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Crystal structure of {*N*,*N*′-bis(4-fluoro-salicylaldehyde)-3,6-dioxa-1,8-diaminooctane-κ^4*O*,*N*,*N*′,*O*′}zinc(II), $C_{20}H_{20}F_2N_2O_4Zn$

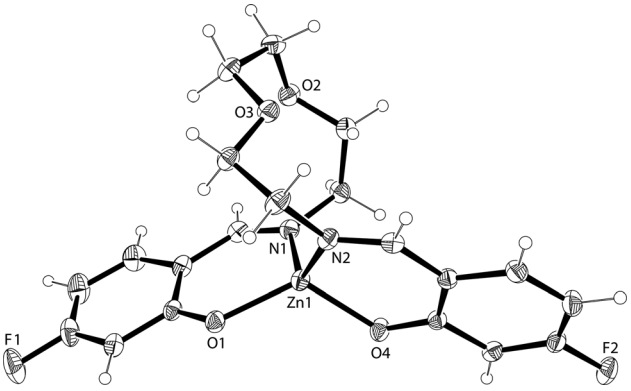

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.19 × 0.17 × 0.16 mm
Wavelength:	CuKα radiation (1.54178 Å)
μ:	2.20 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
θ_{max}, completeness:	72.0°, 98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11394, 3690, 0.036
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3571
$N(param)_{refined}$:	262
Programs:	Bruker [1], SHELX [2], Olex2 [3]

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Abstract

$C_{20}H_{20}F_2N_2O_4Zn$, triclinic, $P\bar{1}$ (no. 2), a = 8.4062(2) Å, b = 10.9987(3) Å, c = 11.8247(3) Å, α = 97.969(1)°, β = 103.217(1)°, γ = 110.601(1)°, V = 967.04(4) Å^3, Z = 2, $R_{gt}(F)$ = 0.0415, $wR_{ref}(F^2)$ = 0.1167, T = 173(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All reagents and chemicals were purchased from commercial sources and used without further purification. The title complex was prepared according to the literature reported earlier [4, 5]. A solution of zinc acetate dihydrate (219.51 mg, 1 mmol) in methanol (2 mL) was added to a stirring solution of the *N*,*N*′-bis(4-fluoro-salicylaldehyde)-3,6-dioxa-1,8- diaminooctane (392.40 mg, 1 mmol) in dichloromethane (2 mL). The colour of the mixture immediately turned yellow, and the stirring was continued at room temperature for 1 h. The product was filtered and the filtrate was allowed to stand at room temperature 12 days in a quiet environment. Several clear yellow block crystals were obtained.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

For many years, multidentate Schiff base metal complexes are a growing field of research because of their application in many fields [6–10 and cited references]. Multidentate Schiff base ligands contain many more N and O coordination sites, so they can form complexes with transition metals or lanthanide metals. Recently, we have also prepared the title complex, and we predict that this complex has excellent spectral properties similar to the literature known ones [11].

The title crystal structure is shown in the figure. Compared with reported structures, all bond lengths and bond angles are within the normal ranges [10]. The Zn1 ion is tetracoordinated in a N_2O_2 geometry by two amino

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6846 (3)	0.9298 (2)	0.2137 (2)	0.0285 (5)
C2	0.6696 (4)	1.0543 (3)	0.2338 (3)	0.0361 (6)
H2	0.633688	1.081529	0.300164	0.043*
C3	0.7071 (5)	1.1359 (3)	0.1571 (3)	0.0463 (7)
C4	0.7596 (5)	1.1049 (3)	0.0592 (3)	0.0537 (9)
H4	0.789773	1.166054	0.010463	0.064*
C5	0.7668 (5)	0.9812 (3)	0.0348 (3)	0.0455 (7)
H5	0.797335	0.955332	−0.034523	0.055*
C6	0.7301 (4)	0.8912 (3)	0.1095 (2)	0.0322 (6)
C7	0.7394 (4)	0.7644 (3)	0.0703 (2)	0.0329 (6)
H7	0.765469	0.750482	−0.003329	0.040*
C8	0.7295 (4)	0.5462 (3)	0.0652 (3)	0.0357 (6)
H8A	0.715191	0.543423	−0.020740	0.043*
H8B	0.632556	0.466397	0.071194	0.043*
C9	0.9071 (4)	0.5431 (3)	0.1233 (3)	0.0354 (6)
H9A	0.926699	0.552413	0.210417	0.042*
H9B	0.910776	0.457198	0.088663	0.042*
C10	1.2121 (4)	0.6993 (3)	0.1881 (3)	0.0368 (6)
H10A	1.306114	0.733535	0.149338	0.044*
H10B	1.226477	0.623915	0.219973	0.044*
C11	1.2336 (4)	0.8084 (3)	0.2892 (3)	0.0383 (6)
H11A	1.360062	0.853514	0.338312	0.046*
H11B	1.196177	0.875841	0.257203	0.046*
C12	1.0855 (4)	0.8434 (3)	0.4315 (2)	0.0332 (6)
H12A	1.017571	0.882886	0.379466	0.040*
H12B	1.196564	0.916517	0.485049	0.040*
C13	0.9758 (4)	0.7698 (3)	0.5043 (2)	0.0370 (6)
H13A	1.045644	0.731557	0.556297	0.044*
H13B	0.949102	0.833732	0.556500	0.044*
C14	0.7560 (3)	0.5511 (3)	0.4602 (2)	0.0291 (5)
H14	0.834502	0.545130	0.529028	0.035*
C15	0.5918 (3)	0.4345 (2)	0.4039 (2)	0.0274 (5)
C16	0.4495 (3)	0.4272 (2)	0.3074 (2)	0.0267 (5)
C17	0.2940 (3)	0.3073 (3)	0.2666 (2)	0.0303 (5)
H17	0.194219	0.300117	0.204673	0.036*
C18	0.2885 (4)	0.2017 (3)	0.3170 (3)	0.0338 (6)
C19	0.4230 (4)	0.2052 (3)	0.4112 (3)	0.0383 (6)
H19	0.412742	0.130188	0.444844	0.046*
C20	0.5728 (4)	0.3225 (3)	0.4538 (3)	0.0339 (6)
H20	0.667141	0.328573	0.519427	0.041*
F1	0.6934 (4)	1.2556 (2)	0.1812 (2)	0.0699 (7)
F2	0.1385 (2)	0.08663 (16)	0.27148 (17)	0.0455 (4)
N1	0.7165 (3)	0.6681 (2)	0.12347 (19)	0.0299 (5)
N2	0.8083 (3)	0.6620 (2)	0.42807 (19)	0.0291 (5)
O1	0.6553 (2)	0.85776 (18)	0.29196 (16)	0.0318 (4)
O2	1.0417 (3)	0.6525 (2)	0.10150 (18)	0.0368 (4)
O3	1.1259 (2)	0.75036 (19)	0.36098 (17)	0.0331 (4)
O4	0.4515 (2)	0.52519 (18)	0.25539 (17)	0.0339 (4)
Zn1	0.66208 (4)	0.68391 (3)	0.27930 (3)	0.02869 (14)

nitrogen (N1 and N2) atoms and two phenoxo oxygen (O1 and O4) atoms from the deprotonated L^{2-} unit. The Zn1—O1 bond length is 1.9191(19) Å and the Zn1—O4 is 1.9289(18) Å. The Zn1—N1 bond length is 1.997(2) Å and the Zn1—N2 is 2.000(2) Å. The angle of O1—Zn1—N1 is 97.39(8)°, O4—Zn1—N1 is 104.77(9)°, O1—Zn1—N2 is 114.31(8)° and O1—Zn1—O4 is 121.89(8)°, respectively.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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