Supplementary Information

Table S1. Crystal data and structure refinement for $[Ga_{30}(\mu_4\text{-}O)_{12}(\mu_3\text{-}O)_4(\mu_3\text{-}OH)_4(\mu_2\text{-}OH)_{42}(H_2O)_{16}](2,6\text{-}NDS)_6 \ 47H_2O$. The structure is filed in the Cambridge Structural Database as CCDC 1038690.

Identification code	mn2113
Empirical formula[a]	$C_{60}H_{208}Ga_{30}O_{161}S_{12}$
Formula weight[a]	5982.57
Temperature	100(2) K
Wavelength[b]	0.7749 Å, synchrotron radiation
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 16.0487(7) Å; a= 112.7753(16)°
	b = 17.6742(7) Å; b= 105.1611(18)°
	c = 18.6218(8) Å; g = 94.7401(18)°
Volume	4599.2(3) $Å^3$
Z	1
Density (calculated)	2.160 Mg/m^3
Absorption coefficient	5.761 mm^{-1}
F(000)	2978
Crystal size	0.094 × 0.094 × 0.075 mm^3
Crystal color and habit	colorless block
Diffractometer	Bruker D8 with Photon 100 detector
Θ range for data collection	2.183 to 40.222°.
Index ranges	$-26 \le h \le 26$, $-29 \le k \le 29$, $-30 \le l \le 31$
Reflections collected	105735
Independent reflections	43758 [*R*(int) = 0.0340]
Observed reflections ($I > 2\sigma(I)$)	31256
Completeness to Θ = 27.706°	99.70%
Absorption correction	multi-scan
Max. and min. transmission	0.749 and 0.675
Solution method	SHELXS (Sheldrick, 2013)
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)
Data / restraints / parameters	43758/391/1477
Goodness-of-fit on F2	1.046
Final R indices [$I > 2\sigma$(I)]	R_1 = 0.0539, wR_2 = 0.1484
R indices (all data)	$\mathbf{R}_1$ = 0.0839, wR_2 = 0.1704
Extinction coefficient	n/a
Largest diff. peak and hole	3.502 and −2.774 e.$Å^{-3}$

[a] Includes missing hydrate hydrogen atoms.