Supporting Information for

The role of non-covalent interactions on vanadium tellurite chain connectivities

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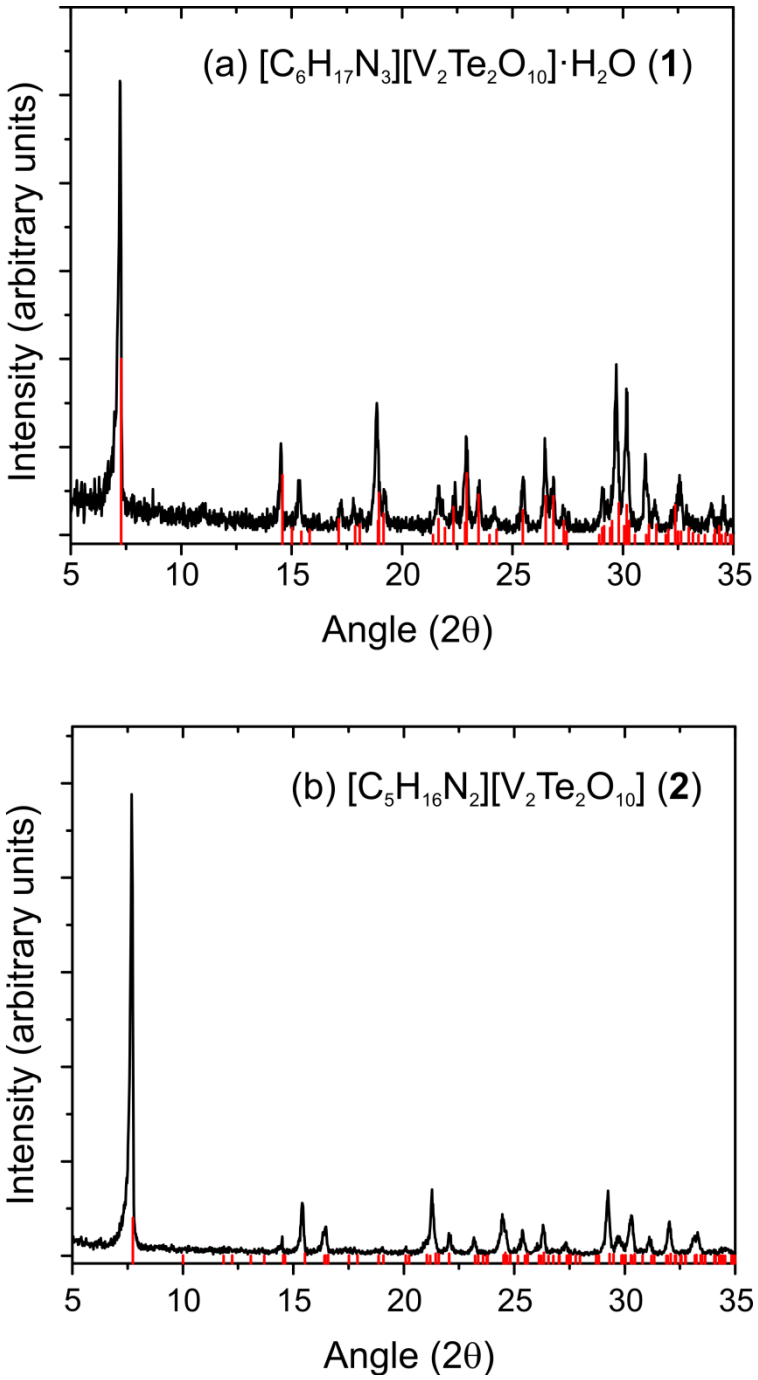

Figure S1. Powder diffraction patterns for (a) **1** and (b) **2**.

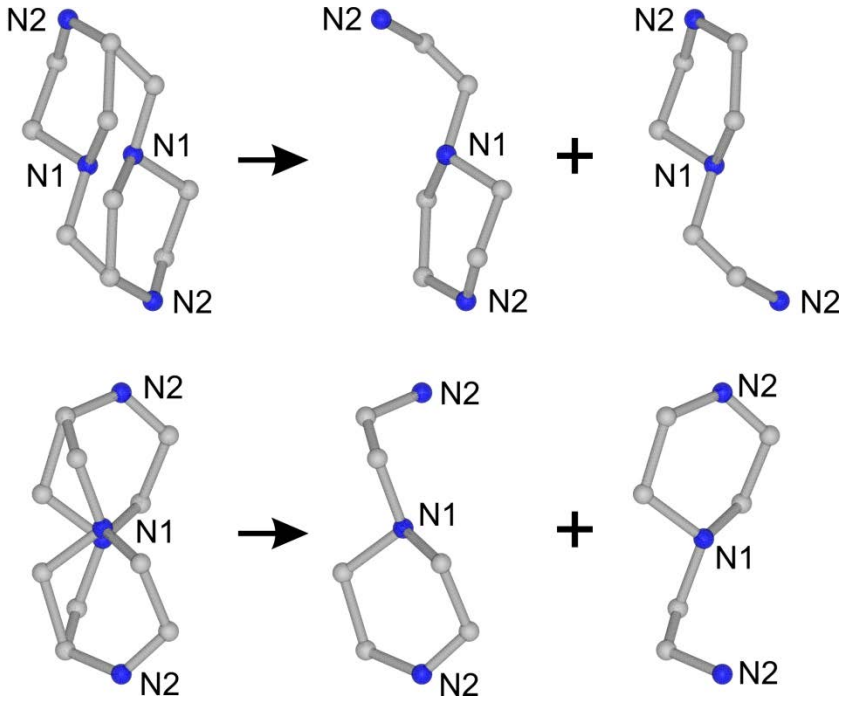

Figure S2. Two views of the $[aepH_2]^{2+}$ cation disorder mechanism in $[C_6H_{17}N_3][V_2Te_2O_{10}]\cdot H_2O$ (**1**).

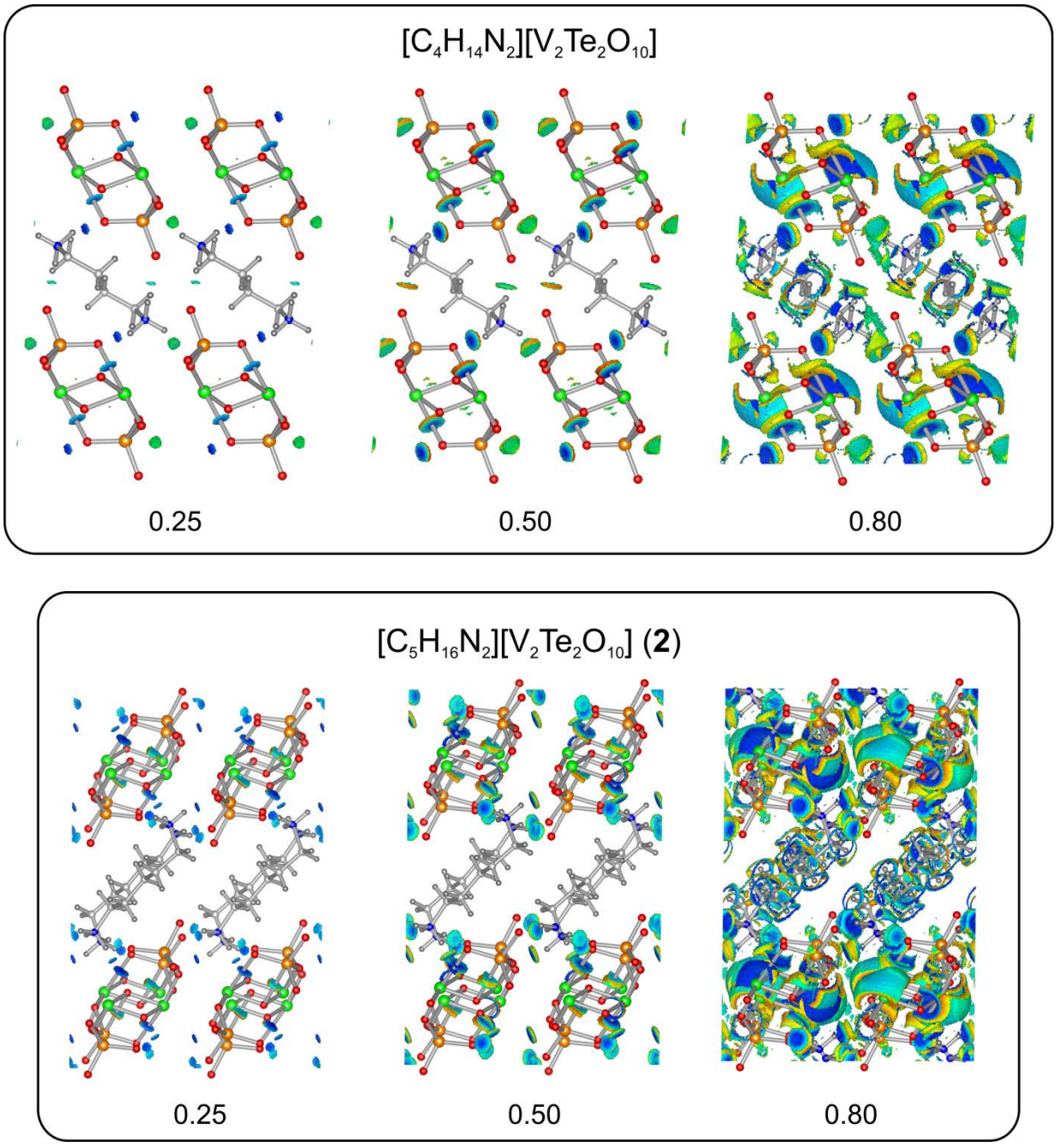

Figure S3. Isosurface as a function of reduced density gradient cutoff for (a) $[C_4H_{14}N_2][V_2Te_2O_{10}]$ and (b) $[C_5H_{16}N_2][V_2Te_2O_{10}]$ (**2**). Surface coloring indicates relative strength (sign(λ_2)ρ) from red = weaker to blue = stronger.

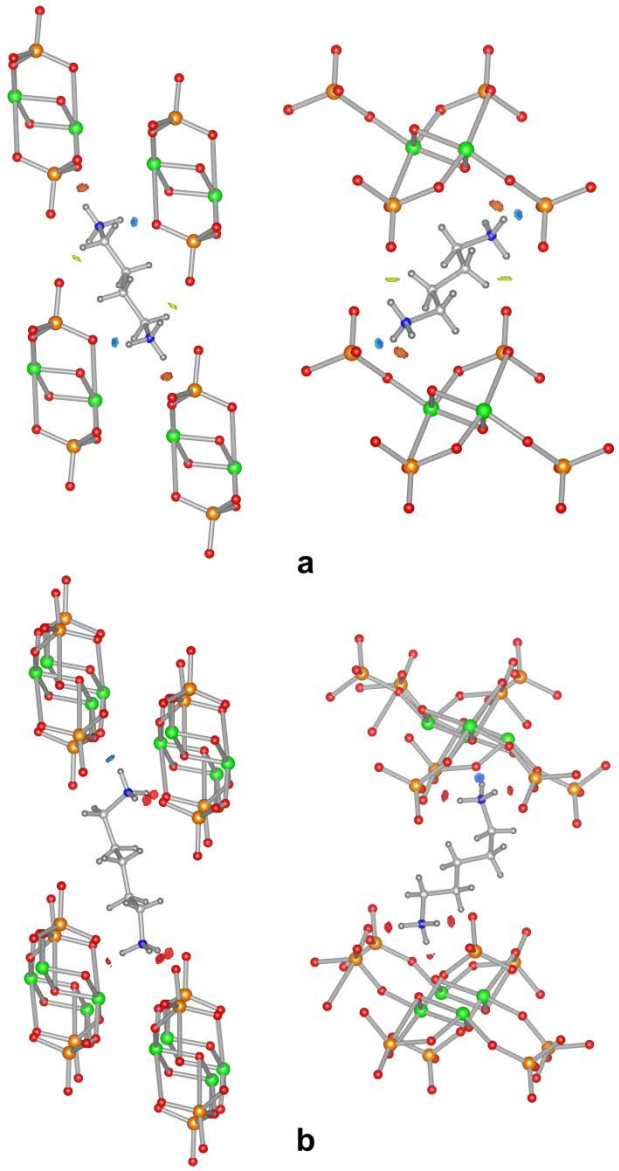

Figure S4. Isosurfaces representing N – H ⋯ O hydrogen bonds in (a) $[C_4H_{14}N_2][V_2Te_2O_{10}]$ and (b) $[C_5H_{16}N_2][V_2Te_2O_{10}]$ (**2**). Surface coloring indicates relative strength (sign(λ_2)ρ) from red = weaker to blue = stronger.

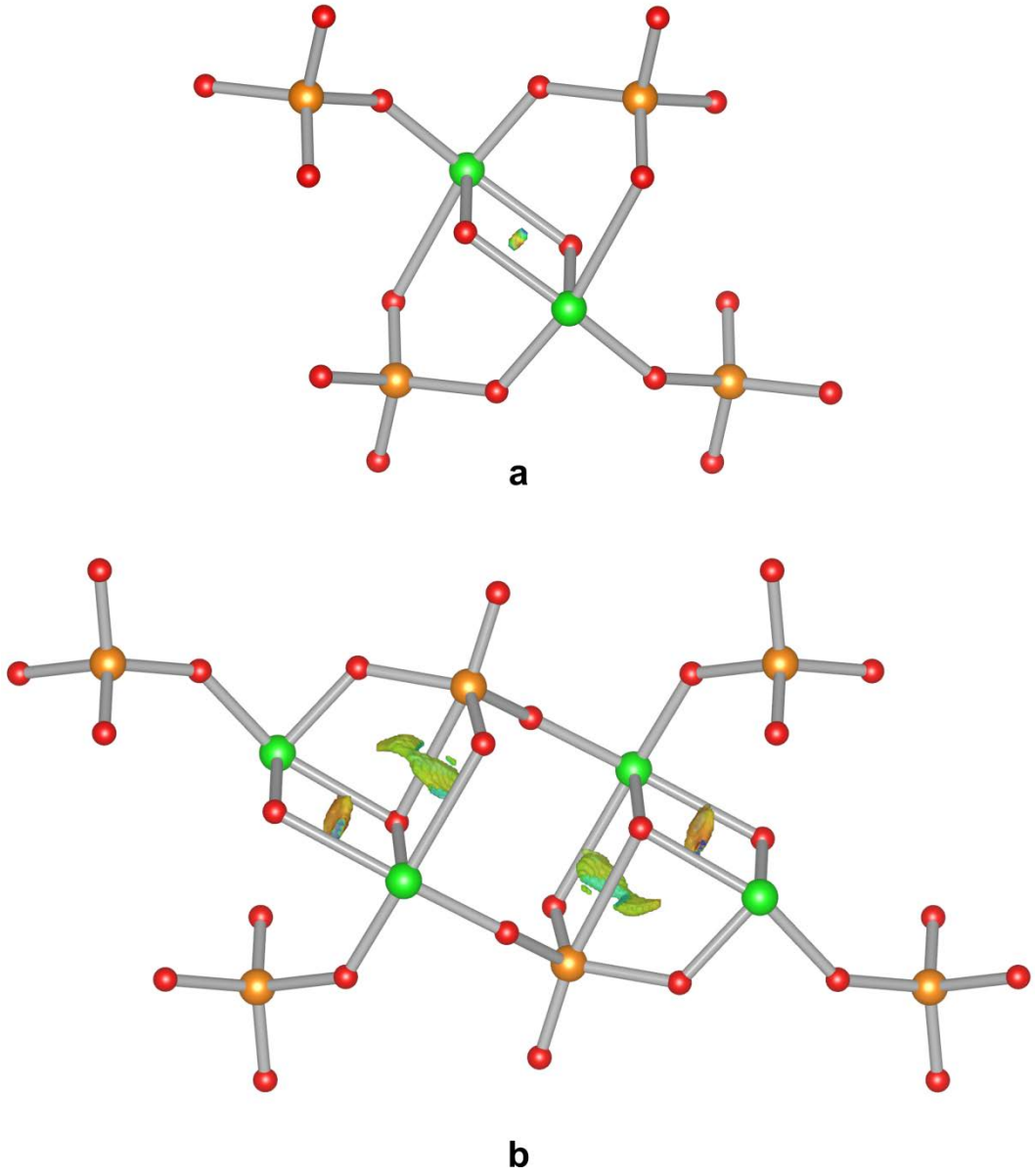

Figure S5. Isosurfaces representing the moderate density repulsions in (a) $[C_4H_{14}N_2][V_2Te_2O_{10}]$ and (b) $[C_5H_{16}N_2][V_2Te_2O_{10}]$ (**2**). Surface coloring indicates relative strength (sign(λ_2)ρ) from red = weaker to blue = stronger.

Table S1. Bond valence sums for $[C_6H_{17}N_3][V_2Te_2O_{10}]\cdot H_2O$ (**1**).

S_i	V1	Te1	Hydrogen bonds	ΣS_i	V- ΣS_i
O1	1.59			1.59	-0.41*
O2	1.47	0.14		1.61	-0.39*
O3	0.89	1.12		2.01	0.01
O4	1.01	0.88		1.89	-0.11*
O5		1.25 0.56		1.81	-0.19
O6			1.6	1.6	-0.40*
ΣS_i	4.96	3.95			

* Hydrogen bond acceptor (determined by N – O and O – O distances).

Table S2. Bond valence sums for $[C_5H_{16}N_2][V_2Te_2O_{10}]$ (**2**).

S_i	V1	V2	Te1	Te2	ΣS_i	V- ΣS_i
O1	1.58				1.58	-0.42*
O2	0.86		1.16		2.02	0.02*
O3	1.47			0.18	1.65	-0.53*
O4	1.00			1.14	2.13	0.13
O5	0.12		0.50	1.31	1.93	-0.07
O6		1.52			1.52	-0.48*
O7		1.55			1.55	-0.45*
O8		0.93		1.17	2.10	0.10
O9		1.03	1.05		2.08	0.08
O10			1.34	0.34	1.69	-0.31*
ΣS_i	5.03	5.03	4.05	4.15		

* Hydrogen bond acceptor (determined by N – O and O – O distances).

Table S3. Hirshfeld-I partial atomic charges for $[V_2Te_2O_{10}]_n^{2n-}$ chain atoms in **1**.

Atom	Iterative-Hirshfeld charge
V1	1.374
Te1	1.371
O1	-0.574
O2	-0.651
O3	-0.712
O4	-0.762
O5	-0.652
O6	-0.875

Table S4. Hirshfeld-I partial atomic charges in **2**.

Atom	Iterative-Hirshfeld charge	Atom	Iterative-Hirshfeld charge
V1	1.470	C1	0.017
V2	1.329	C2	-0.343
Te1	1.329	C3	-0.281
Te2	1.370	C4	-0.323
O1	-0.593	C5	-0.061
O2	-0.696	H1	0.428
O3	-0.656	H2	0.426
O4	-0.732	H3	0.433
O5	-0.670	H4	0.141
O6	-0.626	H5	0.151
O7	-0.586	H6	0.164
O8	-0.696	H7	0.159
O9	-0.708	H8	0.138
O10	-0.693	H9	0.141
N1	-0.979	H10	0.165
N2	-0.952	H11	0.151
		H12	0.160
		H13	0.152
		H14	0.431
		H15	0.424
		H16	0.417

Table S5. Hirshfeld-I partial atomic charges in $[C_4H_{14}N_2][V_2Te_2O_{10}]$.

Atom	Iterative-Hirshfeld charge
V1	1.398
Te1	1.343
O1	-0.638
O2	-0.710
O3	-0.726
O4	-0.650
O5	-0.570
N1	-1.005
C1	0.008
C3	-0.349
H1	0.448
H2	0.440
H3	0.436
H4	0.148
H5	0.129
H6	0.153
H7	0.146

Table S6. Attractive and repulsive interaction energy ratios as a function of reduced density gradient cutoff for $[C_5H_{16}N_2][V_2Te_2O_{10}]$ (**2**) : $[C_4H_{14}N_2][V_2Te_2O_{10}]$.

Reduced density gradient cutoff	Attractive interactions			Repulsions.
	Strong + weak	Strong	Weak	
0.125	2.053	2.548	1.714	1.183
0.175	2.033	2.384	1.780	1.272
0.225	2.070	2.302	1.883	1.359
0.275	2.049	2.145	1.960	1.408
0.325	2.059	2.091	2.028	1.380
0.375	2.089	2.101	2.077	1.356
0.425	2.125	2.113	2.138	1.364
0.475	2.160	2.131	2.195	1.390
0.525	2.162	2.101	2.237	1.409
0.575	2.190	2.133	2.263	1.433
0.625	2.215	2.150	2.303	1.444
0.675	2.350	2.355	2.343	1.428
0.725	2.719	2.933	2.368	1.412
0.775	2.684	2.809	2.409	1.434
0.825	2.607	2.653	2.471	1.445
0.875	2.495	2.475	2.570	1.464
0.925	2.371	2.289	2.739	1.501
0.975	2.305	2.173	2.914	1.548
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