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Synthesis, characterization, molecular modeling and applications on complexes of some azine derivatives

A Thesis Submitted by

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Master of the Teacher's Preparation in Science
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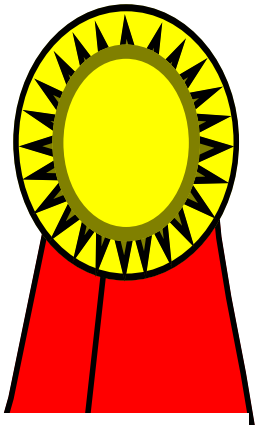

Dedication

To

My little sweet kid Leen& my wife

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1- A.Taha[a], A.A.M.Farag[b*], MagdyShebl [a], O. M. I. Adly [a] and **H.M.Ahmed[a]**, Molecular structure 1142-16:42-(2017) **".**

2- A.Taha[a], A.A.M.Farag[b,c*], O. M. I. Adly[a], N.Roushdy[d],MagdyShebl[a] and **H.M.Ahmed[a]** Molecular structure 31-42-1139(2017)

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List of abbreviations

DSSC	dye sensitized solar cells
DHT	5, 6 di phenyl-3-hydrazino-1, 2,4 triazine
HBDHT	2-Benzylidene-1-(5,6-diphenyl-1,2,4-triazin-3-yl)hydrazine
o-HBDHT	2-benzylidene-3-hydroxy -1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
p-HBDHT	2-benzylidene-P-hydroxy -1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
p-ClBDHT	2-benzylidene-P-Cl -1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
p-MBDHT	2-benzylidene-P-CH_3 -1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
p-NBDHT	2-benzylidene-P-NO_2 -1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
HBzDHT	3-(α-Benzoylbenzylidenehydrazino)-5,6 diphenyl-1,2,4-triazine
o-HACBDHT	2-benzylidene-3-hydroxy –CH_3-1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
VBDHT	2-benzylidene-p-OH –m-OCH_3-1-(5,6-diphenyl-1,2,4-

	triazine-3-yl)hydrazine
DHBDHT	2-benzylidene-2,4-hydroxy -1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
Me_2NBDHT	2-benzylidene-p-$N(CH_3)_2$ -1-(5,6-diphenyl-1,2,4-triazine-3-yl)hydrazine
λ_{max}	The higher wave length
λ_{ex}	Excitation wave length
λem	Emission wavelength
λ-stokes	λem- λex
Q_Y	Quantum yield
fst	the areas under the fluorescence emission curves of the samples and the standard
ε	the extinction coefficient
η	Hardness
μ	Potential reactivity
ω	electrophilic index
B3LYP	Becke's 3-parameter hybrid exchange functional and Lee, Yang, and Parr correlation functional
DFT	Density functional theory
MO	Molecular orbital
ΔH_f	Heat of formation
HOMO	High occupied molecular orbital
LUMO	Low unoccupied molecular orbital
V_{oc}	Open circuit voltage
PCBM	Phenyl C61 butric acid methyl ester
IP	Ionization potential
EA	Electron affinity

J_{sc}	the short-circuit current
BHJ	the bulk hetero-junction solar cell
SEM	Scanning electron microscopy
ε	the real dielectric constant
tanδ	the loss factor
α	the absorption coefficient
δ	the skin depth
V	the applied voltage
η	The ideality factor
R_s	The series resistance
J_o	the reverse saturation current density
Φ_b	the zero-bias barrier height
A^*	the Richardson constant
P	the illumination intensity
J_{sc}	short circuit current density
J_{ph}	photocurrent density
EDTA-Na_2	Ehylenediaminetetraacetic acid disodium salt dihydrate
DMSO	Dimethylsulphoxide
DMF	Dimethylformamide
TGA	Thermal gravimetric analysis
DTA	Differential thermal analysis

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