Molecular Engineering of Sensitizers for Solar Cell Applications

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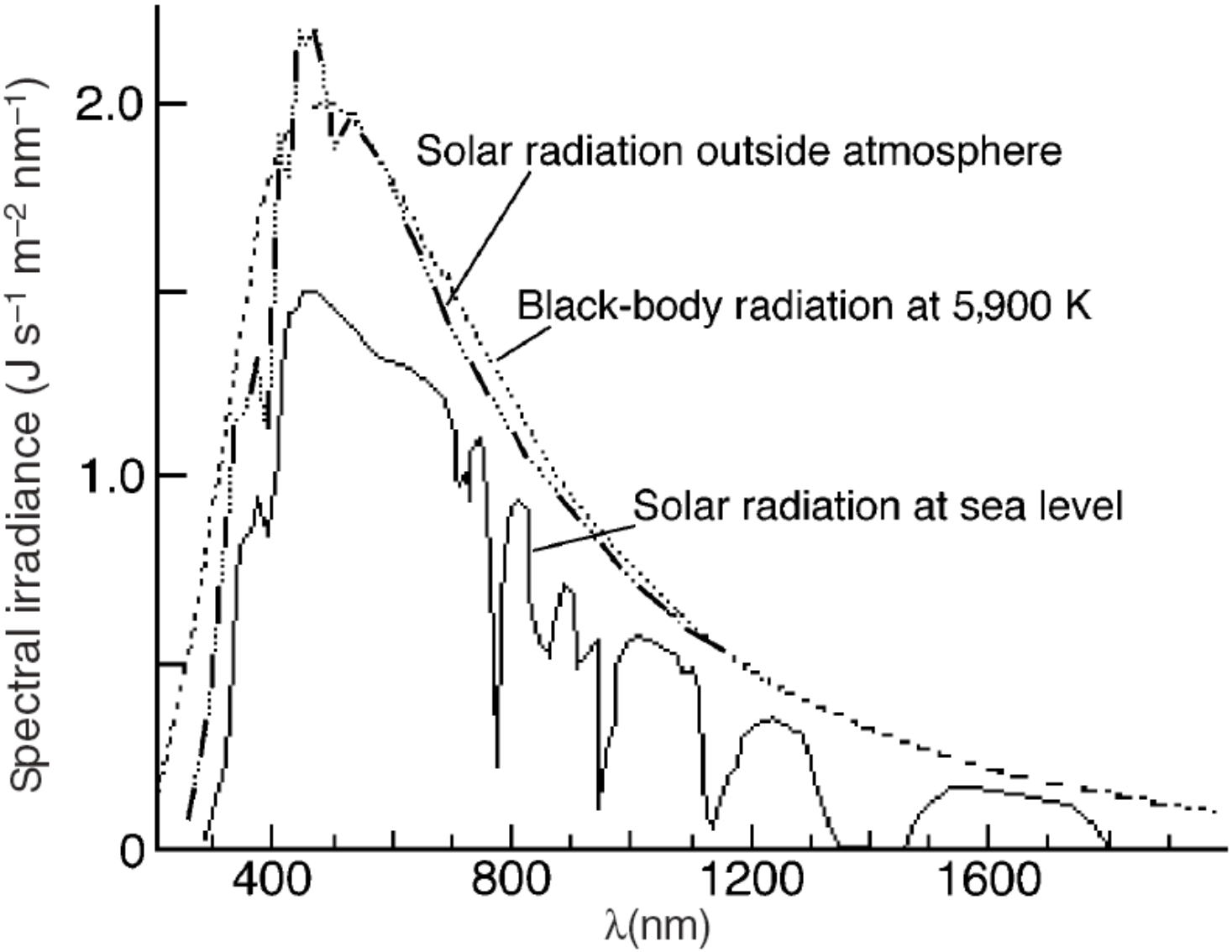
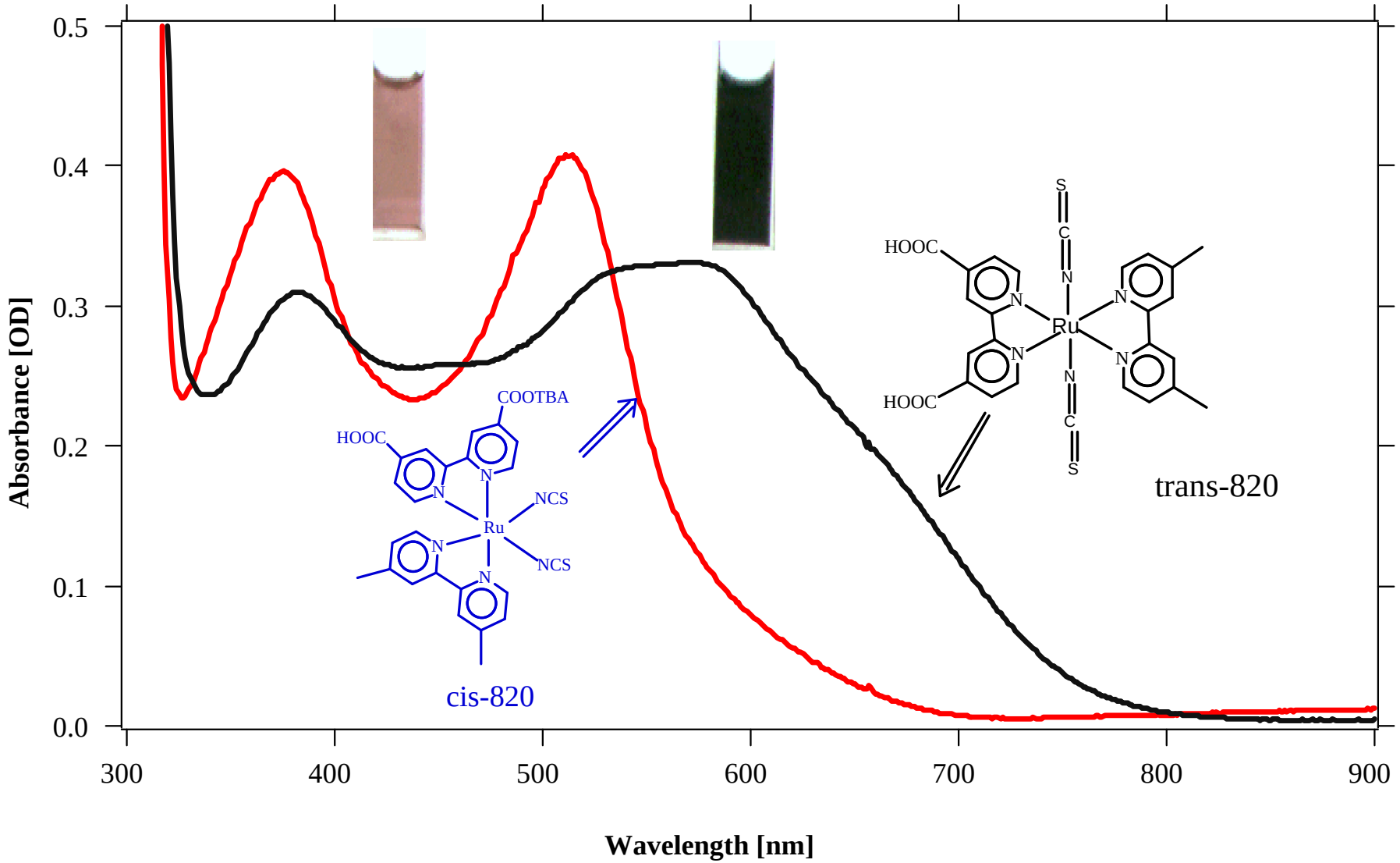
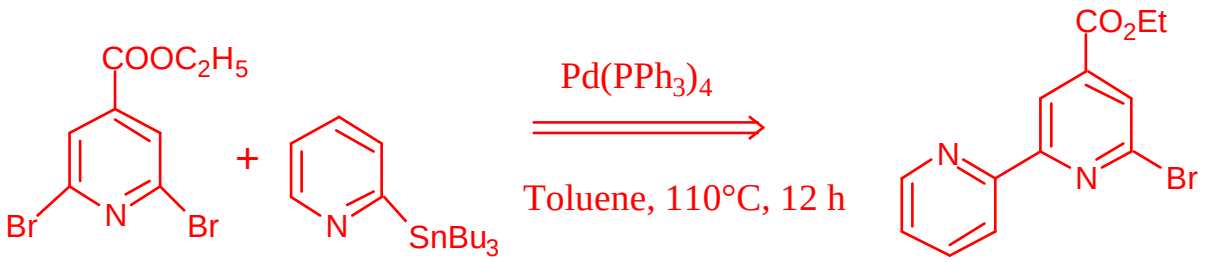
Spectral irradiance of the Sun at mean Earth-Sun separation

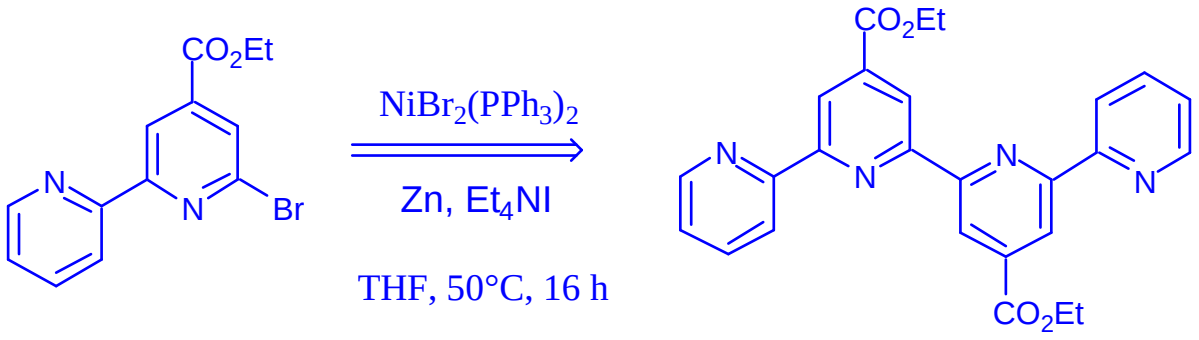


Cis- and trans-Isomers of N820



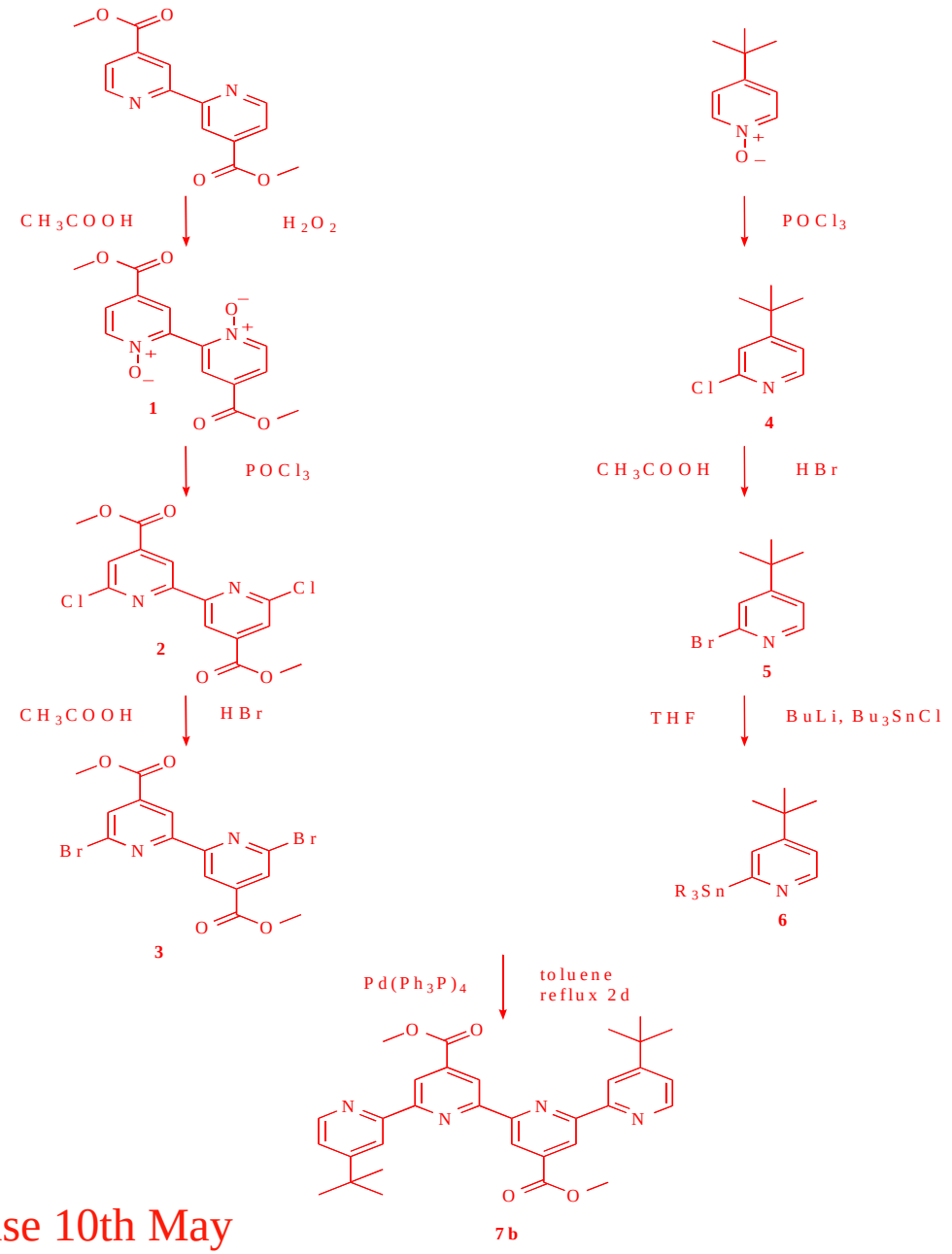
Synthesis of 4’,4’’-Diethoxycarbonyl-2,2':6',2'':6'',2'''-quaterpyridine





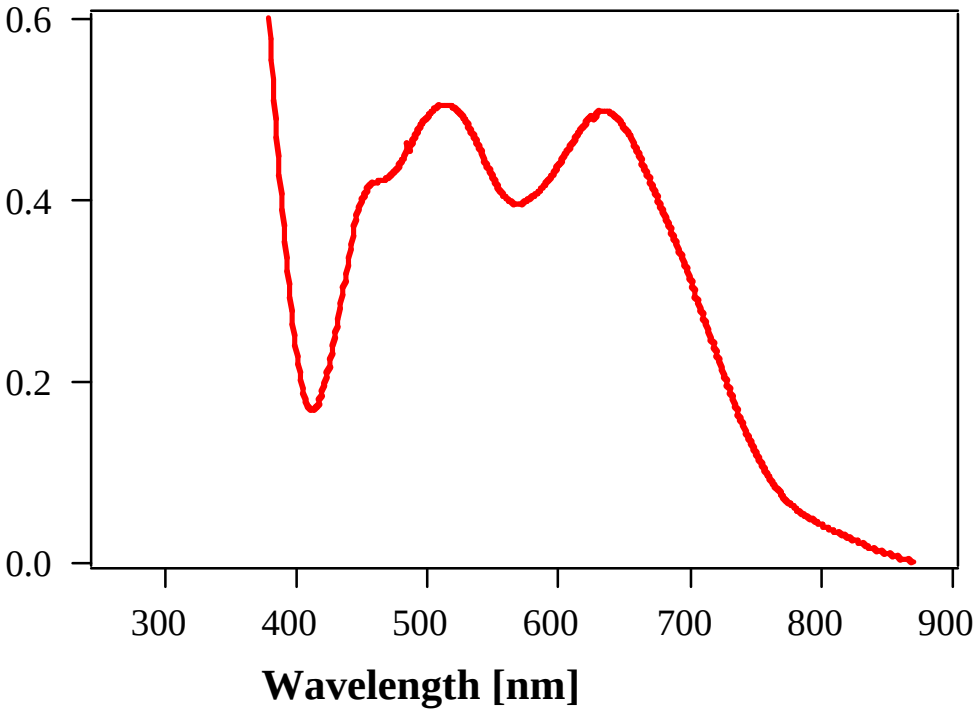
(L^4)

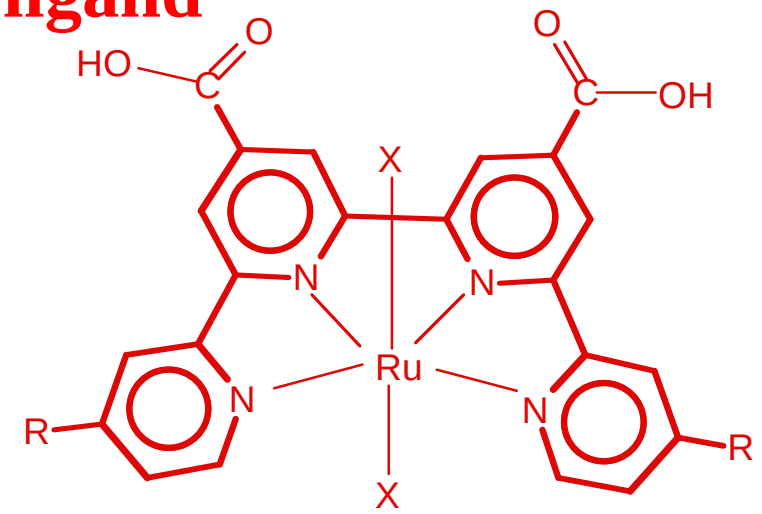
Inorg. Chem.2002,41,367-378



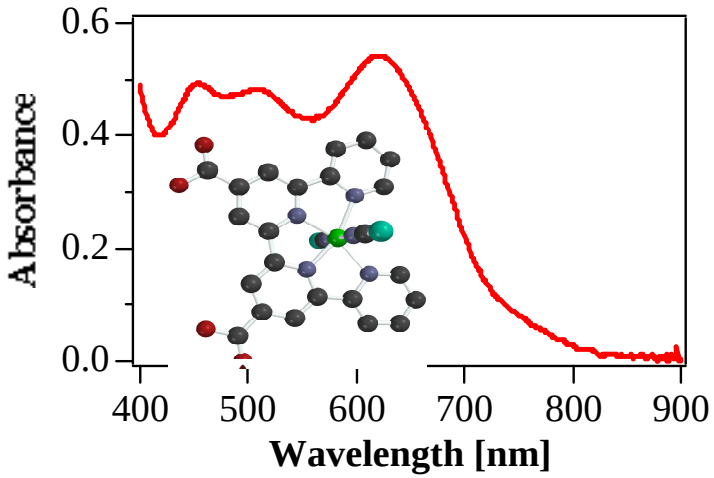
Inorg. Chem 2006, web release 10th May

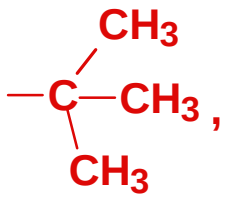
Ruthenium Sensitizer with Functionalized Tetradentate ligand

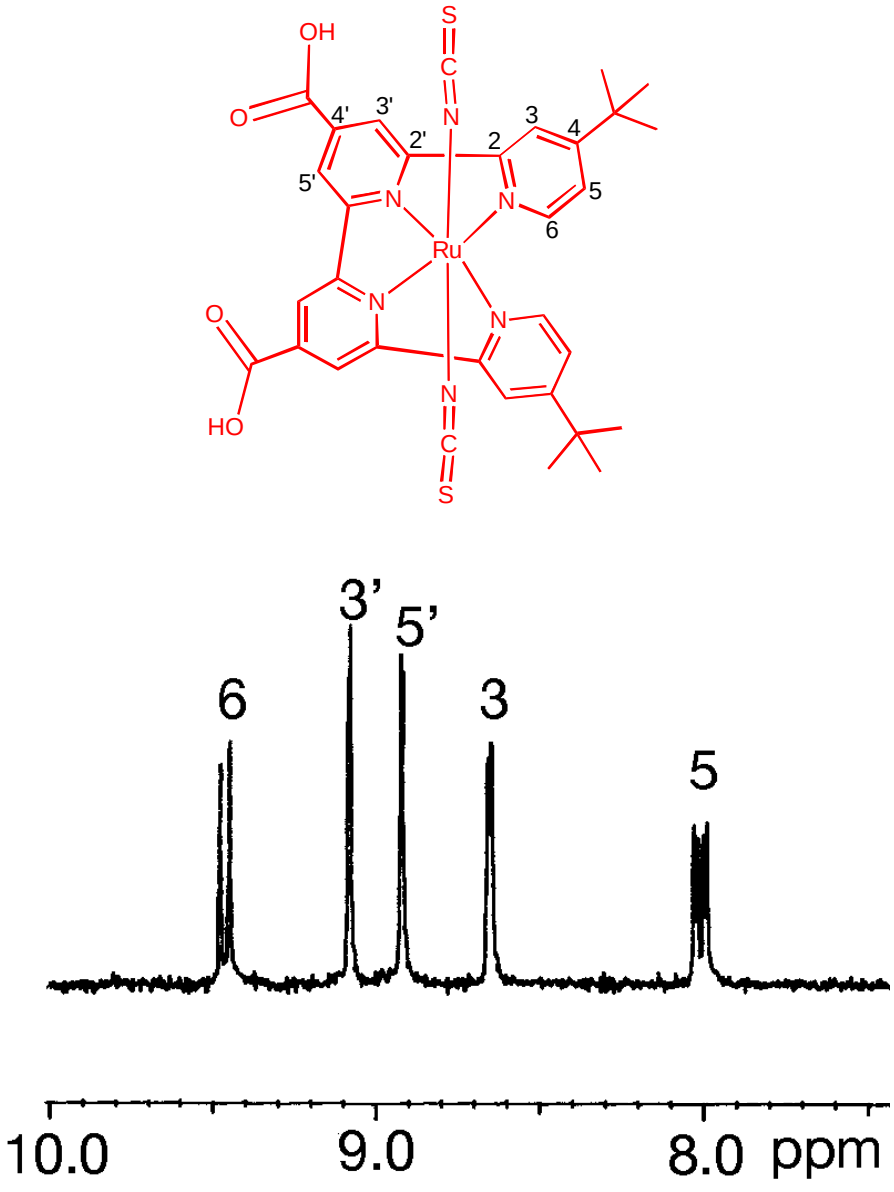




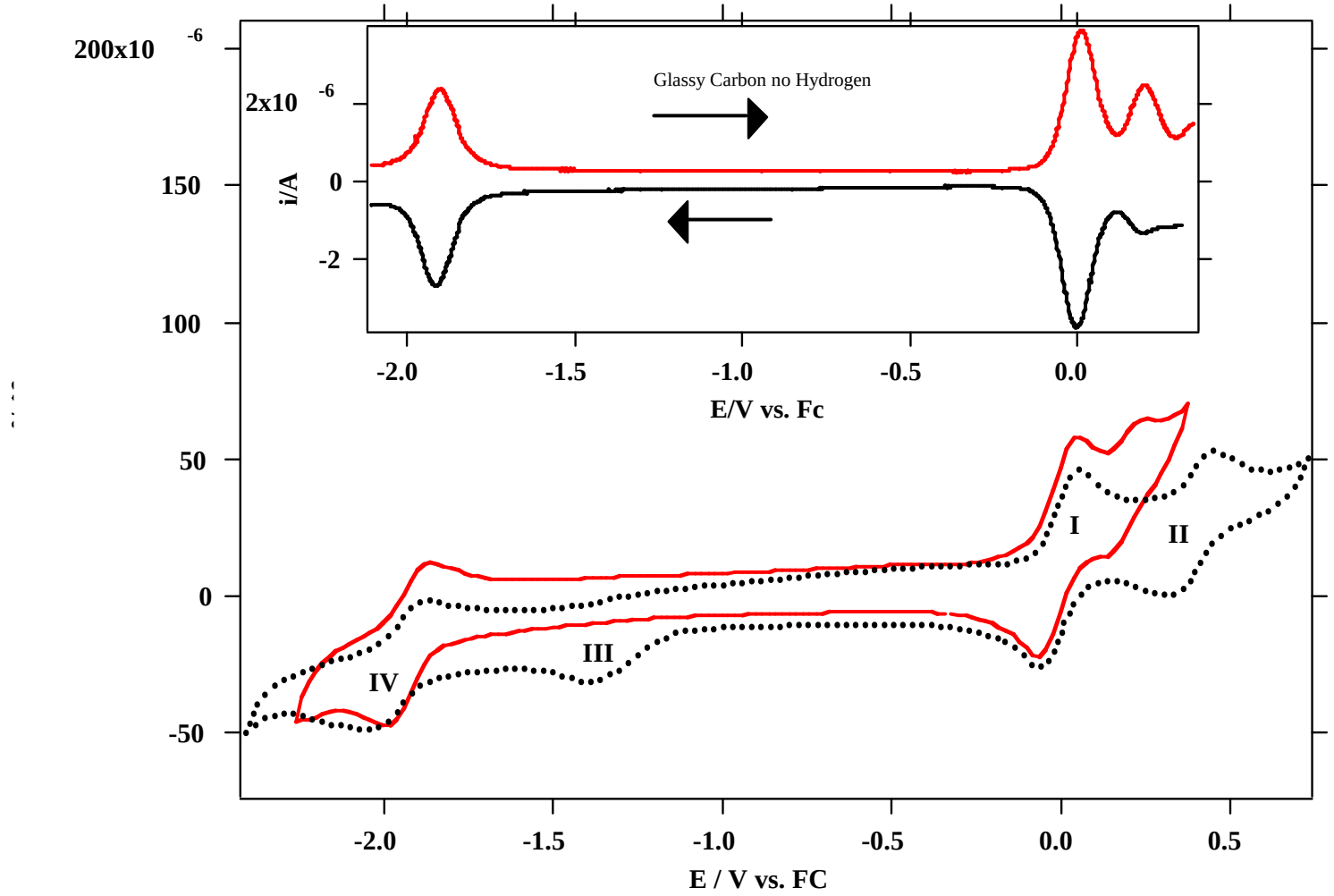
X = Cl⁻, NCS⁻ and CN⁻



R = CH3,  , $-C_9H_{19}$

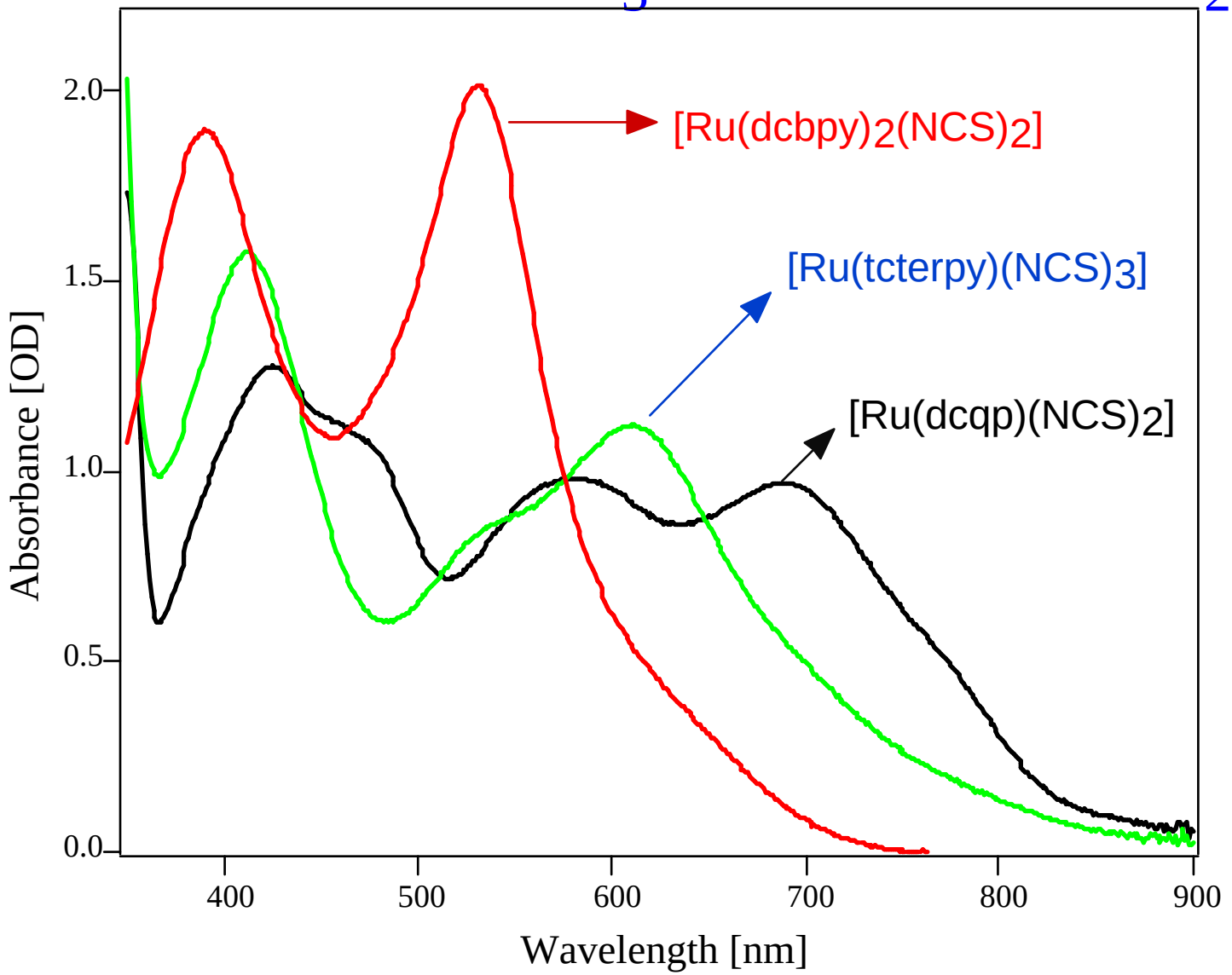

OH
O
S
C
N
4'
3'
2'
2
3
4
5'
5
6
Ru
HO
3’
5’
6
3
5
10.0
9.0
8.0 ppm

Cyclic voltammogram of N886 complex in protonated (black line) and deprotonated state (red line) measured in DMF solution

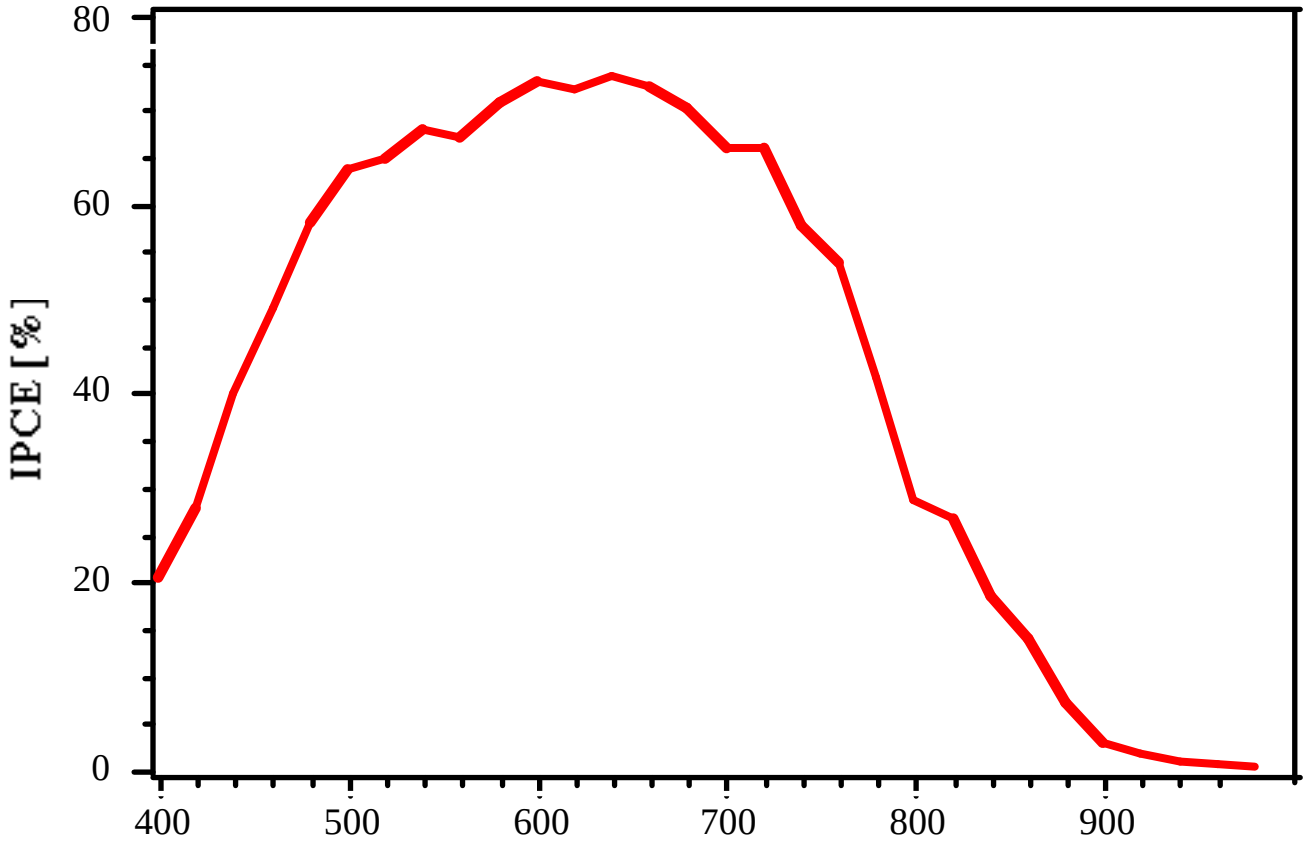


Comparison of UV-vis absorption spectra of the complexes

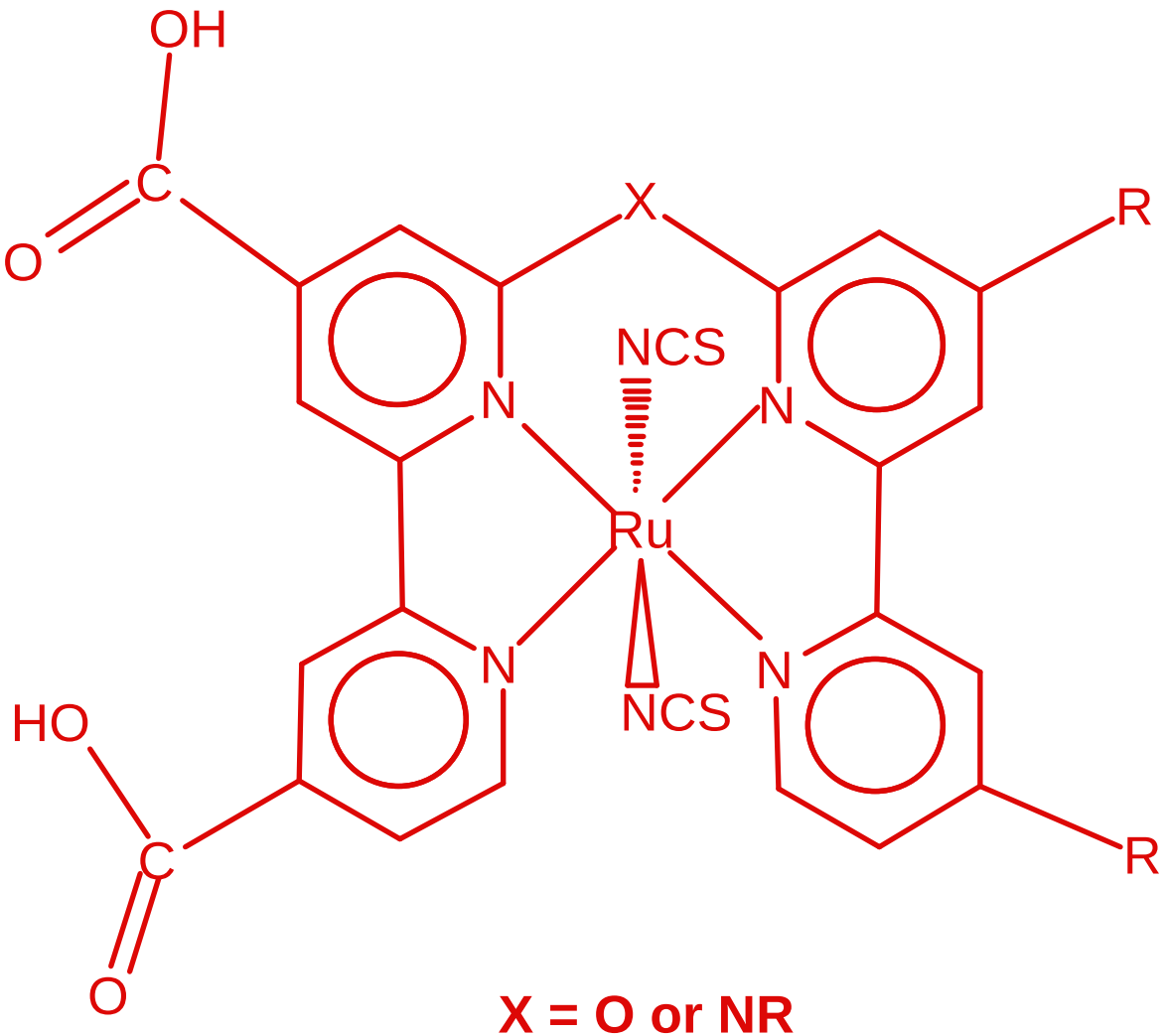
N3, [Ru(Htcterpy)(NCS)$_3$] and *trans*-[Ru(L)(NCS)$_2$]



Photocurrent action spectrum obtained with [Ru(4,4 ’dcqpy)$(NCS)_2$] complex attached to nanocrystalline TiO_2 films



New Ligands and Sensitizers

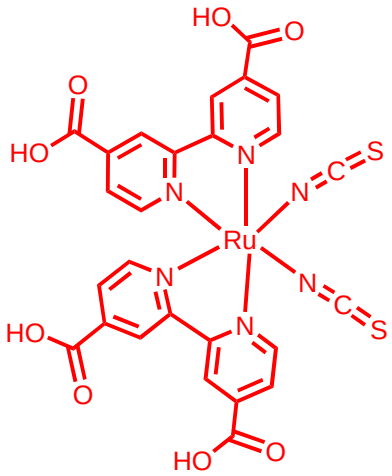


X = O or NR

R = C(nH2n+1)

Dr. F. P. Rotzinger

New Sensitizers with extended π-system



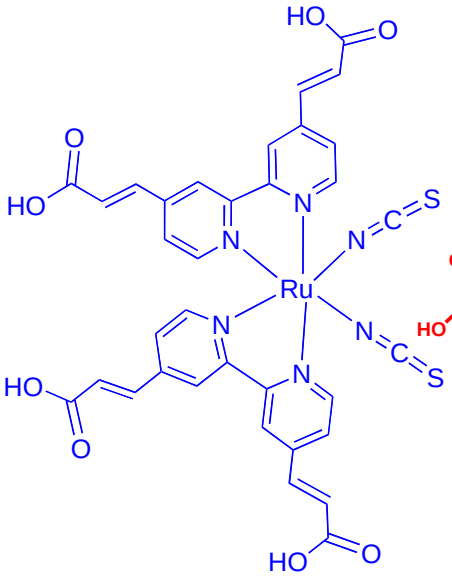
N3

λmax 535 nm

ε= : 13800 $M^{-1}cm^{-1}$

Em. λ_{max} : 780 nm

E_{ox} = 0.85 (irrev)



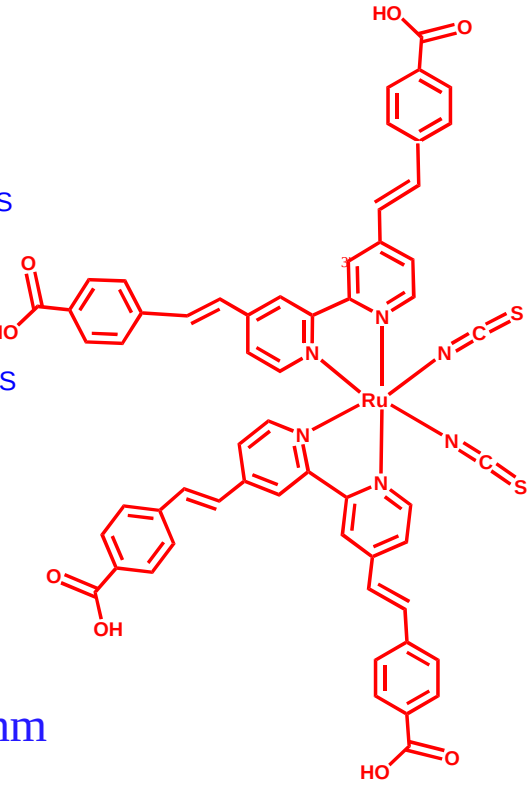
K-8

Abs. λ_{max} : 555 nm

ε: 17600 $M^{-1}cm^{-1}$

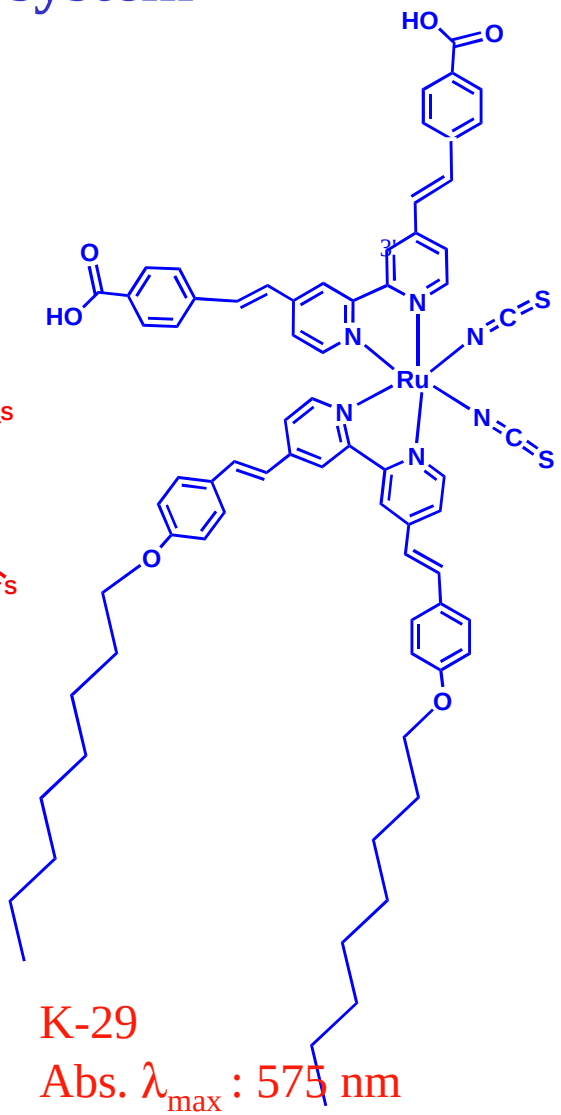
Em. λ_{max} : 840 nm

E_{ox} = 0.77 (rev)



K-27

Abs. λ_{max} : 566 nm

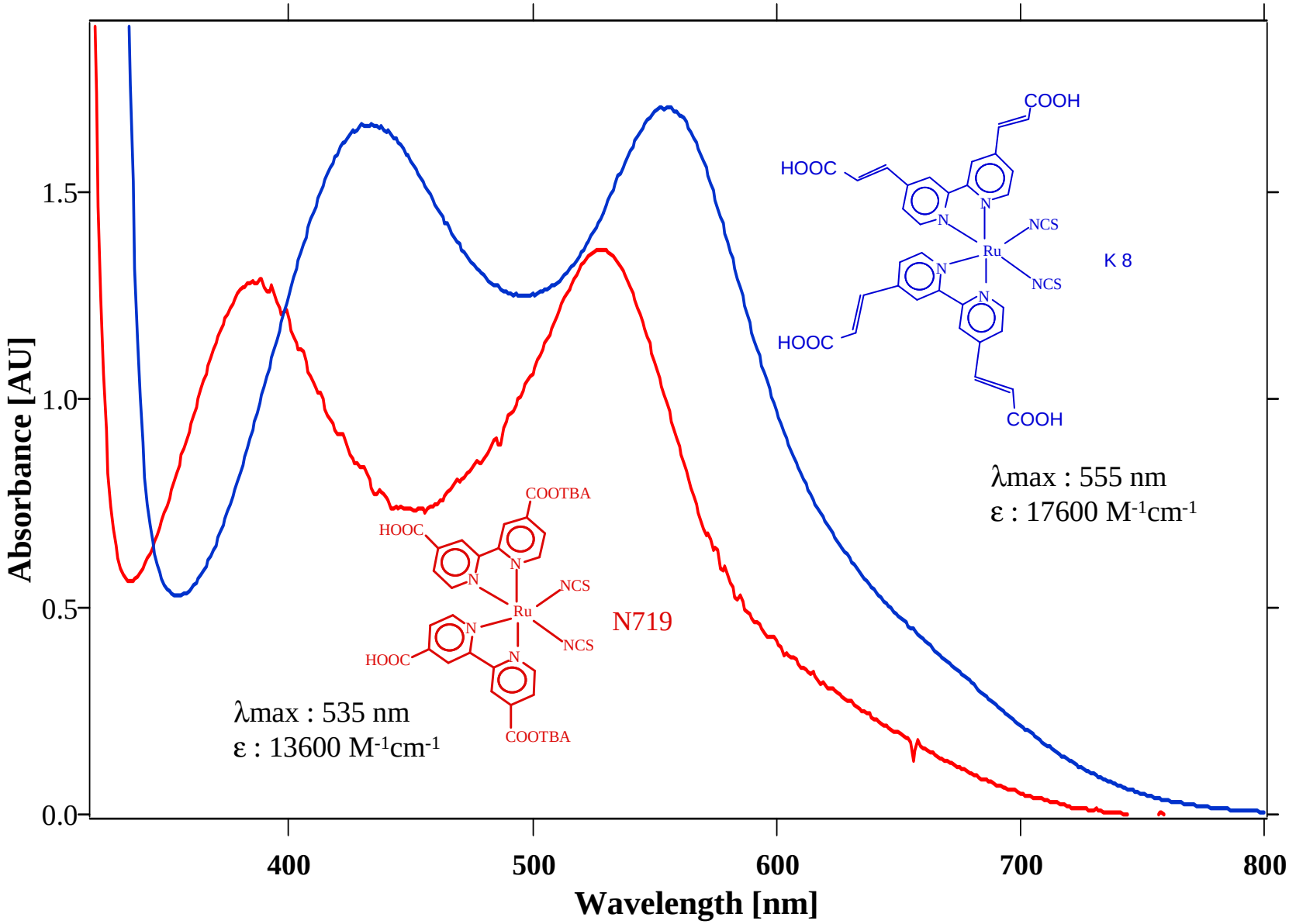


K-29

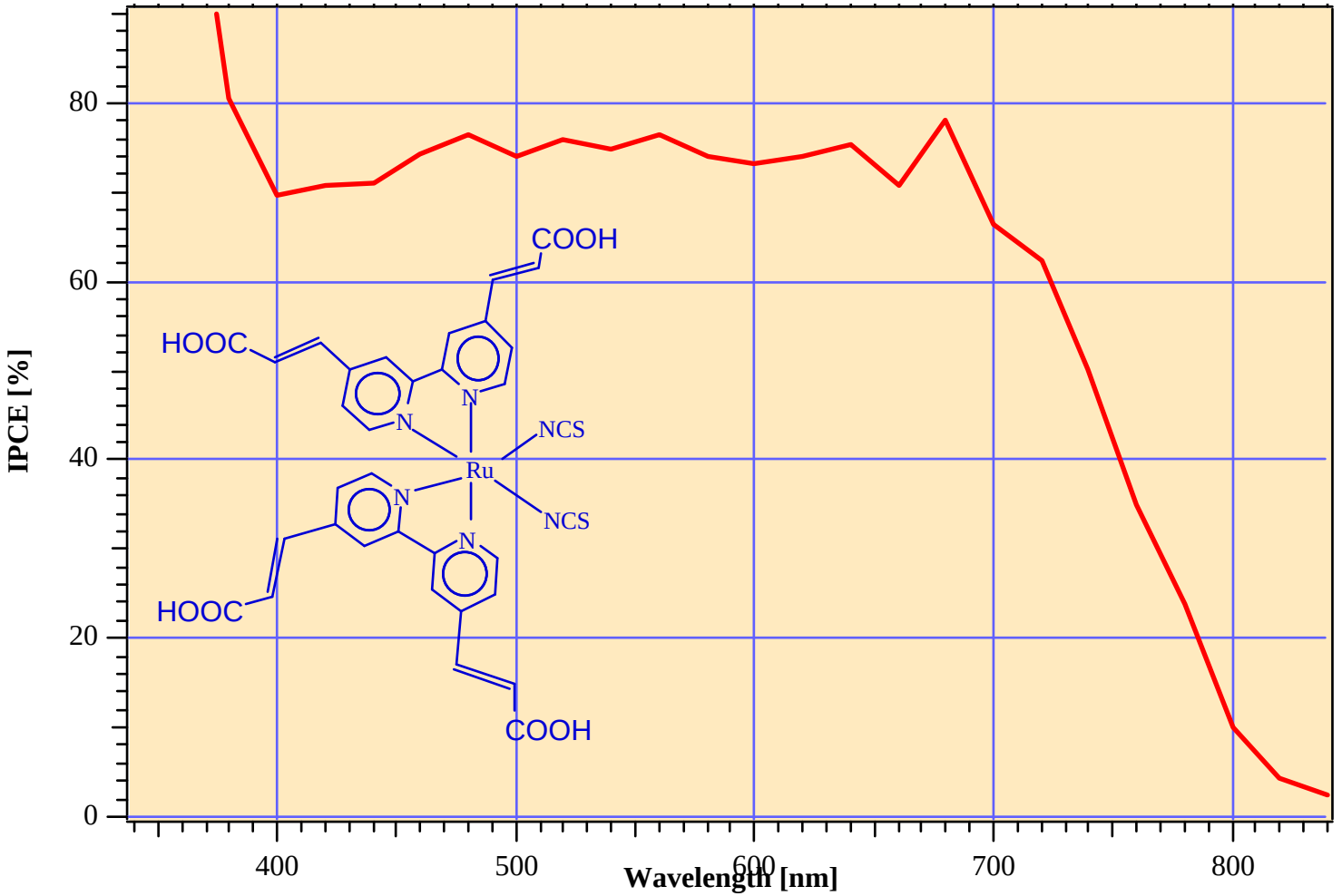
Abs. λ_{max} : 575 nm

ε: 17600 $M^{-1}cm^{-1}$

UV/Vis Spectra of N719 and K8 Sensitizers



Incident Photon to Current Conversion Efficiency of K 8 Sensitizer



Solar AM 1.5 (1000 W/cm^2) is 18 - 19 mA/cm^2

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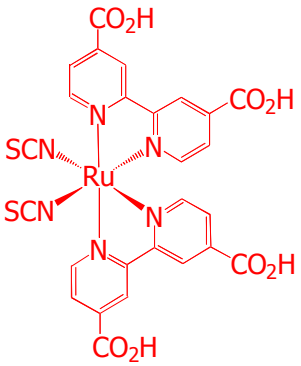
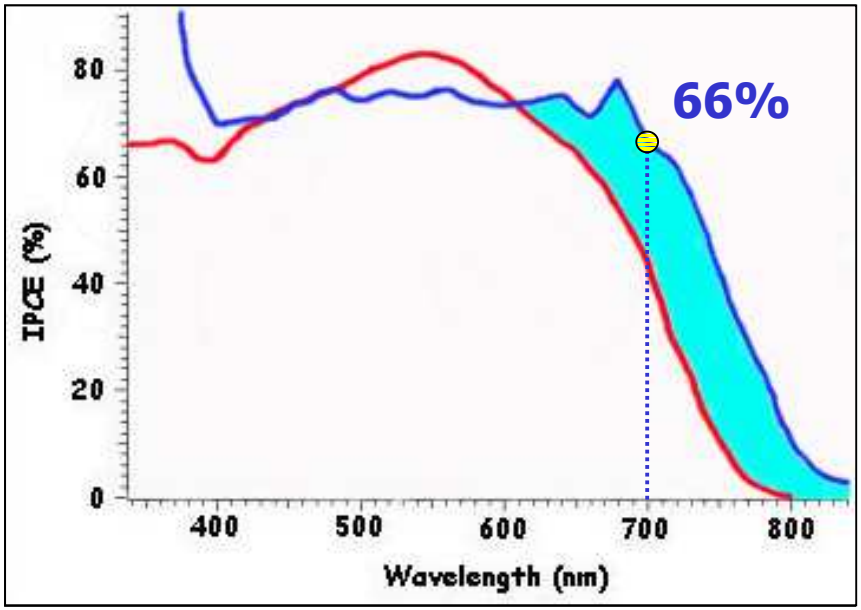
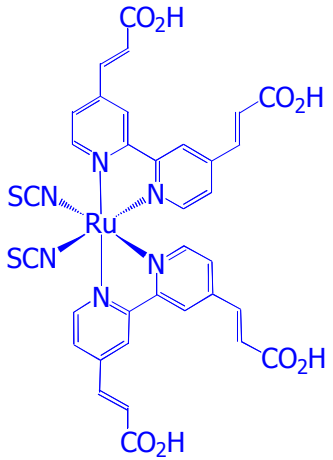
Extension of the π-system on the anchoring ligand

IPCE measurement :



N_3



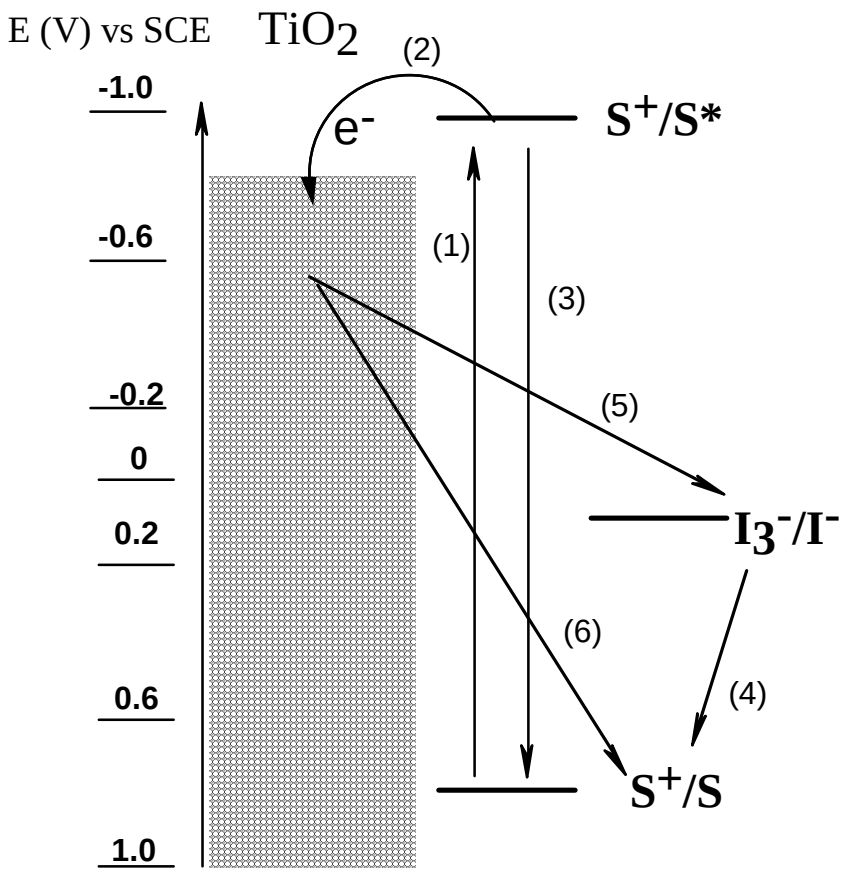


K_8

Performance Characteristics of Photovoltaic cells based on Nanocrystalline TiO_2 films sensitized by K8

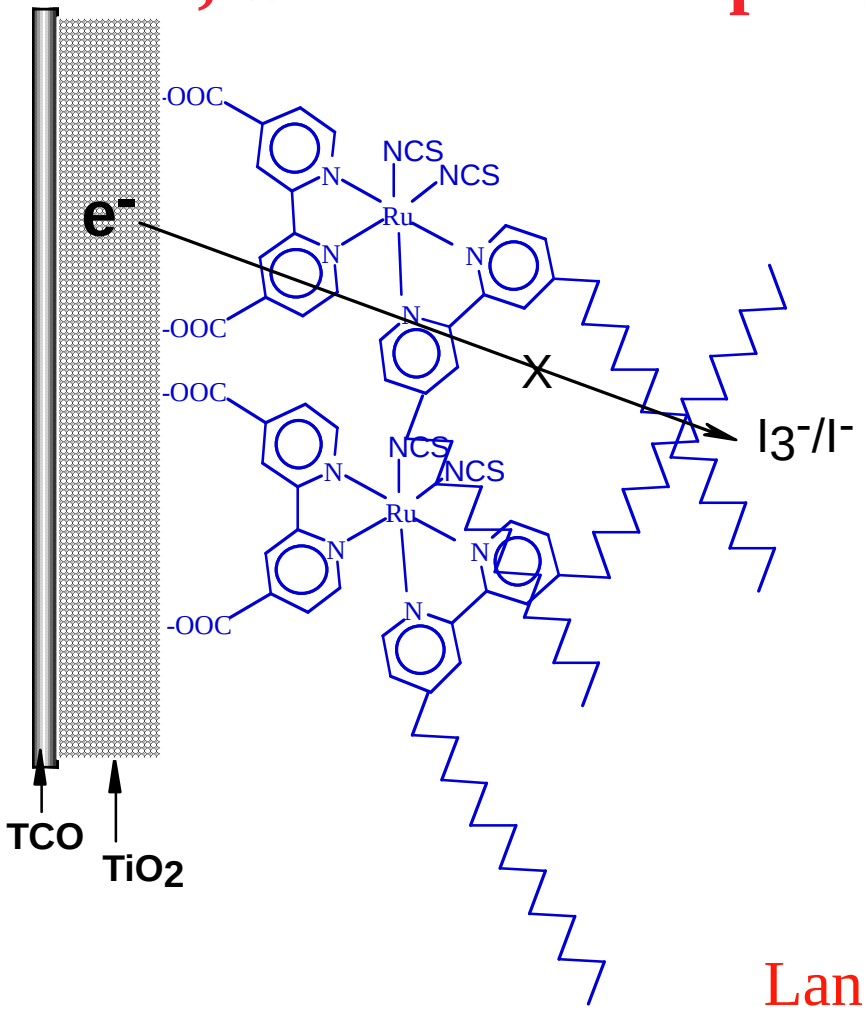
TiO_2 Layer thickness (μm)	Current mA/cm^2	Potential (mV)	Fill Factor	Efficiency
8 + 4	16.9 ± 0.3	665 ± 30	0.73 ± 0.05	8.20
10 + 4	17.7 ± 0.3	645 ± 20	0.74 ± 0.05	8.45
12 + 4	18.0 ±0.3	640 ±20	0.75±0.05	8.64
16 + 4	18.0 ± 0.3	638 ± 50	0.72 ±0.05	8.26

Illustration of the interfacial charge transfer processes in nanocrystalline dye sensitized solar cell.



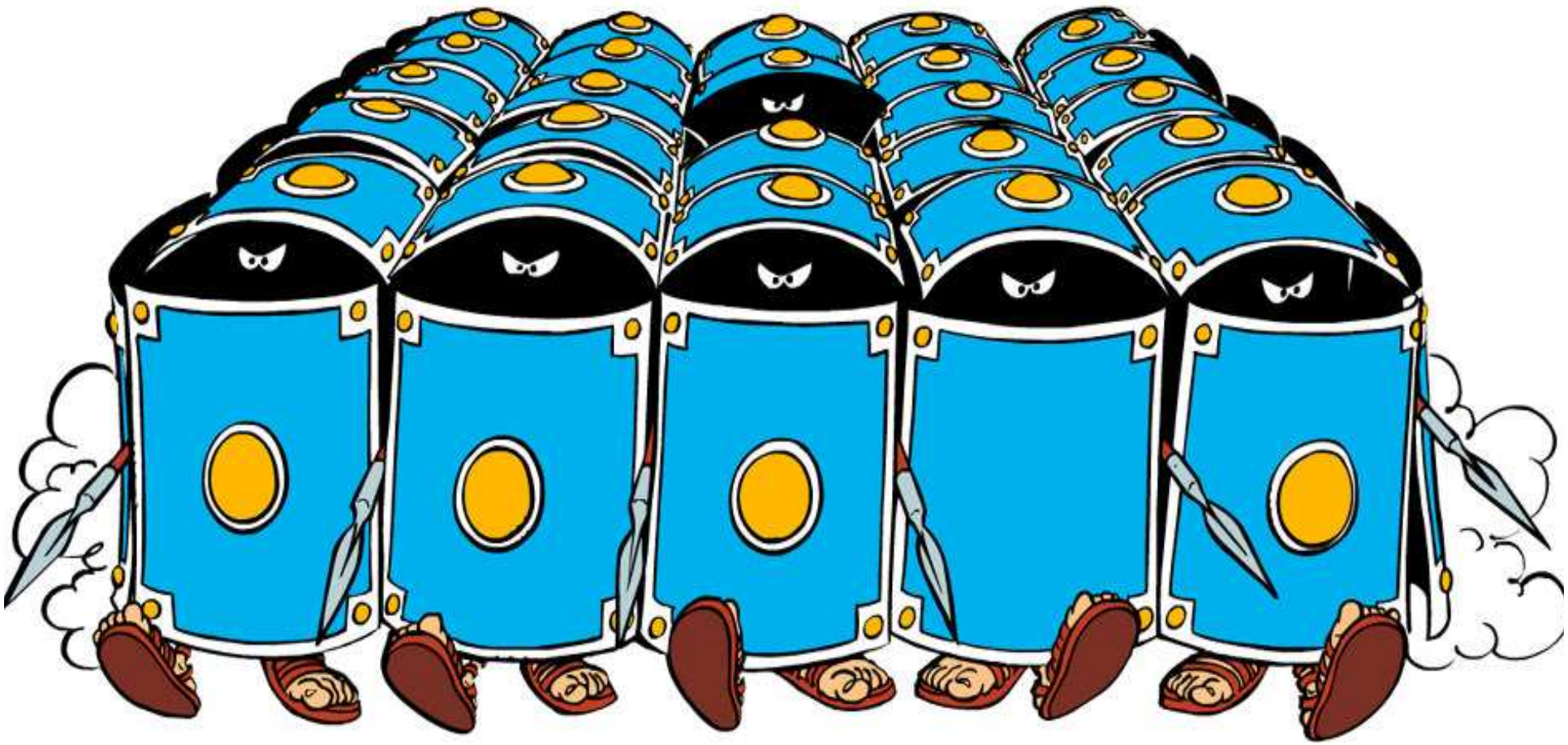
(1) An excited state: (2) electron injection onto the conduction band of TiO_2. (3) The oxidized sensitizer gets reduced by I^- / I_3^- redox couple. (4) The injected electrons into the conduction band may react either with the oxidized redox couple (5) or with oxidized dye molecule (6).

Pictorial representation of blocking of the oxidized redox couple I_3^- reaching onto the surface of TiO_2 for conduction band electrons using hydrophobic sensitizers, which forms aliphatic net work.



Langmuir 2002. 18, 952-954

Interface Engineering in Dye-Sensitised Solar Cells



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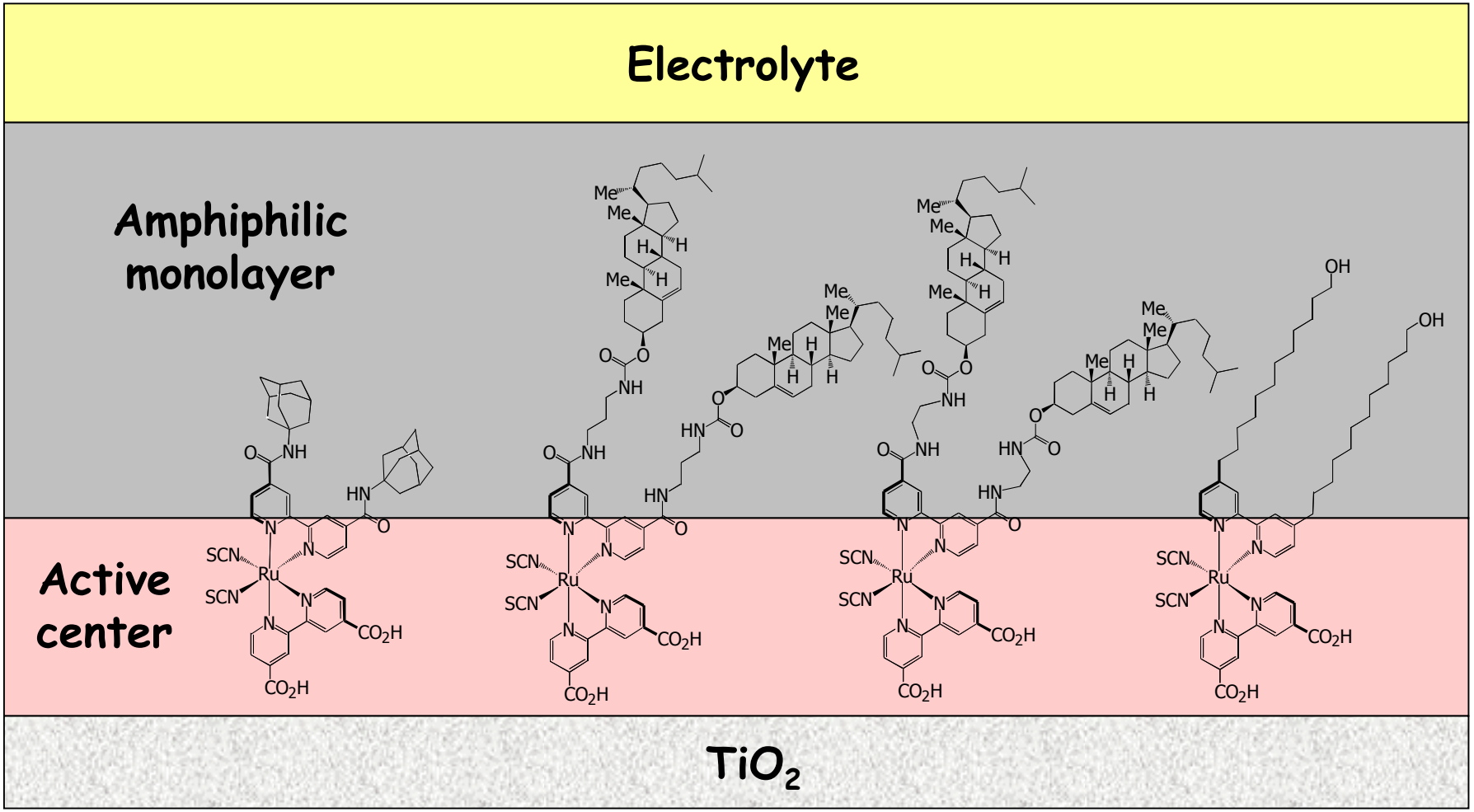
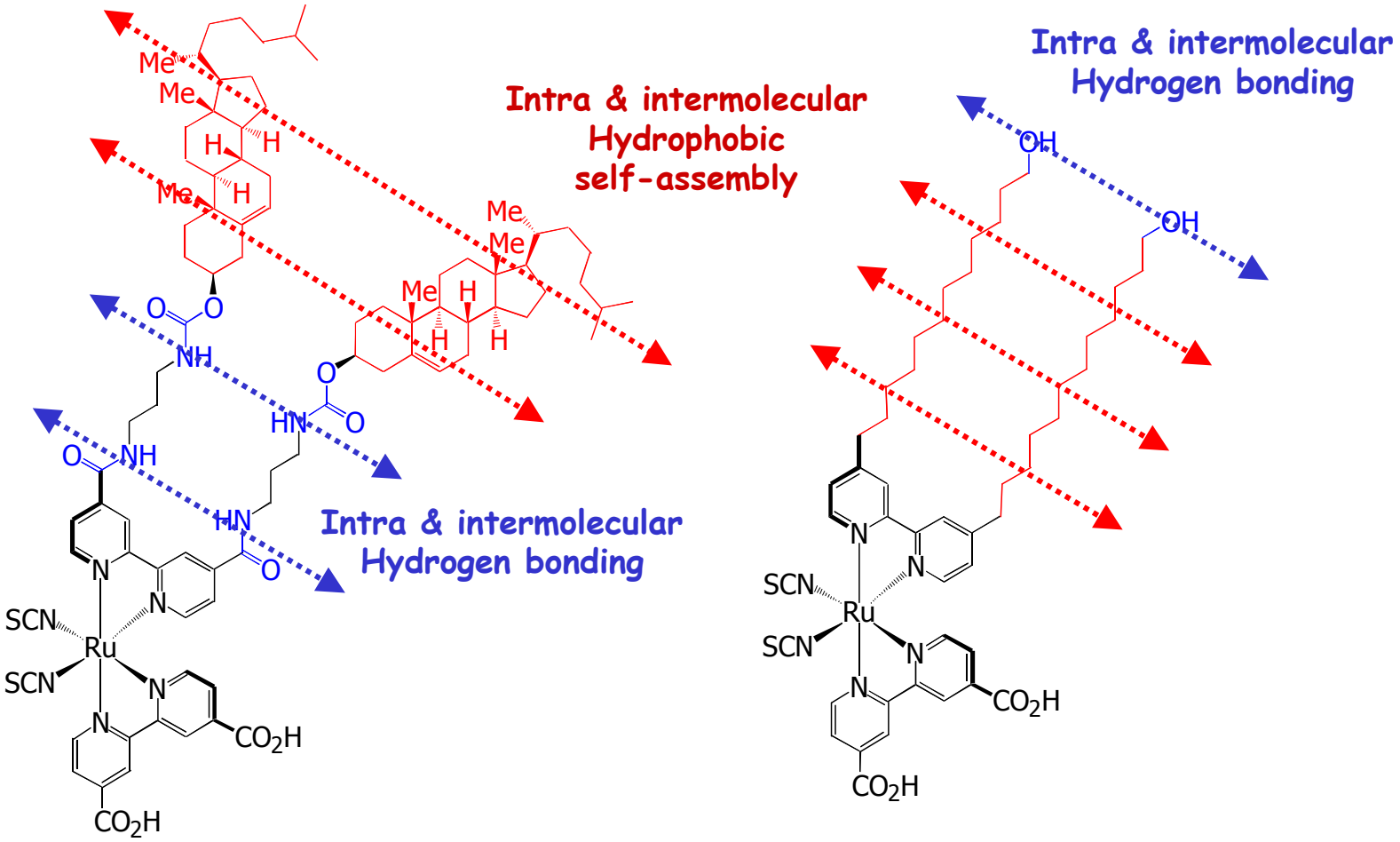
Amphiphilic Ruthenium-based sensitizers



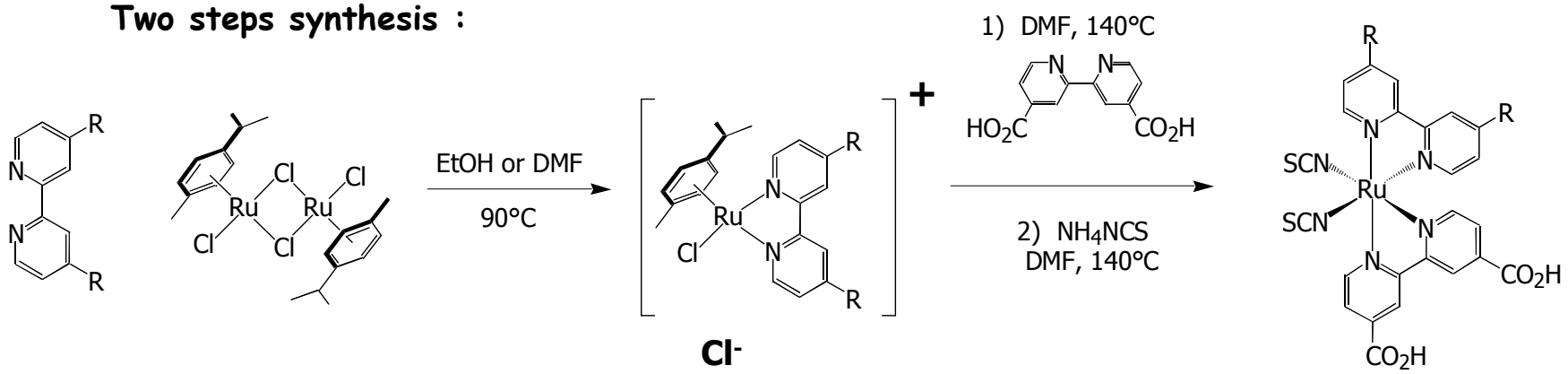
Amphiphilic Ruthenium-based sensitizers



Amphiphilic Ruthenium-based sensitizers

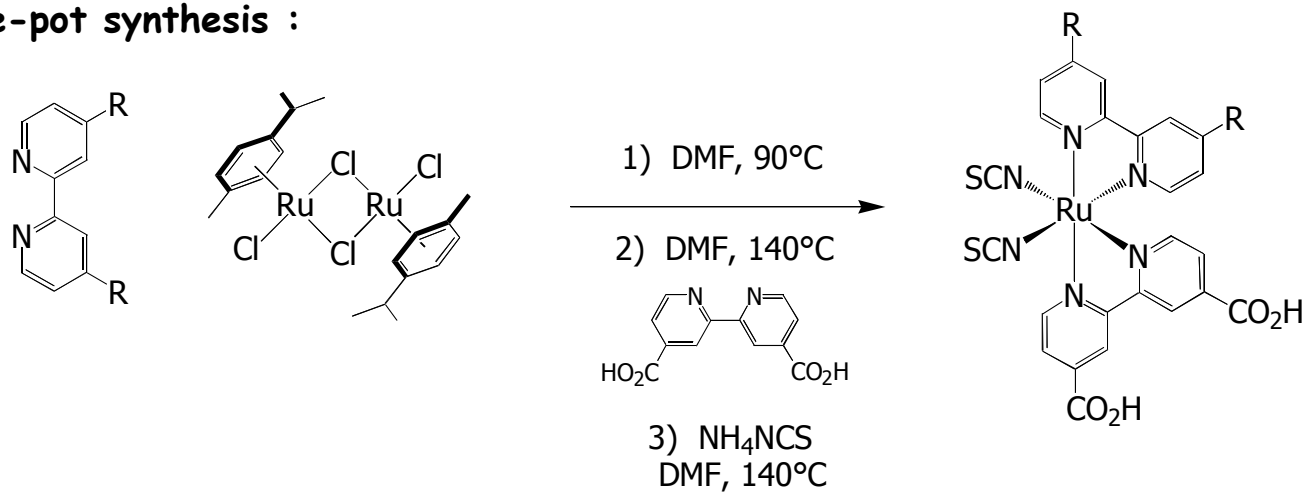
Synthesis of heteroleptic complexes :

Two steps synthesis :

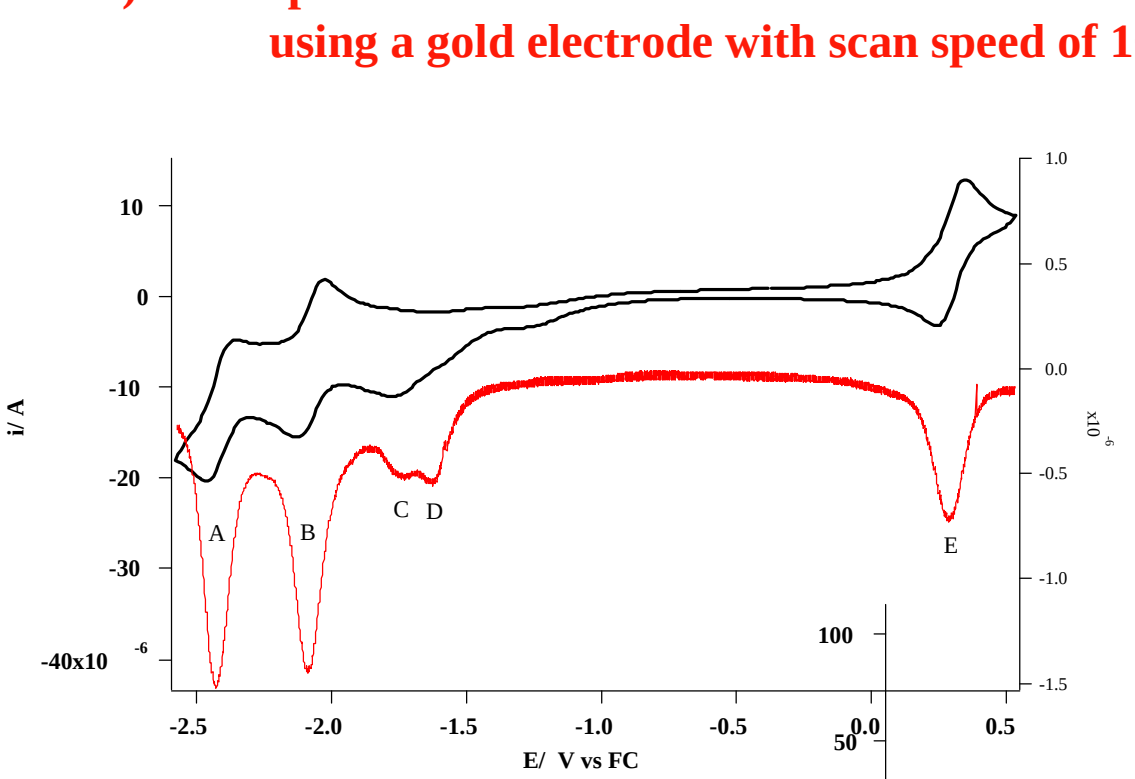


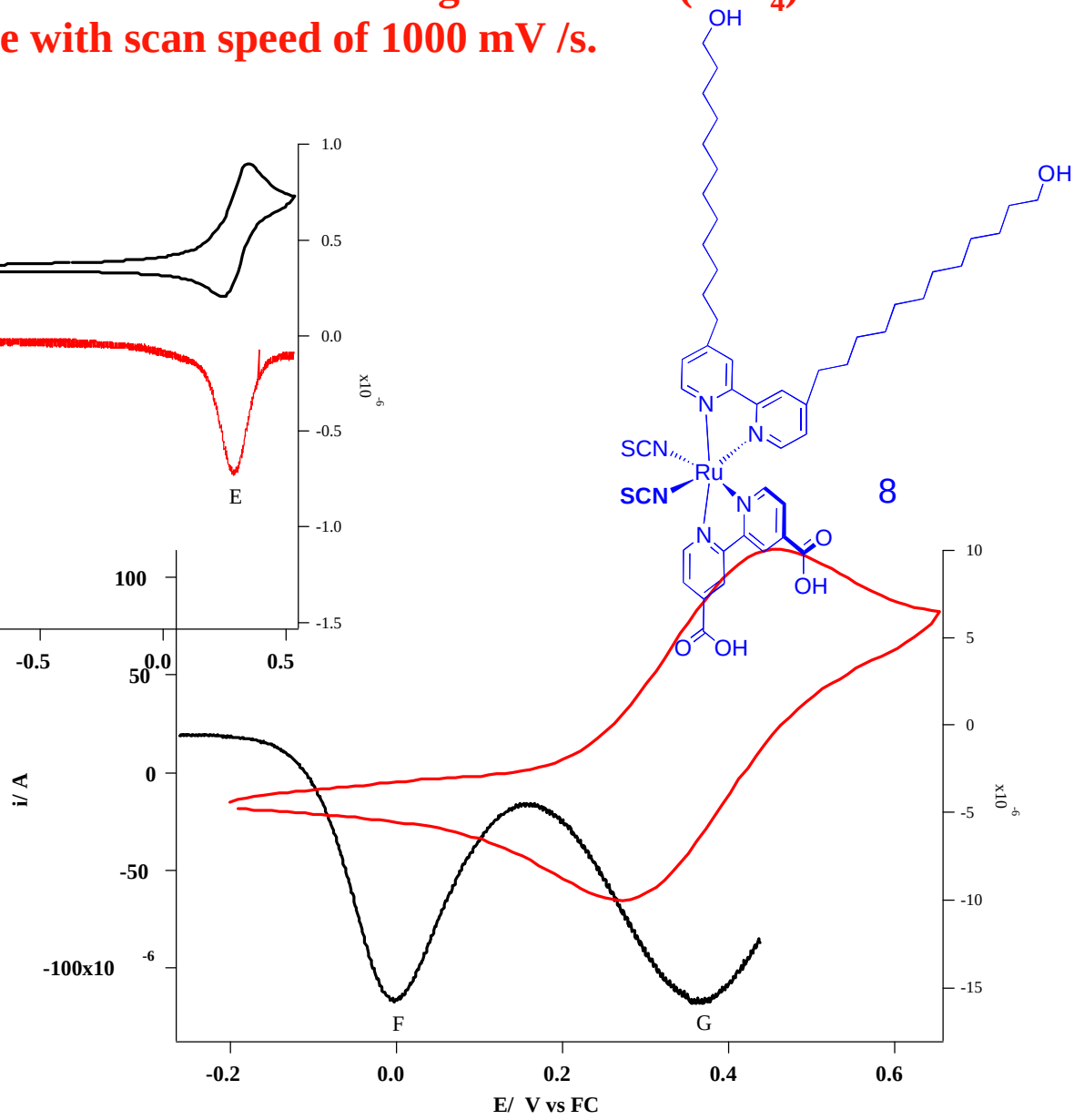
Cl$^-$

One-pot synthesis :

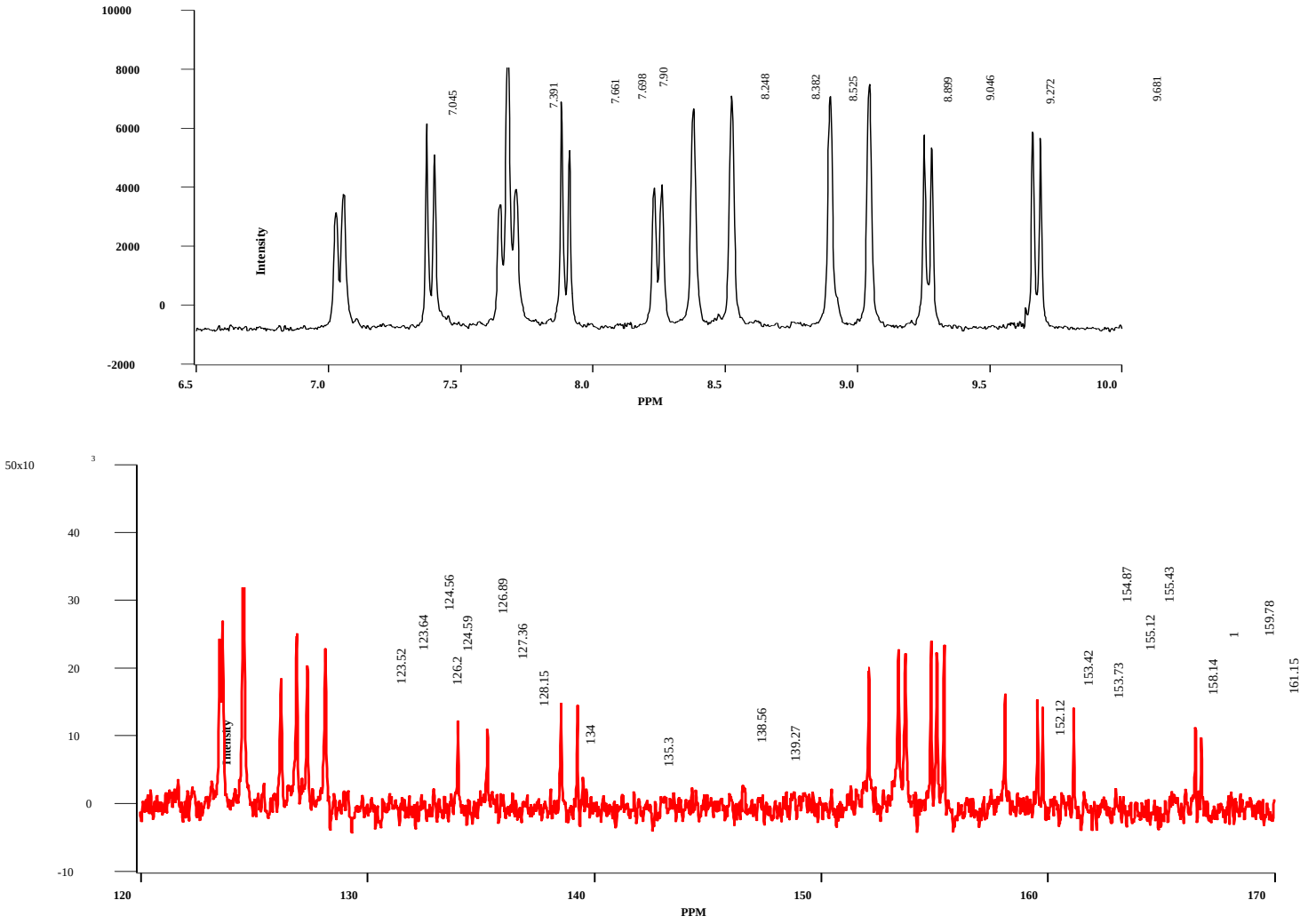


Cyclic voltammogram (black line) and the square wave voltammogram (red line) of complex 8 measured in DMF solution containing 0.1 M TBA(ClO_4) using a gold electrode with scan speed of 1000 mV /s.





A part of ^{1}H and ^{13}C NMR spectrum of the complex **8** in CD_3OD. For clarity the peaks in the aliphatic region is not included.



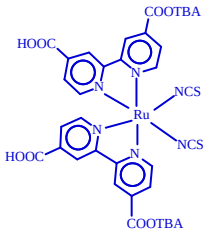
The advantages of heteroleptic hydrophobic sensitizers are:

(1) Improves the interface between the sensitizer and the hole conducting material (spirobifluorene, Co-complex)

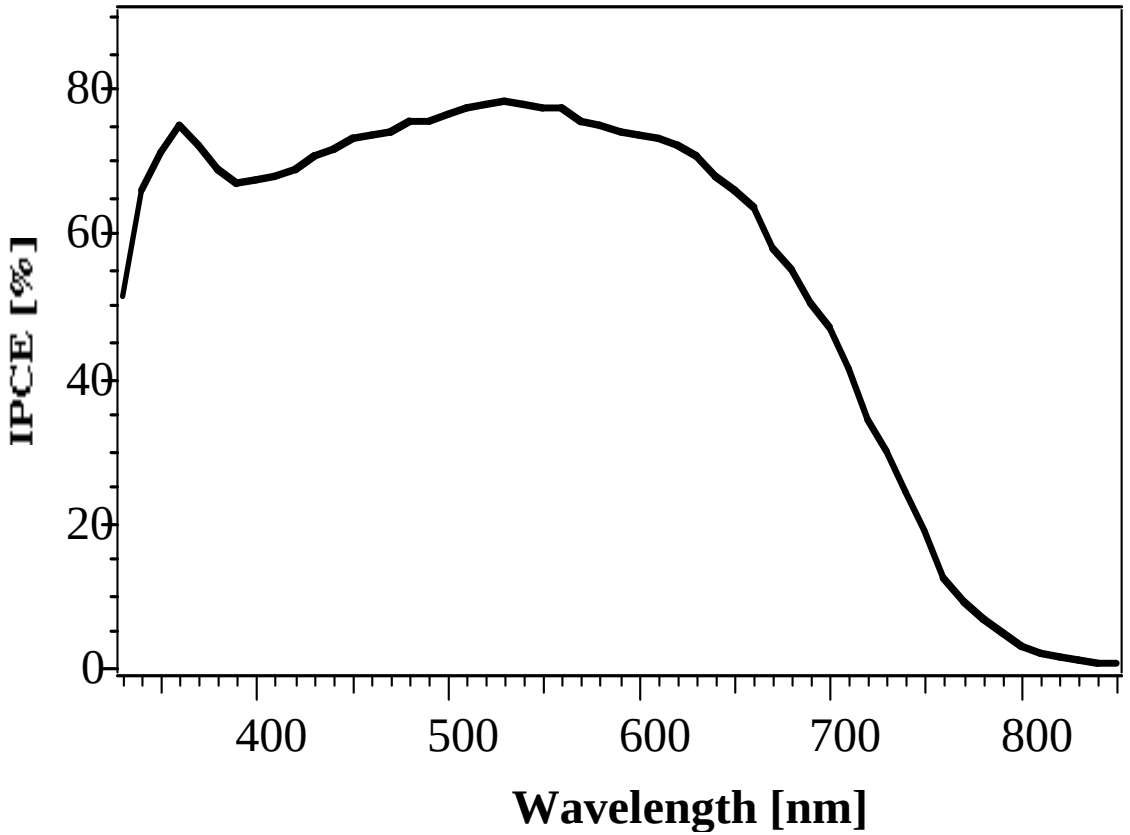
(2) Increased ground state pK_a of the heteroleptic sensitizer increases the dye uptake

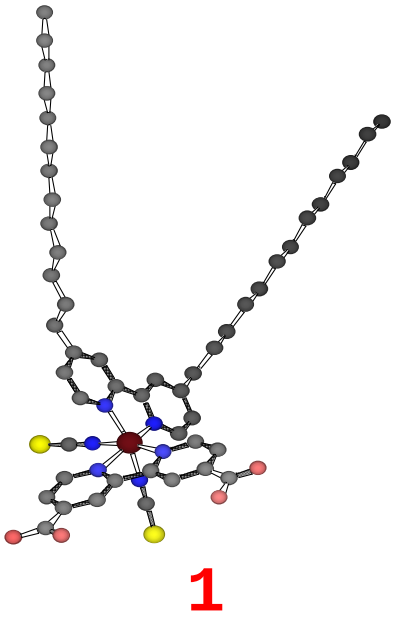
(3) The decreased electrostatic repulsion enhances sensitizer adsorption onto TiO_2

(1) No desorption occurs in the presence of water containg electrolytes, which enhances the long-term stability of the cell.



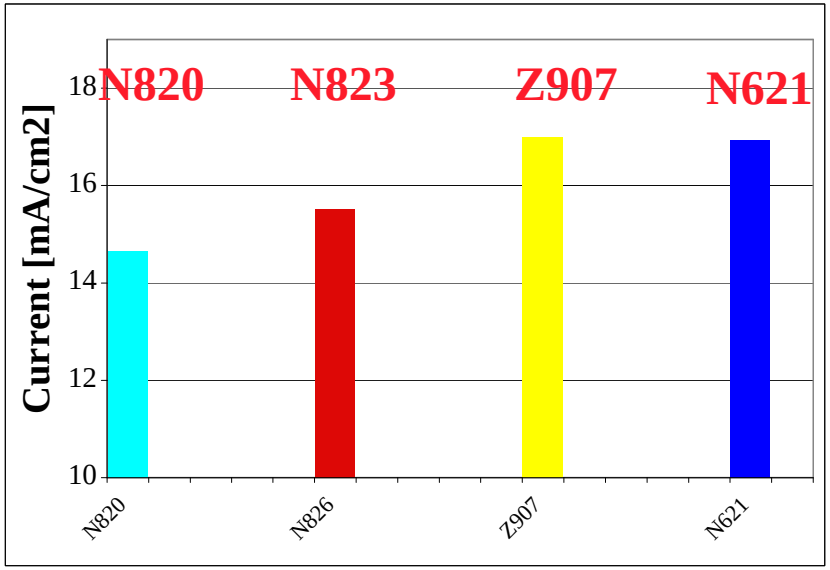
Photocurrent action spectrum obtained with Complex 1 attached to TiO_2 films

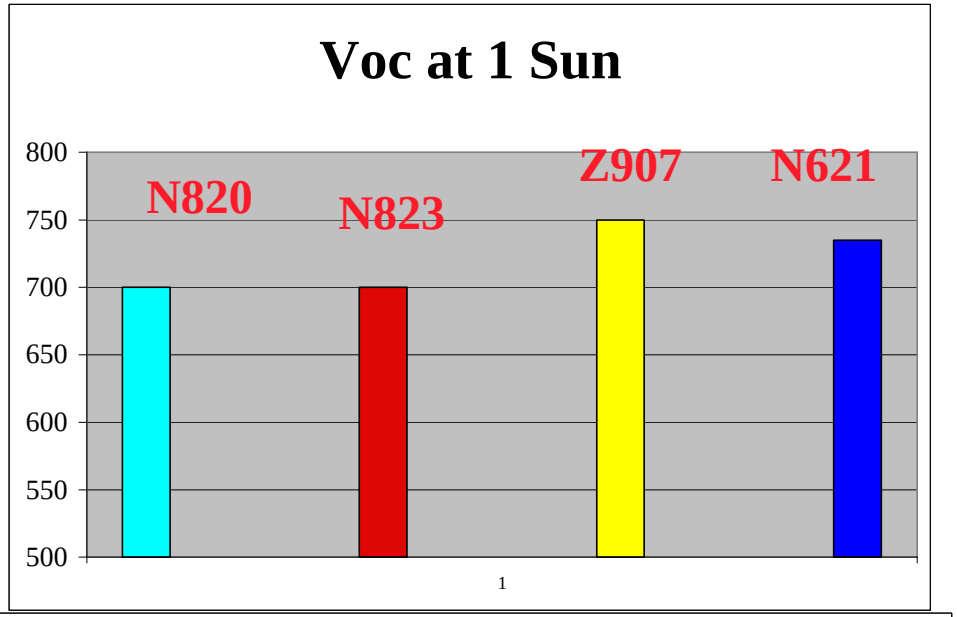


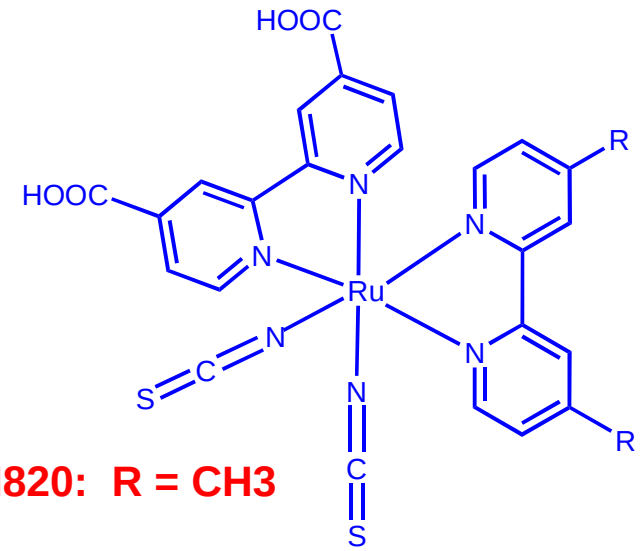


1

(Langmuir 2002, 18, 952 - 954)





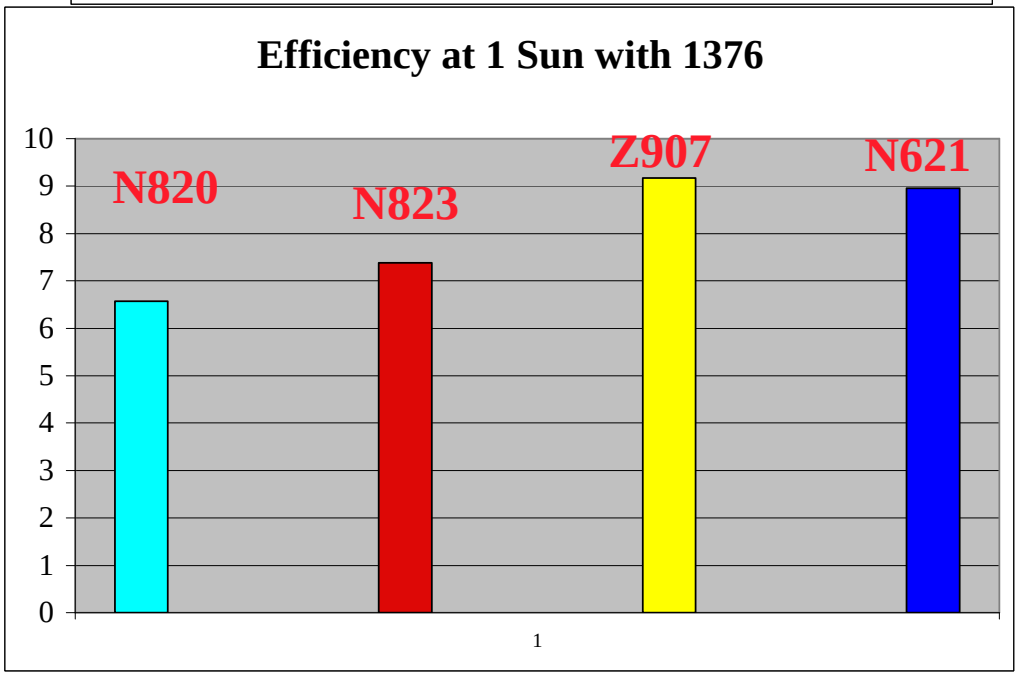


N820: R = CH3

N823: R = C6H13

Z907: R = C9H19

N621: R = C13H27



1376 = 0.6 M NMBII, 0.05 M iodine, 0.05 M LiI and 0.5 M tbpy in 50:50 (v/v) mixture of valeronitirile and acetonitrile

ATR-FTIR spectra of the hydrophobic complexes adsorbed on a 2 μm thick nanocrystalline TiO_2 film

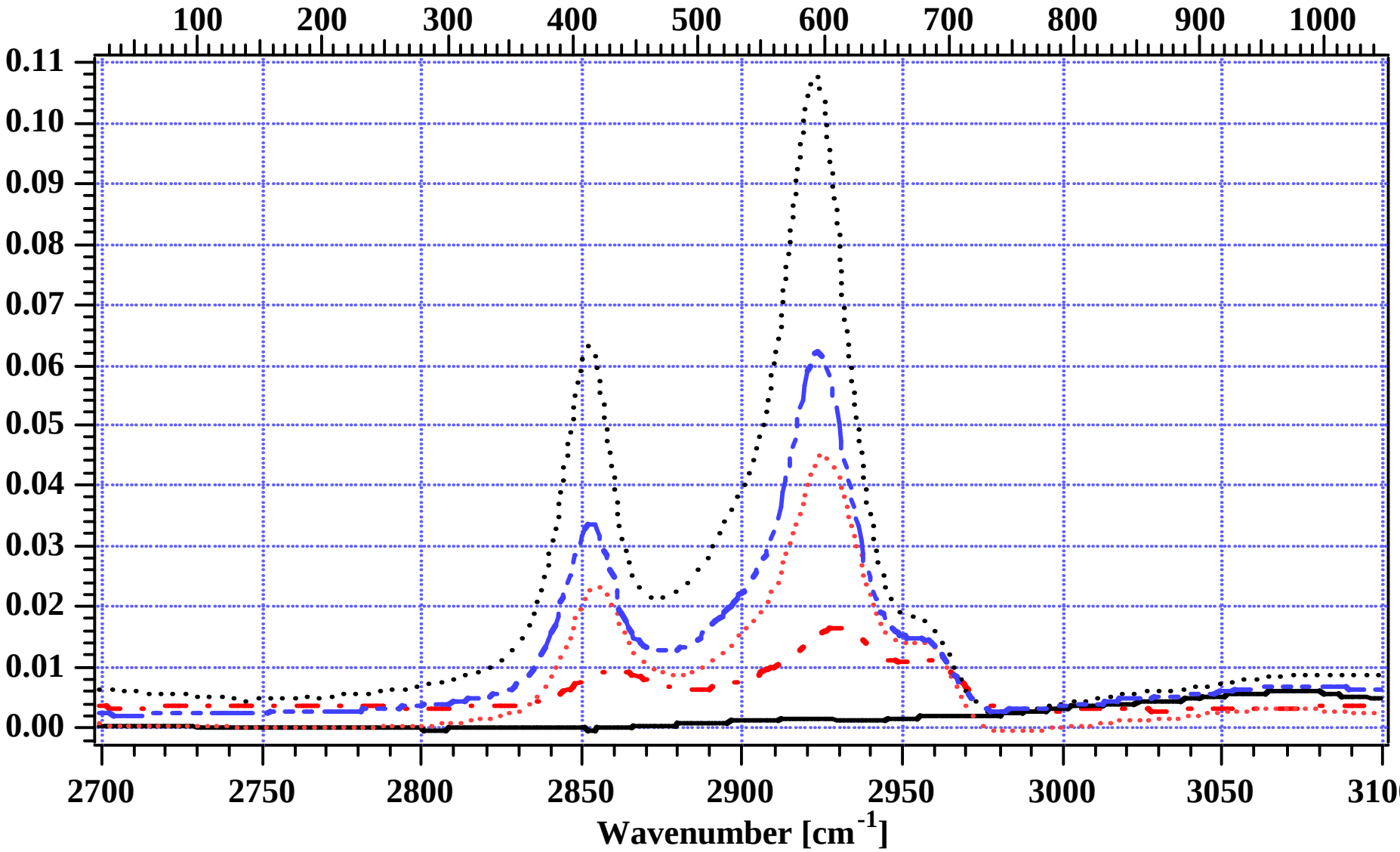
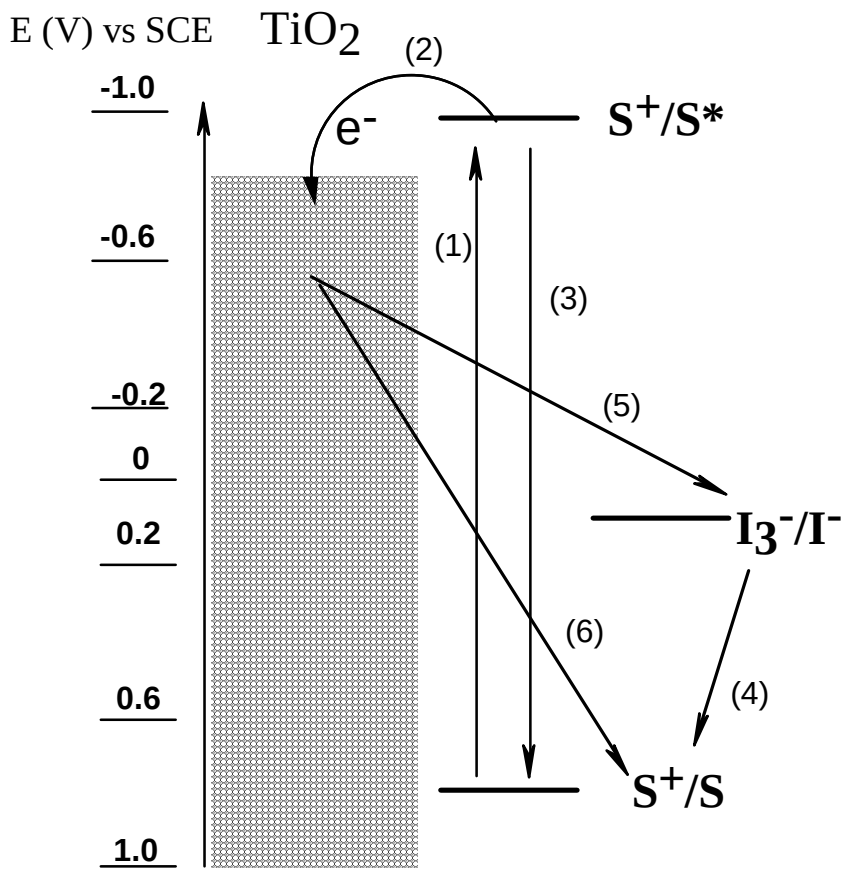
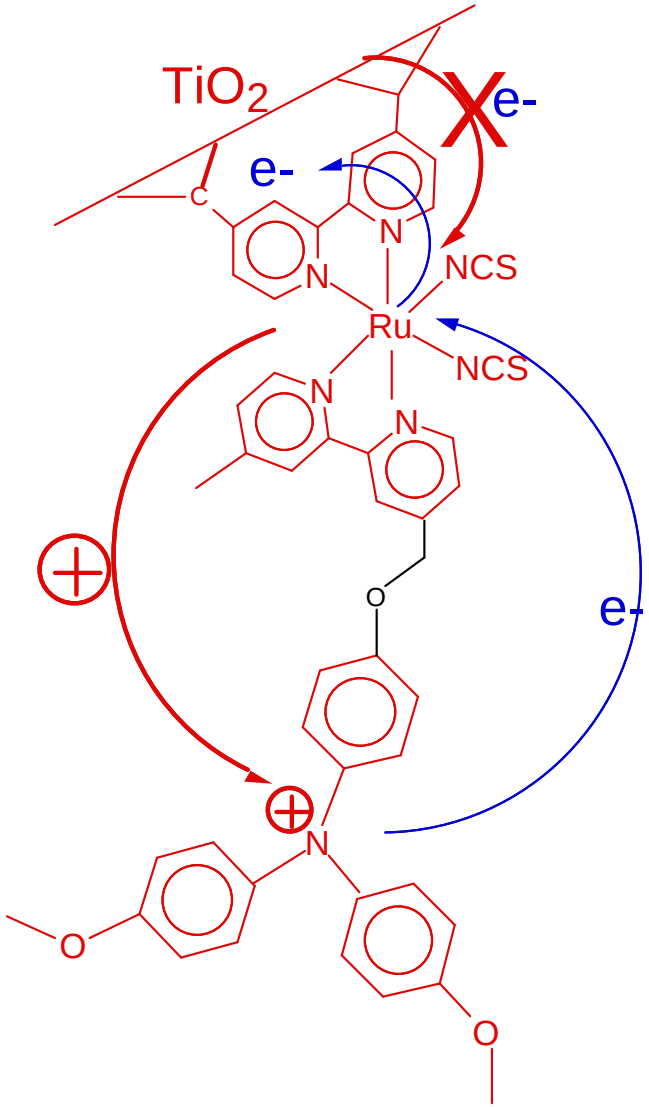


Illustration of the interfacial charge transfer processes in nanocrystalline dye sensitized solar cell.



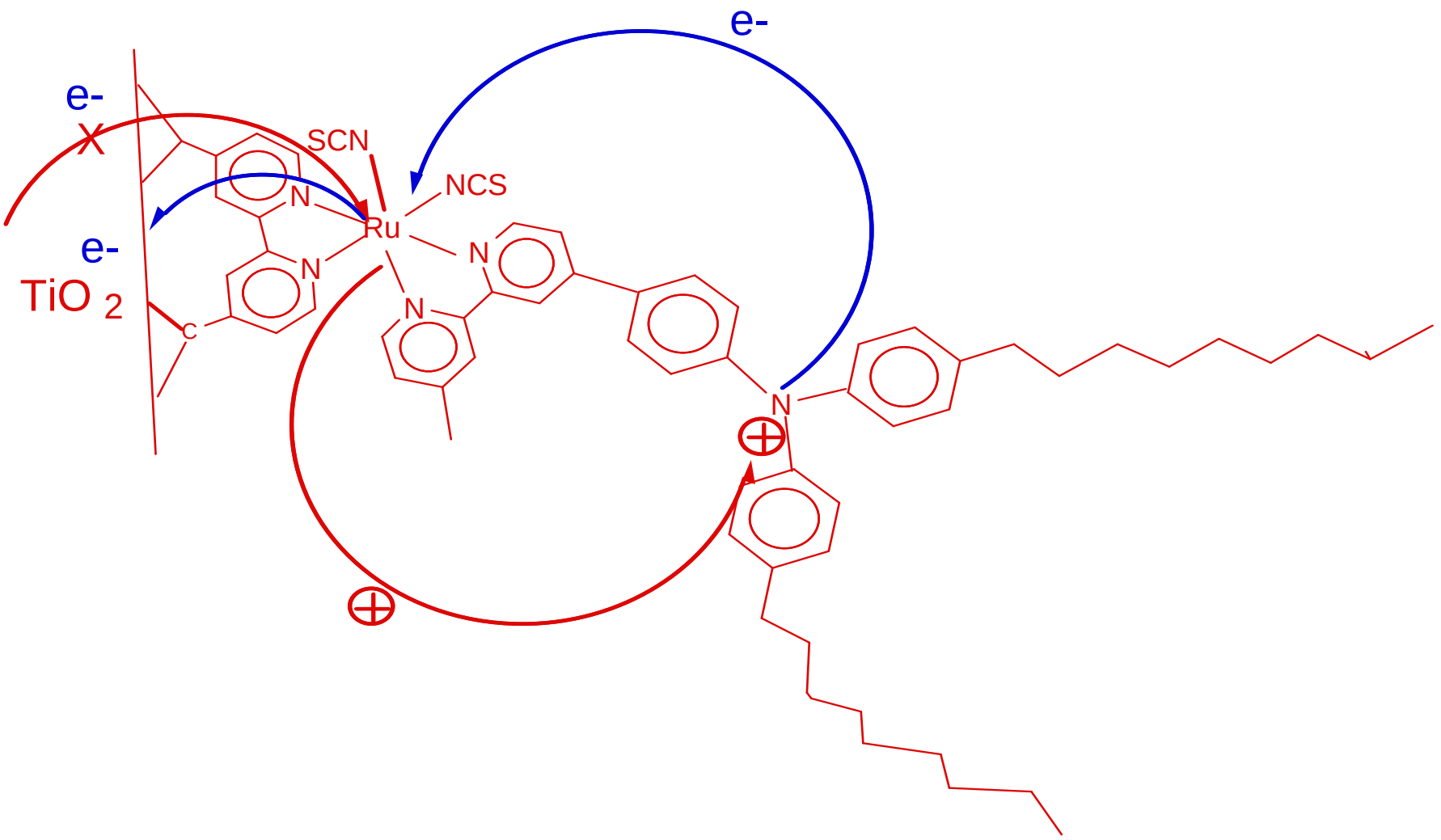
(1) An excited state: (2) electron injection onto the conduction band of TiO_2. (3) The oxidized sensitizer gets reduced by I^- / I_3^- redox couple. (4) The injected electrons into the conduction band may react either with the oxidized redox couple (5) or with oxidized dye molecule (6).

Ruthenium Sensitizer Containing Donor-Acceptor Ligands

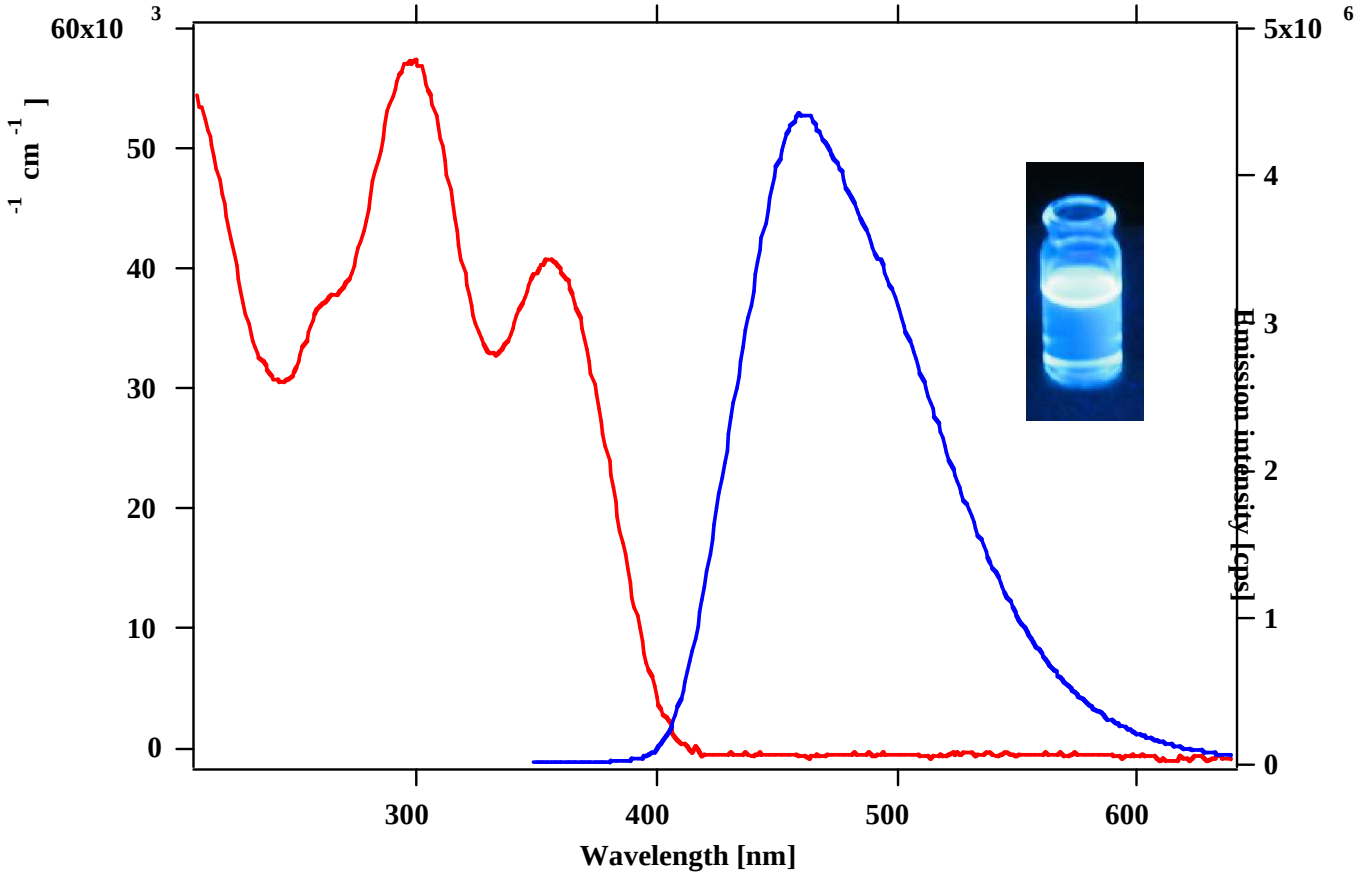


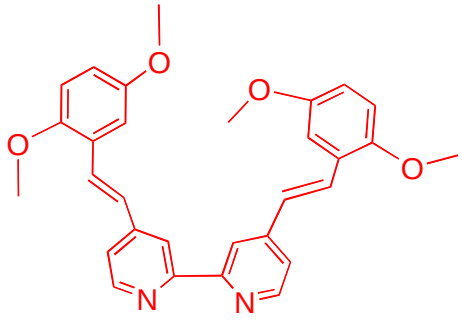
[a]Complex	[b]Abs. max. (nm) (ε/10^4 M^{-1} Cm^{-1})			$E^{1/2}_{ox}$ V vs. SCE	$E^{1/2}_{ox}$ V vs. SCE	$E^{1/2}_{red}$ V vs. SCE
	π–π*L 1	π–π*L 2	dπ-π*	**Donor L^1**	**Ru $^{III/II}$**	**L^2/L^{2-}**
$RuL^1L^2NCS_2$	296 (5.52)	312 (4.41)	400 (1.05) 545 (1.1)	**0.600**	**0.800**	**-1.6**

Engineering of Sensitizers to modulate interfacial properties

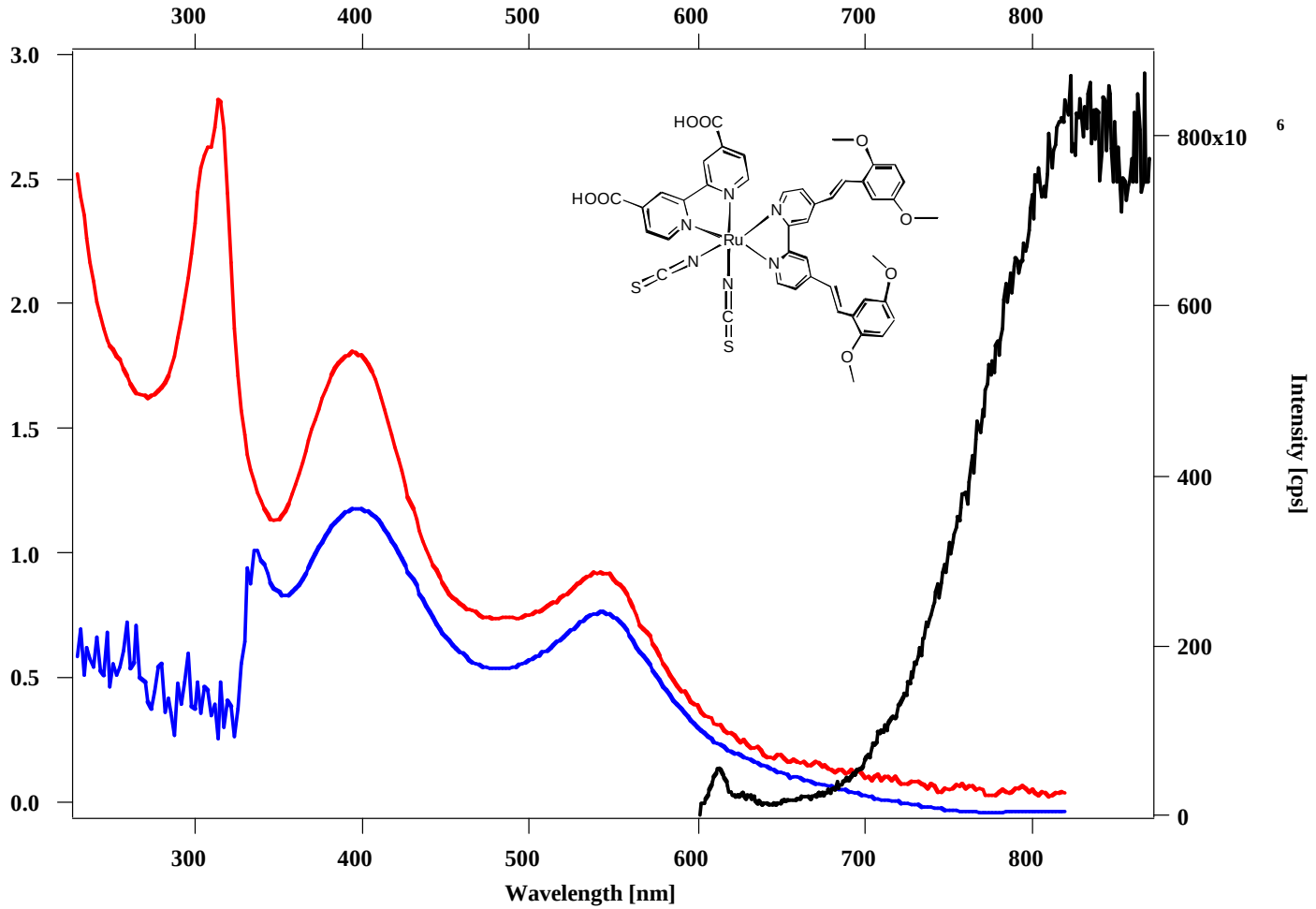


Absorption (red line) and emission (blue line) spectra of the 4,4'-di-(2-(3,6-dimethoxyphenyl)ethenyl)-2,2'-bipyridine in dichloromethane solution λ_{ex} 350 nm, at 298 K.

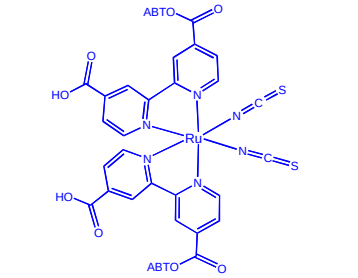


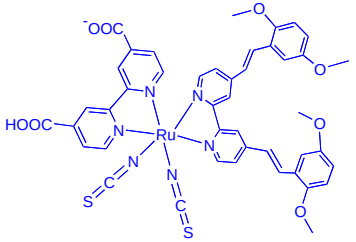


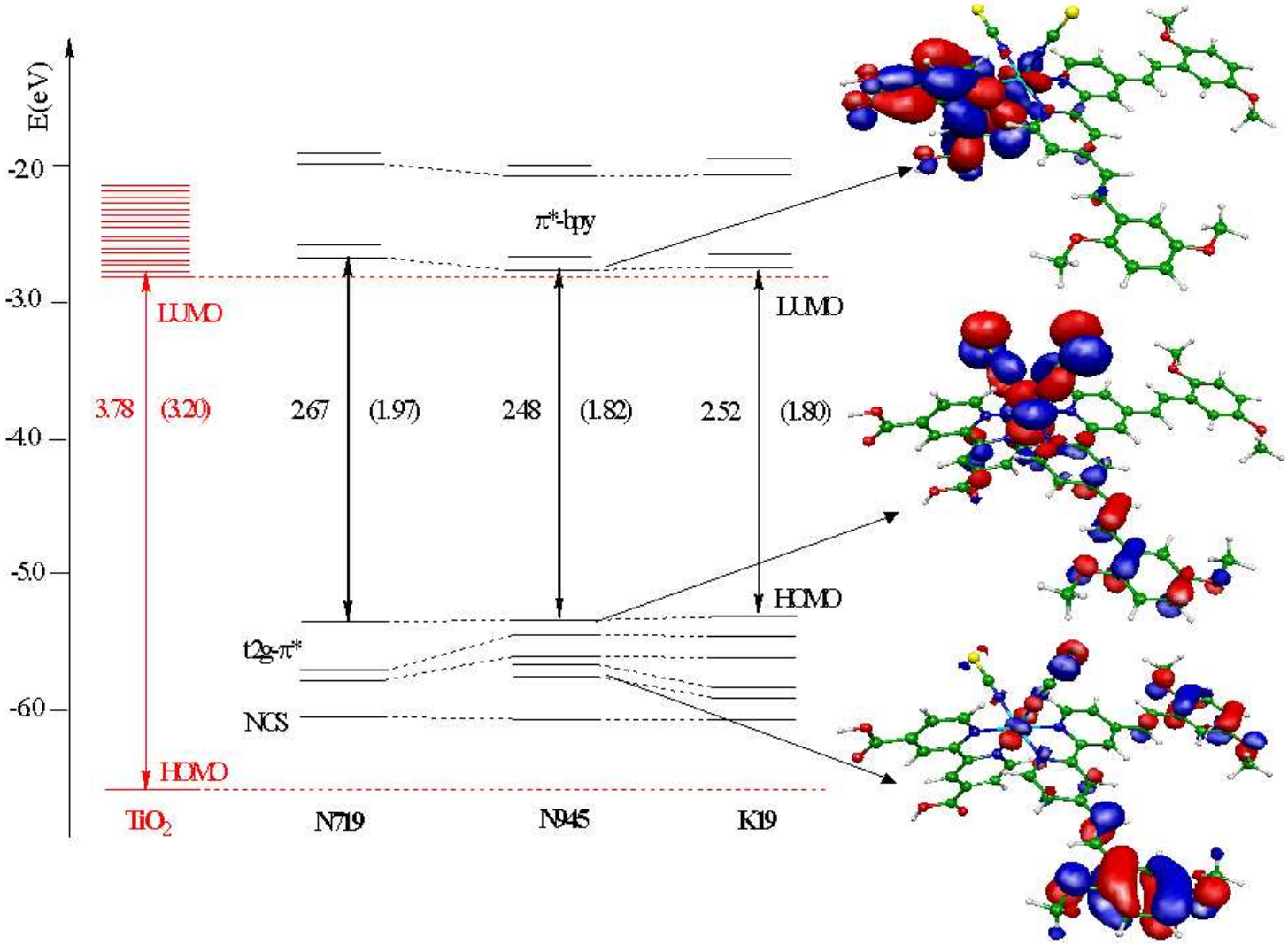
UV/Vis absorption spectra of N945 complex (red line) and adsorbed on a nanocrystalline 2 μm thick transparent TiO_2 film (blue line)

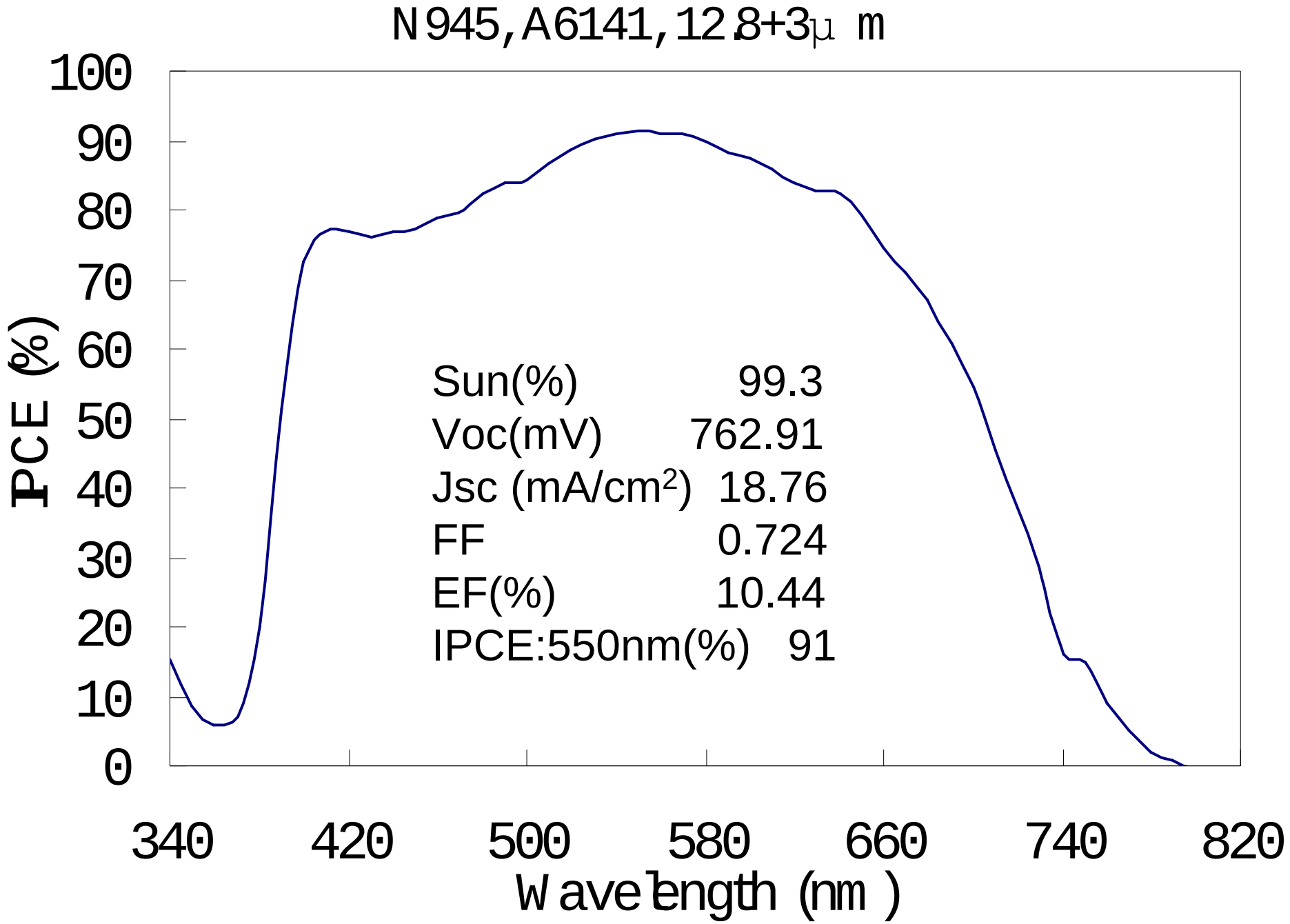


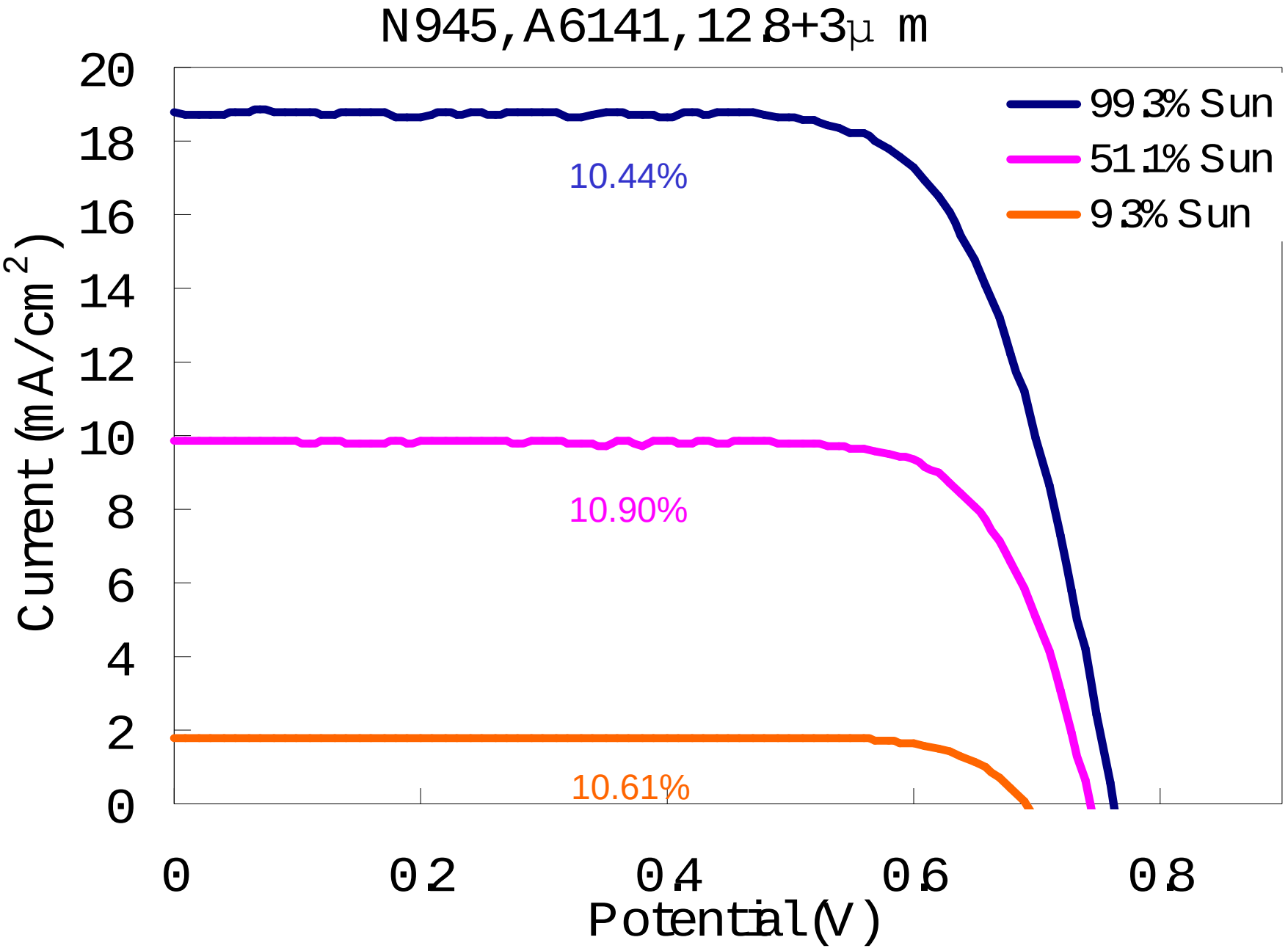
Molecular orbital energy diagram of N719, N945 and K19 compared to that of a TiO_2 nanoparticle model








N945,A6141,12.8+3μm
100
90
80
70
60
50
40
30
20
10
0
IPCE (%)
Sun(%) 99.3
Voc(mV) 762.91
Jsc (mA/cm2) 18.76
FF 0.724
EF(%) 10.44
IPCE:550nm(%) 91
340
420
500
580
660
740
820
Wavelength (nm)


N945,A6141,128+3μm
99.3% Sun
51.1% Sun
9.3% Sun
10.44%
10.90%
10.61%
Current (mA/cm²)
Potential(V)
0
2
4
6
8
10
12
14
16
18
20
0
0.2
0.4
0.6
0.8