Table VII. Dual descriptors evaluated at the wB97XD/6-311++G(2d,2p) level of theory employing the PCM solvation model according to equation (13). In all cases the isosurfaces were obtained at 0.01 e/u.a.3

|  |  |  |
| --- | --- | --- |
|  | **-chloro** | **-without chloro** |
| **TB** |  |  |
| **TBS** |  |  |
| **TBSu** |  |  |