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THEORETICAL AND EXPERIMENTAL STUDIES OF SOME SCHIFF BASE

BAZI SCHIFF BAZLARIN TEORİK VE DENEYSEL ÇALIŞMALARI

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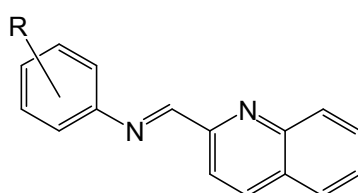
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ABSTRACT

The electrophilic carbon atoms of aldehydes can be targets of nucleophilic attack by amines. The end result of this reaction is a compound in which the C=O double bond is replaced by a C=N double bond. This type of compound is known as a Schiff base.

In this study some Schiff bases were synthesized from 2-quinoline aldehyde and some aniline derivatives and the molecules were characterized with spectroscopic methods. The pKa values of the molecules calculated with potentiometric methods and DFT calculated methods. The spectroscopic and the potentiometric results were compared with the calculated results.



R= 4-OH, 4-NO₂, 4-Cl, 4-CH₃

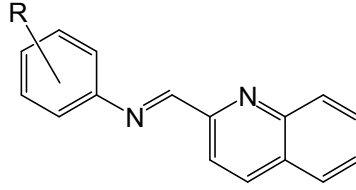
Figure 1. The general structure of the calculated molecules.

Keywords

Schiff bases, DFT calculation, pKa.

ÖZET

Aldehitlere ait karbonlar aminlerin nükleofilik saldırmasına uygundur. Bu reaksiyonun sonunda üründe C=O çiftli bağı yerine C=N bağı oluşur. Bu tip birleşiklere Schiff bazı denir. Bu çalışmada Schiff bazları 2-kinolin aldehit ve bazı anilin türevlerinden sentezlenmiştir. Sentezlenen moleküller bazı spektroskopik yöntemlerle karakterize edilmiştir. Moleküllerin pKa değerleri potansiyometrik metod ve DFT metoduyla hesaplanmıştır. Spektroskopik ve teorik sonuçlar karşılaştırılmıştır.



Şekil 1. Hesaplama yapılan moleküllerin genel yapısı

Anahtar Kelimeler

Schiff bazları, DFT hesaplamaları, pKa.

Kaynaklar / References

[1] Esmailzadeh, S., Azimian, L., Shekoohi, K., Mohammadi, K., Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Volume 133, 10 December 2014, Pages 579-590