Supramolecular Structure and Antimicrobial Activity of Ni(II) Complexes with s-Triazine/Hydrazine Type Ligand

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Physical measurements

All the chemicals were bought from Sigma-Aldrich and used without additional purifications. CHN analyses were carried out using a PerkinElmer 2400 Elemental Analyzer. The amount of Ni was determined with the aid of a Shimadzu atomic absorption spectrophotometer (AA-7000 series, Shimadzu, Ltd., Japan). FTIR spectra was recorded at the Central Lab, Faculty of Science, Alexandria University using a Bruker Tensor 37 FT-IR spectrophotometer (Bruker company, Germany) in KBr pellets at 4000-400 cm^{-1}. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of the ligand **DPPT** were performed in deuterated chloroform ($CDCl_3$) as shown in Figures S1 and S2 (Supplementary data).

Crystal structure determination

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 diffractometer using Mo Kα radiation. The *Denzo-Scalepack* [39] software package was used for cell refinements and data reductions. The structures were solved by the intrinsic phasing method using the *SHELXT* software [40]. A multi-scan absorption correction based on equivalent reflections (*SADABS* [41]) was applied to the intensities before the structure solution. Structural refinements were carried out using *SHELXL* [42] software with *SHELXLE* [43] graphical user interface. In **2**, the NO_3^- -anion was disordered over two sites with occupancy ratio of 0.75/0.25. Therefore, the N-O distances in the two disordered nitrate moieties were restraint to be similar. Furthermore, the water of crystallization was partially lost and the water molecule was refined with the occupancy factor of 0.75. All heavy atoms in the nitrate anions and in the water molecule were restrained so that their U_{ij} components approximate to isotropic behavior. The NH hydrogen in **1** was located from the difference Fourier map and refined isotropically. The H_2O hydrogens were also located from the difference Fourier map but the positions were optimized to avoid close H-H contacts and the atoms were constrained to ride on their parent oxygen with U_{iso} = 1.5 U_{eq}(parent oxygen). In **2** both the NH and OH 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).

Method S1. Evaluation of antimicrobial activity [45]

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 negatvie 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 20^{o}C; 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.

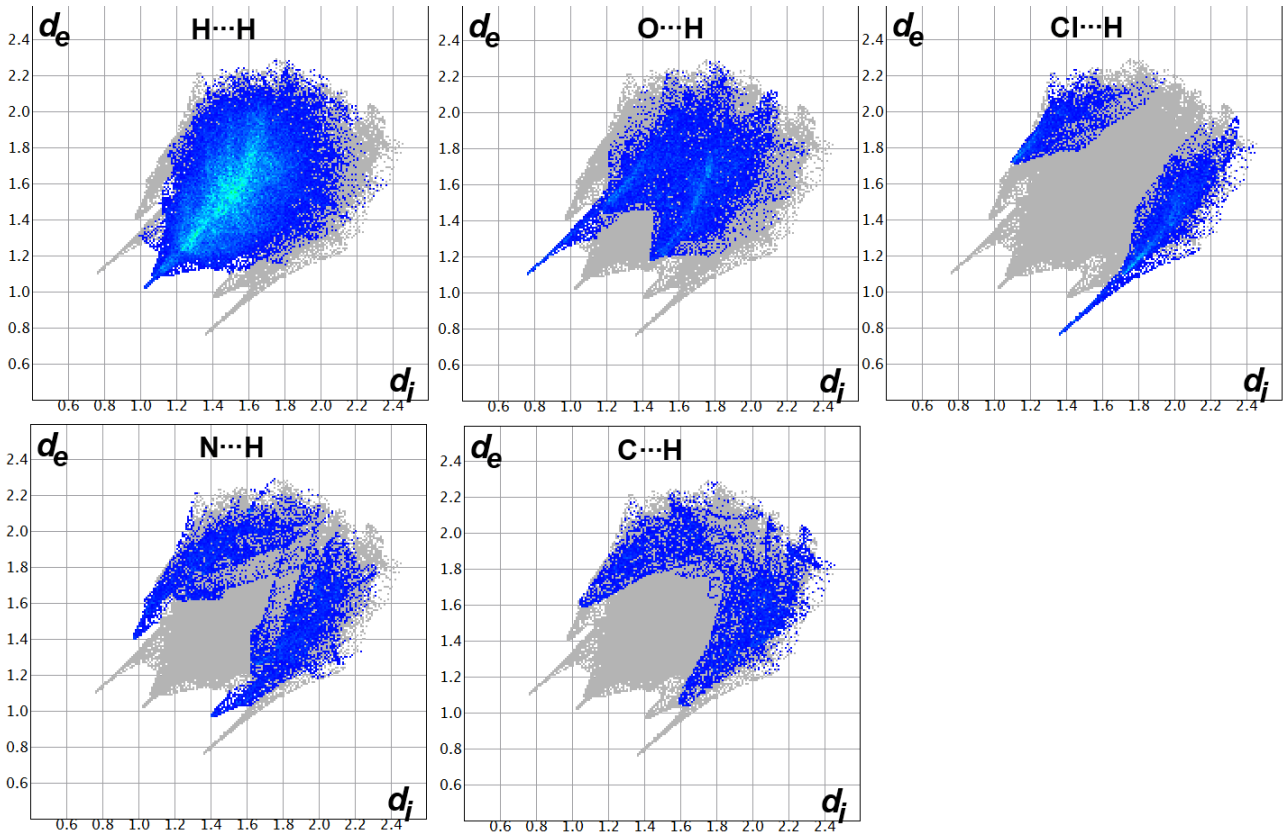

Figure S1. Fingerprint plots for the important interactions in **2**.

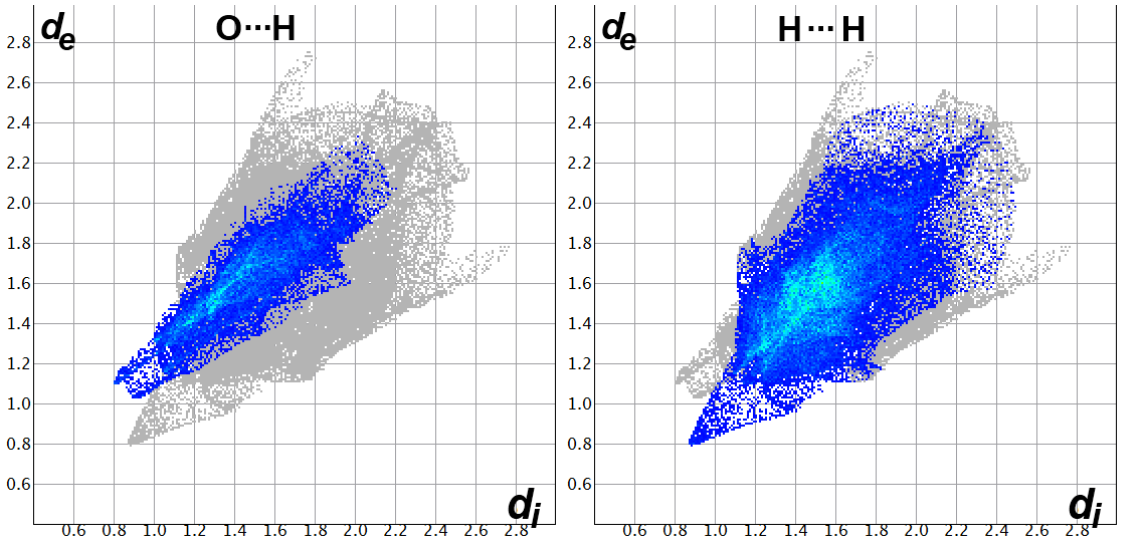

Figure S2. Fingerprint plots for the important interactions in **1**.

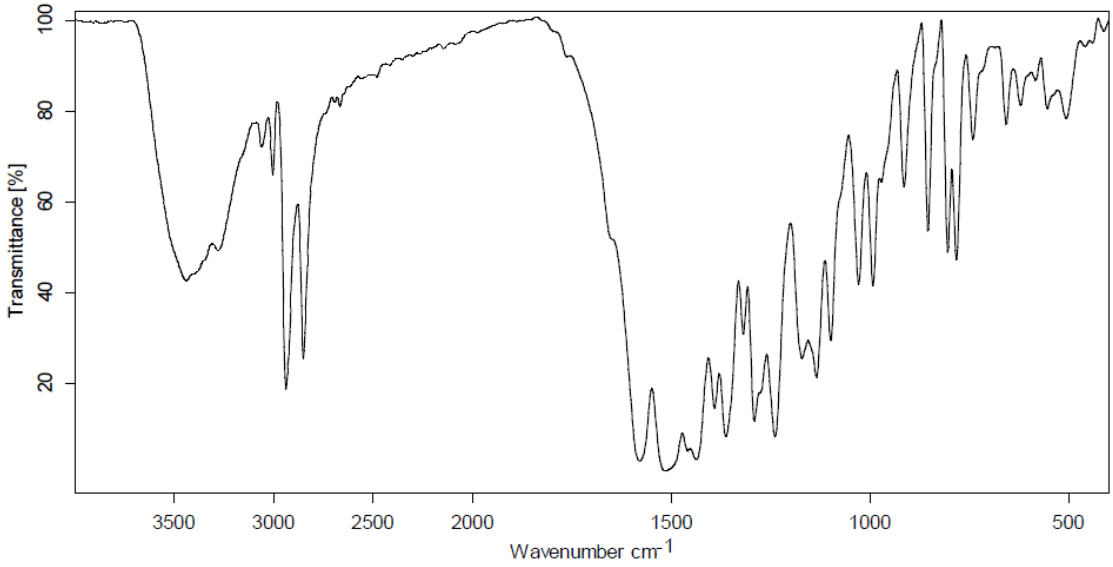

Figure S3. FTIR spectra of **DPPT.**

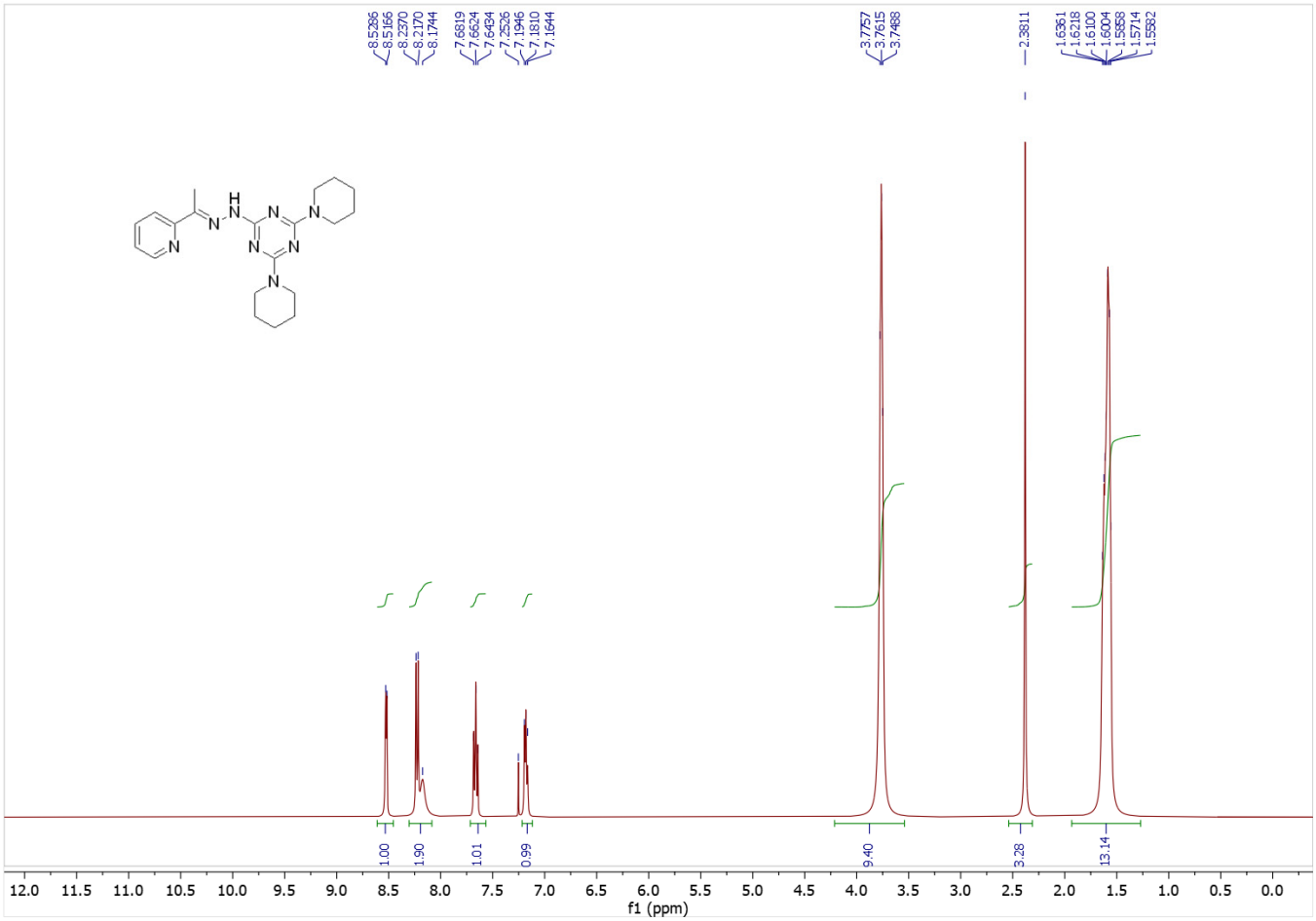

Figure S4. ^{1}H NMR spectra of **DPPT.**

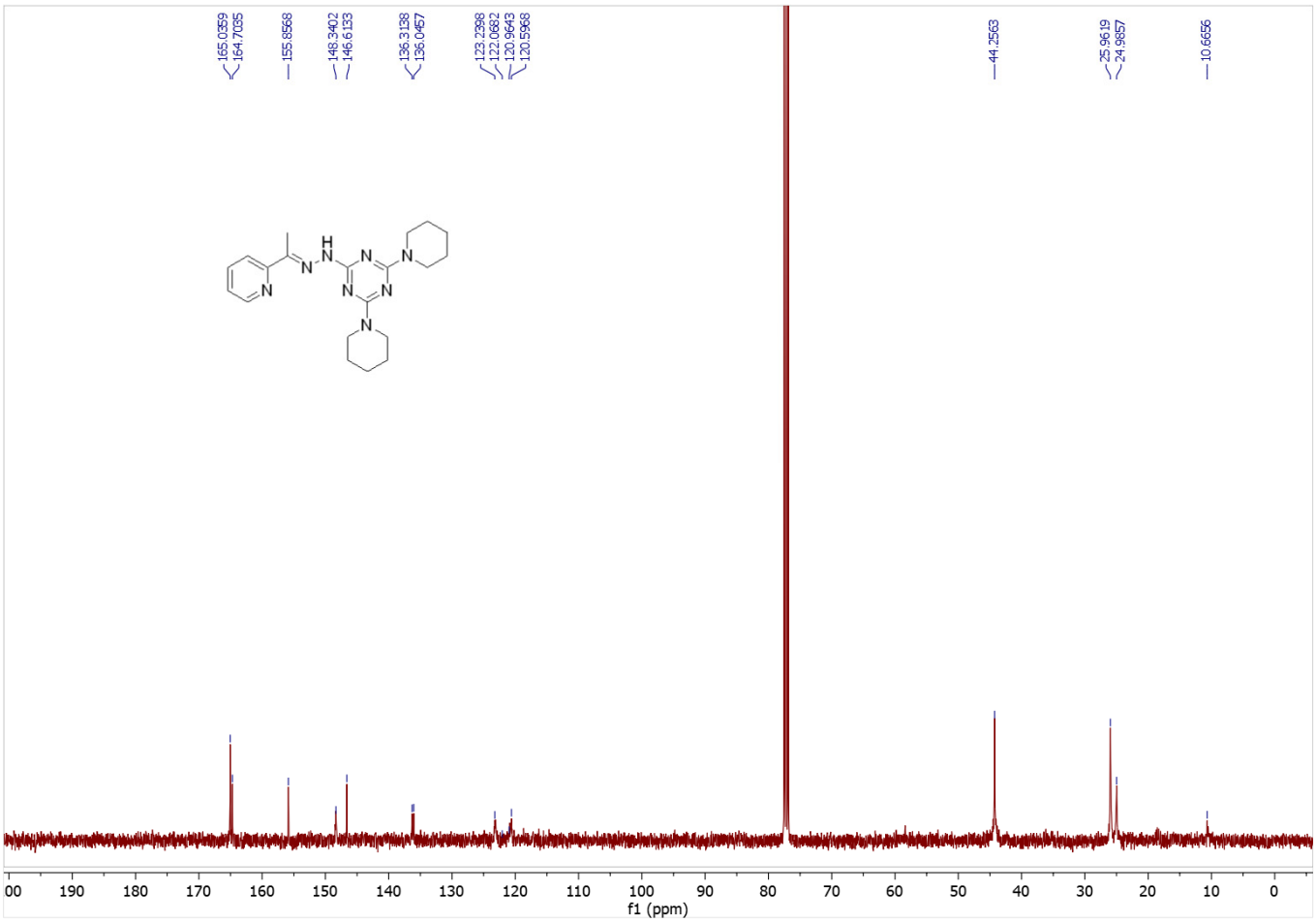

Figure S5. ^{13}C NMR spectra of **DPPT.**