# Template for inter-document cross-referencing: Another part (supporting information)

Andriy Zhugayevych
a.zhugayevych@skoltech.ru

January 29, 2015

## S1 Experimental IP and EA for functional groups

| Group | Name | IP | EA |
|---|---|---|---|
| $NH_2$ | amino | 10.8 | 0.8 |
| $CH_3$ | methyl | 9.8 | 0.1 |
| $OCH_3$ | methoxy | 10.7 | 1.6 |
| $C_2H_3$ | vinyl | 8.3 | 0.7 |
| $C_6H_5$ | phenyl | 8.3 | 1.1 |
| H | hydrogen | 13.6 | 0.8 |

Table S1: Experimental IP and EA (in eV) for the selected functional groups. See Eq. (1) and Eq. (2).

## S2 Single quantum mode fit to transition spectral density


Figure S1: Experimental transition spectral density (amplitude normalized to 1) for emission (left black curve) and absorption (right black curve) of H-OPV3 in chloroform solution. Red curves are the single quantum mode fits.

For a given electronic transition, the transition spectral density (vibrational) is given by

$$f(E) = \sum_{nn'} \rho_n \langle n|n'\rangle^2 \delta(E - E_{nn'}), \tag{S1}$$

## S3 Experimental data

| Group | Solvent | $\lambda_{\max}$(nm) | $E_{\text{vert}}$(eV) | $\sigma_E$(eV) | $\hbar\omega_{\text{Q}}$(eV) | $S_{\text{Q}}$ |
|---|---|---|---|---|---|---|
| Absorption: Dependence on solvent | | | | | | |
| $NO_2$ | thf | 422.4(1) | 2.947(5) | 0.240(3) | 0.20 | 0.9 |
| $NO_2$ | tol | 423.9(4) | 2.944(3) | 0.223(1) | 0.17 | 1.4 |
| $NO_2$ | clf | 426.7(1) | 2.915(4) | 0.240(1) | 0.19 | 1.0 |
| $NO_2$ | clb | 429.4(1) | 2.901(8) | 0.230(4) | 0.18 | 1.1 |
| $NO_2$ | dmso | 430.2(1) | 2.884(2) | 0.254(1) | 0.21 | 0.9 |
| Absorption: Dependence on functional group | | | | | | |
| H | clf | 388.4(2) | 3.217(3) | 0.218(3) | 0.20 | 0.7 |
| $CH_3$ | clf | 389.4(2) | 3.209(3) | 0.216(2) | 0.19 | 0.8 |
| Br | clf | 392.0(2) | 3.187(3) | 0.218(4) | 0.20 | 0.8 |
| $NH_2$ | clf | 396.9(1) | 3.147(6) | 0.223(3) | 0.20 | 0.8 |
| COOH | clf | 400.4(2) | 3.119(4) | 0.225(6) | 0.20 | 0.7 |
| $NO_2$ | clf | 426.7(1) | 2.915(4) | 0.240(1) | 0.19 | 1.0 |
| Emission: Dependence on functional group | | | | | | |
| H | clf | 441.8(4) | 2.646(6) | 0.181(2) | 0.16 | 1.0 |
| $CH_3$ | clf | 442.2(4) | 2.641(10) | 0.182(13) | 0.17 | 1.0 |
| Br | clf | 445.6(11) | 2.608(6) | 0.191(0) | 0.17 | 1.0 |
| $NH_2$ | clf | 473.9(7) | 2.487(2) | 0.199(4) | 0.15 | 1.3 |
| COOH | clf | 474.9(16) | 2.474(2) | 0.193(1) | 0.16 | 1.2 |
| $NO_2$ | clf | 481.9(11) | 2.453(2) | 0.192(3) | 0.15 | 1.3 |

Table S2: Processed experimental UV-Vis absorption and fluorescence data. Here $\lambda_{\max}$ is the absorption/emission peak in the original wavelength scale estimated by a fourth-order polynomial fit to the raw data; $E_{\text{vert}}$, $\sigma_E$, $\hbar\omega_{\text{Q}}$, $S_{\text{Q}}$ are the vertical transition energy, spectral width, energy and Huang–Rhys factor of the quantum mode, all estimated by the single quantum mode fit, see Section S2. The last digit uncertainty is the superposition of the statistical fitting error and the change upon expanding or contracting the fitting range (red curve in Fig. S1) by about 30%. The uncertainties of $\hbar\omega_{\text{Q}}$ and $S_{\text{Q}}$ are comparable to the spread of their values across the table. The measurements are made in chloroform with the solute concentration $10^{-4}$ M for absorption and $10^{-6}$ M for emission. Abbreviations for solvents: clb=chlorobenzene, clf=chloroform, dmso=dimethylsulfoxide, thf=tetrahydrofuran, tol=toluene.

Skoltech
Skolkovo Institute of Science and Technology

Figure S2: Vertical excitation energy, see Table S2.