**Table** S**1.** Geometric parameters of MHTT

|  |  |
| --- | --- |
| Bond length, Å | Bond angle, Degree |
| H(13)-O(12) | 0.9835 | H(10)-C(7)-H(9) | 108.1862 |
| O(12)-N(3) | 1.3622 | H(10)-C(7)-H(8) | 108.6632 |
| S(11)-C(4) | 1.6735 | H(10)-C(7)-C(1) | 111.1968 |
| H(10)-C(7) | 1.0937 | H(9)-C(7)-H(8) | 108.6659 |
| H(9)-C(7) | 1.0937 | H(9)-C(7)-C(1) | 111.1969 |
| H(8)-C(7) | 1.0892 | H(8)-C(7)-C(1) | 108.8658 |
| C(7)-C(1) | 1.4867 | H(6)-N(5)-C(4) | 123.0004 |
| H(6)-N(5) | 1.0081 | H(6)-N(5)-C(1) | 127.7953 |
| N(5)-C(1) | 1.3777 | C(4)-N(5)-C(1) | 109.2043 |
| N(5)-C(4) | 1.3822 | S(11)-C(4)-N(5) | 132.4776 |
| C(4)-N(3) | 1.3510 | S(11)-C(4)-N(3) | 126.6194 |
| N(3)-N(2) | 1.3510 | N(5)-C(4)-N(3) | 100.9031 |
| N(2)-C(1) | 1.3080 | O(12)-N(3)-C(4) | 124.2816 |
|  |  | O(12)-N(3)-N(2) | 119.8977 |
|  |  | C(4)-N(3)-N(2) | 115.8207 |
|  |  | N(3)-N(2)-C(1) | 103.6950 |
|  |  | C(7)-C(1)-N(5) | 124.6376 |
|  |  | C(7)-C(1)-N(2) | 124.9855 |
|  |  | N(5)-C(1)-N(2) | 110.3770 |
|  |  | H(10)-C(7)-H(9) | 108.1862 |

**Table S2.** Some global reactivity parameters of MHTT in various solvents

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Parameters**  | MHTT | MHTT+ACN | MHTT+AC | MHTT+DO | MHTT+DMF |
| Dipole moment,(Debay)  | 5.078 | 11.549 | 8.958 | 6.760 | 10.873 |
| EHOMO (eV)  | -5,997 | -6,097 | -6,12 | -5,894 | -6,101 |
| ELUMO (eV)  | -0,785 | -1,222 | -0,443 | -0,484 | -0,395 |
| EHOMO - ELUMO (eV)  | -5,212 | -4,875 | -5,677 | -5,41 | -5,706 |
| Hardness,η=(EHOMO - ELUMO)/2 (eV)  | -2,606 | -2,4375 | -2,8385 | -2,705 | -2,853 |
| Chemical potential, μ=(EHOMO+ ELUMO)/2 (eV)  | -3,391 | -3,6595 | -3,2815 | -3,189 | -3,248 |
| Global electrophilic index, ω=μ2/2η (eV)  | -2,206 | -2,747 | -1,897 | -1,880 | -1,849 |
| IP = -EHOMO (eV)  | 5,997 | 6,097 | 6,12 | 5,894 | 6,101 |
| EA = -ELUMO (eV)  | 0,785 | 1,222 | 0,443 | 0,484 | 0,395 |

**Table S3.** Excitation state, absorption wavelength, oscillator strength, and percentage contribution of MHTT in solvents computed at the B3LYP/6-311++G(d,p)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Medium | Electronic transitions | Eex (eV) | λ (nm) | f (eV) | Transitions probability (%) |
| MHTT | S0→S1S0→S2S0→S3 | 4.52914.76484.7736 | 273.75260.21259.73 | 0.00490.12220.0000 | H→L (69)H→L+3 (11)H→L+1 (67)H→L+2 (15)H-1→L+1 (55)H-1→L+2 (43) |
| MHTT+ACN | S0→S1S0→S2S0→S3 | 4.98935.01675.0575 | 248.50247.14245.15 | 0.03890.00210.2817 | H-1→L (14)H→L+1 (57)H→L+3 (38)H-1→L (67)H-1→L+2 (14)H→L+1 (53)H→L (64)H→L+2 (27) |
| MHTT+AC | S0→S1S0→S2S0→S3 | 4.31094.64954.8661 | 287.60266.66254.79 | 0.00390.00030.0018 | H→L (71)H-2→L (66)H-1→L (22)H-2→L (22)H→L (64)H→L+1 (19) |
| MHTT+DO | S0→S1S0→S2S0→S3 | 4.77944.89614.9169 | 259.42253.23252.16 | 0.01980.20580.0000 | H→L (64)H→L+3 (29)H→L+1 (68)H→L+2 (14)H-1→L+1 (58)H-1→L+2 (38) |
| MHTT+DMF | S0→S1S0→S2S0→S3 | 4.96895.04025.0893 | 249.52245.99243.62 | 0.04100.00040.2979 | H→L +1 (60)H→L+2 (16)H→L+3 (13)H→L+4 (28)H-1→L (67)H-1→L+2 (17)H→L (63)H→L+2 (14)H→L+3 (25) |