

List of Abbreviations:

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| AC | Arduengo Carbene |
| <i>a</i> NHC | abnormal <i>N</i> -Heterocyclic Carbene |
| BDE | Bond Dissociation Energy |
| CAAC | Cyclic Alkyl Amino Carbene |
| CP | Critical Point |
| DFT | Density Functional Theory |
| ECP | Effective Core Potential |
| GGA | Generalized-Gradient Approximation |
| 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 | <i>N</i> -Heterocyclic Carbene |
| NICS | Nucleus Independent Chemical Shift |
| NMR | Nuclear Magnetic Resonance |
| PA | Proton Affinity |
| PCM | Polarizable Continuum Model |
| PHC | <i>P</i> -Heterocyclic Carbene |
| QTAIM | Quantum Theory of Atoms in Molecules |
| <i>r</i> NHC | Remote <i>N</i> -Heterocyclic Carbene |
| SE | Stabilization Energy |
| TCNE | Tetracyanoethylene |