Supplementary material for:

Excited state dipole moment of two pyridazinium-p-nitro-phenacylids estimated from solvatochromic study

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Table 1S. Angles between bonds and dihedral angles for pyridazinium-p-nitro-phenacylid molecule

|  |  |
| --- | --- |
| angles/dihedral angles | degrees |
| (C10, C12, C13) | 119.86 |
| (C13, N15, O17) | 119.39 |
| (O17, N15, O16) | 121.19 |
| (C4, N6, C7,C8) | 0.16 |
| (N5, N6, C7, H23) | -1.38 |
| (N6, C7, C8, O18) | 1.88 |
| (H23, C7, C8, O18) | 175.87 |
| (C7, C8, C9, C10) | -162.75 |
| (C7, C8, C9, C11) | 18.64 |
| (C14, C13, N15, O16) | -0.06 |

Table 2S. Angles between bonds and dihedral angles for p-phenyl-p’-phenyl-pyridazinium-p-nitro-phenacylid molecule.

|  |  |
| --- | --- |
| angles/dihedral angles | degrees |
| (C24, C26, C27) | 118.62 |
| (C27, N28, O30) | 118.81 |
| (O29, N28, O30) | 121.50 |
| (C6, C4, C7, C8) | 34.94 |
| (C10, C13, N17, N18) | -23.16 |
| (N17, N18, C19, H43) | -1.33 |
| (N17, N18, C19, C20) | 1.38 |
| (O21, C20, C22, C24) | 16.55 |
| (O21, C20, C22, C23) | -162.10 |
| (C26, C27, N28, O30) | -0.20 |
| (H43, C19, C20, O21) | 7.11 |

Table 3S. Regression parameters in relation (1) for pyridazinium-p-nitro-phenacylid (P1) and p-phenyl-p’-phenyl-pyridazinium-p-nitro-phenacylid (P2) molecules.

|  |  |  |  |
| --- | --- | --- | --- |
|  | | | |
| P1 | | P2 | |
| (cm-1) | 19969.68 ± 245.12 | (cm-1) | 19812.32 ± 260.33 |
| *C*1 ± Δ*C*1 | 1390.61 ± 287.31 | *C*1 | 1473.95 ± 306.92 |
| *C*2 ± Δ*C*2 | - 1035.29 ± 382.53 | *C*2 | -1313.00 ± 395.02 |
| *C*3 ± Δ*C*3 | - 308.91 ± 88.23 | *C*3 | -293.67 ± 90.76 |
| *C*4 ± Δ*C*4 | 773.42 ± 136.3 | *C*4 | 761.34 ± 145.6 |
| Adj. R-Square | 0.91 | Adj. R-Square | 0.90 |