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Boolean and fuzzy logic implemented at the molecular level

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Abstract

In this work, it is shown how to implement both hard and soft computing by means of two structurally related heterocyclic compounds: flindersine (FL) and 6(5H)-phenanthridinone (PH). Since FL and PH have a carbonyl group in their molecular skeletons, they exhibit Proximity Effects in their photophysics. In other words, they have an emission power that can be modulated through external inputs such as temperature (T) and hydrogen-bonding donation (HBD) ability of solvents. This phenomenology can be exploited to implement both crisp and fuzzy logic. Fuzzy Logic Systems (FLSs) wherein the antecedents of the rules are connected through the AND operator, are built by both the Mamdani's and Sugeno's models. Finally, they are adopted as approximators of the proximity effect phenomenon and tested for their prediction capabilities. Moreover, FL as photochromic compound is also a multiply configurable crisp logic molecular element.

Keywords: Crisp logic; Fuzzy logic; Proximity effect; Mamdani's and Sugeno's methods; Photochromism

1. Introduction

We are living in societies whose economies are based on intangible assets such as knowledge and its transmission. Scientific community is contributing to the Intangible Economy [1] through the achievements of Information Technology. Information Technology deals with the design and construction of devices and machines able to process, store and convey information, always more effectively.

Computer constitutes an example of machine whereby data can be manipulated. There exists a worldwide race to make microprocessors of computers as much powerful as possible. Their performances can be improved through shrinking electronic components and cramming logic gates onto smaller and smaller wafers of silicon. Over the past few years, some companies [2] and several academic laboratories [3] have started seriously entertaining the idea of constructing computers in which computations are performed by individual molecules. If the logic gates, sculpted from bulk semiconductors, are based exclusively on electrical signals, those defined from single molecules can be extended to optical and chemical inputs and outputs. This means that Boolean binary logic can have not only electrical but also photo-chemical manifestations. Binary logic has the peculiarity of manipulating only precise, objective knowledge, i.e. statements that are true or false, reducible to strings of zeros and ones. However, it is not always possible to store accurate information, for instance when very complex phenomena are to be described. Quite often, the available data and knowledge suffer a certain degree of uncertainty and imprecision, especially when they are based on subjective linguistic statements. In all these cases, it is still possible to process information by abandoning hard computing, based on binary logic and crisp systems, and adopting soft computing, based on fuzzy logic, neural nets and probabilistic reasoning [4]. In the partnership of fuzzy logic, neurocomputing and probabilistic reasoning, fuzzy logic is mainly concerned with imprecision and approximate reasoning; neurocomputing with learning and curve-fitting and probabilistic reasoning with uncertainty and belief propagation. In coming years, soft

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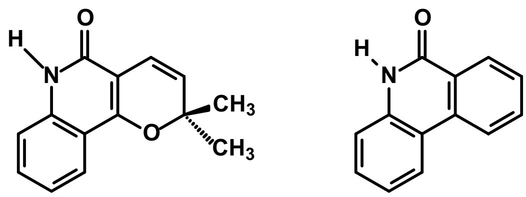
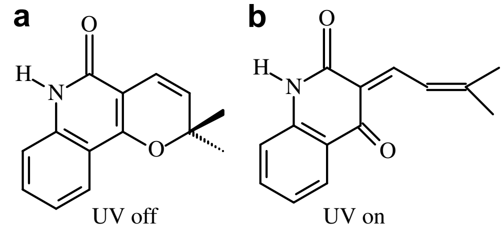


(I) Flindersine (FL) (II) 6(5H)-phenanthridinone (PH)

Scheme 1.



Scheme 2.

computing and particularly fuzzy logic are likely to play an increasingly important role in the conception and design of systems whose machine intelligence quotient is much higher than that of systems designed by conventional methods.

In this work, two fluorescent compounds, flindersine (FL) and 6(5H)-phenanthridinone (PH) (see Scheme 1 for their molecular structures) are proposed as elements whereby not only Boolean but also fuzzy logic can be implemented at the molecular level. This has been accomplished through the sensitivity of both compounds on physical and chemical inputs such as temperature and hydrogen-bonding power of the solvent [5]. Moreover, FL, as photochromic compound, is demonstrated to be an example of multiply configurable crisp logic element.

2. Materials and methods

To compute the prediction capabilities of the different Fuzzy Logic Systems, the Fuzzy Logic Toolbox for Use with MathLab [6] was employed. For the description of the materials and experimental methods adopted to determine the fluorescence quantum yields and the photochromic behaviour of FL, see Ref. [5].

3. Results and discussion

3.1. Crisp logic

In crisp Boolean logic, data processing requires the encoding of information in the form of binary digits [7]. For this purpose, it is necessary to establish a threshold value and a logic convention for each signal. The signals can be simply high or low: digital 1 or 0, respectively, in the positive logic convention, whereas the negative logic convention reverses this relationship.

3.1.1. Photochromism of FL

FL belongs to the compound family of chromenes. Chromenes are photochromic compounds [8]. As any photochrome, FL is a molecular switch [9,10]: in the dark, it exists in the closed uncoloured form (structure a of Scheme 2), whereas upon UV irradiation, it converts to the open coloured form (structure b) [11,5].

As with any switch [12], even with FL it is possible to perform Boolean logic operations. In particular, the dissimilar spectral changes induced at various wavelengths by the optical input, i.e. UV photons, (see Fig. 1) afford to define FL as a multiply configurable Boolean logic element [3a,13].

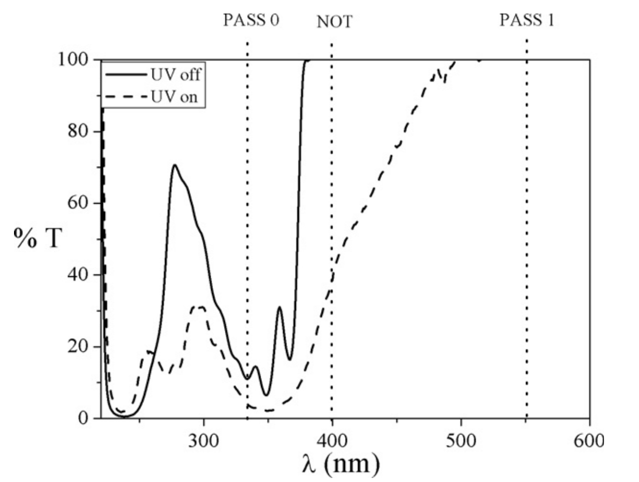


Fig. 1. Transmittance spectra of FL (1 cm optical path length and solute concentration 2×10^{-4} mol dm^{-3}) in 3MP before UV irradiation (solid line) and upon UV irradiation (dashed line); NOT, PASS 1 and PASS 0 logic gates are indicated at three different wavelengths.

NOT logic can be obtained by monitoring the transmittance (%T) at an appropriate wavelength, for instance at 400 nm: when UV is "off", %T is high (100%), but when UV is "on", %T becomes low (40%). Monitoring at wavelengths longer than 500 nm, the molecular system gives 100% transmittance irrespective of the optical input and thus corresponds to the PASS 1 logic element. Monitoring at wavelengths shorter than 370 nm, FL behaves as a PASS 0 logic gate since it exhibits low %T regardless of the input condition. The truth tables with operational parameters are shown in Table 1.

Table 1
Truth tables of the logic elements (NOT, PASS 0, PASS 1) defined for FL by adopting the transmittances (measured with 1 cm optical path length and a FL concentration of 2×10^{-4} mol dm^{-3}) at different wavelengths as optical outputs

Input	Output		
UV	%T (400 nm)	%T (550 nm)	%T (334 nm)
0	1 (high, 100)	1 (high, 100)	0 (low, 11)
1	0 (low, 38.6)	1 (high, 100)	0 (low, 4)
	NOT	PASS 1	PASS 0