X-ray powder diffraction data for lanthanum trilactate trihydrate

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X-ray powder diffraction data, unit cell parameters, and space group for a new organometallic compound, lanthanum trilactate trihydrate, $LaC_9H_{21}O_{12}$, are reported [$a = 9.986(1)$ Å, $b = 9.158(1)$ Å, $c = 11.200(1)$ Å, $\alpha = 115.08(1)$, $\beta = 117.41(1)$, $\gamma = 88.61(1)$, unit cell volume $V = 804.70$ Å^3, $Z = 2$ and space group $P1$]. All measured lines were indexed. No detectable impurity was observed.
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Key words: unit cell parameters, space group, X-ray powder diffraction data, lanthanum trilactate trihydrate

I. INTRODUCTION

Lanthanum is an important rare earth element used in many applications such as hydride batteries, high temperature superconductors or heavy fluoride glass. Recently, rare earth fluorides have attracted lot of attention because of their unique properties namely luminescent properties in nanoparticle forms.

Various salts of rare earths are used as precursors for nano-fluorides when various organic and inorganic precursors take place (Bartůněk *et al.*, 2013; Zhang *et al.*, 2010; Zhang and Huang, 2010). Studies of rare earths lactates including lanthanum lactate are also important for the advanced nuclear fuel cycles technologies where lactates can play crucial role in actinides and lanthanides separations (Tian *et al.*, 2010; Zalupski *et al.*, 2010).

II. EXPERIMENTAL

A. Sample preparation

Lanthanum trilactate was prepared by neutralization reaction of 50% lactic acid with lanthanum oxide under air atmosphere at approximately 50 °C. Reaction was carried out until neutral pH and the product subsequently filtered and obtained by free crystallization in pure form. Crystals were subsequently dried in a desiccator. Pale blue crystals of tris[2-(hydroxy-κO) propanoato-κO]lanthanum trihydrate (Figure 1) were milled and subsequently analyzed. All chemicals were used in pure form. The water content was determined by single-crystal structure analysis.

B. Diffraction data collection and reduction

The diffraction pattern for the title compound was collected at room temperature using an X'Pert PRO θ–θ powder diffractometer with parafocusing Bragg–Brentano geometry and Cu$K\alpha$ radiation ($\lambda = 1.5418$ Å, generator setting: 40 kV, 30 mA). An ultrafast X'Celerator detector was employed to collect XRD data over the angular range from 4 to 60 °2θ with a step size of 0.017 °2θ and an accumulative counting time of 20.32 s/step. The experimental powder diffraction pattern is depicted in Figure 2. The software package HighScore Plus V 3.0d of PANalytical, Almelo, Netherlands, was used to smooth the data, to fit the background and to eliminate the $K\alpha_2$ component. The top of smoothed peak method was used to determine the peak positions and intensities of the diffraction peaks.

Automatic indexing of the experimental XRD pattern was done using DICVOL06 (Boultif and Louër, 2004).

III. RESULTS

The experimental powder diffraction pattern is depicted in Figure 2. Automatic indexing results obtained by DICVOL06 (Table I) show that the title compound is triclinic with the space group $P1$ and unit cell parameters: $a = 9.986(1)$ Å, $b = 9.158(1)$ Å, $c = 11.200(1)$ Å, $\alpha = 115.08(1)$, $\beta = 117.41(1)$, $\gamma = 88.61(1)$, unit cell volume $V = 804.70$ Å^3, $Z = 2$. The figures of merits are $F_{20} = 59.9(0.0108, 31)$ (Smith and Snyder, 1979) and $M_{20} = 24.0$ (de Wolff, 1968). All lines were indexed and are consistent with the $P1$ space group. Only first two pages of the peak table are presented in the article, the whole Table 1 is available as a supplementary material.

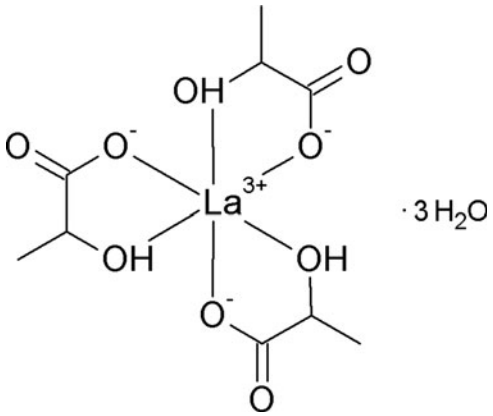

Figure 1. Structural formula of the title compound tris[2-(hydroxy-κO) propanoato-κO]lanthanum trihydrate.

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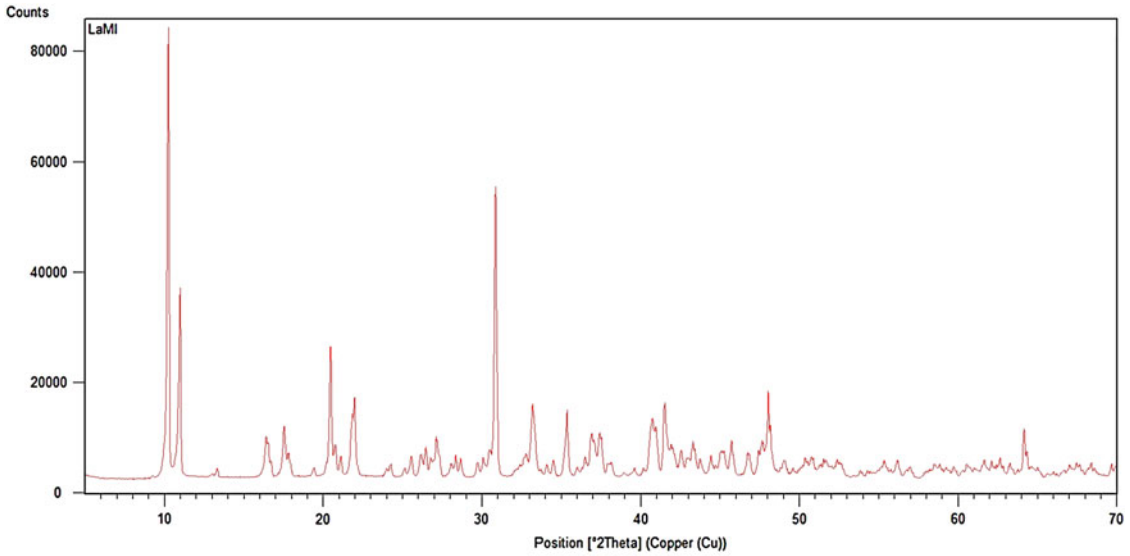

Figure 2. (Color online) X-ray powder diffraction pattern of the title compound using and Cu$K\alpha$ radiation ($\lambda = 1.5418$ Å).

TABLE I. Indexed X-ray powder diffraction data for the title compound, $LaC_9OH_{21}O_{12}$. Only the peaks with I_{rel} of 1 or greater are presented [$a = 9.986(1)$ Å, $b = 9.158(1)$ Å, $c = 11.200(1)$ Å, $\alpha = 115.08(1)$, $\beta = 117.41(1)$, $\gamma = 88.61(1)$, unit cell volume $V = 804.70$ Å^3, $Z = 2$ and space group $P\bar{1}$]. All measured lines were indexed. The d-values were calculated using CuKα_1 radiation ($\lambda = 1.5406$ Å).

$2\theta_{obs}$ (deg)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (deg)	d_{calc} (Å)	$\Delta 2\theta$
10.241	8.63075	100	1	0	−1	10.209	8.65733	0.032
10.981	8.05073	42	0	1	0	10.964	8.06321	0.017
13.018	6.79521	1	1	1	−1	13.008	6.80052	0.010
13.322	6.64082	2	1	−1	0	13.325	6.63937	−0.003
16.413	5.39648	9	1	1	−2	16.407	5.39854	0.006
16.530	5.35854	8	1	1	0	16.534	5.35725	−0.004
16.709	5.30154	4	1	−1	−1	16.724	5.29694	−0.015
17.538	5.05277	11	1	0	−2	17.528	5.05554	0.010
17.812	4.97565	5	2	0	−1	17.812	4.97556	0.000
17.940	4.94044	3	0	1	−2	17.952	4.93717	−0.012
19.428	4.56528	2	0	2	−1	19.432	4.56442	−0.004
20.232	4.38563	3	0	0	2	20.216	4.38907	0.016
20.469	4.33539	29	2	0	−2	20.444	4.34072	0.025
20.776	4.27201	7	2	1	−1	20.764	4.27445	0.012
21.113	4.20458	5	2	−1	−1	21.117	4.20370	−0.004
21.840	4.06623	14	1	2	−1	21.875	4.05983	0.009
21.908	4.05377	14	0	2	−2	21.875	4.05983	0.033
21.977	4.04119	18	0	2	0	21.972	4.04207	0.005
22.177	4.00520	2	1	−2	0	22.192	4.00246	−0.015
24.000	3.70494	2	1	1	−3	24.003	3.70449	−0.003
24.251	3.66716	3	1	−1	−2	24.268	3.66461	−0.017
25.135	3.54015	2	2	1	−3	25.138	3.53973	−0.003
25.562	3.48197	5	2	−1	−2	25.539	3.48512	0.023
26.157	3.40410	5	2	2	−2	26.129	3.40773	0.028
26.467	3.36493	7	1	−2	−1	26.484	3.36284	−0.017
26.783	3.32594	4	2	−2	0	26.776	3.32681	0.007
27.136	3.28347	8	0	1	−3	27.119	3.28552	0.017
27.195	3.27648	8	0	1	2	27.218	3.27375	−0.023
27.353	3.25791	4	3	0	−1	27.339	3.25954	0.014
28.076	3.17564	3	0	2	−3	28.082	3.17493	−0.006
28.350	3.14557	5	3	1	−2	28.348	3.14574	0.002
28.659	3.11235	4	2	−2	−1	28.667	3.11154	−0.008
29.698	3.00578	3	0	3	−2	29.716	3.00400	−0.018
29.777	2.99799	3	0	3	−1	29.771	2.99859	0.006
30.086	2.96790	4	3	1	−3	30.076	2.96885	0.010
30.480	2.93043	6	0	0	3	30.497	2.92884	−0.017
30.865	2.89474	64	1	−3	1	30.877	2.89369	−0.012

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TABLE I. Continued

$2\theta_{obs}$ (deg)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (deg)	d_{calc} (Å)	$\Delta 2\theta$
32.396	2.76135	3	2	1	−4	32.394	2.76151	0.002
32.636	2.74159	4	2	1	1	32.645	2.74087	−0.009
32.799	2.72834	5	2	−1	2	32.827	2.72604	−0.028
33.195	2.69669	16	0	3	0	33.190	2.69709	0.005
33.306	2.68795	12	3	2	−3	33.283	2.68979	0.023
33.721	2.65582	2	2	−2	−2	33.757	2.65304	−0.036
34.093	2.62769	3	3	−2	−1	34.095	2.62756	−0.002
34.510	2.59688	4	2	3	−2	34.521	2.59611	−0.011
35.362	2.53624	15	3	−1	−3	35.357	2.53659	0.005
35.465	2.52911	7	2	0	−4	35.424	2.53194	0.041
36.001	2.49268	2	4	0	−2	36.014	2.49182	−0.013
36.507	2.45928	4	0	2	2	36.487	2.46055	0.020
36.841	2.43775	8	1	0	−4	36.829	2.43850	0.012
36.928	2.43220	10	1	0	3	36.934	2.43185	−0.006
37.059	2.42391	8	0	1	−4	37.043	2.42490	0.016
37.417	2.40153	10	4	0	−3	37.424	2.40112	−0.007
37.520	2.39518	8	4	0	−1	37.541	2.39387	−0.021
37.930	2.37022	3	4	−1	−2	37.947	2.36922	−0.017
38.151	2.35700	3	2	−3	2	38.155	2.35677	−0.004
38.950	2.31047	1	0	3	−4	38.976	2.30901	−0.026
39.612	2.27337	2	3	3	−3	39.609	2.27353	0.003
40.175	2.24280	2	4	1	−4	40.192	2.24187	−0.017
40.623	2.21909	11	1	4	−2	40.606	2.21997	0.017
40.751	2.21242	13	2	2	1	40.723	2.21386	0.028
40.959	2.20166	11	1	−4	2	40.992	2.19998	−0.033
41.468	2.17580	15	2	−1	−4	41.478	2.17532	−0.010
41.551	2.17165	16	2	−1	3	41.571	2.17067	−0.020
41.925	2.15314	7	3	−3	−1	41.947	2.15204	−0.022
42.026	2.14820	6	1	−2	4	42.057	2.14670	−0.031
42.561	2.12242	6	3	−2	−3	42.574	2.12181	−0.013
42.929	2.10508	4	4	−2	−2	42.936	2.10476	−0.007
43.304	2.08771	8	1	−1	−4	43.317	2.08709	−0.013
43.429	2.08199	6	1	3	−5	43.455	2.08081	−0.026
43.749	2.06750	4	1	3	1	43.769	2.06659	−0.020
44.436	2.03712	5	2	4	−2	44.447	2.03664	−0.011
44.721	2.02480	2	0	4	0	44.746	2.02374	−0.025
45.068	2.01001	6	3	0	−5	45.079	2.00956	−0.011
45.240	2.00277	5	2	−4	0	45.213	2.00388	0.027
45.733	1.98232	8	3	−3	−2	45.753	1.98151	−0.020
45.861	1.97708	4	0	2	3	45.866	1.97687	−0.005

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SUPPLEMENTAL DATA

The supplementary material for this article can be found at http://www.journals.cambridge.org/PDJ

Chemical Information File (CIF) of the compound is available online.

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