Table II. Electroaccepting (**+) powers evaluated at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase, employing the PCM solvation model, according to the equation (6).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **  / eV |  |  | **  / eV |
| TB | 0.0195 |  | DTB | 0.0158 |
| TBS | 0.0201 |  | DTBS | 0.0202 |
| TBSu | 0.0204 |  | DTBSu | 0.0167 |