Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary table S1. Summary of data collection conditions and refinement parameters for vyacheslavite based on electron diffraction.

Structural formula	$U(PO_4)(OH)$
Unit–cell parameters	a = 6.96 Å, b = 9.07 Å, c = 12.27 Å
V	774.57 Å^3
Z	8
Space group	*Cmca*
D_{calc} (g cm^{-3})	6.042 (for the formula given above)
Temperature	100 K
Diffractometer	TEM Philips CM120
Radiation (wavelength)	electrons, (0.0335 Å)
Resolution	0.1–0.7 Å^{-1}
Limiting Miller indices	$-9<h<9$, $-12<k<12$, $-17<l<17$
No. of independent reflections (obs/all) – kinematic	433/598
R_{int} (obs/all) – kinematic	0.3185/0.3760
Redundancy	10.784
No. of independent reflections (obs/all) – dynamic	4828/14646
Dynamical refinement by Jana2006	
Reflection selection parameter	R_{Sg}(max) = 0.6
No. of reflections (obs/all)	4010/9607
R, wR (obs)	0.0888, 0.0841
N parameters/N struct. parameters	295/39

Supplementary table S2a. Atom positions, displacement parameters (equivalent/isotropic, in Å^2) and bond-valences (in valence units, *vu*) for the crystal structure of vyacheslavite at 100 K.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{iso} (Å^2)	*BV*
U1	0.0	0.69756(9)	0.06804(7)	0.0219(2)	4.42(2)
P1	0.0	0.5962(3)	0.3596(2)	0.0050(9)	5.03(3)
O1	0.0	0.6548(5)	0.2470(4)	0.0222(17)	2.21(2)
O2	0.0	0.9262(6)	0.1374(5)	0.0285(19)	1.96(2)
O3	0.8284(4)	0.6621(3)	0.4247(3)	0.0129(10)	2.15(1)
O4	0.0	0.4436(7)	0.0940(6)	0.057(3)	2.35(3)
H1	0.0	0.431	0.160	0.038*	1.38(2)

*U_{iso} set to 1.2*U_{iso} of the O4 atom.

Supplementary table S2b. Anisotropic displacement parameters (in Å^2) for the structure of vyacheslavite at 100K.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.0180(4)	0.0258(4)	0.0218(4)	0	0	0.0018(6)
P1	0.0036(14)	0.0065(15)	0.0049(16)	0	0	0.0002(13)
O1	0.020(3)	0.028(3)	0.018(3)	0	0	0.000(3)
O2	0.048(3)	0.006(3)	0.031(3)	0	0	0.008(3)
O3	0.0101(15)	0.0153(18)	0.0132(16)	0.0009(11)	0.0027(16)	−0.0074(17)
O4	0.040(4)	0.037(4)	0.093(7)	0	0	−0.015(4)

Supplementary table S3a. Positions of H atoms from DFT (structure relaxed to the ground state).

Lattice (Å)		6.871	8.9181	12.2203
		x	*y*	*z*
H1 - DFT	8*f*	0.0	0.3993	0.1677
H1 - vdW	8*f*	0.0	0.3991	0.1680

Supplementary table S3b. Symmetry constraint relaxation of all atomic positions for fixed experimental lattice at the DFT+U level of theory.

Lattice (Å)		6.871	8.9181	12.2203
Atom		*x*	*y*	*z*
U1	8*f*	0.0	0.6903	0.0669
P1	8*f*	0.0	0.5898	0.3613
O1	8*f*	0.0	0.6685	0.2517
O2	8*f*	0.0	0.9216	0.1525
O3	16*g*	0.8264	0.6462	0.4322
O4	8*f*	0.0	0.4342	0.0982
H1	8*f*	0.0	0.3954	0.1734

Supplementary table S3b. Selected interatomic distances (in Å) and hydrogen bond geometry in the structure of vyacheslavite at 100K.

U1–O1	2.230(5)	P1–O1	1.480(6)
U1–O2	2.241(5)	P1–O2^{vi}	1.542(6)
U1–O3^{i}	2.478(3)	P1–O3	1.557(3)
U1–O3^{ii}	2.311(3)	P1–O3^{vii}	1.557(3)
U1–O3^{iii}	2.311(3)	*<P1–O>*	1.53
U1–O3^{iv}	2.478(3)		
U1–O4	2.325(6)		
U1–O4^{v}	2.364(7)		
<U1–O>	2.34		
O1–O2	2.804(7)	O2–O3^{ix}	2.566(5)
O1–O2^{vi}	2.512(7)	O2–O3^{iv}	2.980(6)
O1–O3	2.487(5)	O3–O3^{x}	2.674(4)
O1–O3^{vii}	2.487(5)	O3–O3^{vii}	2.390(4)
O1–O4	2.682(8)	O3–O4^{viii}	2.827(6)
O2–O3^{i}	2.980(6)	O4–O4^{v}	2.523(10)
O2–O3^{viii}	2.566(5)		

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O4–H1···O2^{vi}	0.812(7)	2.492(6)	3.300(9)	173.0(4)

Symmetry codes: (i) –*x*+2, –*y*+3/2, *z*–1/2; (ii) –*x*+3/2, *y*, –*z*+1/2; (iii) *x*+1/2, *y*, –*z*+1/2; (iv) *x*, –*y*+3/2, *z*–1/2; (v) *x*, –*y*+1, –*z*; (vi) –*x*+2, *y*–1/2, –*z*+1/2; (vii) –*x*+2, *y*, *z*; (viii) –*x*+2, *y*+1/2, –*z*+1/2; (ix) *x*, *y*+1/2, –*z*+1/2; (x) –*x*+3/2, –*y*+3/2, –*z*+1.

Supplementary table S4a. Hydrogen-bond geometry in the structure of vyacheslavite as obtained from DFT. Positions and lattice were fixed at the experimental parameters (obtained from PED data at 100K), except for hydroxyl hydrogen which were relaxed to its ground state.

DFT+U

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O4–H1···O2^{vi}	0.973	2.420	3.322	153.9
O4-H1…O1	0.973	2.444	2.692	93.9
O4-H1…O1^{xii}	0.973	2.449	3.208	134.6
O4-H1…O3^{xii}	0.973	2.657	2.706	82.4
O4-H1…O3^{xiii}	0.973	2.657	2.706	82.4

Symmetry codes: (vi) –*x*+2, *y*–1/2, –*z*+1/2; (xi) 0,*y*,*z*; (xii) *x*,*y*+1/2,–*z*+1/2; (xiii) –*x*+1,*y*+1/2,–*z*+1/2.

DFT+U+vdW

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O4–H1···O2^{vi}	0.977	2.417	3.322	153.8
O4-H1…O1	0.977	2.445	2.692	93.8
O4-H1…O1^{xii}	0.977	2.445	3.208	134.6
O4-H1…O3^{xii}	0.977	2.657	2.706	82.4
O4-H1…O3^{xiii}	0.977	2.657	2.706	82.4

Symmetry codes: (vi) –*x*+2, *y*–1/2, –*z*+1/2; (xi) 0,*y*,*z*; (xii) *x*, *y*+1/2, –*z*+1/2; (xiii) –*x*+1, *y*+1/2, –z+1/2.

Supplementary table S4b. Selected interatomic distances (in Å) and hydrogen bond geometry in the structure of vyacheslavite. Symmetry constraint relaxation of all atomic positions for fixed experimental lattice at the DFT+U level of theory.

DFT+U

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O4–H1···O2^{vi}	0.981	2.141	3.048	153.1
O4-H1…O1	0.981	2.617	2.807	90.8
O4-H1…O1^{XII}	0.981	2.221	2.996	135.0
O4-H1…O3^{XII}	0.981	2.833	2.856	81.4
O4-H1…O3^{XIII}	0.981	2.833	2.856	81.4

(xi) 0,*y*,*z*; (xii) *x*,*y*+1/2,–*z*+1/2; (xiii) –*x*+1,*y*+1/2,–*z*+1/2.