

Supporting materials

Carbonate and phosphite encaged in the frameworks constructed by square lanthanum aminopolycarboxylates and sodium chlorides

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Figure and Table Options

Figure S1. 2D layered structure of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1) viewed along c axis.

Figure S2. 2D layered structure of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{CO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (2) viewed along c axis.

Figure S3. Schematic descriptions of the equivalent topology frameworks in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1) and $\text{Na}_{12n}[\text{La}(\text{edta})(\text{CO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (2). Color codes: teal for La units, violet for Na units.

Figure S4. (a) Two sodium cations in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1). Symmetry codes: a ($x, 1\frac{1}{2} - y, 1 - z$), b ($\frac{1}{2} + x, -\frac{1}{2} + y, z$), c ($\frac{1}{2} + x, 1 - y, 1 - z$); (b) The plane with sodium chlorides in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1). Symmetry codes: a ($x, 1\frac{1}{2} - y, 1 - z$), b ($\frac{1}{2} + x, -\frac{1}{2} + y, z$), d ($1 - x, \frac{1}{2} + y, 1 - z$).

Figure S5. The site of sodium chloride in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1). Symmetry codes: a ($x, 1\frac{1}{2} - y, 1 - z$), b ($1 - x, 2 - y, 1 - z$), c ($1 - x, \frac{1}{2} + y, z$).

Figure S6. 2D layered structure of $\text{K}_{12n}[\text{La}(\text{cdta})(\text{CO}_3)]_{4n} 35\text{H}_2\text{O}$ (3) viewed along c axis.

Figure S7. Potassium atoms in $\text{K}_{12n}[\text{La}(\text{cdta})(\text{CO}_3)]_{4n} 35\text{H}_2\text{O}$ (3). Symmetry codes: a ($1 - x, y, \frac{1}{2} - z$).

Figure S8. Potassium atoms in $\text{K}_{12n}[\text{La}(\text{cdta})(\text{CO}_3)]_{4n} 35\text{H}_2\text{O}$ (3). Symmetry codes: a ($1 - x, y, \frac{1}{2} - z$), b ($1 - x, 1 + y, \frac{1}{2} - z$), c ($x, 1 + y, z$), d ($\frac{1}{2} - x, -\frac{1}{2} - y, \frac{1}{2} - z$), e ($\frac{1}{2} + x, \frac{1}{2} + y, z$), f ($\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$), g ($\frac{1}{2} + x, -\frac{1}{2} + y, z$).

Figure S9. TG-DTG curves of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1).

Figure S10. TG-DTG curves of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{CO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (2).

Figure S11. TG-DTG curves of $\text{K}_{12n}[\text{La}(\text{cdta})(\text{CO}_3)]_{4n} 35\text{H}_2\text{O}$ (3).

Figure S12. IR spectra of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1), $\text{Na}_{12n}[\text{La}(\text{edta})$

(CO₃)_{4n} 8nNaCl 4nH₂O (2) and K_{12n}[La(cdta)(CO₃)_{4n} 35nH₂O (3).

Table S1. Selected bond distances (Å) and angles (°) for Na_{12n}[La(edta)(HPO₃)_{4n} 8nNaCl 4nH₂O (1).

Table S2. Selected bond distances (Å) and angles (°) for Na_{12n}[La(edta)(CO₃)_{4n} 8nNaCl 4nH₂O (2).

Table S3. Selected bond distances (Å) and angles (°) for K_{12n}[La(cdta)(CO₃)_{4n} 35nH₂O (3).

Table S4. Comparisons of selected bond distances (Å) for **1** ~ **77**.

Table S5. Solid ¹³C NMR data for K_{12n}[La(cdta)(CO₃)_{4n} 35nH₂O (3).

Table S6. Crystal data and structural refinements for **1** ~ **3**.

Figure S1. 2D layered structure of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (**1**) viewed along *c* axis.

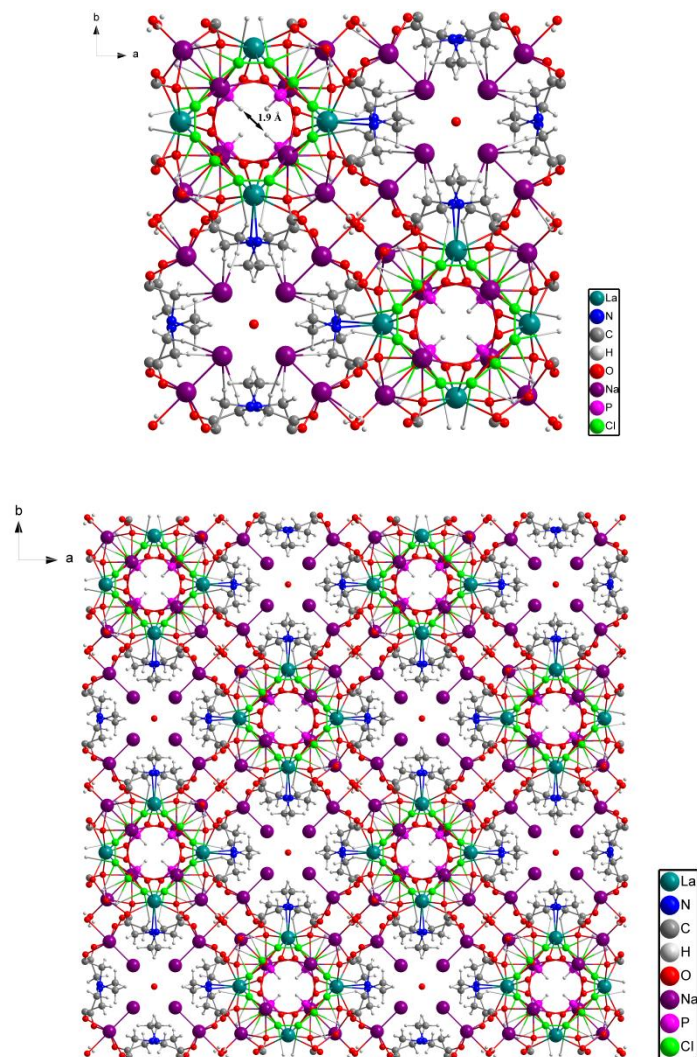


Figure S2. 2D layered structure of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{CO}_3)]_{4n} \cdot 8n\text{NaCl} \cdot 4n\text{H}_2\text{O}$ (2) viewed along c axis.

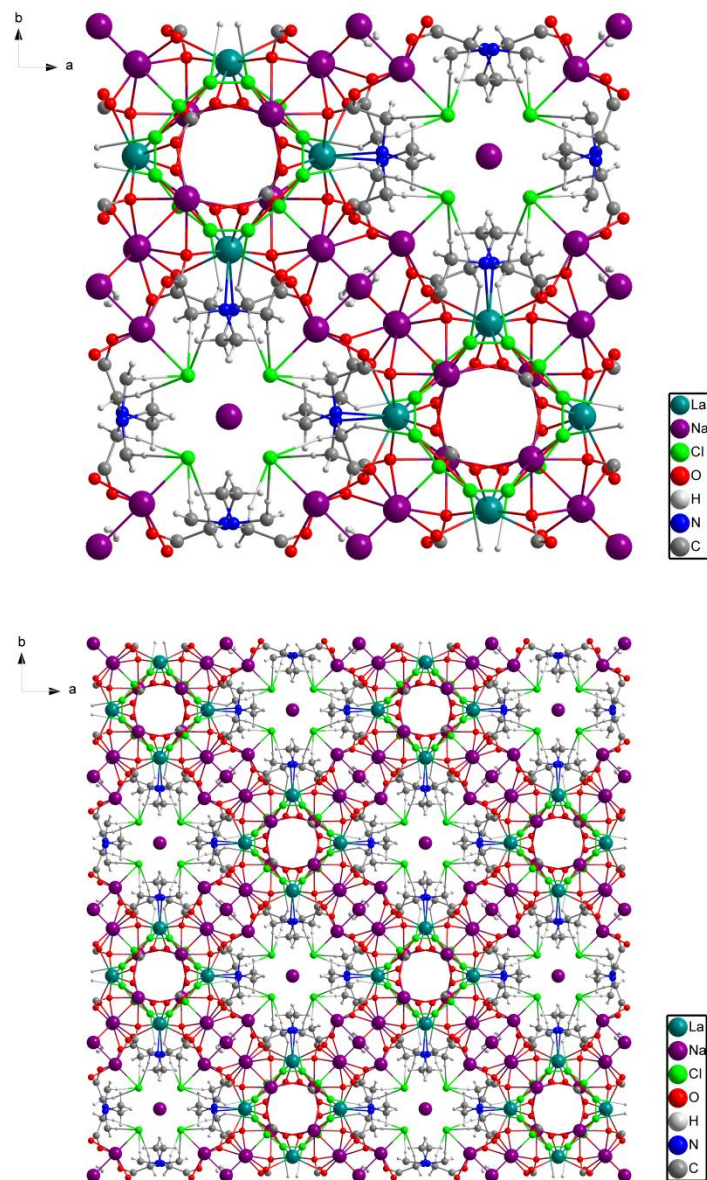


Figure S3. Schematic descriptions of the equivalent topology frameworks in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1) and $\text{Na}_{12n}[\text{La}(\text{edta})(\text{CO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (2). Color codes: teal for La units, violet for Na units.

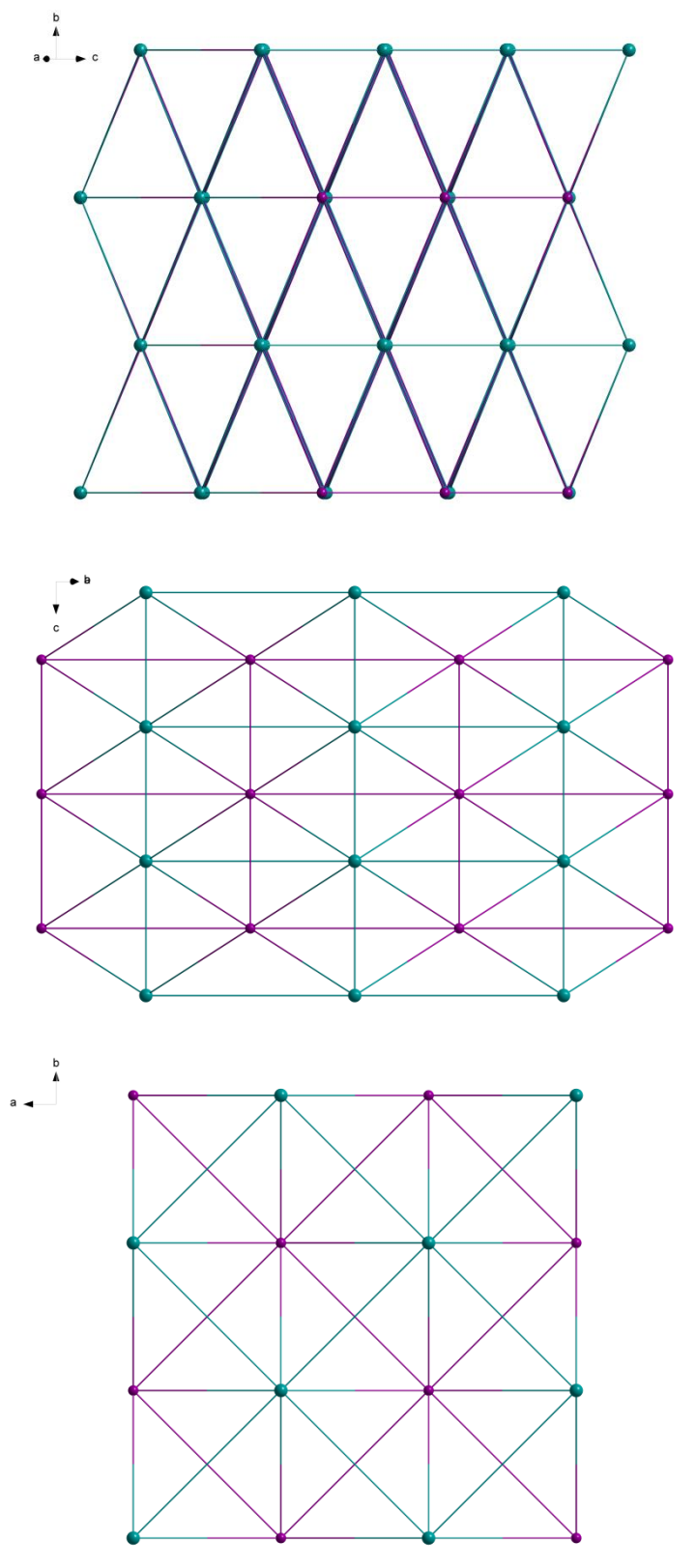


Figure S4. (a) Two sodium cations in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (**1**). Symmetry codes: *a* ($x, 1\frac{1}{2} - y, 1 - z$), *b* ($\frac{1}{2} + x, -\frac{1}{2} + y, z$), *c* ($\frac{1}{2} + x, 1 - y, 1 - z$); (b) The plane with sodium chlorides in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (**1**). Symmetry codes: *a* ($x, 1\frac{1}{2} - y, 1 - z$), *b* ($\frac{1}{2} + x, -\frac{1}{2} + y, z$), *d* ($1 - x, \frac{1}{2} + y, 1 - z$).

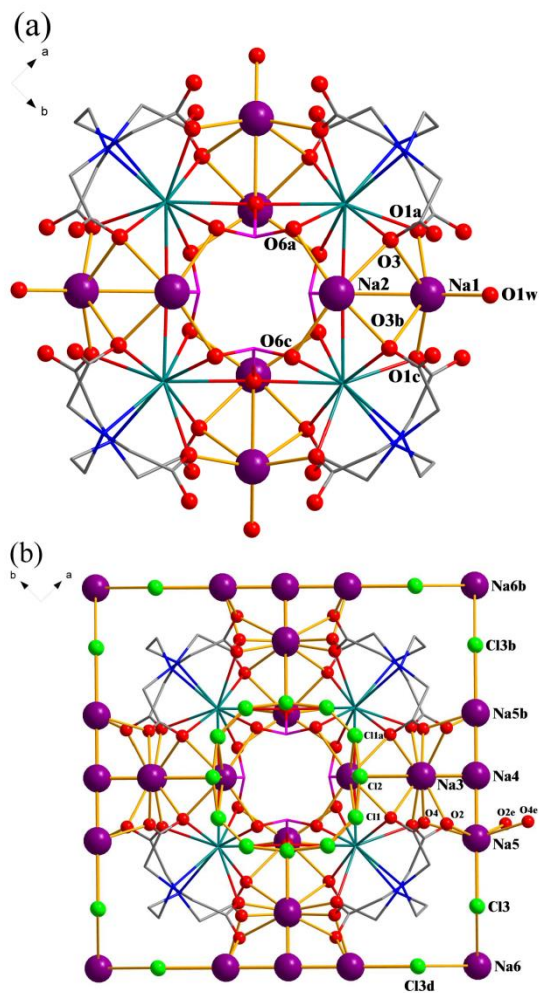


Figure S5. The site of sodium chloride in $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)_4]_{4n} \cdot 8n\text{NaCl} \cdot 4n\text{H}_2\text{O}$ (1). Symmetry codes: a ($x, 1\frac{1}{2} - y, 1 - z$), b ($1 - x, 2 - y, 1 - z$), c ($1 - x, \frac{1}{2} + y, z$).

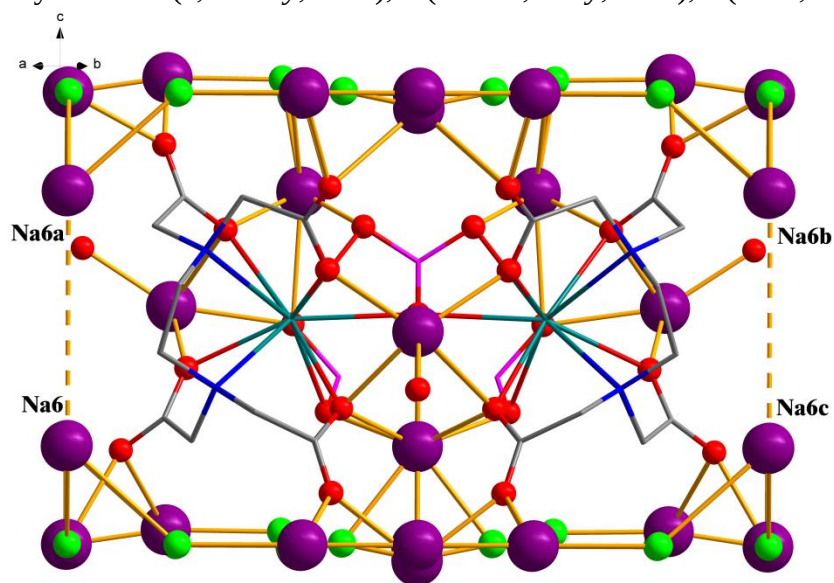


Figure S6. 2D layered structure of $\text{K}_{12n}[\text{La}(\text{cdta})(\text{CO}_3)]_{4n} \cdot 35n\text{H}_2\text{O}$ (**3**) viewed along c axis.

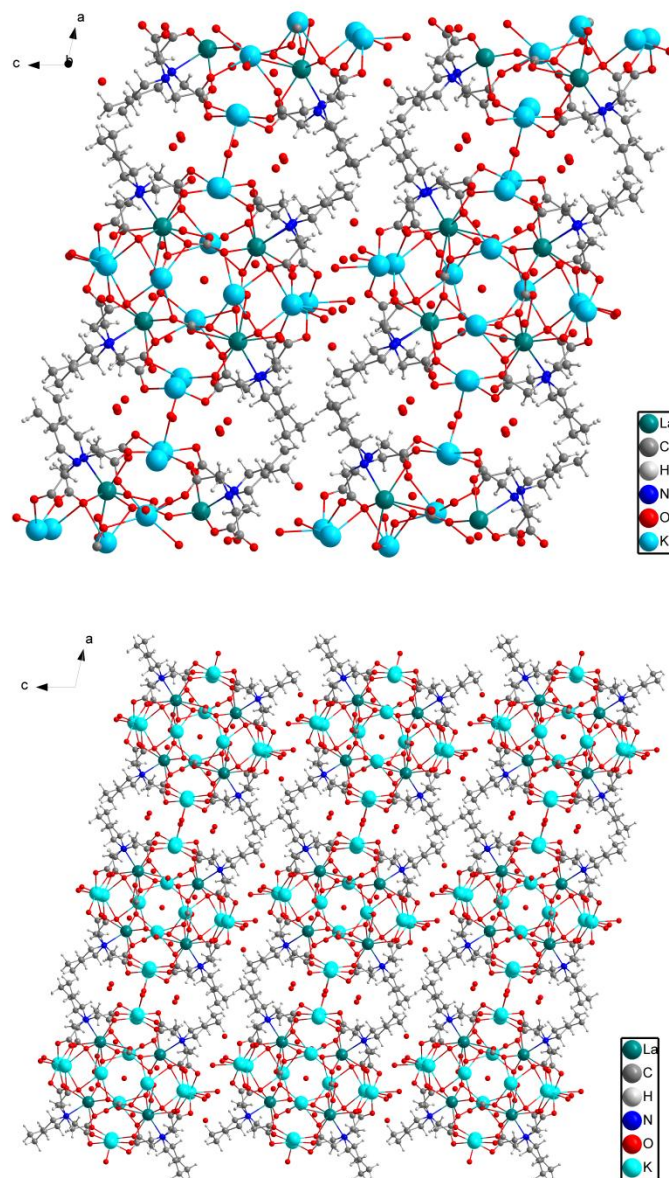


Figure S7. Potassium atoms in $K_{12n}[La(cdta)(CO_3)]_{4n} \cdot 35H_2O$ (**3**). Symmetry codes: *a* $(1 - x, y, \frac{1}{2} - z)$.

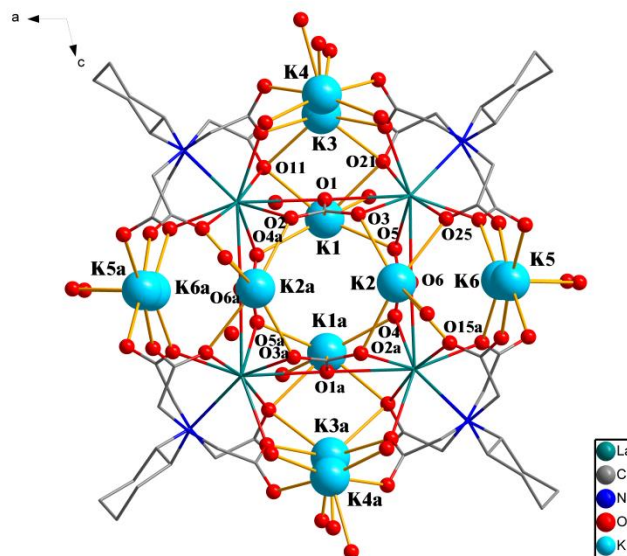


Figure S8. Potassium atoms in $K_{12n}[La(cdta)(CO_3)]_{4n} \cdot 35H_2O$ (**3**). Symmetry codes: *a* $(1 - x, y, \frac{1}{2} - z)$, *b* $(1 - x, 1 + y, \frac{1}{2} - z)$, *c* $(x, 1 + y, z)$, *d* $(\frac{1}{2} - x, -\frac{1}{2} - y, \frac{1}{2} - z)$, *e* $(\frac{1}{2} + x, \frac{1}{2} + y, z)$, *f* $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z)$, *g* $(\frac{1}{2} + x, -\frac{1}{2} + y, z)$.

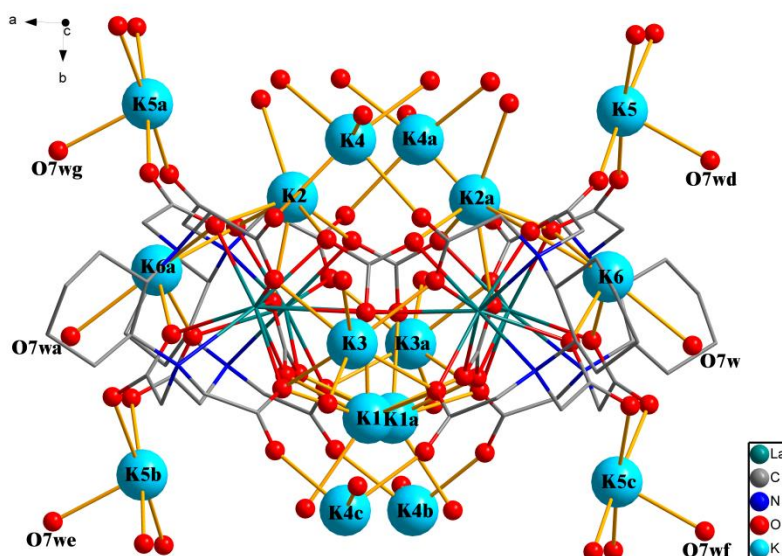


Figure S9. TG–DTG curves of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (1).

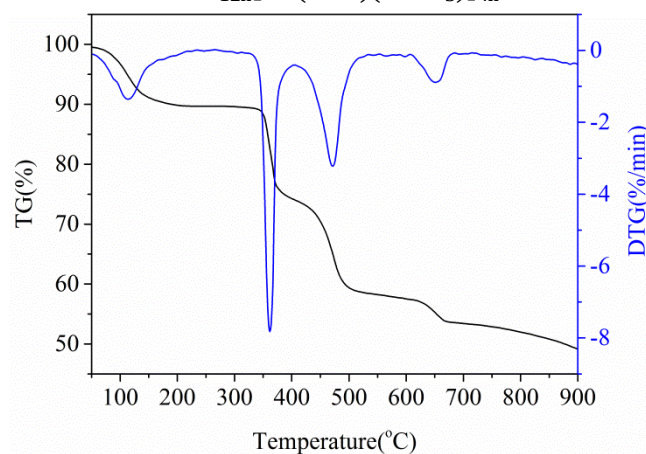


Figure S10. TG–DTG curves of $\text{Na}_{12n}[\text{La}(\text{edta})(\text{CO}_3)]_{4n} 8n\text{NaCl} 4n\text{H}_2\text{O}$ (2).

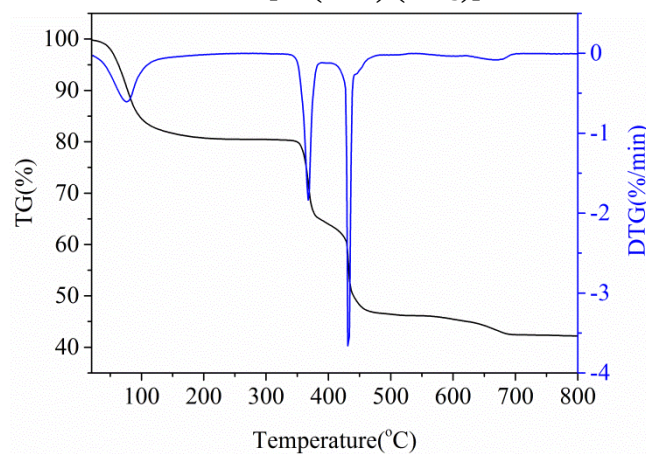


Figure S11. TG–DTG curves of $\text{K}_{12}\text{n}[\text{La}(\text{cdta})(\text{CO}_3)]_{4\text{n}} \cdot 35\text{nH}_2\text{O}$ (**3**).

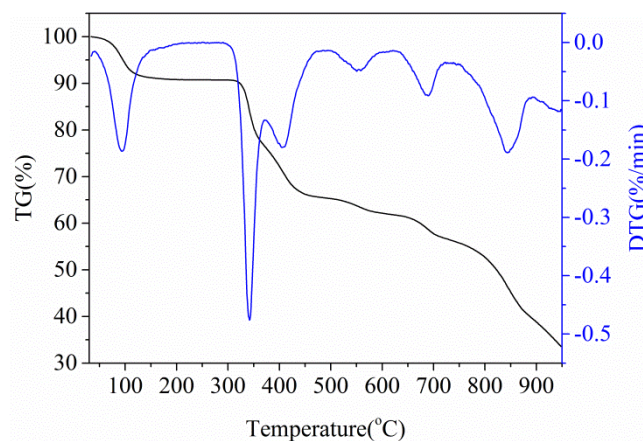


Figure S12. IR spectra of $\text{Na}_{12}\text{n}[\text{La}(\text{edta})(\text{HPO}_3)]_{4\text{n}} \cdot 8\text{nNaCl} \cdot 4\text{nH}_2\text{O}$ (**1**), $\text{Na}_{12}\text{n}[\text{La}(\text{edta})(\text{CO}_3)]_{4\text{n}} \cdot 8\text{nNaCl} \cdot 4\text{nH}_2\text{O}$ (**2**) and $\text{K}_{12}\text{n}[\text{La}(\text{cdta})(\text{CO}_3)]_{4\text{n}} \cdot 35\text{nH}_2\text{O}$ (**3**).

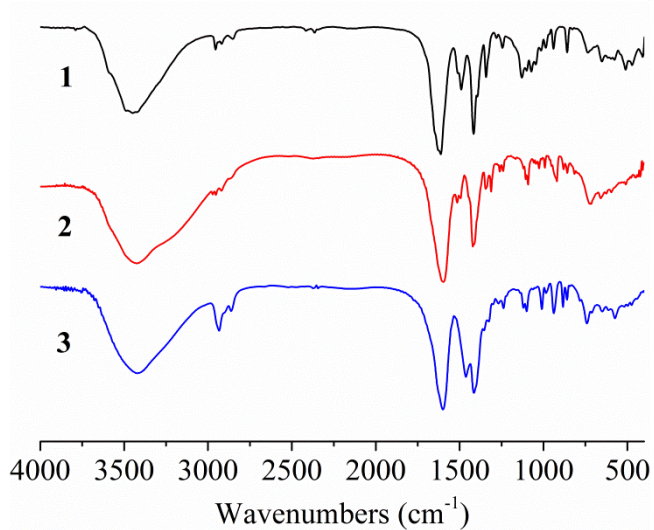


Table S1. Selected bond distances (Å) and angles (°) for Na_{12n}[La(edta)(HPO₃)]_{4n} 8nNaCl 4nH₂O (1).

La(1)–O(1)	2.564(7)	La(1)–P(1)	3.13(1)
La(1)–O(1a)	2.564(7)	La(1)–P(1b)	3.13(1)
La(1)–O(3)	2.577(7)	La(1)–N(1)	2.821(8)
La(1)–O(3a)	2.577(7)	La(1)–N(1a)	2.822(8)
La(1)–O(5)	2.7014(9)	La(1c)–O(5)	2.7014(8)
La(1)–O(5b)	2.7014(9)	La(1c)–P(1)	3.13(1)
La(1)–O(6)	2.606(8)	La(1c)–P(2)	3.15(1)
La(1)–O(6a)	2.606(8)	La(1c)–Na(1)	3.711(5)
O(1)–La(1)–O(1a)	133.4(3)	P(1b)–La(1)–N(1a)	153.7(4)
O(1)–La(1)–O(3)	102.8(2)	N(1)–La(1)–N(1a)	62.5(3)
O(1)–La(1)–O(3a)	73.1(2)	La(1)–P(1)–La(1c)	118.9(7)
O(1a)–La(1)–O(3)	73.1(2)	O(5)–P(1)–La(1)	59.5(3)
O(1a)–La(1)–O(3a)	102.8(2)	O(5)–P(1)–La(1c)	59.5(3)
O(1)–La(1)–O(5)	150.8(4)	O(6)–P(1)–La(1)	55.4(5)
O(1)–La(1)–O(5b)	72.3(3)	O(6d)–P(1)–La(1)	150(1)
O(1a)–La(1)–O(5)	72.3(3)	O(6)–P(1)–La(1c)	150(1)
O(1a)–La(1)–O(5b)	150.8(4)	O(6d)–P(1)–La(1c)	55.4(5)
O(1)–La(1)–O(6)	136.4(2)	P(2)–P(1)–La(1)	83(1)
O(1)–La(1)–O(6a)	76.7(3)	P(2)–P(1)–La(1c)	83(1)
O(1a)–La(1)–O(6)	76.7(3)	La(1)–P(1)–Na(2b)	72.2(1)
O(1a)–La(1)–O(6a)	136.4(2)	La(1)–P(1)–Na(2c)	167.5(6)
O(1)–La(1)–P(1)	143.4(4)	La(1c)–P(1)–Na(2b)	167.5(6)
O(1)–La(1)–P(1b)	82.1(4)	La(1c)–P(1)–Na(2c)	72.2(1)
O(1a)–La(1)–P(1)	82.1(4)	La(1)–P(2)–La(1c)	117.6(8)
O(1a)–La(1)–P(1b)	143.4(4)	O(5)–P(2)–La(1)	58.8(4)
O(1)–La(1)–N(1)	60.0(2)	O(5)–P(2)–La(1c)	58.8(4)
O(1)–La(1)–N(1a)	79.8(2)	O(6)–P(2)–La(1)	54.2(7)
O(1a)–La(1)–N(1)	79.8(2)	O(6d)–P(2)–La(1)	153(2)
O(1a)–La(1)–N(1a)	60.0(2)	O(6)–P(2)–La(1c)	153(2)
O(3)–La(1)–O(3a)	170.1(3)	O(6d)–P(2)–La(1c)	54.2(7)
O(3)–La(1)–O(5)	67.9(3)	P(1)–P(2)–La(1)	80(1)
O(3)–La(1)–O(5b)	120.0(3)	P(1)–P(2)–La(1c)	80(1)
O(3a)–La(1)–O(5)	120.0(3)	La(1)–P(2)–Na(1)	70.2(4)
O(3a)–La(1)–O(5b)	67.9(3)	La(1c)–P(2)–Na(1)	70.2(4)
O(3)–La(1)–O(6)	117.8(2)	La(1)–Na(1)–La(1c)	93.3(2)
O(3)–La(1)–O(6a)	69.0(2)	O(1a)–Na(1)–La(1)	43.2(2)
O(3a)–La(1)–O(6)	69.0(2)	O(1c)–Na(1)–La(1)	117.6(3)
O(3a)–La(1)–O(6a)	117.8(2)	O(1a)–Na(1)–La(1c)	117.6(3)
O(3)–La(1)–P(1)	95.9(4)	O(1c)–Na(1)–La(1c)	43.2(2)
O(3)–La(1)–P(1b)	92.4(4)	O(3)–Na(1)–La(1)	43.9(2)
O(3a)–La(1)–P(1)	92.4(4)	O(3d)–Na(1)–La(1)	101.5(3)

O(3a)–La(1)–P(1b)	95.9(4)	O(3)–Na(1)–La(1c)	101.5(3)
O(3)–La(1)–N(1)	60.6(2)	O(3d)–Na(1)–La(1c)	43.9(2)
O(3)–La(1)–N(1a)	110.1(2)	O(5)–Na(1)–La(1)	46.70(8)
O(3a)–La(1)–N(1)	110.1(2)	O(5)–Na(1)–La(1c)	46.70(8)
O(3a)–La(1)–N(1a)	60.6(2)	O(1w)–Na(1)–La(1)	127.5(2)
O(5b)–La(1)–O(5)	88.2(6)	O(1w)–Na(1)–La(1c)	127.5(2)
O(6)–La(1)–O(5)	51.4(3)	P(2)–Na(1)–La(1)	53.1(3)
O(6a)–La(1)–O(5)	74.1(4)	P(2)–Na(1)–La(1c)	53.1(3)
O(6)–La(1)–O(5b)	74.1(4)	Na(2)–Na(1)–La(1)	62.3(1)
O(6a)–La(1)–O(5b)	51.4(3)	Na(2)–Na(1)–La(1c)	62.3(1)
O(5)–La(1)–P(1)	28.1(4)	C(1)–O(1)–La(1)	123.0(6)
O(5)–La(1)–P(1b)	71.1(5)	Na(1b)–O(1)–La(1)	98.1(3)
O(5b)–La(1)–P(1)	71.1(5)	C(3)–O(3)–La(1)	126.8(6)
O(5b)–La(1)–P(1b)	28.1(4)	Na(1)–O(3)–La(1)	92.1(3)
O(5)–La(1)–N(1)	126.5(3)	Na(2)–O(3)–La(1)	99.6(3)
O(5)–La(1)–N(1a)	129.3(4)	La(1)–O(5)–La(1c)	174.9(6)
O(5b)–La(1)–N(1)	129.3(4)	P(1)–O(5)–La(1)	92.4(3)
O(5b)–La(1)–N(1a)	126.5(3)	P(1)–O(5)–La(1c)	92.4(3)
O(6a)–La(1)–O(6)	102.6(4)	P(2)–O(5)–La(1)	92.4(3)
O(6)–La(1)–P(1)	26.3(4)	P(2)–O(5)–La(1c)	92.4(3)
O(6)–La(1)–P(1b)	81.2(4)	Na(1)–O(5)–La(1)	88.7(3)
O(6a)–La(1)–P(1)	81.2(4)	Na(1)–O(5)–La(1c)	88.7(3)
O(6a)–La(1)–P(1b)	26.3(4)	La(1)–O(5)–Na(2)	87.7(3)
O(6)–La(1)–N(1)	155.5(3)	La(1c)–O(5)–Na(2)	87.7(3)
O(6)–La(1)–N(1a)	99.1(3)	P(1)–O(6)–La(1)	98.3(8)
O(6a)–La(1)–N(1)	99.1(3)	P(2)–O(6)–La(1)	101(1)
O(6a)–La(1)–N(1a)	155.5(3)	Na(2b)–O(6)–La(1)	98.1(3)
P(1)–La(1)–P(1b)	65.8(7)	C(2)–N(1)–La(1)	103.8(6)
P(1)–La(1)–N(1)	153.7(4)	C(4)–N(1)–La(1)	109.8(6)
P(1)–La(1)–N(1a)	122.7(4)	C(5)–N(1)–La(1)	115.2(6)
P(1b)–La(1)–N(1)	122.6(4)		

Symmetry codes: (a) $x, 1\frac{1}{2} - y, 1 - z$; (b) $-\frac{1}{2} + y, 1 - x, 1 - z$; (c) $1 - y, \frac{1}{2} + x, 1 - z$; (d) $-\frac{1}{2} + y, \frac{1}{2} + x, z$.

Table S2. Selected bond distances (Å) and angles (°) for Na_{12n}[La(edta)(CO₃)]_{4n} 8nNaCl 4nH₂O (2).

La(1)–O(1)	2.571(6)	La(1)–C(6)	3.046(6)
La(1)–O(1a)	2.570(6)	La(1)–C(6b)	3.046(6)
La(1)–O(3)	2.574(6)	La(1)–N(1)	2.829(6)
La(1)–O(3a)	2.574(6)	La(1)–N(1a)	2.829(6)
La(1)–O(5)	2.6735(7)	La(1b)–Na(1)	3.692(4)
La(1)–O(5b)	2.6735(7)	La(1c)–Na(2)	3.806(4)
La(1)–O(6)	2.586(6)	La(1c)–O(5)	2.6735(7)
La(1)–O(6a)	2.586(6)	La(1c)–C(6)	3.046(6)
O(1)–La(1)–O(1a)	170.1(3)	C(6b)–La(1)–N(1)	115.6(3)
O(1)–La(1)–O(3)	102.8(2)	C(6b)–La(1)–N(1a)	146.8(3)
O(1)–La(1)–O(3a)	73.1(2)	N(1)–La(1)–N(1a)	62.4(3)
O(1a)–La(1)–O(3)	73.1(2)	La(1)–Na(1)–La(1b)	92.6(1)
O(1a)–La(1)–O(3a)	102.8(2)	Na(2b)–Na(1)–La(1)	61.9(1)
O(1)–La(1)–O(5)	68.7(2)	Na(2b)–Na(1)–La(1b)	61.9(1)
O(1)–La(1)–O(5b)	119.1(2)	O(1a)–Na(1)–La(1)	44.1(1)
O(1a)–La(1)–O(5)	119.1(2)	O(1a)–Na(1)–La(1b)	100.7(2)
O(1a)–La(1)–O(5b)	68.7(2)	O(1b)–Na(1)–La(1)	100.7(2)
O(1)–La(1)–O(6)	117.2(2)	O(1b)–Na(1)–La(1b)	44.1(1)
O(1)–La(1)–O(6a)	69.7(2)	O(3)–Na(1)–La(1)	43.7(2)
O(1a)–La(1)–O(6)	69.7(2)	O(3)–Na(1)–La(1b)	117.4(2)
O(1a)–La(1)–O(6a)	117.2(2)	O(3d)–Na(1)–La(1)	117.4(2)
O(1)–La(1)–C(6)	93.4(2)	O(3d)–Na(1)–La(1b)	43.7(2)
O(1)–La(1)–C(6b)	93.9(2)	O(5b)–Na(1)–La(1)	46.37(7)
O(1a)–La(1)–C(6)	93.9(2)	O(5b)–Na(1)–La(1b)	46.38(7)
O(1a)–La(1)–C(6b)	93.4(2)	O(1w)–Na(1)–La(1)	128.1(2)
O(1)–La(1)–N(1)	60.6(2)	O(1w)–Na(1)–La(1b)	128.1(2)
O(1)–La(1)–N(1a)	110.1(2)	La(1)–Na(2)–La(1c)	89.1(1)
O(1a)–La(1)–N(1)	110.1(2)	Na(1c)–Na(2)–La(1)	58.83(9)
O(1a)–La(1)–N(1a)	60.6(2)	Na(1c)–Na(2)–La(1c)	58.83(9)
O(3)–La(1)–O(3a)	132.9(3)	Na(3e)–Na(2)–La(1)	113.8(2)
O(3)–La(1)–O(5)	151.7(2)	Na(3e)–Na(2)–La(1c)	113.8(2)
O(3)–La(1)–O(5b)	72.1(2)	C(11)–Na(2)–La(1)	133.2(1)
O(3a)–La(1)–O(5)	72.1(2)	C(11)–Na(2)–La(1c)	133.2(1)
O(3a)–La(1)–O(5b)	151.7(2)	C(12)–Na(2)–La(1)	96.8(4)
O(3)–La(1)–O(6)	136.9(2)	C(12)–Na(2)–La(1c)	168.9(4)
O(3)–La(1)–O(6a)	77.1(2)	C(12f)–Na(2)–La(1)	168.9(4)
O(3a)–La(1)–O(6)	77.1(2)	C(12f)–Na(2)–La(1c)	96.8(4)
O(3a)–La(1)–O(6a)	136.9(2)	O(1)–Na(2)–La(1)	41.8(2)
O(3)–La(1)–C(6)	152.6(3)	O(1)–Na(2)–La(1c)	100.4(2)
O(3)–La(1)–C(6b)	72.8(3)	O(1f)–Na(2)–La(1)	100.4(2)
O(3a)–La(1)–C(6)	72.8(3)	O(1f)–Na(2)–La(1c)	41.8(2)

O(3a)–La(1)–C(6b)	152.6(3)	O(5)–Na(2)–La(1)	44.54(6)
O(3)–La(1)–N(1)	59.9(2)	O(5)–Na(2)–La(1c)	44.54(6)
O(3)–La(1)–N(1a)	79.5(2)	O(6a)–Na(2)–La(1)	42.2(2)
O(3a)–La(1)–N(1)	79.5(2)	O(6a)–Na(2)–La(1c)	110.9(2)
O(3a)–La(1)–N(1a)	59.9(2)	O(6c)–Na(2)–La(1)	110.9(2)
O(5)–La(1)–O(5b)	88.2(4)	O(6c)–Na(2)–La(1c)	42.2(2)
O(5)–La(1)–O(6)	49.8(2)	C(3)–O(1)–La(1)	126.5(5)
O(5)–La(1)–O(6a)	74.7(2)	Na(1c)–O(1)–La(1)	91.9(2)
O(5b)–La(1)–O(6)	74.7(2)	Na(2)–O(1)–La(1)	99.2(2)
O(5b)–La(1)–O(6a)	49.8(2)	C(1)–O(3)–La(1)	123.0(5)
O(5)–La(1)–C(6)	25.4(3)	Na(1)–O(3)–La(1)	97.8(3)
O(5)–La(1)–C(6b)	80.7(3)	La(1)–O(5)–La(1c)	173.2(4)
O(5b)–La(1)–C(6)	80.7(3)	C(6)–O(5)–La(1)	93.4(2)
O(5b)–La(1)–C(6b)	25.4(3)	C(6)–O(5)–La(1c)	93.4(2)
O(5)–La(1)–N(1)	127.0(2)	Na(1c)–O(5)–La(1c)	88.5(2)
O(5)–La(1)–N(1a)	128.8(2)	Na(1c)–O(5)–La(1)	88.5(2)
O(5b)–La(1)–N(1)	128.8(2)	Na(2)–O(5)–La(1)	86.9(2)
O(5b)–La(1)–N(1a)	127.0(2)	Na(2)–O(5)–La(1c)	86.9(2)
O(6)–La(1)–O(6a)	101.4(3)	C(6)–O(6)–La(1)	98.5(6)
O(6)–La(1)–C(6)	24.4(2)	Na(2b)–O(6)–La(1)	98.6(2)
O(6)–La(1)–C(6b)	88.4(3)	La(1)–C(6)–La(1c)	122.4(4)
O(6a)–La(1)–C(6)	88.4(3)	O(5)–C(6)–La(1)	61.2(2)
O(6a)–La(1)–C(6b)	24.4(2)	O(5)–C(6)–La(1c)	61.2(2)
O(6)–La(1)–N(1)	155.8(2)	O(6)–C(6)–La(1)	57.1(4)
O(6)–La(1)–N(1a)	99.9(2)	O(6)–C(6)–La(1c)	178.5(9)
O(6a)–La(1)–N(1)	99.9(2)	O(6f)–C(6)–La(1)	178.5(9)
O(6a)–La(1)–N(1a)	155.8(2)	O(6f)–C(6)–La(1c)	57.1(4)
C(6)–La(1)–C(6b)	84.3(5)	C(2)–N(1)–La(1)	103.9(5)
C(6)–La(1)–N(1)	146.8(3)	C(4)–N(1)–La(1)	109.1(5)
C(6)–La(1)–N(1a)	115.6(3)	C(5)–N(1)–La(1)	114.9(5)

Symmetry codes: (a) $\frac{1}{2} - x, y, 1 - z$; (b) $1 - y, \frac{1}{2} + x, 1 - z$; (c) $-\frac{1}{2} + y, 1 - x, 1 - z$; (d) $1 - y, 1 - x, z$; (e) $\frac{1}{2} - y, x, z$; (f) $-\frac{1}{2} + y, \frac{1}{2} + x, z$.

Table S3. Selected bond distances (Å) and angles (°) for $K_{12n}[La(cdta)(CO_3)]_{4n} \cdot 35nH_2O$ (**3**).

La(1)–O(1)	2.914(7)	La(1a)–C(2)	3.11(1)
La(1)–O(2)	2.539(6)	La(2)–O(1)	2.845(7)
La(1)–O(4a)	2.515(7)	La(2)–O(3)	2.532(7)
La(1)–O(6a)	2.889(7)	La(2)–O(5)	2.532(7)
La(1)–O(11)	2.519(7)	La(2)–O(6)	2.880(7)
La(1)–O(13)	2.526(7)	La(2)–O(21)	2.530(7)
La(1)–O(15)	2.509(7)	La(2)–O(23)	2.528(6)
La(1)–O(17)	2.547(7)	La(2)–O(25)	2.501(6)
La(1)–C(1)	3.135(9)	La(2)–O(27)	2.543(7)
La(1)–C(2a)	3.11(1)	La(2)–C(1)	3.105(9)
La(1)–N(1)	2.870(7)	La(2)–C(2)	3.09(1)
La(1)–N(2)	2.875(7)	La(2)–N(3)	2.873(7)
La(1a)–O(4)	2.515(7)	La(2)–N(4)	2.912(8)
La(1a)–O(6)	2.889(7)	La(2a)–K(2)	4.060(3)
O(1)–La(1)–O(2)	47.5(2)	O(27)–La(2)–C(1)	75.2(2)
O(1)–La(1)–O(4a)	75.1(2)	O(27)–La(2)–C(2)	154.4(2)
O(1)–La(1)–O(6a)	89.5(2)	O(27)–La(2)–N(3)	78.1(2)
O(1)–La(1)–O(11)	67.1(2)	O(27)–La(2)–N(4)	59.5(2)
O(1)–La(1)–O(13)	152.5(2)	C(1)–La(2)–C(2)	82.8(3)
O(1)–La(1)–O(15)	119.9(2)	C(1)–La(2)–N(3)	146.7(2)
O(1)–La(1)–O(17)	71.0(2)	C(1)–La(2)–N(4)	118.6(2)
O(1)–La(1)–C(1)	24.2(2)	C(2)–La(2)–N(3)	116.6(2)
O(1)–La(1)–C(2a)	82.3(2)	C(2)–La(2)–N(4)	145.5(2)
O(1)–La(1)–N(1)	125.1(2)	N(3)–La(2)–N(4)	61.0(2)
O(1)–La(1)–N(2)	128.4(2)	La(1)–C(1)–La(2)	134.6(3)
O(2)–La(1)–O(4a)	97.5(2)	O(1)–C(1)–La(1)	68.3(5)
O(2)–La(1)–O(6a)	74.5(2)	O(2)–C(1)–La(1)	51.4(5)
O(2)–La(1)–O(11)	113.8(2)	O(3)–C(1)–La(1)	172.5(7)
O(2)–La(1)–O(13)	139.3(2)	La(1a)–C(2)–La(2)	136.8(4)
O(2)–La(1)–O(15)	72.6(2)	O(4)–C(2)–La(1a)	51.6(5)
O(2)–La(1)–O(17)	76.7(2)	O(5)–C(2)–La(1a)	169.6(8)
O(2)–La(1)–C(1)	23.3(2)	O(6)–C(2)–La(1a)	68.3(6)
O(2)–La(1)–C(2a)	86.3(2)	O(1)–C(1)–La(2)	66.4(5)
O(2)–La(1)–N(1)	155.3(2)	O(2)–C(1)–La(2)	174.0(7)
O(2)–La(1)–N(2)	103.0(2)	O(3)–C(1)–La(2)	52.3(5)
O(4a)–La(1)–O(6a)	47.7(2)	O(4)–C(2)–La(2)	171.6(8)
O(4a)–La(1)–O(11)	71.4(2)	O(5)–C(2)–La(2)	53.1(5)
O(4a)–La(1)–O(13)	77.4(2)	O(6)–C(2)–La(2)	68.6(6)
O(4a)–La(1)–O(15)	115.1(2)	C(11)–N(1)–La(1)	108.6(5)
O(4a)–La(1)–O(17)	138.5(2)	C(13)–N(1)–La(1)	100.9(5)
O(4a)–La(1)–C(1)	86.5(2)	C(19)–N(1)–La(1)	115.3(5)

O(4a)–La(1)–C(2a)	23.9(3)	C(15)–N(2)–La(1)	107.7(5)
O(4a)–La(1)–N(1)	102.7(2)	C(17)–N(2)–La(1)	101.0(5)
O(4a)–La(1)–N(2)	156.0(2)	C(20)–N(2)–La(1)	115.6(5)
O(6a)–La(1)–O(11)	118.8(2)	C(21)–N(3)–La(2)	108.5(5)
O(6a)–La(1)–O(13)	72.7(2)	C(23)–N(3)–La(2)	101.2(5)
O(6a)–La(1)–O(15)	68.5(2)	C(29)–N(3)–La(2)	116.2(5)
O(6a)–La(1)–O(17)	151.2(2)	C(25)–N(4)–La(2)	106.5(5)
O(6a)–La(1)–C(1)	81.5(2)	C(27)–N(4)–La(2)	100.5(5)
O(6a)–La(1)–C(2a)	23.7(2)	C(30)–N(4)–La(2)	116.0(5)
O(6a)–La(1)–N(1)	130.0(2)	La(1)–O(1)–La(2)	176.1(3)
O(6a)–La(1)–N(2)	127.0(2)	C(1)–O(1)–La(1)	87.6(5)
O(11)–La(1)–O(13)	102.9(2)	C(1)–O(1)–La(2)	89.2(5)
O(11)–La(1)–O(15)	170.9(2)	K(1)–O(1)–La(1)	91.2(2)
O(11)–La(1)–O(17)	73.7(2)	K(1)–O(1)–La(2)	92.7(2)
O(11)–La(1)–C(1)	90.8(2)	K(3)–O(1)–La(1)	89.9(2)
O(11)–La(1)–C(2a)	95.3(3)	K(3)–O(1)–La(2)	90.2(2)
O(11)–La(1)–N(1)	60.8(2)	C(1)–O(2)–La(1)	105.4(6)
O(11)–La(1)–N(2)	110.5(2)	K(2)–O(2)–La(1)	98.0(2)
O(13)–La(1)–O(15)	73.4(2)	C(1)–O(3)–La(2)	104.0(6)
O(13)–La(1)–O(17)	132.7(2)	K(2a)–O(3)–La(2)	98.6(2)
O(13)–La(1)–C(1)	154.1(2)	C(2)–O(4)–La(1a)	104.4(6)
O(13)–La(1)–C(2a)	73.0(2)	K(1a)–O(4)–La(1a)	99.9(3)
O(13)–La(1)–N(1)	60.5(2)	C(2)–O(5)–La(2)	102.7(7)
O(13)–La(1)–N(2)	78.9(2)	K(1)–O(5)–La(2)	100.5(2)
O(15)–La(1)–O(17)	102.5(2)	La(1a)–O(6)–La(2)	174.5(3)
O(15)–La(1)–C(1)	95.8(2)	C(2)–O(6)–La(1a)	87.9(6)
O(15)–La(1)–C(2a)	91.6(3)	C(2)–O(6)–La(2)	87.6(6)
O(15)–La(1)–N(1)	110.6(2)	K(2a)–O(6)–La(1a)	92.7(2)
O(15)–La(1)–N(2)	60.8(2)	K(2a)–O(6)–La(2)	92.8(2)
O(17)–La(1)–C(1)	72.1(2)	K(6)–O(6)–La(1a)	89.7(2)
O(17)–La(1)–C(2a)	153.3(2)	K(6)–O(6)–La(2)	89.8(2)
O(17)–La(1)–N(1)	78.8(2)	C(12)–O(11)–La(1)	128.6(7)
O(17)–La(1)–N(2)	60.1(2)	K(1)–O(11)–La(1)	101.1(2)
C(1)–La(1)–C(2a)	84.1(3)	K(3)–O(11)–La(1)	100.6(3)
C(1)–La(1)–N(1)	144.2(2)	C(14)–O(13)–La(1)	124.1(6)
C(1)–La(1)–N(2)	117.0(2)	K(6a)–O(13)–La(1)	106.3(3)
C(2a)–La(1)–N(1)	117.6(2)	C(16)–O(15)–La(1)	127.4(7)
C(2a)–La(1)–N(2)	145.3(3)	K(2)–O(15)–La(1)	100.4(2)
N(1)–La(1)–N(2)	61.5(2)	K(6a)–O(15)–La(1)	101.6(3)
O(1)–La(2)–O(3)	48.1(2)	C(18)–O(17)–La(1)	123.3(6)
O(1)–La(2)–O(5)	74.8(2)	K(3)–O(17)–La(1)	105.0(3)
O(1)–La(2)–O(6)	87.9(2)	C(22)–O(21)–La(2)	128.2(7)
O(1)–La(2)–O(21)	68.6(2)	K(1)–O(21)–La(2)	99.0(2)
O(1)–La(2)–O(23)	151.2(2)	K(3)–O(21)–La(2)	99.6(2)

O(1)–La(2)–O(25)	119.4(2)	C(24)–O(23)–La(2)	123.0(5)
O(1)–La(2)–O(27)	73.9(2)	K(6)–O(23)–La(2)	107.7(2)
O(1)–La(2)–C(1)	24.5(2)	C(26)–O(25)–La(2)	128.7(6)
O(1)–La(2)–C(2)	80.6(2)	K(2a)–O(25)–La(2)	100.0(2)
O(1)–La(2)–N(3)	127.0(2)	K(6)–O(25)–La(2)	100.4(2)
O(1)–La(2)–N(4)	130.3(2)	C(28)–O(27)–La(2)	124.3(6)
O(3)–La(2)–O(5)	99.4(2)	K(3)–O(27)–La(2)	103.2(3)
O(3)–La(2)–O(6)	74.5(2)	O(2)–K(2)–La(2a)	111.7(2)
O(3)–La(2)–O(21)	115.5(2)	O(3a)–K(2)–La(2a)	38.1(1)
O(3)–La(2)–O(23)	137.7(2)	O(6a)–K(2)–La(2a)	45.1(2)
O(3)–La(2)–O(25)	71.5(2)	O(15)–K(2)–La(2a)	104.3(2)
O(3)–La(2)–O(27)	78.6(2)	O(25a)–K(2)–La(2a)	37.3(1)
O(3)–La(2)–C(1)	23.7(2)	O(1w)–K(2)–La(2a)	99.8(6)
O(3)–La(2)–C(2)	86.6(3)	O(5w)–K(2)–La(2a)	144.3(7)
O(3)–La(2)–N(3)	156.3(2)	O(8wb)–K(2)–La(2a)	74.9(4)
O(3)–La(2)–N(4)	103.2(2)	O(9wc)–K(2)–La(2a)	122.8(1)
O(5)–La(2)–O(6)	48.1(2)	O(13wc)–K(2)–La(2a)	163.6(3)
O(5)–La(2)–O(21)	71.3(2)	K(6a)–K(2)–La(2a)	63.31(6)
O(5)–La(2)–O(23)	76.4(2)	La(1)–K(1)–La(2)	90.25(6)
O(5)–La(2)–O(25)	116.5(2)	O(1)–K(1)–La(1)	45.8(1)
O(5)–La(2)–O(27)	139.0(2)	O(4a)–K(1)–La(1)	37.6(2)
O(5)–La(2)–C(1)	86.9(2)	O(5)–K(1)–La(1)	113.0(2)
O(5)–La(2)–C(2)	24.2(3)	O(11)–K(1)–La(1)	37.5(1)
O(5)–La(2)–N(3)	100.8(2)	O(21)–K(1)–La(1)	103.1(2)
O(5)–La(2)–N(4)	154.1(2)	O(8w)–K(1)–La(1)	153.7(6)
O(6)–La(2)–O(21)	119.0(2)	O(9w)–K(1)–La(1)	124.4(1)
O(6)–La(2)–O(23)	71.9(2)	O(13w)–K(1)–La(1)	97.0(3)
O(6)–La(2)–O(25)	69.7(2)	K(1a)–K(1)–La(1)	98.37(7)
O(6)–La(2)–O(27)	153.1(2)	K(3)–K(1)–La(1)	62.21(5)
O(6)–La(2)–C(1)	80.0(2)	O(1)–K(1)–La(2)	44.4(1)
O(6)–La(2)–C(2)	23.9(2)	O(4a)–K(1)–La(2)	112.2(2)
O(6)–La(2)–N(3)	128.8(2)	O(5)–K(1)–La(2)	37.8(2)
O(6)–La(2)–N(4)	127.3(2)	O(11)–K(1)–La(2)	102.6(2)
O(21)–La(2)–O(23)	103.1(2)	O(21)–K(1)–La(2)	38.0(1)
O(21)–La(2)–O(25)	169.5(2)	O(8w)–K(1)–La(2)	98.8(3)
O(21)–La(2)–O(27)	73.0(2)	O(9w)–K(1)–La(2)	126.2(1)
O(21)–La(2)–C(1)	92.5(2)	O(13w)–K(1)–La(2)	156.1(4)
O(21)–La(2)–C(2)	95.3(3)	K(1a)–K(1)–La(2)	100.17(6)
O(21)–La(2)–N(3)	60.6(2)	K(3)–K(1)–La(2)	61.56(6)
O(21)–La(2)–N(4)	109.4(2)	O(6)–K(6)–La(2)	43.1(1)
O(23)–La(2)–O(25)	73.2(2)	O(13a)–K(6)–La(2)	102.2(2)
O(23)–La(2)–O(27)	131.7(2)	O(15a)–K(6)–La(2)	98.2(1)
O(23)–La(2)–C(1)	151.8(2)	O(16a)–K(6)–La(2)	125.6(3)
O(23)–La(2)–C(2)	72.6(2)	O(23)–K(6)–La(2)	34.9(1)

O(23)–La(2)–N(3)	60.3(2)	O(25)–K(6)–La(2)	35.7(1)
O(23)–La(2)–N(4)	78.4(2)	O(26)–K(6)–La(2)	75.4(2)
O(25)–La(2)–O(27)	101.9(2)	O(7w)–K(6)–La(2)	116.2(2)
O(25)–La(2)–C(1)	95.0(2)	C(16a)–K(6)–La(2)	120.3(2)
O(25)–La(2)–C(2)	92.9(3)	C(26)–K(6)–La(2)	53.2(2)
O(25)–La(2)–N(3)	109.8(2)	K(2a)–K(6)–La(2)	59.48(5)
O(25)–La(2)–N(4)	60.5(2)		

Symmetry codes: (a) $1 - x, y, \frac{1}{2} - z$; (b) $1 - x, -1 + y, \frac{1}{2} - z$; (c) $x, -1 + y, z$.

Table S4. Comparisons of selected bond distances (Å) for Na_{12n}[La(edta)(HPO₃)_{4n} 8nNaCl 4nH₂O (1), Na_{12n}[La(edta)(CO₃)_{4n} 8nNaCl 4nH₂O (2), K_{12n}[La(cdta)(CO₃)_{4n} 35H₂O (3), Na[La(edta)(H₂O)₃] 5H₂O (4),¹ {[La(edta)(H₂O)]₂]_n (5),² [IC₁₇H₂₀N₂]₂[La₂(edta)₂(H₂O)₄] 4H₂O (6),³ [La₅Cl₂(edta)₃(H₂O)₁₈]_nCl_n 8nH₂O (7),⁴ K_{3n}[La(edta)(HPO₃)_{3n}] 7nH₂O (8),⁵ Na₈[La₂(CO₃)₃(edta)₂] 20H₂O (9), [La₂(NO₃)₂(edta)(H₂O)₅]_n 3nH₂O (10),⁴ [La₂(SO₄)(edta)(H₂O)₃]_n (11),⁴ K₆[La₂(Hmal)₂(edta)₂] 14H₂O (12),⁶ (NH₄)₈[La₂(Hcit)₂(edta)₂] 9H₂O (13),⁶ K₈[La₂(Hcit)₂(edta)₂] 16H₂O (14),⁶ Na[Gd(edta)(H₂O)₃] 5H₂O (15),⁷ (MnH)[Gd(edta)(H₂O)₃] 4H₂O (16),⁸ Cs[Gd(edta)(H₂O)₃] 4H₂O (17),⁹ Na[Gd(edta)(H₂O)₃]_n 5H₂O (18),¹⁰ K_{3n}[Gd(edta)(HPO₃)_{3n}] 7nH₂O (19),⁵ Na₆[Gd₂(edta)₂(HPO₃)₂] 2.5NaCl 21H₂O (20),⁵ (NH₄)₂Na[Gd(edta)(H₂cit)] 4H₂O (21),⁵ [C(NH₂)₃]₃[Er(edta)(CO₃)] H₂O (22),¹¹ [C(NH₂)₃]₂[Er(edta)(H₂O)₂] ClO₄ 6H₂O (23),¹² [C(NH₂)₃]₄[Th(edta)(CO₃)₂] 5H₂O (24),¹¹ [Th(edta)(H₂O)₄] (25),¹³ (N₂H₅)[Ce(edta)(H₂O)₃] 4H₂O (26),¹⁴ K₄[Ce(O₂)(edta)]₂ 14H₂O (27),¹⁵ Rb₄[Ce(O₂)(edta)]₂ 14H₂O (28),¹⁵ K[Co(NH₃)₆][Ce(O₂)(edta)]₂ 7H₂O (29),¹⁵ K₆[Ce₂(Hmal)₂(edta)₂] 14H₂O (30),⁶ (NH₄)₈[Ce₂(Hcit)₂(edta)₂] 9H₂O (31),⁶ Na[Pr(edta)(H₂O)₃] 5H₂O (32),⁷ (N₂H₅)[Pr(edta)(H₂O)₃] 5H₂O (33),¹⁶ [H₂(PhNHNH₂)₃][Pr₂(EDTA)₂(H₂O)₄] 5H₂O (34),¹⁷ Na[Nd(edta)(H₂O)₃] 5H₂O (35),¹ Na[Nd(edta)(H₂O)₃] 5H₂O (36),¹⁸ K[Nd(edta)(H₂O)₃] 5H₂O (37),¹⁹ (N₂H₅)[Nd(edta)(H₂O)₃] 5H₂O (38),¹⁶ [C(NH₂)₃] [Nd(edta)(H₂O)₃] (39),¹⁸ [Nd(edta)(H₂O)]_n (40),²⁰ Na[Sm(edta)(H₂O)₃] 5H₂O (41),⁷ Na[Sm(edta)(H₂O)₃] 5H₂O (42),²¹ Cs[Sm(edta)(H₂O)₃] 4H₂O (43),⁹ (N₂H₅)[Sm(edta)(H₂O)₃] 5H₂O (44),¹⁶ [Sm₂(H₂cdta)₂(H₂O)₁₂][H₂SiW₁₂O₄₀] 17H₂O (45),²² Na[Eu(edta)(H₂O)₃] 5H₂O (46),¹ (N₂H₅)[Eu(edta)(H₂O)₃] 4H₂O (47),¹⁴ Na[Eu(edta)(H₂O)₃]_n 5H₂O (48),²³ [C(NH₂)₃][Eu(edta)(H₂O)₃] (49),²⁴ Na[Eu(cdta) H₂O] 4H₂O (50),²⁵ [C(NH₂)₃][Eu(cdta)(H₂O)] 2.375H₂O (51),²⁶ [C(NH₂)₃]₃[Eu₂(cdta)₂(H₂O)₂]ClO₄ 7H₂O (52),²⁶ [Eu₂(H₂cdta)₂(H₂O)₁₂][H₂SiW₁₂O₄₀] 17H₂O (53),²² Na[Tb(edta)(H₂O)₃]_n 5H₂O (54),²³ Na[Dy(edta)(H₂O)₃] 5H₂O (55),²⁷ Na[Dy(edta)(H₂O)₃] 3.25H₂O (56),²⁸ Cs[Dy(edta)(H₂O)₂] 3H₂O (57),⁹ Na[Dy(edta)(H₂O)₃]_n 5H₂O (58),²³ (H₃O)_n[Dy(edta)]_n nH₂O (59),²⁹ {[Dy(edta)] 3H₂O}_n (60),³⁰ Na[Ho(edta)(H₂O)₃] 5H₂O (61),³¹ K[Ho(edta)(H₂O)₃] 2H₂O (62),⁹ Cs[Ho(edta)(H₂O)₂] 3H₂O (63),⁹ {(H₃O)[Ho(edta)] nH₂O}_n (64),³² {(H₃O)[Er(edta)] H₂O}_n (65),²⁹ Na[Er(edta)(H₂O)₂] 5H₂O (66),⁹ Na[Er(edta)(H₂O)₃] 5H₂O (67),¹² [Er₂(H₂cdta)₂(H₂O)₁₂][H₂SiW₁₂O₄₀] 17H₂O (68),²² K[Yb(edta)(H₂O)₂] 5H₂O (69),³³ Cs[Yb(edta)(H₂O)₂] 3H₂O (70),²⁷ [C(NH₂)₃]₂[Yb(edta)(H₂O)₂]ClO₄ 6H₂O (71),³⁴ K₃[Yb(edta)(CO₃)](H₂O) H₂O (72),³⁵ K₃[Yb(edta)(CO₃)](H₂O)₄ 2H₂O (73),³⁵ Rb₃[Yb(edta)(CO₃)](H₂O)₄ 2H₂O (74),³⁵ Cs₃[Yb(edta)(CO₃)](H₂O)₄ 2H₂O (75),³⁵ Na[Yb(cdta)(H₂O)₂] 5H₂O (76),³⁶ and [C(NH₂)₃]₂[Yb(cdta)(H₂O)₂] 4H₂O (77).³⁴

Complexes	Ln–O _{carboxy} (av)	Ln–O _{inorganic} (av)	Ln–N(av)	Ln–O _w (av)	P/C–O(av)
1	2.570(7)	2.653(9)	2.822(8)		1.418(7)

2	2.572(6)	2.630(7)	2.829(7)		1.283(7)
3	2.585(7)	2.708(7)	2.882(7)		1.285(7)
4¹	2.493(4)		2.768(4)	2.589(4)	
5²	2.524(3)		2.849(4)	2.655(4)	
6³	2.55(1)		2.83(1)	2.60(1)	
7⁴	2.57(1)		2.82(1)		
8⁵	2.545(7)	2.601(7)	2.793(9)	---	1.526(7)
9	2.573(4)	2.581(4)	2.788(5)	---	1.289(4)
10⁴	2.515(3)	2.657(4)	2.746(3)		1.253(5)
11⁴	2.612(3)	2.609(3)	2.786(4)	2.532(3)	1.474(3)
12⁶	2.563(2)		2.801(2)		
13⁶	2.563(2)		2.814(2)		
14⁶	2.563(7)		2.785(9)		
15⁷	2.399(4)		2.655(4)	2.472(4)	
16⁸	2.41(2)		2.68(2)	2.49(2)	
17⁹	2.39(2)		2.655(8)	2.439(7)	
18¹⁰	2.400(8)		2.65(1)	2.468(9)	
19⁵	2.406(6)	2.308(5)	2.616(6)		1.515(6)
20⁵	2.393(5)	2.319(5)	2.609(6)		1.50(1)
21⁵	2.397(5)		2.656(7)		
22¹¹	2.286(3)	2.329(3)	2.574(4)		1.286(6)
23¹²	2.275(1)		2.591(1)	2.344(1)	
24¹¹	2.491(4)	2.454(4)	2.787(4)		1.286(7)
25¹³	2.428(2)		2.805(2)	2.532(2)	
26¹⁴	2.471(3)		2.731(3)	2.554(3)	
27¹⁵	2.494(3)	2.317(3)	2.563(3)		
28¹⁵	2.484(5)	2.315(5)	2.590(6)		
29¹⁵	2.408(4)	2.331(4)	2.712(5)		
30⁶	2.542(4)		2.782(4)		
31⁶	2.543(4)		2.794(5)		
32⁷	2.458(5)		2.714(6)	2.536(5)	
33¹⁶	2.454(2)		2.713(2)	2.54(1)	
34¹⁷	2.475(4)		2.780(4)	2.524(4)	
35¹	2.451(5)		2.699(6)	2.534(6)	
36¹⁸	2.454(3)		2.694(3)	2.525(3)	

37 ¹⁹	2.436(4)	2.712(4)	2.539(4)
38 ¹⁶	2.439(3)	2.702(3)	2.523(3)
39 ¹⁸	2.445(3)	2.692(4)	2.516(3)
40 ²⁰	2.452(2)	2.776(2)	2.552(2)
41 ⁷	2.422(5)	2.673(5)	2.499(5)
42 ²¹	2.42(1)	2.667(7)	2.494(8)
43 ⁹	2.42(1)	2.67(5)	2.473(5)
44 ¹⁶	2.415(3)	2.679(3)	2.489(3)
45 ²²	2.37(2)		2.43(3)
46 ¹	2.411(6)	2.674(7)	2.494(6)
47 ¹⁴	2.415(3)	2.693(3)	2.493(3)
48 ²³	2.410(3)	2.665(4)	2.480(3)
49 ²⁴	2.415(2)	2.674(2)	2.476(2)
50 ²⁵	2.387(3)	2.636(3)	2.339(3)
51 ²⁶	2.37(1)	2.62(2)	2.44(2)
52 ²⁶	2.361(6)	2.611(6)	2.464(6)
53 ²²	2.36(2)		2.42(2)
54 ²³	2.382(6)	2.643(7)	2.447(7)
55 ²⁷	2.39(2)	2.63(2)	2.46(2)
56 ²⁸	2.381(5)	2.649(6)	2.460(5)
57 ⁹	2.31(1)	2.57(1)	2.39(1)
58 ²³	2.38(1)	2.64(1)	2.46(1)
59 ²⁹	2.325(3)	2.605(4)	
60 ³⁰	2.354(3)	2.627(3)	
61 ³¹	2.363(7)	2.633(6)	2.453(6)
62 ⁹	2.367(8)	2.617(9)	2.446(8)
63 ⁹	2.31(2)	2.59(2)	2.38(2)
64 ³²	2.311(3)	2.592(4)	
65 ²⁹	2.298(4)	2.578(6)	
66 ⁹	2.351(6)	2.620(6)	2.430(6)
67 ¹²	2.351(6)	2.620(6)	2.430(6)
68 ²²	2.32(2)		2.34(2)
69 ³³	2.272(2)	2.519(3)	2.344(2)
70 ²⁷	2.262(6)	2.533(7)	2.369(6)
71 ³⁴	2.254(2)	2.577(3)	2.322(3)

72 ³⁵	2.283(2)	2.306(2)	2.553(3)	1.290(4)
73 ³⁵	2.274(2)	2.303(2)	2.539(2)	1.291(4)
74 ³⁵	2.272(4)	2.299(4)	2.533(5)	1.279(7)
75 ³⁵	2.276(4)	2.294(4)	2.541(5)	1.289(7)
76 ³⁶	2.274(4)		2.528(5)	2.324(4)
77 ³⁴	2.271(3)		2.549(3)	2.317(3)

Table S5. Solid ¹³C NMR data for K_{12n}[La(cdta)(CO₃)]_{4n} 35nH₂O (**3**).

Complex	–CH ₂	–CH ₂ CHN	–CHN	–CH ₂ CO ₂	–CO ₂
3	23.6	25.7	54.4	59.5	179.1

Table S6. Crystal data and structural refinements for **1** ~ **3**.^a

Complexes references	1	2	3
Chemical formula	C ₄₀ H ₆₀ N ₈ O ₄₈ La ₄ Na ₂₀ Cl ₈ P ₄	C ₄₄ H ₅₆ N ₈ O ₄₈ La ₄ Na ₂₀ Cl ₈	C ₆₀ H ₁₁₈ K ₁₂ La ₄ N ₈ O ₆₇
Formula Mass	2843.88	2764.00	3048.46
Temperature/K	173(1)	173(1)	173(1)
Crystal system	Tetragonal	Tetragonal	Monoclinic
Space group	<i>P</i> 4/ <i>n</i> <i>bm</i>	<i>P</i> 4/ <i>n</i> <i>bm</i>	<i>C</i> 2/ <i>c</i>
<i>a</i> /Å	21.0289(2)	21.0220(3)	32.893(1)
<i>b</i> /Å	21.0289(2)	21.0220(3)	9.4679(4)
<i>c</i> /Å	9.5708(2)	9.5449(3)	34.229(1)
<i>α</i> /°	90	90	90
<i>β</i> /°	90	90	102.532(4)
<i>γ</i> /°	90	90	90
Unit cell volume/Å ³	4232.4(1)	4218.1(1)	10406.0(7)
<i>Z</i>	2	2	4
Absorption coefficient, μ/mm ^{−1}	2.514	2.447	2.202
No. of reflections measured	18415	14428	23750
No. of independent reflections	2170	2886	8712
<i>R</i> _{int}	0.0281	0.0435	0.0550
Final <i>R</i> _I values [<i>I</i> > 2σ(<i>I</i>)]	0.0880	0.0805	0.0748
Final w <i>R</i> (<i>F</i> ²) values [<i>I</i> > 2σ(<i>I</i>)]	0.1745	0.1609	0.1435
Final <i>R</i> _I values (all data)	0.0885	0.0917	0.0970
Final w <i>R</i> (<i>F</i> ²) values (all data)	0.1747	0.1657	0.1529
Goodness of fit on <i>F</i> ²	1.259	1.208	1.090

^a $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$, $wR_2 = \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]^{1/2}$

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