بسم الله الرحمن الرحيم

شبكة المعلومات الجامعية

التوثيق الالكتروني والميكروفيلم

شبكة المعلومات الجامعية

جامعة عين شمس

التوثيق الالكتروني والميكروفيلم

قَســـم

نقسم بالله العظيم أن المادة التي تم توثيقها وتسجيلها
علي هذه الأفلام قد اعدت دون آية تغيرات

يجب أن

تحفظ هذه الأفلام بعيداً عن الغبار

في درجة حرارة من 15 – 20 مئوية ورطوبة نسبية من 20-40 %

To be kept away from dust in dry cool place of
15 – 25c and relative humidity 20-40 %

بعض الوثائق

الأصلية تالفة

بالرسالة صفحات

لم ترد بالأصـــــل

SCFMO STUDIES OF SOME SELECTED HYDROGEN BONDED SYSTEMS

A THESIS

Presented to Faculty of Science,
Menoufia University, Shebin El-Koom

BY
AMANI ABD EL-AZIZ SHALABI
B.Sc.
In partial fulfillment of the Requirements for
The Degree of Master of Science
Physical and Inorganic Chemistry

Supervised By

PROF. DR.
FARAG AHMED ALI
Prof. of Inorganic Chemistry
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Benha University

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بسم الله الرحمن الرحيم

﴿ ربنا لا تؤاخذنا إن نسينا أو أخطأنا ربنا ولا تحمل علينا إصرا كما حملته على الذين من قبلنا ربنا ولا تحملنا ما لا طاقة لنا به واعف عنا واغفر لنا وارحمنا أنت مولانا فانصرنا على القوم الكافرين ﴾

صدق الله العظيم

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Amani A. Shalabi

NOTES

Besides the work carried in this thesis, the candidate had attended post-graduate courses for one year in Physical and Inorganic Chemistry, in covering the following topics :

- Solid state.
- Microanalysis.
- Electrochemistry.
- Surface chemistry.
- Theory of complexes.
- Spectroscopy.
- Essay.
- Statistics.
- Computer.
- English.

Head of Chemistry Department

Prof. Dr. IBRAHIM F. ZEID

LIST OF ABBREVIATION

ESR : Electron spin resonance
LMO : Localized molecular orbital
CI : Configuration interaction
SCF : Self-consistent field
GVB : Generalized valence-bond.
CISD : Single and double excitation configuration interaction.
DZP : Double - zeta puls polarization
TZ2P : Triple zeta puls double polarization
BDE$_s$: Bond dissociation energies
CCSD : The single and double excitations couple-cluster
CCSD(T) : The single, double and perturbative triple excitations coupled cluster
IRC : Intrinsic reaction coordinate
MEP : Minimum energy path
MNDO : Modified Neglect of Diatomic Differential Overlap.
CNDO : Complete Neglect of Differential Overlap.
INDO : Intermediate Neglect of Differential Overlap.
NDDO : Neglect of Diatomic Differential Overlap.
MINDO/3 : Is a modified INDO mothod.
MRBW : Multireference Brillouim-Wigner.
VB : Valence Bond theory
MO : Molecular Orbital theory

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CHAPTER III : RESULTS AND DISCUSSION

3-1- Acetylenes

3-2- Disilyens :

Chapter 1
INTRODUCTION

1.1- Literature Survey :

The topology of the potential energy surface of Si_2H_2 reveals some very interesting and intriguing features, both in comparison with C_2H_2 as well as in its own right. The contrasting chemical behavior of silicon and carbon has been known, and a variety of reasons put forth in explanation. Kutzelnigg(1) published a pertinent paper in 1984 that provided an excellent discussion of silicon bonding from the point of view of periodic terends. Chemists have historically pointed all too readily to the availability of d-orbitals in the valence shell of silicon when explaining why it behaves differently than carbon, and quite understandably since it is the valence electrons that engage in bonding and other activities that constitute chemical behavior. However, ab initio calculations have shown that the contribution of silicon d-orbitals to the molecular orbitals is very small. Kutzelnigg(1) suggests that it is rather a difference in the cores of carbon and silicon that distinguishes them. First-row elements such as carbon have only s-orbitals in their cores, while the second - row elements additionally have p-orbitals. Because of carbon's totally symmetric core, its 2s and 2p valence orbitals have about the same spatial extension. This establishes an ideal environment for s-p hybridization that does not exist for silicon. Because the 3s orbital is contracted compared to the 3p, silicon's 3p orbitals carry a large amount of the responsibility in forming bonds, while the 3s orbital is more favored for lone-pair orbitals. Thus silicon exhibits unbalanced hybridization, quite different from the concept of equivalent hybrids. In fact, nonhybridization of the silicon atomic orbitals may be a better representation(2, 3). Two other periodic trends that distinguish carbon and silicon are silicon's greater affinity for the divalent state and its smaller electronegativity. These factors combine to provide a clear distinction between the chemistry of carbon and silicon.