Dedicated to....

My Beloved Parents

and My Dear Teacher Late Santa Pradhan

DECLARATION BY THE CANDIDATE

The thesis entitled "***Theoretical Studies on Monovalent Group 13 and Divalent Group 14 Carbenoids, Metallatranes and Model Systems for Dinitrogen Reduction***" is being submitted to Tezpur University in partial fulfillment for the award of degree of Doctor of Philosophy in Chemical Sciences is a record of bonafide research work accomplished by me under the supervision of ***Prof. Ashwini K. Phukan***.

All helps from various sources have been duly acknowledged.

No part of this thesis has been submitted elsewhere for award of any other degree.

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CERTIFICATE FROM SUPERVISOR

This is to certify that the thesis entitled "***Theoretical Studies on Monovalent Group 13 and Divalent Group 14 Carbenoids***, ***Metallatranes and Model Systems for Dinitrogen Reduction***" submitted to the School of Sciences, Tezpur University in partial fulfillment for the award of the degree of Doctor of Philosophy in the Department of Chemical Sciences is a record of research work carried out by ***Mr. Bijoy Ghosh*** under my supervision and guidance.

All help received by him from various sources have been duly acknowledged. No part of this thesis has been submitted elsewhere for award of any other degree.

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Bijoy Ghosh

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aNHC	Abnormal *N*-heterocyclic Carbene
ASM	Activation Strain Model
cAAC	Cyclic Alkyl Amino Carbene
CP	Critical Point
DAC	Diamido carbene
DFT	Density Functional Theory
ECP	Effective Core Potential
EDA	Energy Decomposition Analysis
GGA	Generalized–Gradient approximation
GTO	Gaussian Type orbital
HF	Hartree-Fock
HOMO	Highest Occupied Molecular Orbital
IRC	Intrinsic Reaction Coordinate
KS	Kohn–Sham
LDA	Local Density Approximation
LSDA	Local Spin Density Approximation
LUMO	Lowest Unoccupied Molecular Orbital
MO	Molecular Orbital
NBO	Natural Bond Orbital
NHC	*N*-Heterocyclic Carbene
PA	Proton Affinity
PCM	Polarizable Continuum Model
PHC	*P*-Heterocyclic Carbene
QTAIM	Quantum Theory of Atoms in Molecules
STO	Slater Type Orbital
TCNE	Tetracyanoethylene
TM	Transition Metal
TS	Transition State
WBI	Wiberg Bond Index