# LIST OF ABBREVIATIONS

| | | |
|---|---|---|
| B3LYP | - | Becke-3 parameter-Lee-Yang-Parr functional |
| BRMP | - | (2E)-1- 4-Bromophenyl -3-(2-methoxyphenyl) prop-2-en-1-one |
| CCL | - | (2E)-1-(3-Chlorophenyl)-3-(4-chlorophenyl) prop-2-en-1-one |
| CCD | - | Charge coupled device |
| CIF | - | Crystal information file |
| CT | - | Charge transfer |
| DFT | - | Density functional theory |
| DIM | - | (2E)-3-(3,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl) prop-2-en-1-one (DIM) |
| DINO | - | (2E)-1-(2, 4-Dichlorophenyl)-3-(4, 5-dimethoxy-2-nitrophenyl)-2-propen-1-one |
| 2-D | - | Two dimensional |
| EA | - | Electron affinity |
| ED | - | Electron density |
| E(2) | - | Energy of hyper conjugative interactions |
| FMO | - | Frontier molecular orbital |
| FT | - | Fourier transform |
| FTIR | - | Fourier transform infrared |
| GTO | - | Gaussian type orbital |
| HF | - | Hatree Fock |
| HOMO | - | Highest occupied molecular orbital |
| ICT | - | Intramolecular charge transfer |
| IR | - | Infrared |
| $I_{IR}$ | - | IR Intensity |
| $I_{Raman}$ | - | Raman Intensity |
| KS | - | Kohn-Sham |
| LDA | - | Local density approximation |
| LED | - | Light emitting diode |

| | | |
|---|---|---|
| LUMO | - | Lowest unoccupied molecular orbital |
| MLR | - | Multi-linear regression |
| MP2 | - | Mooler-Plesset |
| NBO | - | Natural bond orbital |
| NCA | - | Normal coordinate analysis |
| NLO | - | Nonlinear optics |
| NPA | - | Natural population analysis |
| NMR | - | Nuclear magnetic resonance |
| PCM | - | Polarizable continuum model |
| PDB | - | Protein data bank |
| PED | - | Potential energy distribution |
| Ph | - | Phenyl |
| PYR | - | (2E)-3-(3-Bromo-4methoxyphenyl)-1-(pyridin-2-yl) prop-2-en-1-one |
| QSAR | - | Quantitative structure activity relationship |
| QTAIM | - | Quantum theory of atoms in molecule |
| SCF | - | Self-consistent field |
| SHG | - | Second harmonic generation |
| SMD | - | Solvation model on density |
| STO | - | Slater type orbital |
| SQMFF | - | Scaled quantum mechanical force field |
| TD-DFT | - | Time-dependent density functional theory |
| UV-Vis | - | Ultra violet visible |
| XRD | - | X-ray diffraction |