

Synthesis and Theoretical Study of new Schiff base derivatives

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Abstract

The study include preparation two Schiff base compounds , 4-acetoamidobenzylidene-glycine SB-A and 4-acetoamidobenzylidene –nitrourea SB-B . Schiff bases were prepared by condensation of 4-acetanilbenzaldehyde with nitrourea and other with glycin. The products were characterized by both FT- IR and UV-Vis. Spectroscopyphotometry. The biological activities against selected types of bacteria which included gram positive bacteria (*staphylococcus aureus*), and gram negative bacteria (*Escherichia coli*, *proteus sp.*, *pseudomonas aeruginosa*) was studied. Later, theoretical studies by using the optimized geometry molecular structures of both compounds, indicates SB-B is more stable than SB-A.

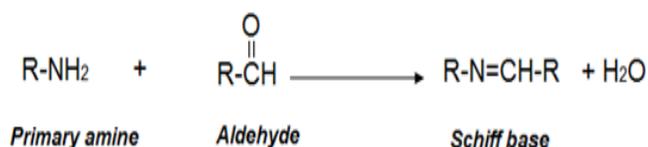
Key words: p-acetamidobenzaldehyde, glycin Schiff base, nitrourea derivatives

الخلاصة

تتضمن الدراسة تحضير مركبين من صنف قواعد شف ٤- اسيتاميدو بنزايليدين-كلايسين SB-B. والآخر ٤- اسيتاميدو بنزايليدين- نيترويوربا SB-A. وقد حضرت قواعد شف بواسطة التكثيف الارجاعي ل ٤- ستاميدوبنزالديهيد مع الكلايسين مرة ونيترويوربا مرة أخرى. شخصت المركبات المحضرة بواسطة مطيافية الأشعة تحت الحمراء ومطيافية الأشعة المرئية وال فوق البنفسجية. كما درست الفعالية البايولوجية لأنواع مختارة من البكتريا وتبين أن كذلك من خلال الدراسة النظرية لاستقرارية SB-A, أكثر فعالية بايولوجية من المركب SB-B. SB-A من المركب هو أكثر أستقرارية SB-B المركبين تبين ان المركب .

1-Introduction:

Compounds containing an azomethine group (-C=N-) are known as Schiff bases⁽¹⁾. They are usually formed by condensation of a primary amine with a carbonyl compound according to the following scheme :



where R may be an aliphatic or an aromatic group. Schiff base compounds have been used as fine chemicals and medicals substrates⁽²⁾. A Schiff base derived from an [aniline](#), where R is a [phenyl](#) or a substituted phenyl, can be called an anil⁽³⁾. Bulter and Hussain reported the reaction of benzaldehyde and substituted benzaldehydes with urea, thiourea and their alkyl/ aryl derivatives in acid media⁽⁴⁾. The reaction of urea with benzaldehyde was first reported by Schiff (5) . Hussain reported Schiff bases products from

reaction of p-dimethylaminobenzaldehyde with urea, thiourea and their alkyl/aryl derivatives(6) .Subsequently, Schiff base products was prepared from reaction of 4-N,N-dimethylamino- cinnamaldehyde with urea, thiourea and their derivatives in acid media(7).Schiff base also have biological importance. An imine linkage between the aldehyde derived from vitamin A and the protein opsin in the retina of the eye plays an important role in the chemistry of vision. Vitamins are also called coenzymes, meaning that they are to the functioning of many enzymes, which are large proteins that catalyze chemical changes in cell (8). Schiff bases have been reported in their biological properties, such as, Schiff bases have also been shown to exhibit a broad range of biological activities, including antifungal(9), antibacterial(10), analgesic(11), anti-tubercular(12), anti-inflammatory(13), antiviral, antipyretic properties (14,15), antioxidant (16) and enzyme inhibitors(17) . They also exhibit significant anticonvulsant activity(18) and antitumor activity(19). Schiff s base complexes play an important role in

designing metal complexes related to synthetic and natural oxygen carriers(20). The main aim of the research is synthesis and characterization of Schiff bases with different in amine side chain (glycin and nitrourea), also compare between its biological against microorganisms.

2-Experimental:

2.1- Instrumentals:

Melting points were measured on Stuart SMP3. The FT-IR spectra (KBr disk) were recorded on Shimadzu spectrophotometer in the rang 400-4000 cm^{-1} , While the U.V. Vis. spectra are measured with UV-1100 spectrophotometer in CHCl_3 .

2.2- Chemicals:

All chemicals and solvents were supplied from Aldrich and Merck chemical companies.

2.3- Methods:

2.3.1- Preparation of urea nitrate (21):

Conc. HNO_3 (10.8 ml) and 8 g (0.1 mmole) of urea (dissolved in 12 ml H_2O) in a 50 ml round-bottomed flask, was stirred at room temperature for 2 hours. The precipitate was filtered and the product is washed with four portions cold water and a white crystalline solid of urea nitrate ($\text{NH}_2\text{CONH}_2 \cdot \text{HNO}_3$) was obtained (m.p.162- 163 $^\circ\text{C}$).

2.3.2- Preparation of nitro urea(22):

Conc. sulfuric acid (14 ml) was cooled to -3 $^\circ\text{C}$ in ice bath, 4 gm (0.038 mmol) dry powdered of urea nitrate was added by fraction to control the temperature below 0 $^\circ\text{C}$. The mixture is poured upon crushed ice, the white divided finally precipitate of nitrourea is form. The product is washed with 4 portions of cold water (m.p. 157-159 $^\circ\text{C}$).

2.3- Preparation of 4-Acetoaminobenzylidene-glycin Schiff base (SB-A)⁽²³⁾:

4-acetoaminebenzaldehyde 0.163 g (1mmol) and 0.075 g (1mmol) of glycin were dissolved in 10 ml 95% ethanol in a 50 ml round bottom flask. 0.5 ml of 10% w/v NaOH were added to the solution and reflux for six hours with stirring. The solution of light yellow colour was then filtered off and the product was recrystallized in methanol (m.p. 127-128 $^\circ\text{C}$) figure (1).

2.4- Preparation of 4-Acetoaminobenzylidene-nitrourea Schiff base (SB-B):

4-acetoaminebenzaldehyde 0.163 g (1mmol) and 0.105 g (1mmol) of nitro urea were dissolved in 10 ml 95% ethanol. 0.5 ml of 10% NaOH were added and allowed to reflux for three hours in an isomental with stirring. The red colour precipitate was then filtered off and then

recrystallized in a mixture of acetone and ethylacetate (1:1) (decomposed at m.p. 220 -222 $^\circ\text{C}$) figure (1).

Results and Discussion:

The two derivatives of 4-acetoamine benzaldehyde with glycin and nitrourea as Schiff base compounds were prepared figure (1). The FT-IR spectra of both Schiff base was showed characteristic functional groups as shows in table (1). FT-IR spectra bands of acetoaminobenzylidene-glycin Schiff base (SB-A) showed strong peak at 1658.67 cm^{-1} which corresponding to carbonyl group of side chain ($\text{CH}_3\text{CONH-}$) band. The band at 1608.52 cm^{-1} confirmed the presence of ($-\text{C}=\text{N}-$) which is the characteristic of Schiff base. While acetoaminobenzylidene- nitrourea Schiff base (SB-B), appearance($-\text{C}=\text{N}-$) band at 1630 cm^{-1} and carbonyl group in ($\text{CH}_3\text{CONH-}$) at 1655 cm^{-1} . From UV-Vis. spectra of both SB-A and SB-B have been studied in chloroform (CHCl_3). The maximum absorption wavelengths for both compounds are shown in table (2). Shift band of compound SB-B is greater than compound SB-A. The enhanced shifting is due to increasing resonance interaction in compound SB-B figure (3).

Antibacterial activity:

The method agar diffusion was used to estimate the biological activity⁽²⁴⁾. The biological activity of both compounds was studied against selected types of bacteria which included gram positive bacteria (*staphylococcus aureus*), and gram negative bacteria (*Escherichia coli*, *proteus sp.*, *pseudomonas aeruginosa*) in nutrient agar media, which is used DMSO as a solvent and as a control for the disc sensitivity test. the results of biological activity in table(3). Compounds SB-A, found have inhibition zone against *S.aureus* with less inhibition against *E.coli* but Compound SB-B more inhibition zone against both the same species. The result was not surprising for SB-B compound, because it contain nitrourea part, which has a pronounced effect on the growth of *E.Coli*. It is apparent that significant inhibition of growth⁽²⁵⁾. The result of antibacterial activity study for Schiff base exhibited antibacterial activity against the studied bacteria. The increased activity of the synthesized compound can be explained electron delocalization over the whole molecule figure(3). This increases the lipophilic character of the molecule and favors its permeation through the lipid layer of the bacterial membranes. The increased lipophilic character of this molecule

