Silicon- and Germanium-Centered Tetrahedral Ligands for Metal-Organic Frameworks

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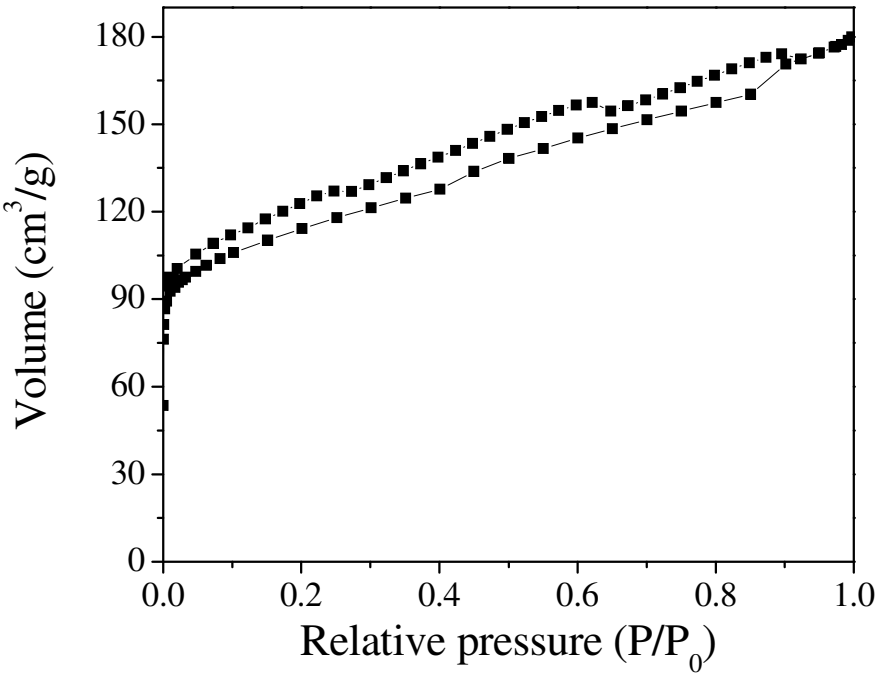
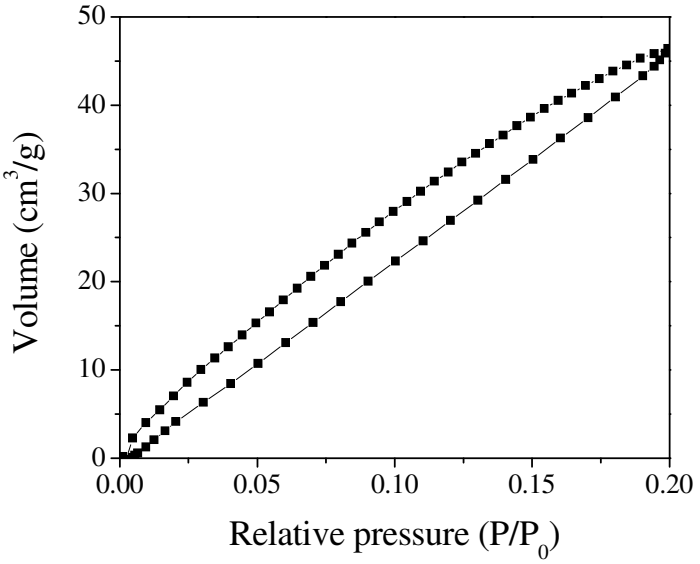
SUPPORTING INFORMATION

Nitrogen Sorption Isotherms of Ge4A-Zn



Carbon Dioxide Sorption Isotherms of Ge4A-Zn



Crystal data and structure refinement for Si4A-Zn

Identification code	Si4A-Zn
Empirical formula	C32.50 H16 N1.50 O11.50 Si Zn2
Formula weight	770.30
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pnna
Unit cell dimensions	a = 12.4868(7) Å
	b = 13.0255(7) Å
	c = 23.7555(13) Å
Volume	3863.8(4) $Å^3$
Z, Calculated density	4, 1.324 Mg/m^3
Absorption coefficient	1.327 mm^{-1}
F(000)	1550
Crystal size	0.540 x 0.318 x 0.262 mm
Theta range for data collection	1.71 to 28.94 º
Limiting indices	-16<=h<=16, -17<=k<=17, -31<=l<=32
Reflections collected / unique	34162 / 4852 [R(int) = 0.0337]
Completeness to theta = 28.94 º	94.7 %
Absorption correction	Integration
Max. and min. transmission	0.7546 and 0.5082
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4852 / 0 / 242
Goodness-of-fit on F^2	1.122
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1802
R indices (all data)	R1 = 0.0633, wR2 = 0.1906
Extinction coefficient	0.0003(3)
Largest diff. peak and hole	1.655 and -0.489 $e.Å^{-3}$

Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Si4A-Zn. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

Atom	X	Y	Z	U(eq)
Zn(1)	0.24070(4)	0.75	0.75	22(1)
Zn(2)	0.75	0	0.29852(2)	22(1)
Si(1)	0.75	0.5	0.53842(5)	21(1)
O(1)	0.7778(2)	0.14939(18)	0.32341(9)	29(1)
O(2)	0.6577(3)	0.0703(2)	0.37567(11)	53(1)
O(3)	0.33891(19)	0.66292(17)	0.70685(9)	30(1)
O(4)	0.3703(2)	0.50861(17)	0.74518(10)	34(1)
O(5)	0.0845(3)	0.75	0.75	38(1)
C(1)	0.7390(2)	0.3864(3)	0.49050(12)	25(1)
C(2)	0.6628(3)	0.3087(3)	0.49549(13)	35(1)
C(3)	0.6579(3)	0.2296(3)	0.45660(14)	39(1)
C(4)	0.7291(3)	0.2268(3)	0.41129(13)	30(1)
C(5)	0.8070(3)	0.3020(3)	0.40609(13)	32(1)
C(6)	0.8117(3)	0.3803(3)	0.44568(13)	31(1)
C(7)	0.7191(3)	0.1444(3)	0.36812(13)	33(1)
C(8)	0.6324(2)	0.5188(2)	0.58606(12)	23(1)
C(9)	0.5999(3)	0.4431(2)	0.62422(13)	29(1)
C(10)	0.5207(3)	0.4617(2)	0.66366(13)	28(1)
C(11)	0.4713(2)	0.5571(2)	0.66618(12)	24(1)
C(12)	0.5015(3)	0.6327(3)	0.62850(16)	40(1)
C(13)	0.5808(3)	0.6137(3)	0.58886(15)	38(1)
C(14)	0.3862(2)	0.5779(2)	0.70955(12)	24(1)
O(6)	0.9487(4)	0.6845(4)	0.8272(2)	35(1)
N(1)	0.8907(16)	0.5368(17)	0.8774(8)	139(6)
C(15)	0.9533(14)	0.6058(13)	0.8343(7)	97(4)
C(16)	0.808(2)	0.596(2)	0.9032(10)	157(8)
C(17)	0.888(3)	0.423(3)	0.8912(13)	207(13)
O(7)	0.8057(19)	0.5464(18)	0.7773(10)	104(6)
N(2)	0.8288(16)	0.3775(14)	0.7711(8)	66(5)
C(18)	0.785(3)	0.455(3)	0.7569(15)	105(10)
C(19)	0.906(3)	0.383(3)	0.8008(17)	123(12)
C(20)	0.790(4)	0.281(5)	0.744(4)	180(20)
O(8)	0.004(2)	0.5599(17)	0.9322(12)	128(10)
O(9)	0.072(3)	0.5407(19)	0.9909(13)	161(13)

Bond lengths [Å] and angles [º] for Si4A-Zn

Bond	Length	Bond	Length
Zn(1)-O(5)	1.951(4)	C(4)-C(5)	1.385(5)
Zn(1)-O(3)#1	1.960(2)	C(4)-C(7)	1.491(4)
Zn(1)-O(3)	1.960(2)	C(5)-C(6)	1.389(4)
Zn(1)-O(1)#2	2.194(2)	C(5)-H(5)	0.95
Zn(1)-O(1)#3	2.194(2)	C(6)-H(6)	0.95
Zn(2)-O(4)#4	1.968(2)	C(8)-C(13)	1.395(4)
Zn(2)-O(4)#5	1.968(2)	C(8)-C(9)	1.399(4)
Zn(2)-O(1)	2.063(2)	C(9)-C(10)	1.384(4)
Zn(2)-O(1)#6	2.063(2)	C(9)-H(9)	0.95
Zn(2)-O(2)#6	2.351(3)	C(10)-C(11)	1.389(4)
Zn(2)-O(2)	2.351(3)	C(10)-H(10)	0.95
Zn(2)-C(7)	2.533(3)	C(11)-C(12)	1.383(4)
Zn(2)-C(7)#6	2.533(3)	C(11)-C(14)	1.505(4)
Si(1)-C(8)#7	1.871(3)	C(12)-C(13)	1.389(5)
Si(1)-C(8)	1.871(3)	C(12)-H(12)	0.95
Si(1)-C(1)	1.872(3)	C(13)-H(13)	0.95
Si(1)-C(1)#7	1.872(3)	O(6)-C(15)	1.041(16)
O(1)-C(7)	1.292(4)	N(1)-C(16)	1.42(3)
O(1)-Zn(1)#2	2.194(2)	N(1)-C(17)	1.52(4)
O(2)-C(7)	1.244(5)	N(1)-C(15)	1.57(2)
O(3)-C(14)	1.257(4)	O(7)-C(18)#7	1.23(4)
O(4)-C(14)	1.253(4)	O(7)-C(18)	1.32(4)
O(4)-Zn(2)#8	1.968(2)	N(2)-C(18)	1.19(4)
C(1)-C(2)	1.395(5)	N(2)-C(19)	1.19(4)
C(1)-C(6)	1.401(4)	N(2)-C(20)	1.49(8)
C(2)-C(3)	1.386(5)	C(18)-O(7)#7	1.23(4)
C(2)-H(2)	0.95	C(18)-C(18)#7	1.47(8)
C(3)-C(4)	1.397(5)	C(20)-C(20)#9	0.85(13)
C(3)-H(3)	0.95		

Bond Angle	Degree	Bond Angle	Degree
O(5)-Zn(1)-O(3)#1	128.73(7)	C(1)-C(2)-H(2)	119.6
O(5)-Zn(1)-O(3)	128.73(7)	C(2)-C(3)-C(4)	120.3(3)
O(3)#1-Zn(1)-O(3)	102.53(15)	C(2)-C(3)-H(3)	119.8

O(5)-Zn(1)-O(1)#2	83.97(7)	C(4)-C(3)-H(3)	119.8
O(3)#1-Zn(1)-O(1)#2	97.81(9)	C(5)-C(4)-C(3)	119.9(3)
O(3)-Zn(1)-O(1)#2	89.76(9)	C(5)-C(4)-C(7)	120.5(3)
O(5)-Zn(1)-O(1)#3	83.97(7)	C(3)-C(4)-C(7)	119.7(3)
O(3)#1-Zn(1)-O(1)#3	89.76(9)	C(4)-C(5)-C(6)	119.2(3)
O(3)-Zn(1)-O(1)#3	97.81(9)	C(4)-C(5)-H(5)	120.4
O(1)#2-Zn(1)-O(1)#3	167.93(13)	C(6)-C(5)-H(5)	120.4
O(4)#4-Zn(2)-O(4)#5	99.86(17)	C(5)-C(6)-C(1)	121.9(3)
O(4)#4-Zn(2)-O(1)	105.01(9)	C(5)-C(6)-H(6)	119
O(4)#5-Zn(2)-O(1)	96.32(9)	C(1)-C(6)-H(6)	119
O(4)#4-Zn(2)-O(1)#6	96.32(9)	O(2)-C(7)-O(1)	120.5(3)
O(4)#5-Zn(2)-O(1)#6	105.01(9)	O(2)-C(7)-C(4)	120.8(3)
O(1)-Zn(2)-O(1)#6	146.69(12)	O(1)-C(7)-C(4)	118.8(3)
O(4)#4-Zn(2)-O(2)#6	153.91(10)	O(2)-C(7)-Zn(2)	67.22(19)
O(4)#5-Zn(2)-O(2)#6	96.07(12)	O(1)-C(7)-Zn(2)	54.18(15)
O(1)-Zn(2)-O(2)#6	93.54(10)	C(4)-C(7)-Zn(2)	166.2(3)
O(1)#6-Zn(2)-O(2)#6	59.42(10)	C(13)-C(8)-C(9)	117.4(3)
O(4)#4-Zn(2)-O(2)	96.07(12)	C(13)-C(8)-Si(1)	120.5(2)
O(4)#5-Zn(2)-O(2)	153.91(10)	C(9)-C(8)-Si(1)	121.8(2)
O(1)-Zn(2)-O(2)	59.42(10)	C(10)-C(9)-C(8)	121.5(3)
O(1)#6-Zn(2)-O(2)	93.54(10)	C(10)-C(9)-H(9)	119.2
O(2)#6-Zn(2)-O(2)	77.54(17)	C(8)-C(9)-H(9)	119.2
O(4)#4-Zn(2)-C(7)	105.16(11)	C(9)-C(10)-C(11)	120.1(3)
O(4)#5-Zn(2)-C(7)	125.37(11)	C(9)-C(10)-H(10)	119.9
O(1)-Zn(2)-C(7)	30.52(11)	C(11)-C(10)-H(10)	119.9
O(1)#6-Zn(2)-C(7)	119.17(11)	C(12)-C(11)-C(10)	119.3(3)
O(2)#6-Zn(2)-C(7)	81.67(12)	C(12)-C(11)-C(14)	120.5(3)
O(2)-Zn(2)-C(7)	29.21(11)	C(10)-C(11)-C(14)	120.3(3)
O(4)#4-Zn(2)-C(7)#6	125.37(11)	C(11)-C(12)-C(13)	120.4(3)
O(4)#5-Zn(2)-C(7)#6	105.16(11)	C(11)-C(12)-H(12)	119.8
O(1)-Zn(2)-C(7)#6	119.17(11)	C(13)-C(12)-H(12)	119.8
O(1)#6-Zn(2)-C(7)#6	30.52(11)	C(12)-C(13)-C(8)	121.3(3)
O(2)#6-Zn(2)-C(7)#6	29.21(11)	C(12)-C(13)-H(13)	119.3
O(2)-Zn(2)-C(7)#6	81.67(12)	C(8)-C(13)-H(13)	119.3
C(7)-Zn(2)-C(7)#6	98.52(16)	O(4)-C(14)-O(3)	126.5(3)
C(8)#7-Si(1)-C(8)	105.54(19)	O(4)-C(14)-C(11)	116.4(3)
C(8)#7-Si(1)-C(1)	108.77(13)	O(3)-C(14)-C(11)	117.1(3)
C(8)-Si(1)-C(1)	114.48(13)	C(16)-N(1)-C(17)	115(2)
C(8)#7-Si(1)-C(1)#7	114.48(13)	C(16)-N(1)-C(15)	109.2(19)
C(8)-Si(1)-C(1)#7	108.77(13)	C(17)-N(1)-C(15)	135(2)
C(1)-Si(1)-C(1)#7	105.1(2)	O(6)-C(15)-N(1)	129.9(17)

C(7)-O(1)-Zn(2)	95.3(2)	C(18)#7-O(7)-C(18)	70(3)
C(7)-O(1)-Zn(1)#2	128.6(2)	C(18)-N(2)-C(19)	119(3)
Zn(2)-O(1)-Zn(1)#2	108.54(9)	C(18)-N(2)-C(20)	116(3)
C(7)-O(2)-Zn(2)	83.6(2)	C(19)-N(2)-C(20)	124(3)
C(14)-O(3)-Zn(1)	141.0(2)	N(2)-C(18)-O(7)#7	108(3)
C(14)-O(4)-Zn(2)#8	126.7(2)	N(2)-C(18)-O(7)	125(4)
C(2)-C(1)-C(6)	117.7(3)	O(7)#7-C(18)-O(7)	93(3)
C(2)-C(1)-Si(1)	124.9(2)	N(2)-C(18)-C(18)#7	162(3)
C(6)-C(1)-Si(1)	117.4(2)	O(7)#7-C(18)-C(18)#7	58(3)
C(3)-C(2)-C(1)	120.9(3)	O(7)-C(18)-C(18)#7	52(3)
C(3)-C(2)-H(2)	119.6	C(20)#9-C(20)-N(2)	132(10)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+3/2,-z+3/2, #2 -x+1,-y+1,-z+1, #3 -x+1,y+1/2,z+1/2, #4 -x+1,y-1/2,z-1/2, #5 x+1/2,-y+1/2,z-1/2, #6 -x+3/2,-y,z, #7 -x+3/2,-y+1,z, #8 x-1/2,-y+1/2,z+1/2, #9 x, -y+1/2,-z+3/2

Anisotropic displacement parameters ($Å^2$ x 10^3) for Si4A-Zn. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U^{11} + ... + 2hka^*b^*U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	26(1)	21(1)	21(1)	-4(1)	0	0
Zn(2)	27(1)	23(1)	17(1)	0	0	1(1)
Si(1)	25(1)	25(1)	12(1)	0	0	4(1)
O(1)	40(1)	29(1)	18(1)	-5(1)	-3(1)	7(1)
O(2)	69(2)	53(2)	36(1)	-20(1)	13(1)	-21(2)
O(3)	36(1)	28(1)	27(1)	2(1)	9(1)	8(1)
O(4)	41(1)	31(1)	30(1)	8(1)	15(1)	7(1)
O(5)	30(2)	36(2)	48(2)	-2(2)	0	0
C(1)	28(1)	32(2)	15(1)	-4(1)	-3(1)	4(1)
C(2)	37(2)	45(2)	22(1)	-9(1)	6(1)	-6(1)
C(3)	44(2)	45(2)	27(2)	-11(1)	5(1)	-13(2)
C(4)	35(2)	37(2)	19(1)	-9(1)	-1(1)	1(1)
C(5)	33(2)	41(2)	21(1)	-8(1)	4(1)	1(1)
C(6)	33(2)	38(2)	24(1)	-8(1)	3(1)	-3(1)
C(7)	41(2)	37(2)	22(2)	-8(1)	-3(1)	2(2)
C(8)	27(1)	28(1)	15(1)	1(1)	1(1)	3(1)
C(9)	40(2)	23(1)	25(1)	2(1)	7(1)	7(1)
C(10)	38(2)	23(1)	23(1)	4(1)	7(1)	3(1)
C(11)	29(1)	24(1)	19(1)	1(1)	2(1)	2(1)
C(12)	48(2)	30(2)	41(2)	14(1)	20(2)	17(2)

C(13)	47(2)	32(2)	35(2)	16(1)	18(2)	14(1)
C(14)	28(1)	26(1)	20(1)	0(1)	1(1)	0(1)
O(8)	128(18)	98(15)	160(20)	39(14)	62(17)	64(14)
O(9)	230(40)	100(17)	150(20)	-17(18)	20(20)	90(20)

Hydrogen coordinates (Å x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Si4A-Zn

Atom	X	Y	Z	U(eq)
H(2)	6135	3101	5260	42
H(3)	6059	1769	4608	46
H(5)	8566	3000	3758	38
H(6)	8658	4312	4423	38
H(9)	6330	3775	6230	35
H(10)	4999	4089	6891	34
H(12)	4677	6980	6297	47
H(13)	6003	6663	5631	46

Crystal data and structure refinement for Ge4A-Zn

Identification code	Ge4A-Zn
Empirical formula	C37 H37 Ge N3 O11 Zn1.50
Formula weight	870.34
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pnnn
Unit cell dimensions	a = 14.2546(9) Å
	b = 23.6813(14) Å
	c = 24.0132(14) Å
Volume	8106.1(8) Å3
Z, Calculated density	8, 1.426 Mg/m3
Absorption coefficient	1.681 mm-1
F(000)	3560
Crystal size	0.378 x 0.348 x 0.040 mm
Theta range for data collection	1.21 to 28.98 º
Limiting indices	-19<=h<=18, -30<=k<=31, -31<=l<=32
Reflections collected / unique	63197 / 10119 [R(int) = 0.0789]
Completeness to theta = 28.98 º	93.9 %
Absorption correction	Integration
Max. and min. transmission	0.9350 and 0.5326
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10119 / 0 / 353
Goodness-of-fit on F^2	0.851
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0882
R indices (all data)	R1 = 0.0681, wR2 = 0.0931
Largest diff. peak and hole	0.515 and -0.412 e.$Å^{-3}$

Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ge4A-Zn. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

Atom	X	Y	Z	U(eq)
Ge(1)	0.563238(19)	0.982971(11)	0.139240(10)	31(1)
Zn(1)	1	1	0	30(1)
Zn(2)	0.56113(2)	0.636441(12)	0.013464(12)	34(1)
O(1)	0.95371(14)	1.14932(8)	0.07674(8)	53(1)
O(2)	0.94949(11)	1.08932(7)	0.00664(6)	34(1)
O(3)	0.6601(5)	0.7239(3)	0.0186(3)	72(1)
O(4)	0.5153(6)	0.7132(3)	0.0302(3)	72(1)
O(3A)	0.6099(5)	0.7134(2)	0.0193(3)	72(1)
O(4A)	0.4694(4)	0.7110(2)	0.0504(2)	72(1)
O(5)	0.11773(13)	1.02367(7)	0.04671(7)	42(1)
O(6)	0.16707(13)	1.11279(8)	0.03334(7)	45(1)
O(7)	0.55539(13)	0.98190(7)	0.42635(7)	39(1)
O(8)	0.59146(14)	0.89152(8)	0.41103(7)	48(1)
C(1)	0.66743(18)	1.02805(10)	0.11220(9)	33(1)
C(2)	0.72565(18)	1.05803(11)	0.14817(10)	39(1)
C(3)	0.80339(19)	1.08686(11)	0.12817(10)	40(1)
C(4)	0.82499(18)	1.08558(10)	0.07207(10)	35(1)
C(5)	0.76562(18)	1.05713(10)	0.03591(10)	36(1)
C(6)	0.68713(18)	1.02964(11)	0.05540(10)	38(1)
C(7)	0.91443(18)	1.11030(11)	0.05171(11)	38(1)
C(8)	0.5659(2)	0.90929(11)	0.10323(11)	43(1)
C(9)	0.6480(2)	0.88158(11)	0.09109(11)	47(1)
C(10)	0.6469(3)	0.82746(13)	0.06968(12)	66(1)
C(11)	0.5669(4)	0.79942(14)	0.06046(14)	77(1)
C(12)	0.4857(4)	0.82739(17)	0.06880(19)	110(2)
C(13)	0.4843(3)	0.88245(15)	0.08931(18)	90(1)
C(14A)	0.5899(6)	0.7412(5)	0.0325(4)	52(2)
C(14B)	0.5399(5)	0.7368(4)	0.0435(3)	52(2)
C(15)	0.44279(18)	1.01618(10)	0.11996(10)	32(1)
C(16)	0.43602(19)	1.05850(11)	0.07978(10)	38(1)
C(17)	0.35037(19)	1.07532(11)	0.05972(10)	38(1)
C(18)	0.26851(17)	1.04899(10)	0.07784(9)	33(1)
C(19)	0.27360(19)	1.00776(12)	0.11893(10)	42(1)
C(20)	0.36037(19)	0.99241(11)	0.14020(10)	40(1)
C(21)	0.17650(19)	1.06258(11)	0.05102(10)	36(1)
C(22)	0.57133(17)	0.97146(10)	0.21936(9)	31(1)

C(23)	0.5295(2)	1.00904(10)	0.25644(11)	40(1)
C(24)	0.53245(19)	0.99953(11)	0.31293(10)	39(1)
C(25)	0.57683(17)	0.95282(11)	0.33409(9)	33(1)
C(26)	0.6190(2)	0.91521(11)	0.29758(10)	43(1)
C(27)	0.6166(2)	0.92469(11)	0.24105(10)	43(1)
C(28)	0.57426(17)	0.94130(11)	0.39536(10)	35(1)

Bond lengths [Å] and angles [º] for Ge4A-Zn

Bond	Length	Bond	Length
Ge(1)-C(1)	1.941(3)	C(2)-H(2)	0.95
Ge(1)-C(15)	1.944(3)	C(3)-C(4)	1.382(3)
Ge(1)-C(22)	1.947(2)	C(3)-H(3)	0.95
Ge(1)-C(8)	1.948(3)	C(4)-C(5)	1.387(3)
Zn(1)-O(7)#1	1.9836(16)	C(4)-C(7)	1.486(4)
Zn(1)-O(7)#2	1.9836(16)	C(5)-C(6)	1.376(3)
Zn(1)-O(5)#3	2.0950(18)	C(5)-H(5)	0.95
Zn(1)-O(5)#4	2.0950(18)	C(6)-H(6)	0.95
Zn(1)-O(2)#5	2.2402(17)	C(8)-C(13)	1.367(4)
Zn(1)-O(2)	2.2402(17)	C(8)-C(9)	1.373(4)
Zn(2)-O(3A)	1.956(6)	C(9)-C(10)	1.381(4)
Zn(2)-O(6)#6	1.9641(17)	C(9)-H(9)	0.95
Zn(2)-O(4)	1.973(6)	C(10)-C(11)	1.338(5)
Zn(2)-O(8)#7	1.9780(17)	C(10)-H(10)	0.95
Zn(2)-O(2)#8	2.0026(17)	C(11)-C(12)	1.349(6)
Zn(2)-O(4A)	2.369(5)	C(11)-C(14A)	1.567(11)
Zn(2)-C(14B)	2.502(9)	C(11)-C(14B)	1.586(9)
Zn(2)-C(14A)	2.557(11)	C(12)-C(13)	1.394(5)
O(1)-C(7)	1.236(3)	C(12)-H(12)	0.95
O(2)-C(7)	1.292(3)	C(13)-H(13)	0.95
O(2)-Zn(2)#9	2.0026(17)	C(14A)-C(14B)	0.767(9)
O(3)-O(3A)	0.758(7)	C(15)-C(20)	1.391(4)
O(3)-C(14A)	1.133(10)	C(15)-C(16)	1.394(3)
O(3)-C(14B)	1.840(9)	C(16)-C(17)	1.372(3)
O(4)-C(14B)	0.732(9)	C(16)-H(16)	0.95
O(4)-O(4A)	0.818(8)	C(17)-C(18)	1.393(3)
O(4)-C(14A)	1.254(12)	C(17)-H(17)	0.95
O(4)-O(3A)	1.373(10)	C(18)-C(19)	1.390(3)
O(3A)-C(14A)	0.785(10)	C(18)-C(21)	1.496(3)
O(3A)-C(14B)	1.280(10)	C(19)-C(20)	1.387(4)

O(4A)-C(14B)	1.188(8)	C(19)-H(19)	0.95
O(4A)-C(14A)	1.910(9)	C(20)-H(20)	0.95
O(5)-C(21)	1.250(3)	C(22)-C(27)	1.384(3)
O(5)-Zn(1)#10	2.0950(18)	C(22)-C(23)	1.393(3)
O(6)-C(21)	1.270(3)	C(23)-C(24)	1.376(4)
O(6)-Zn(2)#11	1.9641(17)	C(23)-H(23)	0.95
O(7)-C(28)	1.245(3)	C(24)-C(25)	1.372(3)
O(7)-Zn(1)#2	1.9836(16)	C(24)-H(24)	0.95
O(8)-C(28)	1.261(3)	C(25)-C(26)	1.387(3)
O(8)-Zn(2)#7	1.9780(17)	C(25)-C(28)	1.497(3)
C(1)-C(2)	1.393(3)	C(26)-C(27)	1.376(3)
C(1)-C(6)	1.393(3)	C(26)-H(26)	0.95
C(2)-C(3)	1.387(4)	C(27)-H(27)	0.95

Bond Angle	Degree	Bond Angle	Degree
C(1)-Ge(1)-C(15)	111.94(10)	C(13)-C(8)-C(9)	116.8(3)
C(1)-Ge(1)-C(22)	111.24(10)	C(13)-C(8)-Ge(1)	120.6(2)
C(15)-Ge(1)-C(22)	110.14(10)	C(9)-C(8)-Ge(1)	122.6(2)
C(1)-Ge(1)-C(8)	109.21(11)	C(8)-C(9)-C(10)	120.8(3)
C(15)-Ge(1)-C(8)	105.90(11)	C(8)-C(9)-H(9)	119.6
C(22)-Ge(1)-C(8)	108.19(11)	C(10)-C(9)-H(9)	119.6
O(7)#1-Zn(1)-O(7)#2	180.000(1)	C(11)-C(10)-C(9)	122.2(3)
O(7)#1-Zn(1)-O(5)#3	95.78(7)	C(11)-C(10)-H(10)	118.9
O(7)#2-Zn(1)-O(5)#3	84.22(7)	C(9)-C(10)-H(10)	118.9
O(7)#1-Zn(1)-O(5)#4	84.22(7)	C(10)-C(11)-C(12)	117.6(3)
O(7)#2-Zn(1)-O(5)#4	95.78(7)	C(10)-C(11)-C(14A)	109.2(5)
O(5)#3-Zn(1)-O(5)#4	180	C(12)-C(11)-C(14A)	132.4(5)
O(7)#1-Zn(1)-O(2)#5	90.73(6)	C(10)-C(11)-C(14B)	135.6(4)
O(7)#2-Zn(1)-O(2)#5	89.27(6)	C(12)-C(11)-C(14B)	106.8(5)
O(5)#3-Zn(1)-O(2)#5	91.91(6)	C(14A)-C(11)-C(14B)	28.1(3)
O(5)#4-Zn(1)-O(2)#5	88.10(6)	C(11)-C(12)-C(13)	121.6(4)
O(7)#1-Zn(1)-O(2)	89.27(6)	C(11)-C(12)-H(12)	119.2
O(7)#2-Zn(1)-O(2)	90.73(6)	C(13)-C(12)-H(12)	119.2
O(5)#3-Zn(1)-O(2)	88.09(6)	C(8)-C(13)-C(12)	120.6(4)
O(5)#4-Zn(1)-O(2)	91.90(6)	C(8)-C(13)-H(13)	119.7
O(2)#5-Zn(1)-O(2)	180	C(12)-C(13)-H(13)	119.7
O(3A)-Zn(2)-O(6)#6	91.9(2)	C(14B)-C(14A)-O(3A)	111.2(18)
O(3A)-Zn(2)-O(4)	40.9(3)	C(14B)-C(14A)-O(3)	150.8(18)
O(6)#6-Zn(2)-O(4)	129.3(3)	O(3A)-C(14A)-O(3)	41.9(6)
O(3A)-Zn(2)-O(8)#7	99.67(19)	C(14B)-C(14A)-O(4)	32.4(11)

O(6)#6-Zn(2)-O(8)#7	105.13(8)	O(3A)-C(14A)-O(4)	81.2(10)
O(4)-Zn(2)-O(8)#7	101.2(2)	O(3)-C(14A)-O(4)	123.0(10)
O(3A)-Zn(2)-O(2)#8	145.0(2)	C(14B)-C(14A)-C(11)	77.3(13)
O(6)#6-Zn(2)-O(2)#8	108.31(7)	O(3A)-C(14A)-C(11)	170.7(12)
O(4)-Zn(2)-O(2)#8	107.4(2)	O(3)-C(14A)-C(11)	129.0(9)
O(8)#7-Zn(2)-O(2)#8	102.01(7)	O(4)-C(14A)-C(11)	107.9(7)
O(3A)-Zn(2)-O(4A)	58.3(2)	C(14B)-C(14A)-O(4A)	15.3(11)
O(6)#6-Zn(2)-O(4A)	148.34(16)	O(3A)-C(14A)-O(4A)	95.9(10)
O(4)-Zn(2)-O(4A)	19.0(3)	O(3)-C(14A)-O(4A)	136.6(9)
O(8)#7-Zn(2)-O(4A)	91.54(16)	O(4)-C(14A)-O(4A)	18.1(4)
O(2)#8-Zn(2)-O(4A)	93.82(15)	C(11)-C(14A)-O(4A)	92.6(5)
O(3A)-Zn(2)-C(14B)	30.4(2)	C(14B)-C(14A)-Zn(2)	77.2(13)
O(6)#6-Zn(2)-C(14B)	121.93(19)	O(3A)-C(14A)-Zn(2)	34.0(8)
O(4)-Zn(2)-C(14B)	13.1(3)	O(3)-C(14A)-Zn(2)	74.8(6)
O(8)#7-Zn(2)-C(14B)	94.61(19)	O(4)-C(14A)-Zn(2)	48.9(5)
O(2)#8-Zn(2)-C(14B)	120.17(18)	C(11)-C(14A)-Zn(2)	153.7(6)
O(4A)-Zn(2)-C(14B)	28.07(18)	O(4A)-C(14A)-Zn(2)	62.1(3)
O(3A)-Zn(2)-C(14A)	13.0(3)	O(4)-C(14B)-C(14A)	113.5(19)
O(6)#6-Zn(2)-C(14A)	104.8(2)	O(4)-C(14B)-O(4A)	42.7(8)
O(4)-Zn(2)-C(14A)	28.6(3)	C(14A)-C(14B)-O(4A)	154.8(17)
O(8)#7-Zn(2)-C(14A)	97.2(2)	O(4)-C(14B)-O(3A)	81.1(11)
O(2)#8-Zn(2)-C(14A)	135.3(2)	C(14A)-C(14B)-O(3A)	34.9(11)
O(4A)-Zn(2)-C(14A)	45.4(2)	O(4A)-C(14B)-O(3A)	120.0(8)
C(14B)-Zn(2)-C(14A)	17.39(19)	O(4)-C(14B)-C(11)	160.2(11)
C(7)-O(2)-Zn(2)#9	107.17(16)	C(14A)-C(14B)-C(11)	74.6(13)
C(7)-O(2)-Zn(1)	123.18(15)	O(4A)-C(14B)-C(11)	130.6(7)
Zn(2)#9-O(2)-Zn(1)	104.69(7)	O(3A)-C(14B)-C(11)	109.4(6)
O(3A)-O(3)-C(14A)	43.7(7)	O(4)-C(14B)-O(3)	100.2(11)
O(3A)-O(3)-C(14B)	33.7(7)	C(14A)-C(14B)-O(3)	17.5(11)
C(14A)-O(3)-C(14B)	11.7(7)	O(4A)-C(14B)-O(3)	138.5(7)
C(14B)-O(4)-O(4A)	100.0(12)	O(3A)-C(14B)-O(3)	19.2(3)
C(14B)-O(4)-C(14A)	34.1(10)	C(11)-C(14B)-O(3)	90.7(5)
O(4A)-O(4)-C(14A)	133.4(10)	O(4)-C(14B)-Zn(2)	37.7(8)
C(14B)-O(4)-O(3A)	67.1(9)	C(14A)-C(14B)-Zn(2)	85.4(13)
O(4A)-O(4)-O(3A)	154.1(11)	O(4A)-C(14B)-Zn(2)	69.8(5)
C(14A)-O(4)-O(3A)	34.4(5)	O(3A)-C(14B)-Zn(2)	50.5(4)
C(14B)-O(4)-Zn(2)	129.2(11)	C(11)-C(14B)-Zn(2)	158.9(5)
O(4A)-O(4)-Zn(2)	109.0(8)	O(3)-C(14B)-Zn(2)	68.7(3)
C(14A)-O(4)-Zn(2)	102.5(6)	C(20)-C(15)-C(16)	118.3(2)
O(3A)-O(4)-Zn(2)	68.9(4)	C(20)-C(15)-Ge(1)	119.94(18)
O(3)-O(3A)-C(14A)	94.4(10)	C(16)-C(15)-Ge(1)	121.11(19)

O(3)-O(3A)-C(14B)	127.2(9)	C(17)-C(16)-C(15)	120.9(2)
C(14A)-O(3A)-C(14B)	33.9(9)	C(17)-C(16)-H(16)	119.6
O(3)-O(3A)-O(4)	158.8(9)	C(15)-C(16)-H(16)	119.6
C(14A)-O(3A)-O(4)	64.4(8)	C(16)-C(17)-C(18)	120.4(2)
C(14B)-O(3A)-O(4)	31.8(4)	C(16)-C(17)-H(17)	119.8
O(3)-O(3A)-Zn(2)	129.9(9)	C(18)-C(17)-H(17)	119.8
C(14A)-O(3A)-Zn(2)	133.0(10)	C(19)-C(18)-C(17)	119.5(2)
C(14B)-O(3A)-Zn(2)	99.1(5)	C(19)-C(18)-C(21)	120.2(2)
O(4)-O(3A)-Zn(2)	70.2(4)	C(17)-C(18)-C(21)	120.2(2)
O(4)-O(4A)-C(14B)	37.4(6)	C(20)-C(19)-C(18)	119.5(2)
O(4)-O(4A)-C(14A)	28.5(7)	C(20)-C(19)-H(19)	120.3
C(14B)-O(4A)-C(14A)	9.8(7)	C(18)-C(19)-H(19)	120.3
O(4)-O(4A)-Zn(2)	52.0(6)	C(19)-C(20)-C(15)	121.3(2)
C(14B)-O(4A)-Zn(2)	82.2(5)	C(19)-C(20)-H(20)	119.4
C(14A)-O(4A)-Zn(2)	72.5(4)	C(15)-C(20)-H(20)	119.4
C(21)-O(5)-Zn(1)#10	141.13(16)	O(5)-C(21)-O(6)	126.3(2)
C(21)-O(6)-Zn(2)#11	122.67(17)	O(5)-C(21)-C(18)	117.7(2)
C(28)-O(7)-Zn(1)#2	141.78(17)	O(6)-C(21)-C(18)	116.0(2)
C(28)-O(8)-Zn(2)#7	122.95(16)	C(27)-C(22)-C(23)	118.1(2)
C(2)-C(1)-C(6)	118.3(2)	C(27)-C(22)-Ge(1)	120.78(17)
C(2)-C(1)-Ge(1)	121.94(18)	C(23)-C(22)-Ge(1)	121.13(18)
C(6)-C(1)-Ge(1)	119.78(19)	C(24)-C(23)-C(22)	120.8(2)
C(3)-C(2)-C(1)	120.8(2)	C(24)-C(23)-H(23)	119.6
C(3)-C(2)-H(2)	119.6	C(22)-C(23)-H(23)	119.6
C(1)-C(2)-H(2)	119.6	C(25)-C(24)-C(23)	120.8(2)
C(4)-C(3)-C(2)	120.3(2)	C(25)-C(24)-H(24)	119.6
C(4)-C(3)-H(3)	119.8	C(23)-C(24)-H(24)	119.6
C(2)-C(3)-H(3)	119.8	C(24)-C(25)-C(26)	118.9(2)
C(3)-C(4)-C(5)	119.0(2)	C(24)-C(25)-C(28)	120.0(2)
C(3)-C(4)-C(7)	120.2(2)	C(26)-C(25)-C(28)	121.0(2)
C(5)-C(4)-C(7)	120.6(2)	C(27)-C(26)-C(25)	120.5(2)
C(6)-C(5)-C(4)	120.9(2)	C(27)-C(26)-H(26)	119.7
C(6)-C(5)-H(5)	119.6	C(25)-C(26)-H(26)	119.7
C(4)-C(5)-H(5)	119.6	C(26)-C(27)-C(22)	120.9(2)
C(5)-C(6)-C(1)	120.6(2)	C(26)-C(27)-H(27)	119.6
C(5)-C(6)-H(6)	119.7	C(22)-C(27)-H(27)	119.6
C(1)-C(6)-H(6)	119.7	O(7)-C(28)-O(8)	125.8(2)
O(1)-C(7)-O(2)	121.3(2)	O(7)-C(28)-C(25)	116.9(2)
O(1)-C(7)-C(4)	121.5(2)	O(8)-C(28)-C(25)	117.3(2)
O(2)-C(7)-C(4)	117.2(2)		

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+2,z-1/2, #2 -x+3/2,y,-z+1/2, #3 x+1,y,z, #4 -x+1,-y+2,-z, #5 -x+2,-y+2,-z, #6 x+1/2,y-1/2,-z, #7 x,-y+3/2,-z+1/2, #8 x-1/2,y-1/2,-z, #9 x+1/2,y+1/2,-z, #10 x-1,y,z, #11 x-1/2,y+1/2,-z

Anisotropic60 displacement parameters ($Å^2$ x 10^3) for Ge4A-Zn. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U^{11} + ... + 2hka^*b^*U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ge(1)	33(1)	33(1)	28(1)	-5(1)	-3(1)	1(1)
Zn(1)	32(1)	33(1)	26(1)	5(1)	-1(1)	-1(1)
Zn(2)	38(1)	30(1)	35(1)	-5(1)	4(1)	-1(1)
O(1)	52(1)	45(1)	63(1)	-15(1)	10(1)	-14(1)
O(2)	35(1)	34(1)	32(1)	6(1)	0(1)	1(1)
O(3)	82(3)	39(1)	97(2)	-29(1)	-5(2)	0(2)
O(4)	82(3)	39(1)	97(2)	-29(1)	-5(2)	0(2)
O(3A)	82(3)	39(1)	97(2)	-29(1)	-5(2)	0(2)
O(4A)	82(3)	39(1)	97(2)	-29(1)	-5(2)	0(2)
O(5)	39(1)	41(1)	46(1)	0(1)	-10(1)	-1(1)
O(6)	44(1)	41(1)	51(1)	8(1)	-15(1)	-2(1)
O(7)	49(1)	39(1)	30(1)	-8(1)	5(1)	-7(1)
O(8)	65(1)	46(1)	33(1)	1(1)	5(1)	15(1)
C(1)	36(2)	34(1)	28(1)	-2(1)	1(1)	5(1)
C(2)	39(2)	48(2)	29(1)	-5(1)	1(1)	-2(1)
C(3)	40(2)	40(2)	39(2)	-7(1)	-3(1)	-2(1)
C(4)	34(2)	32(1)	39(1)	-1(1)	1(1)	7(1)
C(5)	38(2)	40(2)	32(1)	0(1)	0(1)	3(1)
C(6)	37(2)	42(2)	35(1)	-5(1)	-5(1)	1(1)
C(7)	42(2)	34(2)	38(1)	7(1)	-1(1)	5(1)
C(8)	52(2)	35(2)	41(2)	-8(1)	-2(1)	3(1)
C(9)	62(2)	36(2)	44(2)	4(1)	9(1)	10(2)
C(10)	118(3)	44(2)	37(2)	4(1)	18(2)	31(2)
C(11)	129(4)	36(2)	65(2)	-17(2)	-24(2)	25(2)
C(12)	124(4)	54(3)	152(4)	-36(3)	-44(3)	-7(3)
C(13)	70(3)	52(2)	147(4)	-46(2)	-18(3)	1(2)
C(14A)	55(5)	46(3)	54(4)	-1(3)	-5(4)	4(4)
C(14B)	55(5)	46(3)	54(4)	-1(3)	-5(4)	4(4)
C(15)	34(1)	29(1)	32(1)	-3(1)	-6(1)	-1(1)
C(16)	37(2)	41(2)	37(1)	-2(1)	0(1)	-8(1)
C(17)	47(2)	37(2)	32(1)	7(1)	-6(1)	1(1)
C(18)	36(2)	34(1)	30(1)	-4(1)	-6(1)	1(1)

C(19)	36(2)	54(2)	36(1)	7(1)	-3(1)	-2(1)
C(20)	41(2)	45(2)	34(1)	14(1)	-4(1)	7(1)
C(21)	39(2)	39(2)	31(1)	-3(1)	-5(1)	5(1)
C(22)	29(1)	36(1)	27(1)	-3(1)	-1(1)	1(1)
C(23)	50(2)	33(1)	38(2)	-2(1)	-6(1)	12(1)
C(24)	43(2)	39(2)	34(1)	-13(1)	0(1)	8(1)
C(25)	35(2)	34(1)	31(1)	-7(1)	1(1)	1(1)
C(26)	54(2)	41(2)	35(1)	0(1)	0(1)	20(1)
C(27)	51(2)	46(2)	32(1)	-7(1)	2(1)	18(1)
C(28)	34(2)	39(2)	31(1)	-8(1)	1(1)	-4(1)

Hydrogen coordinates (Å x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ge4A-Zn

Atom	X	Y	Z	U(eq)
H(2)	7120	10588	1869	46
H(3)	8420	11076	1531	47
H(5)	7793	10566	-28	44
H(6)	6460	10116	299	45
H(9)	7064	8999	975	57
H(10)	7048	8096	612	80
H(12)	4280	8091	605	132
H(13)	4261	9015	937	108
H(16)	4915	10759	661	45
H(17)	3469	11051	333	46
H(19)	2181	9902	1323	50
H(20)	3636	9651	1691	48
H(23)	4985	10416	2425	48
H(24)	5034	10256	3376	47
H(26)	6498	8826	3117	52
H(27)	6465	8988	2166	52