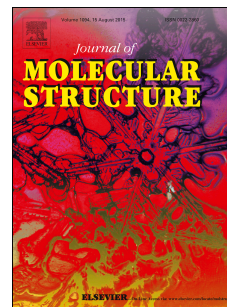


# Accepted Manuscript

Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: A comparative study

Kabiru Haruna, Tawfik A. Saleh, Jameel Al Thagfi, Abdulaziz A. Al-Saadi



PII: S0022-2860(16)30468-9

DOI: [10.1016/j.molstruc.2016.05.021](https://doi.org/10.1016/j.molstruc.2016.05.021)

Reference: MOLSTR 22535

To appear in: *Journal of Molecular Structure*

Received Date: 16 January 2016

Revised Date: 29 April 2016

Accepted Date: 9 May 2016

Please cite this article as: K. Haruna, T.A. Saleh, J. Al Thagfi, A.A. Al-Saadi, Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: A comparative study, *Journal of Molecular Structure* (2016), doi: 10.1016/j.molstruc.2016.05.021.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: a comparative study

Kabiru Haruna, Tawfik A. Saleh, Jameel Al Thagfi and Abdulaziz A. Al-Saadi\*

\* Correspondence to: Abdulaziz A. Al-Saadi, Department of Chemistry, King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, Saudi Arabia; email [asaadi@kfupm.edu.sa](mailto:asaadi@kfupm.edu.sa)

Department of Chemistry, King Fahd University of Petroleum & Minerals (KFUPM), Dhahran, Saudi Arabia

### Abstract

A comparative electronic and spectroscopic analysis of 2,4,6-trichloroaniline (TCA) and 2,4,6-tribromoaniline (TBA) was carried out by theoretical and experimental techniques. The  $\text{NH}_2$  inversion barrier in TCA and TBA molecules was predicted to be three times less than that in aniline and 2,4,6-trifluoroaniline. The size of the halogen substituents in the ortho positions is shown by density functional theory to play an important role in determining the electronic and structural properties of the amino group in the investigated haloaniline derivatives. A thorough interpretation of the infrared and Raman spectra has been performed on the basis of the observed and calculated infrared and Raman spectra as well as calculated potential energy distribution values. In addition, the SERS spectra for both trihaloanilines were successfully collected up to a concentration of  $10^{-6}$  M using aged hydroxylamine-reduced silver colloid as an active substrate for TCA and TBA. SERS intensities of several peaks were found to linearly change with concentration allowing quantitative analyses of TCA and TBA. A relatively stronger interaction in the case of TBA–silver colloids is predicted compared to the TCA analogue.

**Keywords:** Trihaloanilines; Infrared and Raman spectra; Density functional theory (DFT); Surface-enhanced Raman scattering (SERS).

Download English Version:

<https://daneshyari.com/en/article/7809246>

Download Persian Version:

<https://daneshyari.com/article/7809246>

[Daneshyari.com](https://daneshyari.com)