**DFT Computational Method**

The structure of the Betalain dye was generated using Avogadro [1] with a preliminary energy minimisation performed using the Universal Force Field. The dye was optimised in the ground state without any symmetry constraint in the gas phase based on DFT method with the B3LYP functional and the 6-311G(d) basis set for all atoms. Frequency calculation were performed at the same level of theory to confirm that all the optimised geometries were located at the minima point of the potential energy surface.

Ab initio computation was performed using the ORCA program package version 5.0.4 [2]. The RIJCOSX algorithm and the tight criterion of SCF convergence were used in the computations [3-4]. The processing of input and output files was carried out using Avogadro and visualisation was carried out using Chemcraft [5] after which the total energy was extracted.

**Reference**

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