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

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For

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Dedication

To

My little sweet kid Leen& my wife

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List of abbreviations

dye sensitized solar cells
5, 6 di phenyl-3-hydrazino-1, 2,4 triazine
2-Benzylidene-1-(5,6-diphenyl-1,2,4-triazin-3-
yl)hydrazine
2-benzylidene-3-hydroxy -1-(5,6-diphenyl-1,2,4-
triazine-3-yl)hydrazine
2-benzylidene-P-hydroxy -1-(5,6-diphenyl-1,2,4-
triazine-3-yl)hydrazine
2-benzylidene-P-Cl -1-(5,6-diphenyl-1,2,4-triazine-3-
yl)hydrazine
2-benzylidene-P-CH ₃ -1-(5,6-diphenyl-1,2,4-triazine-3-
yl)hydrazine
2-benzylidene-P-NO ₂ -1-(5,6-diphenyl-1,2,4-triazine-3-
yl)hydrazine
3-(α-Benzoylbenzylidenehydrazino)-5,6 diphenyl-
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triazine-3-yl)hydrazine
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

Me₂NBDHT 2-benzylidene-p-N(CH₃)₂ -1-(5,6-diphenyl-1,2,4-

triazine-3-yl)hydrazine

 λ_{ex} Excitation wave length

λem Emission wavelength

 λ -stokes λ em- λ ex

Q_Y Quantum yield

fst the areas under the fluorescence emission curves of the

samples and the standard

 ϵ the extinction coefficient

 $\eta \qquad \qquad \text{Hardness}$

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 potentialEA Electron affinity

 $J_{sc} \\$ the short-circuit current BHJ the bulk hetero-junction solar cell **SEM** Scanning electron microscopy the real dielectric constant 3 the loss factor $tan\delta$ the absorption coefficient α the skin depth δ V the applied voltage The ideality factor η The series resistance R_{s} the reverse saturation current density J_{o} 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 Ehylenediaminetetraacetic acid disodium salt dihydrate EDTA-Na₂ **DMSO** Dimethylsulphoxide **DMF** Dimethylformamide **TGA** Thermal gravimetric analysis DTA Differential thermal analysis

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