Electronic supplementary information for

Understanding structural adaptability: a reactant informatics approach to experiment design

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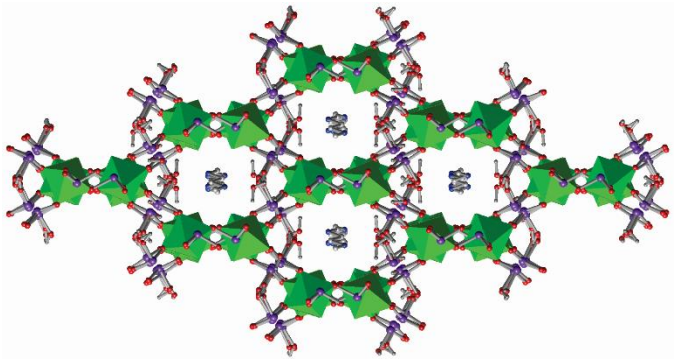

Figure S1. Three dimensional packing of $[C_4H_{14}N_2]_2[VO(SeO_3)(HSeO_3)]_6 \cdot 5H_2O$ (**1**). Green octahedra represent $[VO_6]$ while purple, red, blue, white and gray spheres represent selenium oxygen, nitrogen, carbon and hydrogen atoms, respectively. Selected hydrogen atoms have been removed for clarity.

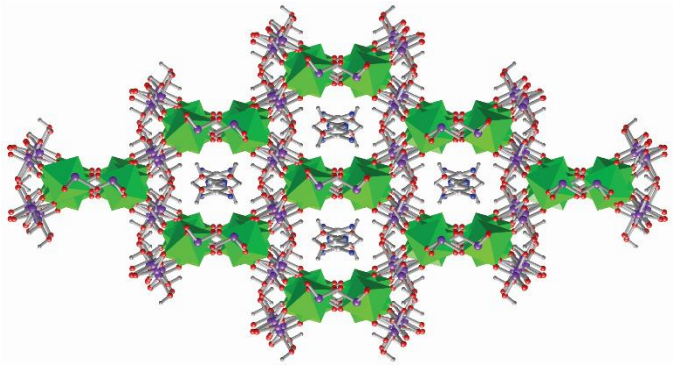

Figure S2. Three dimensional packing of $[C_8H_{26}N_4][VO(SeO_3)(HSeO_3)]_6 \cdot 6H_2O$ (**3**). Green octahedra represent $[VO_6]$ while purple, red, blue, white and gray spheres represent selenium oxygen, nitrogen, carbon and hydrogen atoms, respectively. Selected hydrogen atoms have been removed for clarity.

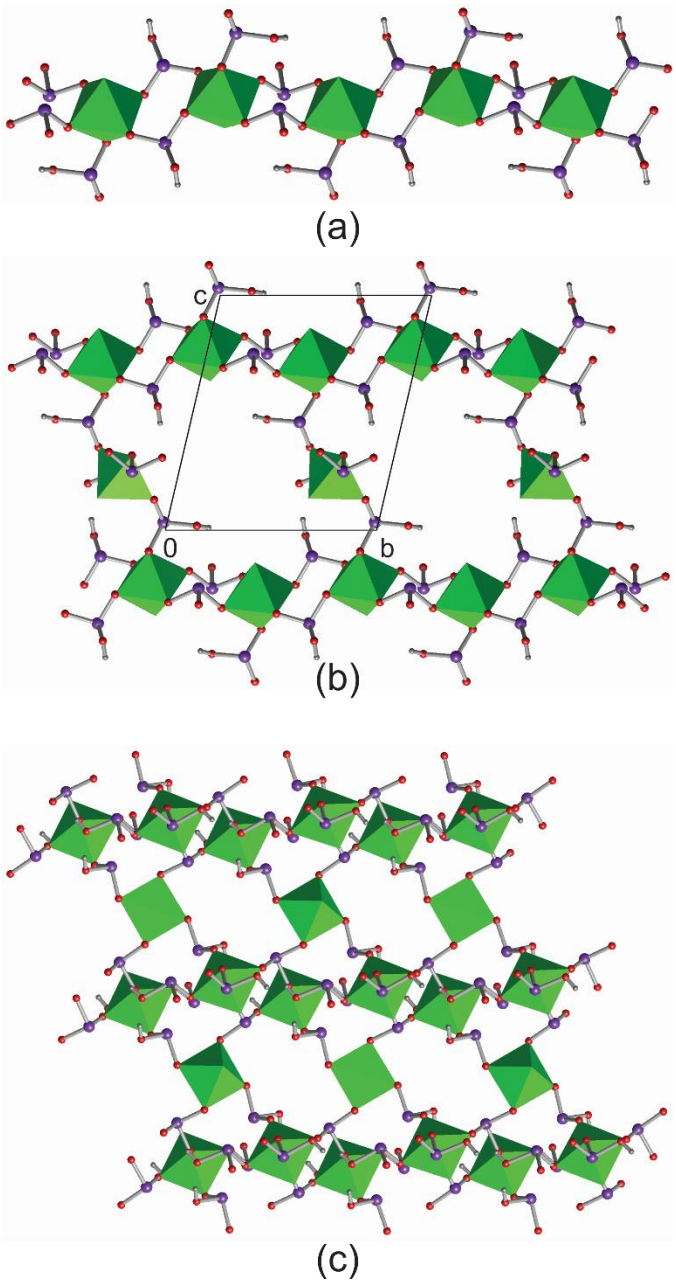

Figure S3. (a) One-dimensional chain SBU and (b) and (c) two slice connectivities in $[C_4H_{12}N_2][(VO)_3(SeO_3)(HSeO_3)_4]\cdot H_2O$ (4). Green polyhedra represent $[VO_6]$ and $[VO_5]$ while purple, red, and gray spheres represent selenium oxygen, and hydrogen atoms, respectively.

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Time taken to build model: 0.03 seconds

=== Stratified cross-validation ===
=== Summary ===

Correctly Classified Instances         114               89.0625 %
Incorrectly Classified Instances        14               10.9375 %
Kappa statistic                          0.5475
Mean absolute error                      0.1174
Root mean squared error                  0.2857
Relative absolute error                 47.6831 %
Root relative squared error             82.1076 %
Coverage of cases (0.95 level)          96.875  %
Mean rel. region size (0.95 level)      65.2344 %
Total Number of Instances              128

=== Detailed Accuracy By Class ===

                 TP Rate  FP Rate  Precision  Recall   F-Measure  MCC
                 0.936    0.389    0.936      0.936    0.936      0.547
                 0.611    0.064    0.611      0.611    0.611      0.547
Weighted Avg.    0.891    0.343    0.891      0.891    0.891      0.547

=== Confusion Matrix ===

   a   b   <-- classified as
 103   7 |   a = 0
   7  11 |   b = 1
```

Figure S4. 10-fold cross validation results for the decision trees in this study.

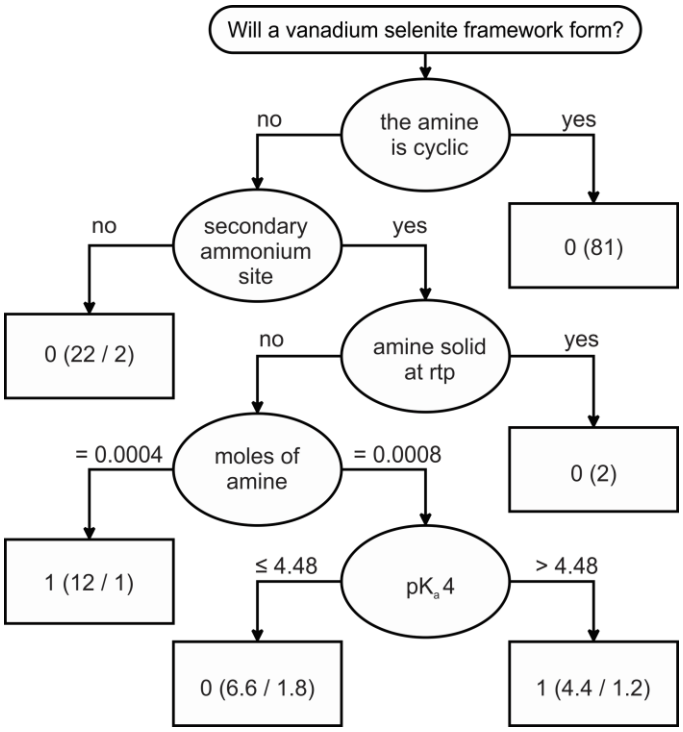

Figure S5. Decision tree containing the 75 historical reactions and the 128 reactions from the fractional factorial analysis. Each reaction bin contains a specific outcome value and number of reactions correctly and incorrectly assigned to that bin, respectively.

Table S1. Descriptors used in the historical reaction set.

Name	Description
amine_abbreviation	abbreviation for the amine used in the reaction
carbon_nitrogen_ratio	ratio of carbon to nitrogen atoms in the amine
pKa1	amine pK_a 1
pKa2	amine pK_a 2
pKa3	amine pK_a 3, if applicable
pKa4	amine pK_a 4, if applicable
min_pKa	minimum amine pK_a value
mw	amine molecular weight (g / mol)
length	length of longest chain in the molecule
nitrogenCount	number of nitrogen atoms in each amine molecule
has_primary	presence (1) or absence (0) of a primary amine in the organic reactant
has_secondary	presence (1) or absence (0) of a secondary amine in the organic reactant
is_cyclic	presence (1) or absence (0) of a ring in the amine
is_spherical	presence (1) or absence (0) of a bicylic structure in the amine
bond_count	number of bonds in the neutral amine
solid_at_rtp	amine exists as a solid (1) or liquid (0) at room temperature
maxproj_N	maximal projection area per N ("inverse charge density")
actual_V_amount	moles of vanadium in the reaction
actual_Se_amount	moles of selenium in the reaction
actual_amine_amount	moles of amine in the reaction
actual_water_amount	mass (g) of vanadium in the reaction
actual_pH	initial reaction pH
Na_present	(1) $NaVO_3$ is the vanadium source or (0) $NaVO_3$ is not the vanadium source
NH4_present	(1) NH_4VO_3 is the vanadium source or (0) NH_4VO_3 is not the vanadium source
temp	maximum reaction temperature in ºC
outcome	coded during data entry: 1 for no solid product, 2 for an amorphous solid, 3 for a polycrystalline sample, 4 for single crystals with average crystallite dimensions exceeding approximately 0.01 mm
purity	coded during data entry: 1 for multiple solid phases present, 2 for a single solid phase

Table S2. Amine specifications.

Name	Abbreviation	Source	Purity (%)
piperazine	pip	Sigma-Aldrich	99
1-methylpiperazine	1-mpip	Sigma-Aldrich	99
2-methylpiperazine	2-mpip	Sigma-Aldrich	95
1,4-dimethylpiperazine	1,4-dmpip	Sigma-Aldrich	98
2,5-dimethylpiperazine	2,5-dmpip	Sigma-Aldrich	98
2,6-dimethylpiperazine	2,6-dmpip	Sigma-Aldrich	97
2-piperazinoethylamine	aep	Sigma-Aldrich	99
1,4-bis(3-aminopropyl)piperazine	bapp	Sigma-Aldrich	≥ 99
1-(2-aminoethyl)pyrrolidine	1-2-aep	Sigma-Aldrich	98
1-(2-aminoethyl)piperidine	1-2-aepip	Sigma-Aldrich	98
1,4-diazabicyclo[2.2.2]octane	dabco	Sigma-Aldrich	≥ 99
ethylenediamine	en	Sigma-Aldrich	≥ 99.5
N-methylethylenediamine	N-meda	Sigma-Aldrich	95
N,N'-dimethylethylenediamine	dmed	Sigma-Aldrich	99
N,N-dimethylethylenediamine	N,N-dmed	Sigma-Aldrich	95
N,N,N'N'-tetramethylethylenediamine	tmed	Sigma-Aldrich	99
diethylenetriamine	deta	Sigma-Aldrich	99
triethylenetetramine	teta	Sigma-Aldrich	≥ 97
1,2-bis(3-aminopropylamino)ethane	Bape	Sigma-Aldrich	94
tetraethylenepentamine	tepa	Sigma-Aldrich	tech.
pentaethylenehexamine	peha	Sigma-Aldrich	80-90
N,N_-bis(3-aminopropyl)-1,4-diaminobutane	spermine	Sigma-Aldrich	≥ 97
tris(2-aminoethyl)amine	tren	Sigma-Aldrich	96
N,N-dimethyl-p-phenylenediamine	dmPhd	Sigma-Aldrich	97
m-phenylenediamine	m-Phd	Sigma-Aldrich	99
N,N'-diphenylethylenediamine	dPhen	Sigma-Aldrich	98
4-aminopiperidine	4-apip	Sigma-Aldrich	≥ 88
N,N,N_,N_-tetramethyl-1,3-propanediamine	tmpda	Sigma-Aldrich	≥ 99
N,N_-diisopropylethylenediamine	N,N'-dipeda	Sigma-Aldrich	99
3-(dimethylamino)-1-propylamine	3-dmpa	Sigma-Aldrich	99
1,3-diaminopropane	1,3-dap	Sigma-Aldrich	≥ 99
N-methyl-1,3-diaminopropane	N-m-1,3-dap	Sigma-Aldrich	98
4-(1-pyrrolidinyl)piperidine	4-1-pp	Sigma-Aldrich	95
1-amino-4-methylpiperidine	1-amino-4-mpip	Sigma-Aldrich	95
3-aminoquinuclidine dihydrochloride	aqnHCl	Sigma-Aldrich	98
N,N-dibutyl-1,3-propanediamine	3-dbapa	Sigma-Aldrich	98
bis(3-aminopropyl)amine	bapa	Sigma-Aldrich	98
1,2-diaminopropane	1,2-dap	Sigma-Aldrich	99
2-amino-1-dimethylaminopropane	dmapa	Sigma-Aldrich	98
diethylamine	diethylamine	Sigma-Aldrich	≥ 99.5
1,4-diaminobutane	1,4-dab	Sigma-Aldrich	99
N-propylethylenediamine	N-peda	Sigma-Aldrich	≥ 97

Table S3. Minimum projection distances, polar surface areas and product structure family designations.

Amine	Minimum projection distance (Å)	Polar surface area (Å^2)	Product structure family*
pip	6.54	33.22	3
1-mpip	7.14	21.05	4
2-mpip	6.54	33.22	1 type-1
1,4-dmpip	7.02	8.88	2
2,5-dmpip	6.68	33.22	1 type-1
2,6-dmpip	7.68	33.22	2
aep	7.28	48.69	amine decomposition
bapp	7.96	64.16	amine decomposition
1-2-aep	6.46	32.08	4
1-2-aepip	6.94	32.08	4
dabco	6.88	8.88	2
en	5.3	55.28	1 type-2
N-meda	5.22	44.25	1 type-2
dmed	5.28	33.22	1 type-2
N,N-dmed	6.64	32.08	2
tmed	7.02	8.88	4
deta	6.14	71.89	1 type-2
teta	6.1	88.5	1 type-2
Bape	7.74	88.5	1 type-2
tepa	8.08	105.11	1 type-2
peha	10.22	121.72	1 type-2
spermine	8.2	88.5	2
tren	8.94	87.36	amine decomposition
dmPhd	6.72	32.08	4
m-Phd	7.78	55.28	4
dPhen	7.5	33.22	4
4-apip	7.18	44.25	2
tmpda	6.52	8.88	4
N,N'-dipeda	7.44	33.22	4
3-dmpa	6.66	32.08	2
1,3-dap	5.78	55.28	2
N-m-1,3-dap	5.74	44.25	2
4-1-pp	6.9	21.05	4
1-amino-4-mpip	6.84	36.52	4
aqnHCl	7.22	32.08	2
3-dbapa	10.92	32.08	2
bapa	6.28	71.89	2
1,2-dap	6.3	55.28	2
dmapa	6.5	32.08	2
diethylamine	5.6	16.61	2
1,4-dab	5.72	55.28	2

N-peda	6.22	44.25	2

*note: Product structure family designations: 1 = [$VO(SeO_3)(HSeO_3)$] frameworks with two modifications (type-1 and type-2); 2 = [$V_3O_5(SeO_3)_3$] layers[1]; 3 = other connectivities; 4 = no templated vanadium selenites observed.

Table S4. Bond valence sums for $[C_4H_{14}N_2]_2[VO(SeO_3)(HSeO_3)]_6 \cdot 5H_2O$ (**1**).

S_i	V1	V2	V3	V4	V5	V6	Se1	Se2	Se3	Se4	Se5	Se6	Se7	Se8	Se9	Se10	Se11	Se12	Se13	Hydrogen bonds	ΣS_i	$V - \Sigma S_i$
O1	1.62						1.42														1.62	-0.38
O2	0.54							1.38													1.96	-0.04
O3	0.51								1.43												1.89	-0.11
O4	0.52												1.38								1.96	-0.04
O5	0.54												1.47								1.92	-0.08
O6	0.32																				1.79	-0.21
O7		1.75																			1.75	-0.25
O8		0.77						1.24													2.01	0.01
O9		0.84							1.13												1.96	-0.04
O10		0.66								1.31											1.97	-0.03
O11		0.57															1.38				1.95	-0.05
O12		0.34																1.46	1.46		1.80	-0.20
O13			1.62																		1.62	-0.38
O14			0.50						1.41												1.91	-0.09
O15			0.53							1.32											1.85	-0.15
O16			0.53								1.39										1.92	-0.08
O17			0.54											1.38							1.92	-0.08
O18			0.29												1.51						1.79	-0.21
O19				1.63																	1.63	-0.37
O20				0.53						1.42											1.95	-0.05
O21				0.54							1.33										1.87	-0.13
O22				0.50								1.42									1.92	-0.08
O23				0.50												1.35					1.85	-0.15
O24				0.30												1.50					1.80	-0.20
O25					1.61																1.61	-0.39
O26					0.51							1.44									1.96	-0.04
O27					0.51		1.35														1.86	-0.14
O28					0.53																1.82	-0.18
O29					0.53			1.42													1.95	-0.05
O30					0.32													1.58	1.26		1.79	-0.21
O31						1.78															1.78	-0.22
O32						0.85						1.12					1.48				1.97	-0.03
O33						0.65					1.29										1.84	-0.16
O34						0.52															1.85	-0.15
O35						0.79	1.19														1.97	-0.03
O36						0.35								1.55							1.90	-0.10
O37													1.15							0.8	1.95	-0.05
O38														1.17						0.8	1.97	-0.03
O39															1.31					0.8	2.11	0.11
O40															0.98					0.8	1.78	-0.22
O41																1.18				0.8	1.98	-0.02
O42																	1.13			0.8	1.93	-0.07
O43																		1.09		0.8	1.89	-0.11
O44																			1.14	0.8	1.94	-0.06
O45																				1.6	1.6	-0.4
O46																				1.6	1.6	-0.4
O47																				1.6	1.6	-0.4
O48																				1.6	1.6	-0.4
O49																				1.6	1.6	-0.4
O50																				1.6	1.6	-0.4
O51																				1.6	1.6	-0.4
ΣS_I	4.05	4.94	4.01	4.00	4.02	4.94	3.96	4.03	3.96	4.05	4.01	3.99	4.00	4.10	4.15	4.02	3.98	3.83	3.88			

Table S5. Bond valence sums for $[C_8H_{26}N_4][VO(SeO_3)(HSeO_3)]_6 \cdot 6H_2O$ (**2**).

S_i	V1	V2	V3	Se1	Se2	Se3	Se4	Se5	Se6	Se7	Hydrogen bonds	ΣS_i	$V - \Sigma S_i$
O1	1.58									disordered		1.58	-0.42
O2	0.53			1.36								1.89	-0.11
O3	0.52			1.35								1.88	-0.12
O4	0.53						1.36					1.89	-0.11
O5	0.54				1.46							2.00	0
O6	0.33						1.50					1.83	-0.17
O7		1.72										1.72	-0.28
O8		0.65		1.28								1.93	-0.07
O9		0.82			1.12							1.94	-0.06
O10		0.77				1.18						1.94	-0.06
O11		0.57							1.22			1.79	-0.21
O12		0.37						1.52				1.89	-0.11
O13			1.58									1.58	-0.32
O14			0.50			1.36						1.87	-0.13
O15			0.54					1.35				1.90	-0.10
O16			0.53		1.39							1.93	-0.07
O17			0.53			1.38						1.91	-0.09
O18			0.29						1.48			1.77	-0.23
O19							1.16					1.96	-0.04
O20								1.15				1.95	-0.05
O21									1.04			1.84	-0.16
O22											1.6	1.6	-0.4
O23											1.6	1.6	-0.4
O24											1.6	1.6	-0.4
ΣS_I	4.04	4.90	3.99	4.00	3.98	3.92	4.01	4.03	3.74				

Table S6. Bond valence sums for $[C_4H_{16}N_2]_2[VO(SeO_3)(HSeO_3)]_8 \cdot 9.333H_2O$ (**3**).

S_i	V1	V2	V3	V4	V5	V6	V7	V8	Se1	Se2	Se3	Se4	Se5	Se6	Se7	Se8	Se9	Se10	Se11	Se12	Se13	Se14	Se15	Se16	Hydrogen bonds	ΣS_i	V – ΣS_i
O1	1.74																									1.74	-0.26
O2	0.81								1.15																	1.96	-0.04
O3	0.81									1.21																2.02	0.02
O4	0.64																	1.35								1.96	-0.04
O5	0.66															1.28										1.94	-0.06
O6	0.34																					1.48				1.82	-0.18
O7		1.60																								1.60	-0.40
O8		0.54									1.32															1.86	-0.14
O9		0.54										1.43														1.96	-0.04
O10		0.53																				1.34				1.87	-0.13
O11		0.54								1.44																1.98	-0.02
O12		0.33																					1.53			1.86	-0.14
O13			1.59																							1.59	-0.41
O14			0.53							1.35																1.88	-0.12
O15			0.52						1.42																	1.94	-0.06
O16			0.52																1.34							1.86	-0.14
O17			0.32														1.50									1.82	-0.18
O18			0.55								1.32															1.87	-0.13
O19				1.59								1.31														1.59	-0.41
O20				0.53							1.34															1.84	-0.16
O21				0.54																						1.88	-0.12
O22				0.51									1.41											1.34		1.85	-0.15
O23				0.52																						1.92	-0.08
O24				0.32									1.18					1.47								1.79	-0.21
O25					1.73									1.21												1.73	-0.27
O26					0.78																					1.96	-0.04
O27					0.82							1.28														2.03	0.03
O28					0.66																1.33					1.99	-0.01
O29					0.67																					1.95	-0.05
O30					0.32															1.51						1.83	-0.17
O31						1.59																				1.59	-0.41
O32						0.52										1.40										1.92	-0.08
O33						0.50														1.31						1.82	-0.18
O34						0.52								1.45												1.97	-0.03
O35						0.54									1.32											1.86	-0.14
O36						0.34													1.52							1.86	-0.14
O37							1.59																			1.59	-0.41
O38							0.52							1.35												1.88	-0.12
O39							0.52						1.42													1.94	-0.06
O40							0.52																1.35			1.89	-0.11
O41							0.60								1.35											1.95	-0.05
O42							0.32																	1.52		1.85	-0.15
O43								1.60																		1.60	-0.40
O44								0.51								1.32										1.83	-0.17
O45								0.55							1.38											1.93	-0.07
O46								1.51	1.42																	1.92	-0.08
O47								0.51									1.38									1.89	-0.11
O48								0.31													1.48					1.79	-0.21
O49																	1.11								0.8	1.91	-0.09
O50																		1.16							0.8	1.96	-0.04
O51																			1.18						0.8	1.98	-0.02
O52																				1.17					0.8	1.97	-0.03
O53																					1.18				0.8	1.98	-0.02
O54																						1.18			0.8	1.98	-0.02
O55																							1.19		0.8	1.99	-0.01
O56																								1.13	0.8	1.83	-0.17
O57																									1.6	1.6	-0.4
O58																									1.6	1.6	-0.4
O59																									1.6	1.6	-0.4
O60																									1.6	1.6	-0.4
O61																									1.6	1.6	-0.4
O62																									1.6	1.6	-0.4
O63																									1.6	1.6	-0.4
O64																									1.6	1.6	-0.4
O65																									1.6	1.6	-0.4
O66																									1.6	1.6	-0.4
O67																									1.6	1.6	-0.4
ΣS_i	4.97	4.03	4.03	4.01	4.99	4.02	4.07	3.99	3.99	4.00	3.98	4.02	4.00	4.01	4.05	4.00	4.00	3.98	4.04	3.99	3.99	3.99	4.07	3.77			

Table S7. Bond valence sums for $[C_4H_{12}N_2][(VO)_3(SeO_3)(HSeO_3)_4]\cdot H_2O$ (**4**).

S_i	V1	V2	V3	Se1	Se2	Se3	Se4	Se5	Se6	Hydrogen bonds	ΣS_i	$V - \Sigma S_i$
O1	1.58										1.58	-0.42
O2	0.52			1.26							1.78	-0.22
O3	0.53				1.35						1.88	-0.12
O4	0.51					1.42					1.93	-0.07
O5	0.54						1.33				1.87	-0.13
O6	0.33								1.46		1.79	-0.21
O7		1.62									1.62	-0.38
O8		0.52				1.35					1.87	-0.13
O9		0.51			1.44						1.95	-0.05
O10		0.55		1.35							1.90	-0.10
O11		0.50					1.29				1.79	-0.21
O12		0.29						1.49			1.79	-0.21
O13			1.65								1.65	-0.35
O14			0.58				1.35				1.93	-0.07
O15			0.60					1.35			1.95	-0.05
O16			0.56	1.35							1.91	-0.09
O17			0.61						1.38		1.99	-0.01
O18						1.15				0.8	1.95	-0.05
O19									1.09	0.8	1.89	-0.11
O20					1.19					0.8	1.99	-0.01
O21								1.05		0.8	1.85	-0.15
O22										1.6	1.6	-0.4
ΣS_I	4.00	3.98	3.99	3.97	3.92	3.97	3.90	3.93				

Table S8. Bond valence sums for $[C_4H_{12}N_2][(VO)_2O_2(SeO_3)_2]$ (**5**).

S_i	V1	Se1	ΣS_i	$V - \Sigma S_i$
O1	1.62		1.62	-0.38
O2	1.44		1.74	-0.26
	0.31			
O3	0.62	1.25	1.88	-0.12
O4	0.63	1.28	1.91	-0.09
O5	0.35	1.39	1.74	-0.26
ΣS_I	4.97	3.93		

Table S9. Bond valence sums for vanadium centers in compounds **1 – 5**, $[C_6H_{16}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$, $[C_5H_{14}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$, $[(S)\text{-}C_5H_{14}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$ and $[(R)\text{-}C_5H_{14}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$.

Compound	V1	V2	V3	V4	V5	V6	V7	V8
$[C_4H_{14}N_2]_2[VO(SeO_3)(HSeO_3)]_6 \cdot 5H_2O$ (**1**)	4.05	4.94	4.01	4.00	4.02	4.94	-	-
$[C_8H_{26}N_4][VO(SeO_3)(HSeO_3)]_6 \cdot 6H_2O$ (**2**)	4.04	4.90	3.99	-	-	-	-	-
$[C_4H_{16}N_2]_2[VO(SeO_3)(HSeO_3)]_8 \cdot 9.333H_2O$ (**3**)	4.97	4.06	4.03	4.01	4.99	4.02	4.07	3.99
$[C_4H_{12}N_2][(VO)_3(SeO_3)(HSeO_3)_4] \cdot H_2O$ (**4**)	4.00	3.98	3.99	-	-	-	-	-
$[C_4H_{12}N_2][(VO)_2O_2(SeO_3)_2]$ (**5**)	4.97							
$[C_6H_{16}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$[2]	3.93	-	-	-	-	-	-	-
$[C_5H_{14}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$[2]	4.02	3.94	-	-	-	-	-	-
$[(S)\text{-}C_5H_{14}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$[2]	3.97	3.97	-	-	-	-	-	-
$[(R)\text{-}C_5H_{14}N_2][VO(SeO_3)(HSeO_3)]_2 \cdot 2H_2O$[2]	3.95	3.96	-	-	-	-	-	-

(1) Adler, P. D. F.; Xu, R.; Olshansky, J. H.; Smith, M. D.; Elbert, K. C.; Yang, Y.; Ferrence, G. M.; Zeller, M.; Schrier, J.; Norquist, A. J. Probing structural adaptability in templated vanadium selenites *Polyhedron* **2016**, *114*, 184-193.

(2) Olshansky, J. H.; Thao Tran, T.; Hernandez, K. J.; Zeller, M.; Halasyamani, P. S.; Schrier, J.; Norquist, A. J. Role of Hydrogen-Bonding in the Formation of Polar Achiral and Nonpolar Chiral Vanadium Selenite Frameworks *Inorg. Chem.* **2012**, *51*, 11040-11048.

Table S10. Fractional factorial analysis study results.

Condition	Outcome
Number of amines involved in reactions resulting in type-2 [$VO(SeO_3)(HSeO_3)$] frameworks	10
Amines involved in reactions resulting in type-2 [$VO(SeO_3)(HSeO_3)$] frameworks	aep, bape, deta, dmed, en, n-meda, peha, tepa, teta, tren
Number of individual reactions resulting in type-2 [$VO(SeO_3)(HSeO_3)$] frameworks	27
Number of individual reactions resulting in type-2 [$VO(SeO_3)(HSeO_3)$] frameworks without amine decomposition	19
Amines involved in decomposition reactions	aep, tren
Number of unique compounds synthesized that contain type-2 [$VO(SeO_3)(HSeO_3)$] frameworks	8

Table S11. Number of reactions from the fractional factorial analysis that produced compounds containing both type-2 [$VO(SeO_3)(HSeO_3)$] frameworks and the following amines.

Amine	Number of reactions
bis-aminopropylethylenediamine (bape)	3
diethyltriamine (deta)	10
ethylenediamine (en)	5
n-methylethylenediamine (n-meda)	2
pentaethylhexamine (peha)	2
tetraethylpentamine (tepa)	1
triethyltetramine (teta)	1

Table S12. Confusion matrix for the historical decision tree.

	True positive	True negative
Predicted positive	18	2
Predicted negative	2	53

Table S13. Confusion matrix for the [$VO(SeO_3)(HSeO_3)$] type-2 framework decision tree (26 amines).

	True positive	True negative
Predicted positive	7	0
Predicted negative	3	16

Table S14. Confusion matrix for the [$VO(SeO_3)(HSeO_3)$] type-2 framework decision tree (42 amines).

	True positive	True negative
Predicted positive	7	1
Predicted negative	1	33

Table S15. Decision tree confusion matrix values.

Measure	Historical decision tree	$[VO(SeO_3)(HSeO_3)]$ type-2 framework decision tree (26 amines)	$[VO(SeO_3)(HSeO_3)]$ type-2 framework decision tree (42 amines)
Sensitivity	0.9000	0.7000	0.8750
Specificity	0.9636	1.000	0.9706
Precision	0.9000	1.000	0.8750
Negative predictive value	0.9636	0.8421	0.9706
False positive rate	0.0364	0.000	0.0294
False discovery rate	0.1000	0.000	0.1250
False negative rate	0.1000	0.3000	0.1250
Accuracy	0.9467	0.8846	0.9524
F1 score	0.9000	0.8335	0.8750
Matthews correlation coefficient	0.8636	0.7678	0.8456