



Al-Qadisiyah Journal of Pure Science

Al-Qadisiyah Journal of Pure Science

ISSN(Printed): 1997-2490

ISSN(Online): 2411-3514

DOI: /10.29350/jops.

<http://qu.edu.iq/journalsc/index.php/JOPS>

Synthesis, and studying effect of a solvent on the $^1\text{H-NMR}$ chemical shifts of 4-Azido-N-(6-chloro-3-pyridazinyl)benzenesulfonamide

<p>Authors Names Sadiq M. Hasan</p> <p>Article History Received on: 3/7/2021 Revised on: 30/7/2021 Accepted on: 5/8/2021</p> <p>Keywords: Polarity, azido, $^1\text{H-NMR}$, dielectric constants, correlation coefficient</p> <p>DOI: https://doi.org/10.29350/jops.2021.26.3.1429</p>	<p>ABSTRACT</p> <p>The compound 4-Azido-N-(6-chloro-3-pyridazinyl)benzenesulfonamide was synthesized and studied using FTIR, and $^1\text{H-NMR}$. The influence of a solvent on the experimental $^1\text{H-NMR}$ chemical shifts of title compound is discussed. Small chemical shift $\Delta\delta < 0.1$ ppm were observed when switching from DMSO-d₆ to CD₃OD. Record a marked change in chemical shifts values $\Delta\delta > 0.3$ ppm when transform from high-polar solvents (DMSO-d₆, and CD₃OD) to low-polar solvent (CDCl₃). The $^1\text{H-NMR}$ chemical shifts of C₂-H and C₆-H were shown to have excellent linear correlation with the dielectric constants of the solvents DMSO-d₆, CD₃OD, and CDCl₃ ($r = 0.995$). The $^1\text{H-NMR}$ chemical shifts of C₁₈-H shows a perfect relationship with solvatochromic parameter β ($r = 0.999$).</p>
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1. Introduction

Organic azides play a distinct role in organic chemistry, they are highly effective compounds that have a major role in many organic chemical reactions such as Curtius rearrangement [19,23], azo-Wittig reaction [14,24], and Staudinger reduction [15, 16] synthesis of triazoles and tetrazoles through 1,3 dipolar cycloaddition reaction to alkynes [4,12] and nitriles [28], as well in natural product synthesis [30].

As reactive molecules, organic azides exhibit many interesting properties such as cross-linkers [29] and photoaffinity labels [17,18]. Using azidonucleosides as a treatment of Acquired immunodeficiency syndrome (AIDS) has attracted specialist in this field, and azidothymidine (AZT) is one of the first treatments for AIDS [5]. Furthermore, AZT gold (I) complex has been shown to act as an anti-inflammatory agent, and as an inhibitor to HIV-1, as well [26].

A number of studies have been carried based on practical and theoretical usefulness of organic azides. Najafi et al synthesis and characterization of performed DFT calculations at B3LYP/6-31G* level on 4-(Sulfonylazide)phenyl-1-azide, and they compared the spectral properties that have been calculated