Supplementary material for:

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

Liliana Mihaela IVAN1, Dan Gheorghe DIMITRIU1\*, Antonina GRITCO-TODIRASCU1, Ana Cezarina MOROSANU1, Dana Ortansa DOROHOI1 and Corina CHEPTEA2

1Faculty of Physics, Alexandru Ioan Cuza University, Iasi, Romania

2Faculty of Medical Bioengineering, “Grigore T. Popa” University of Medicine and Pharmacy, Iasi, Romania

\*corresponding author: *Faculty of Physics, Alexandru Ioan Cuza University, 11 Carol I Blvd., RO-700506 Iasi, Romania,* dimitriu@uaic.ro

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.

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| --- |
|  |
|  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 |