

Supplementary Information

New Heteroleptic [Ni(II) 1,1-Dithiolate-Phosphine] Complexes: Synthesis, Characterization and Electrocatalytic Oxygen Evolution Studies‡

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Table of Contents

Fig. S1: Simulated and experimental PXRD patterns of complexes **1-4**.

Fig. S2: IR spectra of complexes **1-4**.

Fig. S3: ¹H, ¹³C{¹H} and ³¹P{¹H} spectra of complexes **1-4**.

Fig. S4: Non-covalent interactions in complexes **1-4**.

Table S1: Weak secondary interactions and their parameters observed in complexes **1-4**.

Fig. S1: Simulated and experimental PXRD patterns of complexes 1-4.

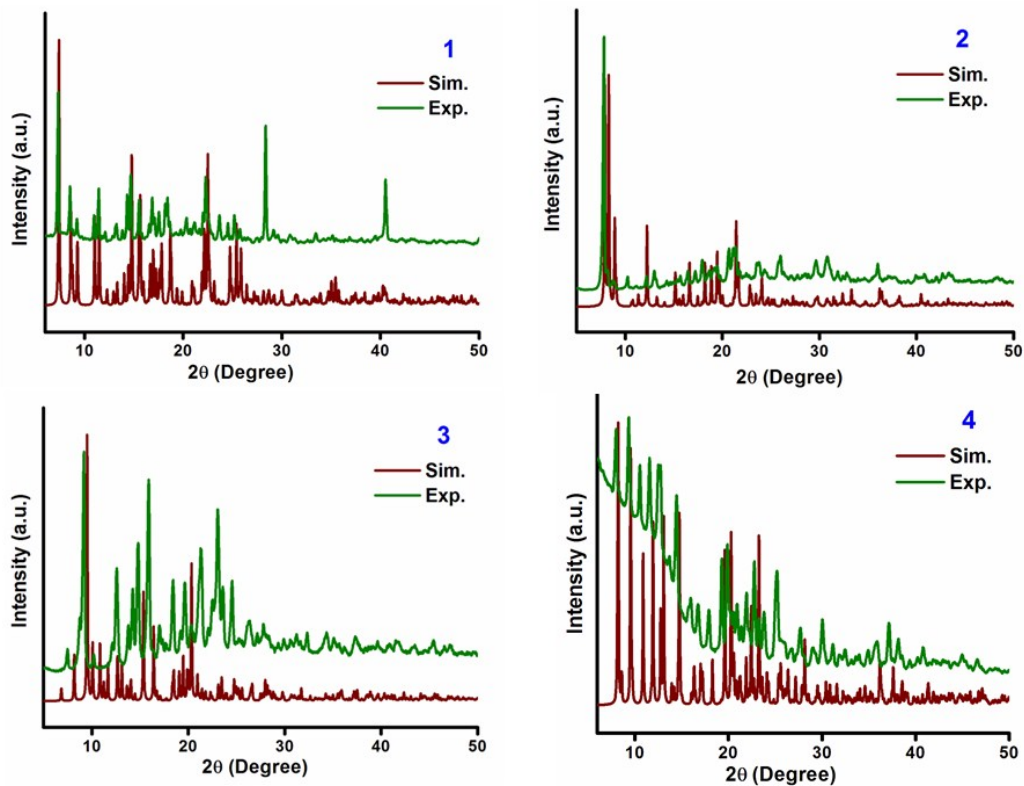
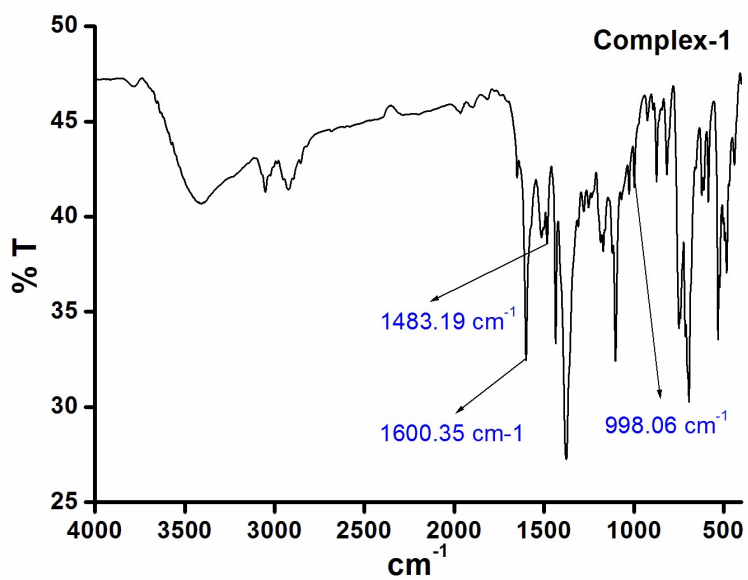
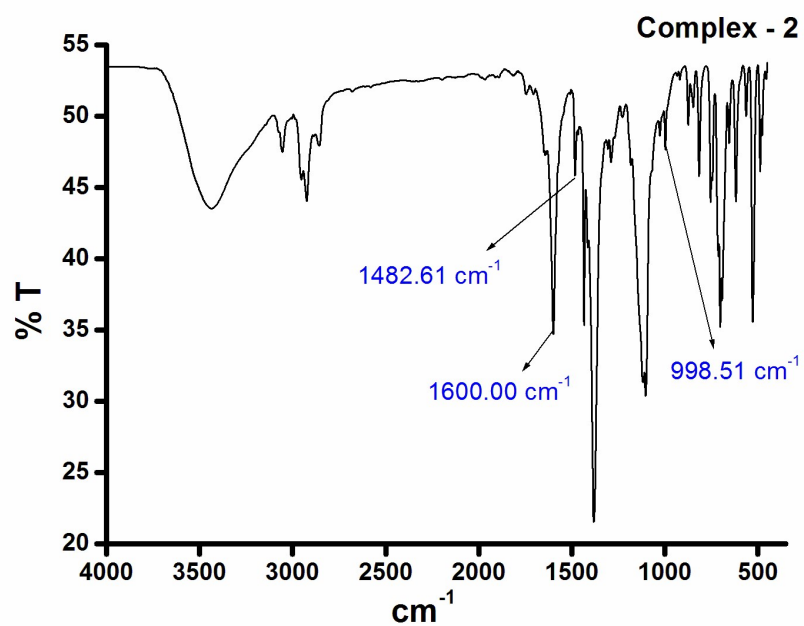


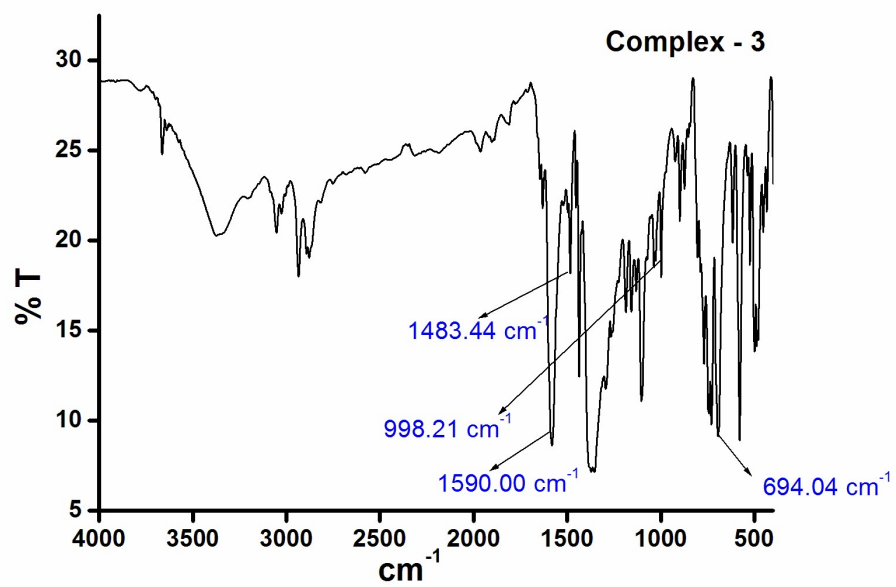
Fig. S2: IR spectra of complexes 1-4.



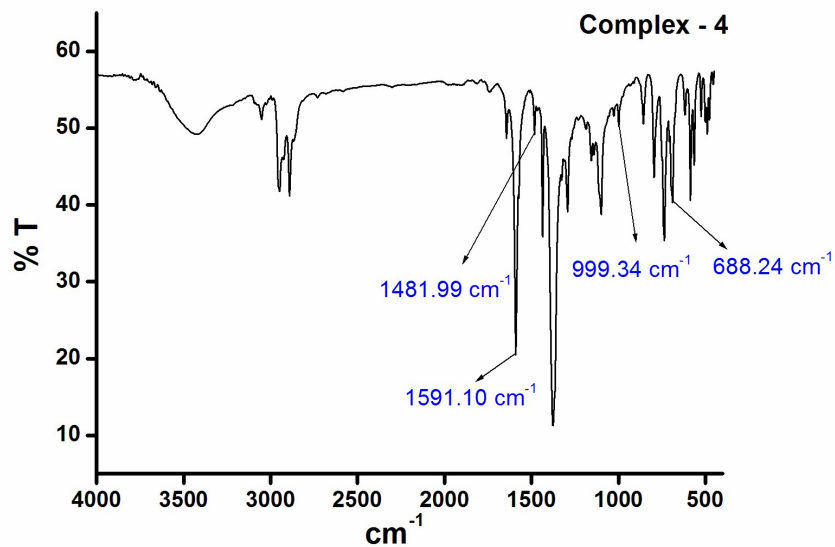
Spectrum a: IR spectrum of complex 1.



Spectrum b: IR spectrum of complex 2.

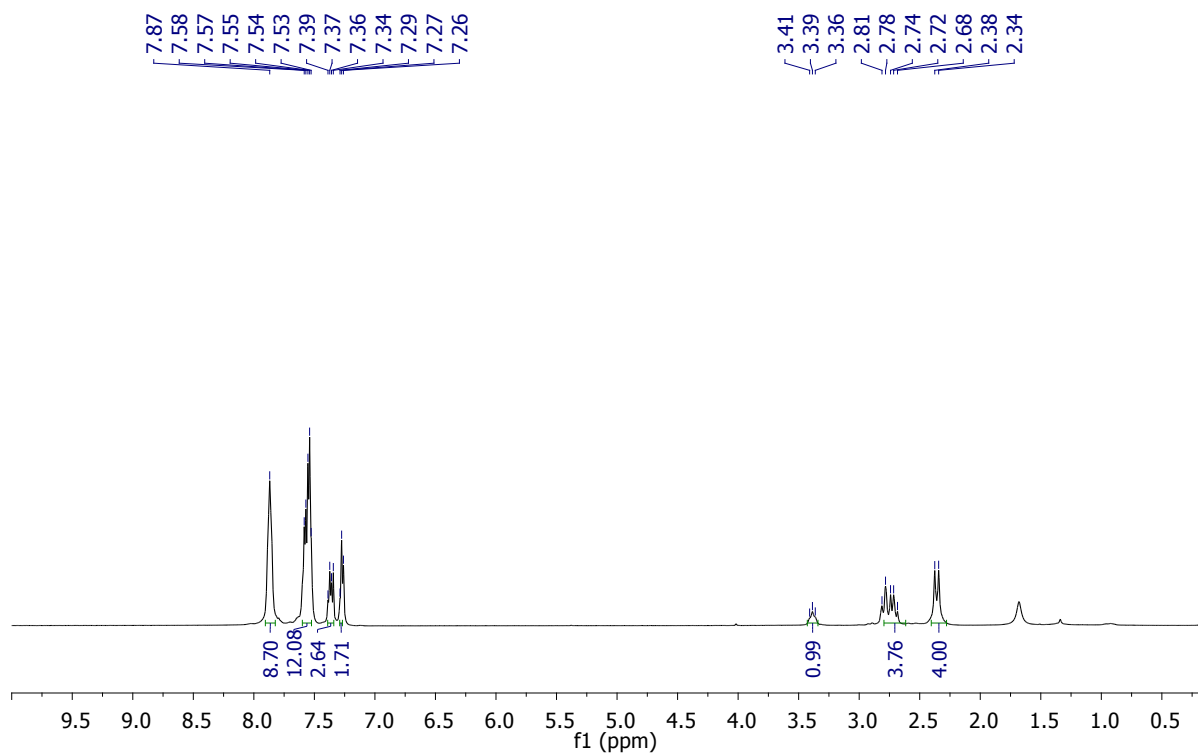


Spectrum c: IR spectrum of complex 3.

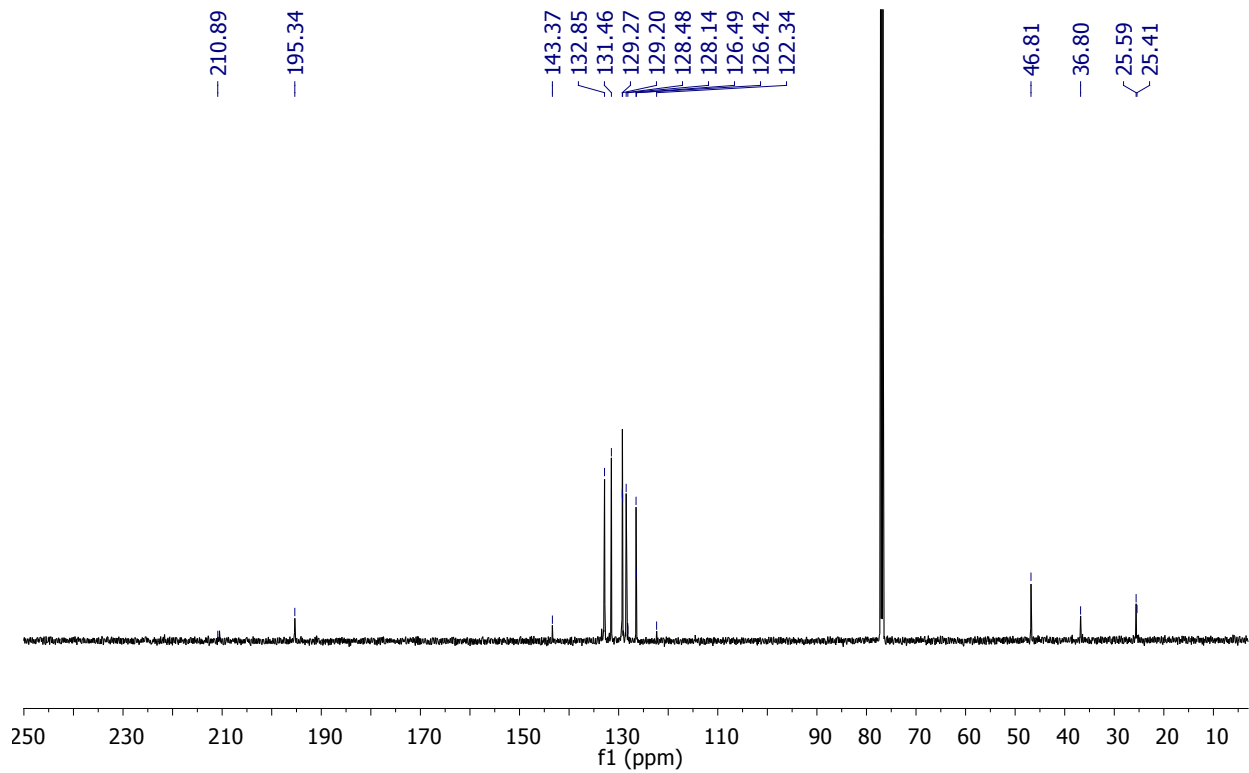


Spectrum d: IR spectrum of complex 4.

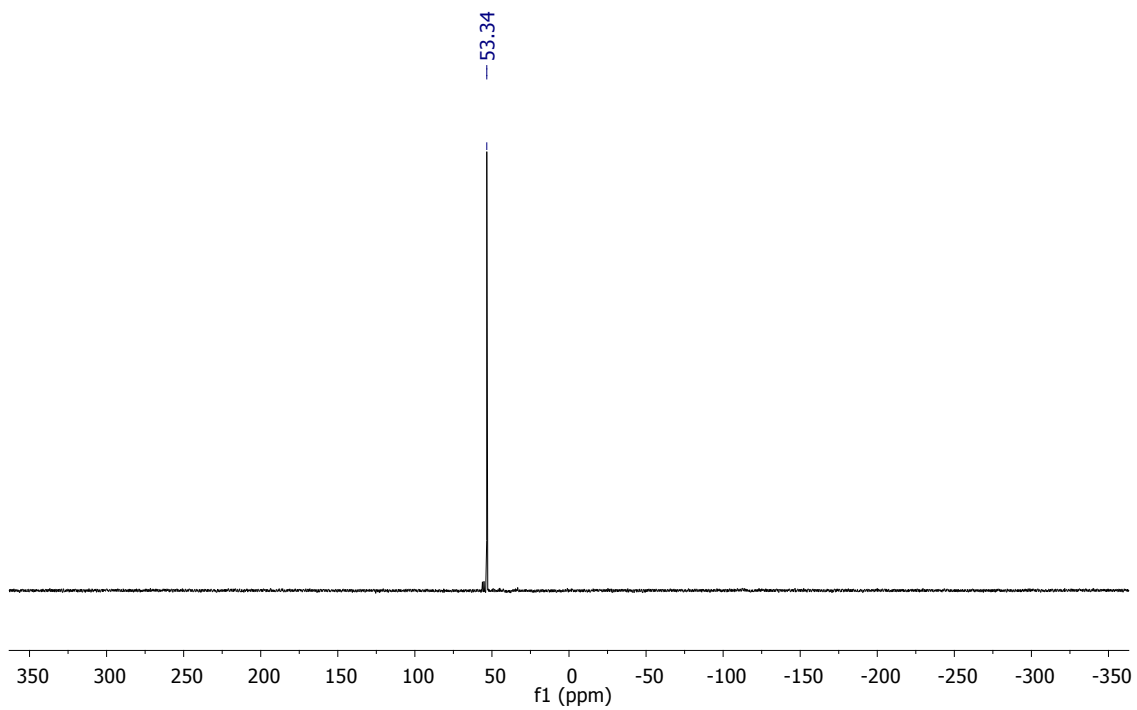
Fig. S3: ^1H , $^{13}\text{C}\{^1\text{H}\}$ and $^{31}\text{P}\{^1\text{H}\}$ spectra of complex 1-4.



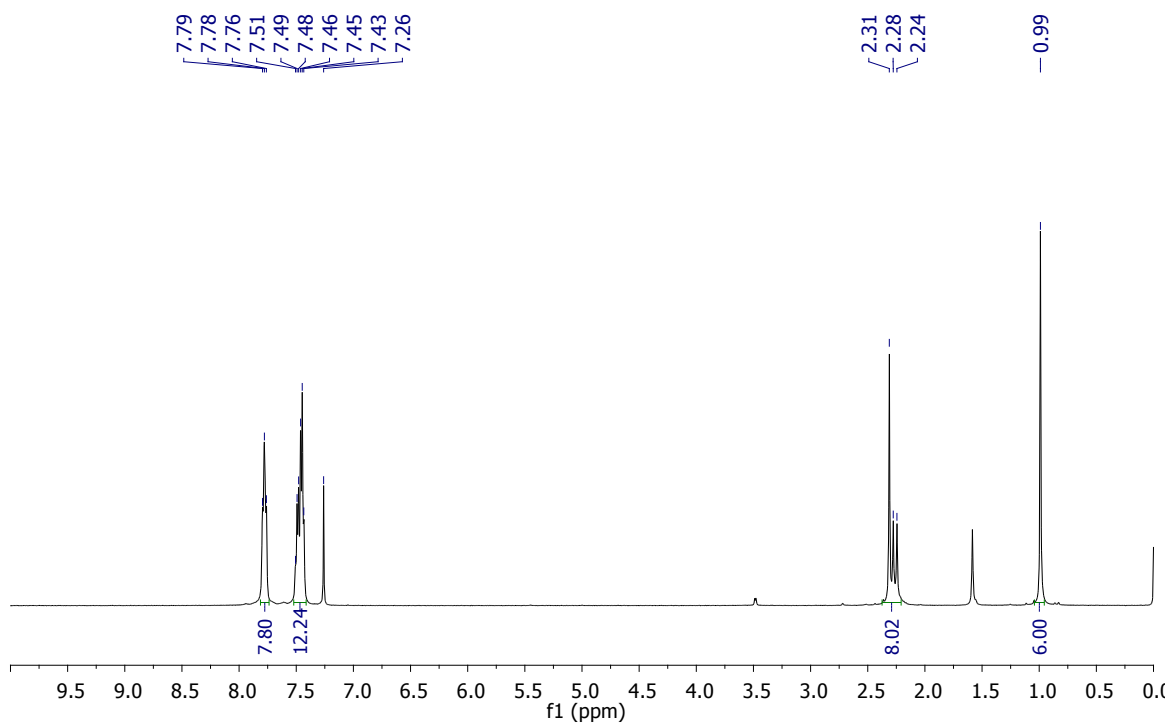
Spectrum 1a: ^1H NMR (500 MHz, CDCl_3) of complex 1



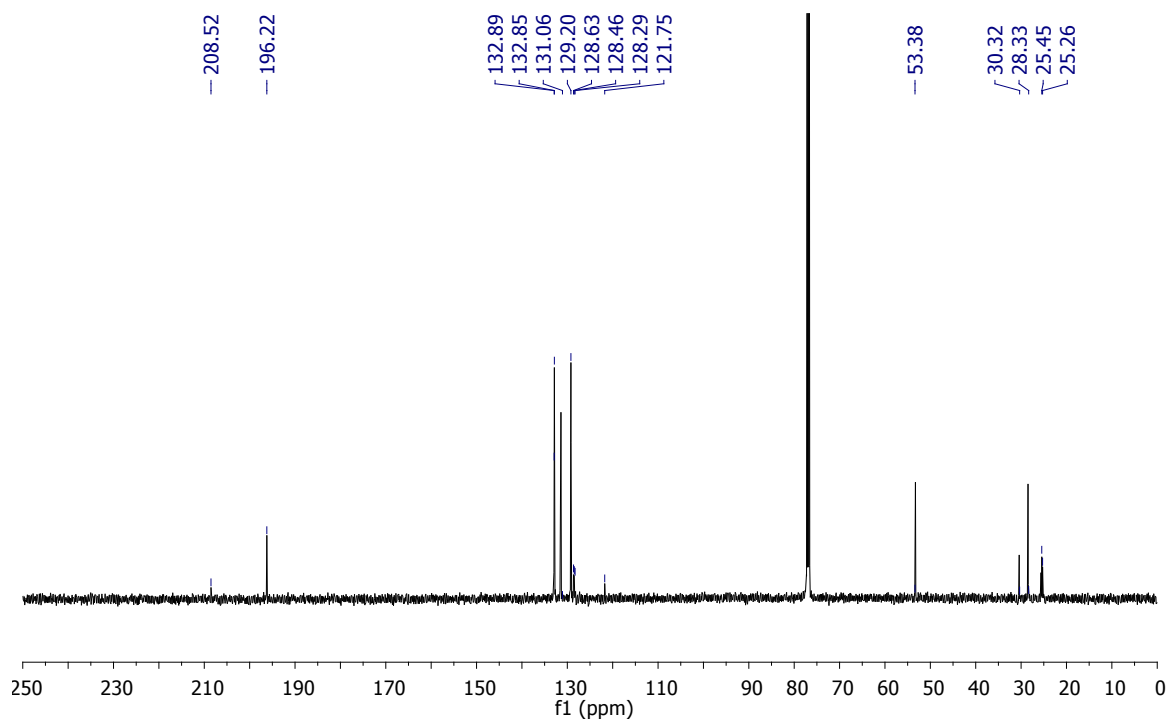
Spectrum 1b: $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of complex **1**



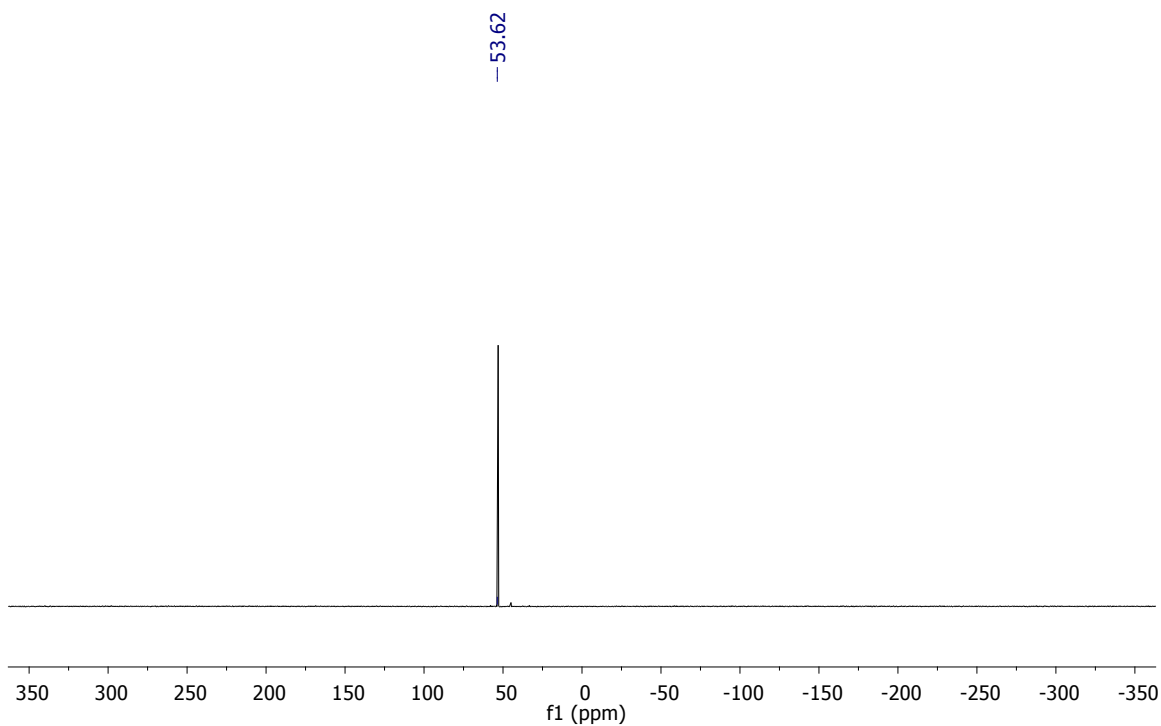
Spectrum 1c: $^3\text{P}\{^1\text{H}\}$ NMR (202 MHz, CDCl_3) of complex **1**



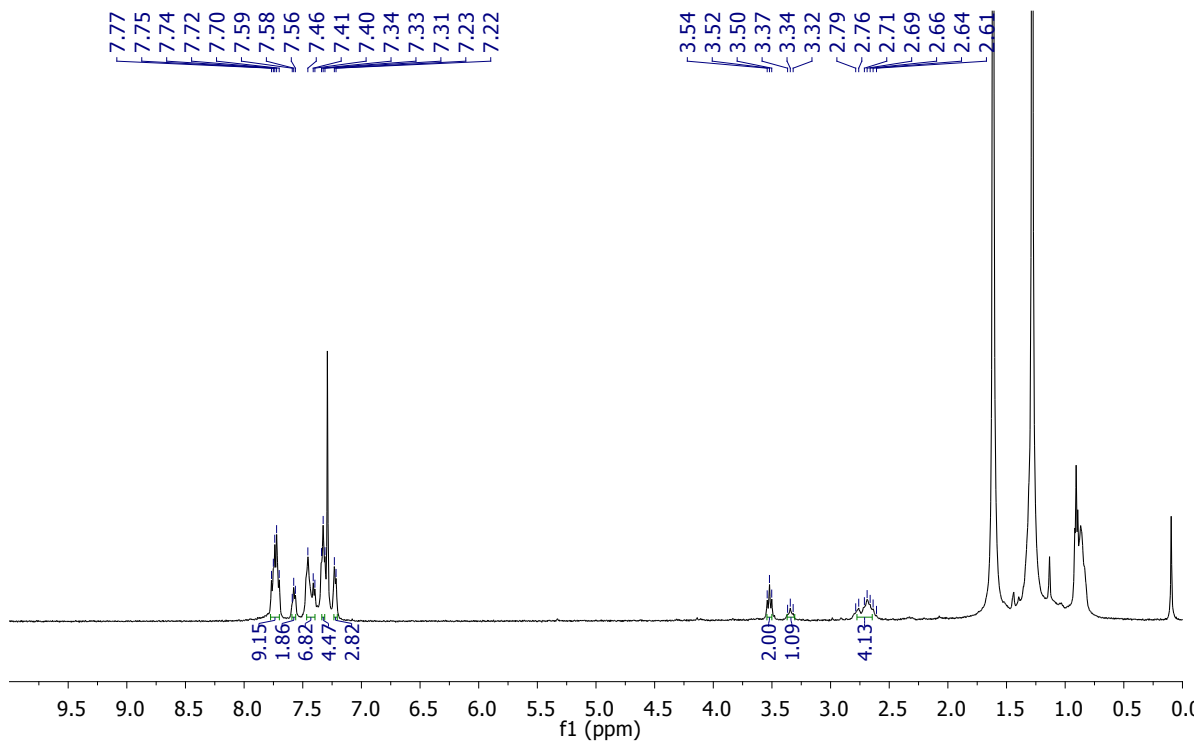
Spectrum 2a: ^{13}C NMR (500 MHz, CDCl_3) of complex **2**.



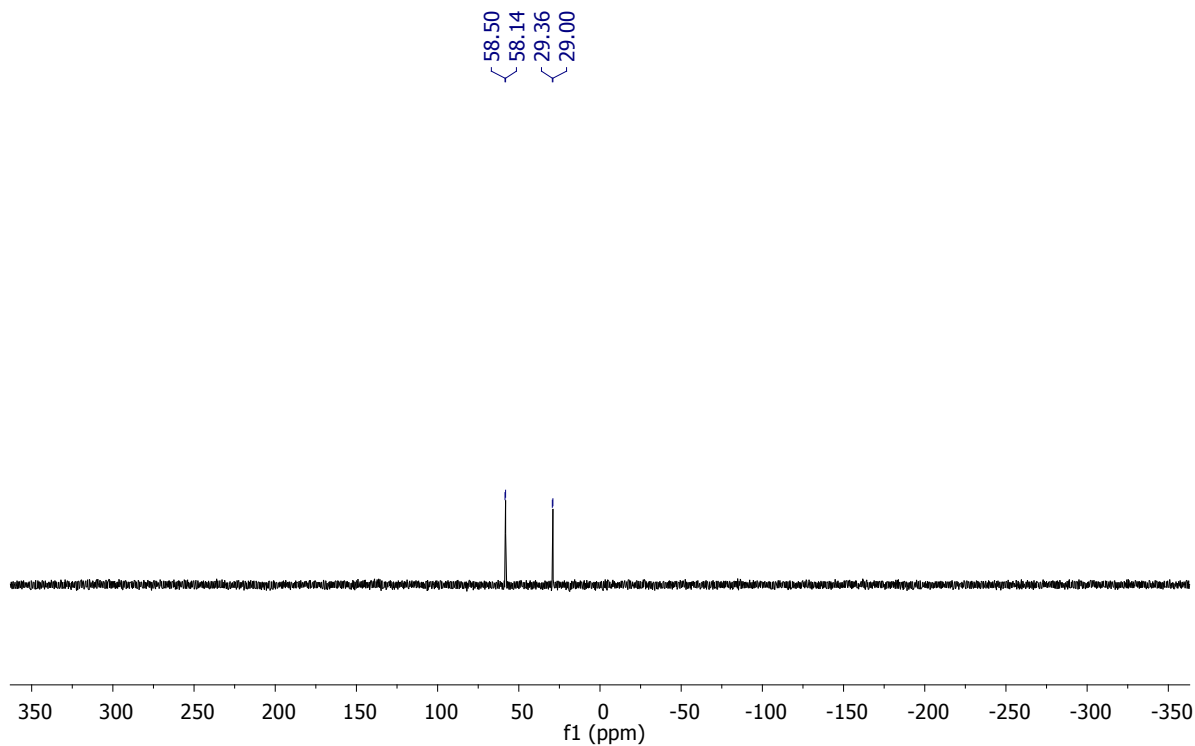
Spectrum 2b: ^{13}C NMR (125 MHz, CDCl_3) of complex **2**.



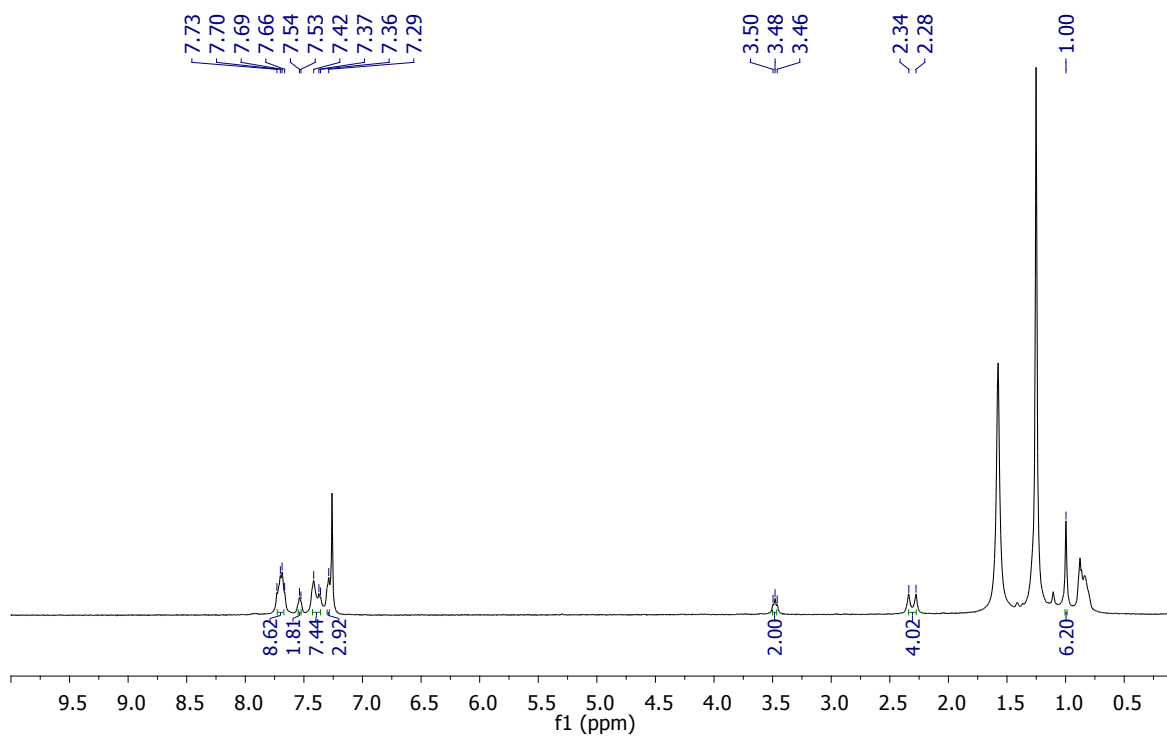
Spectrum 2c: ^1H NMR (202 MHz, CDCl_3) of complex **2**



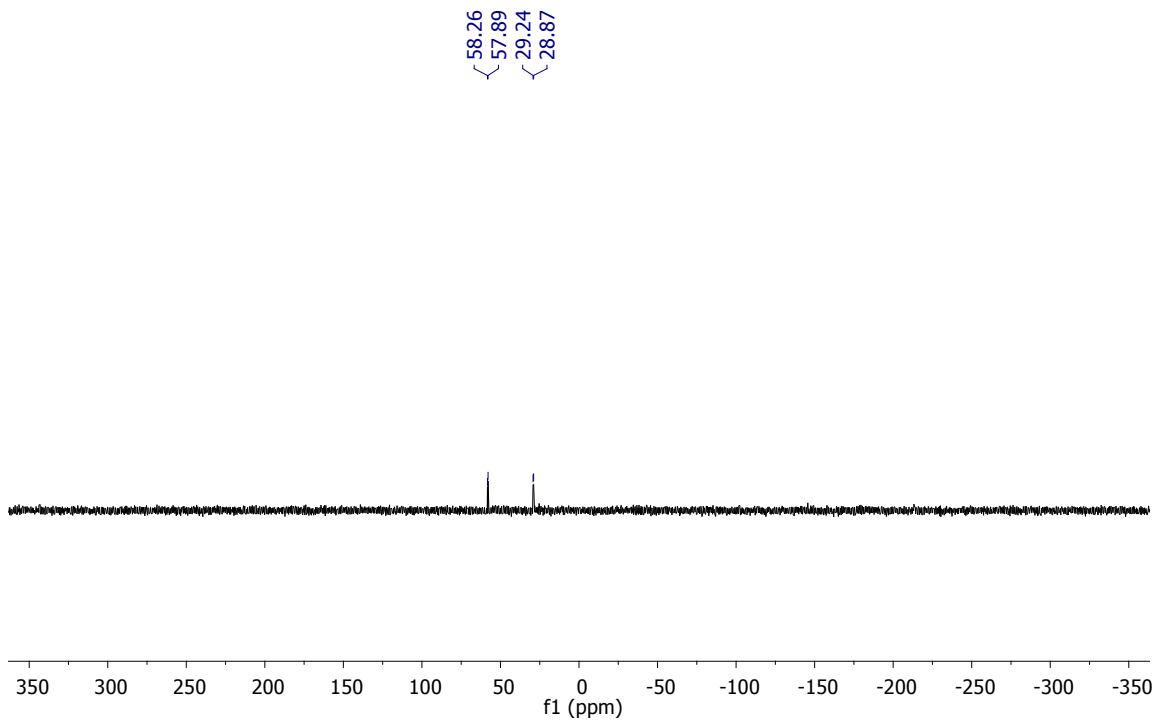
Spectrum 3a: ^1H NMR (500 MHz, CDCl_3) of complex **3**.



Spectrum 3b: $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz, CDCl_3) of complex **3**



Spectrum 4a: ^1H NMR (500 MHz, CDCl_3) of complex **4**.



Spectrum 4b: $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz, CDCl_3) of complex **4**.

Fig. S4 : Non-covalent interactions in complexes **1-4**.

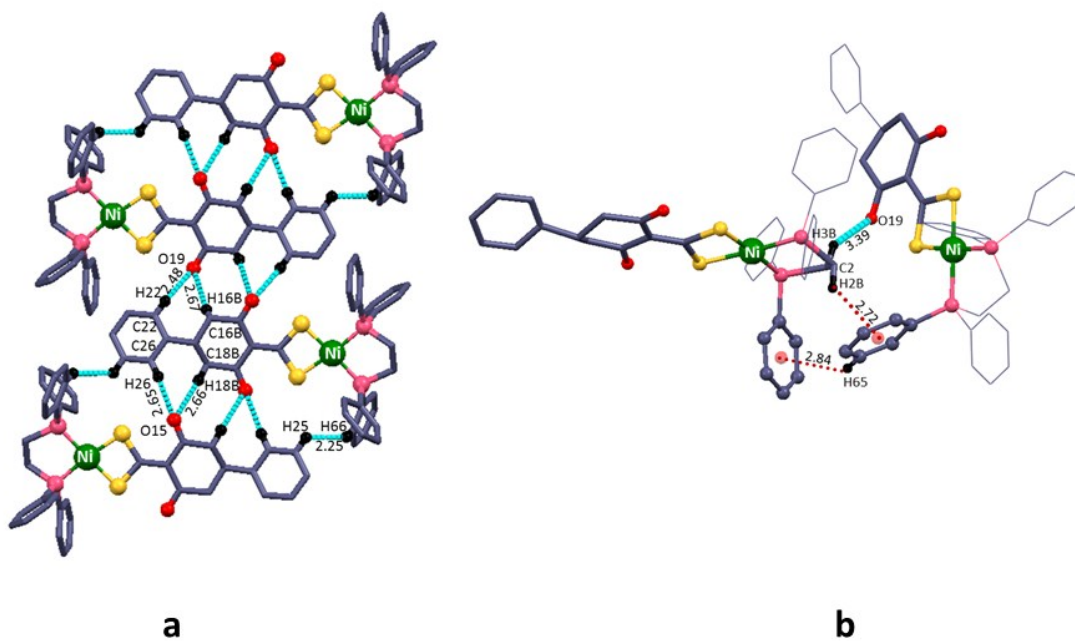


Fig. S4. 1 (a) Supramolecular network sustained via C-H \cdots O, H \cdots H and (b) C-H \cdots π and C-H \cdots O interactions in **1**.

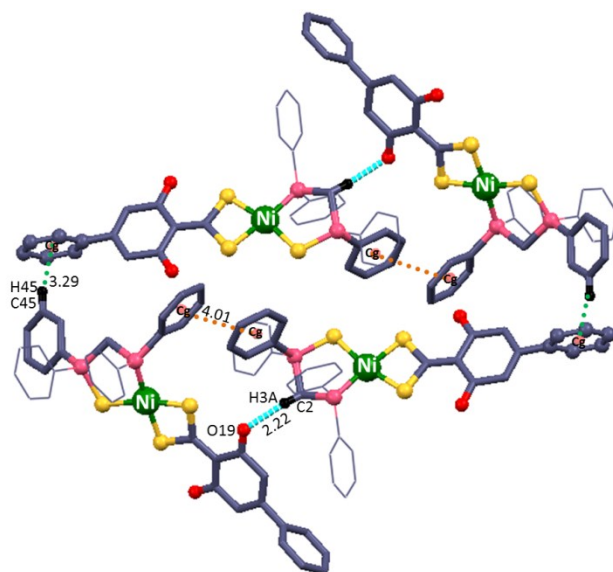


Fig. S4. 2 Supramolecular structure sustained via C-H \cdots O, C-H \cdots π and π \cdots π interactions in **3**.

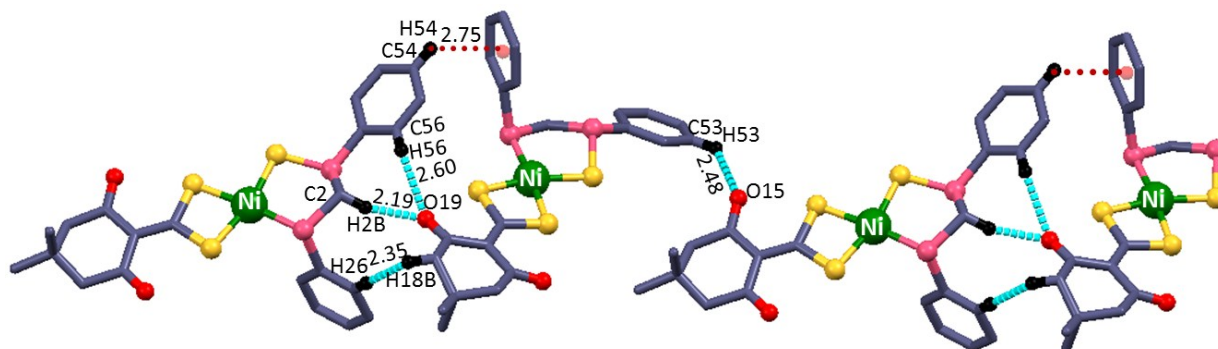


Fig. S4. 3 1-D Polymeric structure of **4** sustained by C-H \cdots O, H \cdots H and C-H \cdots π interactions.

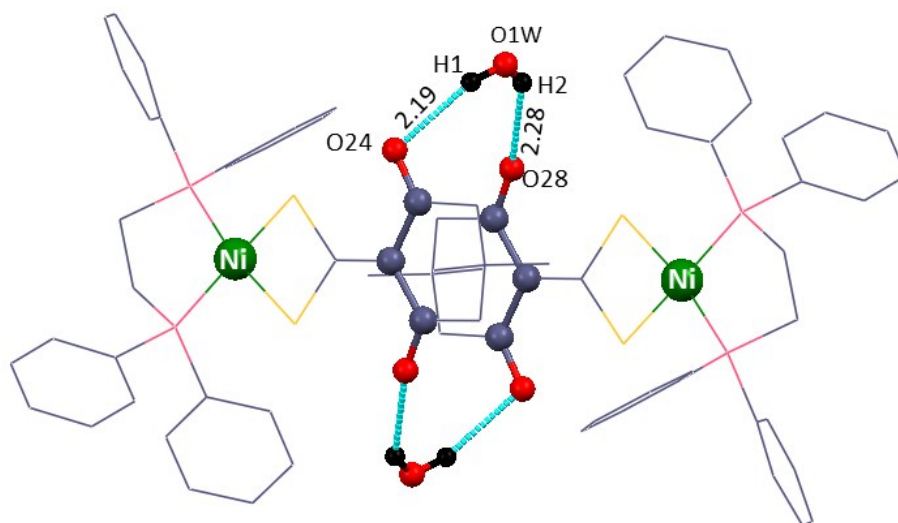


Fig. S4. 4 The C–O···H–O hydrogen bonding interactions in complex **2**.

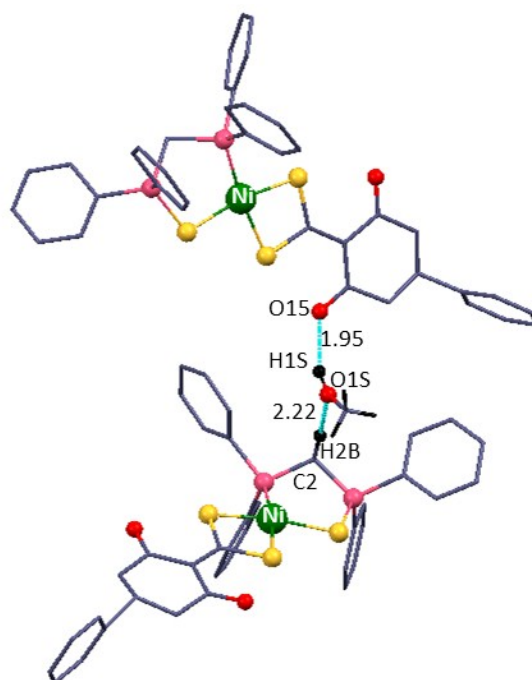


Fig. S4. 5 The C–O···H–O hydrogen bonding interaction and C–H···O interaction in complex **3**.

Table S1: Weak secondary interactions and their parameters observed in compounds **1- 4**.

Donor (D)-acceptor (A) hydrogen bonds (Å, °)					
Complex	D–H···A	d(H···A)	d(D···A)	∠D–H···A	Symmetry Element
1	C(22)–H(22)···O(19)	2.48	3.408(5)	175	-x,-y,1-z
	C(16B)–H(16B)···O(19)	2.67	3.626(4)	167	-x,-y,1-z
	C(26)–H(26)···O(15)	2.65	3.528(5)	157	1-x, -y, 1-z
	C(18A)–H(18C)···O(15)	2.61	3.548(5)	162	1-x,-y,1-z
	C(3)–H(3B)···O(19)	2.39	3.233(4)	145	x, -y+1/2, z-1/2
2	C(54)–H(54)···O(19)	2.37	3.303(4)	176	3/2-x,1/2+y,z
	C(2)–H(2B)···O(15)	2.58	3.209(4)	123	1-x, 1/2+y,1/2-z
3	C(2)–H(2A)···O(19)	2.23	3.097(6)	148	x,1/2-y,z-1/2
	C(2)–H(2B)···O(15)	2.22	3.173(7)	165	x,y,z
4	C(56)–H(56)···O(19)	2.60	3.445(5)	153	1/2-x,y-1/2, 3/2-z
	C(53)–H(53)···O(15)	2.48	3.157(6)	130	3/2-x,y-1/2,3/2-z
	C(2)–H(2B)···O(19)	2.19	3.126(5)	160	1/2-x,y-1/2, 3/2-z
Complex					
Complex	H···H	H···H	Symmetry element		
1	H(66)···H(23)	2.26	-x,-y,1-z		
2	H(43)···H(21B)	2.38	x,1/2-y,-1/2+z		
4	H(26)···H(18B)	2.35	1/2-x,y-1/2,3/2-z		
Complex					
Complex	C–H···π / π ···π	C–H···π/ π ···π	Symmetry element		
1	C(65)–H(65)··· π(C71–C76)	2.84	x,1/2-y, z+1/2		
	C(2)–H(2B)··· π(C61–C66)	2.72	x,1/2-y,z-1/2		
2	C(34)–H(34)··· π(C61–C66)	3.16	1-x,1/2+y,1/2-z		
3	C(45)–H(45)··· π(C21–C26)	3.29	1-x,1/2-y,1/2+z		
π ···π					
4	C(54)–H(54)··· π(C21–C26)	2.75	1/2-x, y-1/2, 3/2-z		