

Electronic Supplementary Information

Introducing organosilicone source into the synthetic system of polyoxovanadates: two novel $\{V_{15}Si_6O_{48}\}$ -based extended chains

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Contents

Fig. S1 a) Ball-and-stick representation of the cluster $\{V^{IV}_{15}Si_6\}$. b) The layered structure of the $\{V^{IV}_{15}Si_6\}$ cluster within which all metal ions are placed in an arrangement of a central large ring sandwiched by two hexagons.

Fig. S2 IR spectra of **1** and **2**.

Fig. S3 XPS spectra: a) for V^{IV} - V^V in compound **1** and b) for V^{IV} in compound **2**.

Table S1 Selected Bond Distances (Å) for Compound **1** and **2**

Table S2 Bond balance sum calculations for Compound **1** and **2**

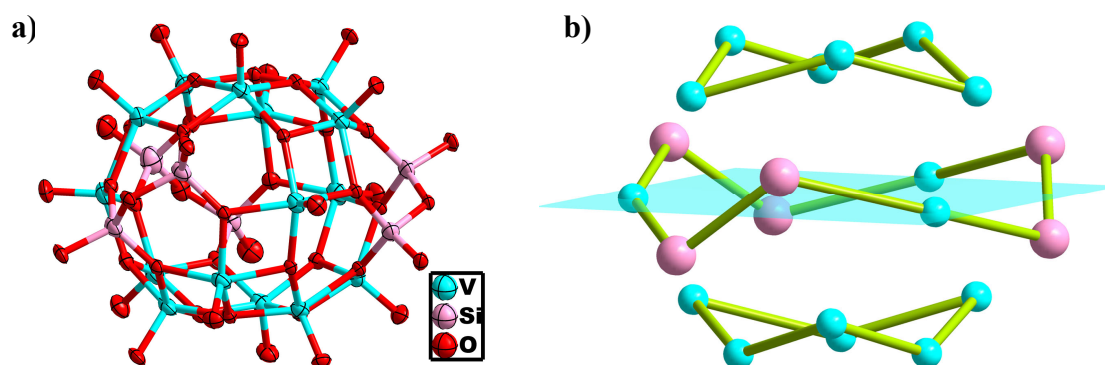


Fig. S1 a) Ball-and-stick representation of the cluster $\{V^{IV}_{15}Si_6\}$. b) The layered structure of the $\{V^{IV}_{15}Si_6\}$ cluster within which all metal ions are placed in an arrangement of a central large ring sandwiched by two hexagons.

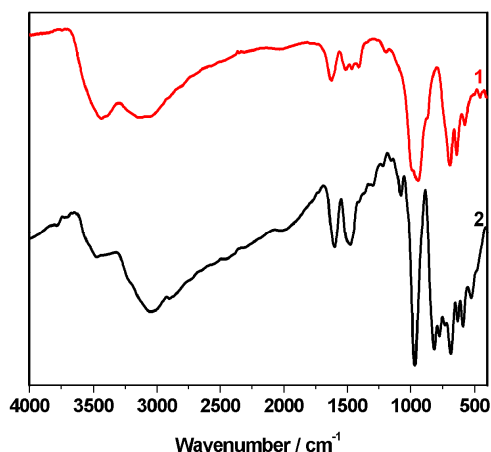


Fig. S2 IR spectra of compounds 1 and 2.

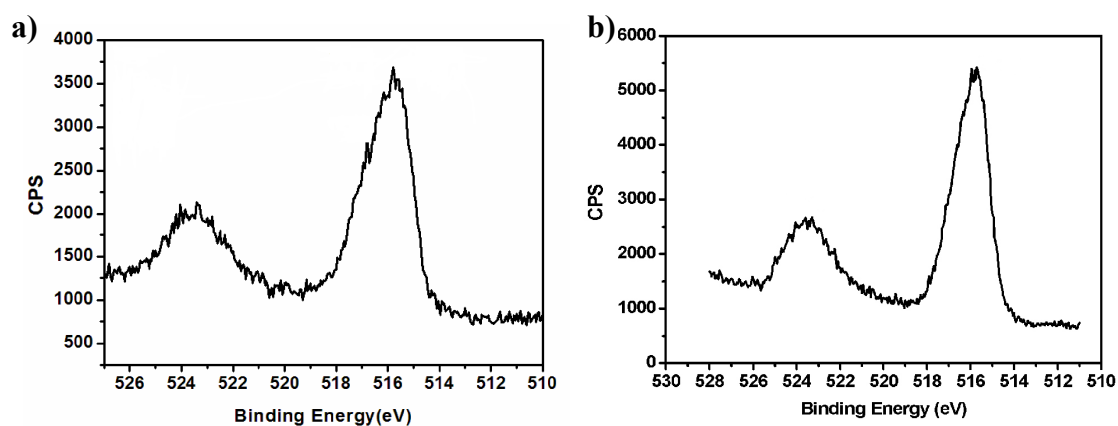


Fig. S3 XPS spectra: a) for V^{IV}-V^V in compound 1 and b) for V^{IV} in compound 2 .

Table S1 Selected Bond Distances (Å) for Compound 1 and 2

Compound 1

V(1)-O(1)	1.622(5)	V(6)-O(15)	1.921(5)
V(1)-O(18)#1	1.923(5)	V(6)-O(13)	1.936(5)
V(1)-O(15)#1	1.924(5)	V(6)-O(10)	1.939(6)
V(1)-O(2)	1.928(5)	V(6)-O(16)	2.002(5)
V(1)-O(3)	2.011(5)	V(6)-V(7)	3.0268(18)
V(1)-V(7)#1	2.8284(17)	V(7)-O(17)	1.611(5)
V(1)-V(2)	3.0226(17)	V(7)-O(15)	1.903(5)
V(2)-O(4)	1.616(6)	V(7)-O(18)	1.913(5)
V(2)-O(2)	1.897(5)	V(7)-O(16)	2.003(5)
V(2)-O(5)	1.918(6)	V(7)-O(19)	2.011(5)
V(2)-O(3)	1.992(5)	V(7)-V(1)#1	2.8284(17)
V(2)-O(6)	2.008(5)	V(7)-V(8)	3.0051(14)
V(2)-V(3)	2.8684(19)	V(8)-O(20)	1.590(8)
V(2)-V(4)	3.0022(18)	V(8)-O(18)	1.929(5)
V(3)-O(7)	1.602(6)	V(8)-O(18)#1	1.929(5)

V(3)-O(2)	1.927(5)	V(8)-O(19)#1	1.992(5)
V(3)-O(5)	1.955(5)	V(8)-O(19)	1.992(5)
V(3)-O(13)#1	1.959(5)	V(8)-V(7)#1	3.0051(14)
V(3)-O(8)	2.005(6)	V(9)-O(26)	1.622(8)
V(3)-V(5)#1	3.018(2)	V(9)-O(24)	1.638(7)
V(4)-O(9)	1.597(6)	V(9)-O(25)	1.794(5)
V(4)-O(10)	1.925(6)	V(9)-O(27)	1.814(6)
V(4)-O(5)	1.938(5)	Si(1)-O(25)#2	1.605(6)
V(4)-O(11)	1.990(6)	Si(1)-O(19)	1.619(5)
V(4)-O(6)	1.998(5)	Si(1)-O(21)	1.622(5)
V(4)-V(5)	2.9853(19)	Si(1)-O(3)	1.622(5)
V(5)-O(12)	1.608(6)	Si(2)-O(27)	1.610(5)
V(5)-O(10)	1.913(5)	Si(2)-O(6)	1.618(6)
V(5)-O(13)	1.921(6)	Si(2)-O(16)	1.623(5)
V(5)-O(11)	1.986(6)	Si(2)-O(21)	1.649(5)
V(5)-O(8)#1	1.990(6)	Si(3)-O(23)	1.610(7)
V(5)-V(6)	2.895(2)	Si(3)-O(8)	1.627(6)
V(5)-V(3)#1	3.018(2)	Si(3)-O(11)	1.638(6)
V(6)-O(14)	1.613(5)	Si(3)-O(22)	1.641(5)

Symmetry transformations used to generate equivalent atoms:

(#1): $-x+1, y, -z+3/2$; (#2): $-x+1, -y, -z+1$.

Compound 2

V(1)-O(1)	1.622(5)	V(9)-O(25)	1.996(5)
V(1)-O(3)	1.917(5)	V(9)-V(10)	3.0128(18)
V(1)-O(5)	1.933(5)	V(10)-O(27)	1.610(6)
V(1)-O(4)	1.954(5)	V(10)-O(24)	1.912(5)
V(1)-O(2)	2.002(5)	V(10)-O(47)	1.914(5)
V(1)-V(12)	2.8783(16)	V(10)-O(25)	1.978(5)
V(1)-V(2)	2.9994(16)	V(10)-O(29)	2.010(5)
V(2)-O(6)	1.616(6)	V(10)-V(15)	2.9926(19)
V(2)-O(3)	1.924(5)	V(11)-O(30)	1.608(6)
V(2)-O(46)	1.932(5)	V(11)-O(31)	1.941(5)
V(2)-O(2)	1.976(5)	V(11)-O(46)	1.941(5)
V(2)-O(7)	1.997(5)	V(11)-O(3)	1.953(5)
V(2)-V(11)	2.8884(17)	V(11)-O(32)	2.025(5)
V(2)-V(6)	3.0129(16)	V(11)-V(14)	3.0425(17)
V(3)-O(9)	1.618(5)	V(12)-O(48)	1.619(6)
V(3)-O(12)	1.908(5)	V(12)-O(5)	1.918(5)
V(3)-O(4)	1.931(5)	V(12)-O(4)	1.930(5)
V(3)-O(10)	1.975(5)	V(12)-O(11)	1.978(5)
V(3)-O(11)	1.978(5)	V(12)-O(34)	1.990(5)
V(3)-V(4)	2.9881(17)	V(12)-V(13)	3.0197(16)
V(3)-V(12)	2.9907(17)	V(13)-O(8)	1.611(5)

V(4)-O(13)	1.599(6)	V(13)-O(31)	1.930(5)
V(4)-O(15)	1.901(5)	V(13)-O(33)	1.934(5)
V(4)-O(12)	1.920(5)	V(13)-O(5)	1.946(5)
V(4)-O(14)	1.997(5)	V(13)-O(34)	2.007(5)
V(4)-O(10)	2.003(5)	V(13)-V(14)	2.8740(17)
V(4)-V(9)	2.8565(17)	V(14)-O(35)	1.608(6)
V(4)-V(5)	3.0197(16)	V(14)-O(31)	1.918(5)
V(5)-O(16)	1.615(5)	V(14)-O(33)	1.924(5)
V(5)-O(15)	1.933(5)	V(14)-O(28)	1.996(6)
V(5)-O(17)	1.938(5)	V(14)-O(32)	2.003(5)
V(5)-O(18)	1.958(5)	V(14)-V(15)	2.9943(19)
V(5)-O(14)	2.006(5)	V(15)-O(36)	1.617(5)
V(5)-V(7)	2.8956(16)	V(15)-O(33)	1.899(5)
V(6)-O(22)	1.609(5)	V(15)-O(47)	1.908(6)
V(6)-O(46)	1.913(5)	V(15)-O(28)	1.985(5)
V(6)-O(18)	1.936(5)	V(15)-O(29)	2.010(5)
V(6)-O(7)	1.983(5)	Si(1)-O(39)	1.580(5)
V(6)-O(21)	1.984(5)	Si(1)-O(10)	1.634(5)
V(6)-V(7)	2.9902(16)	Si(1)-O(37)	1.644(5)
V(7)-O(19)	1.602(5)	Si(1)-O(2)	1.661(5)
V(7)-O(18)	1.931(5)	Si(2)-O(38)	1.609(5)
V(7)-O(17)	1.939(5)	Si(2)-O(14)	1.623(5)
V(7)-O(20)	1.983(5)	Si(2)-O(7)	1.636(5)
V(7)-O(21)	2.000(5)	Si(2)-O(37)	1.636(5)
V(7)-V(8)	3.0396(16)	Si(3)-O(40)	1.585(6)
V(8)-O(23)	1.605(6)	Si(3)-O(32)	1.633(5)
V(8)-O(24)	1.930(5)	Si(3)-O(21)	1.644(5)
V(8)-O(17)	1.944(5)	Si(3)-O(41)	1.648(5)
V(8)-O(47)	1.961(5)	Si(4)-O(42)	1.584(6)
V(8)-O(20)	1.998(5)	Si(4)-O(20)	1.627(5)
V(8)-V(10)	2.9049(17)	Si(4)-O(28)	1.642(6)
V(9)-O(26)	1.604(6)	Si(4)-O(41)	1.649(6)
V(9)-O(24)	1.928(5)	Si(5)-O(43)	1.594(6)
V(9)-O(15)	1.936(5)	Si(5)-O(34)	1.632(5)
V(9)-O(12)	1.953(5)	Si(5)-O(44)	1.634(5)
Co(1)-O(42)#1	2.212(6)	Si(5)-O(29)	1.636(5)
Co(1)-N(7)	2.25(2)	Si(6)-O(45)	1.589(6)
Co(1)-N(6)	2.303(11)	Si(6)-O(25)	1.636(5)
Co(1)-O(1W)	2.349(9)	Si(6)-O(11)	1.645(5)
Co(1)-O(1)#2	2.361(5)	Si(6)-O(44)	1.646(5)
Co(1)-O(36)#1	2.711(6)		

Symmetry transformations used to generate equivalent atoms:

(#1): x+1,y,z; (#2): x,-y+1/2,z-1/2.

Table S2 Bond balance sum calculations for Compound 1 and 2

Compound 1							
Atom	Σs	Atom	Σs	Atom	Σs	Atom	Σs
Si(1)	4.074	V(1)	4.158	V(4)	4.174	V(7)	4.142
Si(2)	3.995	V(2)	4.139	V(5)	4.184	V(8)	4.223
Si(3)	3.951	V(3)	4.148	V(6)	4.181	V(9)	5.217

Compound 2							
Atom	Σs	Atom	Σs	Atom	Σs	Atom	Σs
Si(1)	3.954	V(1)	4.116	V(7)	4.136	V(13)	4.154
Si(2)	3.980	V(2)	4.104	V(8)	4.154	V(14)	4.138
Si(3)	3.972	V(3)	4.163	V(9)	4.194	V(15)	4.166
Si(4)	3.993	V(4)	4.232	V(10)	4.175	Co(1)	1.897
Si(5)	4.007	V(5)	4.093	V(11)	4.094		
Si(6)	3.957	V(6)	4.167	V(12)	4.112		