

**UNIVERSITI TEKNOLOGI MARA**

**SYNTHESIS, CHARACTERIZATION  
AND ANTIBACTERIAL SCREENING  
OF NEW BENZOYLTHIOUREA  
DERIVATIVES AND THEIR Cu(II)  
AND Ni(II) COMPLEXES**

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## ABSTRACT

Three new mono-thiourea ligands namely *N*-(2-methoxybenzoyl)-*N'*-(4-diphenylamino)thiourea (T1), *N*-(3-methoxybenzoyl)-*N'*-(4-diphenylamino)thiourea (T2) and *N*-(4-methoxybenzoyl)-*N'*-(4-diphenylamino)thiourea (T3) have been successfully synthesized and characterized by elemental analysis (CHNS), infrared,  $^1\text{H}$  and  $^{13}\text{C}$  NMR and UV-Vis spectroscopic techniques. The structure of T1 was determined by single crystal X-ray diffraction method and crystallized in the monoclinic system, space group P2(1)/c, with  $a = 7.2647$  (13) Å,  $b = 20.478$  (4) Å,  $c = 12.687$  (2) Å,  $\beta = 101.015$  (4) °,  $V = 1852.6$  (6) Å<sup>3</sup>,  $Z = 4$ . The thiourea moiety maintains its *cis-trans* geometry causing the molecule to be non-planar. The N2-C9 bond length of 1.326(2)Å is shorter than N1-C9 (1.400(3)Å) indicating a double bond character. Thus, the S1-C9-N2 thioamide is delocalized. A series of new bis-thiourea derivatives namely 1,2-bis(*N'*-2-methoxybenzoyl-thioureido)-4-chlorobenzene (T4), 1,2-bis(*N'*-3-methoxybenzoylthioureido)-4-chloro-benzene (T5), 1,2-bis(*N'*-4-methoxybenzoylthioureido)-4-chlorobenzene (T6), 1,2-bis(*N'*-2-methoxybenzoyl-thioureido)-4-nitrobenzene (T7), 1,2-bis(*N'*-3-methoxybenzoylthioureido)-4-nitrobenzene (T8) and 1,2-bis(*N'*-4-methoxybenzoylthioureido)-4-nitrobenzene (T9) has been successfully prepared. The Cu(II) and Ni(II) complexes of T4, T5 and T6 series are also isolated. The structure of the ligands and complexes are elucidated by elemental analysis (CHNS), infrared,  $^1\text{H}$  and  $^{13}\text{C}$  NMR, UV-Vis spectroscopic and magnetic susceptibility determination method. The Ni(II) complexes are suggested to have tetrahedral geometry. All the compounds were screened for their antibacterial activity using disc diffusion method against three Gram-positive bacteria (*Bacillus subtilis* ATCC 6633, *Staphylococcus aureus* ATCC 29213 and *Lactobacillus casei* ATCC 393) and three Gram-negative bacteria (*Escherichia coli* ATCC 25922, *Pseudomonas aeruginosa* ATCC 10145, and *Shigella sonnei* ATCC 9290). The results show that the antibacterial activity of the metal complexes is higher than the ligands. The copper(II) complexes are more active against bacteria than the nickel(II) complexes.

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