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Supporting Information

Auxiliary Ligands-Assisted Structural Diversity of Three Metal-Organic Frameworks Assembled by Potassium 1*H*–1,2,3–Triazole–4,5– Dicarboxylic Acid: Syntheses, Crystal Structures and Luminescence Properties

Ji-Yong Zou,^a Hong-Ling Gao,^{*a} Wei Shi,^b Jian-Zhong Cui^{*a} and Peng Cheng^b

1. Thermogravimetric analysis



Fig. S1 The thermal gravimetric analysis (TGA) data of 1-3.

2. Power X-Ray diffraction

Powder X-ray diffraction measurements were recorded on a D/Max-2500 X-ray diffractometer using Cu/K α radiation.



Fig. S2 Comparison of the experimental PXRD pattern of as-synthesized 1 with the one simulated from its single crystal structure.

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Fig. S3 Comparison of the experimental PXRD pattern of as-synthesized 2 with the one simulated from its single crystal structure



Fig. S4 Comparison of the experimental PXRD pattern of as-synthesized 3 with the one simulated from its single crystal structure

3. Infrared spectra

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4. Crystal Structures



Fig. S6 View of the 3D structure of 1 along (a) the [0, 1, 0] direction, (b) the [0, 0, 1] direction, (c) the space filling of 1 viewed along the [1, 0, 0] direction and (d) the [0, 1, 0] direction, (e) the hcb layers.



Fig. S7 View of the 3D structure of 2 along (a) the [1, 0, 0] direction, (b) the [0,1,0] direction, (c) the space filling of 2 viewed along the [0, 0, 1] direction.



Fig. S8 View of the 3D structure of 3 along (a) the [0, 1, 0] direction, (b) the [0,0,1] direction.

Table S1 Selected	bonds length and	angles for MOFs	1-3
	0	0	

		1	
Zn(1)-O(1)	2.113(3)	$N(6)-Zn(1)-N(6)^{\#1}$	180.0
$Zn(1)-O(1)^{\#1}$	2.113(3)	$N(1)^{#2}$ -Zn(2)-N(1)	180.0
Zn(1)-O(3)	2.091(3)	$N(1)^{#2}$ -Zn(2)-O(2)	101.61(13)
$Zn(1)-O(3)^{\#1}$	2.091(3)	N(1)-Zn(2)-O(2)	78.39(13)
Zn(1)-N(6)	2.149(4)	$N(1)^{#2}$ -Zn(2)-O(2) ^{#2}	78.39(13)
$Zn(1)-N(6)^{\#1}$	2.149(4)	$N(1)-Zn(2)-O(2)^{\#2}$	101.61(13)
Zn(2)-O(2)	2.132(3)	$O(2)-Zn(2)-O(2)^{\#2}$	180.0
$Zn(2)-O(2)^{+2}$	2.132(3)	$N(1)^{*2}$ -Zn(2)-N(4)*2	90.12(14)
Zn(2)-N(1)	2.057(4)	$N(1)-Zn(2)-N(4)^{\frac{\pi}{2}}$	89.88(14)
$Zn(2)-N(1)^{n^2}$	2.057(4)	$O(2)-Zn(2)-N(4)^{n^2}$	94.11(14)
Zn(2)-N(4)	2.219(4)	$O(2)^{-2}-Zn(2)-N(4)^{-2}$	85.90(14)
Zn(2)-N(4) Zn(2) O(4)	2.219(4)	N(1) -Zn(2) - N(4) N(1) -Zn(2) - N(4)	89.88(14)
Zn(3)-O(4)	2.129(3)	N(1)-Zn(2)-N(4) O(2) Zn(2) N(4)	90.12(14)
$Z_{n}(3) - O(4)$ $Z_{n}(3) N(3)$	2.129(3) 2.080(4)	O(2)=ZII(2)=IV(4) $O(2)^{\#2}$ $Zp(2)$ $V(4)$	03.09(14) 04.10(14)
$Zn(3)-N(3)^{\#3}$	2.080(4)	$N(4)^{\#2}$ - $Zn(2)$ - $N(4)$	180.0(2)
Zn(3) - N(5)	2.000(4) 2 176(4)	$N(3)-Zn(3)-N(3)^{\#3}$	180.0
$Zn(3)-N(5)^{\#3}$	2.176(4)	$N(3)-Zn(3)-O(4)^{\#3}$	101.56(14)
$O(3)^{\#1}$ -Zn(1)-O(3)	180.00(19)	$N(3)^{#3}$ -Zn(3)-O(4) ^{#3}	78.44(14)
$O(3)^{\#1}-Zn(1)-O(1)$	87.19(13)	N(3)-Zn(3)-O(4)	78.44(14)
O(3)-Zn(1)-O(1)	92.81(13)	$N(3)^{\#3}$ -Zn(3)-O(4)	101.55(14)
$O(3)^{\#1}$ -Zn(1)-O(1)^{\#1}	92.81(13)	$O(4)^{\#3}$ -Zn(3)-O(4)	180.0
$O(3)-Zn(1)-O(1)^{\#1}$	87.19(13)	N(3)-Zn(3)-N(5)	90.72(15)
$O(1)-Zn(1)-O(1)^{\#1}$	180.0	$N(3)^{#3}$ -Zn(3)-N(5)	89.28(15)
$O(3)^{#1}$ -Zn(1)-N(6)	86.87(14)	$O(4)^{#3}$ -Zn(3)-N(5)	91.77(15)
O(3)-Zn(1)-N(6)	93.13(14)	O(4)-Zn(3)-N(5)	88.23(15)
O(1)-Zn(1)-N(6)	90.37(13)	$N(3)-Zn(3)-N(5)^{\#3}$	89.28(15)
$O(1)^{\#1}$ -Zn(1)-N(6)	89.63(13)	$N(3)^{#3}$ -Zn(3)-N(5) ^{#3}	90.72(15)
$O(3)^{*1}$ -Zn(1)-N(6) ^{*1}	93.13(14)	$O(4)^{#3}$ -Zn(3)-N(5) ^{#3}	88.23(15)
$O(3)-Zn(1)-N(6)^{\#1}$	86.87(14)	$O(4)-Zn(3)-N(5)^{#3}$	91.77(15)
$O(1)-Zn(1)-N(6)^{n}$	89.63(13)	$N(5)-Zn(3)-N(5)^{n}$	180.0
$(J(1)) = Z_1((1) = N(0))$	90.57(15)		
Symmetry transformations used to	generate equivalent atoms:		
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3	generate equivalent atoms: 3 -x,-y,-z		
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3	generate equivalent atoms: 3 -x,-y,-z	2	144.540
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zr(1) O(5)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2 120(5)	2 O(5)-Zn(1)-N(3) O(2)#1.7z (2) O(2)#1	166.5(2)
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(5)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1)	166.5(2) 92.9(2) 174.54(10)
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1)	166.5(2) 92.9(2) 174.54(19) 88.3(2)
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1)	166.5(2) 92.9(2) 174.54(19) 88.3(2) 97.6(2)
Symmetry transformations used to 5 #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.110(6)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1)	166.5(2) 92.9(2) 174.54(19) 88.3(2) 97.6(2) 95.4(2)
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.110(6) 2.125(5)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(1)-Zn(2)-N(1)	$166.5(2) \\92.9(2) \\174.54(19) \\88.3(2) \\97.6(2) \\95.4(2) \\76.9(2)$
Symmetry transformations used to 5 #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(1) Zn(2)-O(2)#1	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.110(6) 2.110(6) 2.125(5) 2.109(5)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(1)-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2	$166.5(2) \\92.9(2) \\174.54(19) \\88.3(2) \\97.6(2) \\95.4(2) \\76.9(2) \\93.7(2)$
Symmetry transformations used to #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(3)#1	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.110(6) 2.125(5) 2.109(5) 2.054(5)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(1)-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2	$166.5(2) \\92.9(2) \\174.54(19) \\88.3(2) \\97.6(2) \\95.4(2) \\76.9(2) \\93.7(2) \\82.9(2)$
Symmetry transformations used to 5 #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(1) Zn(2)-O(1) Zn(2)-O(3)#1 Zn(2)-N(1)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(1)-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2	$166.5(2) \\92.9(2) \\174.54(19) \\88.3(2) \\97.6(2) \\95.4(2) \\76.9(2) \\93.7(2) \\82.9(2) \\91.7(2)$
Symmetry transformations used to 5 #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(1) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(3)#1 Zn(2)-N(1) Zn(2)-N(12)#3	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 N(1)-Zn(2)-N(16)#2	$166.5(2) \\92.9(2) \\174.54(19) \\88.3(2) \\97.6(2) \\95.4(2) \\76.9(2) \\93.7(2) \\82.9(2) \\91.7(2) \\168.6(2)$
Symmetry transformations used to f #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(3)#1 Zn(2)-N(1) Zn(2)-N(1) Zn(2)-N(1)#3 Zn(2)-N(16)#2	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.110(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 N(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2	$166.5(2) \\92.9(2) \\174.54(19) \\88.3(2) \\97.6(2) \\95.4(2) \\76.9(2) \\93.7(2) \\82.9(2) \\91.7(2) \\168.6(2) \\89.4(2)$
$\begin{array}{c} S(y) = 2h(1) + h(0) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(4) \\ Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - N(3) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - N(1) \\ Zn(3) - O(6) \#1 \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5)	$\begin{array}{c} \\ O(5)\text{-}Zn(1)\text{-}N(3)\\ O(3)\#1\text{-}Zn(2)\text{-}O(2)\#1\\ O(3)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}O(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(2)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(2)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(1)\text{-}Zn(2)\text{-}N(16)\#2\\ N(1)\text{-}Zn(2)\text{-}N(16)\#2\\ N(1)\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(2)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(2)\#1\text{-}Zn(2)\#1\text{-}N(12)\#3\\ O(2)\#1\text{-}Zn(2)\#1\text{-}N(12)\#3\\ O(2)\#1\text{-}Zn(2)\#1\text{-}N(12)\#3\\ O(2)\#1\text{-}N(12)\#1\text{-}N(12)\#3\\ O(2)\#1\text{-}N(12)\#1\text{-}N(12)\#3\\ O(2)\#1\text{-}$	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2)
$\begin{array}{c} Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(4) \\ Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - N(3) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ \hline Zn(2) - O(3) \#1 \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(7) \#1 \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5)	$\begin{array}{c} & O(5)\text{-}Zn(1)\text{-}N(3)\\ O(3)\#1\text{-}Zn(2)\text{-}O(2)\#1\\ O(3)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}O(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(2)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(2)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(1)\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(2)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(1)\text{-}Zn(2)\text{-}N(12)\#3\\ O(1)\text{-}Zn(2)\text{-}N(12)\#3\\ O(1)\text{-}Zn(2)\text{-}N(12)\#3\\ \end{array}$	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2) 90.3(2)
$\begin{array}{c} S(y) = 2h(1) + h(0) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(4) \\ Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(8) \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.110(5)	$\begin{array}{c} & O(5)\text{-}Zn(1)\text{-}N(3)\\ O(3)\#1\text{-}Zn(2)\text{-}O(2)\#1\\ O(3)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(2)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(1)\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(1)\text{-}Zn(2)\text{-}N(12)\#3\\ O(1)\text{-}Zn(2)\text{-}N(12)\#3\\ N(1)\text{-}Zn(2)\text{-}N(12)\#3\\ N(1)\text{-}Zn(2)\text{-}N(12)\#3\\ \end{array}$	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2) 90.3(2) 93.2(2)
$\begin{array}{c} S(y) = 2h(1) + h(0) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - N(3) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(2) \#1 \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(6) \\ Zn(3) - O(8) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.161(6)	$\begin{array}{c} & O(5)\text{-}Zn(1)\text{-}N(3)\\ O(3)\#1\text{-}Zn(2)\text{-}O(2)\#1\\ O(3)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}N(1)\\ O(2)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(2)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(1)\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(2)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(1)\text{-}Zn(2)\text{-}N(12)\#3\\ N(1)\text{-}Zn(2)\text{-}N(12)\#3\\ N(1)\text{-}Zn(2)\text{-}N(12)\#3\\ N(16)\#2\text{-}Zn(2)\text{-}N(12)\#3\\ \end{array}$	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2) 90.3(2) 93.2(2) 87.9(2)
Symmetry transformations used to j #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(5) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(2)#1 Zn(2)-N(1) Zn(2)-N(1) Zn(2)-N(1) Zn(3)-O(6)#1 Zn(3)-O(6)#1 Zn(3)-O(6) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(9) Zn(3)-N(9)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.213(6) 2.136(6) 2.137(6) 2.136(6) 2.137(6) 2.157($\begin{array}{c} 2\\ O(5)-Zn(1)-N(3)\\ O(3)\#1-Zn(2)-O(2)\#1\\ O(3)\#1-Zn(2)-O(1)\\ O(2)\#1-Zn(2)-O(1)\\ O(2)\#1-Zn(2)-N(1)\\ O(3)\#1-Zn(2)-N(1)\\ O(1)-Zn(2)-N(1)\\ O(3)\#1-Zn(2)-N(16)\#2\\ O(2)\#1-Zn(2)-N(16)\#2\\ O(1)-Zn(2)-N(16)\#2\\ O(1)-Zn(2)-N(16)\#2\\ O(3)\#1-Zn(2)-N(16)\#2\\ O(3)\#1-Zn(2)-N(16)\#2\\ O(3)\#1-Zn(2)-N(12)\#3\\ O(2)\#1-Zn(2)-N(12)\#3\\ O(2)\#1-Zn(2)-N(12)\#3\\ O(1)-Zn(2)-N(12)\#3\\ N(1)-Zn(2)-N(12)\#3\\ N(16)\#2-Zn(2)-N(12)\#3\\ O(6)\#1-Zn(3)-O(7)\#1\\ O(6)\#1\\ O(6)\#1$	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2) 90.3(2) 93.2(2) 87.9(2) 94.23(19)
Symmetry transformations used to j #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(2)#1 Zn(2)-O(3)#1 Zn(2)-N(1) Zn(2)-N(1) Zn(2)-N(1) Zn(3)-O(6)#1 Zn(3)-O(6)#1 Zn(3)-O(8) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(13) O(2) Zn(3)-N(13) O(2) Zn(3)-N(13)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.213(6) 2.155(6)	$\begin{array}{c} & O(5)\text{-}Zn(1)\text{-}N(3)\\ O(3)\#1\text{-}Zn(2)\text{-}O(2)\#1\\ O(3)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}O(1)\\ O(2)\#1\text{-}Zn(2)\text{-}O(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(2)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(1)\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(2)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(1)\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(16)\#2\\ O(3)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(2)\#1\text{-}Zn(2)\text{-}N(12)\#3\\ O(1)\text{-}Zn(2)\text{-}N(12)\#3\\ N(1)\text{-}Zn(2)\text{-}N(12)\#3\\ N(16)\#2\text{-}Zn(2)\text{-}N(12)\#3\\ O(6)\#1\text{-}Zn(3)\text{-}O(7)\#1\\ O(6)\#1\text{-}Zn(3)\text{-}O(8)\\ O(2)\#1\text{-}Zn(2)\text{-}O(2)\end{array}$	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2) 90.3(2) 93.2(2) 87.9(2) 94.23(19) 171.57(19) 97.5(2)
$\begin{array}{c} Symmetry transformations used to y \\ \#1 -x, -y, -z+1 & \#2 -x, -y-1, -z+1 & \#3 \\ Zn(1)-O(4) \\ Zn(1)-O(5) \\ Zn(1)-O(9) \\ Zn(1)-N(3) \\ Zn(1)-N(4) \\ Zn(1)-N(7) \\ Zn(2)-O(1) \\ Zn(2)-O(2)\#1 \\ Zn(2)-O(3)\#1 \\ Zn(2)-N(1) \\ Zn(2)-N(1) \\ Zn(2)-N(1) \\ Zn(3)-O(6)\#1 \\ Zn(3)-O(6)\#1 \\ Zn(3)-O(6) \\ Zn(3)-N(6) \\ Zn(3)-N(6) \\ Zn(3)-N(6) \\ Zn(3)-N(6) \\ Zn(3)-N(13) \\ O(9)-Zn(1)-N(7) \\ O(0) Zn(1)-N(7) \\ O(0) Zn(1)-N(7) \\ O(0) Zn(1)-N(7) \\ Sn(2)-N(1) \\ Sn(2)-$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.110(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85 1(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(1)-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 N(16)#2-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-O(8) O(7)#1-Zn(3)-O(8)	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2) 90.3(2) 93.2(2) 87.9(2) 94.23(19) 171.57(19) 87.5(2) 94.1(2)
$\begin{array}{c} S(y) = 2h(1) \cdot h(0) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(4) \\ Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - N(3) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(7) \#1 \\ Zn(3) - O(6) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ Zn(3) - N(9) \\ Zn(3) - N(13) \\ O(9) - Zn(1) - N(7) \\ O(9) - Zn(1) - N(4) \\ N(7) Zn(1) \\ N(4) \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.110(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(1)-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(1)#1 O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-O(8) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13)	166.5(2) 92.9(2) $174.54(19)$ 88.3(2) 97.6(2) 95.4(2) 76.9(2) 93.7(2) 82.9(2) 91.7(2) 168.6(2) 89.4(2) 170.7(2) 90.3(2) 93.2(2) 87.9(2) 94.23(19) 171.57(19) 87.5(2) 94.1(2) 82.6(2)
$\begin{array}{c} S(y) = 2h(1) \cdot h(0) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(4) \\ Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - N(3) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - N(12) \#3 \\ Zn(2) - N(16) \#2 \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(7) \#1 \\ Zn(3) - O(8) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ Zn(3) - N(9) \\ Zn(3) - N(13) \\ O(9) - Zn(1) - N(7) \\ O(9) - Zn(1) - N(4) \\ N(7) - Zn(1) - N(4) \\ O(9) - Zn(1) - N(4) \\ O(9) - Zn(1) - N(4) \\ O(9) - Zn(1) - O(4) \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 N(16)#2-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(1)#3 O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(8)-Zn(3)-N(13)	166.5(2) $92.9(2)$ $174.54(19)$ $88.3(2)$ $97.6(2)$ $95.4(2)$ $76.9(2)$ $93.7(2)$ $82.9(2)$ $91.7(2)$ $168.6(2)$ $89.4(2)$ $170.7(2)$ $90.3(2)$ $93.2(2)$ $87.9(2)$ $94.23(19)$ $171.57(19)$ $87.5(2)$ $94.1(2)$ $82.6(2)$
Symmetry transformations used to j #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(9) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(2)#1 Zn(2)-O(3)#1 Zn(2)-N(1) Zn(2)-N(1) Zn(2)-N(1)#1 Zn(3)-O(7)#1 Zn(3)-O(6)#1 Zn(3)-O(7)#1 Zn(3)-O(8) Zn(3)-N(6) Zn(3)-N(9) Zn(3)-N(6) Zn(3)-N(9) Zn(3)-N(13) O(9)-Zn(1)-N(4) N(7)-Zn(1)-N(4) N(7)-Zn(1)-O(4)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.110(6) 2.125(5) 2.054(5) 2.054(5) 2.054(5) 2.048(5) 2.048(5) 2.091(5) 2.110(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 N(16)#2-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-O(8) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13)	166.5(2) $92.9(2)$ $174.54(19)$ $88.3(2)$ $97.6(2)$ $95.4(2)$ $76.9(2)$ $93.7(2)$ $82.9(2)$ $91.7(2)$ $168.6(2)$ $89.4(2)$ $170.7(2)$ $90.3(2)$ $93.2(2)$ $87.9(2)$ $94.23(19)$ $171.57(19)$ $87.5(2)$ $94.1(2)$ $82.6(2)$ $94.3(2)$ $95.1(2)$
$\begin{array}{c} S(y) = 2n(1) \cdot N(6) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - O(9) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(3) - O(3) \#1 \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(7) \#1 \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(6) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ Zn(3) - N(6) \\ Zn(3) - N(9) \\ Zn(3) - N(6) \\ Zn(3) - N(9) \\ Zn(3) - N(13) \\ O(9) - Zn(1) - N(4) \\ N(7) - Zn(1) - N(4) \\ N(7) - Zn(1) - O(4) \\ N(4) - Zn(1) - O(4) \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.110(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-N(13) O(8)-Zn(3)-N(13) O(6)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6)	166.5(2) $92.9(2)$ $174.54(19)$ $88.3(2)$ $97.6(2)$ $95.4(2)$ $76.9(2)$ $93.7(2)$ $82.9(2)$ $91.7(2)$ $168.6(2)$ $89.4(2)$ $170.7(2)$ $90.3(2)$ $93.2(2)$ $87.9(2)$ $94.23(19)$ $171.57(19)$ $87.5(2)$ $94.1(2)$ $82.6(2)$ $94.3(2)$ $95.1(2)$ $99.3(2)$
$\begin{array}{c} S(y) = 2h(1) \cdot h(0) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - O(6) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(2) - N(1) \\ Zn(3) - O(3) \#1 \\ Zn(3) - O(3) \#1 \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(7) \#1 \\ Zn(3) - O(8) \\ Zn(3) - O(6) \#1 \\ Zn(3) - O(7) \#1 \\ Zn(3) - O(1) + O(1) \\ Zn(3) - O(1) - O(1) \\ N(7) - Zn(1) - O(1) \\ N(7) - Zn(1) - O(4) \\ N(7) - Zn(1) - O(4) \\ O(9) - Zn(1) - O(5) \\ \hline \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2) 88.1(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6)	$\begin{array}{c} 166.5(2)\\ 92.9(2)\\ 174.54(19)\\ 88.3(2)\\ 97.6(2)\\ 95.4(2)\\ 76.9(2)\\ 93.7(2)\\ 82.9(2)\\ 91.7(2)\\ 168.6(2)\\ 89.4(2)\\ 170.7(2)\\ 90.3(2)\\ 93.2(2)\\ 87.9(2)\\ 94.23(19)\\ 171.57(19)\\ 87.5(2)\\ 94.1(2)\\ 82.6(2)\\ 94.3(2)\\ 95.1(2)\\ 99.3(2)\\ 76.5(2)\\ \end{array}$
$\begin{array}{c} S(y) = 2h(1) \cdot h(0) \\ Symmetry transformations used to y \\ \#1 - x, -y, -z + 1 & \#2 - x, -y - 1, -z + 1 & \#3 \\ \hline Zn(1) - O(5) \\ Zn(1) - O(5) \\ Zn(1) - O(6) \\ Zn(1) - N(3) \\ Zn(1) - N(4) \\ Zn(1) - N(7) \\ Zn(2) - O(1) \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(2) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - O(3) \#1 \\ Zn(2) - N(10) \#1 \\ Zn(2) - N(10) \#1 \\ Zn(3) - O(7) \#1 \\ Zn(3) - O(1) - O(1) \\ Zn(3) - O(1) - O(1) \\ O(9) - Zn(1) - O(1) \\ O(9) - Zn(1) - O(4) \\ O(9) - Zn(1) - O(4) \\ O(9) - Zn(1) - O(5) \\ N(7) - Zn(1) - O(5) \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.110(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2) 88.1(2) 96.4(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(7)=N(13)-Zn(6) N(13)-Zn(3)-N(6)	166.5(2) $92.9(2)$ $174.54(19)$ $88.3(2)$ $97.6(2)$ $95.4(2)$ $76.9(2)$ $93.7(2)$ $82.9(2)$ $91.7(2)$ $168.6(2)$ $89.4(2)$ $170.7(2)$ $90.3(2)$ $93.2(2)$ $87.9(2)$ $94.23(19)$ $171.57(19)$ $87.5(2)$ $94.1(2)$ $82.6(2)$ $94.3(2)$ $95.1(2)$ $99.3(2)$ $76.5(2)$ $170.4(2)$
Symmetry transformations used to j #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-O(5) Zn(1)-N(3) Zn(1)-N(4) Zn(1)-N(7) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(2)#1 Zn(2)-O(3)#1 Zn(2)-N(1) Zn(2)-N(1) Zn(2)-N(1) Zn(3)-O(6)#1 Zn(3)-O(6)#1 Zn(3)-O(6)#1 Zn(3)-O(6) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(6) Zn(3)-N(13) O(9)-Zn(1)-N(4) N(7)-Zn(1)-N(4) N(7)-Zn(1)-O(4) N(7)-Zn(1)-O(4) N(7)-Zn(1)-O(4) N(7)-Zn(1)-O(5) N(4)-Zn(1)-O(5)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2) 88.1(2) 96.4(2) 77.2(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(7)#1 O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(6)#1-Zn(3)-N(6) O	166.5(2) $92.9(2)$ $174.54(19)$ $88.3(2)$ $97.6(2)$ $95.4(2)$ $76.9(2)$ $93.7(2)$ $82.9(2)$ $91.7(2)$ $168.6(2)$ $89.4(2)$ $170.7(2)$ $90.3(2)$ $93.2(2)$ $87.9(2)$ $94.23(19)$ $171.57(19)$ $87.5(2)$ $94.1(2)$ $82.6(2)$ $94.3(2)$ $95.1(2)$ $99.3(2)$ $76.5(2)$ $170.4(2)$ $93.0(2)$
Symmetry transformations used to j #1 -x,-y,-z+1 #2 -x,-y-1,-z+1 #3 Zn(1)-O(4) Zn(1)-O(5) Zn(1)-N(3) Zn(1)-N(3) Zn(1)-N(4) Zn(2)-O(1) Zn(2)-O(2)#1 Zn(2)-O(2)#1 Zn(2)-O(3)#1 Zn(2)-N(1) Zn(2)-N(1) Zn(2)-N(10)#2 Zn(3)-O(6)#1 Zn(3)-O(6)#1 Zn(3)-O(6)#1 Zn(3)-O(6)#1 Zn(3)-O(6) Zn(3)-N(13) O(9)-Zn(1)-N(4) N(7)-Zn(1)-N(4) N(7)-Zn(1)-N(4) N(7)-Zn(1)-O(4) N(7)-Zn(1)-O(4) N(7)-Zn(1)-O(4) N(7)-Zn(1)-O(5) N(7)-Zn(1)-O(5) N(4)-Zn(1)-O(5) O(4)-Zn(1)-O(5)	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.169(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2) 88.1(2) 96.4(2) 77.2(2) 92.95(18)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(2)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(13) O(6)#1-Zn(3)-O(13) O(6)#1-Zn(3)-O(13) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(6) O(7)#1-Zn(3)-N(6) O(6)#1-Zn(3)-N(6) O(6)#1-Zn(3)-N(9) O(7)#1-Zn(3)-N(9)	$\begin{array}{c} 166.5(2)\\ 92.9(2)\\ 174.54(19)\\ 88.3(2)\\ 97.6(2)\\ 95.4(2)\\ 76.9(2)\\ 93.7(2)\\ 82.9(2)\\ 91.7(2)\\ 168.6(2)\\ 89.4(2)\\ 170.7(2)\\ 90.3(2)\\ 93.2(2)\\ 87.9(2)\\ 94.23(19)\\ 171.57(19)\\ 87.5(2)\\ 94.1(2)\\ 82.6(2)\\ 94.3(2)\\ 95.1(2)\\ 99.3(2)\\ 76.5(2)\\ 170.4(2)\\ 93.0(2)\\ 167.9(2)\\ \end{array}$
$\begin{array}{c} Symmetry transformations used to y \\ \#1 -x, -y, -z+1 & \#2 -x, -y-1, -z+1 & \#3 \\ \hline Zn(1)-O(4) \\ Zn(1)-O(5) \\ Zn(1)-O(5) \\ Zn(1)-N(3) \\ Zn(1)-N(3) \\ Zn(1)-N(4) \\ Zn(2)-O(2) \\ Zn(2)-O(2) \\ Zn(2)-O(2) \\ Zn(2)-O(3) \\ Zn(2)-O(3) \\ Zn(2)-N(1) \\ Zn(2)-N(1) \\ Zn(2)-N(1) \\ Zn(2)-N(1) \\ Zn(2)-N(1) \\ Zn(2)-N(1) \\ Zn(3)-O(6) \\ Zn(3)-O(6) \\ Zn(3)-O(6) \\ Zn(3)-O(6) \\ Zn(3)-O(8) \\ Zn(3)-O(7) \\ Zn(3)-O(8) \\ Zn(3)-O(7) \\ Zn(3)-O(8) \\ Zn(3)-O(7) \\ Zn(3)-O(8) \\ Zn(3)-O(7) \\ Zn(3)-O$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.110(5) 2.161(6) 2.213(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2) 88.1(2) 96.4(2) 77.2(2) 92.95(18) 83.1(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(12)#3 O(6)#1-Zn(3)-O(13) O(6)#1-Zn(3)-O(8) O(7)#1-Zn(3)-O(8) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13)	$\begin{array}{c} 166.5(2)\\ 92.9(2)\\ 174.54(19)\\ 88.3(2)\\ 97.6(2)\\ 95.4(2)\\ 76.9(2)\\ 93.7(2)\\ 82.9(2)\\ 91.7(2)\\ 168.6(2)\\ 89.4(2)\\ 170.7(2)\\ 90.3(2)\\ 93.2(2)\\ 87.9(2)\\ 94.23(19)\\ 171.57(19)\\ 87.5(2)\\ 94.1(2)\\ 82.6(2)\\ 94.3(2)\\ 95.1(2)\\ 99.3(2)\\ 76.5(2)\\ 170.4(2)\\ 93.0(2)\\ 167.9(2)\\ 86.7(2)\\ \end{array}$
$\begin{array}{c} Symmetry transformations used to y \\ \#1 -x, -y, -z+1 & \#2 -x, -y-1, -z+1 & \#3 \\ \hline Zn(1)-O(4) \\ Zn(1)-O(5) \\ Zn(1)-O(5) \\ Zn(1)-N(3) \\ Zn(1)-N(4) \\ Zn(1)-N(7) \\ Zn(2)-O(2) \\ \#1 \\ Zn(2)-O(2) \\ \#1 \\ Zn(2)-N(1) \\ Zn(3)-O(6) \\ \#1 \\ Zn(3)-O(6) \\ \#1 \\ Zn(3)-O(6) \\ \#1 \\ Zn(3)-O(6) \\ Zn(3)-N(6) \\ Zn(3)-N(9) \\ Zn(3)-N(13) \\ O(9)-Zn(1)-N(4) \\ O(9)-Zn(1)-N(4) \\ O(9)-Zn(1)-N(4) \\ O(9)-Zn(1)-O(4) \\ N(7)-Zn(1)-O(4) \\ N(4)-Zn(1)-O(5) \\ N(4)-Zn(1)-O(5) \\ O(4)-Zn(1)-O(5) \\ O(9)-Zn(1)-N(3) \\ N(7)-Zn(1)-N(3) \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.110(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2) 88.1(2) 96.4(2) 77.2(2) 92.95(18) 83.1(2) 92.6(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(2)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(12)#3 O(6)#1-Zn(3)-O(12)#3 O(6)#1-Zn(3)-O(13) O(7)#1-Zn(3)-O(8) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N($\begin{array}{c} 166.5(2)\\ 92.9(2)\\ 174.54(19)\\ 88.3(2)\\ 97.6(2)\\ 95.4(2)\\ 76.9(2)\\ 93.7(2)\\ 82.9(2)\\ 91.7(2)\\ 168.6(2)\\ 89.4(2)\\ 170.7(2)\\ 90.3(2)\\ 93.2(2)\\ 87.9(2)\\ 94.23(19)\\ 171.57(19)\\ 87.5(2)\\ 94.1(2)\\ 82.6(2)\\ 94.3(2)\\ 95.1(2)\\ 99.3(2)\\ 76.5(2)\\ 170.4(2)\\ 93.0(2)\\ 167.9(2)\\ 86.7(2)\\ 87.2(2)\\ \end{array}$
$\begin{array}{c} Symmetry transformations used to y \\ \#1 -x, -y, -z+1 & \#2 -x, -y-1, -z+1 & \#3 \\ \hline Zn(1)-O(4) \\ Zn(1)-O(5) \\ Zn(1)-O(9) \\ Zn(1)-N(3) \\ Zn(1)-N(4) \\ Zn(1)-N(7) \\ Zn(2)-O(1) \\ Zn(2)-O(2) \\ \#1 \\ Zn(2)-O(3) \\ \#1 \\ Zn(2)-N(12) \\ Zn(3)-O(6) \\ \#1 \\ Zn(3)-O(6) \\ \#1 \\ Zn(3)-O(8) \\ Zn(3)-N(6) \\ Zn(3)-N(6) \\ Zn(3)-N(6) \\ Zn(3)-N(6) \\ Zn(3)-N(9) \\ Zn(3)-N(13) \\ O(9)-Zn(1)-N(4) \\ N(7)-Zn(1)-O(4) \\ N(7)-Zn(1)-O(4) \\ N(7)-Zn(1)-O(4) \\ N(4)-Zn(1)-O(5) \\ O(9)-Zn(1)-N(3) \\ N(4)-Zn(1)-N(3) \\ N(4)-Zn(1)-N(3) \\ N(4)-Zn(1)-N(3) \\ \end{array}$	generate equivalent atoms: 3 -x,-y,-z 2.123(5) 2.130(5) 2.108(5) 2.108(5) 2.109(6) 2.119(6) 2.119(6) 2.125(5) 2.109(5) 2.054(5) 2.138(6) 2.211(6) 2.147(6) 2.048(5) 2.091(5) 2.161(6) 2.213(6) 2.155(6) 175.6(2) 85.1(2) 95.8(2) 87.1(2) 92.7(2) 167.7(2) 88.1(2) 96.4(2) 77.2(2) 92.95(18) 83.1(2) 92.6(2) 112.0(2)	2 O(5)-Zn(1)-N(3) O(3)#1-Zn(2)-O(2)#1 O(3)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(2)#1-Zn(2)-O(1) O(3)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(1) O(3)#1-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(1)-Zn(2)-N(16)#2 O(3)#1-Zn(2)-N(12)#3 O(2)#1-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(1)-Zn(2)-N(12)#3 O(6)#1-Zn(3)-O(12)#3 O(6)#1-Zn(3)-O(12)#3 O(6)#1-Zn(3)-O(13) O(7)#1-Zn(3)-O(13) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N(13) O(6)#1-Zn(3)-N(13) O(7)#1-Zn(3)-N	$\begin{array}{c} 166.5(2)\\ 92.9(2)\\ 174.54(19)\\ 88.3(2)\\ 97.6(2)\\ 95.4(2)\\ 76.9(2)\\ 93.7(2)\\ 82.9(2)\\ 91.7(2)\\ 168.6(2)\\ 89.4(2)\\ 170.7(2)\\ 90.3(2)\\ 93.2(2)\\ 87.9(2)\\ 94.23(19)\\ 171.57(19)\\ 87.5(2)\\ 94.1(2)\\ 82.6(2)\\ 94.3(2)\\ 95.1(2)\\ 99.3(2)\\ 76.5(2)\\ 170.4(2)\\ 93.0(2)\\ 167.9(2)\\ 86.7(2)\\ 87.2(2)\\ 89.7(2)\\ \end{array}$

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z-1/2 #2 x-1/2,-y+2,-z+1/2 #3 -x,-y+2,-z+2

		3	
Cd(1)-O(1)	2.498(4)	O(9)-K(1)-O(4) ^{#6}	84.60(9)
Cd(1)-O(5)	2.301(4)	O(6)-K(1)-O(6) ^{#3}	60.93(15)
Cd(1)-O(7)	2.243(5)	O(9)-K(1)-O(6) ^{#3}	107.85(9)
Cd(1)-N(1)	2.314(4)	$O(4)^{\#6}$ -K(1)-O(6)^{\#3}	154.21(13)
$Cd(1)-N(2)^{\#1}$	2.285(5)	O(6)-K(1)-O(8)	114.76(13)
Cd(1)-N(4)	2.260(4)	O(9)-K(1)-O(8)	76.63(14)
$K(1)-O(4)^{\#6}$	2.807(4)	O(4) ^{#6} -K(1)-O(8)	80.49(9)
$K(1)-O(6)^{\#3}$	2.861(5)	$O(6)^{\#3}$ -K(1)-O(8)	80.64(10)
K(1)-O(8)	2.970(4)	O(6)-K(1)-N(5) ^{#8}	75.22(11)
K(1)-O(9) ^{#7}	2.805(4)	$O(9)-K(1)-N(5)^{\#8}$	86.11(11)
K(1)-O(6)	2.754(5)	$O(4)^{\#6}$ -K(1)-N(5) ^{#8}	130.72(11)
$K(1)-N(3)^{\#6}$	3.106(5)	$O(6)^{#3}$ -K(1)-N(5) ^{#8}	73.78(11)
K(1)-N(5) ^{#8}	3.102(5)	O(8)-K(1)-N(5) ^{#8}	142.95(7)
K(2)-O(3) ^{#9}	2.908(4)	$O(6)-K(1)-N(3)^{\#6}$	80.67(13)
$K(2)-O(3)^{\#10}$	2.908(4)	O(9)-K(1)-N(3) ^{#6}	102.63(12)
$K(2)-O(5)^{\#6}$	2.818(4)	$O(4)^{\#6}$ -K(1)-N(3)^{\#6}	55.93(12)
K(2)-O(5)	2.818(4)	$O(6)^{#3}$ -K(1)-N(3) ^{#6}	137.40(13)
O(7)-Cd(1)-N(4)	99.16(17)	O(8)-K(1)-N(3) ^{#6}	135.99(10)
$O(7)-Cd(1)-N(2)^{\#1}$	83.4(2)	$N(5)^{#8}$ -K(1)-N(3) ^{#6}	79.44(10)
$N(4)-Cd(1)-N(2)^{\#1}$	100.01(16)	O(5)-K(2)-O(5) ^{#6}	180.0
O(7)-Cd(1)-O(5)	170.13(18)	O(5)-K(2)-O(3) ^{#9}	70.11(11)
N(4)-Cd(1)-O(5)	72.74(14)	$O(5)^{#6}$ -K(2)-O(3) ^{#9}	109.88(11)
$N(2)^{\#1}-Cd(1)-O(5)$	103.32(15)	$O(5)-K(2)-O(3)^{\#10}$	109.89(11)
O(7)-Cd(1)-N(1)	98.20(16)	$O(5)^{\#6}$ -K(2)-O(3)^{\#10}	70.11(11)
N(4)-Cd(1)-N(1)	157.48(17)	$O(3)^{\#9}$ -K(2)-O(3) ^{#10}	180.0
$N(2)^{\#1}-Cd(1)-N(1)$	96.13(15)	O(5)-K(2)-O(7) ^{#8}	68.68(12)
O(5)-Cd(1)-N(1)	88.37(14)	O(5) ^{#6} -K(2)-O(7) ^{#8}	111.33(12)
O(7)-Cd(1)-O(1)	96.79(18)	O(3) ^{#9} -K(2)-O(7) ^{#8}	109.27(11)
N(4)-Cd(1)-O(1)	94.61(14)	$O(3)^{\#10}$ -K(2)-O(7) ^{\#8}	70.73(12)
$N(2)^{#1}-Cd(1)-O(1)$	165.17(13)	$O(5)-K(2)-O(7)^{\#1}$	111.32(12)
O(5)-Cd(1)-O(1)	78.61(14)	$O(5)^{#6}$ -K(2)-O(7) ^{#1}	68.68(12)
N(1)-Cd(1)-O(1)	69.13(14)	$O(3)^{#9}$ -K(2)-O(7) ^{#1}	70.73(12)
O(6)-K(1)-O(9)	160.19(12)	$O(3)^{\#10}$ -K(2)-O(7) $^{\#1}$	109.27(11)
O(6)-K(1)-O(4) ^{#6}	112.53(13)	$O(7)^{#8}$ -K(2)-O(7) ^{#1}	180.00(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x-1,y,z #3 -x+3/2,y,-z+3/2 #4 x,y+1,z #5 -x+3/2,y+1,-z+3/2 #6 -x+1,-y,-z+1 #7 -x+5/2,y,-z+3/2 #8 x,y-1,z #9 x+1,y,z #10 -x,-y,-z+1