Table S.1.- Details of the crystal data, structural resolution and refinement procedure for $Ni_3(C_4H_4N_2)_3(V_8O_{23})$.

Formula	C6 H6 N3 Ni1.5 O11.5 V4
Molecular weight, g·mol^{-1}	595.96
Crystalline system	Triclinic
Space group (Nº.)	P-1 (2)
a, Å	8.556(2)
b, Å	9.117(2)
c, Å	12.619(3)
α, º	71.05(2)
β, º	83.48(2)
γ, º	61.32(3)
V, Å^3	815.7(3)
Z	2
ρ_{obs}, ρ_{calc}, gr·cm^{-3}	2.41(1), 2.426
F(000)	578
Collection data	
Temperature, K	293(2)
Diffractometer	Oxford Diffraction Xcalibur2
μ, mm^{-1}	3.962
Radiation, λ(Mo Kα), Å	0.71073
Cristal size, mm	0.12 x 0.06 x 0.04
Range θ, º	2.87-26.37
Interval h, k, l	-10≤ h≤8, -11≤ k≤10, -15≤ l≤15
Nº of measured refelctions	6134
Nº of independent reflections	3269
R (int)	0.0376
Refinement	
Data/Restrictions/Parameter	3269/0/238
R factors [I>2σ(I)]	R1=0.0272, wR2=0.0409
R factors [all data]	R1=0.0460, wR2=0.0439
Máx. y min. of electronic residual density, e.Å^{-3}	0.411, -0.359
G. O. F	0.901

$$R1 = \frac{\sum \left| |F_O| - |F_C| \right|}{\sum |F_O|} \; ; \; wR2 = \sqrt{\frac{\sum w\left(|F_O| - |F_C|\right)^2}{\sum w|F_O|^2}}$$

$w= 1/[\sigma^2|F_o|^2 + (xp)^2 + yp]$ with $p= [\max|F_o|^2 + 2|F_c|^2]/3$, where x= 0.0045, y= 0

Table S.2.- Selected bond distances (Å) and angles (º) for $Ni_3(C_4H_4N_2)_3(V_8O_{23})$.

Bond distances

$Ni(1)O_4N_2$ octahedron		*$Ni(2)O_4N_2$ octahedron*		*$V(1)O_4$ tetrahedron*	
N1-O(7)^{i}	2.028(2)	Ni2-O(11)	2.034(2)	V1-O(2)^{iv}	1.648(2)
Ni1-O(7)^{ii}	2.028(2)	Ni2-O(4)	2.058(2)	V1-O(4)	1.659(2)
Ni1-O(6)^{i}	2.054(2)	Ni2-O(2)	2.069(2)	V1-O(3)	1.800(2)
Ni1-O(6)^{ii}	2.054(2)	Ni2-N(1)	2.080(2)	V1-O(1)	1.831(2)
Ni1-N(2)	2.095(2)	Ni2-O(10)	2.091(2)		
Ni1-N(2)^{iii}	2.095(2)	Ni2-N(3)	2.106(2)		

$V(2)O_4$ tetrahedron		*$V(3)O_4$ tetrahedron*		*$V(4)O_4$ tetrahedron*	
V2-O(10)	1.649(2)	V3-O(7)	1.643(2)	V4-O(9)	1.599(2)
V2-O(6)	1.663(2)	V3-O(11)	1.658(2)	V4-O(5)	1.770(2)
V2-O(3)^{iv}	1.790(2)	V3-O(12)	1.7833(9)	V4-O(1)^{v}	1.773(2)
V2-O(5)	1.819(2)	V3-O(8)	1.821(2)	V4-O(8)^{vi}	1.781(2)

$(C_4H_4N_2)$ pyrazine					
N(1)-C(1)	1.337(4)	N(1)-C(4)	1.351(4)	N(2)-C(3)	1.338(4)
N(2)-C(2)	1.349(4)	N(3)-C(5)	1.332(4)	N(3)-C(6)^{x}	1.347(4)
C(1)-C(2)	1.393(4)	C(5)-C(6)	1.387(4)	C(6)-N(3)^{x}	1.347(4)

Bond angles

$Ni(1)O_4N_2$ octahedron		*$Ni(2)O_4N_2$ octahedron*	
O(7)^{i}-Ni1-O(7)^{ii}	180.0(0)	O(11)-Ni2-O(4)	178.49(8)
O(7)^{i}-N1-O(6)^{i}	90.14(9)	O(11)-Ni2-O(4)	90.29(8)
O(7)^{ii}-Ni1-O(6)^{i}	89.86(9)	O(4)-Ni2-O(2)	89.50(8)
O(7)^{i}-Ni1-O(6)^{ii}	89.86(9)	O(11)-Ni2-N(1)	91.91(9)
O(7)^{ii}-Ni1-O(6)^{ii}	90.14(9)	O(4)-Ni2-N(1)	88.43(9)
O(6)^{i}-Ni1-O(6)^{ii}	180.0(0)	O(2)-Ni2-N(1)	174.95(9)
O(7)^{i}-Ni1-N(2)	99.14(9)	O(11)-Ni2-O(10)	89.26(8)
O(7)^{ii}-Ni1-N(2)	90.86(9)	O(4)-Ni2-O(10)	92.23(8)
O(6)^{i}-Ni1-N(2)	88.71(9)	O(2)-Ni2-O(10)	89.48(8)
O(6)^{ii}-Ni1-N(2)	91.29(9)	N(1)-Ni2-O(10)	86.00(9)
O(7)^{i}-Ni1-N(2)^{iii}	90.86(9)	O(11)-Ni2-N(3)	89.34(9)
O(7)^{ii}-Ni1-N(2)^{iii}	89.14(9)	O(4)-Ni2-N(3)	89.16(9)
O(6)^{i}-Ni1-N(2)^{iii}	91.29(9)	O(2)-Ni2-N(3)	86.02(9)
O(6)^{ii}-Ni1-N(2)^{iii}	88.71(9)	N(1)-Ni2-N(3)	98.55(9)
N(2)-Ni1-N(2)^{iii}	180.0(0)	O(10)-Ni2-N(3)	175.28(9)

V(1)O_4 tetrahedron		*V(2)O_4 tetrahedron*	
O(2)^{iv}-V1-O(4)	111.5(1)	O(10)-V2-O(6)	111.3(1)
O(2)^{iv}-V1-O(3)	107.6(1)	O(10)-V2-O(3)^{iv}	107.8(1)
O(4)-V1-O(3)	106.1(1)	O(6)-V2-O(3)^{iv}	107.2(1)
O(2)^{iv}-V1-O(1)	108.8(1)	O(10)-V2-O(5)	109.9(1)
O(4)-V1-O(1)	114.1(1)	O(6)-V2-O(5)	108.4(1)
O(3)-V1-O(1)	108.41(9)	O(3)^{iv}-V2-O(5)	112.39(9)

V(3)O_4 tetrahedron		*V(4)O_4 tetrahedron*	
O(7)-V3-O(11)	109.3(1)	O(9)-V4-O(5)	110.2(1)
O(7)-V3-O(12)	110.05(8)	O(9)-V4-O(1)^{v}	109.4(1)
O(11)-V3-O(12)	109.71(8)	O(5)-V4-O(1)^{v}	108.5(1)
O(7)-V3-O(8)	105.4(1)	O(9)-V4-O(8)^{vi}	107.7(2)
O(11)-V3-O(8)	108.2(1)	O(5)-V4-O(8)^{vi}	109.1(1)
O(12)-V3-O(8)	113.96(8)	O(1)^{v}-V4-O(8)^{vi}	112.0(1)

($C_4H_4N_2$) pyrazine	
C(1)-N1-C(4)	117.1(3)
C(1)-N1-Ni(2)	118.4(2)
C(4)-N1-Ni(2)	124.4(2)
C(3)-N2-C(2)	116.9(3)
C(3)-N2-Ni(1)	122.7(2)
C(2)-N2-Ni(1)	120.5(2)
C(5)-N3-C(6)^{x}	116.1(2)
C(5)-N3-Ni(2)	119.7(2)
C(6)^{x}-N3-Ni(2)	123.6(2)
N(1)-C1-C(2)	121.8(3)
N(2)-C2-C(1)	120.9(3)
N(2)-C3-C(4)	122.4(3)
N(1)-C4-C(3)	120.9(3)
N(3)-C5-C(6)	123.0(3)
N(3)^{x}-C6-C(5)	120.9(3)

Symmetry codes :

i= -x+2,-y+1,-z	ii= x,y+1,z	iii= -x+2,-y+2,-z	iv= -x+2,-y,-z+1
v= -x+3,-y,-z+1	vi= x+1,y,z	vii=x,y-1,-z+1	viii= x-1,-y+1,-z
ix= -x+1,-y+1,-z	x= -x+1,-y+1,-z+1		