

Supporting information

β - $\text{Ca}_3(\text{PO}_4)_2$ -related structure and dielectric properties of $\text{Ca}_8\text{CdLa}(\text{PO}_4)_7$

Elena V. Sipina¹, Evgeniya S. Zhukovskaya², Vladimir A. Morozov², Sergey Yu. Stefanovich²,
Vadim V. Grebenev³, Alexei A. Belik⁴, Bogdan I. Lazoryak², Dina V. Deyneko²

¹ Physics Department, Moscow State University, 119991 Moscow, Russia

² Chemistry Department, Moscow State University, 119991 Moscow, Russia

³ A.V. Shubnikov Institute of Crystallography of the Kurchatov Complex Crystallography and Photonics of the NRC "Kurchatov Institute", 119333, Moscow, Russia

⁴ Research Center for Materials Nanoarchitectonics (MANA), Namiki 1-1, Tsukuba, Ibaraki, 305-0044, Japan

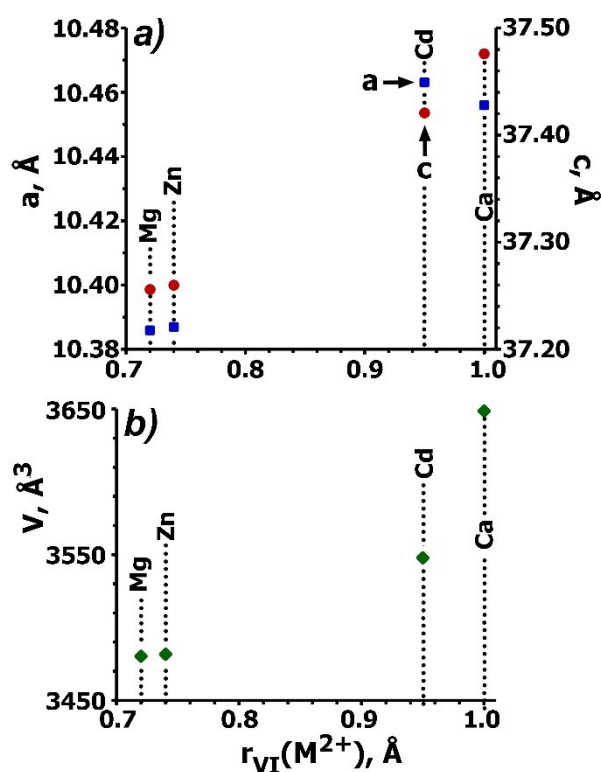


Fig. S1. The lattice cell parameters of $\text{Ca}_8\text{MLa}(\text{PO}_4)_7$ ($M = \text{Mg}, \text{Zn}, \text{Ca}$) and $\text{Ca}_{8.61}\text{Cd}_{0.70}\text{La}_{0.82}(\text{PO}_4)_7$: a and c (a); V (b).

Table S1. Fractional atomic coordinates, site symmetry, isotropic displacement atomic parameters (U_{iso}), site occupation, and BVS values for $\text{Ca}_{8.61}\text{Cd}_{0.70}\text{La}_{0.82}(\text{PO}_4)_7$ from synchrotron SXRD data.

Atom	M	x	y	z	U_{iso}	BVS
$M1$	0.972(3) Ca^{2+} 0.028(3) La^{3+}	0.7241(3)	0.8554(5)	0.43483(6)	0.0077(8)	1.77(2) (Ca) 2.95(3) (La)
$M2$	Ca^{2+}	0.6179(3)	0.8199(5)	0.23494(7)	0.0090(7)	1.98(2)
$M3$	0.754(3) Ca^{2+} 0.246(3) La^{3+}	0.1445(10) 0.1256(9)	0.2966(4) 0.2666(4)	0.3291(2) 0.3279(2)	0.0038(5) 0.0038(5)	1.59(2)(Ca) 2.54(3)(La)
$M4$	0.128(6) Ca^{2+}	0	0	0.1847(9)	0.016(11)	0.505(5)
$M5$	0.692(6) Cd^{2+} 0.308(6) Ca^{2+}	0 0	0 0	0.0025(2) 0	0.0029(5) 0.0029(5)	1.94(2)(Cd) 2.47(3)(Ca)
P1	1P	0	0	0.2718(2)	0.014(1)	4.23(5)
P2	1P	0.6820(3)	0.8537(6)	0.1357(2)	0.009(1)	4.50(5)
P3	1P	0.6505(4)	0.8433(5)	0.0344(2)	0.0087(1)	4.94(6)
O1	1O	0	0	0.3125(4)	0.026(2)	1.89(4)
O2	1O	-0.1487(7)	-0.013(9)	0.2571(3)	0.026(2)	1.62(2)
O3	1O	0.7188(8)	0.8912(8)	0.1751(2)	0.0091(3)	1.44(2)
O4	1O	0.7609(13)	0.7710(1)	0.1214(3)	0.0091(3)	1.74(4)
O5	1O	0.7417(3)	0.0110(1)	0.1186(3)	0.0091(3)	2.07(3)
O6	1O	0.5095(8)	0.7548(6)	0.1293(2)	0.0091(3)	2.04(4)
O7	1O	0.6055(1)	0.9483(9)	0.0497(3)	0.0051(2)	2.00(4)
O8	1O	0.5810(1)	0.6844(2)	0.0515(3)	0.0051(2)	1.65(3)
O9	1O	0.8176(7)	0.9182(3)	0.0457(2)	0.0051(2)	1.83(2)
O10	1O	0.6325(6)	0.8277(9)	-0.0051(2)	0.0051(2)	2.15(3)

Table S2. Selected distances (Å), distortion indexes (DI), and the tetrahedral distortion parameters Δd and $\Delta\alpha$ in $\text{Ca}_{8.61}\text{Cd}_{0.70}\text{La}_{0.82}(\text{PO}_4)_7$ from SXRD data.

Polyhedra	Distance,	d, Å	Polyhedra	Distance,	d, Å
$M1\text{O}_8$	$M1\text{-O}2$	2.473(9)	$M2\text{O}_8$	$\text{Ca}2\text{-O}2$	2.332(7)
	$M1\text{-O}4$	2.846(16)		$\text{Ca}2\text{-O}3$	2.428(8)
	$M1\text{-O}5$	2.692(19)		$\text{Ca}2\text{-O}4$	2.370(12)
	$M1\text{-O}6$	2.465(13)		$\text{Ca}2\text{-O}5$	2.357(12)
	$M1\text{-O}6$	2.389(18)		$\text{Ca}2\text{-O}7$	2.600(16)
	$M1\text{-O}7$	2.418(14)		$\text{Ca}2\text{-O}8$	2.707(13)
	$M1\text{-O}8$	2.326(13)		$\text{Ca}2\text{-O}9$	2.440(14)
	$M1\text{-O}10$	2.398(6)		$\text{Ca}2\text{-O}9$	2.395(11)
	$\langle M1\text{-O} \rangle$	2.501		$\langle \text{Ca}2\text{-O} \rangle$	2.454
	DI(M1-O)	0.054		DI(Ca2-O)	0.041
$M3\text{O}_9$	$\text{Ca}3\text{-O}1$	2.759(5)	$M3\text{O}_9$	$\text{La}3\text{-O}1$	2.484(5)
	$\text{Ca}3\text{-O}2$	3.087(12)		$\text{La}3\text{-O}2$	2.944(12)
	$\text{Ca}3\text{-O}3/$	2.725(15)		$\text{La}3\text{-O}3$	2.893(14)
	$\text{Ca}3\text{-O}4$	2.410(14)		$\text{La}3\text{-O}4$	2.557(13)
	$\text{Ca}3\text{-O}5/$	2.257(17)		$\text{La}3\text{-O}5$	2.327(17)
	$\text{Ca}3\text{-O}7$	2.467(15)		$\text{La}3\text{-O}7$	2.528(14)
	$\text{Ca}3\text{-O}8$	2.556(13)		$\text{La}3\text{-O}8$	2.525(12)
	$\text{Ca}3\text{-O}10$	2.634(14)		$\text{La}3\text{-O}10$	2.554(14)
	$\text{Ca}3\text{-O}10$	2.768(13)		$\text{La}3\text{-O}10$	2.603(12)
	$\langle \text{Ca}3\text{-O} \rangle$	2.63		$\langle \text{La}3\text{-O} \rangle$	2.60
	DI(Ca3-O)	0.070		DI(La3-O)	0.054
$M5\text{O}_6$	$3\times\text{Cd}5\text{-O}6$	2.185(2)	$M5\text{O}_6$	$3\times\text{Ca}5\text{-O}6$	2.123(2)
	$3\times\text{Cd}5\text{-O}9$	2.315(2)		$3\times\text{Ca}5\text{-O}6$	2.380(2)
	$\langle \text{Cd}5\text{-O} \rangle$	2.25		$\langle \text{Ca}5\text{-O} \rangle$	2.25
	DI(Ca5-O)	0.029		DI(Cd5-O)	0.057
$M4\text{O}_9$	$\text{Ca}4\text{-O}2\times 3$	3.09(3)	$\text{P}1\text{O}_4$	$\text{P}1\text{-O}1$	1.524(15)
	$\text{Ca}4\text{-O}3\times 3$	2.595(8)		$\text{P}1\text{-O}2\times 3$	1.591(9)
	$\text{Ca}4\text{-O}4\times 3$	3.41(2)		$\langle \text{P}1\text{-O} \rangle$	1.57
	$\langle \text{Ca}4\text{-O} \rangle$	3.03		Δd	0.0212
	DI(Ca4-O)	0.0960		$\Delta\alpha$	0.0006
$\text{P}2\text{O}_4$	$\text{P}2\text{-O}3$	1.523(11)	$\text{P}3\text{O}_4$	$\text{P}3\text{-O}7$	1.508(15)
	$\text{P}2\text{-O}4$	1.560(16)		$\text{P}3\text{-O}8$	1.579(12)
	$\text{P}2\text{-O}5$	1.574(13)		$\text{P}3\text{-O}9$	1.574(8)
	$\text{P}2\text{-O}6$	1.587(7)		$\text{P}3\text{-O}10$	1.488(7)
	$\langle \text{P}2\text{-O} \rangle$	1.56		$\langle \text{P}3\text{-O} \rangle$	1.54
	Δd	0.0233		Δd	0.0277
	$\Delta\alpha$	0.0017		$\Delta\alpha$	0.0028
	$\text{Ca}3\text{-La}3$	0.279(5)		$\text{Cd}5\text{-Ca}5$	0.093(6)