

Influence of Surface-Attachment Functionality on the Aggregation, Persistence, and Electron-Transfer Reactivity of Chalcogenorhodamine Dyes on TiO_2

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The sweep width used to acquire the ^{31}P NMR spectra in the published article was too narrow to capture the ^{31}P chemical shift for the hexafluorophosphate anion at -146 ppm. The reported values for the hexafluorophosphate anion are “fold-over” values. The ^{31}P NMR spectra were reacquired at 121.5 MHz and 298.1 K with a sweep width of 48 544 Hz, a relaxation delay of 1.000 s, a 45° pulse, line broadening of 0.5 Hz, and proton decoupling at 300 MHz. Phosphoric acid ($\delta = 0.0$) was used as an internal standard.

For 3,6-Bis(dimethylamino)-9-(5-phosphonothien-2-yl)selenoxanthylum hexafluorophosphate (3-Se): ^{31}P NMR (121.5 MHz, $(\text{CD}_3)_2\text{NC}(\text{O})\text{D}$): δ 5.4 (s), -146 (septet, $J = 717$ Hz).

For 3,6-Bis(dimethylamino)-9-(5-phosphonothien-2-yl)xanthylum hexafluorophosphate (3-O): ^{31}P NMR (121.5 MHz, 1:1 $\text{CD}_3\text{OD}/(\text{CD}_3)_2\text{NC}(\text{O})\text{D}$): δ 11.9 (s), -146 (septet, $J = 717$ Hz).

For 3,6-Bis(dimethylamino)-9-(4-phosphonophenyl)selenoxanthylum hexafluorophosphate (4-Se): ^{31}P NMR (121.5 MHz, $(\text{CD}_3)_2\text{NC}(\text{O})\text{D}$): δ 10.7 (s), -146 (septet, $J = 715$ Hz).

For 3,6-Bis(dimethylamino)-9-(4-phosphonophenyl)xanthylum hexafluorophosphate (4-O): ^{31}P NMR (121.5 MHz, $(\text{CD}_3)_2\text{NC}(\text{O})\text{D}$): δ 11.2 (s), -146 (septet, $J = 715$ Hz).