Supporting Information for:

New Vanadium Tris(*tert*-butoxy)siloxy Complexes and Their Thermolytic Conversions to Vanadia-Silica Materials

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Table of Contents:

*Due to the disorder in the Si and V positions in complex **1**, these values are averaged and should be treated with caution.

Table S1. Crystalographic information for **1** and **2**.

A. Crystal Data	**1**	**2**
Empirical Formula	C_{24} H_{54} O7 Si V	C_{32} H_{72} O_{10} Si_2 V
Formula Weight	533.70	724.02
Crystal Color, Habit	blue, platelike	bright blue, needles
Crystal Dimensions (mm)	0.22 x 0.12 x 0.03	0.23 x 0.16 x 0.07
Crystal System	Monoclinic	Monoclinic
Lattice Type	Primitive	Primitive
Lattice Parameters	a = 9.669(3) Å	a = 9.616(2) Å
	b =16.446(6) Å	b = 16.597(3) Å
	c = 20.417(7) Å	c = 27.803(6) Å
	β = 94.94(6)°	β = 96.78(3)°
	V = 3234.7(19) Å^3	V = 4406.2(15) Å^3
Space Group	$P2_1/n$ (#14)	$P2_1/n$ (#14)
Z value	4	4
D_{calc}	1.096 g cm^{-3}	1.091 g cm^{-3}
F_{000}	1164	1580
$\mu(MoK_\alpha)$	3.8 cm^{-1}	3.2 cm^{-1}

B. Intensity Measurements	**1**	**2**
Diffractometer	SMART CCD	
Radiation	MoK_α (λ = 0.71069 Å) graphite monochromated	
Detector Position	60.00 mm	
Exposure Time	30 seconds per frame.	
Scan Type	ω (0.3° per frame)	
No. of Reflections Measured	Total: 10445	19380
	Unique: 3468	7355
	(Rint = 0.1688)	(Rint = 0.0595)
Corrections	Lorentz-polarization	
T_{max}, T_{min}	0.98, 0.53	0.98, 0.74

C. Structure Solution and Refinement	1	2
Structure Solution	direct (SHELXS-86 (Sheldrick, 1990))	
Refinement	Full-matrix least-squares on F^2 (SHELXTL)	
Least squares function minimized	$\Sigma w(\|Fo^2\| - \|Fc^2\|)^2$	
Least squares weighting scheme	$w = 1/[\sigma^2(Fo^2) + ((p\text{-factor})P)^2 + 0P]$ where $P = (Fo^2 + 2Fc^2)/3$	
p-factor	0.0400	0.0493
Anomalous Dispersion	All non-hydrogen atoms	
No. Unique Reflections (all)	3468	7355
No. Observations (I>2.00σ(I))	1347	3342
No. Variables	298	406
No. Restraints	0	0
Residuals: R_{obs}, $wR2_{obs}$	0.060, 0.102	0.047, 0.096
R_{all}, $wR2_{all}$	0.187, 0.132	0.122, 0.108
GOF_{obs}, GOF_{all}	0.823, 1.104	0.780, 1.058
Max Shift/Error in Final Cycle	0.003	0.000
Maximum peak in Final Diff. Map	0.370 $e^- Å^{-3}$	0.637 $e^- Å^{-3}$
Minimum peak in Final Diff. Map	-0.283 $e^- Å^{-3}$	-0.367 $e^- Å^{-3}$

Table S2. Atomic coordinates and Uiso/Ueq for **1**.

atom	x	y	z	Ueq
V1	0.2334(2)	0.7673(1)	0.9390(1)	0.031(1)
V2	0.2638(2)	0.7516(1)	1.0947(1)	0.030(1)
Si1	0.2638(2)	0.7516(1)	1.0947(1)	0.030(1)
Si2	0.2334(2)	0.7673(1)	0.9390(1)	0.031(1)
O1	0.2796(5)	0.7898(2)	1.0192(2)	0.031(2)
O2	0.3395(5)	0.6926(3)	0.9157(3)	0.045(2)
O3	0.2494(5)	0.8503(3)	0.8882(2)	0.031(2)
O4	0.0622(5)	0.7390(3)	0.9262(2)	0.030(1)
O5	0.2014(5)	0.6545(3)	1.0883(2)	0.033(2)
O6	0.1500(5)	0.8073(3)	1.1366(2)	0.032(2)
O7	0.4185(5)	0.7528(3)	1.1438(2)	0.038(2)
C1	0.3219(10)	0.6154(5)	0.8836(4)	0.036(3)
C2	0.2400(10)	0.6249(5)	0.8197(4)	0.081(4)
C3	0.2510(9)	0.5594(5)	0.9281(4)	0.065(3)
C4	0.4715(9)	0.5854(4)	0.8764(4)	0.055(3)
C10	0.3604(9)	0.9117(5)	0.8885(4)	0.032(2)
C11	0.3463(8)	0.9495(5)	0.8215(4)	0.050(3)
C12	0.5021(8)	0.8726(4)	0.9042(4)	0.054(3)
C13	0.3316(8)	0.9737(4)	0.9406(4)	0.047(3)
C20	-0.0698(8)	0.7821(5)	0.9240(4)	0.032(2)
C21	-0.1785(8)	0.7185(4)	0.9352(4)	0.053(3)
C22	-0.0607(8)	0.8483(5)	0.9766(4)	0.051(3)

C23	-0.0941(7)	0.8195(4)	0.8563(4)	0.040(2)
C30	0.1315(9)	0.6018(5)	1.1317(5)	0.037(3)
C31	0.2028(9)	0.6067(4)	1.2020(4)	0.048(3)
C32	-0.0212(8)	0.6303(4)	1.1320(4)	0.045(3)
C33	0.1383(8)	0.5165(4)	1.1036(4)	0.048(3)
C40	0.1677(8)	0.8837(5)	1.1733(4)	0.032(2)
C41	0.2374(9)	0.8641(4)	1.2410(4)	0.047(3)
C42	0.0179(8)	0.9165(5)	1.1767(4)	0.057(3)
C43	0.2527(8)	0.9431(4)	1.1355(4)	0.046(3)
C50	0.5578(8)	0.7223(5)	1.1309(4)	0.031(2)
C51	0.6149(8)	0.6834(4)	1.1953(4)	0.046(3)
C52	0.5476(8)	0.6632(5)	1.0736(4)	0.050(3)
C53	0.6425(8)	0.7990(4)	1.1167(4)	0.054(3)
H2A	0.2887(10)	0.6617(5)	0.7917(4)	0.121
H2B	0.1487(10)	0.6476(5)	0.8266(4)	0.121
H2C	0.2283(10)	0.5717(5)	0.7982(4)	0.121
H3A	0.3074(9)	0.5544(5)	0.9701(4)	0.098
H3B	0.2394(9)	0.5058(5)	0.9075(4)	0.098
H3C	0.1597(9)	0.5816(5)	0.9358(4)	0.098
H4A	0.5215(9)	0.5802(4)	0.9201(4)	0.082
H4B	0.5195(9)	0.6246(4)	0.8502(4)	0.082
H4C	0.4681(9)	0.5324(4)	0.8544(4)	0.082
H11A	0.3653(8)	0.9085(5)	0.7886(4)	0.075
H11B	0.4126(8)	0.9943(5)	0.8199(4)	0.075
H11C	0.2517(8)	0.9703(5)	0.8121(4)	0.075
H12A	0.5069(8)	0.8487(4)	0.9483(4)	0.082
H12B	0.5747(8)	0.9139(4)	0.9025(4)	0.082
H12C	0.5158(8)	0.8299(4)	0.8719(4)	0.082
H13A	0.3414(8)	0.9479(4)	0.9840(4)	0.071
H13B	0.2369(8)	0.9947(4)	0.9319(4)	0.071
H13C	0.3979(8)	1.0187(4)	0.9396(4)	0.071
H21A	-0.1601(8)	0.6953(4)	0.9794(4)	0.080
H21B	-0.1752(8)	0.6752(4)	0.9024(4)	0.080
H21C	-0.2707(8)	0.7437(4)	0.9312(4)	0.080
H22A	-0.0449(8)	0.8233(5)	1.0201(4)	0.076
H22B	-0.1478(8)	0.8791(5)	0.9739(4)	0.076
H22C	0.0163(8)	0.8851(5)	0.9694(4)	0.076
H23A	-0.0223(7)	0.8603(4)	0.8505(4)	0.059
H23B	-0.1856(7)	0.8454(4)	0.8517(4)	0.059
H23C	-0.0901(7)	0.7769(4)	0.8229(4)	0.059
H31A	0.1964(9)	0.6624(4)	1.2185(4)	0.071
H31B	0.3006(9)	0.5913(4)	1.2016(4)	0.071
H31C	0.1566(9)	0.5695(4)	1.2307(4)	0.071
H32A	-0.0233(8)	0.6854(4)	1.1502(4)	0.068
H32B	-0.0715(8)	0.5932(4)	1.1591(4)	0.068

H32C	-0.0652(8)	0.6304(4)	1.0870(4)	0.068
H33A	0.0921(8)	0.5156(4)	1.0590(4)	0.072
H33B	0.0916(8)	0.4785(4)	1.1314(4)	0.072
H33C	0.2356(8)	0.5003(4)	1.1024(4)	0.072
H41A	0.1795(9)	0.8259(4)	1.2634(4)	0.070
H41B	0.2494(9)	0.9142(4)	1.2668(4)	0.070
H41C	0.3284(9)	0.8394(4)	1.2365(4)	0.070
H42A	-0.0233(8)	0.9284(5)	1.1322(4)	0.086
H42B	0.0208(8)	0.9664(5)	1.2031(4)	0.086
H42C	-0.0384(8)	0.8756(5)	1.1970(4)	0.086
H43A	0.2040(8)	0.9540(4)	1.0923(4)	0.069
H43B	0.3438(8)	0.9193(4)	1.1298(4)	0.069
H43C	0.2649(8)	0.9941(4)	1.1602(4)	0.069
H51A	0.6190(8)	0.7242(4)	1.2304(4)	0.070
H51B	0.7083(8)	0.6624(4)	1.1906(4)	0.070
H51C	0.5541(8)	0.6387(4)	1.2063(4)	0.070
H52A	0.5103(8)	0.6914(5)	1.0337(4)	0.075
H52B	0.4859(8)	0.6182(5)	1.0830(4)	0.075
H52C	0.6401(8)	0.6418(5)	1.0672(4)	0.075
H53A	0.6462(8)	0.8354(4)	1.1548(4)	0.081
H53B	0.5980(8)	0.8272(4)	1.0781(4)	0.081
H53C	0.7369(8)	0.7832(4)	1.1081(4)	0.081

Ueq is defined as one third of the orthoganalized Uij tensor

Table S3. Anisotropic displacement parameters for **1**.

atom	U11	U22	U33	U12	U13	U23
V1	0.019(1)	0.027(1)	0.047(1)	-0.004(1)	0.000(1)	0.000(1)
V2	0.022(1)	0.024(1)	0.044(1)	-0.002(1)	-0.002(1)	0.001(1)
Si1	0.022(1)	0.024(1)	0.044(1)	-0.002(1)	-0.002(1)	0.001(1)
Si2	0.019(1)	0.027(1)	0.047(1)	-0.004(1)	0.000(1)	0.000(1)
O1	0.020(4)	0.027(3)	0.045(4)	0.000(3)	0.007(3)	-0.001(3)
O2	0.022(4)	0.028(4)	0.087(5)	-0.020(3)	0.013(4)	-0.007(3)
O3	0.015(3)	0.031(3)	0.043(4)	0.010(3)	-0.013(3)	-0.004(3)
O4	0.010(3)	0.020(3)	0.058(4)	0.005(3)	-0.003(3)	0.000(3)
O5	0.024(4)	0.026(3)	0.048(4)	-0.004(3)	-0.008(3)	-0.005(3)
O6	0.019(4)	0.031(4)	0.047(4)	-0.012(3)	0.005(3)	-0.007(3)
O7	0.033(4)	0.034(3)	0.044(4)	-0.010(3)	-0.008(3)	0.002(3)
C1	0.044(8)	0.030(7)	0.036(7)	0.008(5)	0.012(6)	-0.008(5)
C2	0.080(9)	0.110(9)	0.047(7)	-0.024(6)	-0.023(7)	0.040(7)
C3	0.048(7)	0.043(6)	0.103(9)	-0.016(6)	0.001(7)	-0.002(6)
C4	0.046(7)	0.038(6)	0.081(8)	-0.014(5)	0.006(6)	0.005(5)
C10	0.025(6)	0.025(6)	0.044(7)	-0.003(5)	-0.009(5)	-0.003(5)
C11	0.038(6)	0.054(6)	0.054(7)	0.017(5)	-0.020(6)	-0.032(5)
C12	0.017(6)	0.045(6)	0.101(8)	0.009(5)	0.008(6)	-0.001(5)
C13	0.043(7)	0.038(6)	0.058(7)	0.001(5)	-0.008(6)	-0.007(5)
C20	0.025(6)	0.033(6)	0.035(6)	-0.001(5)	-0.008(5)	0.012(5)
C21	0.020(6)	0.059(7)	0.079(7)	0.015(5)	-0.008(5)	0.003(5)
C22	0.029(6)	0.059(6)	0.060(7)	-0.024(6)	-0.021(5)	0.014(5)
C23	0.012(6)	0.045(6)	0.060(7)	0.005(5)	-0.007(5)	0.005(4)
C30	0.034(7)	0.015(6)	0.063(8)	0.010(5)	0.011(6)	-0.004(5)
C31	0.046(7)	0.047(6)	0.047(7)	0.013(5)	-0.016(6)	-0.008(5)
C32	0.034(7)	0.030(5)	0.073(7)	0.002(5)	0.013(6)	0.000(5)
C33	0.030(6)	0.033(6)	0.079(7)	-0.001(5)	-0.004(6)	-0.006(5)
C40	0.022(6)	0.020(6)	0.053(7)	-0.017(5)	0.007(6)	-0.003(5)
C41	0.046(7)	0.046(6)	0.046(7)	0.001(5)	-0.009(6)	-0.001(5)
C42	0.042(7)	0.057(7)	0.074(8)	-0.006(5)	0.007(6)	0.014(5)
C43	0.043(6)	0.033(6)	0.063(7)	-0.005(5)	0.002(6)	-0.003(5)
C50	0.012(6)	0.027(6)	0.056(7)	0.000(5)	0.004(5)	0.000(4)
C51	0.028(6)	0.053(6)	0.055(7)	0.017(5)	-0.010(5)	0.001(5)
C52	0.029(6)	0.055(6)	0.065(7)	-0.019(6)	-0.004(5)	0.013(5)
C53	0.028(6)	0.048(6)	0.085(8)	0.013(5)	0.004(6)	-0.002(5)

The general temperature factor expression:

$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl)$

Table S4. Bond lengths (Å) for **1**.

atom	atom	distance
V1	O2	1.694(5)
V1	O1	1.700(5)
V1	O4	1.718(5)
V1	O3	1.730(5)

V2	O1	1.683(5)
V2	O5	1.708(5)
V2	O6	1.717(5)
V2	O7	1.728(5)
Si1	O1	1.683(5)
Si1	O5	1.708(5)
Si1	O6	1.717(5)
Si1	O7	1.728(5)
Si2	O2	1.694(5)
Si2	O1	1.700(5)
Si2	O4	1.718(5)
Si2	O3	1.730(5)
O2	C1	1.433(8)
O3	C10	1.474(8)
O4	C20	1.457(8)
O5	C30	1.448(8)
O6	C40	1.465(8)
O7	C50	1.482(8)
C1	C2	1.476(10)
C1	C3	1.500(10)
C1	C4	1.547(10)
C10	C11	1.499(9)
C10	C13	1.517(9)
C10	C12	1.522(10)
C20	C23	1.513(9)
C20	C21	1.515(9)
C20	C22	1.527(9)
C30	C33	1.519(9)
C30	C31	1.540(10)
C30	C32	1.550(10)
C40	C41	1.520(10)
C40	C43	1.529(10)
C40	C42	1.553(10)
C50	C52	1.516(9)
C50	C51	1.521(9)
C50	C53	1.546(9)

Table S5. Bond angles (°) for **1**.

atom	atom	atom	angle
O2	V1	O1	108.3(3)
O2	V1	O4	111.1(3)
O1	V1	O4	112.0(2)
O2	V1	O3	108.4(3)
O1	V1	O3	112.1(2)

O4	V1	O3	104.9(2)
O1	V2	O5	109.8(2)
O1	V2	O6	111.8(2)
O5	V2	O6	107.4(2)
O1	V2	O7	112.6(2)
O5	V2	O7	109.7(2)
O6	V2	O7	105.3(2)
O1	Si1	O5	109.8(2)
O1	Si1	O6	111.8(2)
O5	Si1	O6	107.4(2)
O1	Si1	O7	112.6(2)
O5	Si1	O7	109.7(2)
O6	Si1	O7	105.3(2)
O2	Si2	O1	108.3(3)
O2	Si2	O4	111.1(3)
O1	Si2	O4	112.0(2)
O2	Si2	O3	108.4(3)
O1	Si2	O3	112.1(2)
O4	Si2	O3	104.9(2)
Si1	O1	V2	0.0(2)
Si1	O1	Si2	139.7(3)
V2	O1	Si2	139.7(3)
Si1	O1	V1	139.7(3)
V2	O1	V1	139.7(3)
Si2	O1	V1	0.0(2)
C1	O2	V1	136.1(5)
C1	O2	Si2	136.1(5)
V1	O2	Si2	0.0(2)
C10	O3	V1	129.9(5)
C10	O3	Si2	129.9(5)
V1	O3	Si2	0.0(2)
C20	O4	V1	134.7(4)
C20	O4	Si2	134.7(4)
V1	O4	Si2	0.0(2)
C30	O5	V2	134.0(5)
C30	O5	Si1	134.0(5)
V2	O5	Si1	0.0(2)
C40	O6	V2	131.4(4)
C40	O6	Si1	131.4(4)
V2	O6	Si1	0.0(2)
C50	O7	V2	130.4(5)
C50	O7	Si1	130.4(5)
V2	O7	Si1	0.0(2)
O2	C1	C2	110.1(7)
O2	C1	C3	108.0(7)
C2	C1	C3	111.2(8)

O2	C1	C4	104.6(7)
C2	C1	C4	112.6(8)
C3	C1	C4	110.0(7)
O3	C10	C11	105.7(6)
O3	C10	C13	106.6(7)
C11	C10	C13	110.7(7)
O3	C10	C12	110.7(6)
C11	C10	C12	112.1(8)
C13	C10	C12	110.7(7)
O4	C20	C23	107.0(6)
O4	C20	C21	106.1(6)
C23	C20	C21	111.3(7)
O4	C20	C22	109.2(6)
C23	C20	C22	110.3(6)
C21	C20	C22	112.7(7)
O5	C30	C33	106.6(7)
O5	C30	C31	110.1(7)
C33	C30	C31	111.7(7)
O5	C30	C32	108.4(6)
C33	C30	C32	110.7(7)
C31	C30	C32	109.3(8)
O6	C40	C41	107.8(6)
O6	C40	C43	109.5(7)
C41	C40	C43	112.3(7)
O6	C40	C42	104.7(6)
C41	C40	C42	112.1(7)
C43	C40	C42	110.2(7)
O7	C50	C52	110.7(6)
O7	C50	C51	104.9(7)
C52	C50	C51	113.0(6)
O7	C50	C53	105.1(6)
C52	C50	C53	112.2(7)
C51	C50	C53	110.3(7)

Table S6. Atomic coordinates and Uiso/Ueq for **2**.

atom	x	y	z	Ueq
V1	0.3348(1)	0.1396(1)	0.1314(1)	0.033(1)
Si1	0.3947(1)	0.1735(1)	0.2508(1)	0.032(1)
Si2	0.3099(1)	0.2855(1)	0.0493(1)	0.035(1)
O1	0.1982(2)	0.0728(1)	0.1116(1)	0.036(1)
O2	0.4926(2)	0.0940(1)	0.1199(1)	0.046(1)
O3	0.3412(2)	0.1499(1)	0.1954(1)	0.037(1)
O4	0.3043(2)	0.2298(1)	0.0971(1)	0.043(1)
O5	0.2672(2)	0.1674(1)	0.2839(1)	0.037(1)

O6	0.5179(2)	0.1150(1)	0.2749(1)	0.041(1)
O7	0.4596(2)	0.2630(1)	0.2485(1)	0.038(1)
O8	0.1611(2)	0.3307(1)	0.0346(1)	0.040(1)
O9	0.3554(2)	0.2264(1)	0.0077(1)	0.037(1)
O10	0.4277(2)	0.3557(1)	0.0584(1)	0.039(1)
C1	0.1923(4)	-0.0030(2)	0.0863(1)	0.038(1)
C2	0.2723(4)	-0.0658(2)	0.1183(1)	0.057(1)
C3	0.2556(4)	0.0066(2)	0.0386(1)	0.056(1)
C4	0.0368(4)	-0.0243(2)	0.0769(1)	0.056(1)
C11	0.6380(4)	0.1178(2)	0.1252(1)	0.039(1)
C12	0.7120(5)	0.0599(3)	0.1616(2)	0.092(2)
C13	0.6866(5)	0.1073(3)	0.0763(2)	0.079(2)
C14	0.6537(4)	0.2039(2)	0.1422(2)	0.075(1)
C21	0.1220(4)	0.1921(2)	0.2755(1)	0.041(1)
C22	0.0791(5)	0.2015(4)	0.3262(2)	0.128(2)
C23	0.0400(5)	0.1239(3)	0.2514(2)	0.112(2)
C24	0.1041(5)	0.2665(3)	0.2482(2)	0.131(3)
C31	0.5137(4)	0.0377(2)	0.2986(1)	0.049(1)
C32	0.6563(5)	-0.0005(3)	0.2953(2)	0.094(2)
C33	0.4903(5)	0.0506(2)	0.3509(1)	0.073(1)
C34	0.3980(5)	-0.0146(2)	0.2729(2)	0.082(2)
C41	0.5467(4)	0.3112(2)	0.2840(1)	0.041(1)
C42	0.5105(4)	0.3980(2)	0.2716(1)	0.064(1)
C43	0.5155(4)	0.2910(2)	0.3350(1)	0.053(1)
C44	0.6984(4)	0.2934(3)	0.2780(2)	0.077(1)
C51	0.0168(4)	0.3053(2)	0.0307(2)	0.049(1)
C52	-0.0623(4)	0.3669(3)	-0.0017(2)	0.105(2)
C53	-0.0310(5)	0.3067(3)	0.0805(2)	0.088(2)
C54	0.0012(4)	0.2214(2)	0.0098(2)	0.067(1)
C61	0.4002(4)	0.2420(2)	-0.0394(1)	0.040(1)
C62	0.5554(4)	0.2639(2)	-0.0329(1)	0.058(1)
C63	0.3762(4)	0.1632(2)	-0.0674(1)	0.060(1)
C64	0.3144(4)	0.3105(2)	-0.0650(1)	0.055(1)
C71	0.4305(4)	0.4285(2)	0.0865(1)	0.048(1)
C72	0.3517(5)	0.4939(2)	0.0569(1)	0.067(1)
C73	0.3689(5)	0.4141(2)	0.1337(1)	0.084(2)
C74	0.5850(5)	0.4499(3)	0.0967(2)	0.088(2)
H2A	0.3715(4)	-0.0509(2)	0.1238(1)	0.086
H2B	0.2628(4)	-0.1185(2)	0.1023(1)	0.086
H2C	0.2342(4)	-0.0687(2)	0.1494(1)	0.086
H3A	0.2028(4)	0.0474(2)	0.0185(1)	0.085
H3B	0.2510(4)	-0.0450(2)	0.0213(1)	0.085
H3C	0.3536(4)	0.0236(2)	0.0454(1)	0.085
H4A	-0.0124(4)	0.0171(2)	0.0563(1)	0.084
H4B	-0.0027(4)	-0.0269(2)	0.1078(1)	0.084

H4C	0.0259(4)	-0.0766(2)	0.0607(1)	0.084
H12A	0.6783(5)	0.0680(3)	0.1932(2)	0.138
H12B	0.8131(5)	0.0697(3)	0.1645(2)	0.138
H12C	0.6925(5)	0.0044(3)	0.1508(2)	0.138
H13A	0.6751(5)	0.0509(3)	0.0662(2)	0.119
H13B	0.7855(5)	0.1225(3)	0.0779(2)	0.119
H13C	0.6308(5)	0.1418(3)	0.0527(2)	0.119
H14A	0.6212(4)	0.2090(2)	0.1741(2)	0.113
H14B	0.5977(4)	0.2391(2)	0.1191(2)	0.113
H14C	0.7524(4)	0.2197(2)	0.1443(2)	0.113
H22A	-0.0925(5)	0.1502(4)	0.3436(2)	0.192
H22B	0.0197(5)	0.2172(4)	0.3239(2)	0.192
H22C	0.1368(5)	0.2431(4)	0.3437(2)	0.192
H23A	0.0558(5)	0.0753(3)	0.2713(2)	0.169
H23B	0.0703(5)	0.1142(3)	0.2195(2)	0.169
H23C	-0.0599(5)	0.1374(3)	0.2477(2)	0.169
H24A	0.1600(5)	0.3092(3)	0.2656(2)	0.197
H24B	0.0051(5)	0.2820(3)	0.2444(2)	0.197
H24C	0.1353(5)	0.2587(3)	0.2162(2)	0.197
H32A	0.6694(5)	-0.0083(3)	0.2612(2)	0.141
H32B	0.6611(5)	-0.0527(3)	0.3119(2)	0.141
H32C	0.7300(5)	0.0350(3)	0.3107(2)	0.141
H33A	0.5655(5)	0.0844(2)	0.3670(1)	0.110
H33B	0.4903(5)	-0.0016(2)	0.3674(1)	0.110
H33C	0.4000(5)	0.0774(2)	0.3523(1)	0.110
H34A	0.4145(5)	-0.0225(2)	0.2391(2)	0.123
H34B	0.3073(5)	0.0119(2)	0.2739(2)	0.123
H34C	0.3976(5)	-0.0671(2)	0.2891(2)	0.123
H42A	0.4122(4)	0.4079(2)	0.2757(1)	0.096
H42B	0.5256(4)	0.4087(2)	0.2380(1)	0.096
H42C	0.5705(4)	0.4336(2)	0.2932(1)	0.096
H43A	0.5396(4)	0.2346(2)	0.3422(1)	0.079
H43B	0.4157(4)	0.2995(2)	0.3374(1)	0.079
H43C	0.5711(4)	0.3260(2)	0.3583(1)	0.079
H44A	0.7192(4)	0.2369(3)	0.2862(2)	0.116
H44B	0.7596(4)	0.3284(3)	0.2996(2)	0.116
H44C	0.7146(4)	0.3035(3)	0.2444(2)	0.116
H52A	-0.0300(4)	0.3652(3)	-0.0338(2)	0.158
H52B	-0.0456(4)	0.4207(3)	0.0123(2)	0.158
H52C	-0.1627(4)	0.3548(3)	-0.0046(2)	0.158
H53A	0.0215(5)	0.2664(3)	0.1010(2)	0.132
H53B	-0.1312(5)	0.2943(3)	0.0779(2)	0.132
H53C	-0.0142(5)	0.3603(3)	0.0948(2)	0.132
H54A	0.0540(4)	0.1833(2)	0.0318(2)	0.100
H54B	0.0375(4)	0.2202(2)	-0.0217(2)	0.100
H54C	-0.0980(4)	0.2062(2)	0.0056(2)	0.100

H62A	0.5690(4)	0.3145(2)	-0.0149(1)	0.087
H62B	0.5881(4)	0.2702(2)	-0.0648(1)	0.087
H62C	0.6088(4)	0.2209(2)	-0.0150(1)	0.087
H63A	0.2761(4)	0.1501(2)	-0.0712(1)	0.090
H63B	0.4288(4)	0.1199(2)	-0.0496(1)	0.090
H63C	0.4081(4)	0.1691(2)	-0.0994(1)	0.090
H64A	0.2150(4)	0.2958(2)	-0.0689(1)	0.082
H64B	0.3452(4)	0.3197(2)	-0.0969(1)	0.082
H64C	0.3280(4)	0.3597(2)	-0.0455(1)	0.082
H72A	0.3936(5)	0.5019(2)	0.0268(1)	0.101
H72B	0.3571(5)	0.5443(2)	0.0754(1)	0.101
H72C	0.2535(5)	0.4780(2)	0.0492(1)	0.101
H73A	0.4218(5)	0.3715(2)	0.1521(1)	0.126
H73B	0.2707(5)	0.3977(2)	0.1265(1)	0.126
H73C	0.3743(5)	0.4639(2)	0.1527(1)	0.126
H74A	0.6345(5)	0.4069(3)	0.1159(2)	0.133
H74B	0.5952(5)	0.5007(3)	0.1148(2)	0.133
H74C	0.6247(5)	0.4558(3)	0.0660(2)	0.133

Ueq is defined as one third of the orthoganalized Uij tensor

Table S7. Anisotropic displacement parameters for **2**.

atom	U11	U22	U33	U12	U13	U23
V1	0.032(1)	0.037(1)	0.028(1)	-0.001(1)	0.000(1)	0.001(1)
Si1	0.032(1)	0.036(1)	0.026(1)	-0.001(1)	-0.001(1)	0.002(1)
Si2	0.032(1)	0.039(1)	0.032(1)	0.005(1)	-0.001(1)	-0.001(1)
O1	0.034(2)	0.036(2)	0.037(1)	-0.009(1)	0.004(1)	-0.005(1)
O2	0.028(2)	0.050(2)	0.061(2)	-0.017(1)	0.005(1)	0.005(1)
O3	0.039(2)	0.047(2)	0.025(1)	0.000(1)	0.002(1)	0.000(1)
O4	0.044(2)	0.045(2)	0.039(2)	0.011(1)	0.004(1)	0.002(1)
O5	0.036(2)	0.044(2)	0.034(1)	0.002(1)	0.009(1)	0.004(1)
O6	0.038(2)	0.043(2)	0.041(2)	0.005(1)	-0.003(1)	0.008(1)
O7	0.036(2)	0.040(2)	0.037(1)	-0.001(1)	-0.005(1)	-0.005(1)
O8	0.028(2)	0.040(2)	0.050(2)	0.006(1)	0.001(1)	0.001(1)
O9	0.035(2)	0.044(2)	0.032(1)	0.001(1)	0.001(1)	-0.001(1)
O10	0.038(2)	0.038(2)	0.039(1)	0.000(1)	-0.007(1)	-0.007(1)
C1	0.039(3)	0.033(2)	0.040(2)	-0.004(2)	-0.001(2)	-0.002(2)
C2	0.050(3)	0.050(3)	0.071(3)	0.008(2)	0.006(2)	0.006(2)
C3	0.067(3)	0.060(3)	0.043(3)	-0.011(2)	0.007(2)	-0.005(2)
C4	0.047(3)	0.052(3)	0.066(3)	-0.015(2)	-0.004(2)	-0.007(2)
C11	0.026(2)	0.053(3)	0.039(2)	0.006(2)	0.005(2)	0.002(2)
C12	0.056(3)	0.105(4)	0.106(4)	0.044(3)	-0.026(3)	-0.005(3)
C13	0.068(4)	0.112(4)	0.062(3)	-0.004(3)	0.024(3)	-0.006(3)
C14	0.048(3)	0.075(3)	0.106(4)	-0.026(3)	0.025(3)	-0.019(3)
C21	0.032(3)	0.051(3)	0.040(2)	-0.004(2)	0.008(2)	0.000(2)
C22	0.066(4)	0.241(7)	0.081(4)	-0.029(4)	0.025(3)	0.034(4)
C23	0.052(3)	0.091(4)	0.184(6)	-0.026(4)	-0.027(3)	-0.018(3)
C24	0.051(4)	0.108(5)	0.239(7)	0.108(5)	0.037(4)	0.038(3)
C31	0.051(3)	0.041(3)	0.050(3)	0.002(2)	-0.007(2)	0.011(2)
C32	0.092(4)	0.096(4)	0.092(4)	0.032(3)	0.002(3)	0.058(3)
C33	0.113(4)	0.059(3)	0.046(3)	0.008(2)	0.001(3)	-0.004(3)
C34	0.109(4)	0.044(3)	0.087(4)	0.002(2)	-0.018(3)	0.000(3)
C41	0.034(3)	0.041(3)	0.044(2)	-0.009(2)	-0.006(2)	-0.006(2)
C42	0.070(3)	0.052(3)	0.064(3)	0.001(2)	-0.011(2)	-0.017(3)
C43	0.060(3)	0.048(3)	0.045(3)	-0.013(2)	-0.016(2)	-0.002(2)
C44	0.036(3)	0.097(4)	0.096(4)	-0.030(3)	-0.003(3)	-0.010(3)
C51	0.025(3)	0.045(3)	0.077(3)	0.004(2)	0.004(2)	-0.002(2)
C52	0.038(3)	0.084(4)	0.188(6)	0.052(4)	-0.015(3)	0.003(3)
C53	0.069(4)	0.099(4)	0.104(4)	-0.021(3)	0.042(3)	-0.015(3)
C54	0.040(3)	0.066(3)	0.092(3)	-0.015(3)	0.003(2)	-0.011(2)
C61	0.035(3)	0.048(3)	0.035(2)	0.002(2)	0.001(2)	0.002(2)
C62	0.044(3)	0.080(3)	0.051(3)	0.008(2)	0.008(2)	-0.004(2)
C63	0.074(3)	0.063(3)	0.043(3)	-0.009(2)	0.004(2)	0.005(2)
C64	0.060(3)	0.065(3)	0.039(2)	0.010(2)	0.005(2)	0.011(2)
C71	0.050(3)	0.045(3)	0.045(3)	-0.003(2)	-0.011(2)	-0.005(2)
C72	0.079(4)	0.049(3)	0.070(3)	0.004(2)	-0.010(3)	-0.001(3)

C73	0.142(5)	0.059(3)	0.048(3)	-0.015(2)	-0.001(3)	0.003(3)
C74	0.078(4)	0.065(3)	0.111(4)	-0.006(3)	-0.041(3)	-0.016(3)

The general temperature factor expression:

$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S8. Bond lengths (Å) for **2**.

atom	atom	distance
V1	O1	1.757(2)
V1	O2	1.758(2)
V1	O4	1.779(2)
V1	O3	1.781(2)
Si1	O3	1.615(2)
Si1	O7	1.616(2)
Si1	O6	1.615(2)
Si1	O5	1.620(2)
Si2	O9	1.615(2)
Si2	O10	1.622(2)
Si2	O8	1.624(2)
Si2	O4	1.626(2)
O1	C1	1.437(4)
O2	C11	1.444(4)
O5	C21	1.448(4)
O6	C31	1.444(4)
O7	C41	1.454(4)
O8	C51	1.442(4)
O9	C61	1.450(4)
O10	C71	1.439(4)
C1	C2	1.519(4)
C1	C4	1.529(5)
C1	C3	1.533(4)
C11	C13	1.501(5)
C11	C14	1.507(5)
C11	C12	1.512(5)
C21	C24	1.449(5)
C21	C23	1.492(5)
C21	C22	1.522(5)
C31	C33	1.514(5)
C31	C34	1.522(5)
C31	C32	1.523(5)
C41	C42	1.512(5)
C41	C44	1.517(5)
C41	C43	1.522(4)
C51	C52	1.507(5)
C51	C53	1.509(5)
C51	C54	1.511(5)

C61	C62	1.525(5)
C61	C63	1.526(4)
C61	C64	1.530(4)
C71	C72	1.512(5)
C71	C73	1.520(5)
C71	C74	1.521(5)

Table S9. Bond angles (°) for **2**.

atom	atom	atom	angle
O1	V1	O2	107.45(11)
O1	V1	O4	107.08(11)
O2	V1	O4	110.93(11)
O1	V1	O3	108.03(10)
O2	V1	O3	107.02(11)
O4	V1	O3	116.01(10)
O3	Si1	O7	105.49(12)
O3	Si1	O6	112.69(12)
O7	Si1	O6	107.55(13)
O3	Si1	O5	110.46(13)
O7	Si1	O5	113.68(12)
O6	Si1	O5	107.06(12)
O9	Si2	O10	107.70(13)
O9	Si2	O8	113.96(12)
O10	Si2	O8	106.58(12)
O9	Si2	O4	106.09(12)
O10	Si2	O4	111.78(12)
O8	Si2	O4	110.78(13)
C1	O1	V1	133.6(2)
C11	O2	V1	135.2(2)
Si1	O3	V1	161.15(15)
Si2	O4	V1	153.76(15)
C21	O5	Si1	132.2(2)
C31	O6	Si1	131.7(2)
C41	O7	Si1	132.3(2)
C51	O8	Si2	134.0(2)
C61	O9	Si2	132.2(2)
C71	O10	Si2	131.0(2)
O1	C1	C2	109.1(3)
O1	C1	C4	105.5(3)
C2	C1	C4	111.0(3)
O1	C1	C3	109.6(3)
C2	C1	C3	110.6(3)
C4	C1	C3	110.9(3)
O2	C11	C13	106.1(3)

O2	C11	C14	110.6(3)
C13	C11	C14	111.3(3)
O2	C11	C12	105.5(3)
C13	C11	C12	111.2(3)
C14	C11	C12	111.8(3)
O5	C21	C24	112.2(3)
O5	C21	C23	107.7(3)
C24	C21	C23	112.8(4)
O5	C21	C22	104.0(3)
C24	C21	C22	111.7(4)
C23	C21	C22	107.8(4)
O6	C31	C33	109.2(3)
O6	C31	C34	110.6(3)
C33	C31	C34	110.4(4)
O6	C31	C32	105.6(3)
C33	C31	C32	110.7(3)
C34	C31	C32	110.3(4)
O7	C41	C42	105.7(3)
O7	C41	C44	107.7(3)
C42	C41	C44	111.0(3)
O7	C41	C43	110.5(3)
C42	C41	C43	110.8(3)
C44	C41	C43	110.9(3)
O8	C51	C52	105.1(3)
O8	C51	C53	108.7(3)
C52	C51	C53	110.6(4)
O8	C51	C54	110.5(3)
C52	C51	C54	112.0(4)
C53	C51	C54	109.8(3)
O9	C61	C62	109.1(3)
O9	C61	C63	105.4(3)
C62	C61	C63	110.5(3)
O9	C61	C64	110.6(3)
C62	C61	C64	110.2(3)
C63	C61	C64	111.0(3)
O10	C71	C72	109.3(3)
O10	C71	C73	110.7(3)
C72	C71	C73	111.2(3)
O10	C71	C74	104.7(3)
C72	C71	C74	110.5(3)
C73	C71	C74	110.3(3)