Table III. Isosurfaces of the Fukui Functions for nucleophilic (), electrophilic () and free radical attacks () on TB and DTB according to equations (10), (11) and (12) at the wB97XD/6-311++G(2d,2p) level of theory, employing the PCM solvation model. In all cases the isosurfaces were obtained at 0.01 e/u.a.3

|  |  |  |
| --- | --- | --- |
|  | **TB** | **DTB** |
|  | f+.tif | f+.tif |
|  | f-.tif | f-.tif |
|  | f+.tif | f0.tif |