Supplementary Material

Crystal Structure, Topological and Hirshfeld Surface Analysis of a Zn(II) Zwitterionic Schiff base Complex Exhibiting Non-linear Optical (NLO) Properties Using Z-Scan Technique

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Single crystal X-ray studies

Good quality single crystal of complex **1** were selected and mounted on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 100(2) K during data collection using Mo Kα radiation at λ = 0.71073 Å. Crystal structure was determined by using Olex-2 [1], the structure was solved with the olex-2.solve [2] structure solution program using Charge Flipping and refined with the olex-2.refine refinement package [2] using Gauss-Newton minimisation. All non-hydrogen atoms were refined with anisotropic displacement parameter.

Topological analysis

The analysis was performed with the topcryst.com [3]. The RCSR three-letter codes [4] were used to designate the network topologies. Those nets, that are absent in the RCSR, are designated with the TOPOS NDn nomenclature [5], where N is a sequence of coordination numbers of all non-equivalent nodes of the net, D is periodicity of the net (D=M, C, L, T for 0-,1-,2-,3-periodic nets), and n is the ordinal number of the net in the set of all non-isomorphic nets with the given ND sequence. To calculate the underlying nets, we used algorithms, the application of which for specific structures of complex **1** [6]. The TTD collection [7] was used to determine the topological type of the crystal structure.

Hirshfeld surface analysis

Hirshfeld surface associated with 2D finger plot were generated using Crystal information file (CIF), imported in the Crystal Explorer version 3.1 [8]. Hirshfeld surface analysis is a unique tool for the quantitative information of intermolecular interaction within crystal structure packing. Hirshfeld surface represented by the 2D finger plot relative to their particular contribution of different intermolecular interaction present in the crystal structure. Structural Surface are mapped over the d_{norm}, shape index and curvedness, a view of red color scale shows (shorter distance than van der Waals radii from nucleus), white (equal to van der Waals separation radii) and blue color represent a longer distance than van der Waals radii from nuclei) [9–11]. The decomposed finger plot has been shown in term of d_e is the external distance to the nearest nucleus to the surface and d_i is the internal distance to the nearest nucleus to the surface ($d_e > d_i$, upper case spike shows donor system, $d_e < d_i$ lower case spike represent acceptor system) [10].
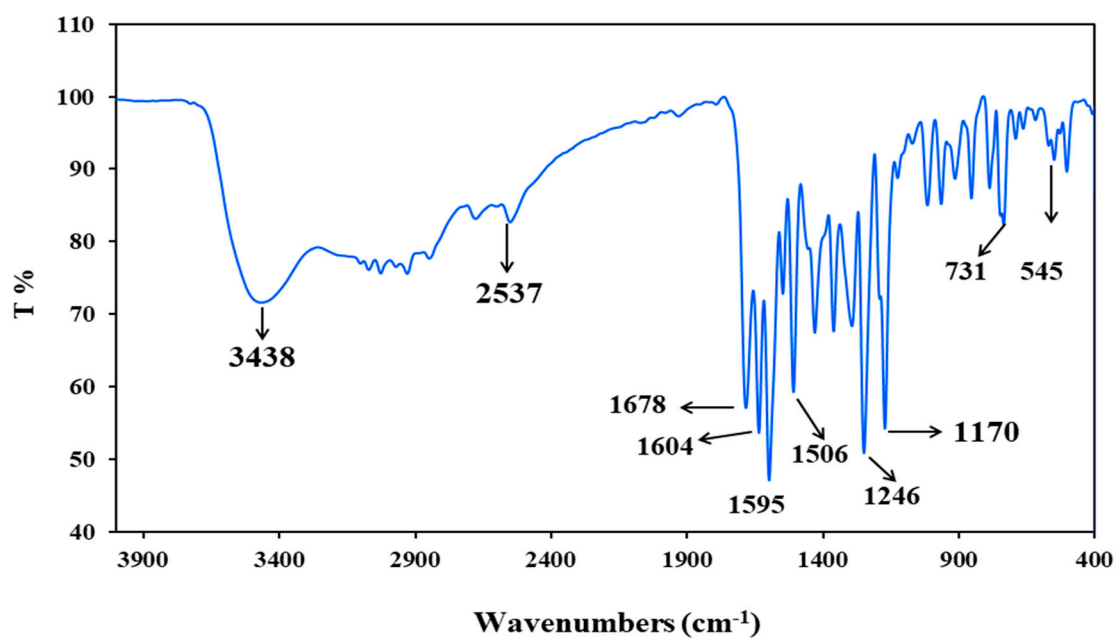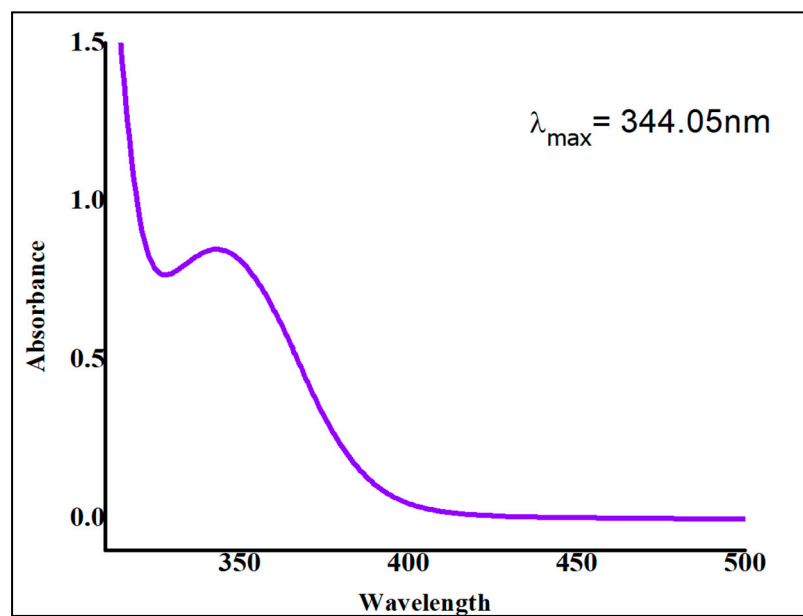
Figure 1. FTIR spectrum of complex **1**.

Figure 2. UV-visible spectrum of complex **1.**

Table 1. Selected Bond Lengths (Å) and Angles (deg) for complex **1**.

Bond Lengths (Å)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	Cl1	2.258(4)	C2	C7	1.425(17)
Zn1	Cl2	2.210(4)	C3	C4	1.399(18)
Zn1	O1	1.990(8)	C4	C5	1.377(17)
Zn1	O5	2.120(10)	C5	C6	1.403(17)
Zn1	O2	2.407(8)	C6	C7	1.422(17)
O1	C7	1.312(13)	C6	C8	1.417(17)
O2	C1	1.401(16)	C9	C10	1.396(16)
O2	C2	1.349(15)	C9	C14	1.387(16)
O3	C15	1.242(15)	O4	C15	1.274(15)
O5	C16	1.52(2)	C11	C12	1.387(17)
N1	C8	1.325(15)	C10	C11	1.377(17)
C12	C13	1.395(17)	N1	C9	1.428(14)
C12	C15	1.490(16)	C2	C3	1.368(17)
C13	C14	1.369(17)			

Bond Angle (degree).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	Zn1	Cl1	116.88(14)	C8	C6	C7	120.8(11)
O1	Zn1	Cl1	123.0(3)	C2	C7	O1	120.7(10)
O1	Zn1	Cl2	118.5(3)	C6	C7	O1	121.5(10)
O5	Zn1	Cl1	96.1(3)	C6	C7	C2	117.8(10)
O5	Zn1	Cl2	98.7(3)	C6	C8	N1	122.0(11)
O5	Zn1	O1	88.0(4)	C10	C9	N1	115.3(10)
C7	O1	Zn1	122.7(7)	C14	C9	N1	123.6(10)
C2	O2	C1	119.8(10)	C14	C9	C10	121.0(11)
C16	O5	Zn1	127.4(9)	C11	C10	C9	119.7(11)
C9	N1	C8	127.7(10)	C12	C11	C10	119.7(11)
C3	C2	O2	126.8(11)	C13	C12	C11	119.9(10)
C7	C2	O2	113.1(10)	C15	C12	C11	120.3(11)
C7	C2	C3	120.1(11)	C15	C12	C13	119.9(11)
C4	C3	C2	121.4(11)	C14	C13	C12	121.0(11)
C5	C4	C3	120.4(11)	C13	C14	C9	118.8(11)
C6	C5	C4	119.4(12)	O4	C15	O3	123.9(11)
C7	C6	C5	121.0(11)	C12	C15	O3	119.6(11)
C8	C6	C5	118.3(11)	C12	C15	O4	116.6(11)

Table S2. Hydrogen Atom Coordinates ($Å×10^4$) and Isotropic Displacement Parameters ($Å^2×10^3$) for complex **1.**

Atom	x	y	z	U(eq)
H5	4580(160)	3870(50)	3600(300)	40.1(11)
H1	8305(11)	3756(3)	5059(15)	19(3)
H1a	6220(90)	2590(5)	11650(90)	41(5)
H1b	6610(70)	3000(20)	13200(20)	41(5)
H1c	4990(30)	2960(20)	11610(90)	41(5)
H3	8856(14)	2700(4)	12588(18)	20(3)
H4a	11298(14)	2701(4)	12180(20)	24(3)
H5a	11892(14)	3060(4)	9286(18)	20(3)
H8	11188(13)	3500(4)	6144(18)	19(3)
H10	7272(13)	4156(4)	2125(19)	22(3)
H11	7487(13)	4552(4)	−900(19)	22(3)
H13	11866(14)	4246(4)	340(20)	23(3)
H14	11671(13)	3858(4)	3371(19)	21(3)
H16a	3930(90)	4592(6)	3560(120)	77(7)
H16b	4530(140)	4562(6)	6140(90)	77(7)
H16c	5680(50)	4587(6)	4600(200)	77(7)
H4	11180(150)	4850(50)	−4200(200)	20(40)

Table S3. Fractional Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for sk1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Zn1	5165.1(16)	3542.9(5)	7196(2)	21.1(4)
Cl1	4422(4)	3973.4(12)	9598(6)	32.1(9)
Cl2	3619(4)	3026.3(11)	5697(5)	26.8(8)
O1	7257(9)	3519(3)	6905(13)	17.6(18)
O2	6556(9)	3119(3)	10160(14)	24(2)
O3	8724(10)	4847(3)	−3716(13)	21(2)
O4	11124(10)	4678(3)	−2945(15)	22(2)
O5	4718(11)	3988(3)	4599(14)	31(2)
N1	9214(11)	3747(3)	4863(15)	15(2)
C1	6057(15)	2900(5)	11780(20)	27(3)
C2	7985(14)	3079(4)	10037(19)	18(3)
C3	9087(14)	2856(4)	11426(18)	16(3)
C4	10547(14)	2852(4)	11170(20)	20(3)
C5	10903(14)	3067(4)	9469(18)	17(3)
C6	9791(14)	3294(4)	8010(20)	17(3)
C7	8306(12)	3307(4)	8262(17)	12(2)
C8	10190(13)	3517(4)	6284(18)	16(2)
C9	9462(13)	3981(4)	3050(18)	14(2)
C10	8207(13)	4179(4)	1762(19)	18(3)
C11	8331(13)	4409(4)	−38(19)	19(3)
C12	9692(14)	4431(4)	−588(18)	15(3)
C13	10933(14)	4227(4)	710(20)	19(3)
C14	10826(13)	4000(4)	2509(19)	18(3)
C15	9833(14)	4668(4)	−2560(20)	19(3)
C16	4720(20)	4475(6)	4740(30)	51(5)

Table S4. Anisotropic Displacement Parameters (Å²×10³) for sk1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn1	17.9(8)	28.9(9)	16.8(7)	2.5(6)	4.6(6)	2.3(7)
Cl1	30.7(19)	44(2)	24.7(17)	11.4(16)	12.8(14)	−2.8(16)
Cl2	20.5(16)	32.2(18)	25.5(17)	−0.6(14)	1.4(13)	−0.3(14)
O1	15(4)	24(5)	14(4)	−1(4)	5(3)	6(4)
O2	13(4)	37(6)	23(5)	−5(4)	8(4)	−1(4)
O3	23(5)	27(5)	10(4)	−2(4)	1(4)	5(4)
O4	21(5)	27(5)	19(5)	0(4)	10(4)	6(4)
O5	39(6)	39(6)	12(5)	5(5)	1(4)	1(4)
N1	13(5)	19(5)	14(5)	−2(4)	2(4)	4(4)
C1	21(7)	33(8)	30(8)	4(6)	13(6)	0(6)
C2	23(7)	16(6)	14(6)	−3(5)	3(5)	−3(5)
C3	30(7)	15(6)	5(5)	0(5)	5(5)	0(5)
C4	27(7)	17(6)	12(6)	−1(5)	0(5)	1(5)
C5	20(6)	18(6)	11(6)	3(5)	1(5)	4(5)
C6	22(6)	17(6)	13(6)	1(5)	6(5)	−3(5)
C7	13(6)	18(6)	4(5)	6(5)	−2(4)	2(5)
C8	19(6)	17(6)	10(6)	2(5)	0(5)	−1(5)
C9	20(6)	19(6)	4(5)	4(5)	6(5)	4(5)
C10	11(6)	29(7)	14(6)	0(5)	−1(5)	4(5)
C11	14(6)	26(7)	11(6)	4(5)	−5(5)	10(5)
C12	29(7)	12(6)	4(5)	2(5)	5(5)	4(5)
C13	24(7)	19(7)	18(6)	6(5)	10(5)	1(5)
C14	12(6)	25(7)	15(6)	3(5)	2(5)	13(5)
C15	24(7)	16(6)	17(7)	0(5)	6(6)	−1(5)
C16	52(11)	47(11)	56(11)	2(9)	16(9)	−6(9)

Table S5. Multilevel analysis of molecular complex packing as monomer.

№	Node degrees	Ωi, %	Dimensionality of net	Topological type
1	2-c	18.92	1D [001]	2C1
2	4-c	8.48	1D [001]	(3,6)(1,2)
3	6-c	8.47	2D (010)	(4,4)IIa
4	7-c	6.51	3D	**svk**
5	8-c	4.80	3D	**hex**
6	9-c	4.21	3D	9T269
7	10-c	3.13	3D	bcu-x/ 14-conn;I m -3 m->P 21/c (1/2a+1/2b+1/2c,2a-2b,-c; 1/2,0,1/2);Bond sets: 2,4,5,7,8,9:bcu-x
8	12-c	2.51	3D	bcu-x/ 14-conn;I m -3 m->P 21/c (1/2a+1/2b+1/2c,2a-2b,-c; 1/2,0,1/2);Bond sets: 1,2,4,5,7,8,9:bcu-x
9	14-c	1.44	3D	14T161
10	16-c	0.86	3D	New topology

Table S6. Multilevel analysis of molecular complex packing as dimer.

№	Node degrees	Ωi, %	Dimensionality of net	Topological type
1	2-c	22.80	1D [001]	2C1
2	4-c	9.06	2D(010)	**sql**
3	8-c	4.54	3D	**hex**
4	10-c	4.36	3D	**bct**
5	12-c	2.25	3D	*gsp*1
6	14-c	1.54	3D	14T92
7	18-c	0.46	3D	New topology

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