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Investigating the properties of PODIPY (Phosphorous-Dipyrromethene) with *ab initio tools*: ESI

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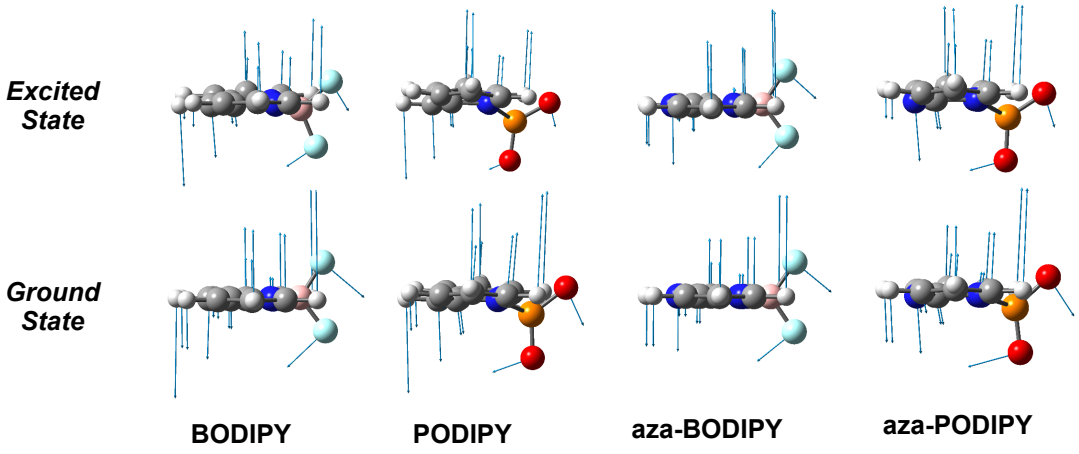

Fig. ESI-1 Representation of the displacements corresponding to the low-frequency vibronic modes (mostly) responsible for the broadening of the spectra.

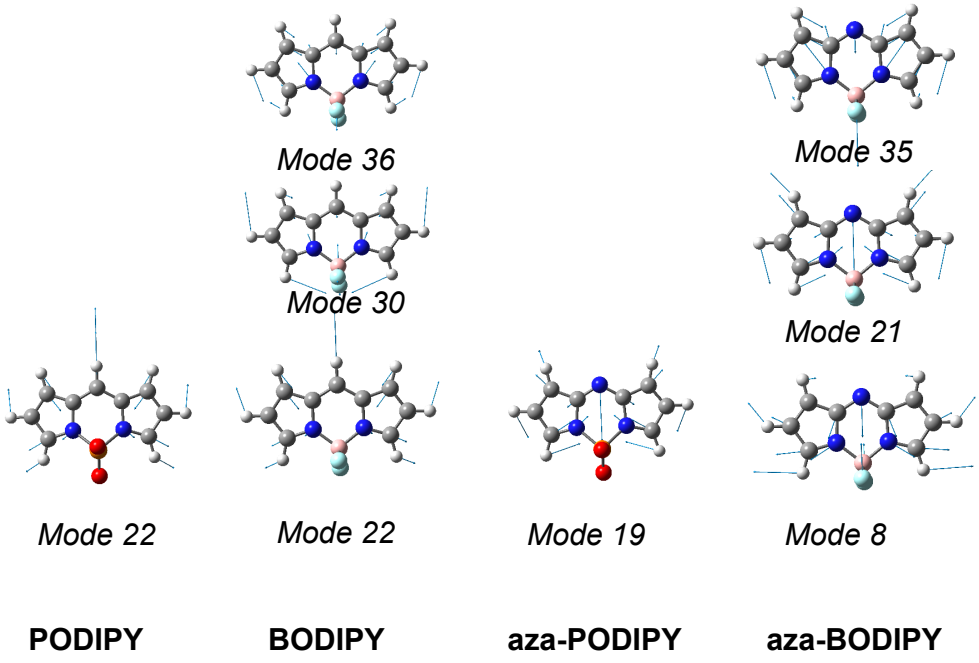

Fig. ESI-2 Representation of the displacements corresponding to the vibronic modes (mostly) responsible for the shoulder in the absorption spectrum. Note that they corresponds to vibration of the excited-state.

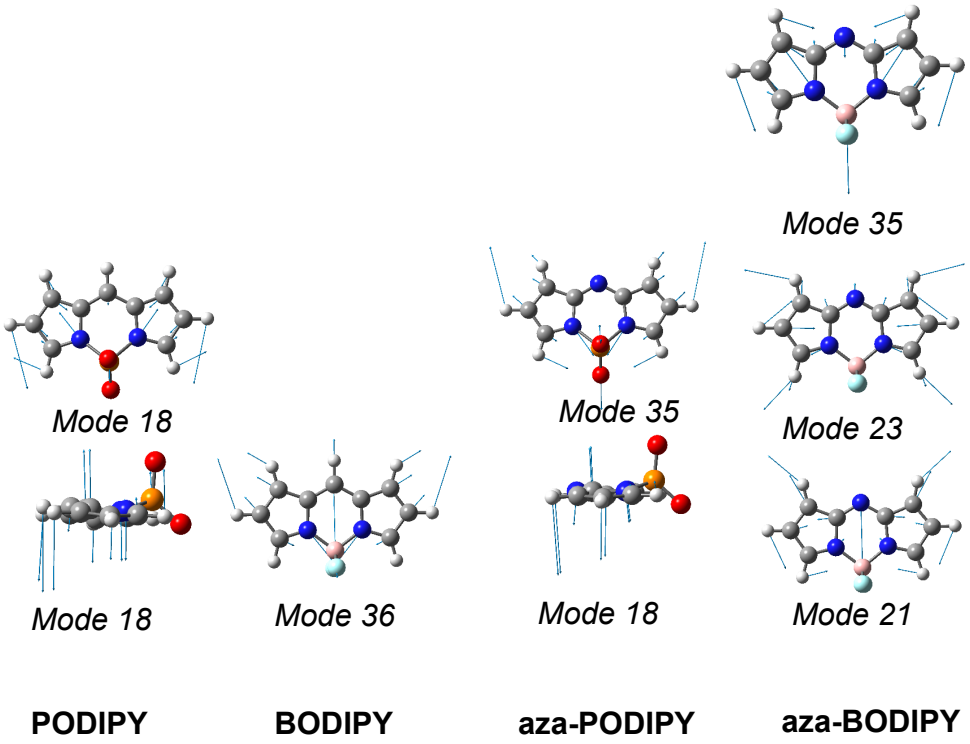

Fig. ESI-3 Representation of the displacements corresponding to the vibronic modes (mostly) responsible for the shoulder in the emission spectrum. Note that they corresponds to vibration of the ground-state.

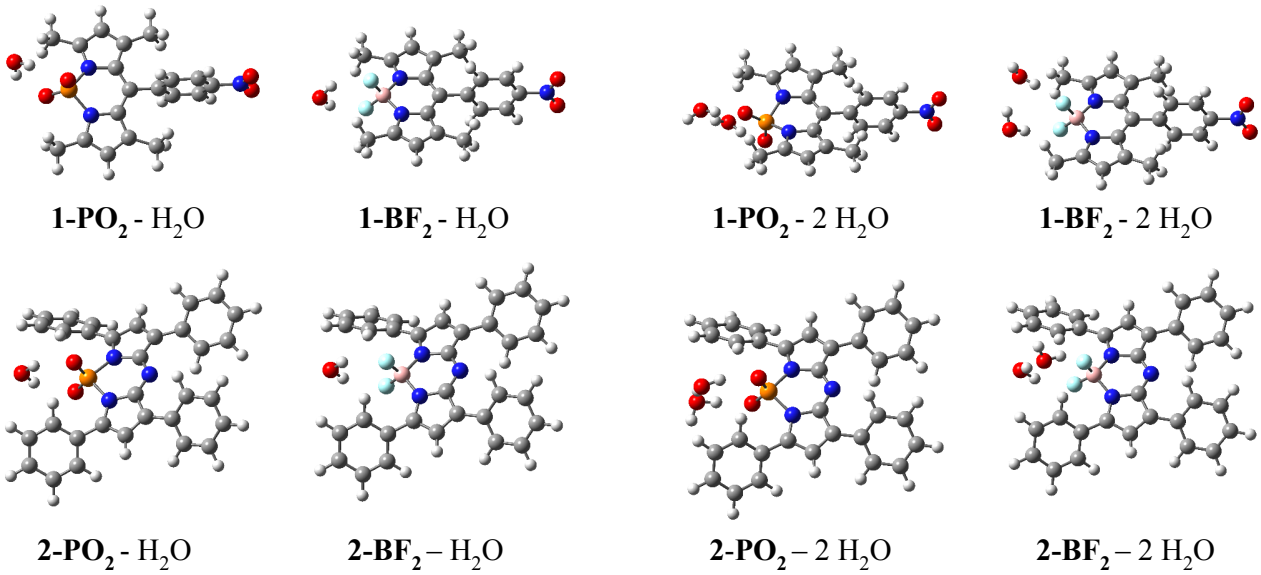

Fig. ESI-4 Equilibrium geometries for water complexes with **1-PO**$_2$, **1-BF**$_2$, **2-PO**$_2$ and **2-BF**$_2$. Structures with one and two water molecules are presented on the left-hand-side and right-hand-side of the figure, respectively.

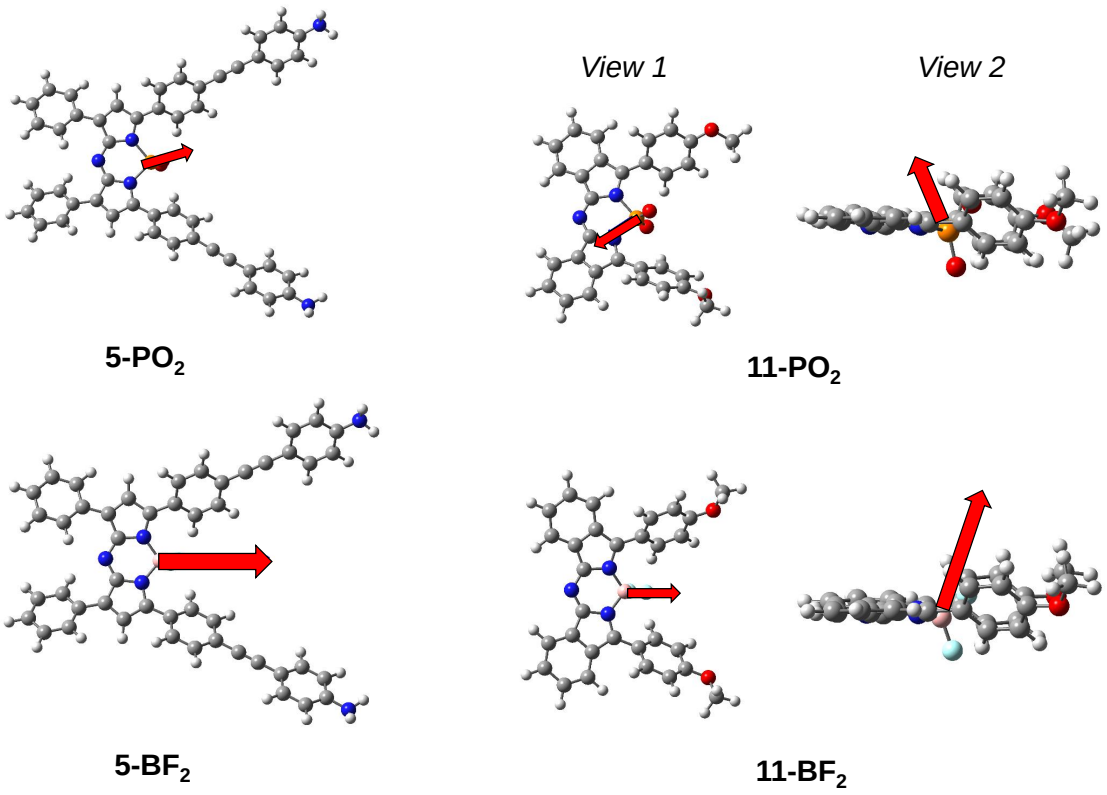

Fig. ESI-5 Ground state total dipole moments in **5** and **11**.