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| Table 7. | | | | | | |
| NBO analysis of HLT based on B3LYP/6–311++G(d,p) | | | | | | |
| BOND (A–B) | ED / Energy | EDA(%) | EDB(%) | NBO | S (%) | P (%) |
| BD (1) C1 – C2 | 1.98628 | 47.01 | 52.99 | 0.6856 (sp1.72)C1 | 36.70 | 63.3 |
|  |  |  |  | 0.7280(sp2.83)C2 | 26.13 | 73.87 |
| BD (1) C1 – O5 | 1.99234 | 31.15 | 68.85 | 0.5581(sp2.51)C1 | 28.5 | 71.5 |
|  |  |  |  | 0.8219(sp2.69)O5 | 27.07 | 72.93 |
| BD (2) C1 – O6 | 1.98849 | 32.44 | 67.56 | 0.5696(sp20.79)C1 | 4.59 | 95.41 |
|  |  |  |  | 0.8219(sp33.09)O6 | 2.93 | 97.07 |
| BD (1) C1 – C3 | 1.96895 | 49.81 | 50.19 | 0.7058(sp2.78)C1 | 26.48 | 73.52 |
|  |  |  |  | 0.7084(sp2.89)C3 | 25.72 | 74.28 |
| BD (1) C2 – O7 | 1.99189 | 34.52 | 65.48 | 0.5876(sp3.98)C2 | 20.09 | 79.91 |
|  |  |  |  | 0.8092(sp2.94)O7 | 25.35 | 74.65 |
| BD (1) C2 – H11 | 1.97371 | 63.41 | 36.59 | 0.7963(sp2.66)C2 | 27.32 | 72.68 |
|  |  |  |  | 0.6049(sp100)H11 | 100 | 0 |
| BD (1) C3 – C4 | 1.97901 | 49.84 | 50.16 | 0.7060(sp2.85)C3 | 25.94 | 74.06 |
|  |  |  |  | 0.7083(sp1.48)C4 | 40.32 | 59.68 |
| BD (1) C3 – O8 | 1.98063 | 35.27 | 64.73 | 0.5939(sp4.11)C3 | 19.59 | 80.41 |
|  |  |  |  | 0.8045(sp2.2)O8 | 23.48 | 76.52 |
| BD (1) C3 – H12 | 1.9789 | 64.92 | 35.08 | 0.8057(sp2.48)C3 | 28.73 | 71.27 |
|  |  |  |  | 0.5923(sp100)H12 | 100 | 0 |
| BD (1) C4 – O9 | 1.99527 | 31.56 | 68.44 | 0.5617(sp2.69)C4 | 27.14 | 72.86 |
|  |  |  |  | 0.8273(sp2.01)O9 | 33.22 | 66.78 |
| BD (1) C4 – O10 | 1.99729 | 33.93 | 66.07 | 0.5825(sp2.09)C4 | 32.38 | 67.62 |
|  |  |  |  | 0.8129(sp1.58)O10 | 38.75 | 61.25 |
| BD (2) C4 – O10 | 1.9906 | 29.35 | 70.65 | 0.5417(sp99.99)C4 | 0.13 | 99.87 |
|  |  |  |  | 0.8405(sp99.99)O10 | 0.06 | 99.94 |
| BD (1) O9 – H15 | 1.98845 | 76.05 | 23.95 | 0.8721(sp4.00)O9 | 19.99 | 80.01 |
|  |  |  |  | 0.4894(sp100)H15 | 100 | 0 |
| BD (1) N16 – N17 | 1.99768 | 54.66 | 45.34 | 0.7393(sp3.67)N16 | 21.42 | 78.58 |
|  |  |  |  | 0.6734(sp4.38)N17 | 18.59 | 81.41 |
| BD (1) N16 – H20 | 1.988 | 86.00 | 14.00 | 0.9273(sp2.92)N16 | 25.53 | 74.47 |
|  |  |  |  | 0.3742(sp100)H20 | 100 | 0 |
| BD (1) N17 – H21 | 1.99272 | 71.87 | 28.13 | 0.9273(sp2.92)N17 | 29.94 | 70.06 |
|  |  |  |  | 0.5304(sp100)H21 | 100 | 0 |
| BD\*(1) C1 – C2 | 0.09421 | 52.99 | 47.01 | 0.7280(sp1.72)C1 | 36.7 | 63.3 |
|  |  |  |  | –0.6856(sp2.83)C2 | 26.13 | 73.87 |
| BD\*(1) C1 – O5 | 0.14019 | 68.85 | 31.15 | 0.8297(sp2.33)C1 | 30.04 | 69.96 |
|  |  |  |  | –0.5581(sp2.69)O5 | 27.07 | 72.93 |
| BD\*(1) C1 – O6 | 0.03923 | 62.56 | 34.44 | 0.8097(sp2.33)C1 | 30.04 | 69.96 |
|  |  |  |  | –0.5868(sp1.76)O6 | 36.22 | 63.78 |
| BD\*(1) C2 – C3 | 0.05425 | 50.19 | 49.81 | 0.7084(sp2.78)C1 | 26.48 | 73.52 |
|  |  |  |  | –0.7058(sp2.89)C3 | 25.72 | 74.28 |
| BD\*(1) C2 – H11 | 0.02517 | 36.59 | 63.41 | 0.6049(sp2.66)C2 | 27.32 | 72.68 |
|  |  |  |  | –0.7963(sp100)H11 | 100 | 0 |
| BD\*(1) C3 – C4 | 0.06833 | 50.16 | 49.84 | 0.7083(sp2.85)C3 | 25.94 | 74.06 |
|  |  |  |  | –0.7060(sp1.48)C4 | 40.32 | 59.68 |
| BD\*(1) C3 – O8 | 0.01963 | 64.73 | 35.27 | 0.8045(sp4.11)C3 | 19.59 | 80.41 |
|  |  |  |  | –0.5939(sp3.26)O8 | 23.48 | 76.52 |
| BD\*(1) C3 – H12 | 0.02621 | 35.08 | 64.92 | 0.5923(sp2.48)C3 | 28.73 | 71.27 |
|  |  |  |  | –0.8057(sp100)H12 | 100 | 0 |
| BD\*(1) C4 – O9 | 0.098 | 68.44 | 31.56 | 0.8273(sp2.69)C4 | 27.14 | 72.86 |
|  |  |  |  | –0.5617(sp2.01)O9 | 33.22 | 66.78 |
| BD\*(1) C4 – O10 | 0.02624 | 66.07 | 33.93 | 0.8129(sp2.09)C4 | 32.38 | 67.62 |
|  |  |  |  | –0.5825(sp1.58)O10 | 38.75 | 61.25 |
| BD\*(2) C4 – O10 | 0.24782 | 70.65 | 29.35 | 0.8405(sp99.99)C4 | 0.13 | 99.87 |
|  |  |  |  | –0.5417(sp99.99)O10 | 0.06 | 99.94 |
| BD\*(1) O9 – H15 | 0.01604 | 23.95 | 76.05 | 0.4894(sp4.00)O9 | 19.99 | 80.01 |
|  |  |  |  | –0.8721(sp100)H15 | 100 | 0 |
| BD\*(1) N16 – N17 | 0.00302 | 45.34 | 54.66 | 0.6734(sp3.67)N16 | 21.42 | 78.58 |
|  |  |  |  | –0.7393(sp4.30)N17 | 18.59 | 81.41 |
| BD\*(1) N16 – H20 | 0.25266 | 14.00 | 86.00 | 0.3742(sp2.92)N16 | 25.53 | 74.47 |
|  |  |  |  | –0.9273(sp100)H20 | 100 | 0 |
| BD\*(1) N17 – H21 | 0.03908 | 28.13 | 71.87 | 0.5304(sp2.34)N17 | 29.94 | 70.06 |
|  |  |  |  | –0.8477(sp100)H21 | 100 | 0 |