Pentacoordinate ternary Zn(II) complexes with flufenamato and niflumato ligands: Crystal structure, spectral characterization and biological properties

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Table S1. Selected bond lengths and angles (A, °) for prepared similar complexes containing carboxylate ligand, N,N'-donor ligand and chloride ligand - [ZnCl(L_1)(L_2)].

CSD refcode	Zn-O_1	Zn-O_2	Zn-N_1	Zn-N_2	Zn-Cl	O_1-Zn-O_2	N_1-Zn-N_2
1A	1.987(2)	2.510(2)	2.081(2)	2.095(2)	2.229(1)	56.95	80.18
1B	2.133(1)	2.179(1)	2.092(1)	2.098(1)	2.221(1)	60.81	80.52
2	2.156(1)	2.158(1)	2.098(1)	2.102(1)	2.219(1)	61.02	79.02
DAMJOS	2.016(2)	2.425(2)	2.052(2)	2.059(2)	2.251(1)	58.01	81.31
DUCRID	1.940(3)	2.970(0)	2.077(5)	2.101(3)	2.219(2)	47.99	89.06
GEQVII	1.976(3)	2.647(3)	2.149(3)	2.153(3)	2.231(1)	54.51	85.75
KEHTOI	2.003(2)	2.343(2)	2.056(2)	2.095(2)	2.229(1)	59.65	80.74
	2.095(2)	2.183(2)	2.082(2)	2.084(3)	2.240(1)	61.28	80.15
KUSDOS	1.960(2)	2.764(0)	2.029(2)	2.060(2)	2.222(1)	52.38	83.01
MEJSEC	2.081(2)	2.204(2)	2.074(2)	2.089(2)	2.218(1)	61.25	78.59
POCXOW	2.027(3)	2.319(3)	2.056(3)	2.078(2)	2.228(1)	60.02	79.75
TARWUF	2.099(1)	2.221(2)	2.056(2)	2.094(2)	2.225(1)	60.7	79.14
YEGDIA	1.988(3)	2.559(3)	2.096(4)	2.112(3)	2.238(1)	56.35	80.02

N_1 represents the nitrogen atom of N,N'-donor ligand closer to central atom, while N_2 is farther. O_1 represents the oxygen atom of carboxylate ligand closer to central atom, while O_2 is farther. Data acquired from CSD database (November 2022) [17].

DAMJOS: L_1 = acetato; L_2 = N-(1,3-dimethyltetrahydropyrimidin-2(1H)-ylidene)quinolin-8-amine; DUCRID: L_1 = benzoate; L_2 = sparteine; GEQVII: L_1 = bis(2,6-dimesitylbenzoato); L_2 = 1,2-bis(t-butyl(methyl)amino)ethane; KEHTOI: L_1 = tolfenamato; L_2 = 1,10-phenanthroline (two crystallographically independent units); KUSDOS: L_1 = but-2-enoato; L_2 = 2,2'-diamino-4,4'-bi-1,3-thiazole; MEJSEC: L_1 = niflumato; L_2 = 2,2'-bipyridine; POCXOW: L_1 = 3-(4-hydroxyphenyl)acrylato; L_2 = 2,2'-bipyridine; TARWUF = L_1 = 4-aminobenzoato; L_2 = 2,2'-bipyridyl; YEGDIA: L_1 = niflumato; L_2 = neocuproine.

Reference:

17. Groom, C. R.; Bruno, I. J.; Lightfoot, M. P.; Ward, S. C. The Cambridge Structural Database. *Acta Crystallog. B: Struct Sci Cryst Eng Mater* **2016**, 72, 171–179. https://doi.org/10.1107/s2052520616003954.

Table S2. Possible intermolecular hydrogen bonding interactions (A, °) for the prepared complexes.

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
1A				
C16-H1c16···F1^{i}	0.96	2.48	3.331(3)	148
C19-H1c19···O2^{ii}	0.96	2.57	3.337(3)	137
1B				
C22-H1c22···Cl1^{iii}	0.96	2.69	3.604(2)	160
C17-H1c17···F3^{iv}	0.96	2.51	3.169(2)	126
2				
C4-H1c4···N2^{v}	0.96	2.60	3.492(2)	155

Symmetry codes: (i) -1+x, y, z; (ii) -2+x, 1+y, z; (iii) x, 1+y, z; (iv) -1+x, y, 1+z; (v) -x, 2-y, 2-z.

Table S3. Selected intermolecular π···π interactions (A, °) for the prepared complexes.

Cg(I)···Cg(J)	d(Cg···Cg)	α	β	γ
1A				
Cg1···Cg2^{i}	3.514(1)	1.78(9)	18.1	16.6
Cg1···Cg3^{ii}	3.652(1)	1.83(10)	17.3	17.9
1B				
Cg1···Cg1^{i}	3.695(1)	0.49(8)	19.4	19.5
Cg1···Cg2^{ii}	3.589(1)	0.02(8)	18.3	18.3
Cg3···Cg3^{i}	3.693(1)	0.03(8)	19.3	19.3
2				
Cg1···Cg2^{i}	3.606(1)	2.57(6)	19.1	18.8
Cg2···Cg2^{ii}	3.734(1)	0.00(6)	20.5	20.5

1A: Cg1 (N2-C25-C24-C23-C22-C21), Cg2 (C8-C9-C10-C11-C12-C13), Cg3 (C18-C19-C20-C21-C25-C26), Symmetry codes: (i) -x, 1-y, -z; (ii) 1+x, y, z.
1B: Cg1 (N3-C15-C16-C17-C18-C26), Cg2 (N2-C25-C24-C23-C22-C21), Cg3 (C18-C19-C20-C21-C25-C26), Symmetry codes: (i) 1-x, 1-y, 1-z; (ii) -x, 1-y, 1-z.
2: Cg1 (N3-C14-C19-C20-C21-C22), Cg2 (N4-C23-C24-C25-C26-C31),
Symmetry codes: (i) 1-x, 1-y, 1-z; (ii) -x, 1-y, 1-z.

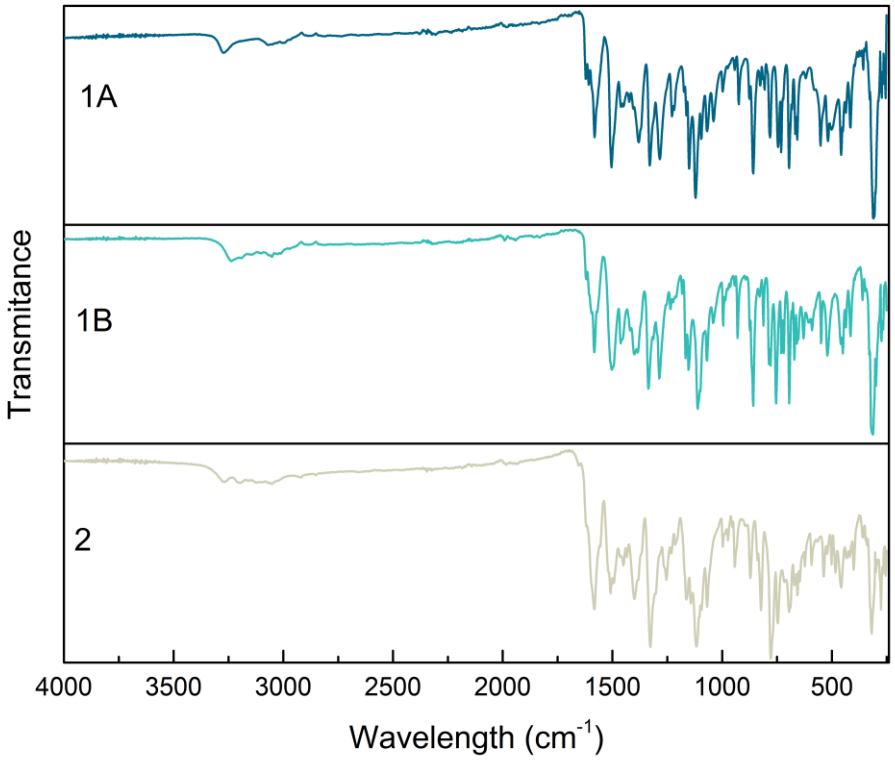

Figure S1. Solid-state FTIR spectra of the prepared complexes.

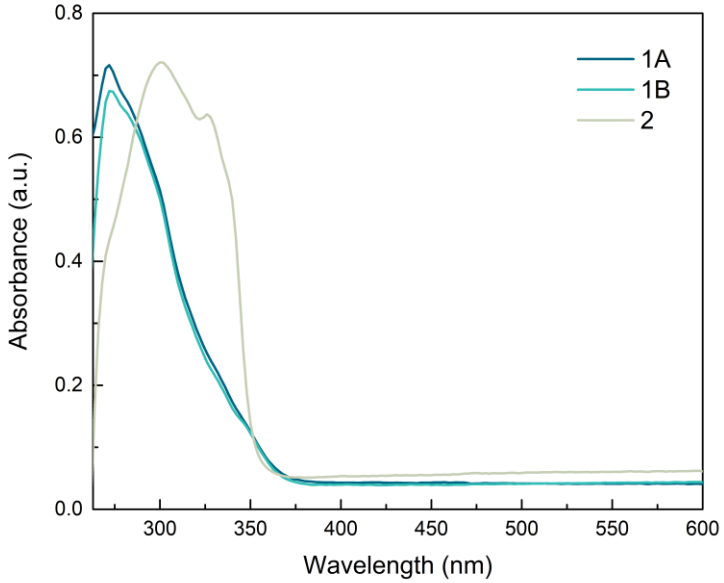

Figure S2. UV-Vis spectra of 10 μM dmso solutions of the prepared complexes.