Electronic Supplementary Information

Structure and stability range of a hexanuclear Th(IV) – glycine complex

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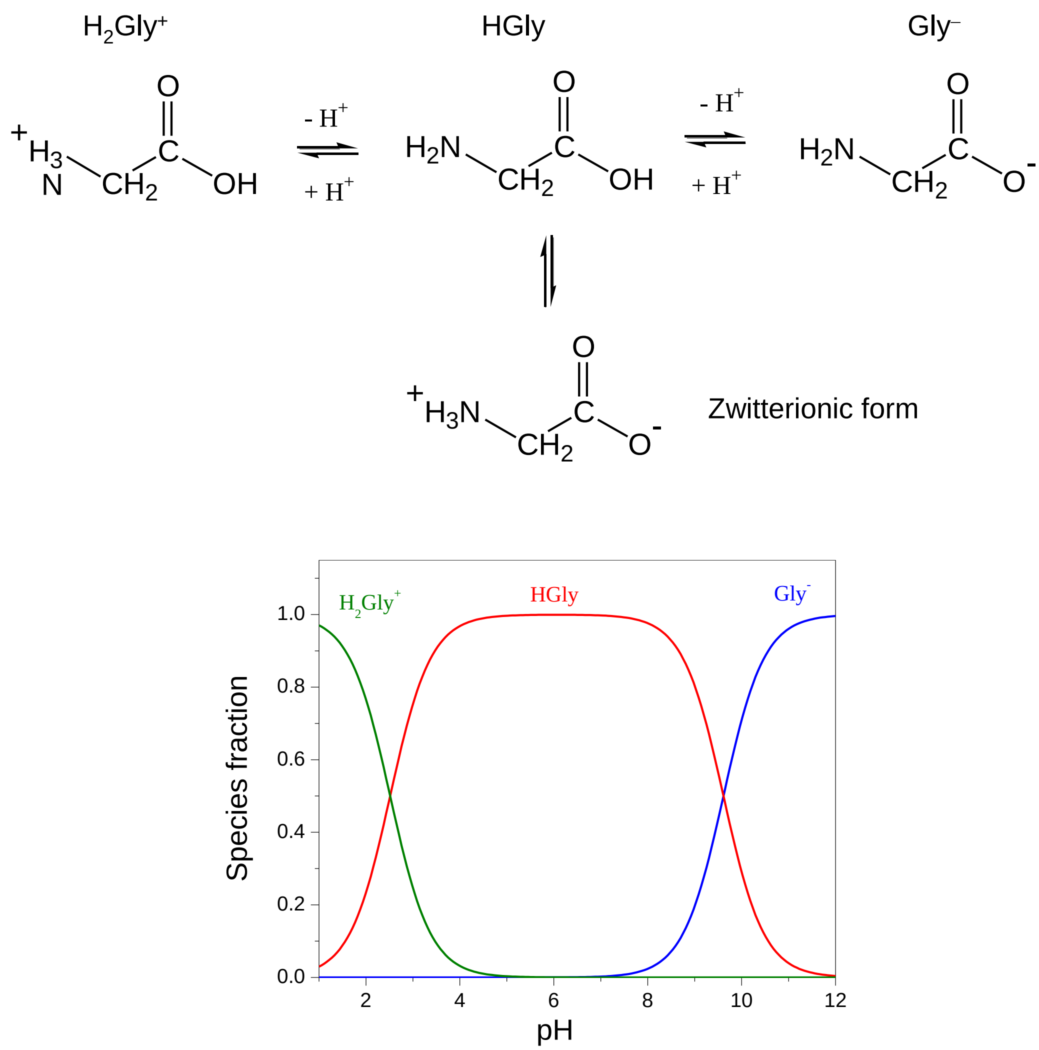

Figure S1: Equilibrium reaction of glycine (top) and species distribution in aqueous solution (bottom) with 1 M glycine, I = 1 M, t = 25°C. The pK_a values are: pK_{COOH} = 2.34, pK_{NH2} = 9.60 at 25°C.

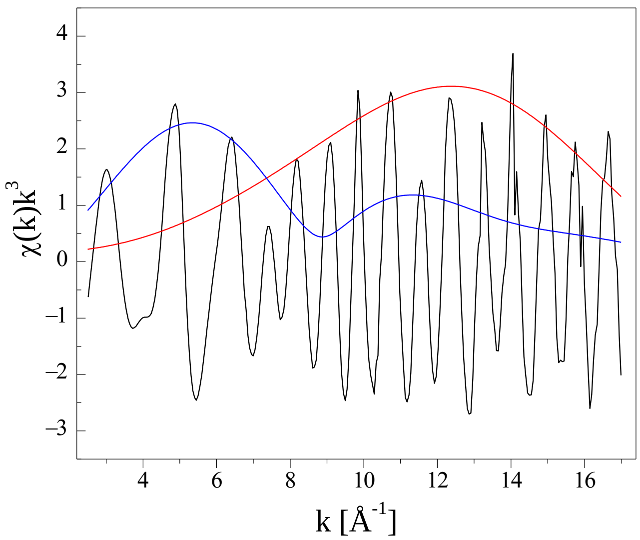

Figure S2. Th L_3-edge k^3-weighted EXAFS data of 0.05 M Th(IV) in 1 M glycine at pH 4.0 (black). In superposition are the scattering amplitude functions of the oxygen (blue) and thorium (red). The low *k*-range oxygen (and carbon) dominates the $\chi(k)$, whereas thorium dominates in the high *k*-range. A restriction of $\chi(k)$ to lower *k*-values promotes the light scattering atoms in the data fit procedure.

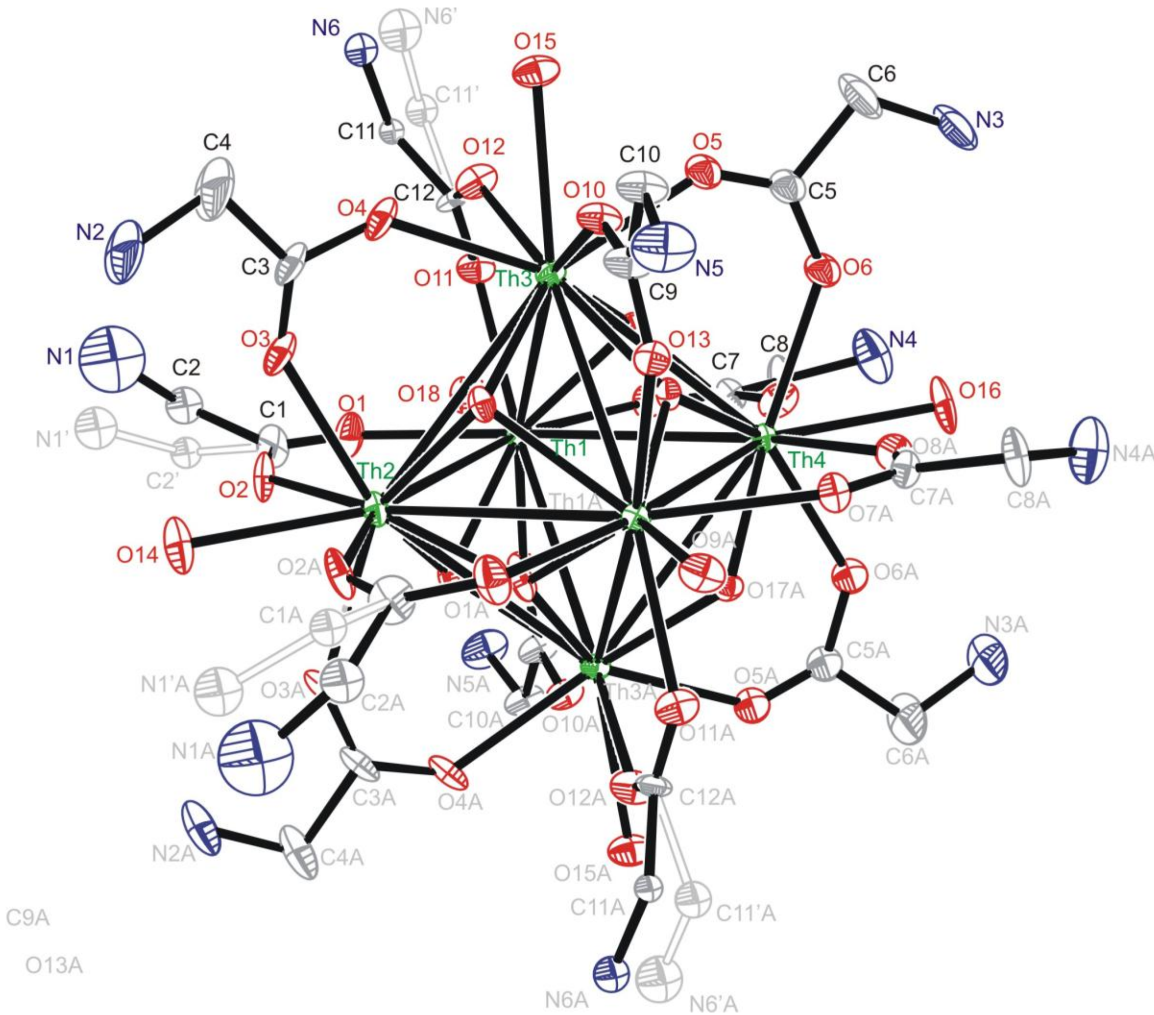

Figure S3: Ortep drawing of **1**, $[Th_6(\mu_3\text{-}O)_4(\mu_3\text{-}OH)_4(H_2O)_6(Gly)_6(HGly)_6](NO_3)_3(ClO_4)_3(H_2O)_3$ with atom labeling used in Table S1.

Table S1: Bond lengths [Å] and angles [deg] of **1**.

Th(1)-O(20)#1	2.307(6)
Th(1)-O(18)	2.335(5)
Th(1)-O(1)	2.482(8)
Th(1)-O(17)	2.501(6)
Th(1)-O(19)#1	2.503(6)
Th(1)-O(13)	2.524(5)
Th(1)-O(11)	2.522(6)
Th(1)-O(7)	2.601(7)
Th(1)-O(9)	2.708(7)
Th(1)-Th(3)#1	3.9366(8)
Th(1)-Th(4)	3.9416(7)
Th(1)-Th(3)	3.9481(8)

Th(2)-O(18)	2.259(6)
Th(2)-O(18)#1	2.259(6)
Th(2)-O(2)	2.507(7)
Th(2)-O(2)#1	2.507(7)
Th(2)-O(19)#1	2.525(5)
Th(2)-O(19)	2.525(5)
Th(2)-O(3)#1	2.546(6)
Th(2)-O(3)	2.546(6)
Th(2)-O(14)	2.708(11)
Th(2)-Th(1)#1	3.9506(7)
Th(2)-Th(3)	3.9535(7)
Th(3)-O(20)	2.297(6)
Th(3)-O(18)	2.318(5)
Th(3)-O(5)	2.488(7)
Th(3)-O(12)	2.502(7)
Th(3)-O(4)	2.503(7)
Th(3)-O(10)	2.514(6)
Th(3)-O(19)	2.518(6)
Th(3)-O(17)	2.525(6)
Th(3)-O(15)	2.712(6)
Th(3)-Th(1)#1	3.9366(8)
Th(3)-Th(4)	3.9461(7)
Th(4)-O(20)#1	2.297(6)
Th(4)-O(20)	2.297(6)
Th(4)-O(6)	2.456(6)
Th(4)-O(6)#1	2.456(6)
Th(4)-O(8)	2.486(7)
Th(4)-O(8)#1	2.486(7)
Th(4)-O(17)	2.538(6)
Th(4)-O(17)#1	2.538(6)
Th(4)-O(16)	2.676(9)
Th(4)-Th(1)#1	3.9416(7)
Th(4)-Th(3)#1	3.9461(7)
C(1)-O(2)	1.208(14)
C(1)-O(1)	1.289(14)
C(1)-C(2')	1.55(2)
C(1)-C(2)	1.59(2)
C(3)-O(3)	1.208(12)
C(3)-O(4)	1.315(13)
C(3)-C(4)	1.543(17)
C(4)-N(2)	1.381(18)
C(5)-O(5)	1.223(13)
C(5)-O(6)	1.345(11)
C(5)-C(6)	1.572(16)
C(6)-N(3)	1.421(17)
C(7)-O(8)	1.253(12)
C(7)-O(7)	1.265(11)
C(7)-C(8)	1.497(15)
C(8)-N(4)	1.418(15)
C(9)-O(10)	1.215(12)
C(9)-O(13)#1	1.245(10)
C(9)-C(10)	1.520(11)
C(10)-N(5)	1.376(14)
C(12)-O(11)	1.232(9)
C(12)-O(12)	1.279(12)
C(12)-C(11)	1.519(18)
C(12)-C(11')	1.69(2)

C(2)-N(1)	1.698(19)
C(11)-N(6)	1.490(13)
C(2')-N(1')	1.696(19)
C(11')-N(6')	1.488(14)
O(13)-C(9)#1	1.245(10)
O(19)-Th(1)#1	2.503(6)
O(20)-Th(1)#1	2.307(6)
N(7)-O(23)	1.225(7)
N(7)-O(22)	1.233(7)
N(7)-O(21)	1.233(7)
N(8)-O(24)	1.211(7)
N(8)-O(26)	1.221(7)
N(8)-O(25)	1.227(8)
N(9)-O(29)	1.220(8)
N(9)-O(27)	1.227(7)
N(9)-O(28)	1.228(8)
Cl(1)-O(33)	1.438(6)
Cl(1)-O(30)	1.442(7)
Cl(1)-O(32)	1.451(7)
Cl(1)-O(31)	1.457(7)
Cl(2)-O(37)	1.451(8)
Cl(2)-O(36)	1.451(7)
Cl(2)-O(34)	1.450(7)
Cl(2)-O(35)	1.453(7)
Cl(3)-O(40)	1.448(7)
Cl(3)-O(38)	1.454(7)
Cl(3)-O(41)	1.449(8)
Cl(3)-O(39)	1.454(6)

O(20)#1-Th(1)-O(18)	87.1(2)
O(20)#1-Th(1)-O(1)	141.3(2)
O(18)-Th(1)-O(1)	80.1(2)
O(20)#1-Th(1)-O(17)	69.60(18)
O(18)-Th(1)-O(17)	69.9(2)
O(1)-Th(1)-O(17)	136.02(19)
O(20)#1-Th(1)-O(19)#1	69.3(2)
O(18)-Th(1)-O(19)#1	68.17(18)
O(1)-Th(1)-O(19)#1	72.0(2)
O(17)-Th(1)-O(19)#1	121.48(19)
O(20)#1-Th(1)-O(13)	81.1(2)
O(18)-Th(1)-O(13)	139.7(2)
O(1)-Th(1)-O(13)	85.6(2)
O(17)-Th(1)-O(13)	137.7(2)
O(19)#1-Th(1)-O(13)	71.62(19)
O(20)#1-Th(1)-O(11)	139.7(2)
O(18)-Th(1)-O(11)	83.0(2)
O(1)-Th(1)-O(11)	74.9(2)
O(17)-Th(1)-O(11)	70.3(2)
O(19)#1-Th(1)-O(11)	139.0(2)
O(13)-Th(1)-O(11)	129.0(2)
O(20)#1-Th(1)-O(7)	81.9(2)
O(18)-Th(1)-O(7)	143.00(18)
O(1)-Th(1)-O(7)	128.2(2)
O(17)-Th(1)-O(7)	73.16(18)
O(19)#1-Th(1)-O(7)	137.13(18)
O(13)-Th(1)-O(7)	73.07(19)
O(11)-Th(1)-O(7)	83.0(2)

O(20)#1-Th(1)-O(9)	138.1(2)
O(18)-Th(1)-O(9)	134.9(2)
O(1)-Th(1)-O(9)	64.2(2)
O(17)-Th(1)-O(9)	118.2(2)
O(19)#1-Th(1)-O(9)	120.3(2)
O(13)-Th(1)-O(9)	66.65(19)
O(11)-Th(1)-O(9)	62.39(18)
O(7)-Th(1)-O(9)	64.0(2)
O(20)#1-Th(1)-Th(3)#1	31.16(14)
O(18)-Th(1)-Th(3)#1	79.75(15)
O(1)-Th(1)-Th(3)#1	110.17(17)
O(17)-Th(1)-Th(3)#1	95.57(13)
O(19)#1-Th(1)-Th(3)#1	38.51(14)
O(13)-Th(1)-Th(3)#1	70.27(16)
O(11)-Th(1)-Th(3)#1	160.74(14)
O(7)-Th(1)-Th(3)#1	105.94(14)
O(9)-Th(1)-Th(3)#1	136.83(11)
O(20)#1-Th(1)-Th(4)	31.06(13)
O(18)-Th(1)-Th(4)	80.60(15)
O(1)-Th(1)-Th(4)	159.76(18)
O(17)-Th(1)-Th(4)	38.88(13)
O(19)#1-Th(1)-Th(4)	95.16(14)
O(13)-Th(1)-Th(4)	105.56(16)
O(11)-Th(1)-Th(4)	108.63(16)
O(7)-Th(1)-Th(4)	71.81(14)
O(9)-Th(1)-Th(4)	135.56(17)
Th(3)#1-Th(1)-Th(4)	60.118(10)
O(20)#1-Th(1)-Th(3)	80.48(13)
O(18)-Th(1)-Th(3)	31.82(14)
O(1)-Th(1)-Th(3)	104.59(15)
O(17)-Th(1)-Th(3)	38.43(14)
O(19)#1-Th(1)-Th(3)	95.02(12)
O(13)-Th(1)-Th(3)	160.17(16)
O(11)-Th(1)-Th(3)	70.67(14)
O(7)-Th(1)-Th(3)	111.23(12)
O(9)-Th(1)-Th(3)	133.06(11)
Th(3)#1-Th(1)-Th(3)	90.109(15)
Th(4)-Th(1)-Th(3)	60.021(11)
O(18)-Th(2)-O(18)#1	86.6(3)
O(18)-Th(2)-O(2)	80.6(2)
O(18)#1-Th(2)-O(2)	140.4(2)
O(18)-Th(2)-O(2)#1	140.4(2)
O(18)#1-Th(2)-O(2)#1	80.6(2)
O(2)-Th(2)-O(2)#1	130.7(3)
O(18)-Th(2)-O(19)#1	68.90(18)
O(18)#1-Th(2)-O(19)#1	68.6(2)
O(2)-Th(2)-O(19)#1	71.8(2)
O(2)#1-Th(2)-O(19)#1	136.7(2)
O(18)-Th(2)-O(19)	68.6(2)
O(18)#1-Th(2)-O(19)	68.90(18)
O(2)-Th(2)-O(19)	136.7(2)
O(2)#1-Th(2)-O(19)	71.8(2)
O(19)#1-Th(2)-O(19)	120.3(3)
O(18)-Th(2)-O(3)#1	137.1(2)
O(18)#1-Th(2)-O(3)#1	81.3(2)
O(2)-Th(2)-O(3)#1	83.0(2)
O(2)#1-Th(2)-O(3)#1	77.8(2)

O(19)#1-Th(2)-O(3)#1	68.3(2)
O(19)-Th(2)-O(3)#1	140.1(2)
O(18)-Th(2)-O(3)	81.3(2)
O(18)#1-Th(2)-O(3)	137.1(2)
O(2)-Th(2)-O(3)	77.8(2)
O(2)#1-Th(2)-O(3)	83.0(2)
O(19)#1-Th(2)-O(3)	140.1(2)
O(19)-Th(2)-O(3)	68.3(2)
O(3)#1-Th(2)-O(3)	132.9(3)
O(18)-Th(2)-O(14)	136.69(15)
O(18)#1-Th(2)-O(14)	136.69(15)
O(2)-Th(2)-O(14)	65.34(16)
O(2)#1-Th(2)-O(14)	65.34(16)
O(19)#1-Th(2)-O(14)	119.86(13)
O(19)-Th(2)-O(14)	119.86(13)
O(3)#1-Th(2)-O(14)	66.46(17)
O(3)-Th(2)-O(14)	66.46(17)
O(18)-Th(2)-Th(1)	31.26(12)
O(18)#1-Th(2)-Th(1)	79.79(16)
O(2)-Th(2)-Th(1)	69.93(16)
O(2)#1-Th(2)-Th(1)	159.22(16)
O(19)#1-Th(2)-Th(1)	38.03(13)
O(19)-Th(2)-Th(1)	94.67(14)
O(3)#1-Th(2)-Th(1)	105.82(17)
O(3)-Th(2)-Th(1)	107.10(19)
O(14)-Th(2)-Th(1)	135.173(10)
O(18)-Th(2)-Th(1)#1	79.79(16)
O(18)#1-Th(2)-Th(1)#1	31.26(12)
O(2)-Th(2)-Th(1)#1	159.22(16)
O(2)#1-Th(2)-Th(1)#1	69.93(16)
O(19)#1-Th(2)-Th(1)#1	94.67(14)
O(19)-Th(2)-Th(1)#1	38.03(13)
O(3)#1-Th(2)-Th(1)#1	107.10(19)
O(3)-Th(2)-Th(1)#1	105.82(17)
O(14)-Th(2)-Th(1)#1	135.173(10)
Th(1)-Th(2)-Th(1)#1	89.654(19)
O(18)-Th(2)-Th(3)	30.68(13)
O(18)#1-Th(2)-Th(3)	80.16(14)
O(2)-Th(2)-Th(3)	104.60(16)
O(2)#1-Th(2)-Th(3)	109.82(14)
O(19)#1-Th(2)-Th(3)	94.53(13)
O(19)-Th(2)-Th(3)	38.32(14)
O(3)#1-Th(2)-Th(3)	158.43(17)
O(3)-Th(2)-Th(3)	68.65(17)
O(14)-Th(2)-Th(3)	135.107(10)
Th(1)-Th(2)-Th(3)	59.934(14)
Th(1)#1-Th(2)-Th(3)	59.742(14)
O(20)-Th(3)-O(18)	87.0(2)
O(20)-Th(3)-O(5)	80.6(2)
O(18)-Th(3)-O(5)	142.2(2)
O(20)-Th(3)-O(12)	142.1(2)
O(18)-Th(3)-O(12)	78.9(2)
O(5)-Th(3)-O(12)	89.4(3)
O(20)-Th(3)-O(4)	138.3(2)
O(18)-Th(3)-O(4)	84.0(2)
O(5)-Th(3)-O(4)	127.8(2)
O(12)-Th(3)-O(4)	75.3(3)

O(20)-Th(3)-O(10)	81.1(2)
O(18)-Th(3)-O(10)	138.9(2)
O(5)-Th(3)-O(10)	74.1(2)
O(12)-Th(3)-O(10)	131.12(18)
O(4)-Th(3)-O(10)	79.5(2)
O(20)-Th(3)-O(19)	69.2(2)
O(18)-Th(3)-O(19)	67.9(2)
O(5)-Th(3)-O(19)	136.6(2)
O(12)-Th(3)-O(19)	133.3(2)
O(4)-Th(3)-O(19)	69.7(2)
O(10)-Th(3)-O(19)	71.1(2)
O(20)-Th(3)-O(17)	69.4(2)
O(18)-Th(3)-O(17)	69.72(19)
O(5)-Th(3)-O(17)	72.5(2)
O(12)-Th(3)-O(17)	72.7(2)
O(4)-Th(3)-O(17)	141.7(2)
O(10)-Th(3)-O(17)	138.3(2)
O(19)-Th(3)-O(17)	120.91(16)
O(20)-Th(3)-O(15)	135.8(2)
O(18)-Th(3)-O(15)	136.9(2)
O(5)-Th(3)-O(15)	61.7(2)
O(12)-Th(3)-O(15)	64.0(2)
O(4)-Th(3)-O(15)	66.7(2)
O(10)-Th(3)-O(15)	67.7(2)
O(19)-Th(3)-O(15)	123.9(2)
O(17)-Th(3)-O(15)	115.2(2)
O(20)-Th(3)-Th(1)#1	31.32(15)
O(18)-Th(3)-Th(1)#1	79.50(16)
O(5)-Th(3)-Th(1)#1	105.04(18)
O(12)-Th(3)-Th(1)#1	157.85(13)
O(4)-Th(3)-Th(1)#1	107.03(18)
O(10)-Th(3)-Th(1)#1	70.03(13)
O(19)-Th(3)-Th(1)#1	38.24(14)
O(17)-Th(3)-Th(1)#1	95.33(13)
O(15)-Th(3)-Th(1)#1	137.70(15)
O(20)-Th(3)-Th(4)	30.81(15)
O(18)-Th(3)-Th(4)	80.69(14)
O(5)-Th(3)-Th(4)	70.44(15)
O(12)-Th(3)-Th(4)	111.51(15)
O(4)-Th(3)-Th(4)	161.49(16)
O(10)-Th(3)-Th(4)	105.63(16)
O(19)-Th(3)-Th(4)	94.80(13)
O(17)-Th(3)-Th(4)	38.92(14)
O(15)-Th(3)-Th(4)	131.76(18)
Th(1)#1-Th(3)-Th(4)	60.003(12)
O(20)-Th(3)-Th(1)	80.23(14)
O(18)-Th(3)-Th(1)	32.09(14)
O(5)-Th(3)-Th(1)	110.24(15)
O(12)-Th(3)-Th(1)	69.11(12)
O(4)-Th(3)-Th(1)	109.91(16)
O(10)-Th(3)-Th(1)	159.76(14)
O(19)-Th(3)-Th(1)	94.84(12)
O(17)-Th(3)-Th(1)	38.00(13)
O(15)-Th(3)-Th(1)	132.23(15)
Th(1)#1-Th(3)-Th(1)	89.891(15)
Th(4)-Th(3)-Th(1)	59.907(10)
O(20)#1-Th(4)-O(20)	87.5(3)

O(20)#1-Th(4)-O(6)	139.6(2)
O(20)-Th(4)-O(6)	82.1(2)
O(20)#1-Th(4)-O(6)#1	82.1(2)
O(20)-Th(4)-O(6)#1	139.6(2)
O(6)-Th(4)-O(6)#1	128.8(3)
O(20)#1-Th(4)-O(8)	80.6(2)
O(20)-Th(4)-O(8)	139.0(2)
O(6)-Th(4)-O(8)	82.2(2)
O(6)#1-Th(4)-O(8)	77.4(2)
O(20)#1-Th(4)-O(8)#1	139.0(2)
O(20)-Th(4)-O(8)#1	80.6(2)
O(6)-Th(4)-O(8)#1	77.4(2)
O(6)#1-Th(4)-O(8)#1	82.2(2)
O(8)-Th(4)-O(8)#1	131.7(4)
O(20)#1-Th(4)-O(17)	69.07(18)
O(20)-Th(4)-O(17)	69.1(2)
O(6)-Th(4)-O(17)	70.8(2)
O(6)#1-Th(4)-O(17)	139.1(2)
O(8)-Th(4)-O(17)	70.0(2)
O(8)#1-Th(4)-O(17)	138.34(18)
O(20)#1-Th(4)-O(17)#1	69.1(2)
O(20)-Th(4)-O(17)#1	69.07(18)
O(6)-Th(4)-O(17)#1	139.1(2)
O(6)#1-Th(4)-O(17)#1	70.8(2)
O(8)-Th(4)-O(17)#1	138.34(18)
O(8)#1-Th(4)-O(17)#1	70.0(2)
O(17)-Th(4)-O(17)#1	120.8(3)
O(20)#1-Th(4)-O(16)	136.26(14)
O(20)-Th(4)-O(16)	136.26(14)
O(6)-Th(4)-O(16)	64.39(17)
O(6)#1-Th(4)-O(16)	64.39(17)
O(8)-Th(4)-O(16)	65.84(19)
O(8)#1-Th(4)-O(16)	65.84(19)
O(17)-Th(4)-O(16)	119.60(14)
O(17)#1-Th(4)-O(16)	119.60(14)
O(20)#1-Th(4)-Th(1)	31.20(14)
O(20)-Th(4)-Th(1)	80.38(15)
O(6)-Th(4)-Th(1)	108.44(18)
O(6)#1-Th(4)-Th(1)	107.17(17)
O(8)-Th(4)-Th(1)	69.23(19)
O(8)#1-Th(4)-Th(1)	159.06(19)
O(17)-Th(4)-Th(1)	38.19(12)
O(17)#1-Th(4)-Th(1)	94.98(14)
O(16)-Th(4)-Th(1)	135.043(10)
O(20)#1-Th(4)-Th(1)#1	80.38(15)
O(20)-Th(4)-Th(1)#1	31.20(14)
O(6)-Th(4)-Th(1)#1	107.17(17)
O(6)#1-Th(4)-Th(1)#1	108.44(18)
O(8)-Th(4)-Th(1)#1	159.06(19)
O(8)#1-Th(4)-Th(1)#1	69.23(19)
O(17)-Th(4)-Th(1)#1	94.98(14)
O(17)#1-Th(4)-Th(1)#1	38.19(12)
O(16)-Th(4)-Th(1)#1	135.043(9)
Th(1)-Th(4)-Th(1)#1	89.914(19)
O(20)#1-Th(4)-Th(3)#1	30.80(15)
O(20)-Th(4)-Th(3)#1	80.63(13)
O(6)-Th(4)-Th(3)#1	160.60(17)

O(6)#1-Th(4)-Th(3)#1	70.61(17)
O(8)-Th(4)-Th(3)#1	105.45(16)
O(8)#1-Th(4)-Th(3)#1	108.20(16)
O(17)-Th(4)-Th(3)#1	94.72(13)
O(17)#1-Th(4)-Th(3)#1	38.67(13)
O(16)-Th(4)-Th(3)#1	135.000(10)
Th(1)-Th(4)-Th(3)#1	59.879(14)
Th(1)#1-Th(4)-Th(3)#1	60.071(14)
O(2)-C(1)-O(1)	127.4(11)
O(2)-C(1)-C(2')	116.8(12)
O(1)-C(1)-C(2')	111.1(11)
O(2)-C(1)-C(2)	118.5(11)
O(1)-C(1)-C(2)	114.0(11)
C(2')-C(1)-C(2)	26.2(9)
O(3)-C(3)-O(4)	124.4(10)
O(3)-C(3)-C(4)	121.8(11)
O(4)-C(3)-C(4)	108.5(9)
N(2)-C(4)-C(3)	106.1(12)
O(5)-C(5)-O(6)	127.2(10)
O(5)-C(5)-C(6)	120.4(9)
O(6)-C(5)-C(6)	111.8(10)
N(3)-C(6)-C(5)	114.0(11)
O(8)-C(7)-O(7)	127.0(9)
O(8)-C(7)-C(8)	116.0(10)
O(7)-C(7)-C(8)	117.0(9)
N(4)-C(8)-C(7)	112.9(11)
O(10)-C(9)-O(13)#1	129.7(8)
O(10)-C(9)-C(10)	115.6(8)
O(13)#1-C(9)-C(10)	114.7(9)
N(5)-C(10)-C(9)	114.5(8)
O(11)-C(12)-O(12)	125.8(9)
O(11)-C(12)-C(11)	115.1(9)
O(12)-C(12)-C(11)	119.1(8)
O(11)-C(12)-C(11')	113.5(9)
O(12)-C(12)-C(11')	117.4(8)
C(11)-C(12)-C(11')	20.7(10)
C(1)-C(2)-N(1)	105.1(16)
C(12)-C(11)-N(6)	110.9(12)
C(1)-C(2')-N(1')	100.3(14)
N(6')-C(11')-C(12)	104.5(16)
C(1)-O(1)-Th(1)	135.3(7)
C(1)-O(2)-Th(2)	135.8(7)
C(3)-O(3)-Th(2)	139.6(7)
C(3)-O(4)-Th(3)	133.9(6)
C(5)-O(5)-Th(3)	136.4(6)
C(5)-O(6)-Th(4)	134.6(7)
C(7)-O(7)-Th(1)	130.8(6)
C(7)-O(8)-Th(4)	141.0(7)
C(9)-O(10)-Th(3)	135.7(5)
C(12)-O(11)-Th(1)	133.2(7)
C(12)-O(12)-Th(3)	137.5(5)
C(9)#1-O(13)-Th(1)	134.1(6)
Th(1)-O(17)-Th(3)	103.6(2)
Th(1)-O(17)-Th(4)	102.93(17)
Th(3)-O(17)-Th(4)	102.4(2)
Th(2)-O(18)-Th(3)	119.5(3)
Th(2)-O(18)-Th(1)	118.6(2)

Th(3)-O(18)-Th(1)	116.1(2)
Th(1)#1-O(19)-Th(2)	103.55(18)
Th(1)#1-O(19)-Th(3)	103.2(2)
Th(2)-O(19)-Th(3)	103.2(2)
Th(3)-O(20)-Th(4)	118.4(3)
Th(3)-O(20)-Th(1)#1	117.5(2)
Th(4)-O(20)-Th(1)#1	117.7(2)
O(23)-N(7)-O(22)	120.3(6)
O(23)-N(7)-O(21)	119.8(6)
O(22)-N(7)-O(21)	119.8(6)
O(24)-N(8)-O(26)	120.3(7)
O(24)-N(8)-O(25)	120.4(6)
O(26)-N(8)-O(25)	119.3(6)
O(29)-N(9)-O(27)	119.8(7)
O(29)-N(9)-O(28)	119.8(7)
O(27)-N(9)-O(28)	119.2(7)
O(33)-Cl(1)-O(30)	110.5(5)
O(33)-Cl(1)-O(32)	109.8(5)
O(30)-Cl(1)-O(32)	109.4(5)
O(33)-Cl(1)-O(31)	109.4(5)
O(30)-Cl(1)-O(31)	109.1(5)
O(32)-Cl(1)-O(31)	108.6(5)
O(37)-Cl(2)-O(36)	109.5(5)
O(37)-Cl(2)-O(34)	109.6(5)
O(36)-Cl(2)-O(34)	109.5(5)
O(37)-Cl(2)-O(35)	109.3(5)
O(36)-Cl(2)-O(35)	109.4(5)
O(34)-Cl(2)-O(35)	109.4(5)
O(40)-Cl(3)-O(38)	109.6(5)
O(40)-Cl(3)-O(41)	109.9(5)
O(38)-Cl(3)-O(41)	109.4(5)
O(40)-Cl(3)-O(39)	109.4(5)
O(38)-Cl(3)-O(39)	109.1(5)
O(41)-Cl(3)-O(39)	109.4(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+1/2

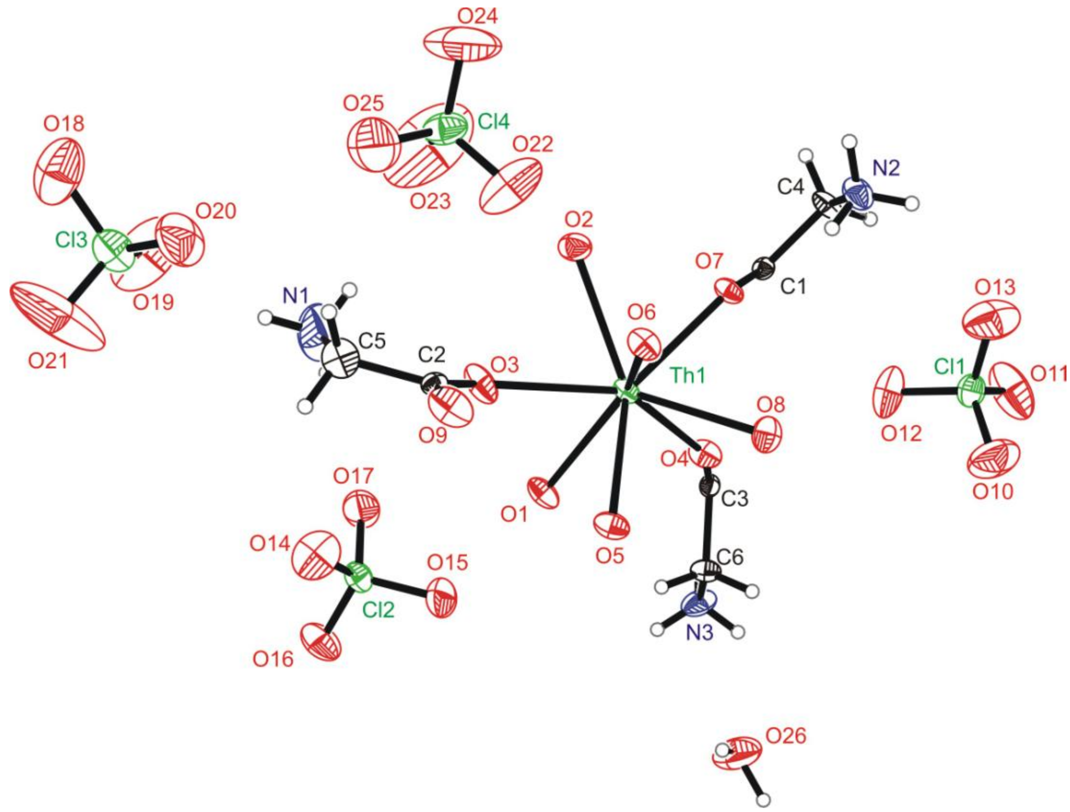

Figure S4: Ortep drawing of **2,** $[Th(H_2O)_3(Gly)_3]\cdot(ClO_4)_4H_2O$ with atom labeling used in Table S2.

Table S2: Bond lengths [Å] and angles [deg] of **2**.

Th(1)-O(6)	2.351(5)
Th(1)-O(4)	2.374(5)
Th(1)-O(9)#1	2.377(6)
Th(1)-O(7)	2.469(4)
Th(1)-O(5)	2.483(5)
Th(1)-O(3)	2.493(5)
Th(1)-O(2)	2.516(5)
Th(1)-O(8)	2.528(5)
Th(1)-O(1)	2.537(5)
N(1)-C(5)	1.363(13)
N(2)-C(4)	1.455(9)
N(3)-C(6)	1.464(9)
O(3)-C(2)	1.224(8)
O(4)-C(3)	1.242(7)
O(5)-C(3)#2	1.229(7)
O(6)-C(1)#2	1.243(7)
O(7)-C(1)	1.240(7)
O(9)-C(2)	1.213(8)

O(9)-Th(1)#2	2.377(6)
C(1)-O(6)#1	1.243(7)
C(1)-C(4)	1.522(9)
C(2)-C(5)	1.538(12)
C(3)-O(5)#1	1.229(7)
C(3)-C(6)	1.492(9)
Cl(1)-O(10)	1.384(8)
Cl(1)-O(12)	1.406(7)
Cl(1)-O(11)	1.427(8)
Cl(1)-O(13)	1.430(8)
Cl(2)-O(14)	1.405(8)
Cl(2)-O(16)	1.417(6)
Cl(2)-O(15)	1.431(6)
Cl(2)-O(17)	1.437(7)
Cl(3)-O(19)	1.351(10)
Cl(3)-O(21)	1.366(12)
Cl(3)-O(20)	1.380(8)
Cl(3)-O(18)	1.450(10)
Cl(4)-O(24)	1.328(10)
Cl(4)-O(23)	1.338(11)
Cl(4)-O(25)	1.379(11)
Cl(4)-O(22)	1.389(9)
O(6)-Th(1)-O(4)	136.42(18)
O(6)-Th(1)-O(9)#1	139.6(2)
O(4)-Th(1)-O(9)#1	75.6(2)
O(6)-Th(1)-O(7)	86.93(16)
O(4)-Th(1)-O(7)	75.10(17)
O(9)#1-Th(1)-O(7)	78.38(19)
O(6)-Th(1)-O(5)	80.09(17)
O(4)-Th(1)-O(5)	89.43(17)
O(9)#1-Th(1)-O(5)	132.67(19)
O(7)-Th(1)-O(5)	141.04(17)
O(6)-Th(1)-O(3)	77.88(17)
O(4)-Th(1)-O(3)	141.16(18)
O(9)#1-Th(1)-O(3)	86.1(2)
O(7)-Th(1)-O(3)	134.68(18)
O(5)-Th(1)-O(3)	78.12(18)
O(6)-Th(1)-O(2)	70.69(18)
O(4)-Th(1)-O(2)	132.35(18)
O(9)#1-Th(1)-O(2)	68.9(2)
O(7)-Th(1)-O(2)	67.59(16)
O(5)-Th(1)-O(2)	138.14(17)
O(3)-Th(1)-O(2)	67.09(19)
O(6)-Th(1)-O(8)	69.53(17)
O(4)-Th(1)-O(8)	67.06(18)
O(9)#1-Th(1)-O(8)	135.8(2)
O(7)-Th(1)-O(8)	70.07(17)
O(5)-Th(1)-O(8)	70.97(18)
O(3)-Th(1)-O(8)	138.03(18)
O(2)-Th(1)-O(8)	122.19(19)
O(6)-Th(1)-O(1)	136.34(17)
O(4)-Th(1)-O(1)	71.26(18)
O(9)#1-Th(1)-O(1)	67.58(19)
O(7)-Th(1)-O(1)	136.73(15)
O(5)-Th(1)-O(1)	65.09(16)
O(3)-Th(1)-O(1)	70.12(18)

O(2)-Th(1)-O(1)	119.55(17)
O(8)-Th(1)-O(1)	118.23(18)
C(2)-O(3)-Th(1)	142.6(5)
C(3)-O(4)-Th(1)	150.4(5)
C(3)#2-O(5)-Th(1)	145.4(4)
C(1)#2-O(6)-Th(1)	176.1(5)
C(1)-O(7)-Th(1)	141.0(4)
C(2)-O(9)-Th(1)#2	174.3(6)
O(7)-C(1)-O(6)#1	126.4(6)
O(7)-C(1)-C(4)	117.9(6)
O(6)#1-C(1)-C(4)	115.6(6)
O(9)-C(2)-O(3)	127.6(7)
O(9)-C(2)-C(5)	107.9(7)
O(3)-C(2)-C(5)	124.5(6)
O(5)#1-C(3)-O(4)	125.8(6)
O(5)#1-C(3)-C(6)	119.7(6)
O(4)-C(3)-C(6)	114.5(6)
N(2)-C(4)-C(1)	112.2(6)
N(1)-C(5)-C(2)	113.2(9)
N(3)-C(6)-C(3)	114.1(6)
O(10)-Cl(1)-O(12)	110.3(6)
O(10)-Cl(1)-O(11)	108.6(6)
O(12)-Cl(1)-O(11)	107.6(5)
O(10)-Cl(1)-O(13)	108.7(5)
O(12)-Cl(1)-O(13)	109.9(5)
O(11)-Cl(1)-O(13)	111.7(6)
O(14)-Cl(2)-O(16)	112.0(5)
O(14)-Cl(2)-O(15)	108.2(5)
O(16)-Cl(2)-O(15)	110.2(5)
O(14)-Cl(2)-O(17)	109.3(5)
O(16)-Cl(2)-O(17)	109.3(5)
O(15)-Cl(2)-O(17)	107.8(4)
O(19)-Cl(3)-O(21)	118.2(11)
O(19)-Cl(3)-O(20)	112.4(8)
O(21)-Cl(3)-O(20)	109.2(7)
O(19)-Cl(3)-O(18)	105.2(7)
O(21)-Cl(3)-O(18)	104.6(10)
O(20)-Cl(3)-O(18)	106.3(6)
O(24)-Cl(4)-O(23)	110.6(11)
O(24)-Cl(4)-O(25)	104.9(8)
O(23)-Cl(4)-O(25)	112.9(12)
O(24)-Cl(4)-O(22)	115.1(9)
O(23)-Cl(4)-O(22)	107.2(8)
O(25)-Cl(4)-O(22)	106.1(7)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z

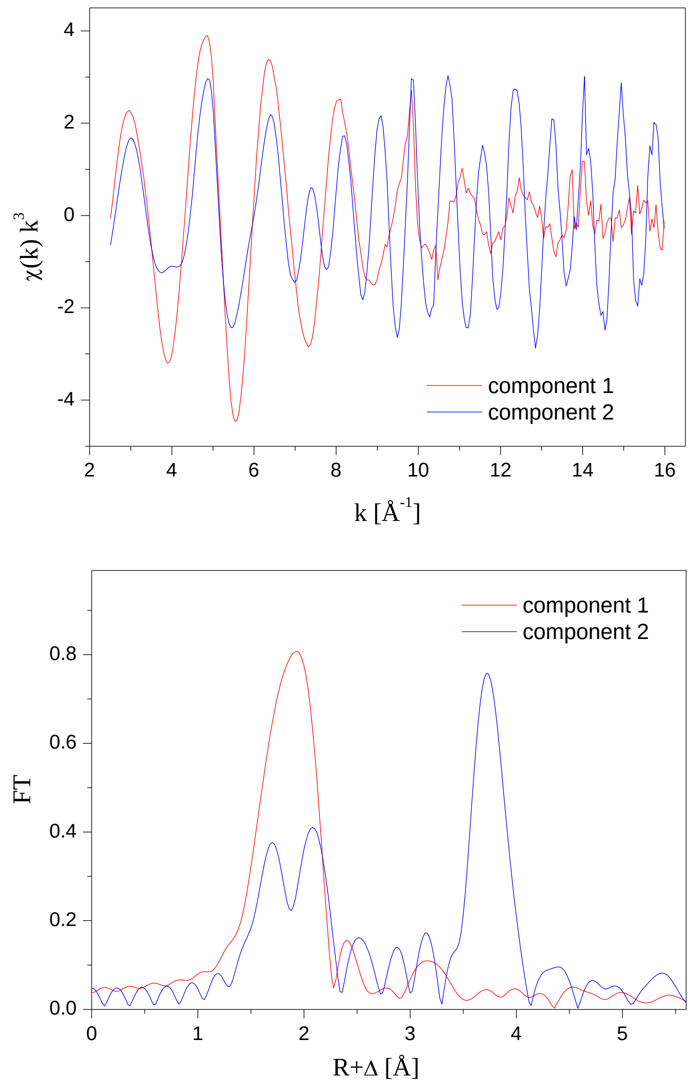

Figure S5. All spectra (13 solutions, and the solid compound) can be reproduced by 2 spectral components in the principal component analysis (PCA). The two limiting components are shown here: EXAFS spectra (top) and the corresponding Fourier transforms (bottom). **Component 1** represents the summary over all mononuclear species, **component 2** represents the hexanuclear complex. The analysis was performed with the program ITFA (A. Rossberg, T. Reich, G. Bernhard, Anal. Bioanal. Chem. **2003**, 376, 631-638.)

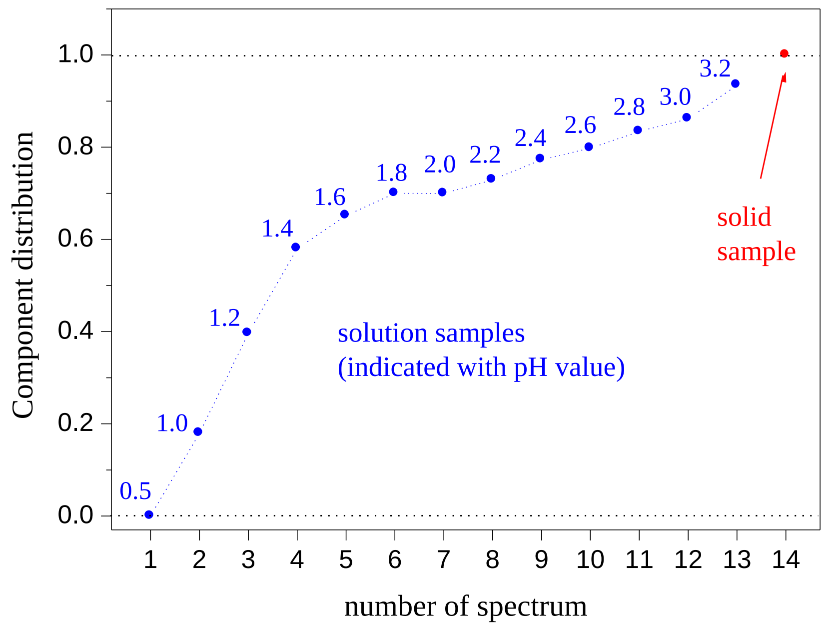

Figure S6. The species distribution of **component 2**. The extracted component distribution including the solid sample. Note the very close similarity with Figure 3 of the manuscript. There, the distribution function was extracted only by the intensity of the Th peak.