Supporting information for article:

Incommensurate structures and radiation damage in Rb2V3O8 and K2V3O8 mixed-valence vanadate fresnoites

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Table S1   Experimental data for the measurement on the (3+1)-*d* structure of $K_2V_3O_8$ at 100 K (● = 0.69127 Å).

Superspace group	*Cmm*2(0*β*1/2)*s*00
a (Å)	12.6452(9)
b (Å)	12.6452(9)
c (Å)	5.2235(5)
V (Å^3)	835.2
Z	4
D_c (g cm^{-3})	2.855
Twin volume (1,2)	0.469(2), 0.531(2)
G_{iso}	0.214(6)
Modulation vector **q**	0, 0.626, 0.5

Data collection

No. measured refl.	8351
No. main refl.	1575
No. satellite refl. ± (1,0)	6776
Range of *hkl*	-16 < *h* < 15
	-16 < *k* < 16
	-6 < *l* < 6
	-1 < *m* < 1
No. observed refl. (all, main, satellites)[a]	1929, 762, 1167
R_{int}(obs/all)	1.58/1.61

Refinement [b]

$R_{obs/all}$ (all refl.)	1.58/2.40
$wR_{obs/all}$ (all refl.)	1.98/2.09
$R_{obs/all}$ (main refl.)	1.34/1.39
$wR_{obs/all}$ (main refl.)	1.80/1.83
$R_{obs/all}$ (satellite refl. ± (1,0))	4.09/8.48
$wR_{obs/all}$ (satellite refl. ± (1,0))	4.49/5.31
No. parameters	144

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[a] Criterion for observed reflections is $|F_{obs}| > 3$♦

[b] All agreement factors are given in %, weighing scheme $1/[♦^2(F_{obs}) + (0.01\ F_{obs})^2]$

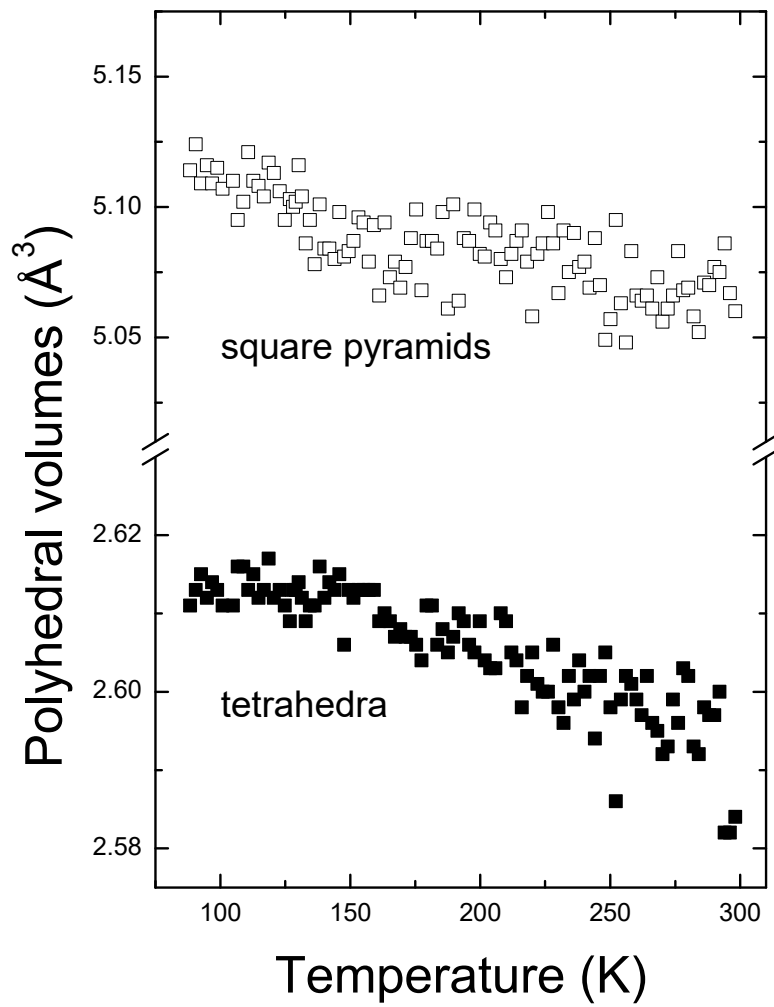**Figure S1**   Volume of the tetrahedra and square pyramids as a function of temperature in $K_2V_3O_8$.
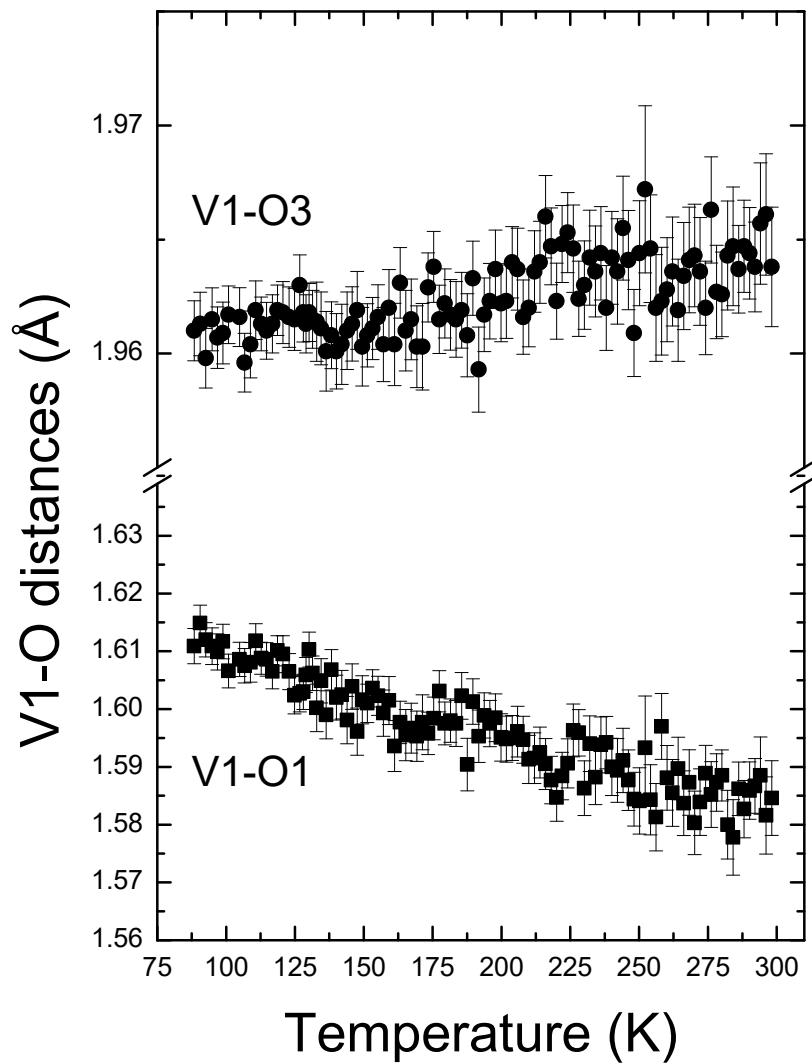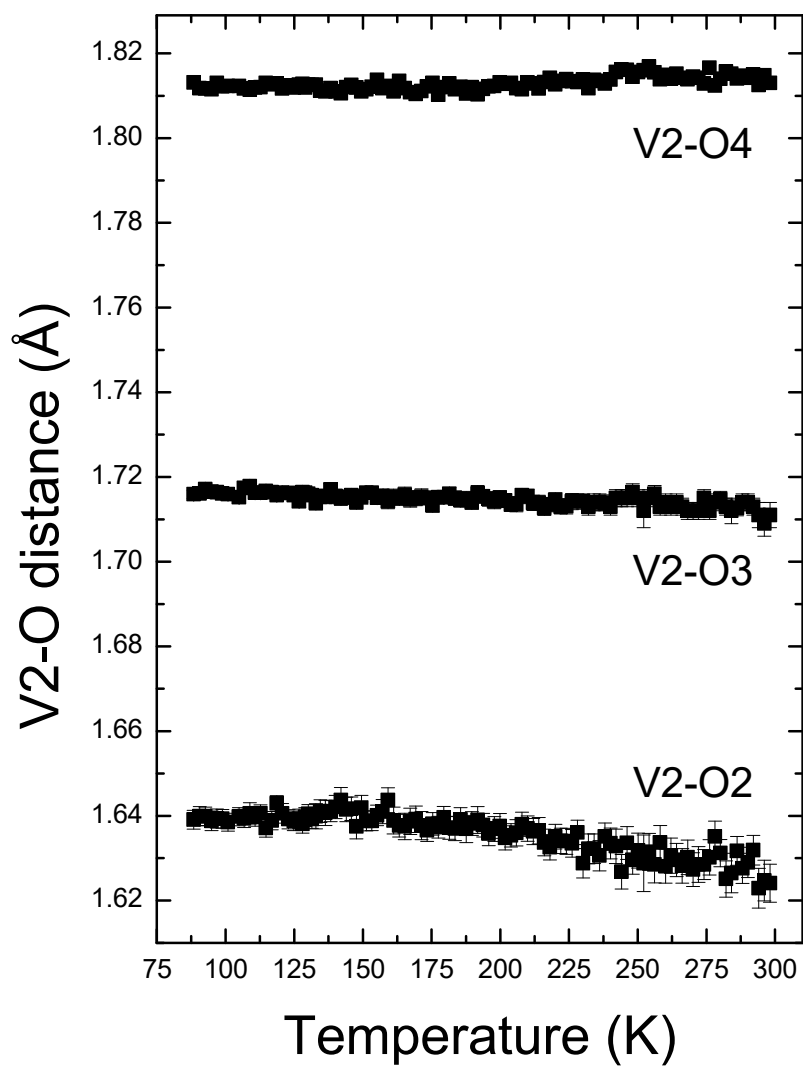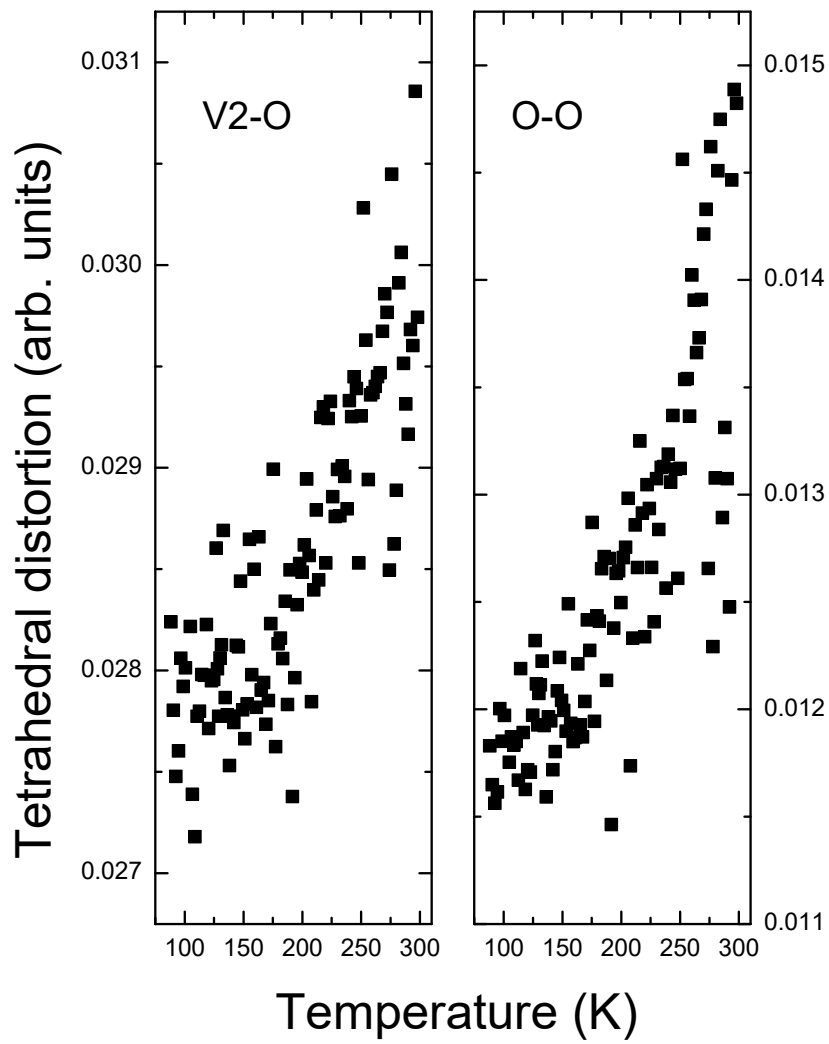
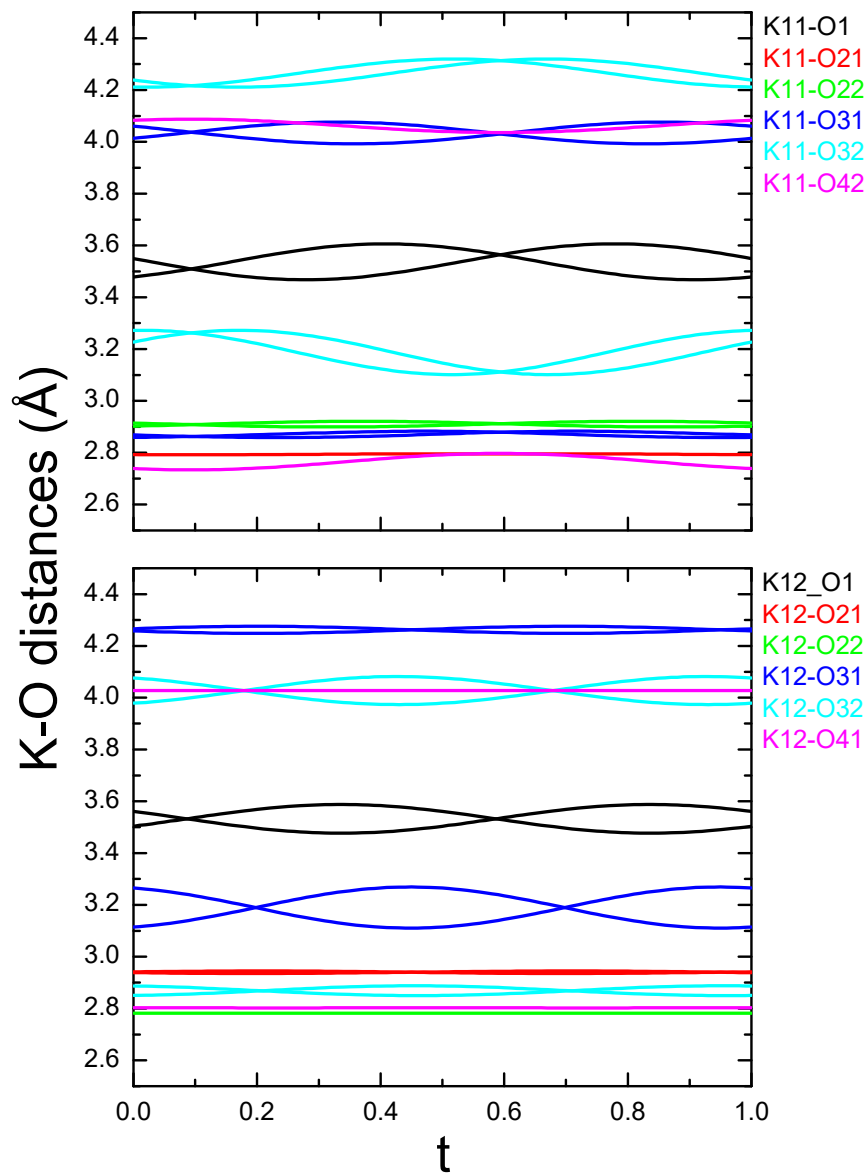**Figure S2**   V1-O interatomic distances in the VO_5 square pyramid as a function of temperature in $K_2V_3O_8$.

Figure S3   V2-O interatomic distances in the VO_4 tetrahedra as a function of temperature in $K_2V_3O_8$. The standard deviations are drawn when larger than the size of the symbols.

Figure S4   V2-O bond-length and O-O distance tetrahedral distortions in $K_2V_3O_8$.

Figure S5   K-O distances in the (3+1)-d structure of $K_2V_3O_8$ at 100 K as a function of the internal coordinate t.
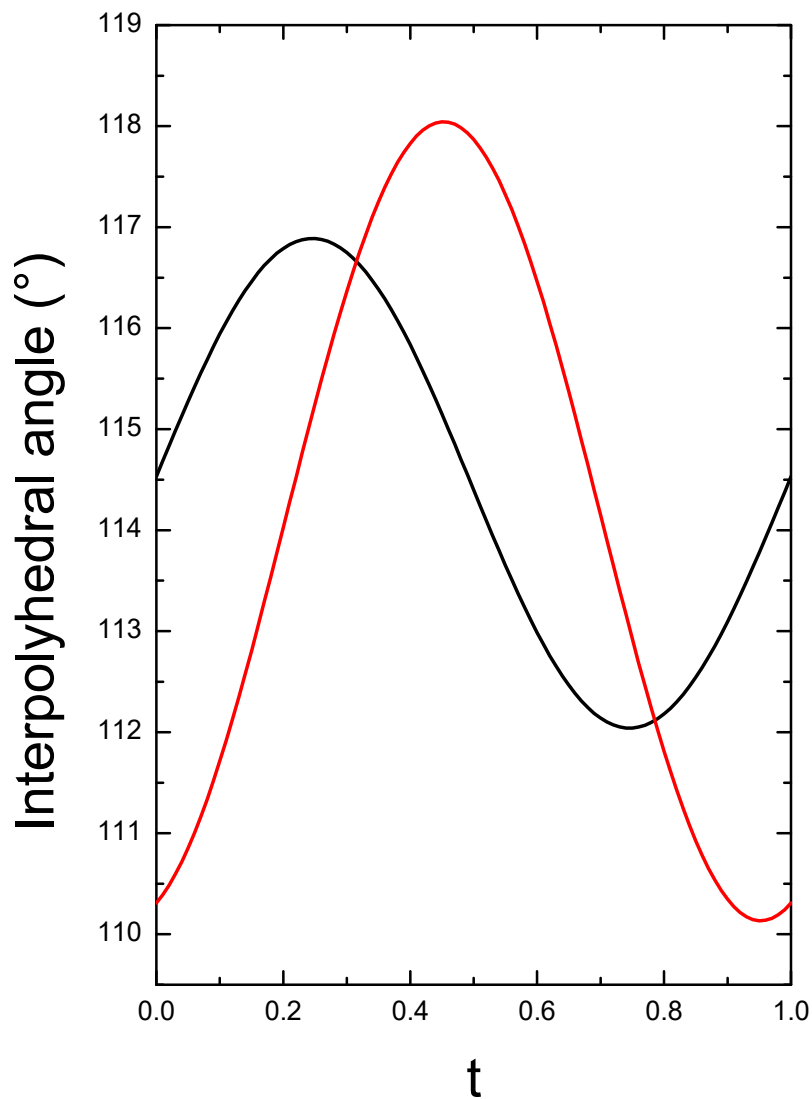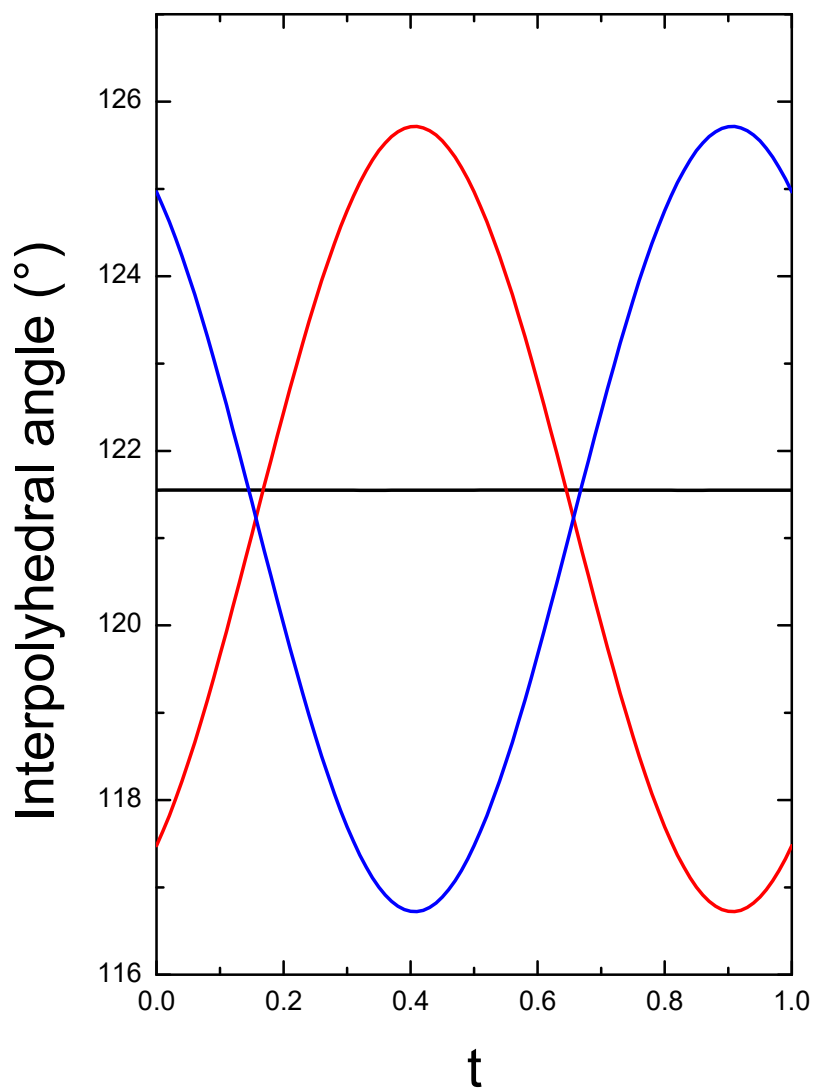
Figure S6   O31-O31-O32 (black line) and O31-O32-O32 (red line) interpolyhedral angles in the

(3+1)-*d* model as a function of the internal coordinate *t*.

Figure S7   O31-O41-O31 (black line), O32-O42-O32 (red line), and O32-O42-O32 (blue line)

interpolyhedral angles in the (3+1)-*d* model as a function of the internal coordinate *t*.