Synthesis, crystal structure, optical properties and quantum chemical studies of novel organic–inorganic material based on Polyoxodecavanadate

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Table S1. Parallel examination of selected bond distances (Å) in vanadate via XRD.

	XRD		**XRD**
V1—O1	1.594 (2)	V5—V9	3.0898 (7)
V1—O2	1.825 (2)	V5—V8	3.1100 (6)
V1—O6	1.8278 (19)	V6—O10	1.6729 (19)
V1—O4	1.9270 (19)	V6—O19	1.6887 (19)
V1—O8	2.037 (2)	V6—O15	1.8626 (18)
V1—O9	2.3830 (19)	V6—O16	2.0499 (18)
V1—V5	3.0631 (7)	V6—O9	2.0964 (18)

V1—V2	3.0753 (7)	V6—O18	2.1041 (17)
V1—V4	3.1057 (7)	V6—V10	3.0356 (7)
V2—O3	1.594 (2)	V7—O20	1.5986 (19)
V2—O2	1.836 (2)	V7—O22	1.7986 (18)
V2—O5	1.8617 (19)	V7—O24	1.8748 (19)
V2—O7	1.8850 (19)	V7—O13	1.9381 (19)
V2—O10	2.058 (2)	V7—O15	1.9985 (18)
V2—O9	2.3135 (18)	V7—O18	2.3303 (18)
V2—V6	3.0723 (7)	V7—V9	3.0766 (6)
V2—V4	3.0948 (6)	V7—V10	3.0894 (6)
V2—V3	3.1065 (6)	V8—O21	1.6176 (18)
V3—O11	1.5947 (18)	V8—O23	1.7136 (18)
V3—O7	1.7795 (19)	V8—O14	1.9180 (19)
V3—O6	1.8577 (19)	V8—O25	1.947 (2)
V3—O15	1.9919 (19)	V8—O16	2.1173 (19)
V3—O13	2.0227 (18)	V8—O18	2.1990 (17)
V3—O9	2.2922 (18)	V8—V9	3.0795 (6)
V3—V7	3.0291 (7)	V9—O26	1.595 (2)
V3—V6	3.1049 (6)	V9—O27	1.796 (2)
V4—O12	1.6226 (19)	V9—O22	1.8425 (18)
V4—O4	1.7391 (19)	V9—O23	1.9724 (19)
V4—O5	1.8406 (18)	V9—O17	2.028 (2)
V4—O14	1.9864 (18)	V9—O18	2.3262 (18)
V4—O16	2.1167 (19)	V9—V10	3.0732 (6)
V4—O9	2.2294 (17)	V10—O28	1.597 (2)
V5—O8	1.6785 (19)	V10—O24	1.7902 (19)
V5—O17	1.6880 (19)	V10—O27	1.8542 (19)
V5—O13	1.9085 (18)	V10—O25	2.0088 (19)
V5—O14	1.9540 (18)	V10—O19	2.0114 (19)
V5—O9	2.0783 (18)	V10—O18	2.2857 (18)
V5—O18	2.1447 (18)	—	—

Table S2. Parallel examination of selected bond angles (°) in vanadate via XRD.

	XRD		**XRD**
O1—V1—O2	105.14 (10)	O10—V6—O19	107.12 (9)

O1—V1—O6	102.02 (10)	O10—V6—O15	100.46 (9)
O2—V1—O6	93.16 (9)	O19—V6—O15	99.85 (9)
O1—V1—O4	103.06 (10)	O10—V6—O16	93.83 (8)
O2—V1—O4	88.38 (8)	O19—V6—O16	94.11 (8)
O6—V1—O4	153.53 (9)	O15—V6—O16	156.04 (8)
O1—V1—O8	100.36 (10)	O10—V6—O9	87.62 (8)
O2—V1—O8	154.16 (8)	O19—V6—O9	163.86 (8)
O6—V1—O8	85.53 (8)	O15—V6—O9	83.44 (7)
O4—V1—O8	81.79 (8)	O16—V6—O9	78.01 (7)
O1—V1—O9	173.69 (9)	O10—V6—O18	164.39 (8)
O2—V1—O9	81.03 (8)	O19—V6—O18	86.78 (8)
O6—V1—O9	78.67 (7)	O15—V6—O18	83.65 (7)
O4—V1—O9	75.47 (7)	O16—V6—O18	77.76 (7)
O8—V1—O9	73.40 (7)	O9—V6—O18	77.84 (7)
O3—V2—O2	103.47 (10)	O20—V7—O22	102.22 (9)
O3—V2—O5	101.43 (9)	O20—V7—O24	102.12 (9)
O2—V2—O5	91.68 (9)	O22—V7—O24	93.15 (8)
O3—V2—O7	102.13 (9)	O20—V7—O13	101.90 (9)
O2—V2—O7	91.22 (9)	O22—V7—O13	92.11 (8)
O5—V2—O7	154.88 (8)	O24—V7—O13	153.70 (8)
O3—V2—O10	100.14 (10)	O20—V7—O15	101.51 (9)
O2—V2—O10	156.36 (8)	O22—V7—O15	155.61 (8)
O5—V2—O10	84.73 (8)	O24—V7—O15	87.31 (8)
O7—V2—O10	82.67 (8)	O13—V7—O15	77.54 (7)
O3—V2—O9	173.75 (10)	O20—V7—O18	176.52 (8)
O2—V2—O9	82.77 (8)	O22—V7—O18	81.08 (7)
O5—V2—O9	77.82 (7)	O24—V7—O18	78.66 (7)
O7—V2—O9	77.80 (7)	O13—V7—O18	76.74 (7)
O10—V2—O9	73.62 (7)	O15—V7—O18	75.10 (7)
O11—V3—O7	104.49 (9)	O16—V8—O18	74.32 (7)
O11—V3—O6	103.46 (9)	O21—V8—O23	105.19 (9)
O7—V3—O6	94.54 (9)	O21—V8—O14	101.96 (9)
O11—V3—O15	99.23 (9)	O23—V8—O14	96.74 (8)
O7—V3—O15	91.75 (8)	O21—V8—O25	98.89 (9)
O6—V3—O15	154.08 (8)	O23—V8—O25	94.56 (9)

O11—V3—O13	100.20 (9)	O14—V8—O25	152.72 (8)
O7—V3—O13	153.84 (8)	O21—V8—O16	95.87 (8)
O6—V3—O13	87.93 (8)	O23—V8—O16	158.71 (8)
O15—V3—O13	75.77 (7)	O14—V8—O16	75.50 (7)
O11—V3—O9	173.21 (9)	O25—V8—O16	85.08 (8)
O7—V3—O9	80.42 (7)	O21—V8—O18	169.87 (8)
O6—V3—O9	80.56 (7)	O23—V8—O18	84.76 (8)
O15—V3—O9	75.73 (7)	O14—V8—O18	78.30 (7)
O13—V3—O9	74.30 (7)	O25—V8—O18	78.11 (7)
O12—V4—O4	104.65 (9)		104.99 (10)
O12—V4—O5	102.77 (9)	O26—V9—O22	102.65 (9)
O4—V4—O5	97.63 (9)	O27—V9—O22	93.71 (9)
O12—V4—O14	99.02 (9)	O26—V9—O23	100.16 (9)
O4—V4—O14	93.27 (8)	O27—V9—O23	89.70 (8)
O5—V4—O14	152.22 (8)	O22—V9—O23	155.18 (8)
O12—V4—O16	97.71 (9)	O26—V9—O17	100.14 (10)
O4—V4—O16	155.88 (8)	O27—V9—O17	154.44 (8)
O5—V4—O16	85.97 (8)	O22—V9—O17	85.27 (8)
O14—V4—O16	74.15 (7)	O23—V9—O17	81.22 (8)
O12—V4—O9	170.77 (9)	O26—V9—O18	173.45 (9)
O4—V4—O9	83.28 (8)	O27—V9—O18	80.48 (7)
O5—V4—O9	80.48 (7)	O22—V9—O18	80.32 (7)
O14—V4—O9	75.50 (7)	O23—V9—O18	76.02 (7)
O16—V4—O9	73.76 (7)	O17—V9—O18	74.16 (7)
O8—V5—O17	107.25 (9)	O28—V10—O24	105.48 (10)
O8—V5—O13	98.25 (8)	O28—V10—O27	104.13 (10)
O17—V5—O13	97.56 (8)	O24—V10—O27	93.75 (8)
O8—V5—O14	96.87 (8)	O28—V10—O25	97.74 (9)
O17—V5—O14	95.62 (8)	O24—V10—O25	156.23 (9)
O13—V5—O14	155.99 (8)	O27—V10—O25	85.31 (8)
O8—V5—O9	89.31 (8)	O28—V10—O19	99.56 (9)
O17—V5—O9	163.29 (8)	O24—V10—O19	88.33 (8)
O13—V5—O9	81.84 (7)	O27—V10—O19	154.70 (8)
O14—V5—O9	79.80 (7)	O25—V10—O19	82.82 (8)
O8—V5—O18	166.48 (8)	O28—V10—O18	171.13 (9)

O17—V5—O18	86.03 (8)	O24—V10—O18	81.55 (8)
O13—V5—O18	82.08 (7)	O27—V10—O18	80.43 (8)
O14—V5—O18	78.90 (7)	O25—V10—O18	74.86 (7)
O9—V5—O18	77.33 (7)	O19—V10—O18	74.93 (7)

Table S3. Hydrogen bond geometry (Å, °) of vanadate.

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	**<*(D*—H···*A)*°**
O16—H16*O*···O21^{i}	0.78 (3)	1.92 (3)	2.696 (2)	170 (3)
O25—H26*O*···O12^{i}	0.72 (4)	1.98 (4)	2.696 (3)	171 (4)
N1—H1*N*···O6^{ii}	0.88	1.80	2.639 (3)	159
C1—H1···O7^{iii}	0.95	2.14	3.009 (3)	151
C1—H1···O11^{iii}	0.95	2.57	3.209 (3)	125
C2—H2···O8	0.95	2.57	3.447 (3)	154
C3—H3···O4	0.95	2.30	2.970 (3)	127
C3—H3···O12	0.95	2.62	3.481 (3)	151
C4—H4···O3^{iii}	0.95	2.57	3.506 (3)	168
N3—H3*N*···O2*W*	0.88	1.91	2.759 (4)	162
C6—H6···O22^{iv}	0.95	2.25	3.104 (3)	149
C7—H7···O1	0.95	2.42	3.118 (4)	131
C8—H8···O13^{ii}	0.95	2.24	3.173 (3)	168
C10—H10*A*···O20^{ii}	0.95	2.66	3.324 (4)	127
C10—H10*B*···O4WA^{iii}	0.95	2.60	3.474 (9)	154
C10—H10*B*···O4WB^{iii}	0.95	2.63	3.130 (10)	114
N5—H5*N*···O5^{v}	0.88	1.84	2.706 (3)	166
C11—H11···O25^{vi}	0.95	2.37	3.215 (3)	148
C11—H11···O27^{vi}	0.95	2.51	3.271 (3)	137
C12—H12···O3^{v}	0.95	2.48	3.095 (3)	123
C12—H12···O26^{ii}	0.95	2.34	3.253 (3)	161
C13—H13···O23^{ii}	0.95	2.47	3.172 (3)	131
C14—H14···O27^{vi}	0.95	2.64	3.324 (3)	130
N7A—H7AN···O3*W*	0.88	1.89	2.745 (7)	164
C16A—H16A···O14^{ii}	0.95	2.21	3.124 (5)	161
C16A—H16A···O17^{ii}	0.95	2.65	3.346 (5)	130
C17A—H17A···O20^{vii}	0.95	2.40	3.073 (5)	127
C17A—H17A···O2*W*^{v}	0.95	2.66	3.441 (6)	140

C18A—H18A···O15^{vii}	0.95	2.41	3.224 (5)	144
C19A—H19A···O21^{ii}	0.95	2.59	3.287 (4)	130
N7B—H7BN···O3*W*	0.88	1.59	2.329 (17)	140
C16B—H16B···O14^{ii}	0.95	2.46	3.35 (2)	156
C16B—H16B···O23^{ii}	0.95	2.53	3.30 (2)	138
C18B—H18B···O11^{vii}	0.95	2.58	3.26 (2)	129
C18B—H18B···O15^{vii}	0.95	2.47	3.357 (17)	155
C18B—H18B···O20^{vii}	0.95	2.23	2.884 (16)	126
O1*W*—H1*O*···O24^{iv}	0.80 (1)	1.98 (1)	2.774 (3)	172 (4)
O1*W*—H1*P*···O28^{i}	0.80 (1)	2.29 (1)	3.033 (3)	155 (2)
O2*W*—H2*P*···O2	0.80 (1)	2.27 (1)	2.995 (3)	151 (3)
O2*W*—H2*P*···O4	0.80 (1)	2.63 (3)	3.182 (3)	128 (3)
O2*W*—H2*P*···O5	0.80 (1)	2.65 (2)	3.328 (3)	143 (3)
O2*W*—H2*O*···O1*W*	0.80 (1)	1.97 (1)	2.758 (4)	171 (3)
O3*W*—H3*P*···O4WA^{v}	0.80 (1)	1.81 (2)	2.543 (11)	152 (3)
O3*W*—H3*O*···O3^{v}	0.80 (1)	2.53 (1)	3.300 (5)	163 (3)
O3*W*—H3*O*···O26^{ii}	0.80 (1)	2.57 (2)	3.113 (5)	126 (3)
O4WA—H4O···O2	0.80 (1)	2.06 (1)	2.829 (8)	161 (4)
O4WA—H4P···O4WA^{v}	0.80 (1)	1.60 (2)	2.386 (17)	165 (6)
O4WB—H5O···O1	0.80 (1)	2.58 (2)	3.206 (7)	136 (3)
O4WB—H5O···N7B	0.80 (1)	2.38 (3)	3.028 (18)	139 (4)
O4WB—H5P···O6	0.80 (1)	2.20 (2)	2.927 (7)	151 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) *x*+1, *y*−1, *z*; (v) −*x*+1, −*y*, −*z*+1; (vi) *x*, *y*−1, *z*+1; (vii) −*x*, −*y*+1, −*z*+1.