The experimental and simulated X-ray powder diffraction patterns for JLG-12.

Figure S2 Thermogravimetric (TG) curve of JLG-12.

Figure S3 Infrared spectrum of JLG-12.

Table S1 Crystal data and structure refinement for compound **JLG-12**.

Identification code	JLG-12
Empirical formula	C ₁₈₀ H ₆₀₀ Ge _{139.73} N ₆₀ O _{339.45}
Formula weight	19181.40
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, <i>C2/m</i>
Unit cell dimensions	$a = 46.377(9)\text{Å}$ $\alpha = 90^\circ$
	$b = 26.689(5)\text{Å}$ $\beta = 92.84(3)^\circ$
	$c = 12.107(2)\text{Å}$ $\gamma = 90^\circ$
Volume	14967(5) Å ³
Z, Calculated density	1, 2.128 Mg/m ³
Absorption coefficient	6.988 mm ⁻¹
F(000)	9287
Crystal size	0.050 × 0.020 × 0.020 mm ³
Theta range for data collection	2.22 to 24.50°
Limiting indices	-50 ≤ h ≤ 54, -29 ≤ k ≤ 30, -13 ≤ l ≤ 12
Reflections collected / unique	35786 / 12325 [<i>R</i> (int) = 0.1629]
Completeness to theta = 24.50	96.6 %
Absorption correction	CrysAlis
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	12325 / 0 / 347
Goodness-of-fit on F ²	0.907
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0938, <i>wR</i> 2 = 0.2237
R indices (all data)	<i>R</i> 1 = 0.1436, <i>wR</i> 2 = 0.2436
Largest diff. peak and hole	3.602 and -2.397 e. Å ⁻³

* $R_1 = \Sigma(\Delta F / \Sigma(F_o))$; $wR_2 = (\Sigma[w(F_o^2 - F_c^2)]) / \Sigma[w(F_o^2)]^{1/2}$, $w = 1/\sigma^2(F_o^2)$

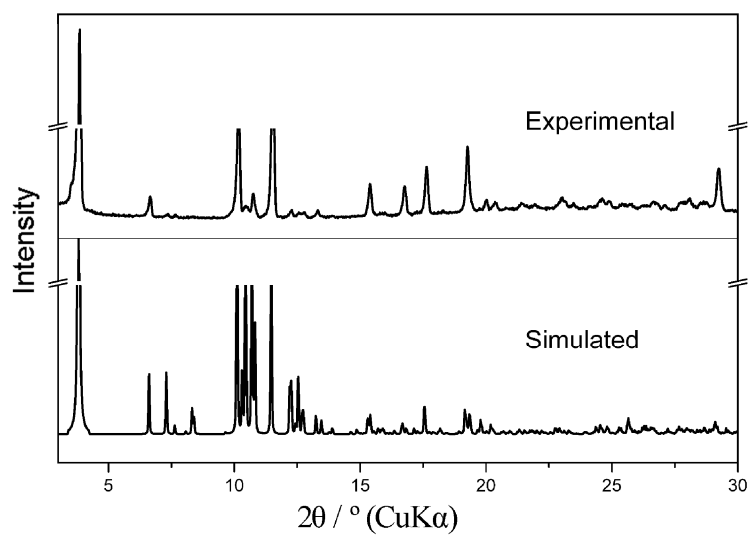


Figure S1 The experimental and simulated X-ray powder diffraction patterns for JLG-12
(Note: The simulated XRD pattern is calculated from the structure model without extra-framework atoms. The discrepancy between the experimental and simulated patterns comes from the ignoring of the contribution of extra-framework species)

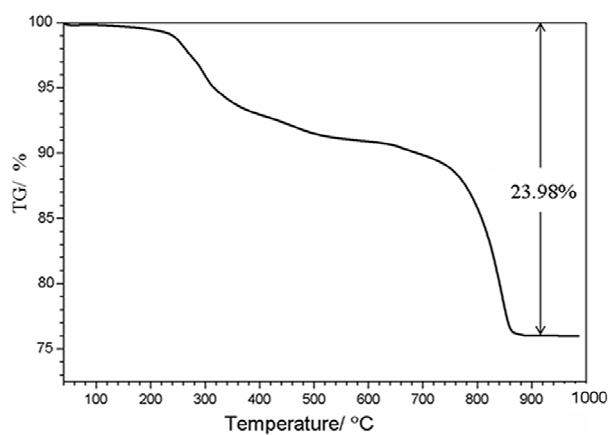


Figure S2 Thermogravimetric (TG) curves of JLG-12 in air. The TG analysis was performed on A Perkin-Elmer TGA 7 unit, with a heating rate of 10°C/min.

(Note: The framework collapses upon heating at 220°C with the decomposition of the occluded template molecules.)

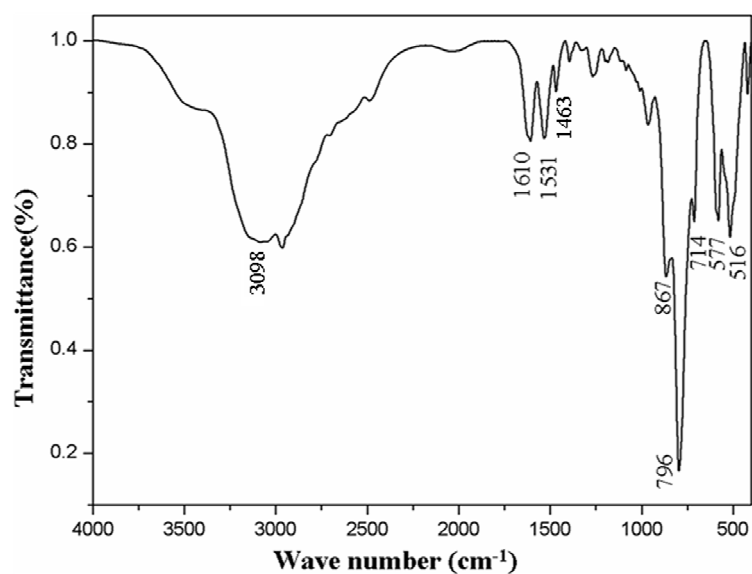


Figure S3 Infrared spectrum of JLG-12. IR (KBr, cm^{-1}): 3098 (OH); 1610, 1531 and 1463 (RNH_3^+); 867, 714, 577 and 516 (Ge-O); 796 (Ge-F).

References:

- (1) Beitone, L.; Loiseau, T.; Férey, G. *Inorg. Chem.* **2002**, 41, 3962.
- (2) Conradsson, T.; Zou, X. D.; Dadachov, M. S. *Inorg. Chem.* **2000**, 39, 1716.
- (2) Paques-Ledent, M. Th. *Spectrochim. Acta* **1976**, 32A, 383.
- (3) Tarte, P.; Pottier, M. J.; Proces, A. M. *Spectrochim. Acta* **1973**, 29A, 1017.