Table ( ) : Results of Lynch correlationsa of 1H chemical shifts of compound fig ( ) with SCS

values for mono substituted benzenes.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | Carbons | Benzene  SCS  (Sb) | Slope | Intercept | rc | nd | Se |
| 1. | H22’ | So | 0.001 | 0.88 | 0.304 | 6 | 0.02 |
|  |  |  |  |  |  |  |  |
| 2. | H33’ | Sm | -0.002 | 0.91 | 0.223 | 6 | 0.008 |
|  |  |  |  |  |  |  |  |
| 3. | H5 | Sp | 0.0002 | 0.92 | 0.689 | 6 | 0.001 |
|  |  |  |  |  |  |  |  |
| 4. | H8 | Sp | 0.0004 | 1.05 | 0.917 | 6 | 0.001 |
|  |  |  |  |  |  |  |  |
| 5. | H10 | Sp | 0.0005 | 1.06 | 0.955 | 6 | 0.001 |

1. SCSX (Y) = a + b SCSX (H)
2. SCS values in Appendix (I)
3. Correlation coefficient
4. Number of data points
5. Standard deviations

**APPENDIX – I**

**Table (10): 13C SCS values for mono substituted benzenes**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| S.No. | Substituents | Z1(Si) | Z2 (So) | Z3 (Sm) | Z4 (Sp) |
|  |  |  |  |  |  |
| 1 | -OME | 30.2 | -14.7 | 0.9 | -8.1 |
|  |  |  |  |  |  |
| 2 | -ME | 9.3 | 0.6 | 0 | -3.1 |
|  |  |  |  |  |  |
| 3 | -H | 0 | 0 | 0 | 0 |
|  |  |  |  |  |  |
| 4 | -Cl | 6.4 | 0.2 | 1 | -2 |
|  |  |  |  |  |  |
| 5 | -Br | -5.4 | 3.3 | 2.2 | -1 |
|  |  |  |  |  |  |
| 6 | -NO2 | 19.6 | -5.3 | 0.8 | 6 |
|  |  |  |  |  |  |