Electronic Supplementary Material (ESI) for CrystEngComm

Assembly of $[V_{15}Sb_6O_{42}(H_2O)]^{6-}$ cluster shells in to higher dimensional aggregates via weak Sb···N/Sb···O intercluster interactions and a new polyoxovanadate with a discrete $[V_{16}Sb_4O_{42}(H_2O)]^{8-}$ cluster

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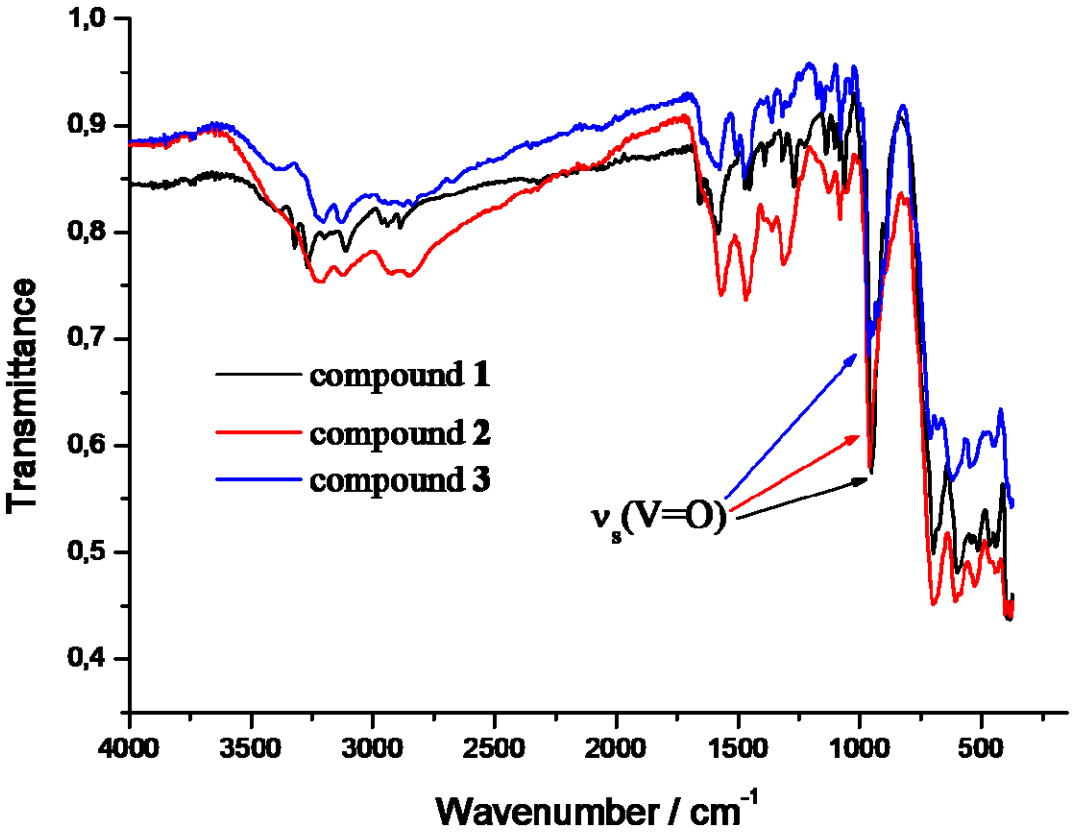

Figure S1: IR spectra of 1, 2 and 3. Some important absorptions modes are marked.

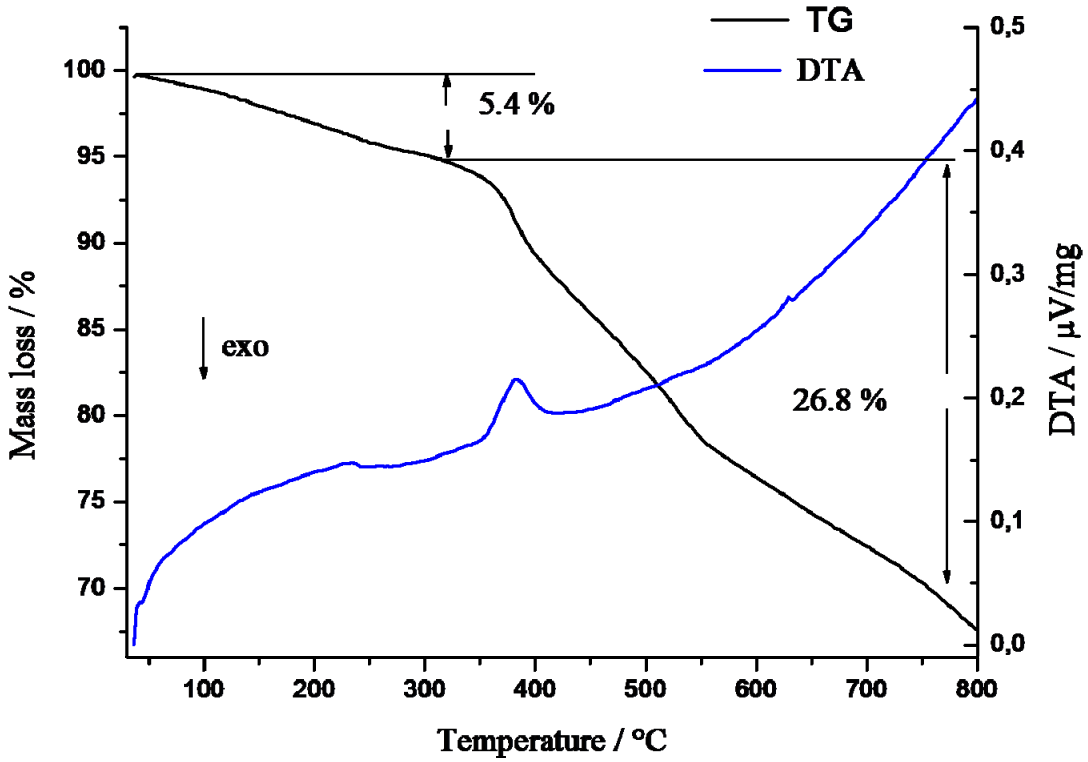

Figure S2: The DTA and TG curves of the thermal decomposition of compound 1.

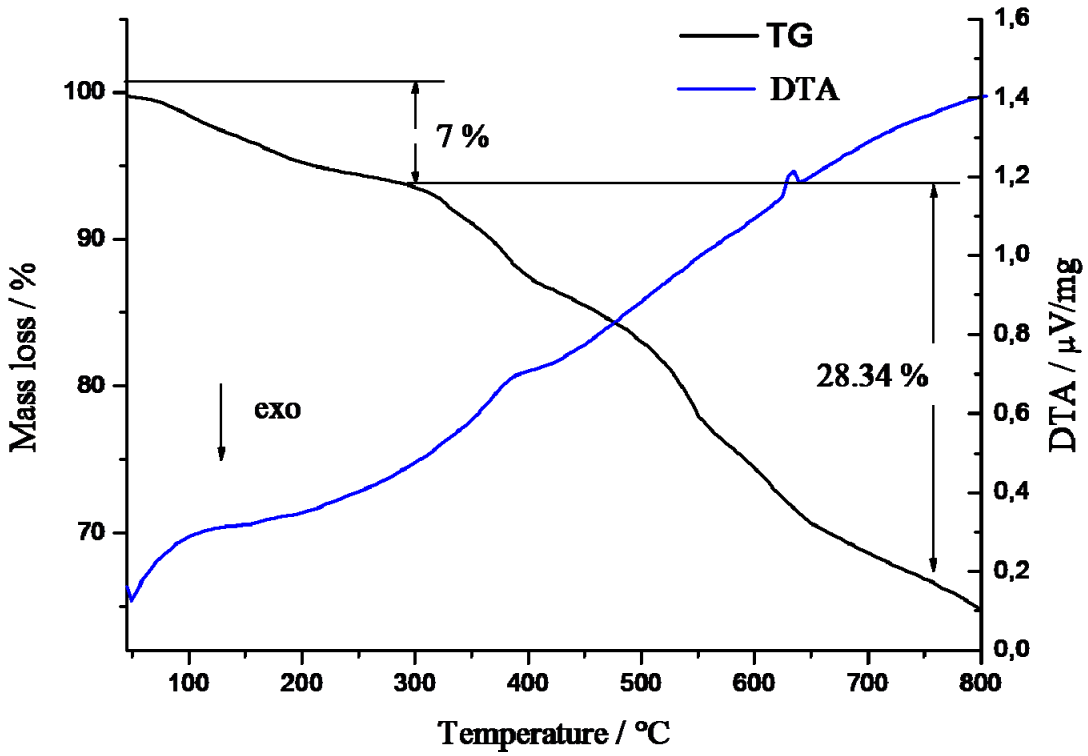

Figure S3: The DTA and TG curves of the thermal decomposition of compound 2.

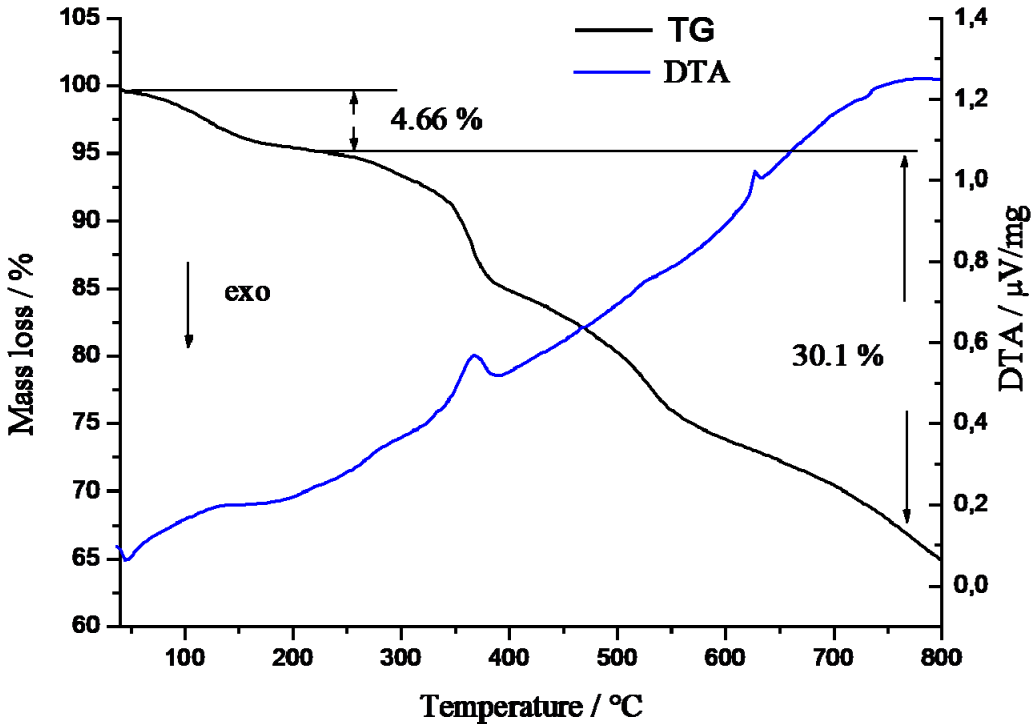

Figure S4: The DTA and TG curves of the thermal decomposition of compound 3.

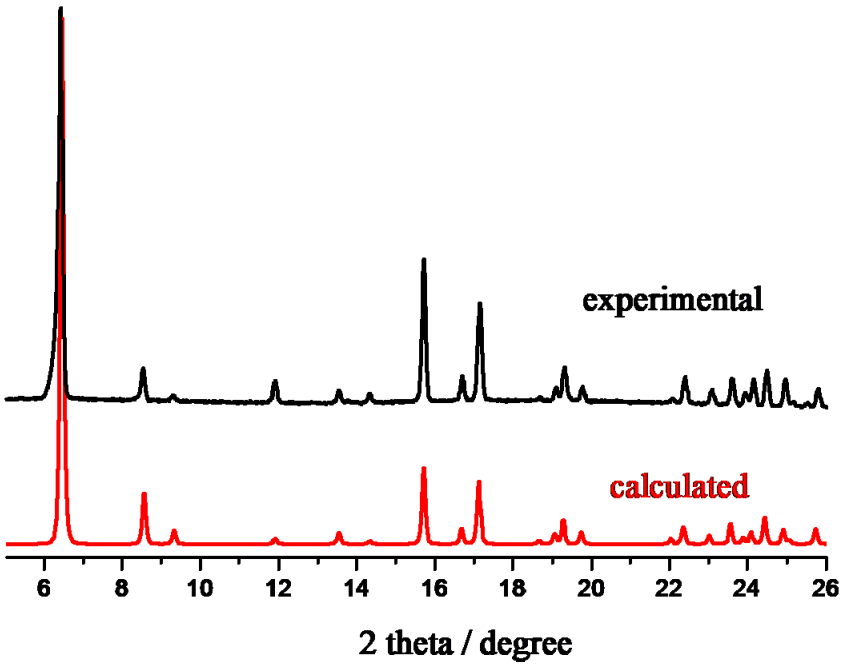

Figure S5: Comparison of measured Powder X-ray diffraction pattern and simulated pattern from single crystal XRD of 1.

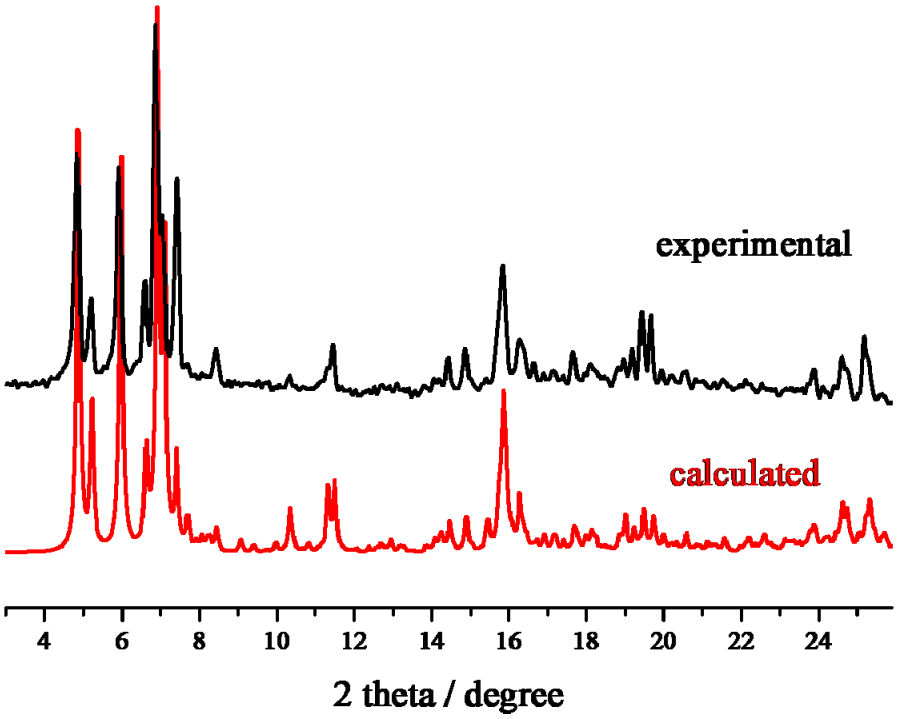

Figure S6: Comparison of measured Powder X-ray diffraction pattern and simulated pattern from single crystal XRD of 2.

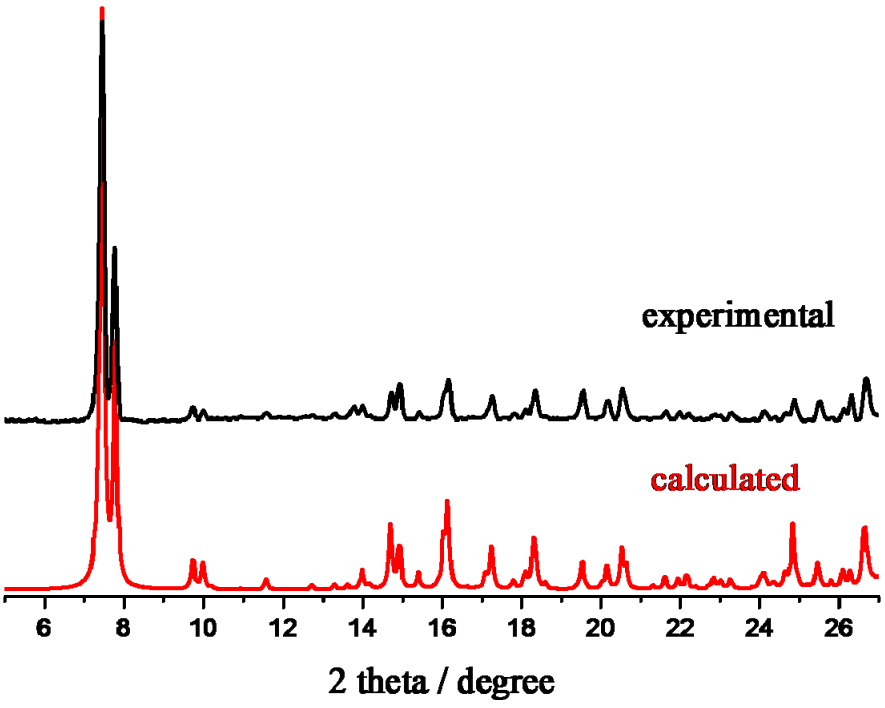

Figure S7: Comparison of measured Powder X-ray diffraction pattern and simulated pattern from single crystal XRD of 3.

Table S1: Bond lengths [Å] of compound 1

A-A	Bond lengths / [Å]	A-A	Bond lengths / [Å]	A-A	Bond lengths / [Å]
V(3)-O(5)	1.984(4)	V(1)-O(7)#1	1.936(4)	Co(1)-N(1)	2.224(9)
V(3)-V(4)	2.9665(12)	V(1)-O(9)#2	1.970(4)	Co(2)-N(12)#5	2.074(6)
V(4)-O(12)	1.624(4)	V(1)-O(3)	2.001(4)	Co(2)-N(12)#6	2.074(6)
V(4)-O(13)	1.919(4)	V(1)-V(2)#2	2.8778(12)	Co(2)-N(12)	2.074(6)
V(4)-O(11)	1.944(4)	V(1)-V(2)	3.0548(12)	Co(2)-O(16)	2.088(10)
V(4)-O(4)#1	1.967(4)	V(2)-O(8)	1.618(4)	Co(2)-N(11)	2.237(10)
V(4)-O(2)#1	1.972(4)	V(2)-O(7)#1	1.908(4)	Co(3)-O(17)	2.045(10)
V(4)-V(5)#2	2.9214(12)	V(2)-O(9)	1.940(4)	Co(3)-N(22)	2.056(5)
V(4)-V(5)	3.0485(12)	V(2)-O(3)	1.963(4)	Co(3)-N(22)#7	2.056(5)
V(5)-O(14)	1.609(4)	V(2)-O(5)	1.997(4)	Co(3)-N(22)#8	2.056(5)
V(5)-O(13)	1.938(4)	V(2)-V(1)#1	2.8778(12)	Co(3)-N(21)	2.251(9)
V(5)-O(13)#1	1.939(4)	V(2)-V(3)	3.0133(13)	N(1)-C(1)	1.479(8)
V(5)-O(11)#1	1.987(4)	V(3)-O(10)	1.622(4)	N(1)-C(1)#3	1.479(8)
V(5)-O(4)#1	2.009(4)	V(3)-O(9)	1.928(4)	N(1)-C(1)#4	1.479(8)
V(5)-V(4)#1	2.9214(12)	V(3)-O(11)	1.940(4)	N(11)-C(11)	1.487(8)
O(2)-V(3)#2	1.967(4)	V(3)-O(2)#1	1.967(4)	N(11)-C(11)#5	1.487(8)
O(2)-V(4)#2	1.972(4)	Sb(1)-O(3)	1.957(4)	N(11)-C(11)#6	1.487(8)
O(4)-V(4)#2	1.967(4)	Sb(1)-O(2)	1.963(4)	C(1)-C(2)	1.461(13)
O(4)-V(5)#2	2.009(4)	Sb(1)-O(1)	1.974(4)	C(2)-N(2)	1.498(10)
O(7)-V(2)#2	1.908(4)	Sb(2)-O(5)	1.945(4)	N(21)-C(21)	1.485(7)
O(7)-V(1)#2	1.936(4)	Sb(2)-O(1)	1.959(4)	N(21)-C(21)#7	1.485(7)
O(9)-V(1)#1	1.970(4)	Sb(2)-O(4)	1.976(4)	N(21)-C(21)#8	1.485(7)
O(11)-V(5)#2	1.987(4)	Co(1)-O(15)	2.075(10)	C(11)-C(12)	1.507(11)
O(13)-V(5)#2	1.939(4)	Co(1)-N(2)	2.080(5)	C(12)-N(12)	1.463(9)
V(1)-O(6)	1.614(4)	Co(1)-N(2)#3	2.080(6)	C(21)-C(22)	1.536(10)
V(1)-O(7)	1.932(4)	Co(1)-N(2)#4	2.080(5)	C(22)-N(22)	1.475(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+y+1,-x+1,z #2 -y+1,x-y,z #3 -y+1,x-y+1,z
#4 -x+y,-x+1,z #5 -y,x-y,z #6 -x+y,-x,z #7 -y+2,x-y+1,z
#8 -x+y+1,-x+2,z

Table S2: Hydrogen bonds of compound 1 with H···A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H··A)	<DHA	d(D··A)	A
N2-H2A	0.900	2.415	135.03	3.117	O8 [-y+1, x-y+1, z]
N2-H2A	0.900	2.636	122.24	3.208	O6 [x, y+1, z]
N2-H2B	0.900	2.292	133.47	2.983	O8 [-x+y, -x+1, z]
N12-H12A	0.900	2.585	128.84	3.226	O12 [x-1, y-1, z]
N12-H12B	0.900	2.357	128.52	3.001	O12 [-x+y, -x+1, z]
N12-H12B	0.900	2.643	157.69	3.493	O4 [-y, x-y, z]
N22-H22A	0.900	2.421	127.50	3.053	O12 [-x+y+2/3, -x+4/3, z+1/3]
N22-H22B	0.900	2.103	165.03	2.981	O14 [x-1/3, y+1/3, z+1/3]

Table S3: Bond lengths [Å] of compound 2

A-A	Bond lenghts / Å	A-A	Bond lenghts / Å	A-A	Bond lenghts / Å
Sb(1)-O(15)	1.946(5)	V(4)-O(21)	1.613(6)	V(12)-V(15)	3.0493(19)
Sb(1)-O(43)	1.960(5)	V(4)-O(32)	1.931(5)	V(13)-O(34)	1.625(6)
Sb(1)-O(9)	2.013(5)	V(4)-O(63)	1.950(5)	V(13)-O(25)	1.931(6)
Sb(1)-N(21)	2.594(7)	V(4)-O(46)	1.961(6)	V(13)-O(29)	1.946(5)
Sb(2)-O(43)	1.964(5)	V(4)-O(30)	2.008(5)	V(13)-O(47)	1.952(5)
Sb(2)-O(11)	1.965(5)	V(4)-V(7)	2.8934(19)	V(13)-O(71)	2.016(6)
Sb(2)-O(75)	1.976(5)	V(4)-V(11)	3.0412(18)	V(13)-V(20)	2.8938(19)
Sb(3)-O(36)	1.940(5)	V(5)-O(40)	1.639(6)	V(13)-V(17)	3.046(2)
Sb(3)-O(20)	1.954(5)	V(5)-O(78)	1.911(5)	V(14)-O(13)	1.611(5)
Sb(3)-O(56)	1.966(5)	V(5)-O(51)	1.938(6)	V(14)-O(52)	1.925(5)
Sb(4)-O(67)	1.946(5)	V(5)-O(35)	1.957(6)	V(14)-O(3)	1.939(5)
Sb(4)-O(56)	1.952(5)	V(5)-O(28)	1.959(5)	V(14)-O(15)	1.970(5)
Sb(4)-O(76)	1.962(6)	V(5)-V(26)	2.9861(19)	V(14)-O(36)	1.997(5)
Sb(5)-O(48)	1.950(5)	V(5)-V(6)	3.0376(18)	V(14)-V(27)	2.9987(18)
Sb(5)-O(1)	1.956(6)	V(6)-O(17)	1.624(6)	V(14)-V(19)	3.0080(19)
Sb(5)-O(6)	1.958(6)	V(6)-O(78)	1.922(5)	V(15)-O(50)	1.633(5)
Sb(6)-O(37)	1.955(6)	V(6)-O(24)	1.934(5)	V(15)-O(41)	1.923(5)
Sb(6)-O(30)	1.960(5)	V(6)-O(72)	1.955(5)	V(15)-O(57)	1.940(6)
Sb(6)-O(6)	1.967(5)	V(6)-O(35)	2.006(5)	V(15)-O(9)	1.961(5)
Sb(7)-O(80)	1.950(5)	V(6)-V(18)	2.8641(18)	V(15)-O(75)	1.967(5)
Sb(7)-O(79)	1.960(5)	V(7)-O(38)	1.620(5)	V(15)-V(30)	2.9874(19)
Sb(7)-O(35)	1.962(5)	V(7)-O(63)	1.930(5)	V(16)-O(44)	1.633(5)
Sb(8)-O(23)	1.945(5)	V(7)-O(46)	1.966(5)	V(16)-O(3)	1.920(5)
Sb(8)-O(80)	1.954(6)	V(7)-O(76)	1.976(5)	V(16)-O(63)	1.933(5)
Sb(8)-O(28)	1.961(5)	V(7)-O(20)	1.981(5)	V(16)-O(39)	1.942(5)
Sb(9)-O(14)	1.955(6)	V(7)-V(23)	3.0312(17)	V(16)-O(20)	2.034(6)
Sb(9)-O(60)	1.962(6)	V(7)-V(16)	3.0673(18)	V(16)-V(19)	2.8127(18)
Sb(9)-O(96)	2.019(5)	V(8)-O(2)	1.621(5)	V(17)-O(58)	1.622(6)
Sb(10)-O(12)	1.953(5)	V(8)-O(41)	1.929(5)	V(17)-O(25)	1.924(6)
Sb(10)-O(14)	1.964(5)	V(8)-O(4)	1.931(5)	V(17)-O(5)	1.956(6)
Sb(10)-O(55)	2.004(5)	V(8)-O(57)	1.950(6)	V(17)-O(59)	1.965(6)
Sb(11)-O(64)	1.945(5)	V(8)-O(1)	2.014(6)	V(17)-O(71)	1.972(6)
Sb(11)-O(71)	1.954(5)	V(8)-V(15)	2.8846(19)	V(17)-V(24)	2.8891(19)
Sb(11)-O(95)	1.964(6)	V(9)-O(33)	1.629(5)	V(17)-V(26)	3.015(2)
Sb(12)-O(49)	1.953(5)	V(9)-O(4)	1.924(5)	V(18)-O(54)	1.626(6)
Sb(12)-O(95)	1.964(6)	V(9)-O(69)	1.936(6)	V(18)-O(24)	1.926(6)
Sb(12)-O(59)	1.971(5)	V(9)-O(16)	1.955(6)	V(18)-O(72)	1.962(5)
V(1)-O(8)	1.619(6)	V(9)-O(67)	2.005(5)	V(18)-O(55)	1.968(6)
V(1)-O(78)	1.920(5)	V(9)-V(27)	3.0636(18)	V(18)-O(60)	1.993(6)
V(1)-O(65)	1.942(5)	V(10)-O(94)	1.627(5)	V(18)-V(28)	3.0038(17)
V(1)-O(51)	1.976(5)	V(10)-O(70)	1.911(6)	V(18)-V(29)	3.0724(19)
V(1)-O(49)	2.013(6)	V(10)-O(61)	1.943(5)	V(19)-O(62)	1.618(5)
V(1)-V(5)	2.8761(18)	V(10)-O(79)	1.988(5)	V(19)-O(39)	1.922(5)
V(1)-V(21)	3.0590(19)	V(10)-O(23)	1.992(6)	V(19)-O(3)	1.935(5)
V(2)-O(74)	1.615(5)	V(10)-V(22)	2.8556(19)	V(19)-O(15)	1.981(5)
V(2)-O(4)	1.918(6)	V(10)-V(28)	3.0170(17)	V(19)-O(11)	1.983(5)
V(2)-O(69)	1.973(5)	V(10)-V(24)	3.0522(19)	V(20)-O(77)	1.625(6)
V(2)-O(37)	1.988(6)	V(11)-O(42)	1.628(6)	V(20)-O(96)	1.937(5)
V(2)-O(1)	1.996(6)	V(11)-O(32)	1.923(5)	V(20)-O(47)	1.938(5)
V(2)-V(9)	2.8377(19)	V(11)-O(45)	1.934(5)	V(20)-O(29)	1.943(5)

Continuation of table S3: Bond lengths [Å] of compound 2.

A-A	Bond lenghts / Å	A-A	Bond lenghts / Å	A-A	Bond lenghts / Å
V(2)-V(23)	3.0181(18)	V(21)-O(64)	1.993(6)	C(11)-C(12)	1.498(16)
V(2)-V(8)	3.0589(19)	V(21)-O(49)	1.998(5)	C(12)-N(8)	1.465(14)
V(3)-O(31)	1.618(5)	V(21)-V(29)	2.8531(19)	Co(2)-N(12)	2.064(7)
V(3)-O(32)	1.933(5)	V(21)-O(22)	1.943(5)	Co(2)-N(9)	2.076(7)
V(3)-O(45)	1.948(5)	O(50)-Co(1)	2.243(5)	Co(2)-N(13)	2.085(6)
V(3)-O(39)	1.958(5)	Co(1)-N(5)	2.094(8)	Co(2)-N(11)	2.090(7)
V(3)-O(11)	2.003(5)	Co(1)-N(2)	2.130(8)	Co(2)-N(10)	2.286(6)
V(3)-V(11)	2.8525(18)	Co(1)-N(4)	2.163(10)	N(9)-C(13)	1.488(10)
V(3)-V(19)	3.0690(18)	Co(1)-N(3)	2.170(11)	C(13)-C(14)	1.528(12)
V(11)-O(30)	1.957(6)	Co(1)-N(1)	2.173(7)	C(14)-N(10)	1.495(11)
V(11)-O(48)	1.976(5)	N(1)-C(1)	1.465(13)	N(10)-C(15)	1.465(11)
V(11)-V(30)	3.0146(19)	C(1)-C(2)	1.454(18)	N(10)-C(17)	1.478(10)
V(12)-O(68)	1.624(6)	C(2)-N(4)	1.486(17)	C(15)-C(16)	1.537(12)
V(12)-O(41)	1.939(5)	N(2)-C(3)	1.54(3)	C(16)-N(11)	1.472(10)
V(12)-O(52)	1.944(5)	C(3)-C(4)	1.52(3)	C(17)-C(18)	1.503(11)
V(12)-O(16)	1.960(5)	C(4)-N(4)	1.418(14)	C(18)-N(12)	1.480(10)
V(12)-O(9)	2.017(5)	N(3)-C(5)	1.352(14)	N(13)-C(19)	1.480(11)
V(12)-V(27)	2.8772(17)	C(5)-C(6)	1.437(15)	C(19)-C(20)	1.548(12)
V(23)-O(69)	1.944(5)	N(4)-C(6)	1.633(12)	C(20)-N(14)	1.486(10)
V(23)-O(37)	1.966(5)	N(5)-C(7)	1.471(12)	N(14)-C(23)	1.456(12)
V(23)-O(76)	1.979(5)	C(7)-C(8)	1.522(14)	C(39)-C(40)	1.498(13)
V(24)-O(19)	1.626(5)	C(8)-N(6)	1.484(12)	C(40)-N(27)	1.471(11)
V(24)-O(70)	1.932(5)	N(6)-C(11)	1.460(13)	N(27)-Co(4)	2.087(7)
V(24)-O(25)	1.940(6)	N(6)-C(9)	1.481(15)	Co(4)-N(31)	2.072(6)
V(24)-O(5)	1.942(6)	C(9)-C(10)	1.47(2)	Co(4)-N(30)	2.078(8)
V(24)-O(23)	2.013(6)	C(10)-N(7)	1.52(3)	Co(4)-N(29)	2.081(7)
V(25)-O(66)	1.607(6)	N(14)-C(21)	1.468(12)	Co(4)-N(28)	2.255(7)
V(25)-O(29)	1.943(5)	C(21)-C(22)	1.535(12)	N(28)-C(41)	1.470(10)
V(25)-O(96)	1.961(6)	C(22)-N(15)	1.470(13)	N(28)-C(45)	1.473(11)
V(25)-O(22)	1.967(6)	C(23)-C(24)	1.519(14)	N(28)-C(43)	1.493(11)
V(25)-O(64)	1.989(6)	C(24)-N(16)	1.489(11)	C(41)-C(42)	1.493(14)
V(26)-O(10)	1.619(6)	N(16)-Co(3)	2.061(7)	C(42)-N(29)	1.485(13)
V(26)-O(51)	1.929(5)	Co(3)-N(18)	2.095(8)	C(43)-C(44)	1.507(13)
V(26)-O(5)	1.952(6)	Co(3)-N(19)	2.099(7)	C(44)-N(30)	1.457(12)
V(26)-O(28)	1.978(6)	Co(3)-N(20)	2.121(8)	C(45)-C(46)	1.512(12)
V(26)-O(59)	1.978(6)	Co(3)-N(17)	2.235(8)	C(46)-N(31)	1.508(11)
V(27)-O(97)	1.619(6)	N(17)-C(27)	1.479(11)	C(47)-C(48)	1.535(11)
V(27)-O(16)	1.929(5)	N(17)-C(25)	1.486(12)	C(48)-N(32)	1.471(11)
V(27)-O(52)	1.931(6)	N(17)-C(29)	1.502(11)	N(32)-Co(5)	2.073(6)
V(27)-O(36)	1.982(5)	C(25)-C(26)	1.481(14)	Co(5)-N(33)	2.053(7)
V(27)-O(67)	1.982(5)	C(26)-N(18)	1.504(13)	Co(5)-N(36)	2.080(7)
V(28)-O(27)	1.615(6)	C(27)-C(28)	1.516(13)	Co(5)-N(35)	2.091(7)
V(28)-O(61)	1.943(5)	C(28)-N(19)	1.481(12)	Co(5)-N(34)	2.273(6)
V(28)-O(72)	1.953(5)	C(29)-C(30)	1.502(14)	N(33)-C(49)	1.472(11)
V(28)-O(55)	1.967(5)	C(30)-N(20)	1.472(14)	C(49)-C(50)	1.522(13)
V(28)-O(79)	1.976(5)	N(21)-C(31)	1.442(13)	C(50)-N(34)	1.475(11)
V(29)-O(18)	1.634(5)	C(31)-C(32)	1.511(14)	N(34)-C(53)	1.472(11)
V(29)-O(24)	1.920(6)	C(32)-N(22)	1.501(15)	N(34)-C(51)	1.482(11)
V(29)-O(22)	1.938(6)	N(22)-C(35)	1.445(17)	C(51)-C(52)	1.496(13)
V(29)-O(65)	1.942(5)	N(22)-C(33)	1.495(19)	C(52)-N(35)	1.471(11)
V(29)-O(60)	2.007(6)	C(33)-C(34)	1.44(2)	C(53)-C(54)	1.517(12)
V(30)-O(7)	1.612(5)	C(34)-N(23)	1.502(18)	C(54)-N(36)	1.467(11)
V(30)-O(75)	1.949(6)	C(35)-C(36)	1.552(17)	Co(6)-N(42)	2.094(7)

Continuation of table S3: Bond lengths [Å] of compound 2.

A-A	Bond lenghts / Å	A-A	Bond lenghts / Å	A-A	Bond lenghts / Å
V(30)-O(45)	1.959(5)	C(36)-N(24)	1.480(16)	Co(6)-N(39)	2.096(11)
V(30)-O(57)	1.960(6)	N(25)-C(37)	1.481(13)	Co(6)-N(37)	2.122(12)
V(20)-O(12)	1.988(5)	C(37)-C(38)	1.503(13)	Co(6)-N(40)	2.165(11)
V(20)-V(25)	2.9201(19)	C(38)-N(26)	1.473(11)	Co(6)-N(41)	2.251(14)
V(20)-V(22)	3.0784(18)	N(26)-C(39)	1.464(10)	Co(6)-N(38)	2.262(11)
V(21)-O(53)	1.622(6)	N(26)-C(47)	1.470(11)	N(37)-C(55)	1.488(18)
V(21)-O(65)	1.912(6)	N(38)-C(57)	1.492(17)	C(55)-C(56)	1.48(2)
C(58)-N(39)	1.49(2)	N(38)-C(59)	1.527(19)	C(56)-N(38)	1.452(16)
C(59)-C(60)	1.577(19)	C(57)-C(58)	1.501(19)	N(41)-C(61)	1.513(16)
C(60)-N(40)	1.460(17)	C(62)-N(42)	1.496(18)	C(61)-C(62)	1.511(16)

Table S4 Hydrogen bonds of compound 2 with H···A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H···A)	<DHA	d(D···A)	A
N1-H1A	0.9	2.135	169.26	3.024	O86 [-x+5/2, y-1/2, -z+1/2]
N1-H1B	0.9	2.132	163.41	3.005	O38 [-x+5/2, y-1/2, -z+1/2]
N2-H2C	0.9	2.491	144.82	3.268	O46 [-x+5/2, y-1/2, -z+1/2]
N3-H3D	0.9	2.37	145.46	3.153	O89 [x-1/2, -y+3/2, z-1/2]
N5-H5C	0.9	2.433	144.9	3.212	O7
N5-H5D	0.9	2.324	113.42	2.806	O26 [-x+5/2, y-1/2, -z+1/2]
N7-H7D	0.89	2.641	136.33	3.342	N23 [-x+5/2, y+1/2, -z+1/2]
N8-H8C	0.89	2.511	151.62	3.321	O77 [x, y-1, z]
N8-H8D	0.89	2.347	113.83	2.826	O14 [x, y-1, z]
N8-H8D	0.89	2.556	134.28	3.241	O56 [-x+5/2, y-1/2, -z+1/2]
N9-H9C	0.9	2.529	126.07	3.145	O8 [-x+3, -y+2, -z]
N9-H9D	0.9	2.127	167.49	3.012	O73 [x+1/2, -y+5/2, z+1/2]
N11-H11C	0.9	2.172	150.39	2.988	O33 [-x+5/2, y+1/2, -z+1/2]
N11-H11D	0.9	2.573	125.64	3.182	O4 [-x+5/2, y+1/2, -z+1/2]
N12-H12C	0.9	1.942	165.15	2.821	O68 [-x+5/2, y+1/2, -z+1/2]
N12-H12D	0.9	2.229	132.67	2.915	O40 [-x+3, -y+2, -z]
N13-H13C	0.9	2.492	125.01	3.097	O8 [-x+3, -y+2, -z]
N13-H13D	0.9	2.27	168.32	3.157	O16 [-x+5/2, y+1/2, -z+1/2]
N15-H15D	0.89	2.65	127.02	3.264	O85 [-x+5/2, y+1/2, -z-1/2]
N15-H15E	0.89	2.336	162.84	3.197	O97 [-x+5/2, y+1/2, -z+1/2]
N16-H16C	0.9	2.117	161.57	2.984	O18
N16-H16D	0.9	2.063	160.35	2.926	O97 [-x+5/2, y+1/2, -z+1/2]
N18-H18D	0.9	2.043	168.67	2.931	O18 [-x+3, -y+2, -z]
N19-H19C	0.9	2.357	135.11	3.062	O13 [-x+5/2, y+1/2, -z+1/2]
N19-H19D	0.9	2.507	167.08	3.39	O22
N20-H20D	0.9	2.531	132.63	3.209	O68 [-x+5/2, y+1/2, -z+1/2]
N21-H21C	0.9	2.148	159.99	3.009	O6 [-x+5/2, y-1/2, -z+1/2]
N21-H21D	0.9	2.251	162.75	3.122	O62
N23-H23C	0.89	2.154	135.85	2.86	O89 [-x+3, -y+1, -z+1]
N23-H23D	0.89	2.527	152.5	3.342	N7 [-x+5/2, y-1/2, -z+1/2]
N24-H24C	0.89	2.441	131.68	3.105	O80 [x, y-1, z+1]
N25-H25C	0.89	2.15	144.85	2.923	O83 [-x+5/2, y-1/2, -z+1/2]
N25-H25D	0.89	2.404	150.62	3.21	O74
N27-H27C	0.9	2.127	159.9	2.988	O39 [-x+5/2, y+1/2, -z+1/2]
N27-H27D	0.9	2.317	115.44	2.824	N26
N27-H27D	0.9	2.41	130.84	3.075	O31 [-x+5/2, y+1/2, -z+1/2]
N29-H29C	0.9	2.301	137.93	3.029	O34 [-x+2, -y+2, -z]
N29-H29D	0.9	2.424	138.35	3.154	O21 [-x+5/2, y+1/2, -z+1/2]
N29-H29D	0.9	2.629	148.67	3.43	O32 [-x+5/2, y+1/2, -z+1/2]
N30-H30C	0.9	2.273	135.71	2.984	O44 [-x+5/2, y+1/2, -z+1/2]
N30-H30C	0.9	2.464	148.3	3.264	O63 [-x+5/2, y+1/2, -z+1/2]
N31-H31C	0.9	2.325	136.76	3.043	O44 [x-1/2, -y+3/2, z-1/2]
N31-H31D	0.9	2.193	154.05	3.028	O77 [-x+2, -y+2, -z]
N32-H32C	0.9	2.399	160.28	3.261	O47 [-x+2, -y+2, -z]

Table S5: Bond lengths [Å] of compound 3

A-A	Bond lenghts / Å	A-A	Bond lenghts / Å	A-A	Bond lenghts / Å
Sb(1)-O(15)	1.950(3)	V(3)-V(6)	2.9811(15)	V(8)-O(2)	1.935(3)
Sb(1)-O(11)	1.951(3)	V(3)-V(4)	3.0316(9)	V(8)-O(1)	2.017(3)
Sb(1)-O(8)	1.955(2)	V(4)-O(17)	1.616(3)	V(8)-V(8)#1	2.7274(13)
Sb(2)-O(10)	1.941(2)	V(4)-O(7)	1.916(3)	O(2)-V(8)#1	1.913(3)
Sb(2)-O(1)	1.943(3)	V(4)-O(5)	1.932(2)	O(4)-V(6)#1	1.914(2)
Sb(2)-O(15)#1	1.943(3)	V(4)-O(10)#1	1.959(3)	O(6)-V(5)#1	1.957(2)
Co(1)-N(3)	2.062(3)	V(4)-O(8)	1.960(3)	O(9)-V(6)#1	1.939(3)
Co(1)-N(2)	2.084(3)	V(5)-O(19)	1.637(3)	O(10)-V(4)#1	1.959(3)
Co(1)-N(4)	2.085(3)	V(5)-O(3)	1.916(3)	O(10)-V(2)#1	2.000(3)
Co(1)-N(5)	2.087(3)	V(5)-O(4)	1.916(3)	O(11)-V(7)#1	2.011(3)
Co(1)-N(1)	2.222(3)	V(5)-O(6)#1	1.957(2)	O(11)-V(5)#1	2.012(3)
V(1)-O(16)	1.629(3)	V(5)-O(11)#1	2.012(3)	O(15)-Sb(2)#1	1.943(3)
V(1)-O(7)	1.916(3)	V(5)-V(6)#1	2.9220(9)	N(1)-C(1)	1.470(5)
V(1)-O(4)	1.937(3)	V(5)-V(7)	3.0580(10)	N(1)-C(3)	1.474(5)
V(1)-O(3)	1.953(3)	V(6)-O(20)	1.642(3)	N(1)-C(5)	1.480(5)
V(1)-O(5)	1.965(3)	V(6)-O(4)#1	1.914(2)	C(1)-C(2)	1.505(7)
V(1)-V(4)	2.9370(11)	V(6)-O(9)	1.936(3)	C(2)-N(2)	1.476(6)
V(1)-V(5)	2.9391(17)	V(6)-O(9)#1	1.939(3)	C(3)-C(4)	1.511(6)
V(2)-O(14)	1.608(3)	V(6)-O(6)	1.980(3)	C(4)-N(3)	1.466(6)
V(2)-O(7)	1.902(2)	V(6)-V(5)#1	2.9220(9)	C(5)-C(6)	1.495(6)
V(2)-O(12)	1.926(3)	V(6)-V(6)#1	2.9609(13)	C(6)-N(4)	1.479(5)
V(2)-O(2)	1.973(3)	V(7)-O(22)	1.602(3)	N(5)-C(7)	1.477(5)
V(2)-O(10)#1	2.000(3)	V(7)-O(12)	1.932(3)	C(7)-C(8)	1.511(6)
V(2)-V(8)	2.9516(16)	V(7)-O(3)	1.953(3)	C(8)-N(6)	1.474(5)
V(2)-V(4)	2.9983(10)	V(7)-O(11)#1	2.011(3)	N(6)-C(9)	1.463(5)
V(3)-O(18)	1.622(3)	V(7)-O(1)	2.015(3)	N(6)-C(11)	1.464(5)
V(3)-O(5)	1.928(2)	V(7)-V(8)	3.0919(9)	C(9)-C(10)	1.517(6)
V(3)-O(9)	1.928(3)	V(8)-O(21)	1.631(3)	C(10)-N(7)	1.476(6)
V(3)-O(6)	1.956(2)	V(8)-O(2)#1	1.913(3)	C(11)-C(12)	1.523(5)
V(3)-O(8)	1.996(2)	V(8)-O(12)	1.919(3)	C(12)-N(8)	1.483(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table S6 Hydrogen bonds of compound 3 with H··A < r (A) + 2.000 Å and <DHA > 110 °

D-H	d(D-H)	d(H··A)	<DHA	d(D··A)	Å
N2-H2C	0.900	2.627	155.95	3.468	O19
N2-H2D	0.900	2.091	144.42	2.871	O17 [-x, -y+1, -z+1]
N3-H3C	0.900	1.952	162.87	2.825	O21 [x, y+1, z]
N3-H3D	0.900	2.309	153.88	3.142	O25 [-x, y, -z+1/2]
N3-H3D	0.900	2.644	110.26	3.074	O20 [-x, y, -z+1/2]
N4-H4C	0.900	2.028	159.70	2.889	O14 [-x, -y+1, -z+1]
N4-H4D	0.900	2.303	147.23	3.098	O22 [x, y+1, z]
N5-H5C	0.900	2.142	170.90	3.034	O16 [-x, -y+1, -z+1]
N5-H5D	0.900	2.367	156.40	3.212	O20 [-x, y, -z+1/2]
N7-H7C	0.890	2.095	165.56	2.965	O20
N7-H7D	0.890	2.433	147.71	3.220	O21 [x, y+1, z]
N7-H7D	0.890	2.527	112.03	2.978	O21 [-x, y+1, -z+1/2]
N7-H7E	0.890	2.291	137.94	3.011	O20 [-x, y, -z+1/2]
N8-H8C	0.890	1.915	160.97	2.772	O16
N8-H8D	0.890	1.950	162.71	2.813	O19 [-x, -y+1, -z+1]
N8-H8E	0.890	2.148	168.05	3.024	O24