Theoretical study of the photophysical processes of a three-input AND molecular logic gate with an enhanced fluorescent output

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The ability of molecules for processing information similar to electronic systems was first demonstrated in 1993 by de Silva [1] and eventually this idea opened up a rapidly growing multidisciplinary research area.[2] Molecular systems that exhibit sequential advanced logic functions such as those for construction of memory devices, delay & storage elements, and finite-state machines have great potential for applications,[3] while, their design is a significant challenge in the field of molecular information technology.[4] In order to be used as a molecular logic gate, a molecular system should meet the following demands: it should exist in several (at least two) thermally stable forms (states), which differ by properties and which can be converted from one to another by some external stimulus.[2-5]

Here, we study theoretically a three-input AND molecular logic gate (**1**) which present the largest fluorescence enhancement to date. **1** is devised in a modular format according to the principles of photoinduced electron transfer systems, Fig. 1. The molecule has been synthesized [6] and it has been proved experimentally that it detects three cations by three different titrimetric methods: H^+ by acid-base chemistry, Na^+ by complexation and Fe^{3+} by redox chemistry. The present study explains why **2** presents such a large fluorescence enhancement, while the remaining seven possible input conditions results in a quenching of the emission.

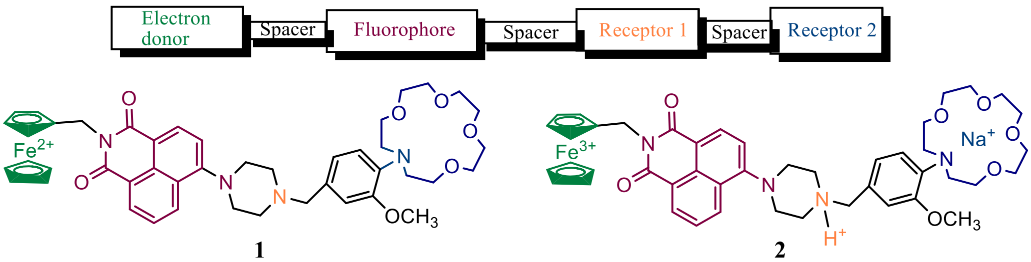

Fig.1

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