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 **Title:** A DFT and TD-DFT Study on Emodin and Purpurin and their Functionalized Molecules to Produce Promising Organic Semiconductor Materials

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|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Emodin | Molecule 1 | Molecule 2 | Molecule 3 | Molecule 4 | Molecule 5 |
| Bond length (˚A) |  |  |  |  |  |
| *C*1-*C*2 | 1.404 | 1.406 | 1.416 | 1.400 | 1.399 |
| *C*2-*C*3 | 1.393 | 1.392 | 1.403 | 1.386 | 1.391 |
| *C*3-*C*4 | 1.399 | 1.400 | 1.393 | 1.396 | 1.400 |
| *C*4-*C*5 | 1.410 | 1.409 | 1.409 | 1.409 | 1.408 |
| *C*5-*C*6 | 1.397 | 1.398 | 1.396 | 1.398 | 1.398 |
| *C*6-*C*1 | 1.401 | 1.399 | 1.399 | 1.399 | 1.392 |
| *C*4-*C*7 | 1.483 | 1.483 | 1.487 | 1.485 | 1.485 |
| *C*7-*C*8 | 1.457 | 1.457 | 1.455 | 1.455 | 1.455 |
| *C*8-*C*9 | 1.420 | 1.419 | 1.421 | 1.420 | 1.420 |
| *C*9-*C*10 | 1.497 | 1.497 | 1.495 | 1.498 | 1.496 |
| *C*8-*C*11 | 1.421 | 1.421 | 1.422 | 1.421 | 1.421 |
| *C*11-*C*12 | 1.402 | 1.402 | 1.402 | 1.402 | 1.402 |
| *C*12-*C*13 | 1.392 | 1.392 | 1.392 | 1.392 | 1.392 |
| *C*13-*C*14 | 1.407 | 1.407 | 1.408 | 1.407 | 1.407 |
| *C*9-*C*14 | 1.385 | 1.385 | 1.384 | 1.384 | 1.384 |
| *C*7-*O*20 | 1.250 | 1.251 | 1.249 | 1.249 | 1.250 |
| *C*10-*O*21 | 1.226 | 1.226 | 1.225 | 1.227 | 1.225 |
| Bond Angle (*◦*) |  |  |  |  |  |
| *C*1*C*2*C*3 | 121.2 | 121.2 | 121.1 | 123.7 | 119.2 |
| *C*2*C*3*C*4 | 120.2 | 120.2 | 120.2 | 118.7 | 120.5 |
| *C*3*C*4*C*5 | 119.2 | 119.2 | 119.3 | 119.6 | 119.5 |
| *C*4*C*5*C*6 | 119.8 | 119.8 | 119.9 | 119.6 | 120.1 |
| *C*5*C*6*C*1 | 121.2 | 121.2 | 121.8 | 122.0 | 119.2 |
| *C*6*C*1*C*2 | 118.1 | 118.1 | 117.5 | 116.2 | 121.3 |
| *C*5*C*4*C*7 | 121.0 | 120.9 | 121.1 | 121.0 | 120.9 |
| *C*4*C*7*C*8 | 118.4 | 118.5 | 118.3 | 118.3 | 118.4 |
| *C*7*C*8*C*9 | 121.6 | 121.6 | 121.8 | 121.7 | 121.7 |
| *C*8*C*9*C*10 | 120.3 | 120.3 | 120.4 | 120.4 | 120.3 |
| *C*9*C*10*C*5 | 117.4 | 117.5 | 117.4 | 117.4 | 117.4 |
| *C*10*C*5*C*4 | 120.9 | 120.9 | 120.9 | 121.0 | 121.0 |
| *C*9*C*8*C*11 | 118.4 | 118.4 | 118.4 | 118.4 | 118.4 |
| *C*8*C*11*C*12 | 120.1 | 120.1 | 120.1 | 120.1 | 120.1 |
| *C*11*C*12*C*13 | 119.8 | 119.8 | 119.8 | 119.7 | 119.8 |
| *C*12*C*13*C*14 | 121.0 | 121.0 | 121.0 | 121.0 | 121.0 |
| *C*13*C*14*C*9 | 119.2 | 119.2 | 119.2 | 119.2 | 119.2 |
| *C*14*C*9*C*8 | 121.2 | 121.1 | 121.2 | 121.1 | 121.2 |

Table 1: Some of the bond lengths (˚A) and bond angle (*◦*) of emodin and its functionalized derivatives calculated at the B3LYP/6-31++G(d,p), for the structures and atom numbering, see Fig 1.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Purpurin | Molecule 1 | Molecule 2 | Molecule 3 | Molecule 4 | Molecule 5 | Molecule 6 |
| Bond length (˚A) |  |  |  |  |  |  |
| *C*1 *− C*2*C*2 *− C*4 | 1.4011.393 | 1.3981.388 | 1.4101.400 | 1.4011.391 | 1.4091.393 | 1.4011.383 |
| *C*4 *− C*12 | 1.400 | 1.398 | 1.397 | 1.398 | 1.396 | 1.400 |
| *C*12 *− C*11 | 1.407 | 1.405 | 1.405 | 1.406 | 1.405 | 1.406 |
| *C*11 *− C*3 | 1.403 | 1.403 | 1.403 | 1.403 | 1.399 | 1.404 |
| *C*12 *− C*6 | 1.503 | 1.506 | 1.506 | 1.505 | 1.503 | 1.503 |
| *C*6 *− C*14 | 1.479 | 1.476 | 1.476 | 1.477 | 1.477 | 1.477 |
| *C*14 *− C*13 | 1.433 | 1.435 | 1.434 | 1.434 | 1.434 | 1.434 |
| *C*13 *− C*5 | 1.467 | 1.465 | 1.466 | 1.469 | 1.468 | 1.468 |
| *C*5 *− C*11 | 1.474 | 1.480 | 1.478 | 1.472 | 1.475 | 1.474 |
| *C*14 *− C*10 | 1.408 | 1.408 | 1.408 | 1.408 | 1.408 | 1.408 |
| *C*10 *− C*9 | 1.409 | 1.410 | 1.410 | 1.409 | 1.410 | 1.410 |
| *C*9 *− C*8 | 1.381 | 1.381 | 1.381 | 1.381 | 1.381 | 1.381 |
| *C*8 *− C*7 | 1.416 | 1.417 | 1.417 | 1.416 | 1.417 | 1.417 |
| *C*7 *− C*13 | 1.400 | 1.401 | 1.401 | 1.400 | 1.400 | 1.400 |
| *C*6 *− O*15 | 1.228 | 1.227 | 1.227 | 1.227 | 1.227 | 1.228 |
| *C*5 *− O*16 | 1.251 | 1.249 | 1.249 | 1.251 | 1.249 | 1.250 |
| Bond Angle (*◦*) |  |  |  |  |  |  |
| *C*1*C*2*C*4 | 120.3 | 122.6 | 120.3 | 121.5 | 120.0 | 120.9 |
| *C*2*C*4*C*12 | 120.2 | 118.7 | 119.9 | 119.3 | 120.5 | 119.3 |
| *C*4*C*12*C*11 | 119.3 | 119.5 | 119.5 | 119.8 | 119.3 | 119.6 |
| *C*12*C*11*C*3 | 120.2 | 120.5 | 120.3 | 119.9 | 120.2 | 120.5 |
| *C*11*C*3*C*1 | 119.9 | 120.1 | 120.1 | 120.3 | 120.1 | 118.9 |
| *C*3*C*1*C*2 | 119.9 | 118.4 | 119.6 | 119.0 | 119.6 | 120.5 |
| *C*12*C*6*C*14 | 117.4 | 117.2 | 117.2 | 117.2 | 117.1 | 117.2 |
| *C*11*C*12*C*6 | 122.0 | 122.2 | 122.1 | 122.1 | 122.2 | 122.2 |
| *C*6*C*14*C*13 | 119.9 | 120.0 | 120.0 | 119.9 | 120.0 | 119.9 |
| *C*14*C*13*C*5 | 121.7 | 121.8 | 121.8 | 121.7 | 121.8 | 121.8 |
| *C*13*C*5*C*11 | 118.7 | 118.7 | 118.7 | 118.7 | 118.5 | 118.6 |
| *C*5*C*11*C*12 | 120.0 | 119.9 | 119.9 | 120.1 | 120.1 | 120.1 |
| *C*13*C*14*C*10 | 117.9 | 117.9 | 117.9 | 117.9 | 117.9 | 117.9 |
| *C*14*C*10*C*9 | 120.6 | 120.6 | 120.6 | 120.6 | 120.6 | 120.6 |
| *C*10*C*9*C*8 | 120.9 | 121.0 | 121.0 | 120.9 | 120.9 | 120.9 |
| *C*9*C*8*C*7 | 119.8 | 119.7 | 119.7 | 119.8 | 119.8 | 119.8 |
| *C*8*C*7*C*13 | 119.8 | 119.7 | 119.8 | 119.8 | 119.7 | 119.7 |
| *C*7*C*13*C*14 | 120.8 | 120.8 | 120.7 | 120.7 | 120.7 | 120.7 |

Table 2: Some of the bond lengths (˚A)and bond angle (*◦*) of purpurin and their functionalized derivatives calculated at the B3LYP/6-31++G(d,p), for the structures and atom numbering, see Fig 1.