Table ( ): Results of statistical treatment of 13C – Chemical shift with σp, σpo, σp+, σp+/ σp,σp+/ σp-,σp+/ σp/ σp-substituent constants using single parameter equation

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | Carbons | Scale | ρ | r | s | F | log δo | n |
| 1 | C4 | σP | 0.04±0.006 | 0.949 | 0.006 | 43.33 | 2.11±0.002 | 7 |
|  | σOP | 0.038±0.01 | 0.882 | 0.008 | 13.99 | 2.11±0.004 | 6 |
|  | σ+P | 0.0320.002 | 0.986 | 0.003 | 179.37 | 2.12±0.001 | 7 |
|  | σ+P/ σP | 0.03±0.006 | 0.924 | 0.007 | 29.11 | 2.12±0.003 | 7 |
|  | σ+P/ σ-P | 0.024±0.002 | 0.989 | 0.003 | 226.34 | 2.12±0.001 | 7 |
|  | σ+P/ σP/ σ-P | 0.026±0.004 | 0.938 | 0.006 | 37.12 | 2.12±0.002 | 7 |
| 2 | C5 | σP | -0.01±0.001 | 0.984 | 0.001 | 152.18 | 2.19±0.0003 | 7 |
|  | σOP | -0.01±0.001 | 0.988 | 0.001 | 163.39 | 2.19±0.0003 | 6 |
|  | σ+P | -0.007±0.001 | 0.916 | 0.002 | 25.94 | 2.19±0.001 | 7 |
|  | σ+P/ σP | -0.008±0.002 | 0.887 | 0.002 | 18.40 | 2.19±0.001 | 7 |
|  | σ+P/ σ-P | -0.006±0.001 | 0.938 | 0.002 | 36.47 | 2.18±0.001 | 7 |
|  | σ+P/ σP/ σ-P | -0.006±0.001 | 0.917 | 0.002 | 26.68 | 2.19±0.001 | 7 |
| 3 | C6 | σP | 0.03±0.004 | 0.950 | 0.004 | 45.95 | 2.07±0.001 | 7 |
|  | σOP | 0.02±0.005 | 0.900 | 0.004 | 17.16 | 2.07±0.002 | 6 |
|  | σ+P | 0.018±0.001 | 0.995 | 0.001 | 508.52 | 2.08±0.0004 | 7 |
|  | σ+P/ σP | 0.02±0.004 | 0.917 | 0.005 | 26.46 | 2.07±0.002 | 7 |
|  | σ+P/ σ-P | 0.014±0.002 | 0.970 | 0.003 | 80.18 | 2.07±0.001 | 7 |
|  | σ+P/ σP/ σ-P | 0.015±0.003 | 0.902 | 0.005 | 21.75 | 2.07±0.002 | 7 |
| 4 | C7 | σP | -0.004±0.002 | 0.722 | 0.001 | 5.43 | 2.21±0.001 | 7 |
|  | σOP | -0.004±0.002 | 0.620 | 0.002 | 2.51 | 2.21±0.001 | 6 |
|  | σ+P | -0.003±0.0008 | 0.820 | 0.001 | 10.24 | 2.21±0.0004 | 7 |
|  | σ+P/ σP | -0.004±0.0007 | 0.917 | 0.001 | 26.41 | 2.21±0.003 | 7 |
|  | σ+P/ σ-P | -0.002±0.001 | 0.775 | 0.001 | 7.51 | 2.21±0.0005 | 7 |
|  | σ+P/ σP/ σ-P | -0.003±0.001 | 0.836 | 0.001 | 11.63 | 2.21±0.0005 | 7 |
| 5 | C11 | σP | -0.003±0.0003 | 0.979 | 0.0003 | 116.72 | 2.21±0.0001 | 7 |
|  | σOP | -0.003±0.0005 | 0.945 | 0.0004 | 33.30 | 2.21±0.0002 | 6 |
|  | σ+P | -0.002±0.0001 | 0.996 | 0.0001 | 640.41 | 2.21±0.0004 | 7 |
|  | σ+P/ σP | -0.002±0.0004 | 0.935 | 0.0005 | 34.80 | 2.21±0.002 | 7 |
|  | σ+P/ σ-P | -0.002±0.0001 | 0.983 | 0.0003 | 145.26 | 2.21±.0001 | 7 |
|  | σ+P/ σP/ σ-P | -0.002±0.0003 | 0.930 | 0.0005 | 32.23 | 2.21±0.0002 | 7 |
| 6 | C22’ | σo | 0.044±0.02 | 0.632 | 0.02 | 3.33 | 2.09±0.008 | 7 |
|  | σo\* | 0.038±0.02 | 0.691 | 0.02 | 3.66 | 2.09±0.01 | 6 |
|  | Es | -0.04±0.013 | 0.825 | 0.016 | 10.69 | 2.13±0.006 | 7 |