for

Bis(2,6-di(pyridin-2-yl)pyridin-4-yl)-6,6'-(1,2diselanediyl)dihexanoate

Evelyn Popa ¹, Adelina A. Andelescu ^{1,*}, Valentin Badea ², Paula Svera (m. Ianăşi)³ and Elisabeta I. Szerb ¹

- ¹ "Coriolan Drăgulescu" Institute of Chemistry, Romanian Academy, 300223 Timisoara, Romania
- ² Department of Applied Chemistry and Organic and Natural Compounds Engineering, Politehnica University Timisoara, 300001 Timisoara, Romania
- ³ National Institute for Research and Development in Electrochemistry and Condensed Matter, 300569 Timisoara, Romania
- * Correspondence: aandelescu@acad-icht.tm.edu.ro



Figure S1. FT-IR spectrum of compound 1



Figure S2. ¹H-NMR spectrum of compound 1 recorded in CDCl₃



Figure S3. ¹³C-NMR spectrum of compound 1 recorded in CDCl₃



Figure S4. ¹H-¹H (COSY) spectrum of compound 1 recorded in CDCl₃



Figure S5. HSQC spectrum of compound 1 recorded in CDCl₃



Figure S6. HMBC spectrum of compound 1 recorded in CDCl₃



Figure S7. Raman spectrum of compound 1

Atom labeling	1H δ/ppm (J/Hz)	13C	COSY	HMBC
		δ/ppm		
С	1.34 - 1.45, m,	28.84	HD	H ^A
	2H			
D	1.61, p, $J = 7.4$	24.13	H ^C	$\mathrm{H}^{\mathrm{A}}\mathrm{H}^{\mathrm{B}}\mathrm{H}^{\mathrm{C}}$
	Hz, 2H			
В	1.69, p, $J = 7.4$	30.56	H ^A	H ^A H ^D
	Hz, 2H			
Е	2.31, t, J = 7.4 Hz,	33.92	HD	$H^{D}H^{C}$
	2H			
А	2.84, t, J = 7.4 Hz,	29.66	H ^B	H ^B
	2H			
G	10.71, br, 1H	180.13	-	H ^{D,E}

Table S1 . 1	D and 2D N	MR of comp	ound 1 recor	ded in CDCl3.



Figure S8. FT-IR spectrum of compound 2 plotted against compound 1



Figure S9. ¹H-NMR spectrum of compound 2 recorded in CDCl₃.



Figure S10. ¹³C-NMR spectrum of compound 2 recorded in CDCl₃.



Figure S11. $^{1}H^{-1}H$ (COSY) spectrum of compound 2



Figure S12. HSQC spectrum of compound 2



Figure S13. HMBC spectrum of compound 2

Atom labeling	1H	13C	COSY	HMBC
С	1.39 – 1.54, m, 2H	28.91	H ^{B,D}	H ^{B,D}
D, B	1.74, q, J = 7.5 Hz, 4H	30.62,	$\mathrm{H}^{\mathrm{A}},\mathrm{H}^{\mathrm{C}},\mathrm{H}^{\mathrm{E}}$	H ^{B,D}
		24.32		
Ε	2.54, t, <i>J</i> = 7.4 Hz, 2H	34.26	H ^{B,D}	H ^C
Α	2.87, t, J = 7.4 Hz, 2H	29.59	H ^{B,D}	H ^C
2	7.23 t (ddd, J = 7.5,	124.12	$\mathrm{H}^{1},\mathrm{H}^{3}$	$\mathrm{H}^{1},\mathrm{H}^{4}$
	4.7, 1.2 Hz, 2H)			
3	7.75 t (td, J = 7.7, 1.8	136.90	$\mathrm{H}^2,\mathrm{H}^4$	H^4
	Hz, 2H)			
7	8.15 (s, 2H)	114.28	-	H^{6}
4	8.51 d (dt, $J = 8.0, 1.1$	121.30	H ³	H^2
	Hz, 2H)			
1	8.59 d (ddd, J = 4.7,	149.14	H^2	$\mathrm{H}^2,\mathrm{H}^3$
	1.8, 0.9 Hz, 2H)			
6	-	155.33	-	${\rm H}^{3}, {\rm H}^{4}, {\rm H}^{7}$
5	-	157.56	-	H ⁴
8	-	159.72	-	H^{7}
F	-	170.85	-	$H^{E}, H^{B,D}$

Table S2. 1D and 2D NMR assignement of compound 2 recorded in CDCl₃.