

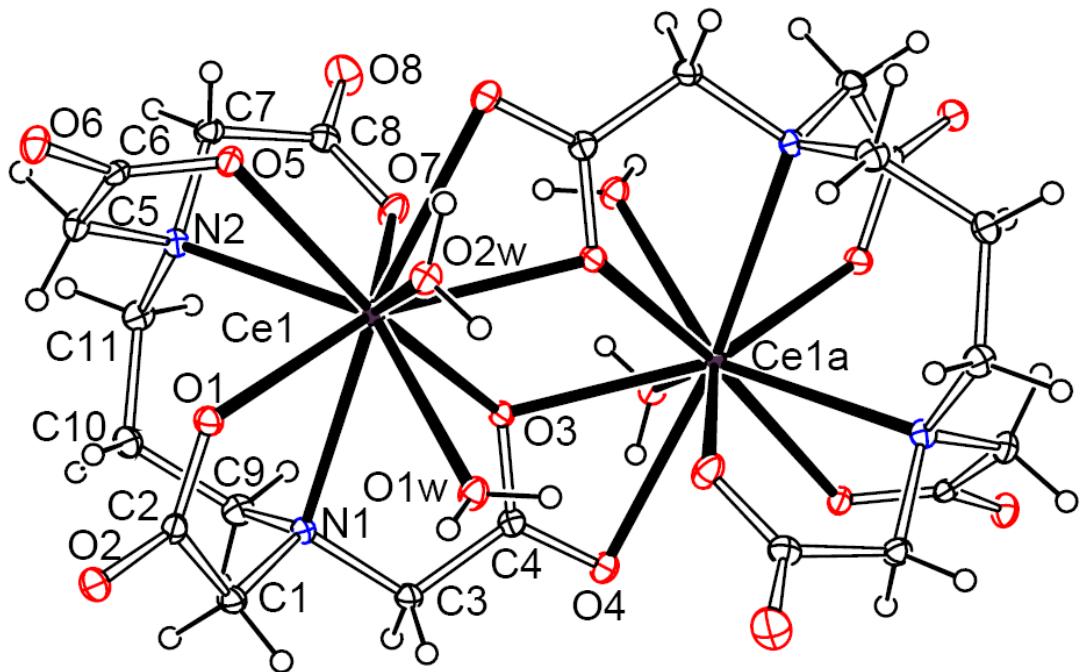
# Dimeric 1,3-propanediaminetetraacetato lanthanides as the precursors of catalysts for the oxidative coupling of methane

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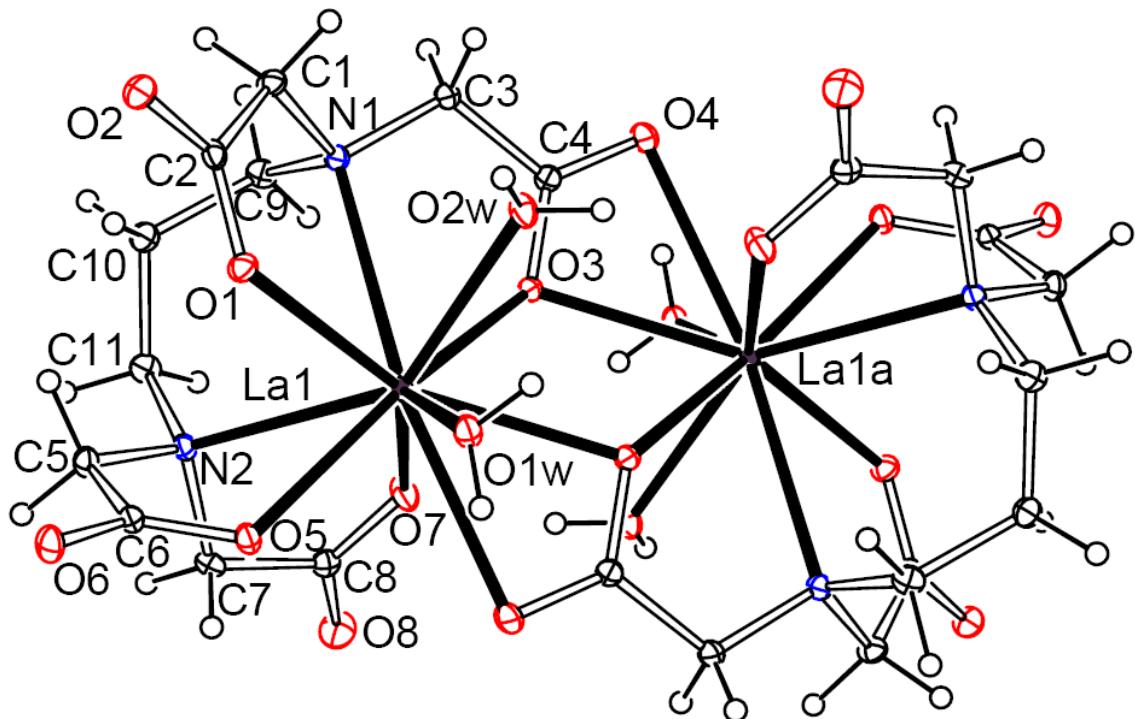
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<b>Fig. S1</b> Anion structure of dimeric complex $(\text{NH}_4)_2[\text{Ce}_2(\text{pdta})_2(\text{H}_2\text{O})_4] \cdot 8\text{H}_2\text{O}$ ( <b>2</b> ) in 30% thermal ellipsoids .....	2
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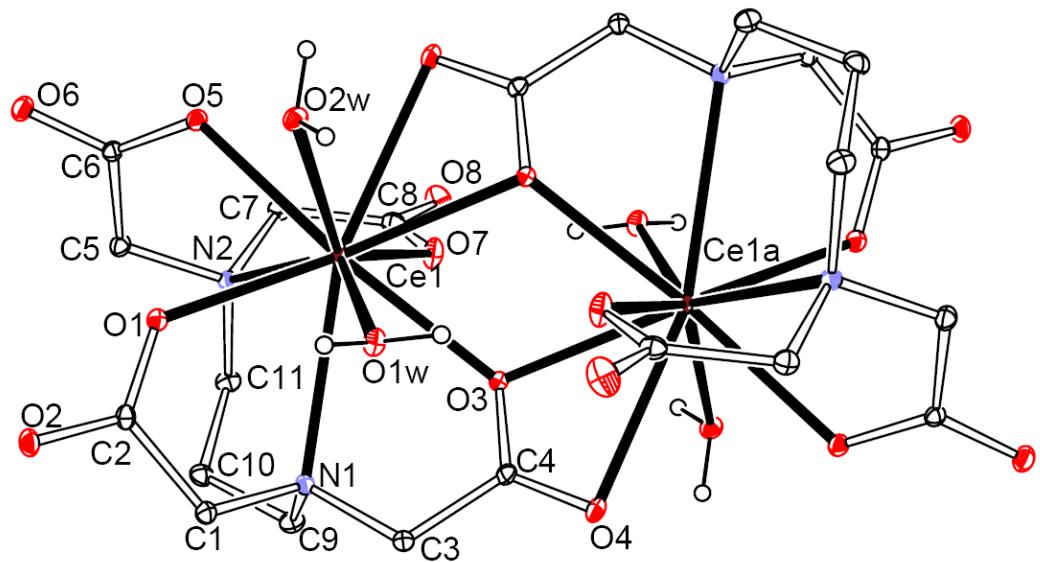


**Fig. S1** Anion structure of dimeric complex  $(\text{NH}_4)_2[\text{Ce}_2(\text{pdta})_2(\text{H}_2\text{O})_4] \cdot 8\text{H}_2\text{O}$  (**2**) in 30% thermal ellipsoids

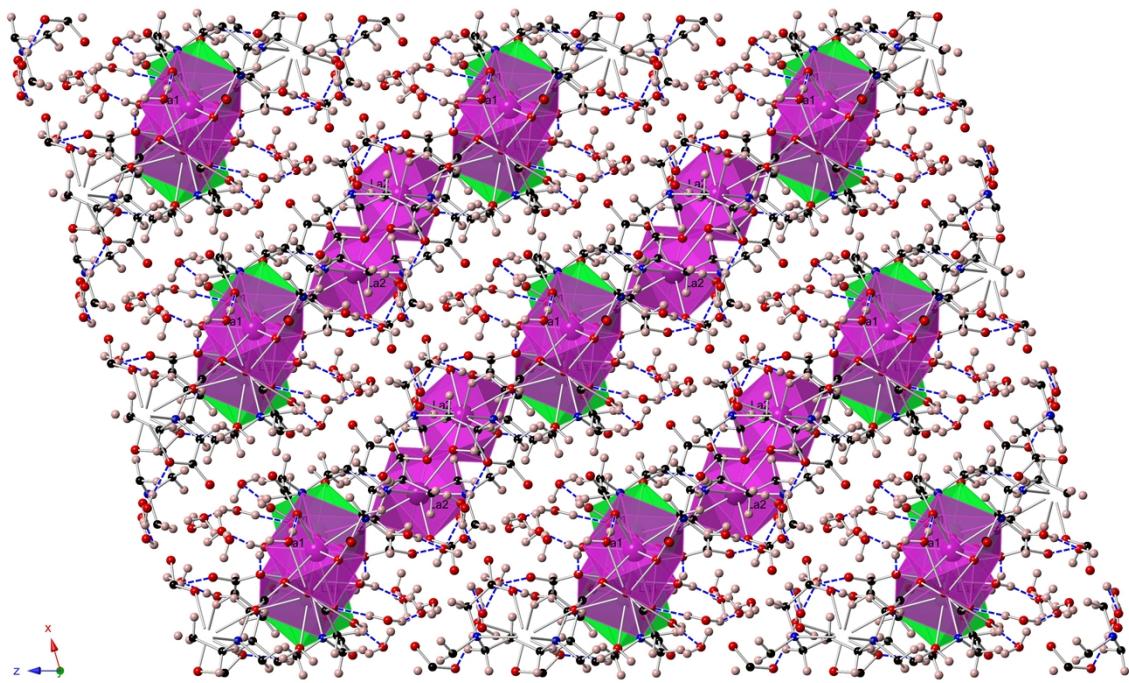


**Fig. S2** Anion structure of dimeric complex  $\text{K}_2[\text{La}_2(\text{pdta})_2(\text{H}_2\text{O})_4] \cdot 11\text{H}_2\text{O}$  (**3**) in 30% thermal ellipsoids

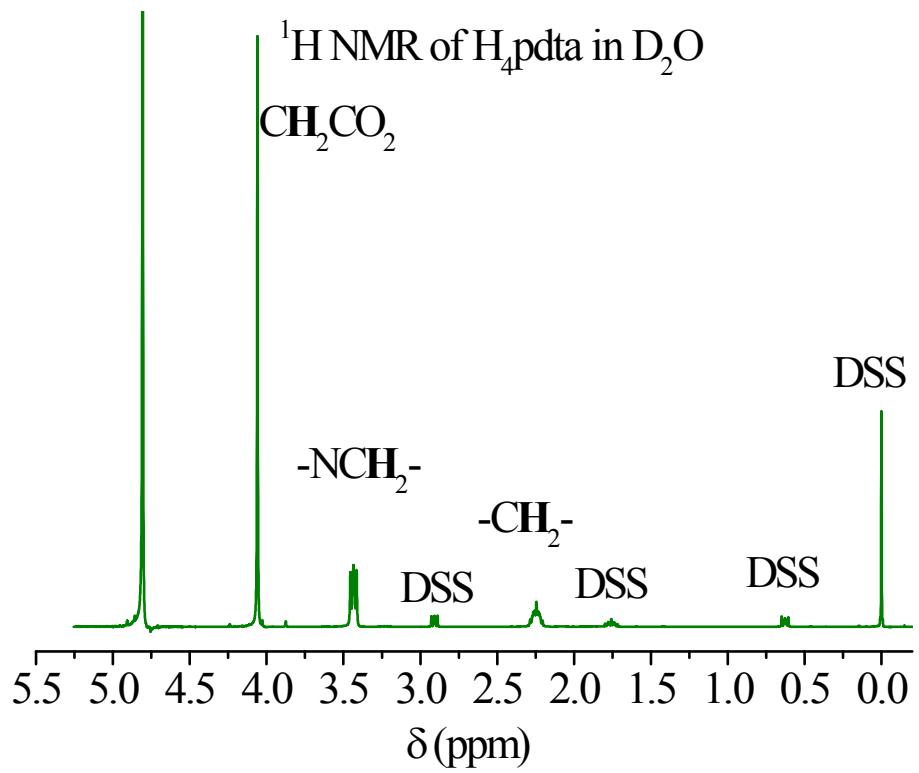
ellipsoids



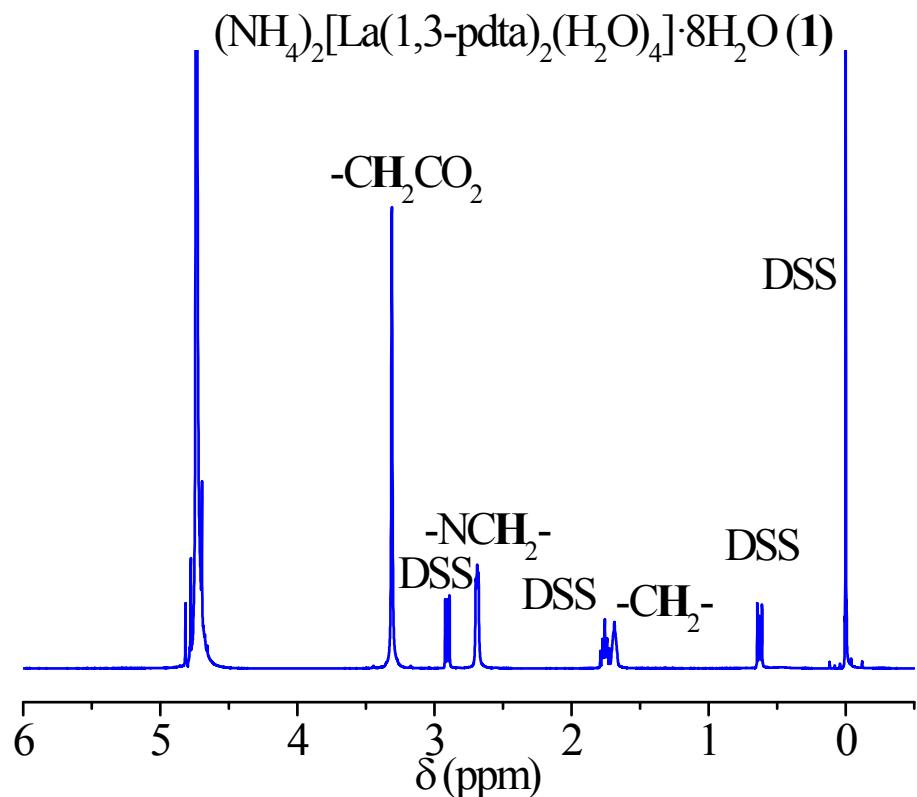
**Fig. S3** Anion structure of dimeric complex  $\text{K}_2[\text{Ce}_2(\text{pdta})_2(\text{H}_2\text{O})_4] \cdot 11\text{H}_2\text{O}$  (**4**) in 30% thermal ellipsoids



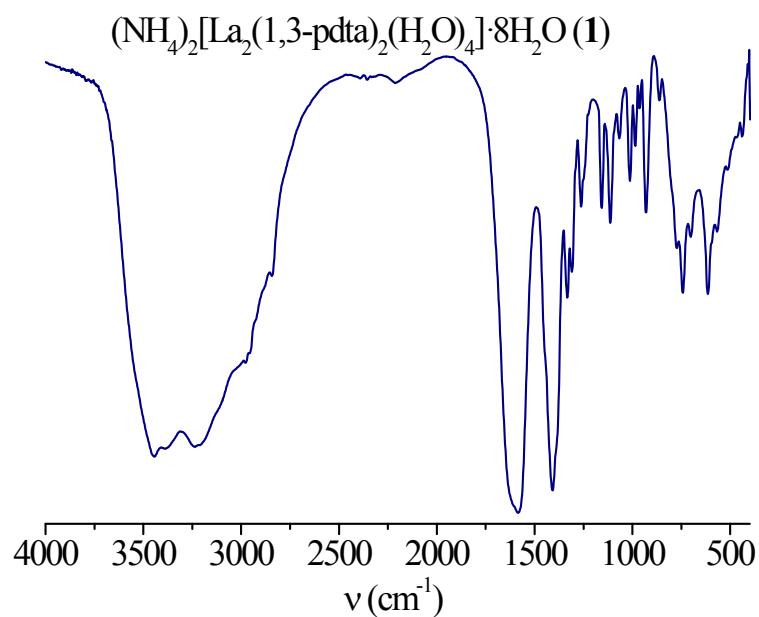
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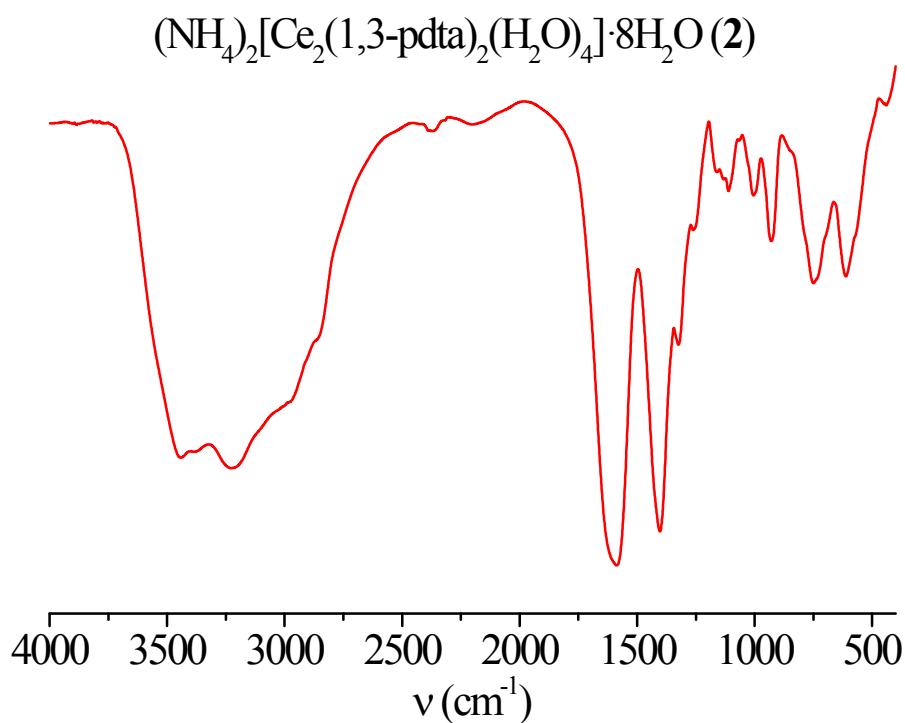
**Fig. S5** <sup>1</sup>H NMR spectrum of H<sub>4</sub>ppta in D<sub>2</sub>O, DSS was used as an internal reference.



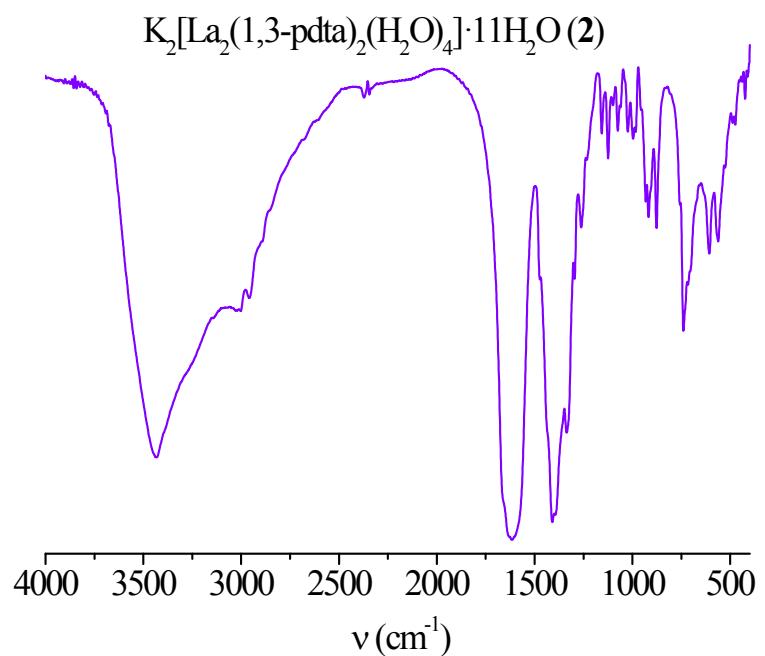
**Fig. S6**  $^1\text{H}$  NMR spectrum of  $(\text{NH}_4)_2[\text{La}_2(\text{pdta})_2(\text{H}_2\text{O})_4]\cdot 8\text{H}_2\text{O}$  (**1**) in  $\text{D}_2\text{O}$ , DSS was used as an internal reference.



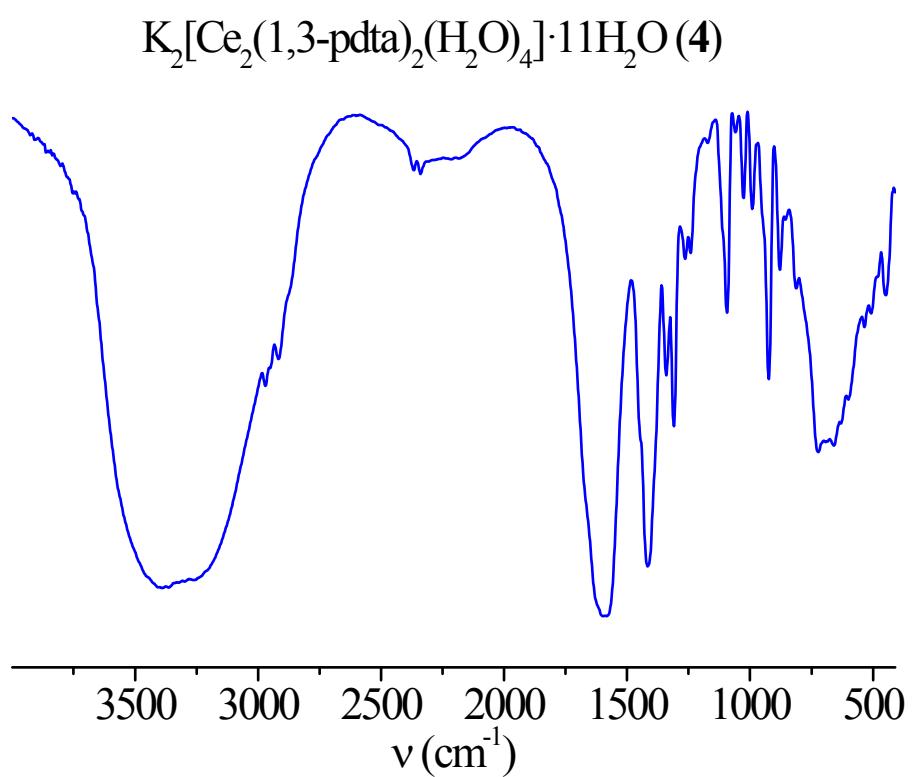
**Fig. S7** IR spectrum of  $(\text{NH}_4)_2[\text{La}_2(1,3\text{-pdta})_2(\text{H}_2\text{O})_4] \cdot 8\text{H}_2\text{O}$  (**1**)



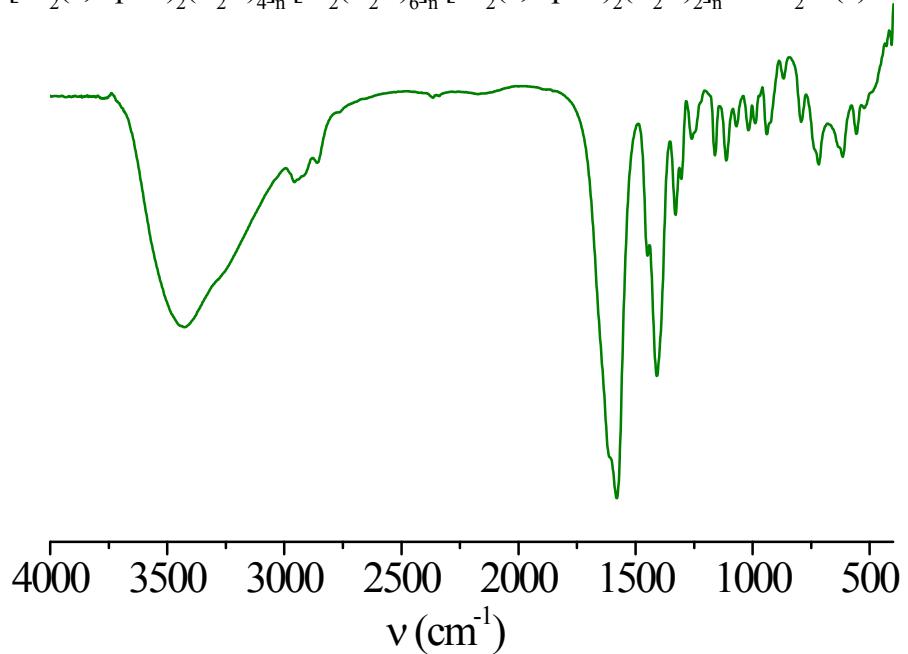
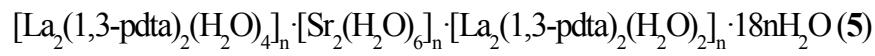
**Fig. S8** IR spectrum of  $(\text{NH}_4)_2[\text{Ce}_2(1,3\text{-pdta})_2(\text{H}_2\text{O})_4] \cdot 8\text{H}_2\text{O}$  (**2**)



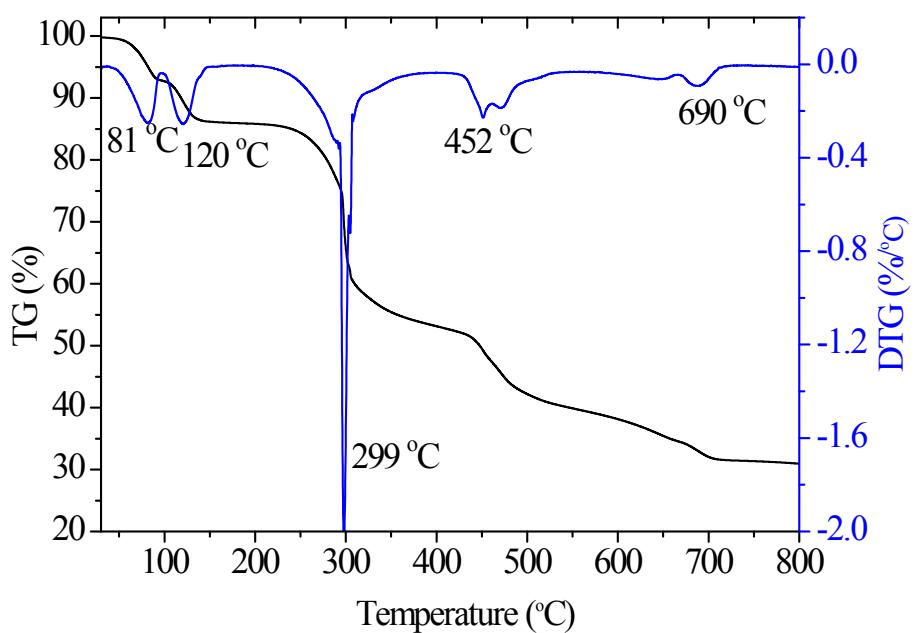
**Fig. S9** IR spectrum of  $\text{K}_2[\text{La}_2(1,3\text{-pdta})_2(\text{H}_2\text{O})_4]\cdot 11\text{H}_2\text{O}$  (**3**)



**Fig. S10** IR spectrum of  $\text{K}_2[\text{Ce}_2(1,3\text{-pdta})_2(\text{H}_2\text{O})_4]\cdot 11\text{H}_2\text{O}$  (**4**)



**Fig. S11** IR spectrum of  $[\text{La}_2(1,3\text{-pdta})_2(\text{H}_2\text{O})_4]_n \cdot [\text{Sr}_2(\text{H}_2\text{O})_6]_n \cdot [\text{La}_2(1,3\text{-pdta})_2(\text{H}_2\text{O})_2]_n \cdot 18n\text{H}_2\text{O}$  (**5**)



**Fig. S12** TG-DTG curves of  $(\text{NH}_4)_2[\text{La}_2(1,3\text{-pdta})_2(\text{H}_2\text{O})_4]\cdot 8\text{H}_2\text{O}$  (**1**)

**Table S1** The catalytic performances of thermal decomposition products from **1** and **5** in oxidative coupling of methane ( $\text{CH}_4/\text{O}_2 = 2.8/1$ , GHSV = 15000  $\text{mL}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ )

Sample	T/°C	Conv CH <sub>4</sub> /%	Sel C <sub>2</sub> /%	Yield C <sub>2</sub> /%
$\text{La}_2\text{O}_2\text{CO}_3$	550	0.0	0.0	0.0
	600	13.10	28.38	3.72
	650	17.36	42.37	7.35
	700	23.02	45.75	10.53
	750	29.62	46.57	13.79
	800	29.93	45.61	13.65
$\text{La}_2\text{O}_3$ , $\text{SrCO}_3$ and $\text{La}_2\text{O}_2\text{CO}_3$	550	12.63	24.05	3.04
	600	26.46	47.17	12.48
	650	29.87	46.31	13.83
	700	29.09	50.25	14.62
	750	29.69	51.74	15.36
	800	30.94	50.71	15.69