Supplementary Material (ESI) for New Journal of Chemistry

Mesogenic, trimeric, halogen-bonded complexes from alkoxystilbazoles and 1,4-diiodotetrafluorobenzene

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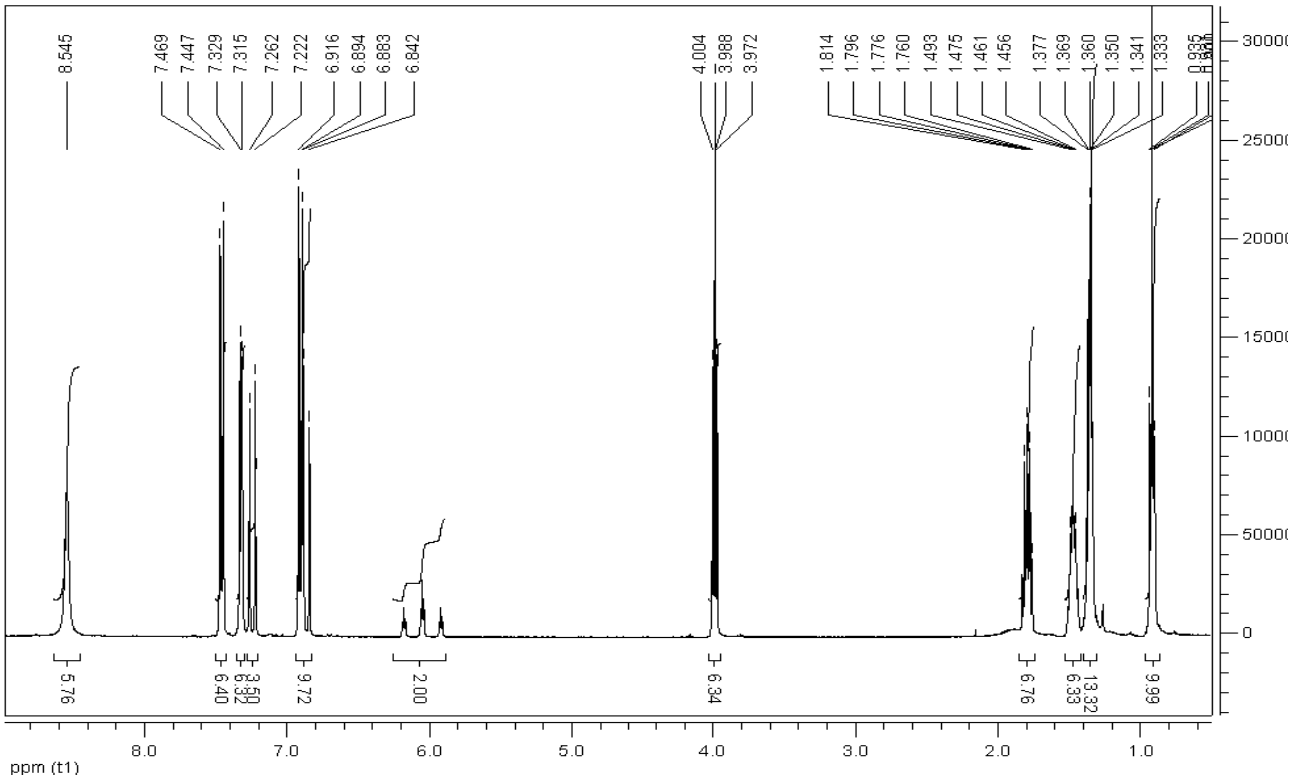
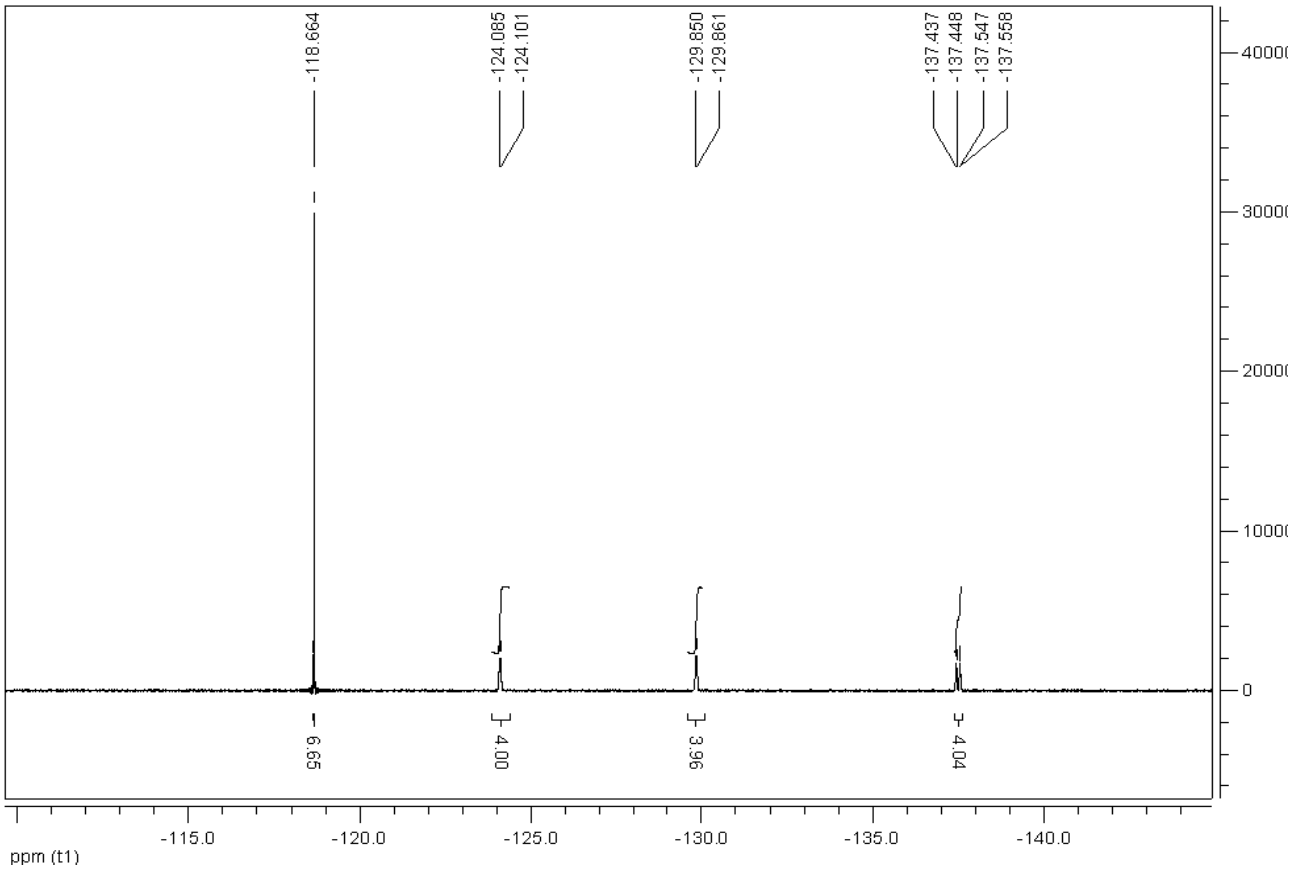
Electronic Supplementary Information

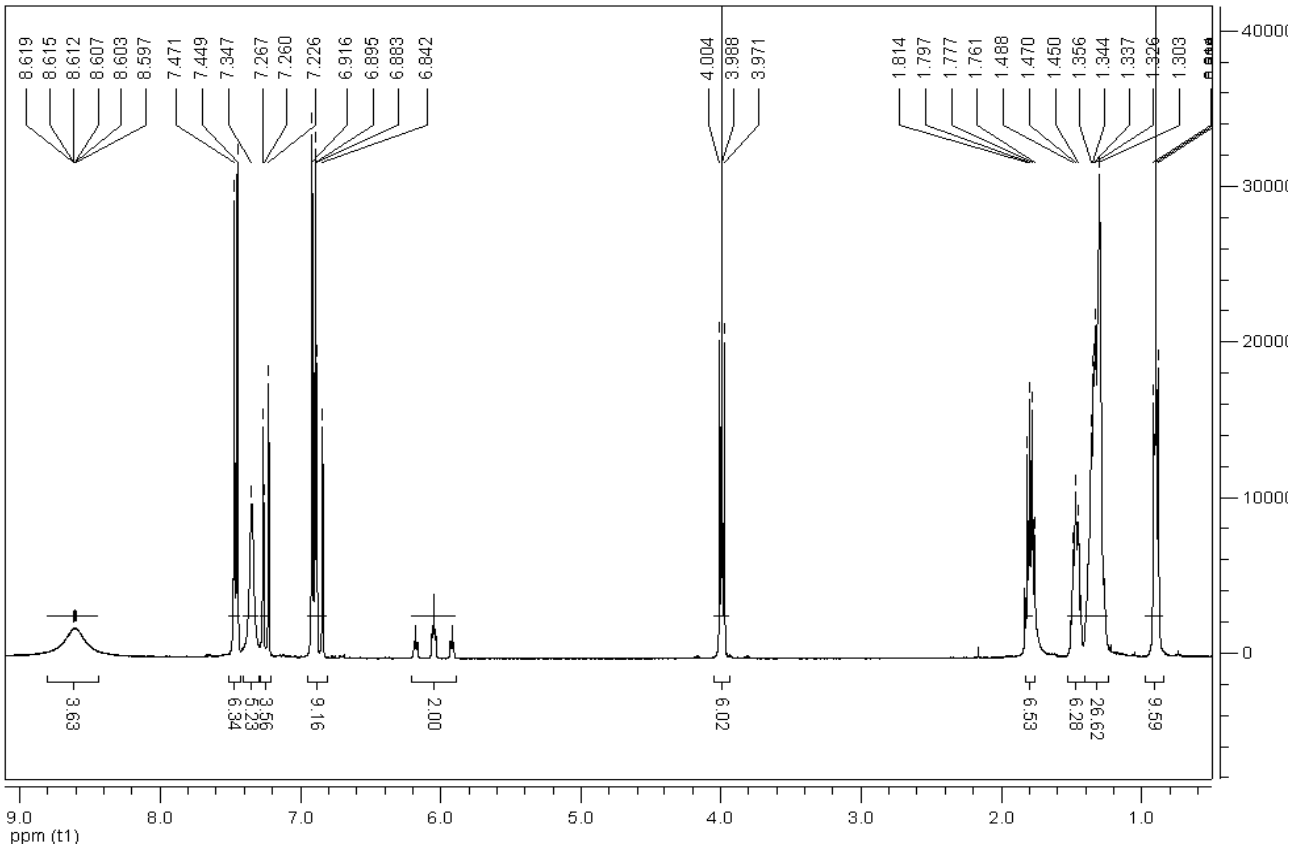
^{1}H-NMR (500 MHz, $CDCl_3$): 3-6 + 1H,6H-perfluorohexane.



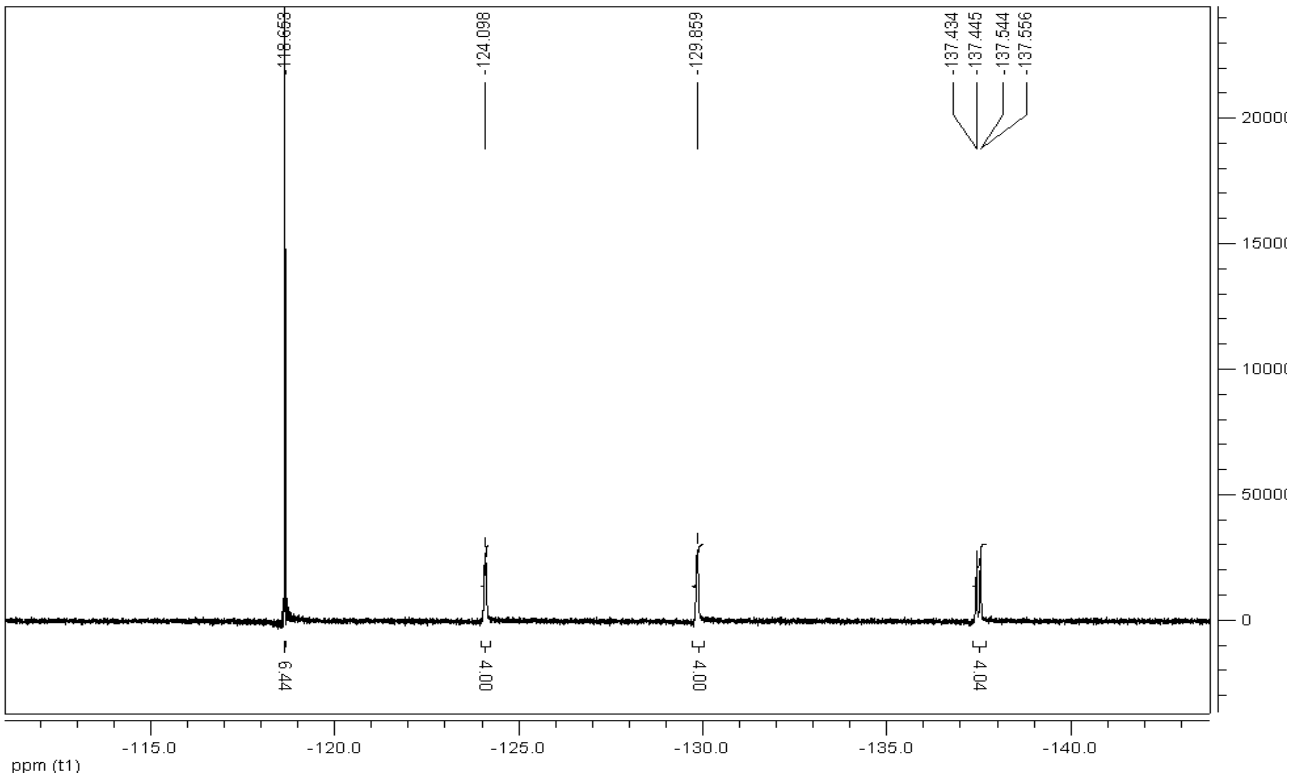
^{19}F-NMR (470 MHz, $CDCl_3$): 3-6 + 1H,6H-perfluorohexane.



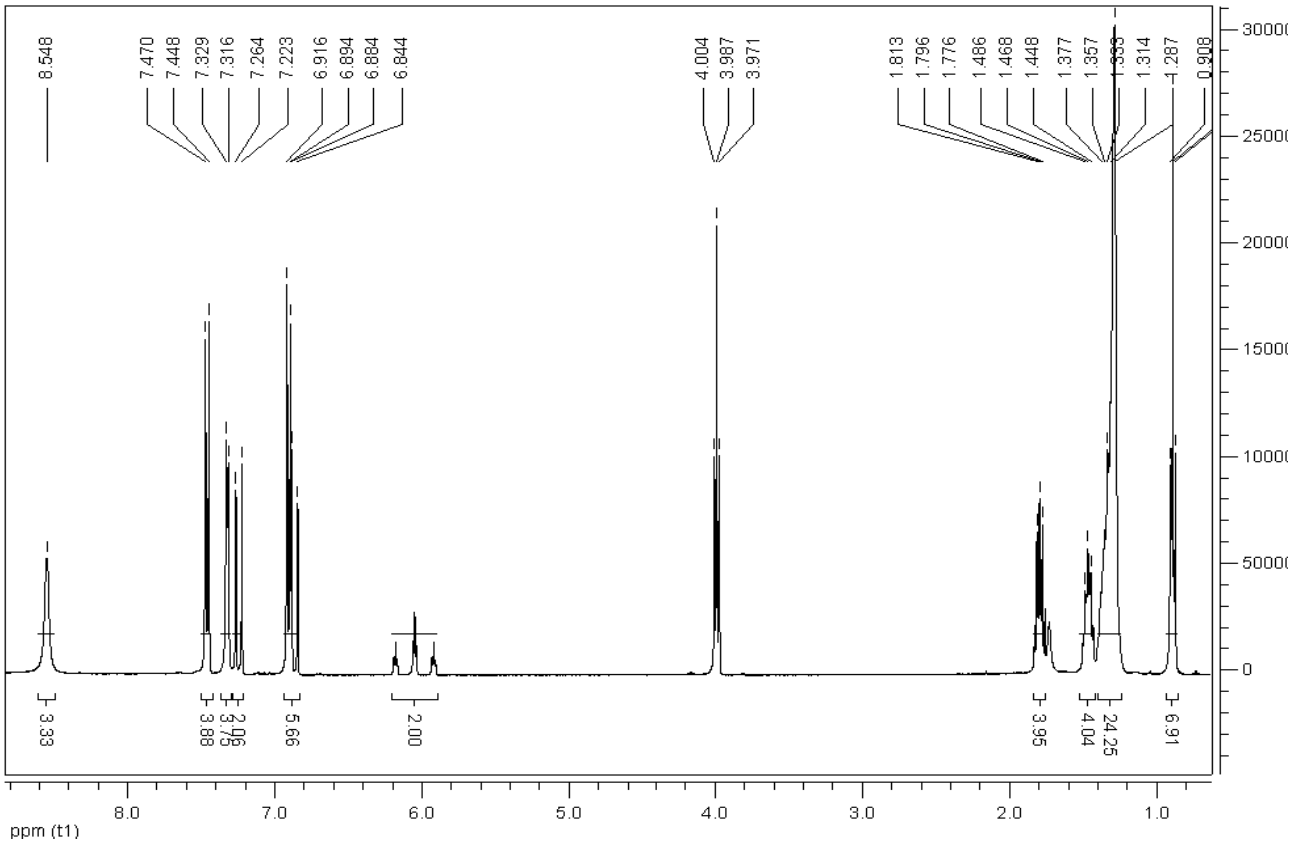
^{1}H-NMR (500 MHz, $CDCl_3$): 3-8 +1H,6H-perfluorohexane.



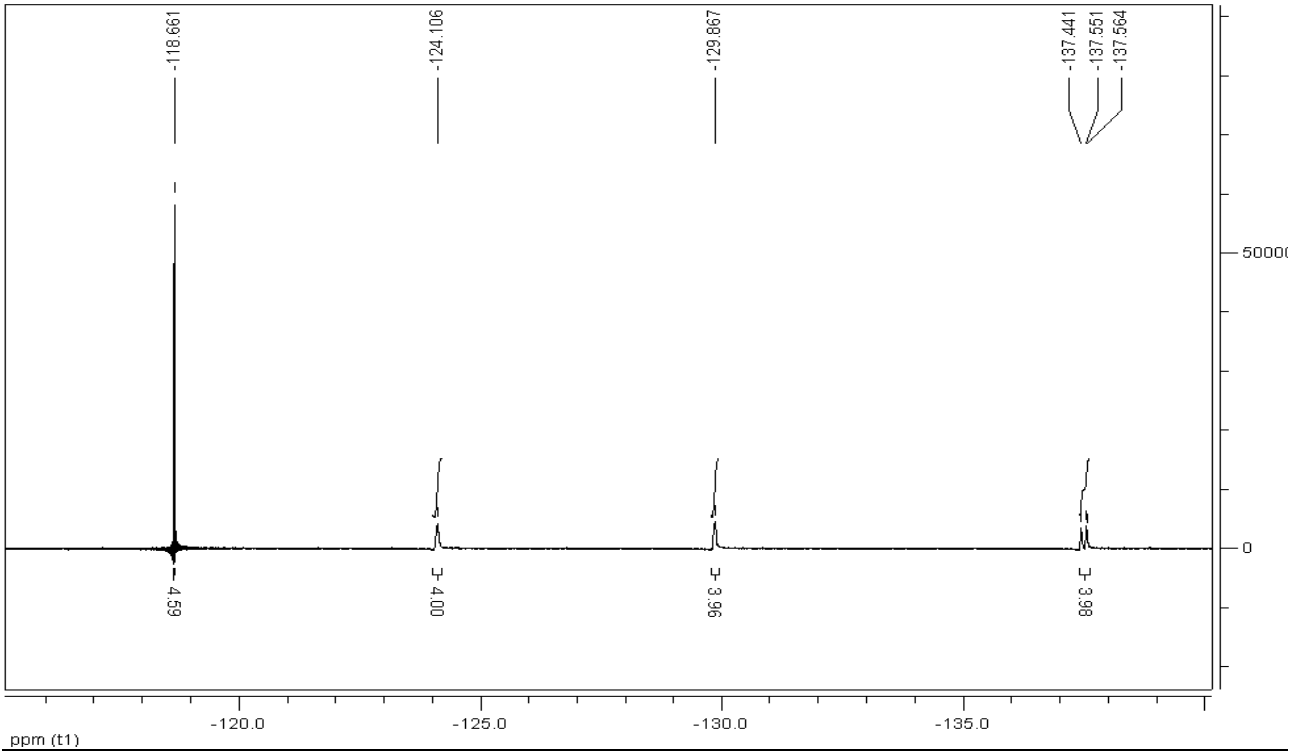
^{19}F-NMR (470 MHz, $CDCl_3$): 3-8 + 1H,6H-perfluorohexane.



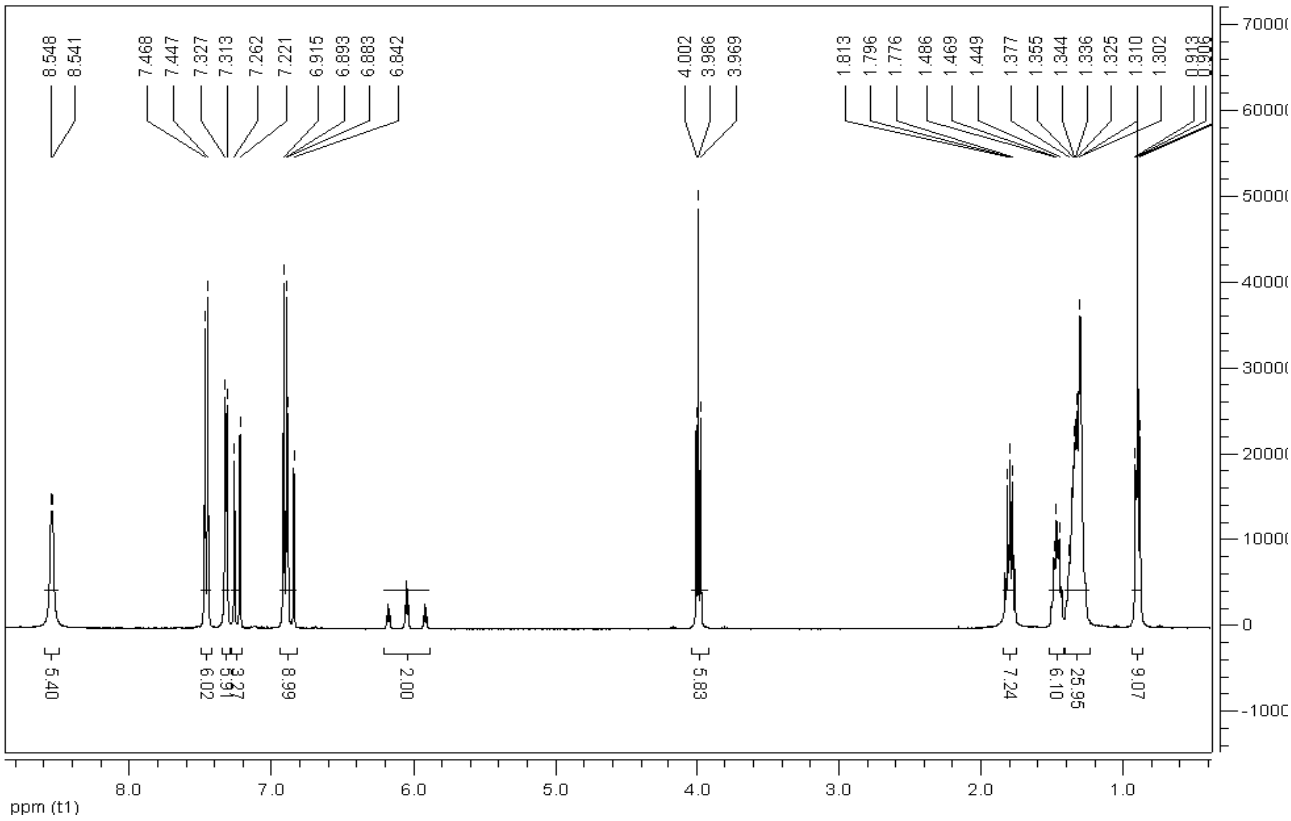
^{1}H-NMR (500 MHz, $CDCl_3$): 3-10 +1H,6H-perfluorohexane.



^{19}F-NMR (470 MHz, $CDCl_3$): 3-10 + 1H,6H-perfluorohexane.



^{1}H-NMR (500 MHz, $CDCl_3$): 4 +1H,6H-perfluorohexane.



^{19}F-NMR (470 MHz, $CDCl_3$): 4 +1H,6H-perfluorohexane.

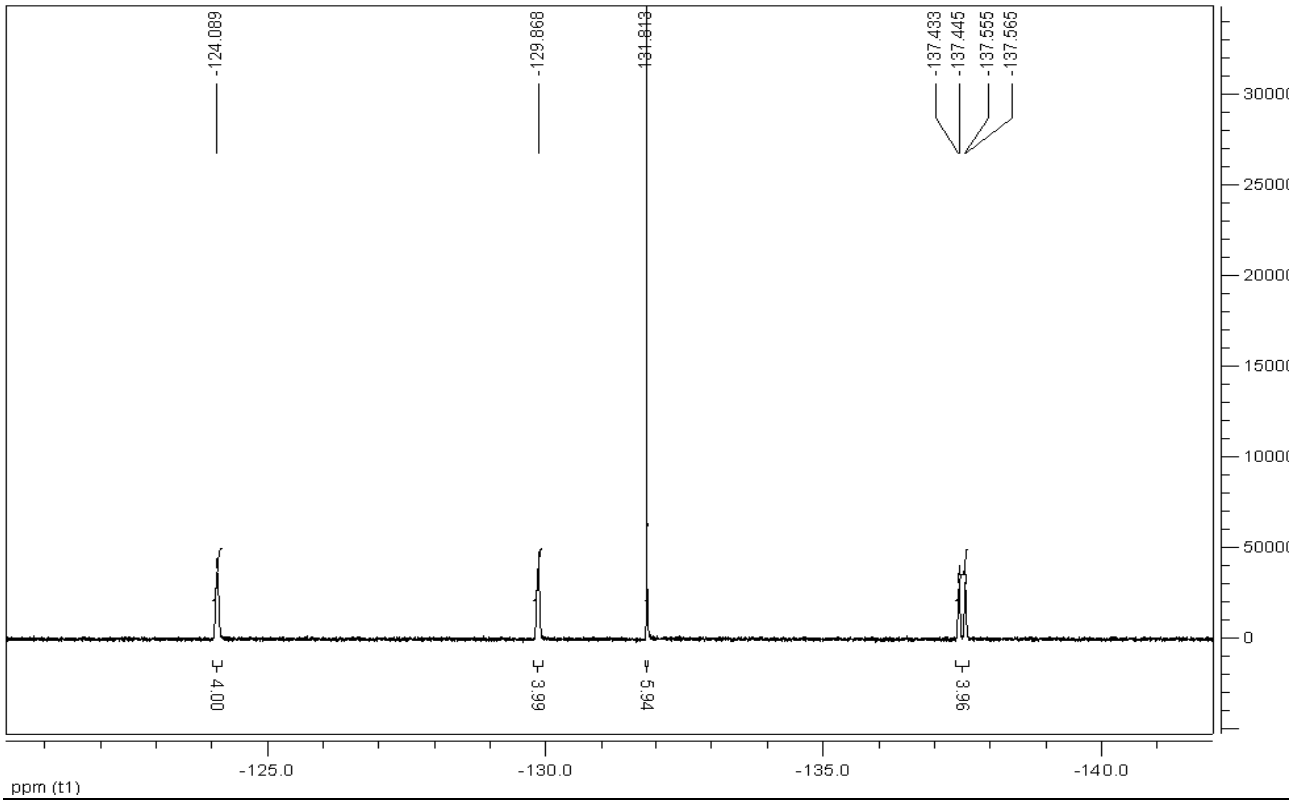


Table 1-ESI. Evaluation ratio stilbazole:dihalotetrafluorobenzene using as internal standard 1H,6H-perfluorohexane.

Entry	H[a]	F[b]	Ratio[c]
3-6	3.33	1.66	2:1
3-8	3.20	1.61	2:1
3-10	2.30	1.15	2:1
4	3.00	1.48	2:1

a: The value was obtained assigning to the signal (tt) at 6.05 ppm, corresponding to the hydrogens in 1H,6H-perfluorohexane, the integral value 2, then the peak at 0.9 ppm, corresponding to the CH_3 of alkyl chain in the stilbazole, was integrated. The acquired value was divided by three, the number of protons in the methyl group of the hydrocarbon molecule.

b: The value was obtained assigning to the signals related to the difluoromethylene groups of 1H,6H-perfluorohexane at -124, -129 and -137 ppm the integral value 4 for each peak, then the peak corresponding to the aromatic –C=C*F*- in the dihaloperfluorobenzene was integrated. The acquired value was divided by four; the number of fluorine atoms in the tetrafluoro arene.

c: Ratio between hydrocarbon molecules (*e.g.* stilbazole) and perfluorocarbon molecules (*e.g.* dihalotetrafluorobenzene) in the samples.

Table 2-ESI. Shift changes of ^{19}F NMR signals of 1,4-diiodotetrafluorobenzene and 1,4-dibromotetrafluorobenzene in the presence of nitrogen donors (4-alkoxy-4'-stilbazoles).[a]

Entry	δ_F (ppm)	$\Delta\delta_F$ (ppm)
3-6	-118.65	0.12
3-8	-118.64	0.11
3-10	-118.64	0.11
4	-131.84	0.03

a: Data are referred to $CDCl_3$ solution wherein the concentrations of pure halogen-bonding donors and related complexes are 0.3 M.

$\Delta\delta_F = \delta$(pure $C_6F_4I_2$) – δ($C_6F_4I_2$ complex).

Pure diiodotetrafluorobenzene: δ = -118.56.

Pure dibromotetrafluorobenzene: δ = -131.83.

Table 3-ESI. Infrared absorptions of electron acceptor and donor modules compared to changes observed in the spectra of complexes **3**-6, **3**-8, **3**-10 and **4**.

Vibrations related to the hydrocarbon compound.

	ν_{C-H} (cm^{-1})		
Entry	**Alkyl chain: C6**	**Alkyl chain: C8**	**Alkyl chain: C10**
stilbazole[a]	3021	3022	3022
3-6	3034		
3-8		3028	
3-10			3031
4		3029	

a: ν_{C-H} (cm^{-1}) of pure compounds

Vibrations related to the fluoro phenyl compound.

Entry	$\nu_{C=CF}$ (cm^{-1})	
diiodotetrafluorobenzene[a]	1457	
dibromotetrafluorobenzene[a]	1479	
3-6	1454	
3-8	1450	
3-10		1450
4	1471	

a: (cm^{-1}) of pure compounds

Entry	$\nu_{C=CF}$ (cm^{-1})	
diiodotetrafluorobenzene[a]	940	
dibromotetrafluorobenzene[a]	952	
3-6	937	
3-8	935	
3-10		935
4	948	

a: (cm^{-1}) of pure compounds

Entry	$\nu_{C=CF}$ (cm^{-1})	
diiodotetrafluorobenzene[a]	758	
dibromotetrafluorobenzene[a]	785	
3-6	750	
3-8	754	
3-10		755
4	785	

a: (cm^{-1}) of pure compounds

Figure 1-ESI. IR spectrum of **3**-6.
Top: region between 3100-2500 cm^{-1}; bottom: region between 1700-550 cm^{-1}.

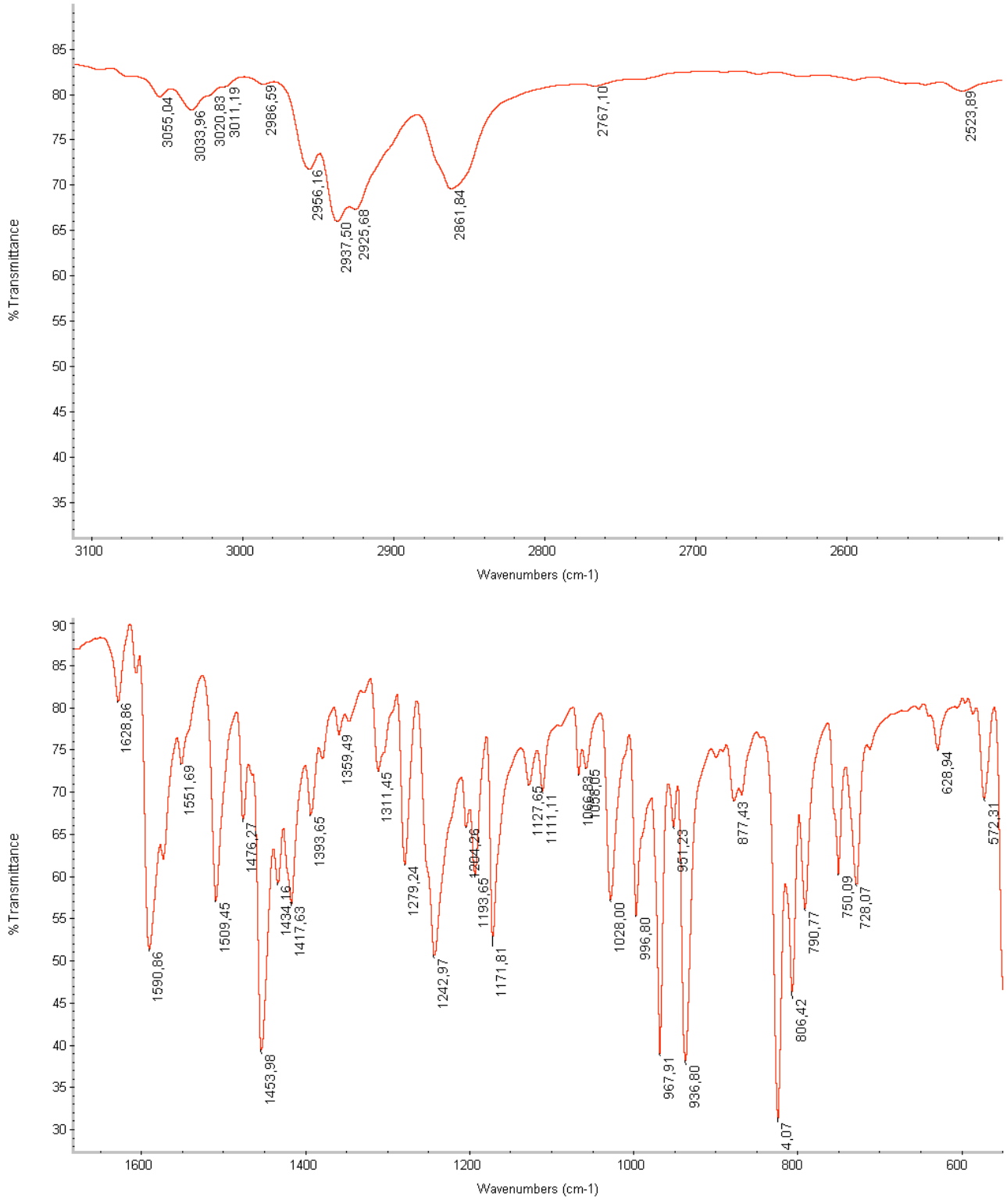


Figure 2-ESI. IR spectrum of **3**-8.
Top: region between 3100-2500 cm^{-1}; bottom: region between 1700-550 cm^{-1}.

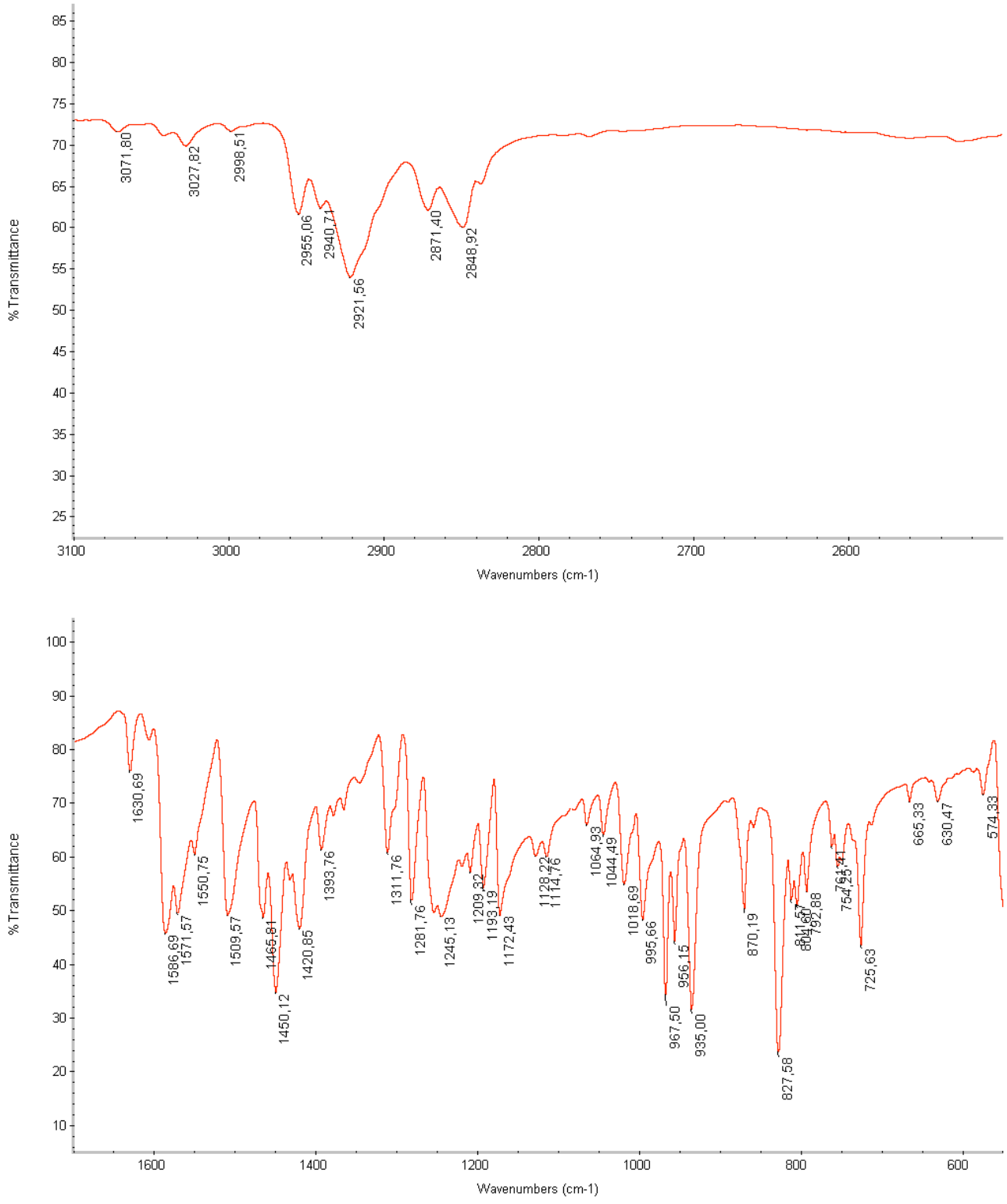


Figure 3-ESI. IR spectrum of **3**-10.
Top: region between 3100-2500 cm^{-1}; bottom: region between 1700-550 cm^{-1}.

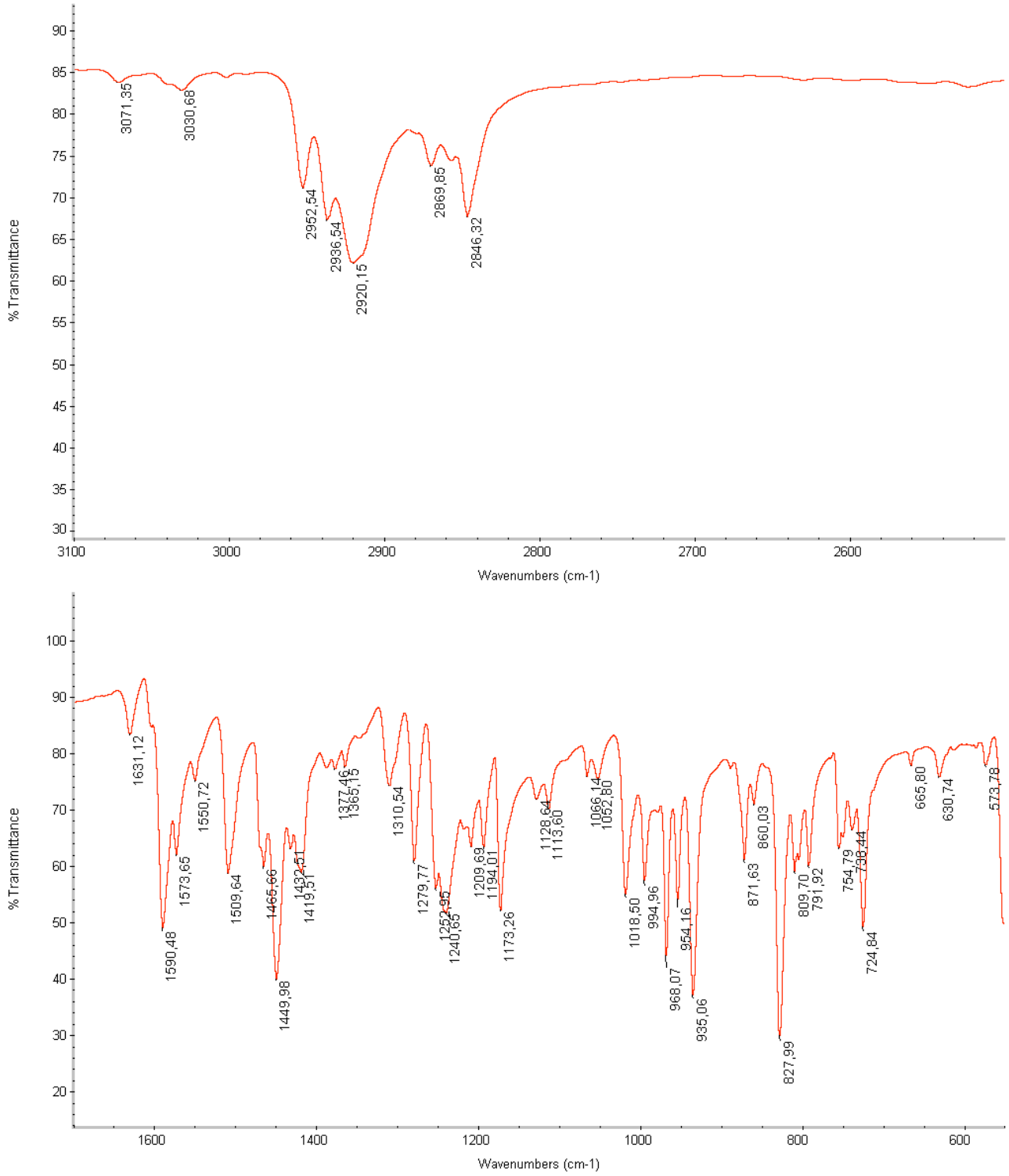


Figure 4-ESI. IR spectrum of **4**.
Top: region between 3100-2500 cm^{-1}; bottom: region between 1700-550 cm^{-1}.