Electronic Supplementary Material (ESI) for Materials Advances.

Full Ce substitution on La in Tl_2LaCl_5: impact and performance

Federico Moretti, Didier Perrodin, Joanna Szornel, and Edith D. Bourret

Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA

Electronic Supplementary Information

Both Tl_2LaCl_5:5 mol% and Tl_2CeCl_5 crystals, grown by the Bridgman-Stockbarger method, cracked into multiple pieces during the cooling phase. Figure S1 reports pictures of some of the largest pieces that could be recovered after opening the ampoules. These pieces appear clear, transparent, and without any coloration. Some haziness can be noticed, though it is related to unevenness of the surface in contact with the quartz growth ampoule.

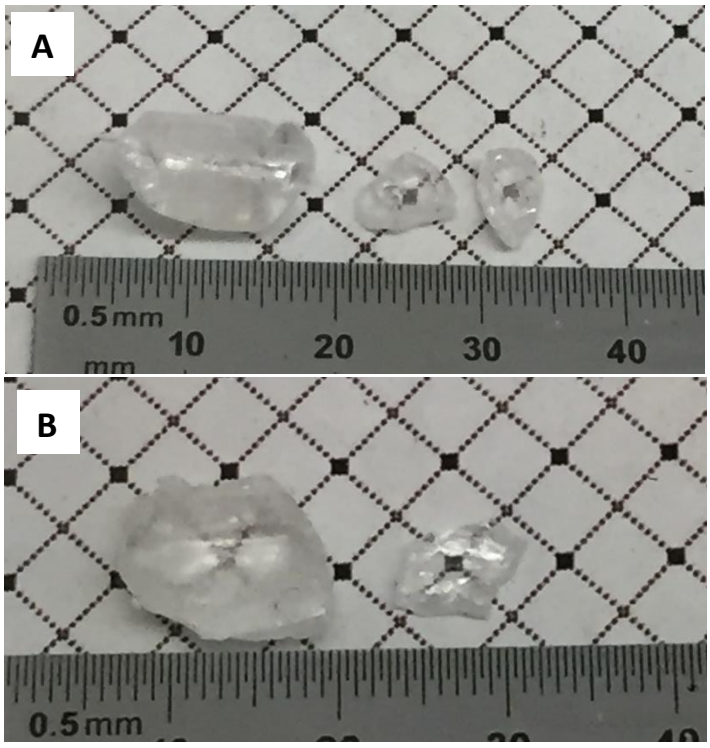

Figure S1: Photographs of single crystal pieces of Tl_2CeCl_5 (panel A) and of Tl_2LaCl_5: 0.5 mol% Ce (panel B). The pieces are as recovered from the growth ampoules without any polishing or lapping process.

Figure S2 reports the powder x-ray diffractograms obtained on Tl_2LaCl_5 and Tl_2CeCl_5 grown crystals. The pieces ground for this characterization were selected from areas of the grown crystals close to the pieces used in the optical and scintillation characterization. The results of Rietveld refinement are reported in table S1. Both crystals have the same orthorhombic crystallographic structure that matches that of Tl_2LaCl_5 previously reported.[1,2] The diffraction data have been obtained using a Bruker D2 Phaser X-ray diffractometer with Cu Kα radiation.

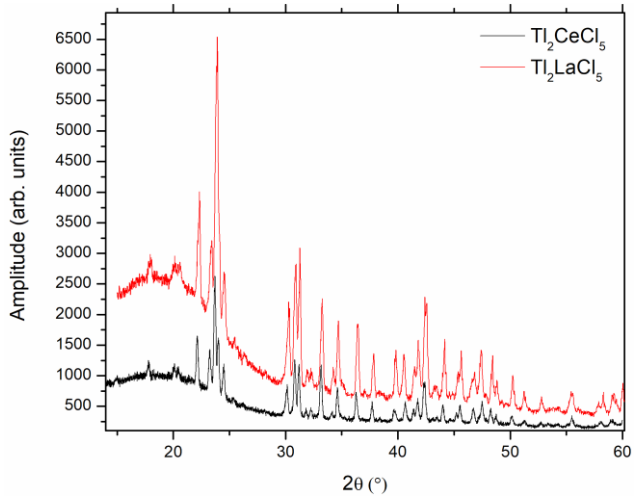

Figure S2: powder x-ray diffraction results obtained on the grown Tl_2LaCl_5:5 mol% Ce and Tl_2CeCl_5 single crystals

Table S1: refined lattice parameter for Tl_2LaCl_5: 5 mol% Ce, and Tl_2CeCl_5.

Empirical formula	Tl_2LaCl_5	Tl_2CeCl_5
Fw (g)	724.91	726.15
Space group	P n m a	P n m a
Space group number	62	62
a (Å)	12.835	12.77
b (Å)	8.967	8.87
c (Å)	8.098	8.04
α=β=γ (°)	90	90
Volume ($Å^3$)	932.0	909.0
Z	4	4

References

1 A. Khan, P. Q. Vuong, G. Rooh, H. J. Kim and S. Kim, *J. Alloys Compd.*, 2020, **827**, 154366.

2 U. Shirwadkar, M. Loyd, M. H. Du, E. van Loef, G. Ciampi, L. Soundara Pandian, L.

Stand, M. Koschan, M. Zhuravleva, C. Melcher and K. Shah, *Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip.*, 2020, **962**, 163684.