Synthesis, X-ray Structure of Two Hexa-Coordinated Ni(II) Complexes with *s*-Triazine Hydrazine Schiff Base Ligand

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X-Ray structure determinations

The crystals of **1** and **2** were immersed in cryo-oil, mounted in a loop, and measured at a temperature of 170 K. The X-ray diffraction data were collected on a Bruker Kappa Apex II (**1**) or Rigaku Oxford Diffraction Supernova (**2**) diffractometer using Mo Kα radiation. The *Denzo-Scalepack* [49] or *CrysAlisPro* [50] software packages were used for cell refinements and data reductions. The structures were solved by the intrinsic phasing method using the *SHELXT* [51] software. A semi-empirical absorption correction based on equivalent reflections (*SADABS* [52]) was applied to the intensities before the structure solution. Structural refinements were carried out using *SHELXL* [53] software with *SHELXLE* [54] graphical user interface. The NH and H_2O hydrogen atoms were located from the difference Fourier map and refined isotropically. All other hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C-H = 0.95 -0.99 Å and Uiso = 1.2-1.5·Ueq (parent atom). The crystallographic details are summarized in Table S**1**.

Table S1. Crystal Data.

	1	**2**
CCDC no.	2261660	2261659
empirical formula	$C_{18}H_{36}N_{10}NiO_{14}$	$C_{18}H_{32}N_{10}NiO_{12}$
fw	675.28	639.24
temp (K)	170(2)	170(2)
λ(Å)	0.71073	0.71073
cryst syst	Monoclinic	Triclinic
space group	$P2_1/n$	$P\bar{1}$
a (Å)	11.4900(2)	8.3135(2)
b (Å)	17.6794(3)	10.9175(2)
c (Å)	14.1294(2)	15.7611(4)
α (deg)	90	71.119(1)
β (deg)	90.110(1)	80.188(1)
γ(deg)	90	84.258(1)
V (Å^3)	2870.19(8)	1332.20(5)
Z	4	2
ρ_{calc} (Mg/m^3)	1.563	1.594
μ(Mo Kα) (mm^{-1})	0.760	0.808
No. reflns.	78229	23437
Completeness to theta = 25.242°	98.3 %	99.7 %

Unique reflns.	7931	7434
GOOF (F^2)	1.091	1.088
R_{int}	0.0398	0.0343
R_1[a] ($I \geq 2\sigma$)	0.0342	0.0469
wR_2[b] ($I \geq 2\sigma$)	0.0732	0.0886

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]]^{1/2}$.

Evaluation of antimicrobial activity [56]

a) Tested pathogenic microbes

The antimicrobial activity of the ligand (**DMPT**) and complexes **1-2** was evaluated against two Gram positive bacteria ((S. aureus (ATCC 25923) and B. subtilis (RCMB015(1)NRR LB-543)), two Gram negative bacteria ((E. coli (ATCC 25922) and P. vulgaris (RCMB 004(1)ATCC 13315)) and two fungi ((A. fumigatus (RCMB 002008) and C. albicans (RCMB 005003(1) ATCC 10231)). Gentamycin was used as standard antibacterial agent. The samples maintained in Brain heart infusion (BHI) at 20ºC; 300 mL of each stock–culture was added to 3 mL of BHI broth. Overnight cultures were kept for 24 h at 37 ºC ± 1ºC and the purity of cultures was checked after 24 h of incubation. After 24 h of incubation, bacterial suspension was diluted with sterile physiological solution, for the diffusion and indirect bioautographic tests, to 108 CFU/mL (turbidity = McFarland barium sulfate standard 0.5). In case of fungi *A. fumigatus* (RCMB 002008) and *C. albicans* (RCMB 005003(1) ATCC 10231), the used medium in antagonistic activity against tested fungi is Potato Dextrose Agar, where Ketoconazole was used standard antifungal agent.

b) Agar well diffusion method

Synthetic compound was prepared at concentration 10 mg/mL dissolved in DMSO as stock solutions. Preparation of sterilized Mueller Hinton agar plates seeded with tested pathogenic bacteria occurred. The wells are done by sterilized cork borer in size 6 mm and hence 100 µL of the synthetic compound was poured in each well comparably with DMSO as control. The plates were incubated at 37 °C for 24-48 h (for bacteria) and at 28 °C for 48 h (for fungi). After incubation period; antimicrobial activity was determined
by inhibition zones.

C) Minimum Inhibitory Concentration (MIC)

Different dilutions of the compound are inoculated with tested pathogenic microbes. After incubation period of 96 well microplate, the results are measured using microplate reader. To determine at what level the MIC endpoint is established; subculture of test samples at different concentrations occurred in nutrient agar plates.

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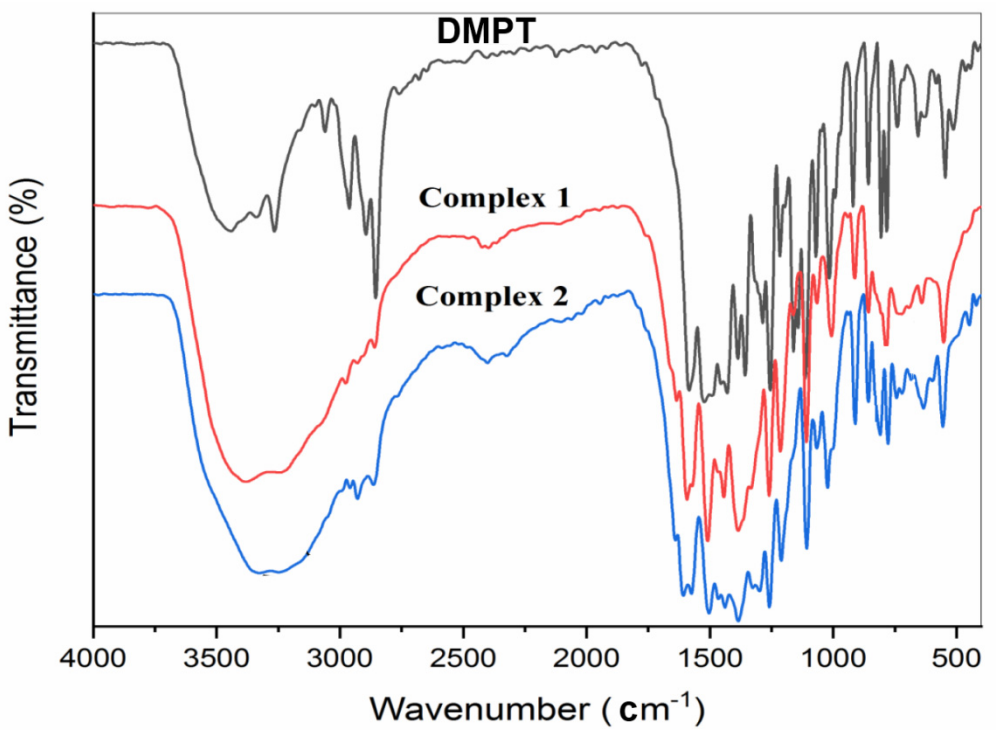

Figure. S1. FTIR spectra of complexes **1** and **2** compared to the free ligand **DMPT**.

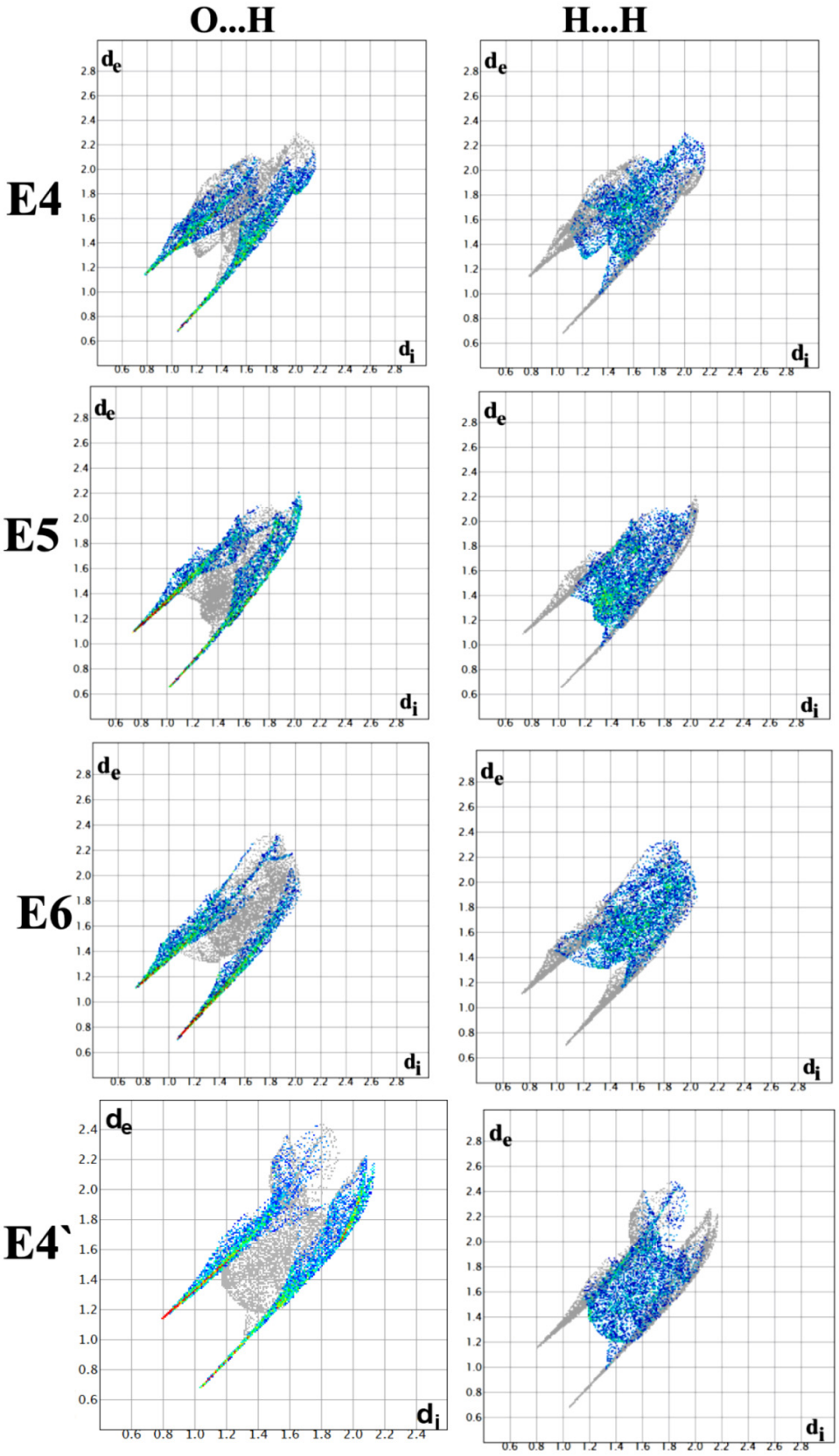

Figure. S2. The 2D fingerprint plots of the major contacts around the water moieties (E4, E5, E6 in complex **1** and E4` in complex **2**).