

Supporting Information

For

The Impact of P-Substituents on the Structures, Spectroscopic Properties, and Reactivities of POCOP-Type Pincer Complexes of Nickel(II)

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List of items :

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3. UV-Vis spectra for complexes $(\text{POCOP}^{i\text{-Pr}})\text{Ni-OCOCH}_3$, $(\text{POCOP}^{i\text{-Pr}})\text{Ni-OSO}_2\text{CF}_3$ and complexes **2-6**

Table 1. ¹H NMR data for complexes 1-6

	<i>o</i> -H (qq)*	<i>m</i> -H (qt)	<i>p</i> -H (t)	H3/H5 (d)	H4 (t)
A	7.68 (8H)	7.16 (8H)	7.13 (8H)	6.98 (8H)	7.03 (8H)
Ni-Br	8.25 (8H)	7.07 (m, 12H) p+m		6.68 (8H)	7.13 (8H)
Ni-CN	8.22 (m)	7.04 (m, 12H) p+m		6.92(8)	7.10(8)
Ni-Otf	8.10(m)	7.13(m, 12H) p+m		6.66(8)	6.94(8)
Ni-Oac	8.2 (m)	7.15(m, 12H) p+m		6.78(8)	7.08(8)
Ni- ONO₂	7.91(m)	6.97(m, 12H) p+m		6.78(8)	6.88(8)
Ni- CCPh	8.40 (qq, 10)	7.07 (m,15H) p+m-H of CCPh		6.99(8)	7.14(8)

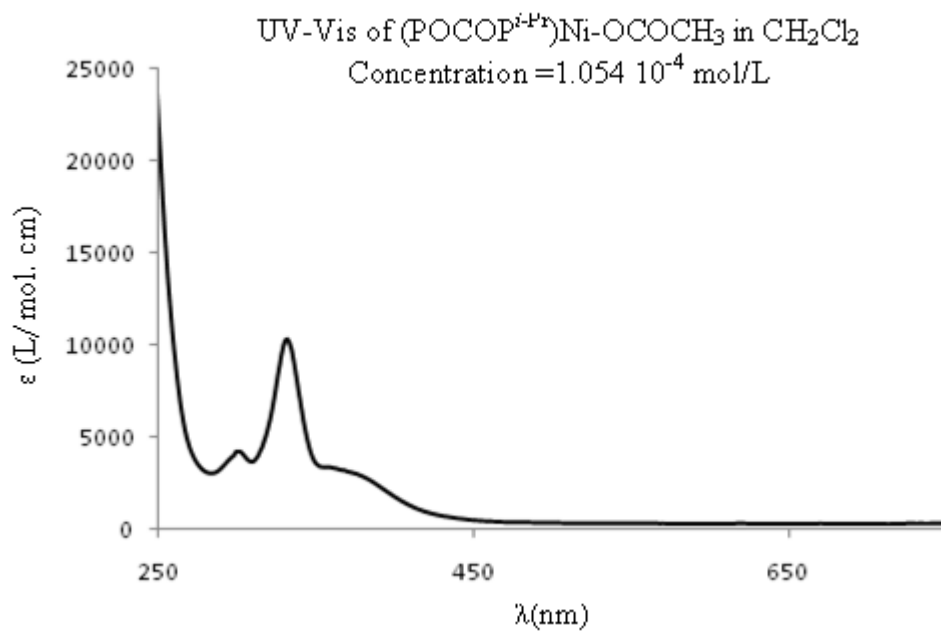
* qq= quasi quartet; qt= quasi triplet

Table 2. $^{13}\text{C}\{^1\text{H}\}$ NMR data for complexes 1-6.

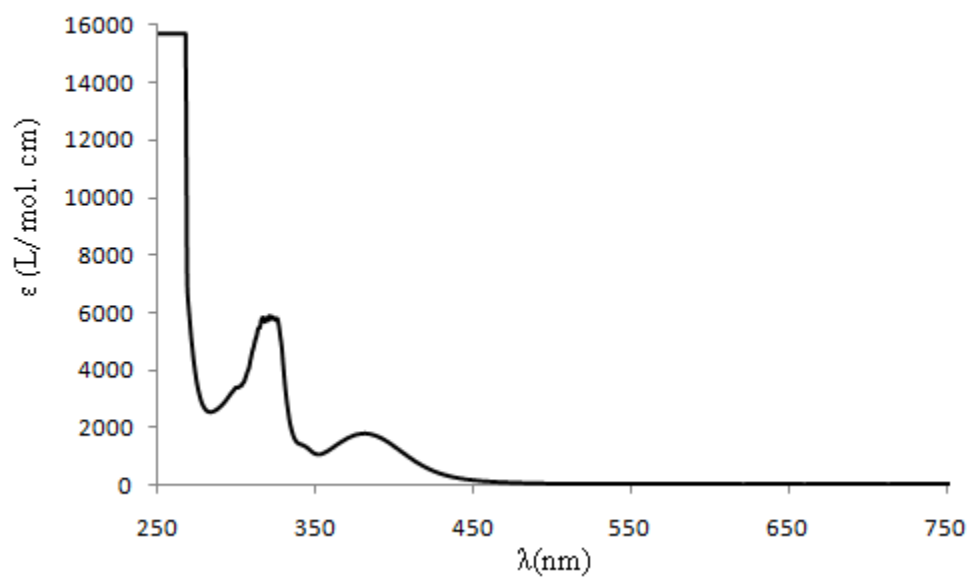
	<i>i</i> -C	<i>o</i> -C	<i>m</i> -C	<i>p</i> -C	C2/C6	C3/C5	C1*	C4
	νt , 4C	νt , 8C	νt , 8C	νt , 4C	νt , 2C	νt , 2C	t , 1C	s , 1C
	(ν) _{P-C}	(ν) _{P-C}	(ν) _{P-C}	(ν) _{C-P}	(ν) _{P-C}	(ν) _{P-C}	(2) _{C-P}	
1	132.0 (15.5)	128.39 (5.3)	131.8 (7)	131.41 (8)	167.05 (11.0)	106.60 (6.8)	128.7 (8.3)	129.4
2	132.27 (28.98)	128.55 (5)	131.33 (4)		167.08 (11.3)	106.29 (7.1)	129.37 (24.4)	130.81
3	131.61 (25.2)	129.3 (7)	132.74 (7)		168.6 (10.8)	107.6 (6.8)	130.48 (4.2)	131.31
4	135.2 (11)	131.37 (9.4)	132.75 (7)		168.71 (10.8)	107.6 (6.8)	130.97 (3.3)	130.4
5	131.23 (9.7)	129.45 (4.8)	132.45 (6.8)		168.72 (2.0)	107.5 (3.0)	129.23 (4.1)	132.8
6	133.7 (24.9)	128.24 (5)	131.6 (7.2)	130.84	167.0	106.0 (6.7)	128.76 (6.2)	130.6

* The signals of the quaternary carbons are very weak.

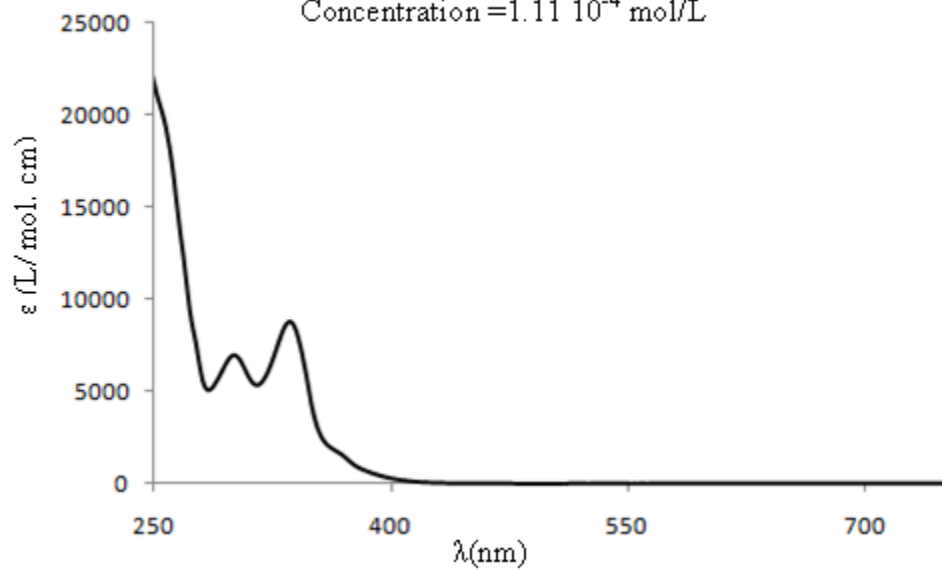
UV-Vis curves for complexes (POCOP^{i-Pr})Ni-OCOCH₃, (POCOP^{i-Pr})Ni-OSO₂CF₃ and complexes 2-6



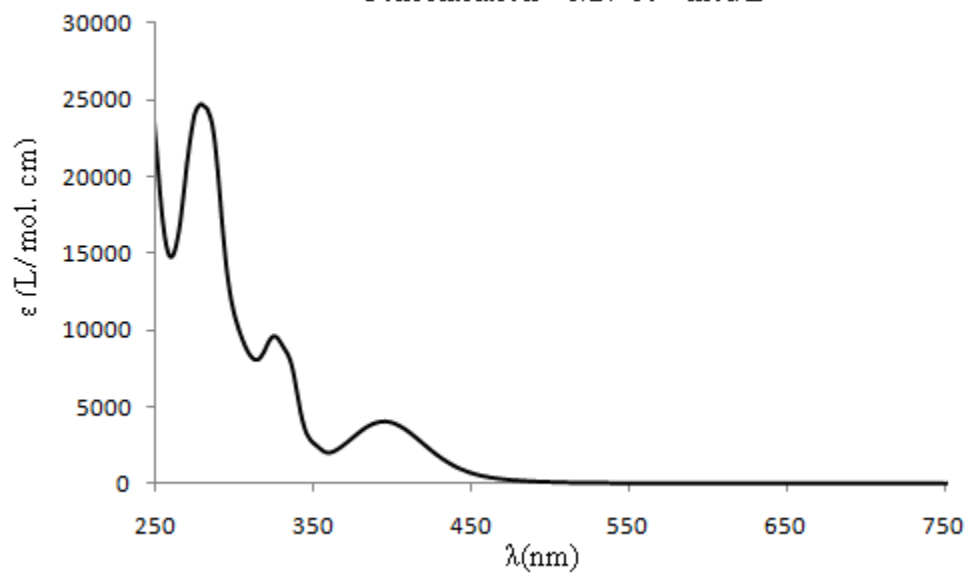
UV-Vis of (POCOPⁱ⁺¹)Ni-OSO₂CF₃ in CH₂Cl₂
Concentration = 1.054 10⁻⁴ mol/L



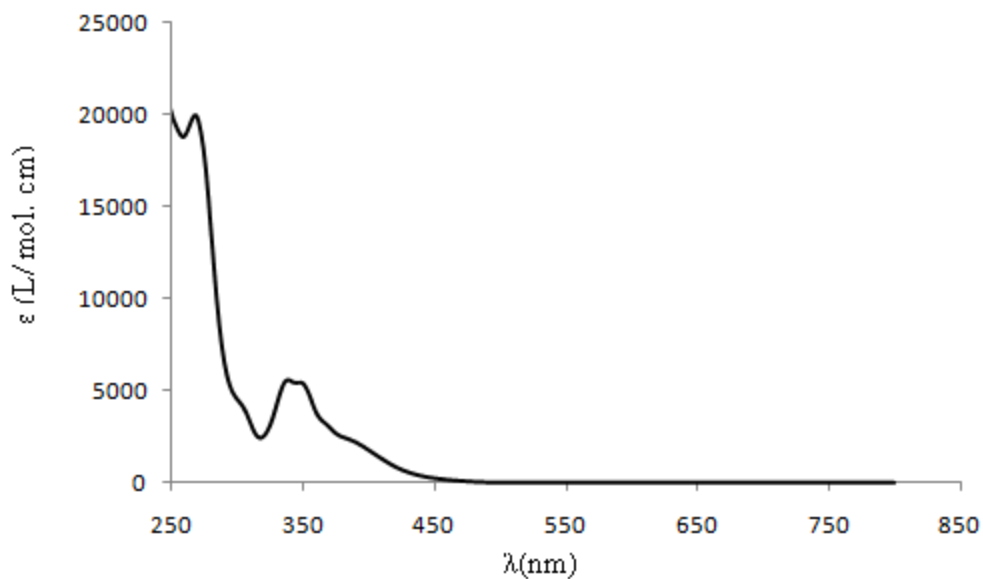
UV-Vis of complex **2** in CH₂Cl₂
Concentration = 1.11 10⁻⁴ mol/L



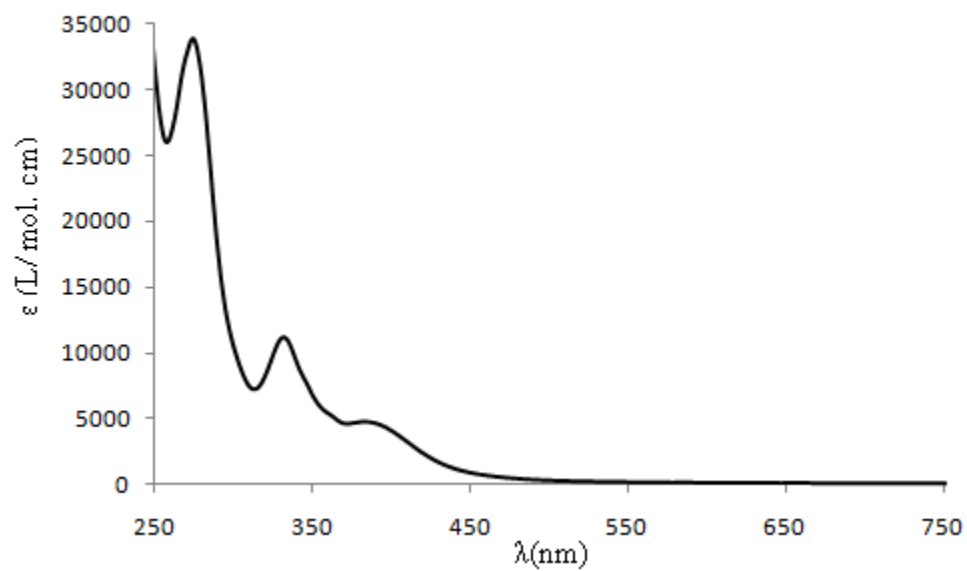
UV-Vis of complex **3** in CH₂Cl₂
Concentration = $1.27 \cdot 10^{-4}$ mol/L



UV-Vis of complex **4** in CH₂Cl₂
Concentration = $5.6 \cdot 10^{-5}$ mol/L



UV-Vis of complex **5** in CH₂Cl₂
Concentration = $5.80 \cdot 10^{-4}$ mol/L



UV-Vis of complex **6** in CH₂Cl₂
Concentration = 7.8510^{-5} mol/L

