Supporting Information

Molecular Engineering of Organic Sensitizers Containing $p$-Phenylene Vinylene Unit for Dye-Sensitized Solar Cells

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**General methods**

All reactions were carried out under an argon atmosphere. Solvents were distilled from appropriate reagents. 1,4-Bis(isopent-ox)-2-methylbenzene,\(^{15}\) 2-(bromomethyl)-1,4-bis(isopentoxy)benzene\(^{16}\) and diethyl (2,5-bis(isopentoxy)phenyl)methylphosphonate,\(^{17}\) diethyl(4-formyl-2,5-bis(isopentoxy)-phenyl)methylphosphonate,\(^{8}\) diethyl(2,5-bis(isopentoxy)-4-(5,5′-dimethyl-1,3-dioxan-2-yl)phenyl)methylphosphonate,\(^{18}\) and 2-iodo-9,9′-dimethylfluorene,\(^{19}\) 4-(N,N-Bis(9,9′-dimethylfluorene-2-yl))benzaldehyde\(^{20}\) were synthesized using a modified procedure of previous references. For general experimental details and instrumentation, see our previous publication.\(^{21}\)
1 (CDCl₃)

^{13}C
$\text{2 (CDCl}_3\text{)}$

$^1\text{H}$
$2 \text{ (CDCl}_3\text{)}$

$^{13}\text{C}$
$3\ (\text{CDCl}_3)$

$^{13}\text{C}$
$^{31}\text{P}$

$3 \text{ (CDCl}_3\text{)}$
$4 \text{ (CDCl}_3\text{)}$

$^1H$
$4 \text{ (CDCl}_3\text{)}$ 

$^{13}\text{C}$
$^31$P NMR spectrum of compound 4 (CDCl₃)
$\textbf{5 (CDCl}_3\textbf{)}$

$^{13}\text{C}$
$^{31}\text{P}$

5 (CDCl$_3$)
$^{31}\text{C}$

6 (CDCl$_3$)
$^1$H NMR spectrum of compound 7 (CDCl$_3$)
$\text{7 (CDCl}_3\text{)}$

$^{13}\text{C}$
$^1$H NMR (CDCl$_3$)
$8 \text{ (CDCl}_3\text{)}$

$^{13}\text{C}$
$9 \text{ (CDCl}_3\text{)}$

$^1H$
$9_{(CDCl_3)}$

$^{13}$C
$^{1}H$

$^{10} (CDCl_{3})$
\[ \text{10 (CDCl}_3) \]

\[ ^{13}\text{C} \]
11 (CDCl₃)

$^1\text{H}$
11 (CDCl₃)

$^{13}$C
12 (CDCl₃)

$^1$H
$^{13}$C
$^{13}\text{C}$

13 (CDCl$_3$)

S32
14 (CDCl₃)

$^1\text{H}$
15 (CDCl$_3$)

$^1$H
15 (CDCl₃)

$^{13}$C
16 (CDCl₃)

$^1$H
$^{13}\text{C}$

16 (CDCl$_3$)

S38
Figure S1. Cyclic voltammogram of the JK-59 measured in THF solution containing 0.1M \((n-C_4H_9)_4NPF_6\) using a glassy carbon as a working and a Pt counter electrode with a scan rate of 50 mVs\(^{-1}\).