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شبكة المعلومات الجامعية

التوثيق الالكتروني والميكروفيلم

شبكة المعلومات الجامعية

جامعة عين شمس

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لم ترد بالاصل

South Valley University
Faculty of Science, Sohag
Chemistry Department

STRUCRURES AND ELECTRONIC STATES OF HETEROPOLYACID CATALYSTS

A THESIS

Submitted to the Faculty of Science (Sohag)
South Valley University

For
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(Chemistry)

By
Tarek Taha Ahmed Ali Saad

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2002

South Valley University
Faculty of Science, Sohag
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Approval

of the Ph. D. thesis and degree

Candidate: *Tarek Taha Ahmed Ali Saad*

Thesis title: **Structures and Electronic States of Heteropolyacid Catalysts.**

Degree: **Ph.D.Chemistry).**

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Examiners

1-
2-
3-
4-

Faculty board of graduate studies

DEDICATION

To

My Inspirator

My Dear Wife
My Lovely Son Amr
Spirit of My Dear Mother

For

Their Continuous Encouragement
And
Their Great Feelings

ACKNOWLEDGEMENT

AKNOWLEDGEMENT

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ABSTRACT

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Thesis Title: Structures and Electronic States of Heteropolyacid Catalysts

Candidate: Tarek Taha Ahmed Ali Saad

Quantum chemical density functional calculations were performed in order to describe the acidity and the catalytic activity of Keggin-type heteropolyacid compounds, i.e. 12-tungstophosphoric ($H_3PW_{12}O_{40}$), 12-molybdophosphoric ($H_3PMo_{12}O_{40}$) and 12-tungstosilicic ($H_4SiW_{12}O_{40}$) acids, as well as to shed light on their physico-chemical properties. Particular attention is paid on the comparison of their proton-donor affinities. The obtained results revealed that the most energetically favorable site for the acidic proton might be an edge-bridging oxygen atom in the anhydrous heteropolyacids. An analysis of harmonic vibrational frequencies as well as of their corresponding normal modes were presented. The adsorption properties of ammonia, pyridine, methanol and water were computed and discussed in relation with the available experimental data. Additionally, the reaction mechanism of methanol hydration was proposed.

Key Words: Heteropolyacids – Density Functional Theory – Proton-donor affinity – Adsorption properties – Methanol conversion.

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