Declaration

I hereby declare that the work presented in this thesis titled '*Redox-active Phenalenyl-based Transition Metal Complexes for Applications in Resistive Memory Device and (Electro)Catalysis*' submitted to the Indian Institute of Technology Jodhpur in partial fulfilment of the requirements for the award of the degree of Doctor of Philosophy, is a bonafide record of the research work carried out under the supervision of Dr. Ramesh K. Metre. The contents of this thesis in full or in parts, have not been submitted to, and will not be submitted by me to, any other Institute or University in India or abroad for the award of any degree or diploma.

Nisha Kamboj
P18CY202

Certificate

This is to certify that the thesis titled '*Redox-active Phenalenyl-based Transition Metal Complexes for Applications in Resistive Memory Device and (Electro)Catalysis*' submitted by Nisha Kamboj (P18CY202) to the Indian Institute of Technology Jodhpur for the award of the degree of Doctor of Philosophy, is a bonafide record of the research work done by her under my supervision. To the best of my knowledge, the contents of this report, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Ramesh K. Metre
Ph. D. Thesis Supervisor
Date:

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"When you want something, all the universe conspires in helping you to achieve it" – Alchemist by Paulo Coelho

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Nisha Kamboj
Ph.D. Student

Dedicated to my Daadu and Naani, who are no more with me, but I have always been protected and guided by their souls.

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List of Symbols

Symbol	*Description*
μ	Bridging
λ	Wavelength
δ	Chemical shift
V	Volume
°	Degree
%	Percentage
d	Interplanar distance
θ	Theta
ν	Frequency
A	Absorbance
s	Second
h	Hour
τ	Addison's parameter
π	Pi
σ	Sigma
Å	Angstrom
I	Current
mV	Millivolt
mA	Miliampere
eV	Electron volt
1D	One-dimensional
2D	Two-dimensional
A	Ampere
V	Potential
η	Overpotential
g	Zeeman factor

List of Abbreviations

Abbreviation	*Full form*
FMO	Frontier Molecular Orbital
POAHs	Polycyclic Odd Alternant Hydrocarbons
PLY	Phenalenyl
NBMO	Non Bonding Molecular Orbitals
LCAO	Linear Combination of Atomic Orbitals
CMOs	Conducting Molecular Orbitals
PAHs	Polycyclic Aromatic Hydrocarbons
DFT	Density Functional Theory
OCP	Open Circuit Potential
PPD	Peak Power Density
CV	Cyclic Voltammetry
NMR	Nuclear Magnetic Resonance Spectroscopy
HRMS	High Resolution Mass Spectrometry
XPS	X-ray Photoelectron Spectroscopy
EPR	Electron paramagnetic resonance spectroscopy
UV-vis	Ultra-violet Visible
FTIR	Fourier Transform Infra-red
AFM	Atomic Force Microscopy
DCM	Dichloromethane
CIF	Crystallographic Information File
TD-DFT	Time-dependent Density Functional Theory
HOMO	Highly Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
SOMO	Singly Occupied Molecular Orbital
HRS	High Resistive State
LRS	Low Resistive State
RRAM	Resistive Random-Access Memory
NPA	Natural Population Analysis
TMC	Transition-Metal Complexes
ECP	Effective Core Potential
WBI	Wiberg Bond Index
NBO	Natural Bond Order
TGA	Thermogravimetric Analysis
TTF	Tetrathiafulvalene
TCNQ	Tetracyanoquinodimethane
NIR	Near Infrared
MLCT	Metal to Ligand Charge Transfer
LLCT	Ligand to Ligand Charge Transfer
HS	High-Spin
LS	Low-Spin
BSLS	Broken-Symmetry Low-Spin
ITO	Indium Tin Oxide
$TBAPF_6$	Tetrabutylammonium Hexafluorophosphate
CCDC	Cambridge Crystallographic Data Centre
TEMPO	2,2,6,6-Tetramethyl-1-piperidinyloxyl
DMF	Dimethyl Formamide
GCE	Glassy Carbon Electrode
OER	Oxygen Evolution Reaction
SEM	Scanning Electron Microscopy
EDS	Energy Dispersive Spectroscopy

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