Design Rules for Solid State Fluorescence Exploiting Excited State Intramolecular Proton Transfer

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Submitted in partial fulfillment of the requirements
of the Degree of Doctor of Philosophy

2018

Abstract

This is the abstract.

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List of Abbreviations

AIE   aggregation induced emission

HC   2'-hydroxychalcone

HP   2-hydroxyphenylpropenone

PES   potential energy surface

1 Connecting Chromophore Design with Crystal Morphorology

1.1 Introduction

In Chapters **??** and **??** the potential energy surfaces (PESs) of a range of 2'-hydroxychalcone (**HC**) derivatives were mapped, in both vacuum and the crystalline form. Through the topology of the PESs and the associated energy differences between states, we determined the radiative and nonradiative relaxation channels and rationalise the observed aggregation induced emission (AIE) of **HC1** and the nonemission of **HC5**. By elucidating the AIE mechanism of **1** and the nonemission of **5**, we isolated three design principles to increase the quantum yield of fluorescence for ESIPT chromophores in the solid state.

In this Chapter, the scope of the study is extended as the design rules established in Chapter **??** are applied to a new set of ESIPT systems. Into the test set we add two fluorene-substituted **HC** derivatives, **HC6** and **7**.[?] . Furthermore, and most pertinently, four completely new compounds with lasing properties are considered. Closely related to **HC**s are the family of 2-hydroxyphenylpropenone (**HP**) derivatives.[?] In contrast to **HC**s, and other organic fluorophores, **HP** compounds contain only a single aryl group and have remarkable QEs, ranging from 0.72-0.84. This has been qualitatively attributed in experimental studies to the herringbone packing mode and molecular rigidity reducing nonradiative decay. The increased quantum yield of the **HP**s, with respect to the **HC**s, make them prime candidates to test the efficacy of our design rules. The eleven compounds studied in this Chapter are summarised in .

Table 1.1: Molecular structures and their QEs (Φ) in the solid state[?][?][?]

	R_1	R_2	Φ		R_3	R_4	Φ
HC1	H	H	0.32	**HP1**	H	H	0.74
HC2	CH_3	H	0.25	**HP2**	F	H	0.84
HC3	OCH_3	CH_3	0.26	**HP3**	H	OCH_3	0.77
HC4	H	CH_3	<0.01	**HP4**	H	F	0.72
HC5	H	OCH_3	<0.01				
HC6	F	H	0.41				
HC7	H	F	0.10				

2 Bibliography

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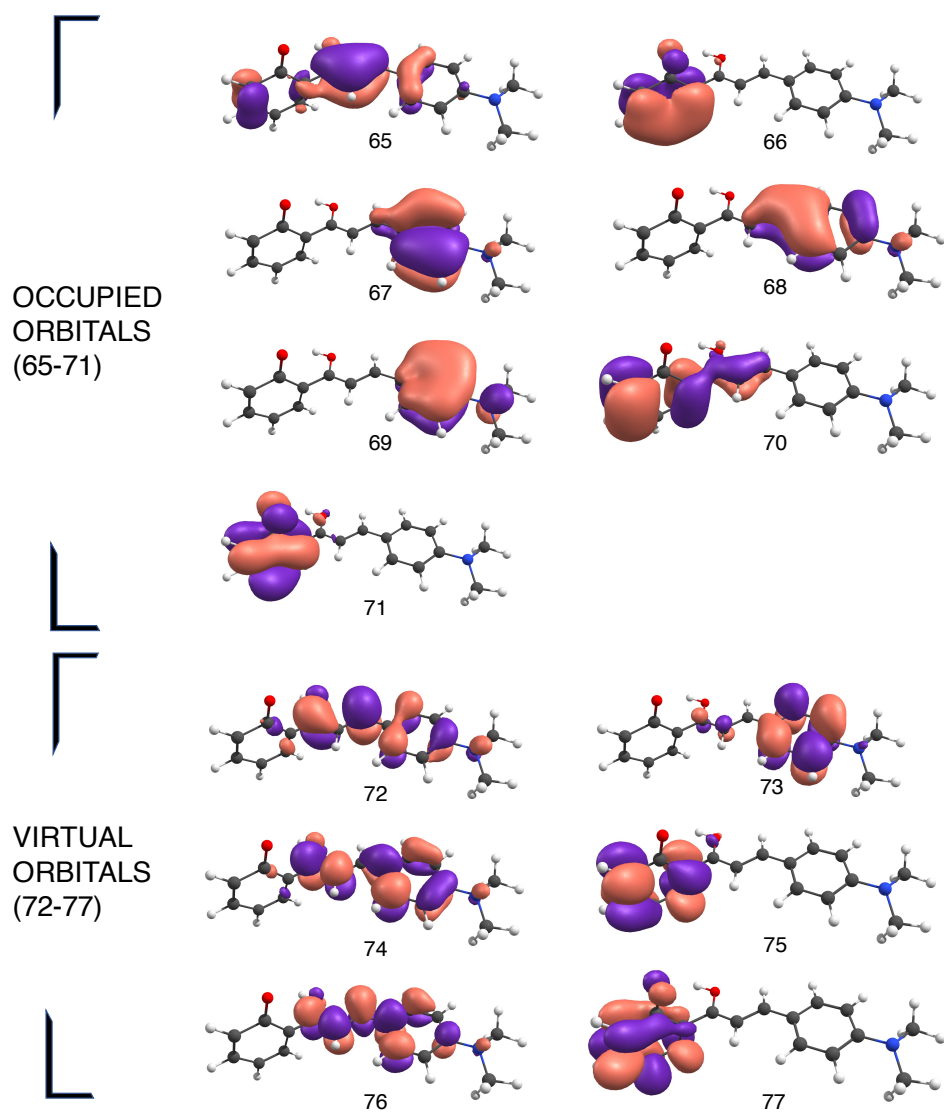
Appendices

Appendix A

Figure A1: CASSCF space used in Chapter **??**.