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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Identification code	Zn(BDC)(H2O).(DMF)
Empirical formula	$C_{11}H_{13}NO_6Zn$
Color	Colorless
Habit	Prismatic
Crystal size	0.31 x 0.27 x 0.22 mm
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 6.718(3) Å α = 90° b = 15.488(7) Å β = 102.83(4)° c = 12.430(8) Å γ = 90°
Volume	1261.0(11) $Å^3$
Cell Refinement	Siemens P3/VAX rel. 4.2
Z	4
Formula weight	320.59
Density (calculated)	1.689 Mg/m^3
Absorption coefficient	1.970 mm^{-1}
F(000)	656

Data Collection

Diffractometer	Siemens R3m/V Autodiffractometer
Collection Software	Siemens P3/VAX rel. 4.2
Wavelength	0.71073 Å
Temperature	293(2) K
Monochromator	Graphite
θ range for data collection	2.13 to 25.04°
Measurement Method	ω scan
Measurement Speed	Variable, 1.50 to 14.65°/min. in ω
Measurement Range	1.60° in ω
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	2
Standards Count Interval	48
Standards Decay	0%
Data Reduction	Siemens XDISK rel. 4.2
Index ranges	$-8 \le h \le 7$ $-1 \le k \le 18$ $-14 \le l \le 7$
Reflections collected	2508
Independent reflections	2219 (R_{int} = 0.0360)
Observed Reflections	1524
Observed Criterion	>2sigma(I)
Absorption correction	Psi-scan
Max. and min. transmission	0.648 and 0.543

Structure Solution and Refinement

Structure Solution	Direct Methods SHELXS-86 (Sheldrick, 1990)
Structure Refinement	Fourier Difference Map SHELXL-93 (Sheldrick, 1993)
Refinement method	Full-matrix least-squares on F^2
Hydrogen Atoms	Riding model
Weighting Scheme	$w=1/[\sigma^2(Fo^2)+(0.0462P)^2+1.1551P]$ where $P=(Fo^2+2Fc^2)/3$
Data / restraints / parameters	2218 / 0 / 172
Final R indices [$I>2\sigma(I)$]	R1 = 0.0458, wR2 = 0.0923
R indices (all data)	R1 = 0.0842, wR2 = 0.1092
Goodness-of-fit on F^2	1.079
Largest and Mean Δ/σ	-0.001, 0.000
Largest diff. peak and hole	0.631 and -0.613 $e\text{Å}^{-3}$
Molecular Graphics	Siemens SHELXTL PC rel. 5.03
Publication Material	Siemens SHELXTL PC rel. 5.03

Table 1. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $C_{11}H_{13}NO_6Zn$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zn(1)	2003(1)	5050(1)	5771(1)	17(1)
O(1)	-600(6)	3952(3)	3669(3)	41(1)
O(2)	2442(6)	4030(3)	4791(3)	41(1)
O(3)	2841(6)	796(3)	587(3)	43(1)
O(4)	5876(6)	805(3)	1715(3)	44(1)
O(5)	4830(5)	5213(2)	6569(3)	29(1)
C(1)	1948(8)	2990(3)	3372(4)	22(1)
C(2)	599(8)	2584(3)	2513(4)	25(1)
C(3)	1280(8)	1960(3)	1895(4)	25(1)
C(4)	3324(8)	1713(3)	2125(4)	22(1)
C(5)	4671(8)	2112(3)	3003(4)	26(1)
C(6)	3991(8)	2743(3)	3617(4)	28(1)
C(7)	1213(8)	3706(3)	3998(4)	22(1)
C(8)	4067(8)	1054(3)	1419(4)	22(1)
O(1S)	6439(7)	4869(3)	8628(3)	53(1)
N(1S)	6382(9)	3967(4)	10052(4)	49(1)
C(2S)	5644(11)	4286(4)	9060(5)	47(2)
C(3S)	5375(13)	3279(5)	10506(7)	74(2)
C(4S)	8278(12)	4285(6)	10706(6)	73(3)

Table 2. Bond lengths [Å] for $C_{11}H_{13}NO_6Zn$.

Zn(1)-O(5)	1.954(4)	Zn(1)-O(1)#1	2.014(4)
Zn(1)-O(4)#2	2.025(4)	Zn(1)-O(2)	2.055(4)
Zn(1)-O(3)#3	2.068(4)	Zn(1)-Zn(1)#1	2.940(2)
O(1)-C(7)	1.255(6)	O(1)-Zn(1)#1	2.014(4)
O(2)-C(7)	1.243(6)	O(3)-C(8)	1.236(6)
O(3)-Zn(1)#4	2.068(4)	O(4)-C(8)	1.250(6)
O(4)-Zn(1)#5	2.025(4)	C(1)-C(2)	1.388(7)
C(1)-C(6)	1.392(7)	C(1)-C(7)	1.500(7)
C(2)-C(3)	1.375(7)	C(3)-C(4)	1.392(7)
C(4)-C(5)	1.397(7)	C(4)-C(8)	1.502(7)
C(5)-C(6)	1.379(7)	O(1S)-C(2S)	1.231(8)
N(1S)-C(2S)	1.319(8)	N(1S)-C(4S)	1.437(9)
N(1S)-C(3S)	1.442(9)		

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1/2,y-1/2,-z+1/2 #5 x+1/2,-y+1/2,z-1/2

Table 3. Bond angles [°] for $C_{11}H_{13}NO_6Zn$.

O(5)-Zn(1)-O(1)#1	101.7(2)	O(5)-Zn(1)-O(4)#2	103.7(2)
O(1)#1-Zn(1)-O(4)#2	92.1(2)	O(5)-Zn(1)-O(2)	98.5(2)
O(1)#1-Zn(1)-O(2)	159.2(2)	O(4)#2-Zn(1)-O(2)	87.8(2)
O(5)-Zn(1)-O(3)#3	97.0(2)	O(1)#1-Zn(1)-O(3)#3	88.0(2)
O(4)#2-Zn(1)-O(3)#3	158.8(2)	O(2)-Zn(1)-O(3)#3	84.6(2)
O(5)-Zn(1)-Zn(1)#1	169.50(10)	O(1)#1-Zn(1)-Zn(1)#1	80.50(12)
O(4)#2-Zn(1)-Zn(1)#1	86.42(13)	O(2)-Zn(1)-Zn(1)#1	78.73(12)
O(3)#3-Zn(1)-Zn(1)#1	72.69(12)	C(7)-O(1)-Zn(1)#1	128.0(3)
C(7)-O(2)-Zn(1)	128.6(4)	C(8)-O(3)-Zn(1)#4	135.9(4)
C(8)-O(4)-Zn(1)#5	119.7(4)	C(2)-C(1)-C(6)	119.2(5)
C(2)-C(1)-C(7)	120.0(5)	C(6)-C(1)-C(7)	120.8(5)
C(3)-C(2)-C(1)	120.5(5)	C(2)-C(3)-C(4)	120.9(5)
C(3)-C(4)-C(5)	118.5(5)	C(3)-C(4)-C(8)	120.4(5)
C(5)-C(4)-C(8)	121.0(5)	C(6)-C(5)-C(4)	120.6(5)
C(5)-C(6)-C(1)	120.4(5)	O(2)-C(7)-O(1)	124.1(5)
O(2)-C(7)-C(1)	118.2(5)	O(1)-C(7)-C(1)	117.6(5)
O(3)-C(8)-O(4)	124.8(5)	O(3)-C(8)-C(4)	117.5(5)
O(4)-C(8)-C(4)	117.7(5)	C(2S)-N(1S)-C(4S)	120.2(6)
C(2S)-N(1S)-C(3S)	122.1(7)	C(4S)-N(1S)-C(3S)	117.7(6)
O(1S)-C(2S)-N(1S)	125.0(7)		

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1/2,y-1/2,-z+1/2 #5 x+1/2,-y+1/2,z-1/2

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for $C_{11}H_{13}NO_6Zn$. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Zn(1)	17(1)	19(1)	16(1)	0(1)	6(1)	1(1)
O(1)	31(3)	44(3)	41(2)	-22(2)	-3(2)	15(2)
O(2)	32(2)	45(3)	44(3)	-29(2)	3(2)	6(2)
O(3)	35(3)	57(3)	36(2)	-27(2)	5(2)	4(2)
O(4)	37(3)	52(3)	44(3)	-23(2)	8(2)	15(2)
O(5)	21(2)	43(2)	20(2)	0(2)	2(2)	-1(2)
C(1)	26(3)	22(3)	19(3)	-1(2)	10(2)	1(2)
C(2)	21(3)	28(3)	27(3)	0(2)	7(2)	9(2)
C(3)	24(3)	24(3)	25(3)	-5(2)	4(2)	0(2)
C(4)	24(3)	23(3)	20(3)	0(2)	9(2)	0(2)
C(5)	19(3)	29(3)	30(3)	-3(3)	4(2)	4(2)
C(6)	29(3)	29(3)	24(3)	-9(2)	3(2)	4(2)
C(7)	31(3)	15(3)	26(3)	6(2)	17(3)	3(2)
C(8)	27(3)	19(3)	24(3)	1(2)	14(2)	-4(2)
O(1S)	63(3)	64(3)	28(2)	5(2)	2(2)	0(3)
N(1S)	63(4)	47(3)	39(3)	8(3)	13(3)	8(3)
C(2S)	62(5)	45(4)	32(4)	-6(3)	7(3)	9(4)
C(3S)	103(7)	55(5)	69(5)	4(4)	31(5)	-3(5)
C(4S)	80(6)	92(6)	42(4)	22(4)	-2(4)	-10(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $C_{11}H_{13}NO_6Zn$.

	x	y	z	U(eq)
H(51)	5545(5)	4831(2)	6395(3)	43
H(52)	5456(5)	5068(2)	7205(3)	43
H(21)	-775(8)	2736(3)	2354(4)	30
H(31)	363(8)	1699(3)	1315(4)	30
H(53)	6038(8)	1950(3)	3175(4)	31
H(61)	4903(8)	3005(3)	4198(4)	33
H(2S1)	4432(11)	4053(4)	8655(5)	56
H(3S1)	6145(13)	3138(5)	11231(7)	111
H(3S2)	5282(13)	2779(5)	10040(7)	111
H(3S3)	4029(13)	3461(5)	10548(7)	111
H(3S4)	4159(13)	3114(5)	9981(7)	111
H(3S5)	5022(13)	3473(5)	11173(7)	111
H(3S6)	6275(13)	2791(5)	10665(7)	111
H(4S1)	8592(12)	3986(6)	11400(6)	110
H(4S2)	8159(12)	4892(6)	10834(6)	110
H(4S3)	9350(12)	4189(6)	10322(6)	110
H(4S4)	8809(12)	4725(6)	10304(6)	110
H(4S5)	9241(12)	3819(6)	10870(6)	110
H(4S6)	8051(12)	4522(6)	11382(6)	110