Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Information for:

Synthesis and Structure of $A_4V_6[Te_2^{4+}Te^{6+}]O_{24}$ (A =K, Rb) — Two New Quaternary Mixed-Valent Tellurium Oxides

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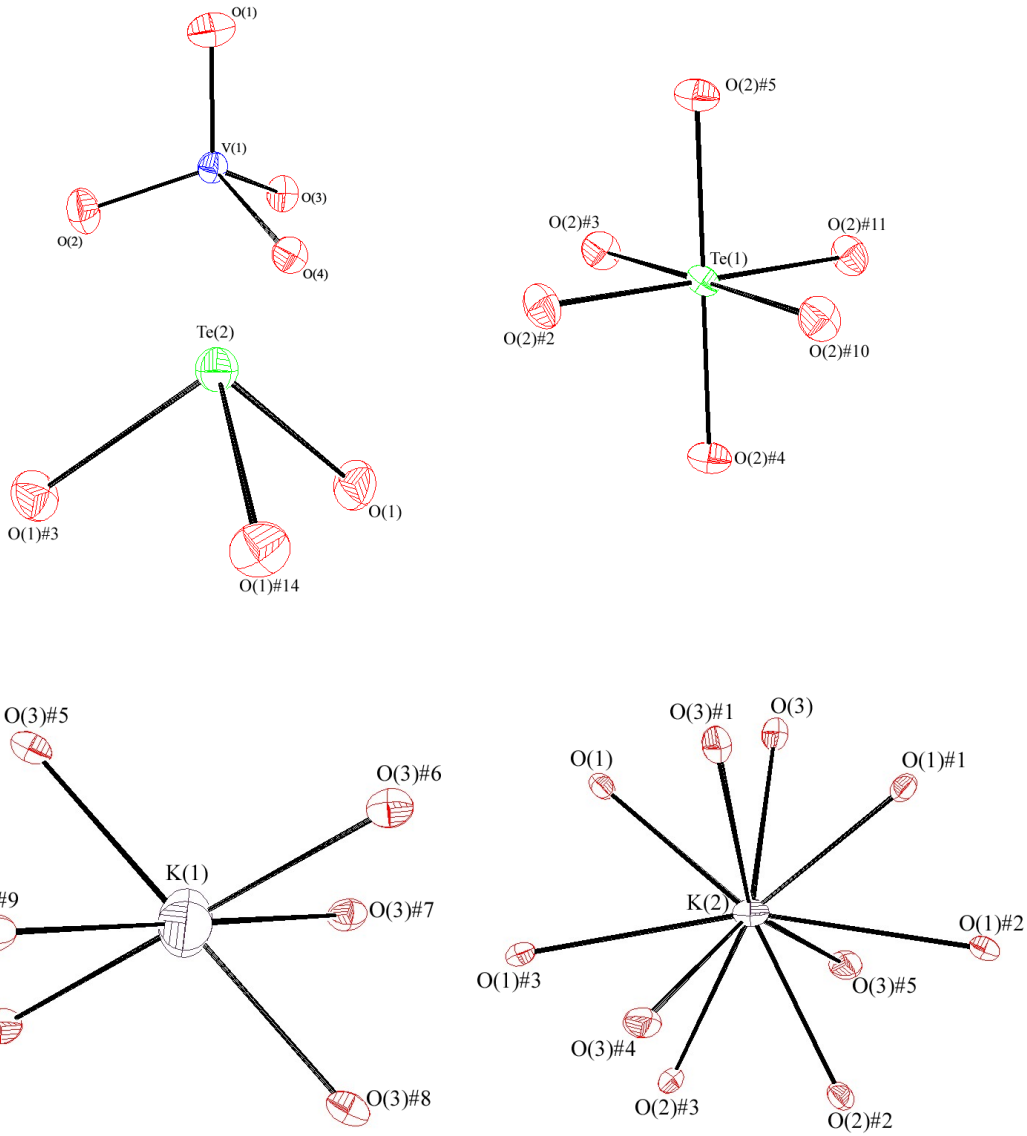
S1. ORTEP (50% probability level ellipsoids) diagrams for the VO_4, TeO_3 and TeO_6 polyhedra and the KO_6, KO_{10} polyhedra for $K_4V_6Te_3O_{24}$



Symmetry transformations used to generate equivalent atoms:

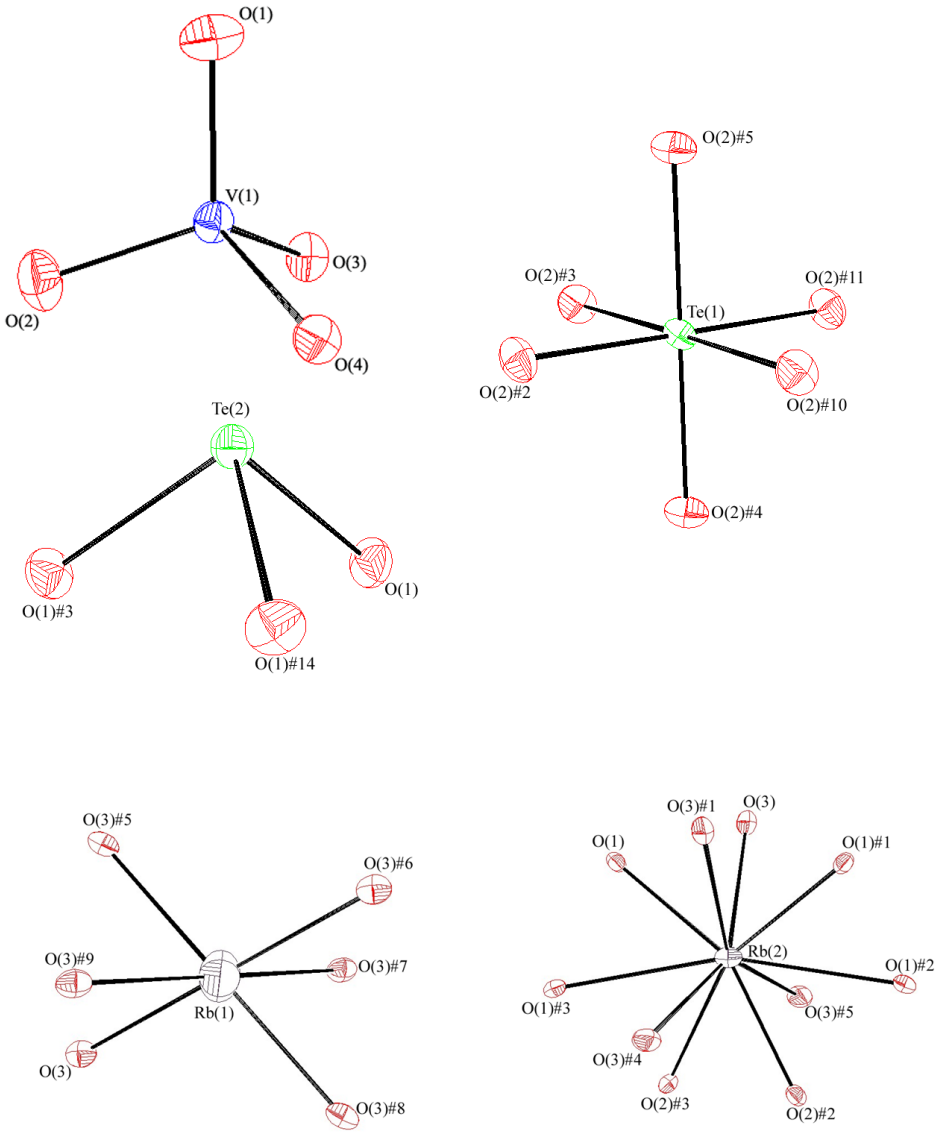
#1 x-y+1/3,-y+2/3,-z+1/6 #2 y+1/3,x-4/3,-z+1/6 #3 -x+y+2,-x+2,z

#4 -x+7/3,-x+y+5/3,-z+1/6 #5 -y+1,x-y-1,z #6 -x+2,-y,-z #7 -x+y+2,-x+1,z

#8 y+1,-x+y+1,-z #9 x-y,x-1,-z #10 x-y-2/3,-y+2/3,-z+1/6 #11 x-1,y,z

#12 -x+y+1,-x+1,z #13 -y+1,x-y,z #14 -y+2,x-y,z #15 x+1,y,z

S2. ORTEP (50% probability level ellipsoids) diagrams for the VO_4, TeO_3 and TeO_6 polyhedra and the RbO_6, RbO_{10} polyhedra for $Rb_4V_6Te_3O_{24}$



Symmetry transformations used to generate equivalent atoms:

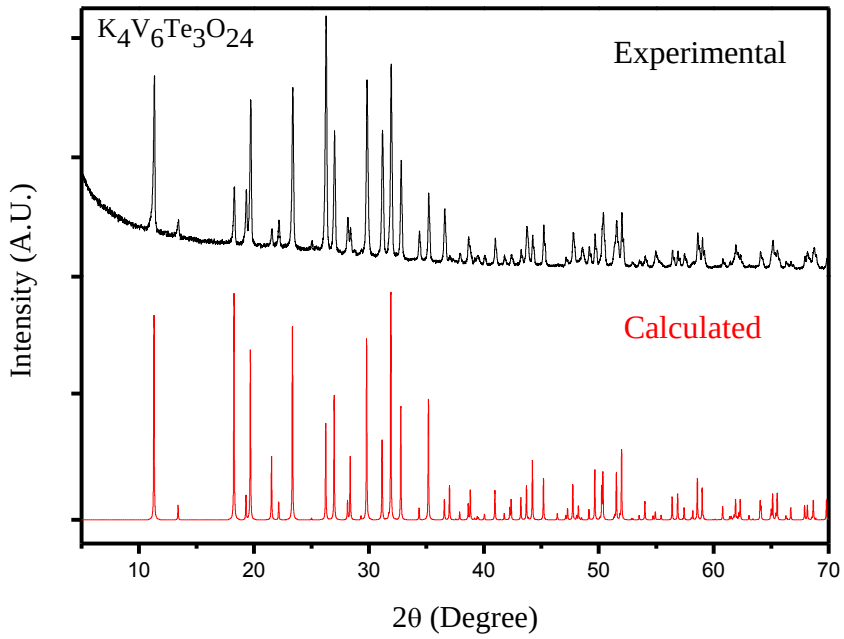
#1 x-y+1/3,-y+2/3,-z+1/6 #2 y+1/3,x-4/3,-z+1/6 #3 -x+y+2,-x+2,z

#4 -x+7/3,-x+y+5/3,-z+1/6 #5 -y+1,x-y-1,z #6 -x+2,-y,-z #7 -x+y+2,-x+1,z

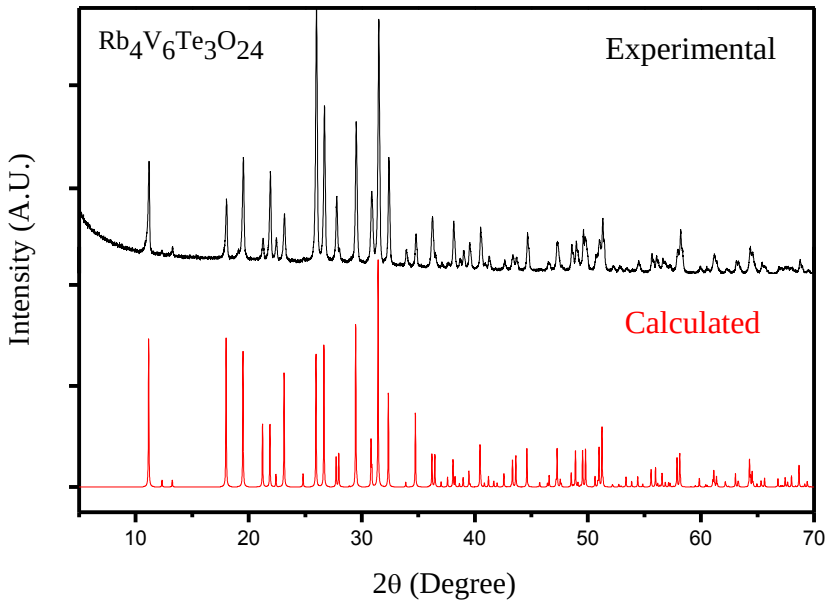
#8 y+1,-x+y+1,-z #9 x-y,x-1,-z #10 x-y-2/3,-y+2/3,-z+1/6 #11 x-1,y,z

#12 -x+y+1,-x+1,z #13 -y+1,x-y,z #14 -y+2,x-y,z #15 x+1,y,z

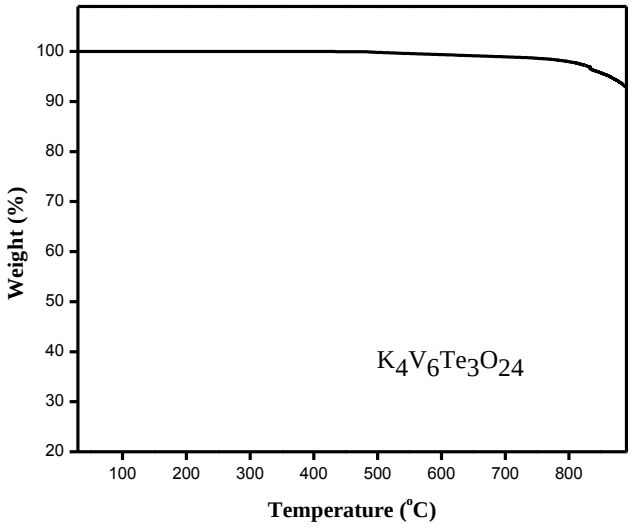
S3. Experimental and calculated powder X-ray diffraction patterns for $K_4V_6Te_3O_{24}$

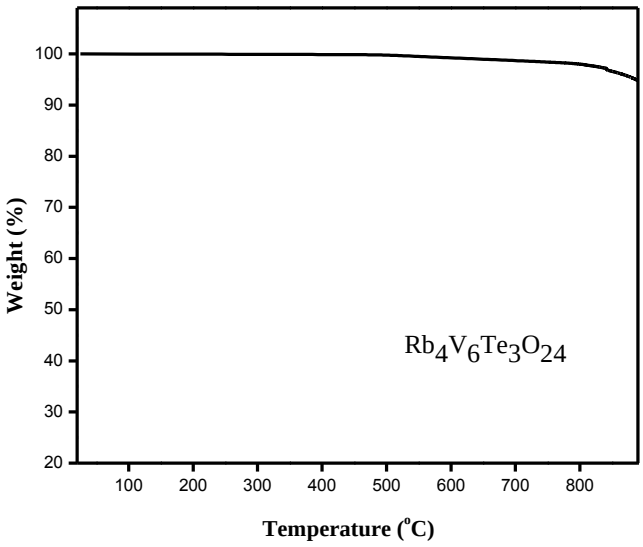


S4. Experimental and calculated powder X-ray diffraction patterns for $Rb_4V_6Te_3O_{24}$



S5.Thermogravimetric plots for $K_4V_6Te_3O_{24}$, $Rb_4V_6Te_3O_{24}$.





S6. Bond strain index (BSI), global instability index (GII) and bond valence data for $K_4Te_3V_6O_{24}$ and $Rb_4Te_3V_6O_{24}$

Compound		**$K_4V_6Te_3O_{24}$**	**$Rb_4V_6Te_3O_{24}$**
BSI		0.076	0.072
GII		0.146	0.141
BVS	**Te^{4+}**	3.80	3.80
	Te^{6+}	6.16	6.08
	V^{5+}	5.06	5.10
	$O(1)^{2-}$	2.38	2.37
	$O(2)^{2-}$	2.09	2.09
	$O(3)^{2-}$	1.89	1.92
	$O(4)^{2-}$	1.54	1.57