Electronic Supplementary Material (ESI) for Dalton Transactions.

Preparation and Crystal Structure of $K_2Ce(PO_4)_2$: A New Complex Phosphate of Ce(IV) Having Structure With One-Dimensional Channels

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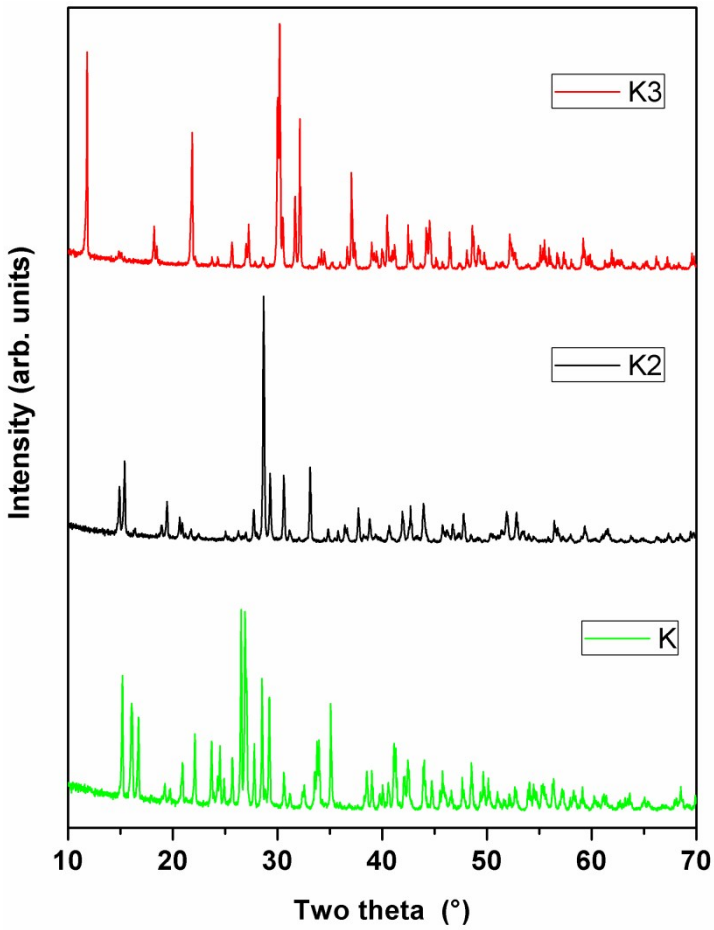
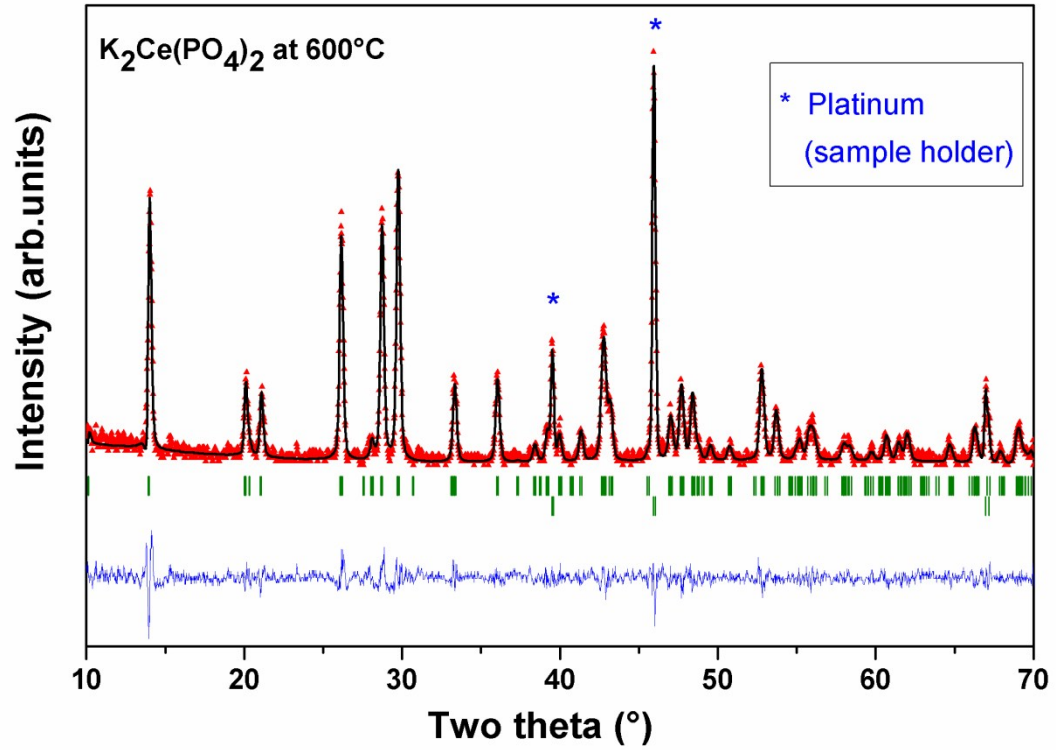
Electronic Supplementary Information

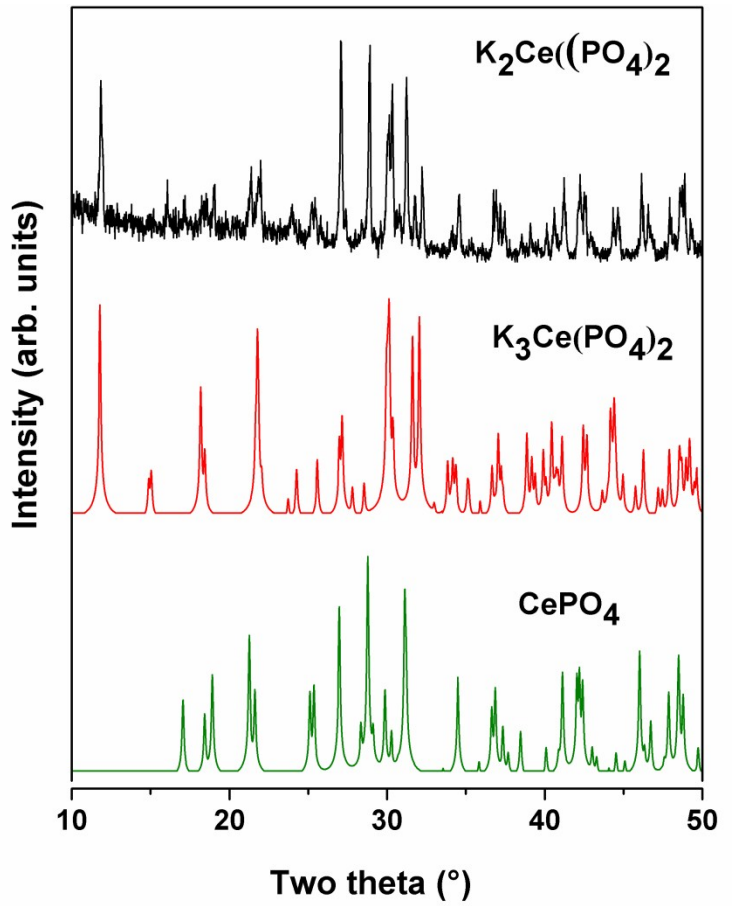


ESI-1. Powder XRD patterns of different phosphates with different K:Ce ratio. (1:1 K, 2:1 K2, 3:1 K3)



ESI-2. Typical XRD pattern of $K_2Ce(PO_4)_2$ recorded at 600°C. The profile was fitted with space group: Imma. The vertical ticks indicate Bragg positions (upper row for $K_2Ce(PO_4)_2$ and lower are for platinum sample holder.

Unit cell parameters of high temperature phase of $K_2Ce(PO_4)_2$ are : a = 6.829(1), b = 6.811(2), c = 17.487(2) Å, V = 813.4(3) $Å^3$.



ESI-3. Typical XRD pattern of $K_2Ce(PO_4)_2$ recorded after heating a 900°C for 5h (upper panel). The calculated XRD patterns of $K_3Ce(PO_4)_2$ and $CePO_4$ are shown in the lower panels. Structural data for $K_3Ce(PO_4)_2$ and $CePO_4$ are taken from references. *J. J. Zah-Letho, P. Houeneou, and R. Eholie, Comptes Rendus Hebdo. des Seances, Ser 2. 1988, 307, 1177 and Y.-X. Ni, J. M. Hughes, and A. N. Mariano, Am. Mineral. 1995, 80, 21.*

ESI-4. Table of motifs of mutual adjunction of $K_2Ce(PO_4)_2$ and related compounds.

(a). $K_2Ce(PO_4)_2$ (Space group: $P2_1/n$)

	O11	**O12**	**O13**	**O14**	**O21**	**O22**	**O23**	**O24**	CN
Ce1	1/ 1	1/ 1	1/ 1	1/ 1	1/ 1	1/ 1	1/ 1	1/ 1	8
K1	2/ 2	1/ 1	1/ 1	0/ 0	1/ 1	1/ 1	1/ 1	2/ 2	8+1
K2	1/ 1	1/ 1	1/ 1	2/ 2	1/ 1	2/ 2	1/ 1	0/ 0	8+1
P1	1/ 1	1/ 1	1/ 1	1/ 1	0/ 0	0/ 0	0/ 0	0/ 0	4
P2	0/ 0	0/ 0	0/ 0	0/ 0	1/ 1	1/ 1	1/ 1	1/ 1	4
CN	5	4	4	4	4	5	4	4	

(b). $Na_2Th(PO_4)_2$ (Space group: $P2_1/n$)

	O1	**O2**	**O3**	**O4**	**O5**	**O6**	**O7**	**O8**	**O9**	**O10**	**O11**	**O12**	**O13**	**O14**	**O15**	**O16**	**CN**
Th1	0/ 0	0/ 0	1/ 1	1/ 1	1/ 1	1/ 1	0/ 0	0/ 0	1/ 1	1/ 1	1/ 1	1/ 1	0/ 0	0/ 0	1/ 1	1/ 1	8+2
Th2	1/ 1	1/ 1	1/ 1	2/ 2	0/ 0	0/ 0	1/ 1	1/ 1	0/ 0	0/ 0	0/ 0	0/ 0	1/ 1	1/ 1	0/ 0	0/ 0	8+1
P1	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	4
P2	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	4
P3	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	4
P4	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	0/ 0	1/ 1	4
Na1	1/ 1	0/ 0	0/ 0	0/ 0	1/ 1	1/ 1	0/ 0	0/ 0	1/ 1	0/ 0	1/ 1	1/ 1	0/ 0	1/ 1	0/ 0	2/ 1	9
Na2	0/ 0	1/ 1	0/ 0	0/ 0	1/ 1	1/ 1	0/ 0	0/ 0	0/ 0	1/ 1	1/ 1	1/ 1	1/ 1	0/ 0	2/ 1	0/ 0	9
Na3	0/ 0	2/ 2	0/ 0	1/ 1	1/ 1	0/ 0	2/ 2	1/ 1	0/ 0	1/ 1	0/ 0	0/ 0	1/ 1	1/ 1	0/ 0	0/ 0	10
Na4	2/ 2	0/ 0	1/ 1	0/ 0	0/ 0	1/ 1	1/ 1	2/ 2	1/ 1	0/ 0	0/ 0	0/ 0	1/ 1	1/ 0	0/ 0	0/ 0	10
CN	5	5	4	4	5	5	5	5	4	4	4	4	5	5	4	4	

(c). $Na_2Th(PO_4)_2$ (Space group: C2/c)

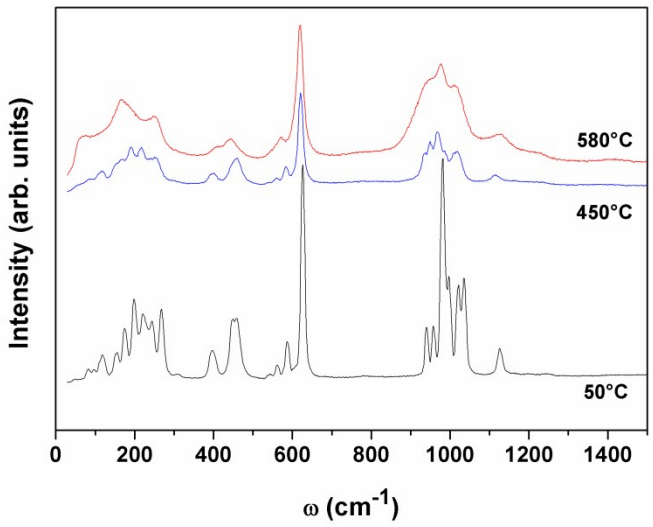
	O1	**O2**	**O3**	**O4**	**O5**	**O6**	**O7**	**O8**	CN
Th1	0/ 0	2/ 1	2/ 1	0/ 0	2/ 2	2/ 1	0/ 0	2/ 1	8+2
Th2	2/ 2	2/ 1	0/ 0	2/ 1	0/ 0	0/ 0	2/ 1	0/ 0	8
P1	1/ 1	1/ 1	1/ 1	1/ 1	0/ 0	0/ 0	0/ 0	0/ 0	4
P2	0/ 0	0/ 0	0/ 0	0/ 0	1/ 1	1/ 1	1/ 1	1/ 1	4
Na1	1/ 1	0/ 0	2/ 2	0/ 0	1/ 1	2/ 2	1/ 1	1/ 1	9
Na2	2/ 2	1/ 1	1/ 1	3/ 3	1/ 1	0/ 0	1/ 1	0/ 0	9
CN	5	4	5	5	5	4	4	4	

(d). $K_2CeZr(PO_4)_2$ (Space group: $I4_1/amd$)

	O1	**O2**	CN
Ce/Zr1	4/ 1	4/ 1	8
P1	2/ 1	2/ 1	4
K1	4/ 2	4/ 2	8
CN	4	4	

a. Present study
b. Galesic, N.; Matkovic, B.; Topic, M.; Coffou, E.; Sljukic, M. *Croat. Chem. Acta* **1984**, *57*, 597-608.
c. Ogorodnyk, I. V.; Zatovsky, I. V.; Baumer, V. N.; Slobodyanik, N. S.; Shishkin, O. V. *Acta Cryst.* C **2006**, *62*, i100-i102.

*CN : Coordination number



ESI-5. Typical Raman spectra of $K_2Ce(PO_4)_2$ recorded at different temperatures.