TABLE 1.The quantum chemical parameters for all compounds

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| --- | --- | --- | --- | --- | --- |
|  | **3** | **4** | **6** | **8** | **11** |
| EHOMO(eV) | -6.8348 | -6.0204 | -0.4212 | -5.7635 | -4.7811 |
| ELUMO(eV) | -3.2312 | -2.0804 | -4.0627 | -2.5709 | -1.7451 |
| Energy gap “∆E” | 3.6036 | 3.9400 | -3.6416 | 3.1925 | 3.0359 |
| Ionization potential “IP(eV)” | 6.8348 | 6.0204 | 0.4212 | 5.7635 | 4.7811 |
| Electron affinity “A(eV)” | 3.2312 | 2.0804 | 4.0627 | 2.5709 | 1.7451 |
| Chemical hardness “η(eV)” | 3.6036 | 3.9400 | -3.6415 | 3.1926 | 3.0360 |
| Chemical softness “S” | 0.2775 | 0.2538 | -0.2746 | 0.3132 | 0.3294 |
| Electronegativity “χ(eV)” | 5.0330 | 4.0504 | 2.2419 | 4.1672 | 3.2631 |
| Transferred electrons fraction “(ΔN)” | 0.2729 | 0.3743 | -0.6533 | 0.4437 | 0.6154 |
| Dipole moment “µ(debye)” | 9.0896 | 3.9613 | 2.6511 | 6.5956 | 3.8746 |
| Electrophilicity index “(ω)” | 11.4636 | 1.9913 | -0.9650 | 6.8129 | 2.4724 |
| ΔE back donation | -0.9009 | -0.985 | 0.9103 | -0.7981 | -0.7590 |