**APPENDIX – I**

13C SCS values for mono substituted benzenes1

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| S.No. | Substituents  X | Z1(Si) | Z2 (So) | Z3 (Sm) | Z4 (Sp) |
|  |  |  |  |  |  |
| 1 | -NMe2 | 22.0 | -16.0 | 0.3 | -12.0 |
|  |  |  |  |  |  |
| 2 | -OCH3 | 30.2 | -14.7 | 0.9 | -8.1 |
|  |  |  |  |  |  |
| 3 | -CH3 | 9.3 | 0.6 | 0 | -3.1 |
|  |  |  |  |  |  |
| 4 | -H | 0 | 0 | 0 | 0 |
|  |  |  |  |  |  |
| 5 | -F | 34.9 | -14.5 | 0.7 | -4.6 |
|  |  |  |  |  |  |
| 6 | -Cl | 6.4 | 0.2 | 1.0 | -2.0 |
|  |  |  |  |  |  |
| 7 | -Br | -5.4 | 3.3 | 2.2 | -1.0 |
|  |  |  |  |  |  |
| 8 | -NO2 | 19.6 | -5.3 | 0.8 | 6.0 |
|  |  |  |  |  |  |

**APPENDIX II**

Substituent constants used in LFER equations

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | Substittuents  X | σp2 | σpo3 | σp+ | σp- | σo 4 | σo\*4 | Es4 |
|  |  |  |  |  |  |  |  |  |
| 1. | -NMe2 | -0.83 | **--** | -1.7 | -- | -- | -- | -- |
|  |  |  |  |  |  |  |  |  |
| 2. | -OCH3 | -0.27 | -0.12 | -0.78 | -- | -0.39 | -0.22 | 0.99 |
|  |  |  |  |  |  |  |  |  |
| 3. | -OH | -0.37 | -- | -0.92 | -- | 0.04 | -- | 0.32 |
|  |  |  |  |  |  |  |  |  |
| 4. | -CH3 | -0.17 | -0.14 | -0.31 | -- | -0.17 | 0 | 0 |
|  |  |  |  |  |  |  |  |  |
| 5. | -H | 0 | 0 | 0 | -- | 0 | 0 | 0 |
|  |  |  |  |  |  |  |  |  |
| 6. | -Cl | 0.23 | 0.34 | 0.11 | -- | 0.2 | 0.37 | 0.18 |
|  |  |  |  |  |  |  |  |  |
| 7. | -Br | 0.23 | 0.22 | 0.15 | -- | 0.21 | 0.38 | 0 |
|  |  |  |  |  |  |  |  |  |
| 8. | -CHO | 0.42 | -- | 0.73 | 1.03 | -- | -- | -- |
|  |  |  |  |  |  |  |  |  |
| 9. | -COOH | 0.45 | 0.44 | 0.42 | 0.77 | -- | -- | -- |
|  |  |  |  |  |  |  |  |  |
| 10. | -NO2 | 0.75 | 0.81 | 0.79 | 1.27 | 0.8 | 0.97 | -0.75 |
|  |  |  |  |  |  |  |  |  |

**APPENDIX III**

Substituent constants used for dual-parameter correlations

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | Substituents  X | σI3 | σR3 | σRo | σR+ | σR- | F2 | R2 | ν5 |
|  |  |  |  |  |  |  |  |  |  |
| 1. | -NMe2 | 0.1 | -0.83 | -- | -1.7 | -0.34 | -- | -- | -- |
|  |  |  |  |  |  |  |  |  |  |
| 2. | -OCH3 | 0.26 | -0.61 | -0.41 | -1.02 | -0.45 | 0.29 | -0.56 | 0.36 |
|  |  |  |  |  |  |  |  |  |  |
| 3. | -OH | 0.27 | -0.43 | -- | -0.44 | -- | 0.33 | -0.7 | 0.32 |
|  |  |  |  |  |  |  |  |  |  |
| 4. | -CH3 | -0.05 | -0.11 | -0.1 | -1.25 | -0.11 | 0.01 | -0.18 | 0.52 |
|  |  |  |  |  |  |  |  |  |  |
| 5. | -H | 0 | 0 | 0 | 0 | 0 | 0.03 | 0 | 0 |
|  |  |  |  |  |  |  |  |  |  |
| 6. | -Cl | 0.47 | -0.23 | -0.21 | -0.23 | -0.35 | 0.42 | -0.19 | 0.55 |
|  |  |  |  |  |  |  |  |  |  |
| 7. | -Br | 0.45 | -0.19 | -0.61 | -0.19 | -0.3 | 0.45 | -0.22 | 0.65 |
|  |  |  |  |  |  |  |  |  |  |
| 8. | -COOH | 0.3 | -0.08 | -- | 0.43 | 0.06 | -- | -- | -- |
|  |  |  |  |  |  |  |  |  |  |
| 9. | -NO2 | 0.64 | 0.15 | 0.19 | 0.15 | 0.46 | 0.65 | 0.13 | 1.39 |
|  |  |  |  |  |  |  |  |  |  |

References

1. D.H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 4th edn., Tata McGraw-Hill, 1988.
2. C.Hansch, A. Leo, R.W. Taft, *Chem. Rev*., **91**, 165, (1991).
3. S. Ehrenson, R.T.C. Brownlee and R.W. Taft. *Prog. Phys. Org. Chem*., **10**,1, (1973).
4. J. Shorter, ‘*Correlation Analysis in Organic Chemistry, an introduction to linear free energy relationship’*, Clenden Press, London, 1973.
5. M.Charton, *Prog.Phys. Org. Chem*., 13, 1981