

## Combining organic photochromism and Inorganic Paramagnetism - Optical Tuning of the Iron(II) Spin State

K. Sénéchal-David,<sup>a</sup> N. Zaman,<sup>a</sup> M. Walko,<sup>b</sup> E. Halza,<sup>b</sup> E. Rivière,<sup>a</sup> R. Guillot,<sup>c</sup> B. L. Feringa,<sup>b</sup> M.-L. Boillot,<sup>a</sup>

<sup>a</sup> ICMMO - Equipe Chimie Inorganique, UMR 8182, Univ. Paris-Sud, 91405 ORSAY cedex, France.

fax : (+33) (0)169 15 47 54 E-mail : [mboillot@icmo.u-psud.fr](mailto:mboillot@icmo.u-psud.fr)

<sup>b</sup> Stratingh Institute for Chemistry & Zernike Centre for Advanced Materials, Faculty of Mathematics and Natural Science, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands.

<sup>c</sup> ICMMO, UMR 8182, Univ. Paris-Sud, 91405 ORSAY cedex, France.

**X-ray crystallography:** CCDC 614028 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif). The crystal data collection and refinement parameters are given in Table S1.

**Table S1.** Crystallographic data for complexe **2o**

formula	C <sub>106</sub> H <sub>68</sub> F <sub>24</sub> Fe N <sub>6</sub> S <sub>10</sub> . 2(CH <sub>3</sub> OH). 2(CH <sub>2</sub> Cl <sub>2</sub> )
Fw	2492.15
crystal system	tetragonal
space group	<i>P</i> 4 <sub>2</sub> /n
<i>a</i> [Å]	34.6061(8)
<i>b</i> [Å]	34.6061(8)
<i>c</i> [Å]	9.4842(5)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	11358.1(7)
<i>Z</i>	4
<i>F</i> (000)	5072
$\lambda$ [Å]	0.71075
<i>T</i> [K]	100(1)
$\rho_{\text{calcd}}$ [Mg m <sup>-3</sup> ]	1.457
$\mu$ (MoK $\alpha$ ) [mm <sup>-1</sup> ]	0.502
$\theta$ range [° min-max]	2.45 -22.46
no. of data collected	50 563
no. of unique data	7 357
<i>R</i> (int)	0.057
no. of variable parameters	696
no. of obsd. refl. <sup>[a]</sup>	7 357
<i>R</i> <sup>[b]</sup> obsd., all	0.079 , 0.096
<i>Rw</i> <sup>[c]</sup> obsd., all	0.192, 0.211
<i>S</i>	1.050
( $\Delta/\sigma$ ) <sub>max</sub>	0.083
( $\Delta/\rho$ ) <sub>max, min</sub> [e Å <sup>-3</sup> ]	0.753 , -0.653

**[a]** Data with  $F_o > 4\sigma(F_o)$ . **[b]**  $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ . **[c]**  $Rw = [\sum w(|F_o|^2) -$

$$|F_c^2| / \sum w |F_o^2|^{1/2}$$

**Table S2.** Intermolecular contacts: Selected measured distances for compound **2o** and comparison with the sum of Van der Waals radii :  $\Sigma r_i$

Labels		Measured distances [Å]	$\Sigma r_i$ [Å]
F <sub>13(1A)</sub>	F <sub>13(1A)</sub>	2.582	2.94
F <sub>8(1A)</sub>	H <sub>45B(1A)</sub>	2.634	2.67
F <sub>9(1A)</sub>	H <sub>76(1B)</sub>	2.531	2.67
F <sub>16(1B)</sub>	H <sub>64(1A)</sub>	2.426	2.67
F <sub>2(1B)</sub>	Cl <sub>1</sub>	3.180	3.22
H <sub>74C(1B)</sub>	Cl <sub>1</sub>	2.661	2.95
H <sub>74C(1B)</sub>	C <sub>500</sub>	2.626	2.90

Fig S1 : RT UV-Vis spectra of the iron(II) complex (**2o**) before (—) and after irradiation at 365 nm(· · · ·) and 650 nm(- - - -).

