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双二茂铁基吡咯衍生物电荷交互通道

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Channel of Electronic Interactions in Diferrocenyl Pyrrole Derivatives

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1. 化合物(2)与(3)晶体测定条件

晶体结构测定选取 0.2mm×0.05mm×0.05mm (**2**)，0.4mm×0.3mm×0.01mm (**3**)的单晶，在 Bruker SMART APEX CCD 衍射仪上，采用 φ 角和ω角扫描技术，Mo-K (λ =0.71073Å)于 296(2)K 下收集化合物(**2**)衍射数据，用 Cu-K (λ =1.54184Å)于 293(2)K 下收集化合物(**3**)衍射数据，用直接法和差值傅立叶技术解析结构，几何法确定氢原子位置，吸收校正采用 SADABS 程序，数据收集、处理和晶胞参数的确定及修正采用 Bruker SAINT 和 Smart 软件，结构计算和精修采用 SHELXSL 97 软件。

晶体数据存放于剑桥晶体数据中心，化合物(**2**)的 CCDC 号为 **878311，**化合物(**3**)的 CCDC 号为 **947276**。

2. 化合物(2)与(3)晶体结构

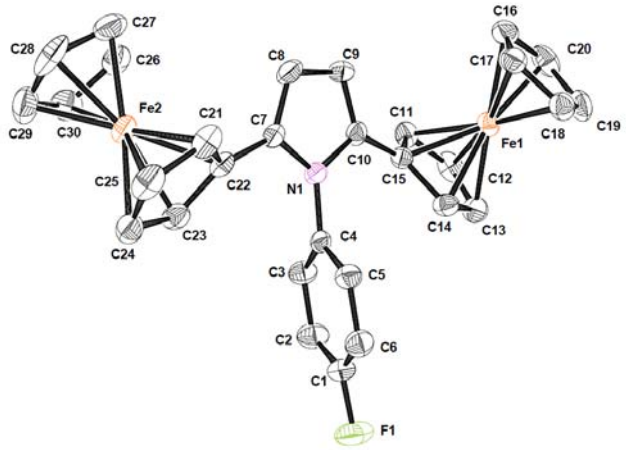

Fig.S1　The molecular structure of compound 2

The H atoms have been omitted for clarity

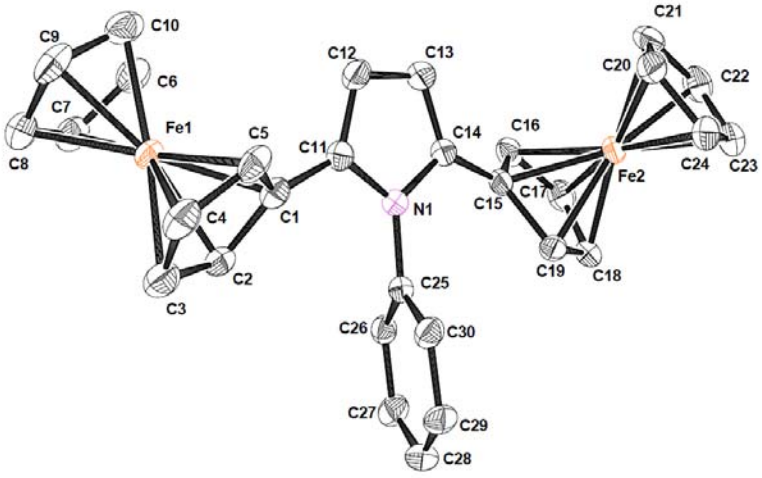

Fig.S2　The molecular structure of compound 3

The H atoms have been omitted for clarity

3. 化合物(2)与(3)晶体结构参数及选择键长、键角、扭角数据

Table S1 Crystal data and relevant structural parameters of compounds 2and 3

compounds	**2**	**3**
Empirical formula	$C_{30}H_{24}FFe_2N$	$C_{30}H_{25}Fe_2N$
Formula weight	529.20	511.21
Temperature (K)	296(2)	293(2)
Wavelength (Å)	0.71073	1.54184
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a(Å)	5.9056(9)	5.9217(4)
b(Å)	12.2523(19)	13.2228(10)
c(Å)	16.612(3)	15.8550(14)
α(º)	75.101(2)	66.798(8)
β(º)	80.710(2)	85.360(6)
γ(º)	80.508(2)	77.503(6)
Volume ($Å^3$),Z	1136.7(3),2	1114.00(15), 2
Density (Mg/m^3)	1.546	1.524
μ(mm^{-1}), F(000)	1.304, 544	10.572, 528
Crystal size (mm)	0.20 x 0.05 x 0.05	0.40 x 0.30 x 0.01
θ range	1.90 to 28.34	3.03 to 67.24
Limiting indices	-7≤h≤7, -15≤k≤16, 0≤l≤22	-7≤h≤7, -14≤ k≤15, -16≤l≤18
Reflections collected	10852	3970
Independent eflections	4424	3970
Completeness to θ	99.5 %	99.8%
Max. and min.	0.9377 and 0.7805	0.9016 and 0.1012
Data / restraints / parameters	10852/0/308	3970/1014/229
Goodness-of-fit on F^2	0.948	1.087
Final Rindices[I > 2σ(I)]	R1 = 0.0733, wR2 = 0.1470	R_1=0.1044, wR_2=0.2812
Rindices (all data)	R1 = 0.2032, wR2 = 0.1982	R_1= 0.1278, wR_2=0.3040
Largest diff. peak/ hole ($e.Å^{-3}$)	0.585/-0.760	1.327/-1.152

Table S2 Selected bond lengths (Å) and Selected angles (º) of compounds 2 and 3

compounds	bond lengths						Bond angles			
2	C22-C7	1.468(6)	C7-C8	1.360(6)	C8-C9	1.404(6)	N1-C10-C15	122.3(4)	N1-C7-C22	122.8(4)
	C9-C10	1.372(6)	C10-C15	1.469(6)	N1-C7	1.384(5)	C7- N1-C10	109.1(3)	C10-C9-C8	107.9(4)
3	C14-C15	1.471(12)	C13-C14	1.356(13)	C12-C13	1.413(14)	N1-C14-C15	123.0(7)	N1-C11-C1	122.7(8)
	C11-C12	1.373(13)	C11-C1	1.476(13)	N1-C11	1.387(12)	C14-N1-C11	109.5(7)	C12-C13-C12	108.7(9)

Table S3 Selected torsion angles (°) of compounds 2 and 3

compounds	torsion angles							
2	Fe1-C15-C10-N1	-142.24	Fe2-C22-C7-N1	-138.94	Fe1-C15-C10-C9	40.17	Fe2-C22-C7-C8	43.38
	C3-C4-N1-C10	-74.02	N1-C10-C15-C14	-49.25	N1-C7-C22-C23	-47.09	C9-C10-N1-C7	-0.31
3	Fe1-C1-C11-N1	-138.34	Fe2-C15-C14-N1	-133.01	Fe1-C1-C11-C12	41.22	Fe2-C15-C14-C13	51.13
	C14-N1-C25-C26	-66.54	N1-C14-C15-C19	-39.73	N1-C11-C1-C2	-47.25	C12-C11-N1-C14	0.73

4. 化合物(2)与(3)各平面间二面角

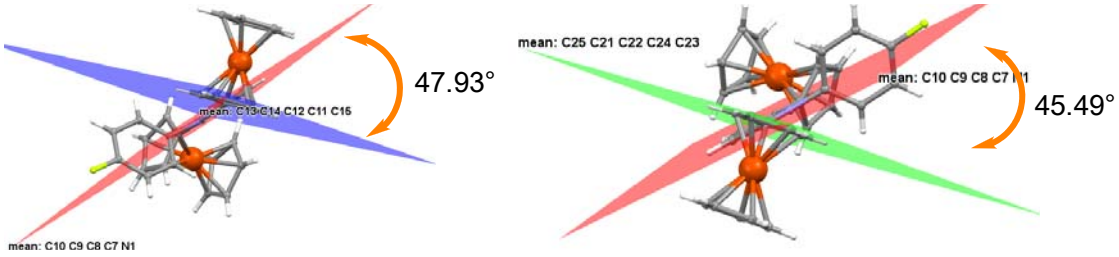

Fig.S3 The pyrrole plane N1-C7-C8-C9-C10 (red), cyclopentadiene plane C11-C12-C13-C14-C15 (blue) and cyclopentadiene plane C21-C22-C23-C24-C25 (green) of compound 2

The dihedral angle of N1-C7-C8-C9-C10 and C11-C12-C13-C14-C15 is 47.93°, the dihedral angle of N1-C7-C8-C9-C10 and C21-C22-C23-C24-C25 is 45.49°

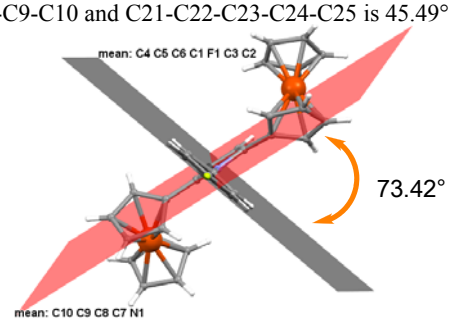

Fig.S4 The pyrrole plane N1-C7-C8-C9-C10 (red), Benzene plane C1-C2-C3-C4-C5-C6 (black) of compound 2

The dihedral angle of N1-C7-C8-C9-C10 and C1-C2-C3-C4-C5-C6 is 73.42°

Fig.S5 The pyrrole plane N1-C11-C12-C13-C14 (red), cyclopentadiene plane C15-C16-C17-C18-C19 (blue) and cyclopentadiene plane C1-C2-C3-C4-C5 (green) of compound 3

The dihedral angle of N1-C11-C12-C13-C14 and C15-C16-C17-C18-C19 is 40.11°, the dihedral angle of N1-C11-C12-C13-C14 and C1-C2-C3-C4-C5 is 47.35°

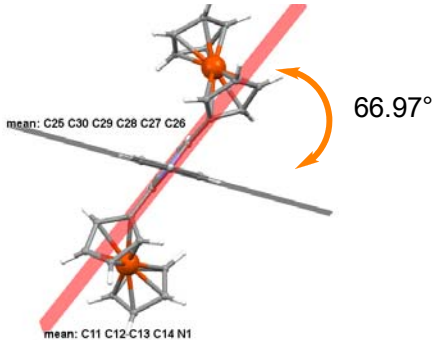

Fig.S6　The pyrrole plane N1-C11-C12-C13-C14 (red), Benzene plane C25-C26-C27-C28-C29-C30 (black) of compound 3

The dihedral angle of N1-C11-C12-C13-C14 and C25-C26-C27-C28-C29-C30 is 66.97°

5. 化合物(1) ^{1}H NMR 与 ^{13}C NMR 数据

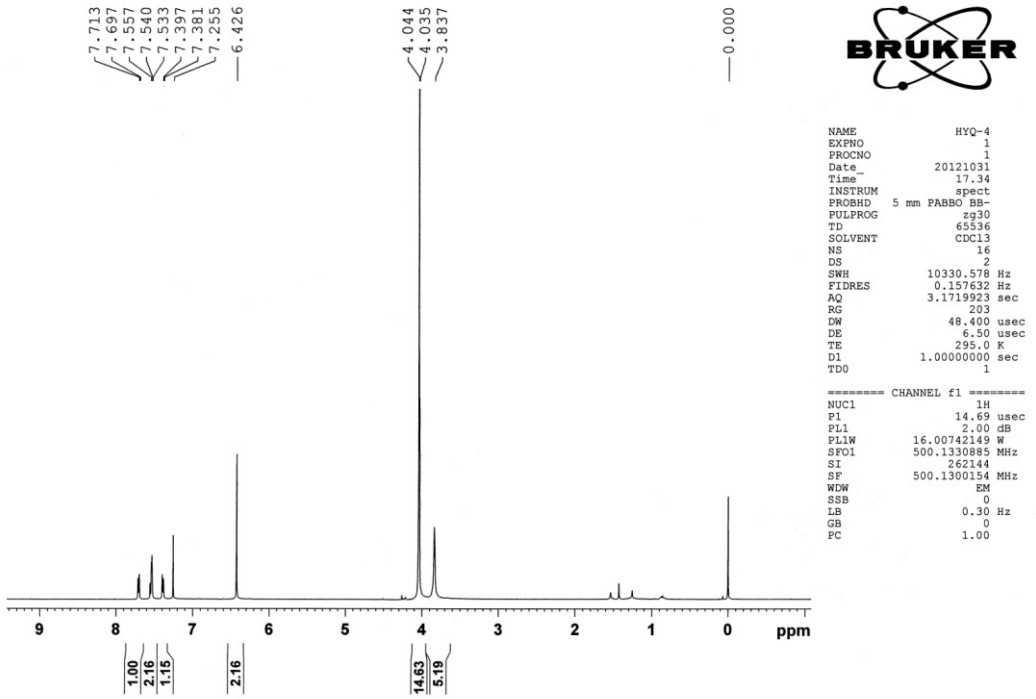

Fig.S7　The ^{1}H NMR spectrum of compound 1 in $CDCl_3$ at 25 °C

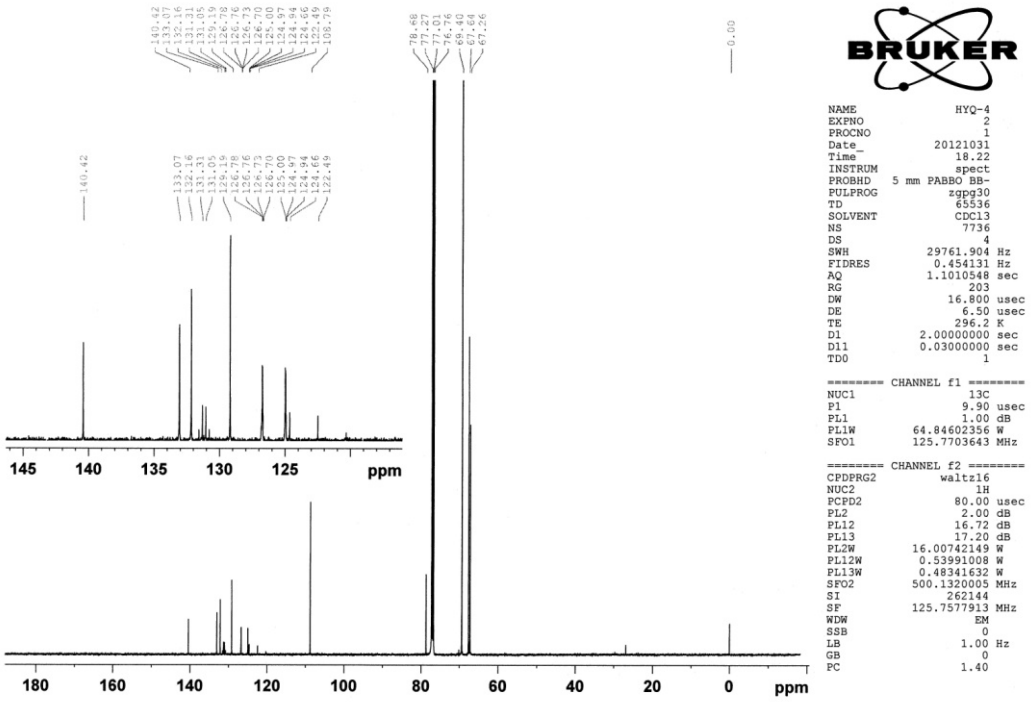

Fig.S8 The ^{13}C NMR spectrum of compound 1 in $CDCl_3$ at 25 °C

6. 化合物(2) ^{1}H NMR 与 ^{13}C NMR 数据

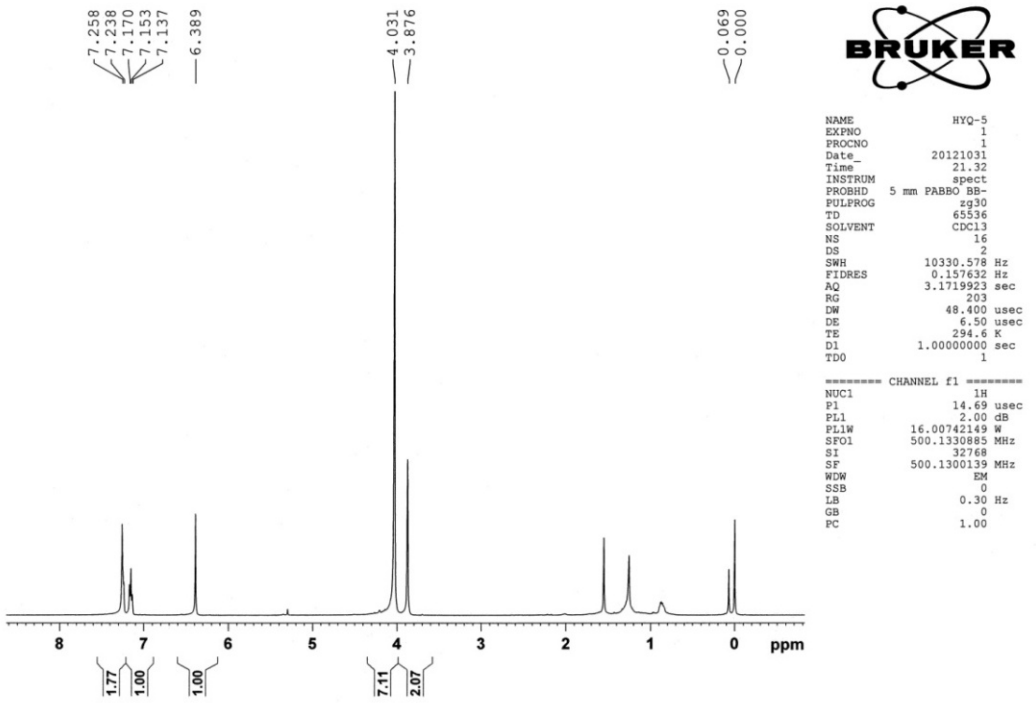

Fig.S9 The ^{1}H NMR spectrum of compound 2 in $CDCl_3$ at 25 °C

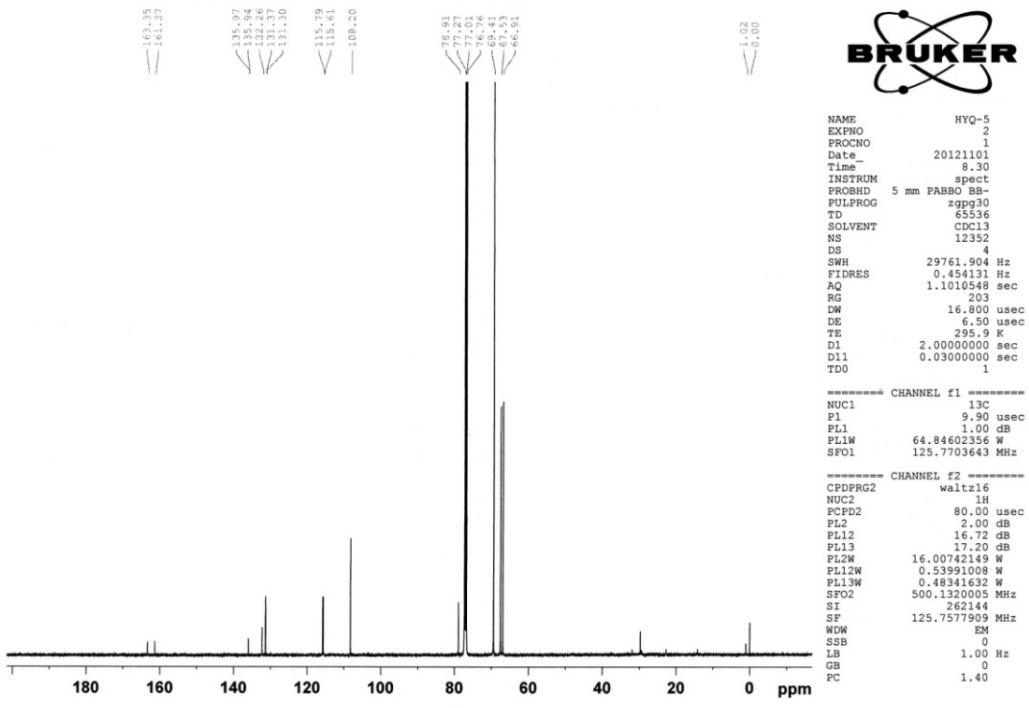

Fig.S10 The ^{13}C NMR spectrum of compound 2 in $CDCl_3$ at 25 °C

7 化合物(3) ^{1}H NMR 与 ^{13}C NMR 数据

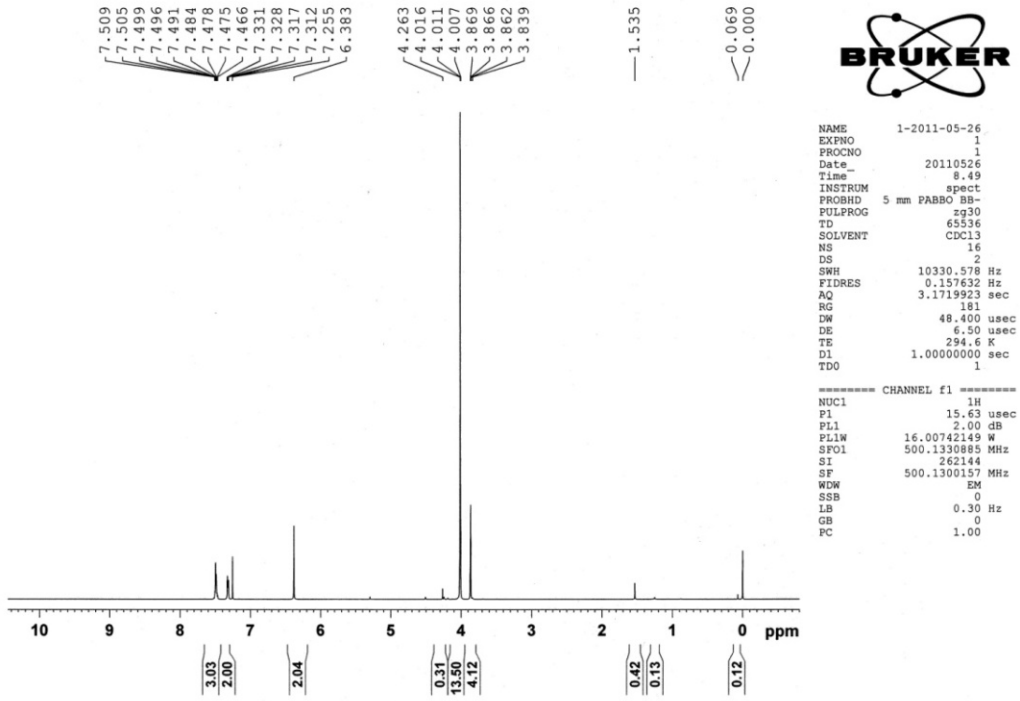

Fig.S11 The ^{1}H NMR spectrum of compound 3 in $CDCl_3$ at 25 °C

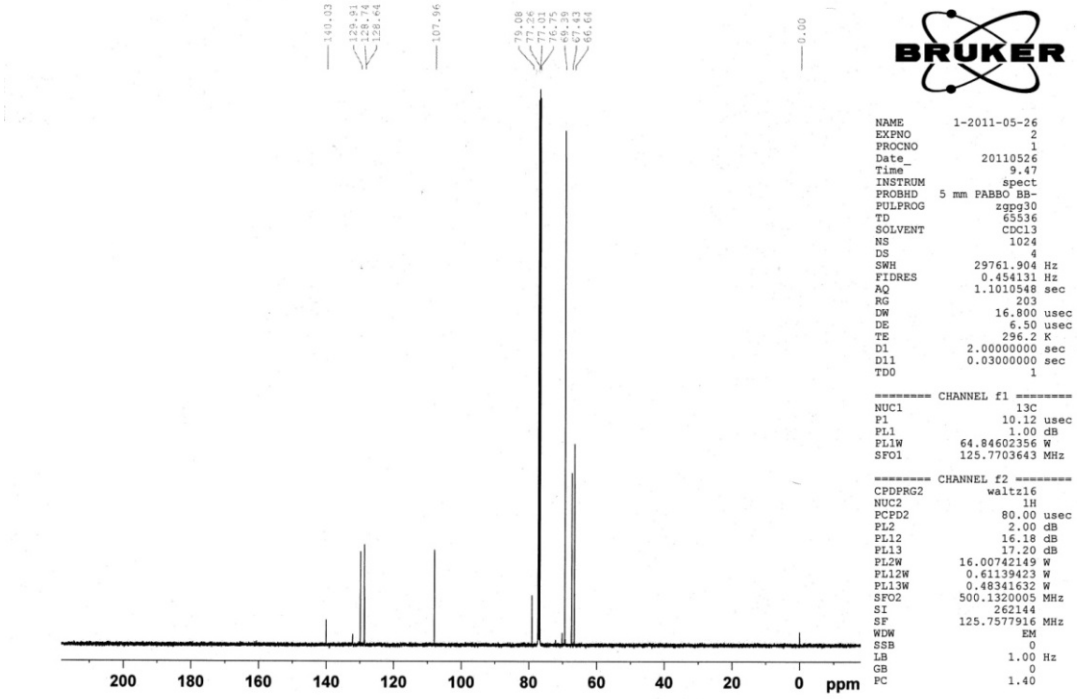

Fig.S12 The ^{13}C NMR spectrum of compound 3 in $CDCl_3$ at 25 °C

8. 化合物(4) ^{1}H NMR 与 ^{13}C NMR 数据

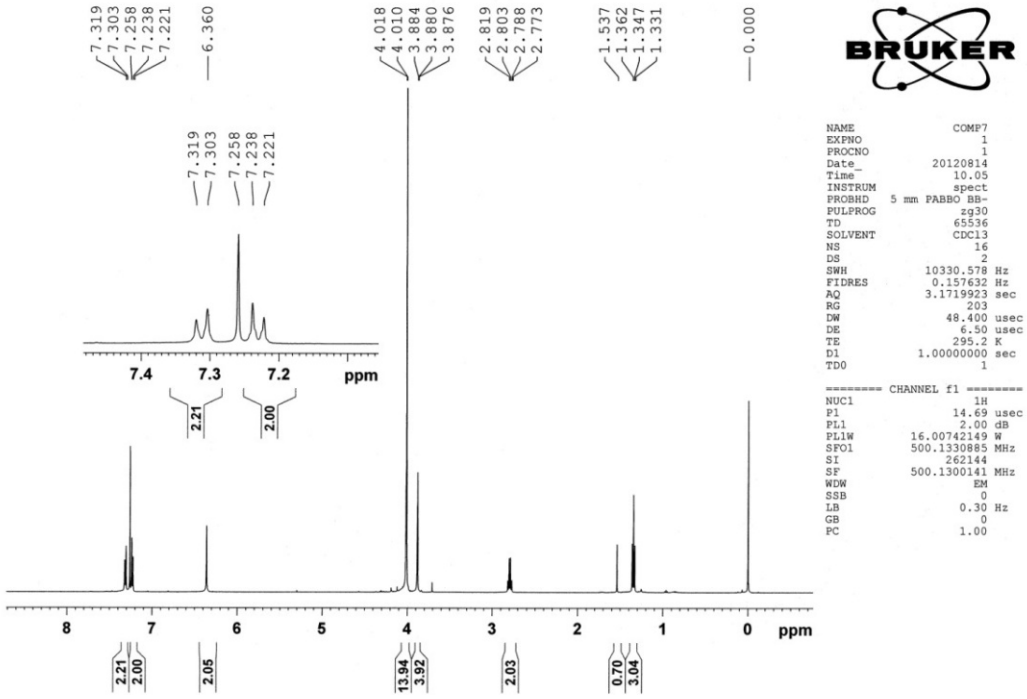

Fig.S13 The ^{1}H NMR spectrum of compound 4 in $CDCl_3$ at 25 °C

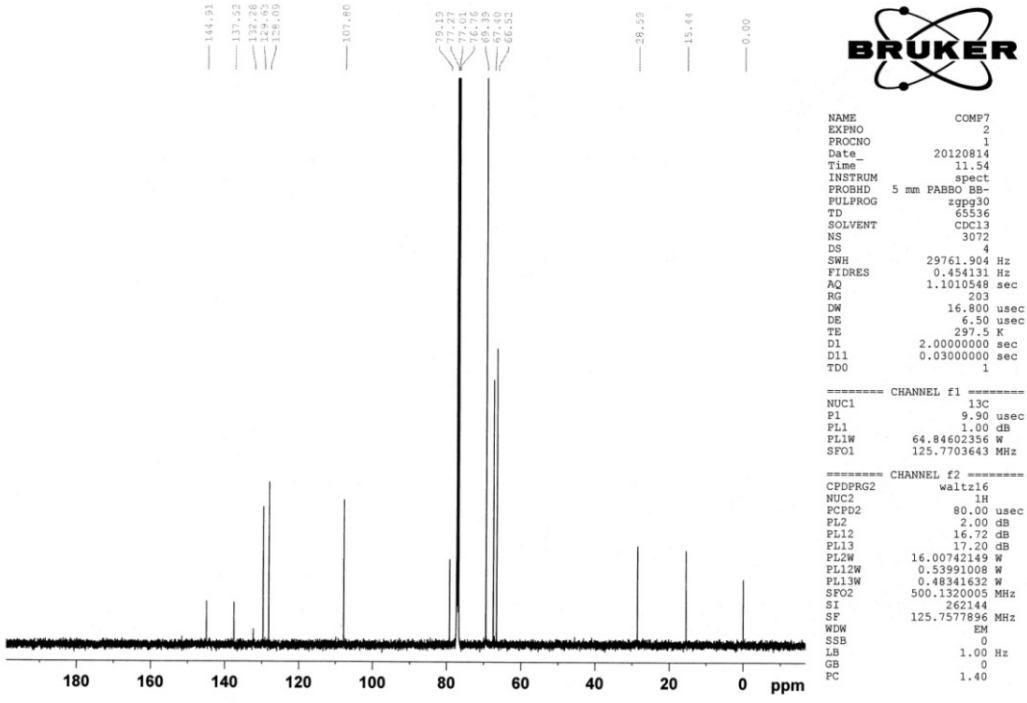

Fig.S14 The ^{13}C NMR spectrum of compound 4 in $CDCl_3$ at 25 °C

9. 化合物(5) ^{1}H NMR 与 ^{13}C NMR 数据

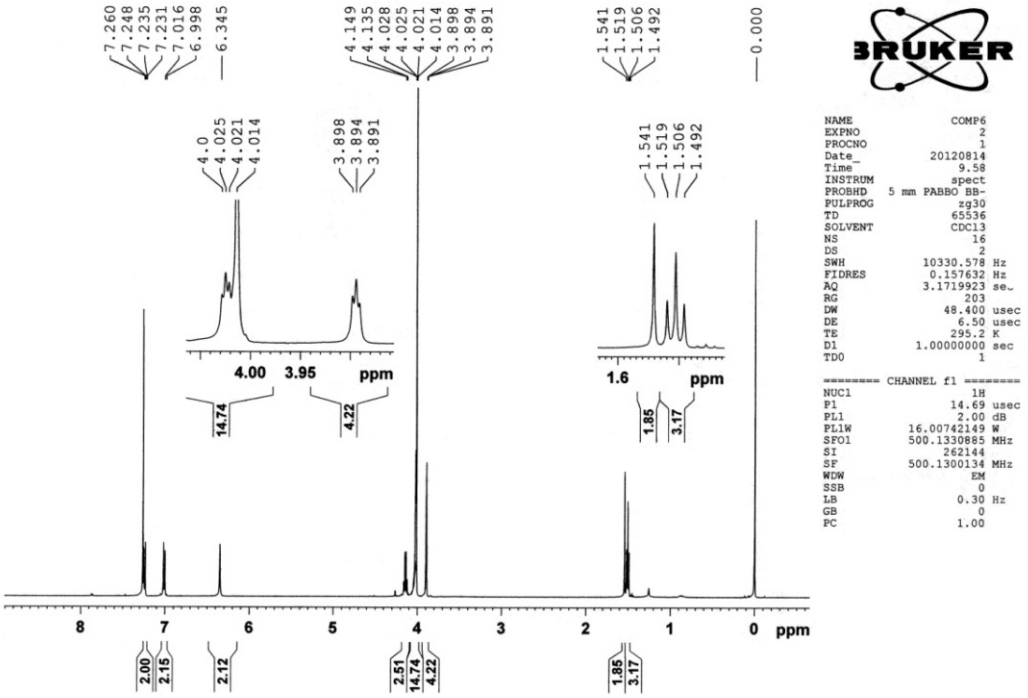

Fig.S15 The ^{1}H NMR spectrum of compound 5 in $CDCl_3$ at 25 °C

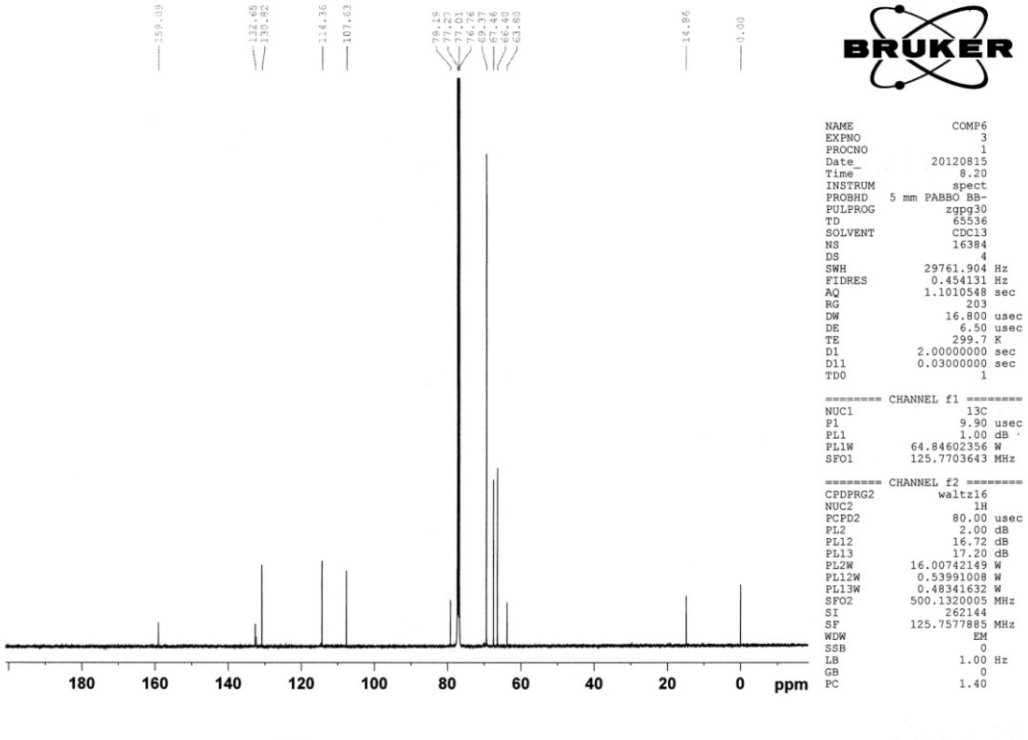

Fig.S16 The ^{13}C NMR spectrum of compound 5 in $CDCl_3$ at 25 °C