

Web of Science

Search

Search Results

My Tools ▾

Search History

Marked List

47 of 455

Eclipsed Acetaldehyde as a Precursor for Producing Vinyl Alcohol

By: [Osman, OI](#) (Osman, Osman I.)^[1]; [Alyoubi, AO](#) (Alyoubi, Abdulrahman O.)^[1]; [Elroby, SAK](#) (Elroby, Shabaan A. K.)^[1]; [Hilal, RH](#) (Hilal, Rifaat H.)^[1]; [Aziz, SG](#) (Aziz, Saadullah G.)^[1]

[View ResearcherID and ORCID](#)

INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES

Volume: 13 Issue: 11 Pages: 15360-15372

DOI: 10.3390/ijms131115360

Published: NOV 2012

[View Journal Impact](#)

Abstract

The MP2 and DFT/B3LYP methods at 6-311++ G(d, p) and aug-cc-pdz basis sets have been used to probe the origin of relative stability preference for eclipsed acetaldehyde over its bisected counterpart. A relative energy stability range of 1.02 to 1.20 kcal/mol, in favor of the eclipsed conformer, was found and discussed. An NBO study at these chemistry levels complemented these findings and assigned the eclipsed acetaldehyde preference mainly to the vicinal antiperiplanar hyperconjugative interactions. The tautomeric interconversion between the more stable eclipsed acetaldehyde and vinyl alcohol has been achieved through a four-membered ring transition state (TS). The obtained barrier heights and relative stabilities of eclipsed acetaldehyde and the two conformers of vinyl alcohol at these model chemistries have been estimated and discussed.

Keywords

Author Keywords: acetaldehyde; eclipsed; bisected; vinyl alcohol; tautomerization; hyperconjugation; MP2; B3LYP; NBO

KeyWords Plus: HYDROXYETHYLIDENE CH₃-C-OH; MICROWAVE-SPECTRUM; DIPOLE-MOMENT; ACETONE

Author Information

Reprint Address: Osman, OI (reprint author)

King Abdulaziz Univ, Fac Sci, Dept Chem, POB 80203, Jeddah 21589, Saudi Arabia.

Organization-Enhanced Name(s)

King Abdulaziz University

Addresses:

[1] King Abdulaziz Univ, Fac Sci, Dept Chem, Jeddah 21589, Saudi Arabia

Organization-Enhanced Name(s)

King Abdulaziz University

E-mail Addresses: oabdelkarim@kau.edu.sa; aalyoubi@kau.edu.sa; Skamel@kau.edu.sa; rhilal@kau.edu.sa; saziz@kau.edu.sa

Funding

Funding Agency	Grant Number
King Abdulaziz University, Jeddah	D7-130-/1432
DSR	

Citation Network

2 Times Cited

28 Cited References

[View Related Records](#)



Create Citation Alert

(data from Web of Science Core Collection)

All Times Cited Counts

2 in All Databases

2 in Web of Science Core Collection

0 in BIOSIS Citation Index

0 in Chinese Science Citation Database

0 in Data Citation Index

0 in Russian Science Citation Index

0 in SciELO Citation Index

Usage Count

Last 180 Days: 0

Since 2013: 21

[Learn more](#)

Most Recent Citation

Hussein, M. A. Photoreactivity, Optical Behavior and DFT Studies of 2,5-Bis[4-choloro-acetyl(thiophen-2-ylmethylene)]cyclopentanone BCTCP in Different Solvents . JOURNAL OF FLUORESCENCE, MAY 2017.

[View All](#)

This record is from:

Web of Science Core Collection
- Science Citation Index Expanded

Suggest a correction

If you would like to improve the quality of the data in this record, please [suggest a correction](#).

[View funding text](#)

Publisher

MDPI AG, POSTFACH, CH-4005 BASEL, SWITZERLAND

Categories / Classification

Research Areas: Biochemistry & Molecular Biology; Chemistry

Web of Science Categories: Biochemistry & Molecular Biology; Chemistry, Multidisciplinary

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000311425000098

PubMed ID: 23203130

ISSN: 1422-0067

Other Information

IDS Number: 041TV

Cited References in Web of Science Core Collection: **28**

Times Cited in Web of Science Core Collection: **2**