Synthesis, Characterization, and Green to Orange Luminescence Properties of Copper(I) Complexes with 3-bdppmapy Ligand-Containing Phenanthroline and Its Derivatives

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Caption of Figure

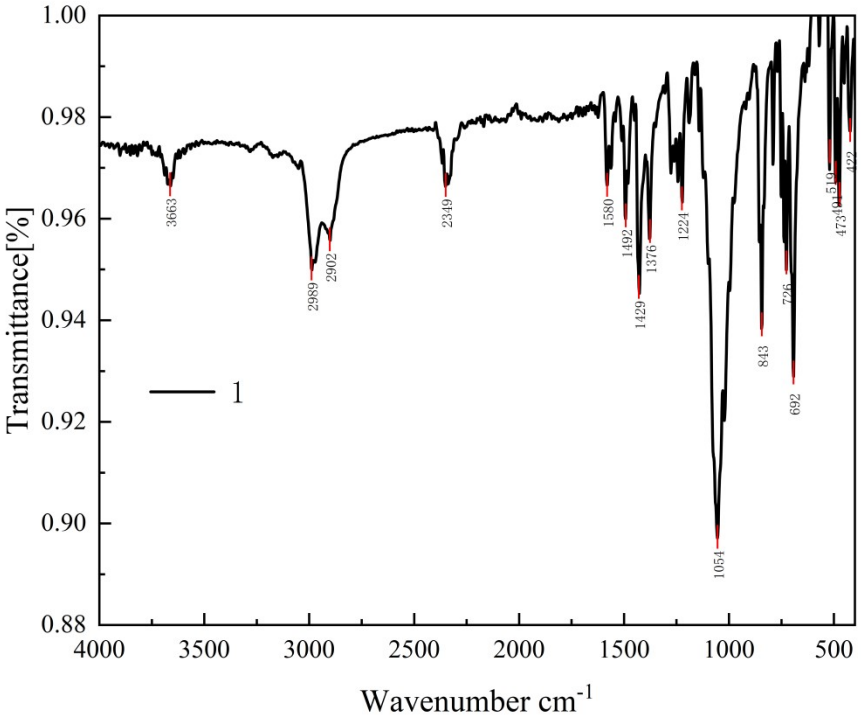

Fig. S1 The IR spectra for complex **1**

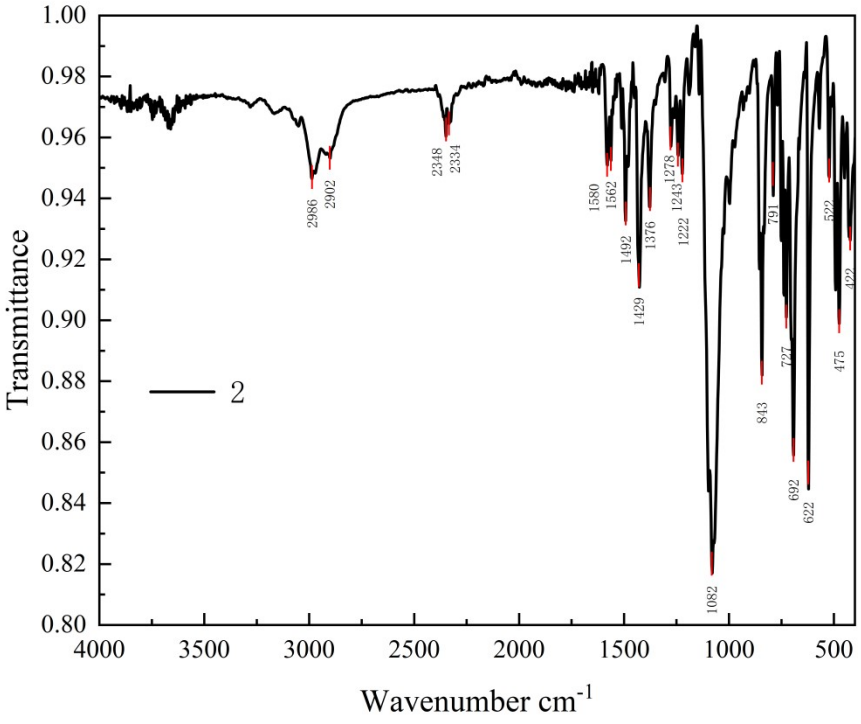

Fig. S2 The IR spectra for complex **2**

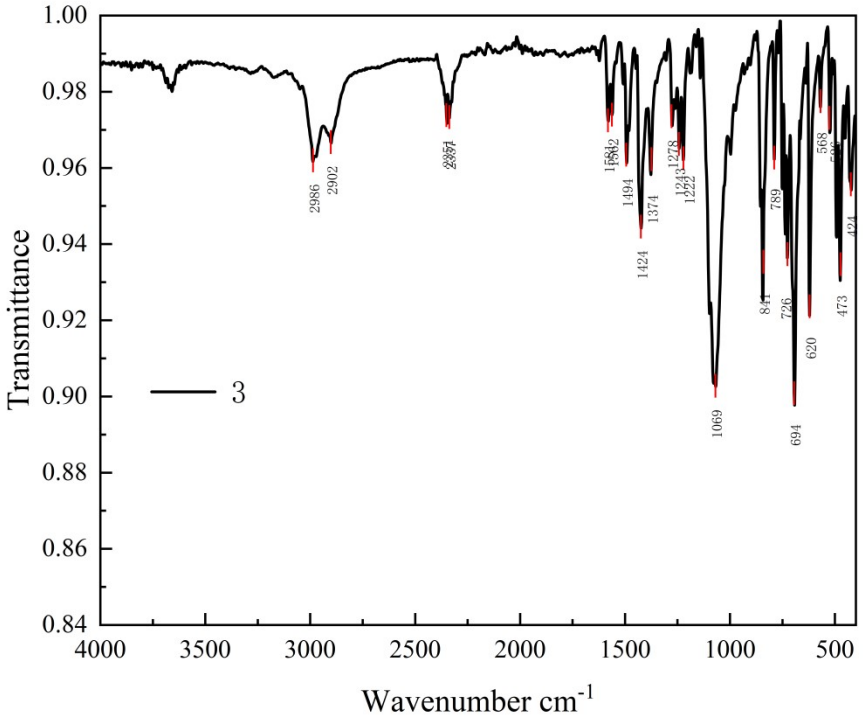

Fig. S3 The IR spectra for complex **3**

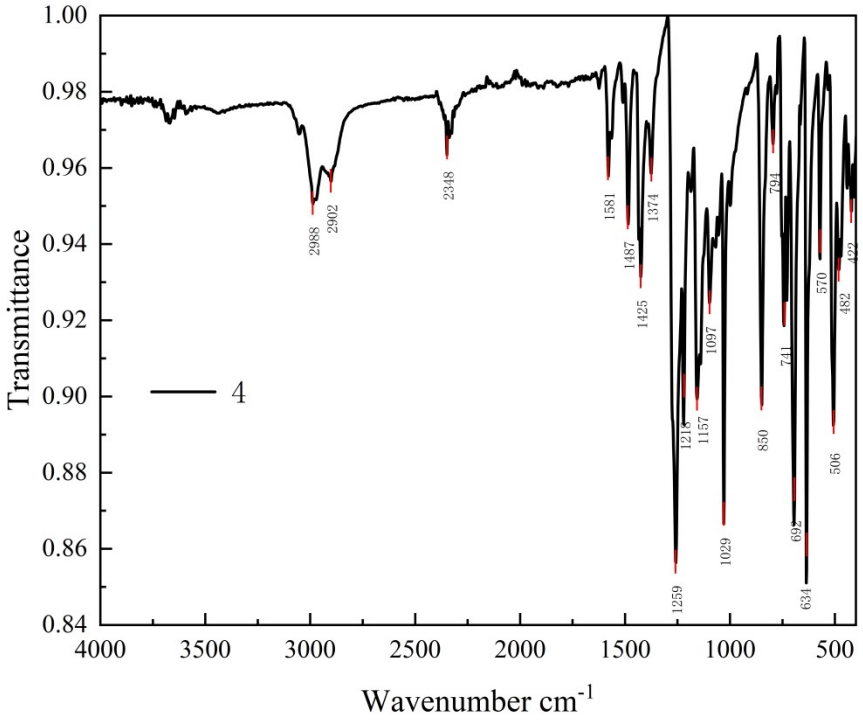

Fig. S4 The IR spectra for complex **4**

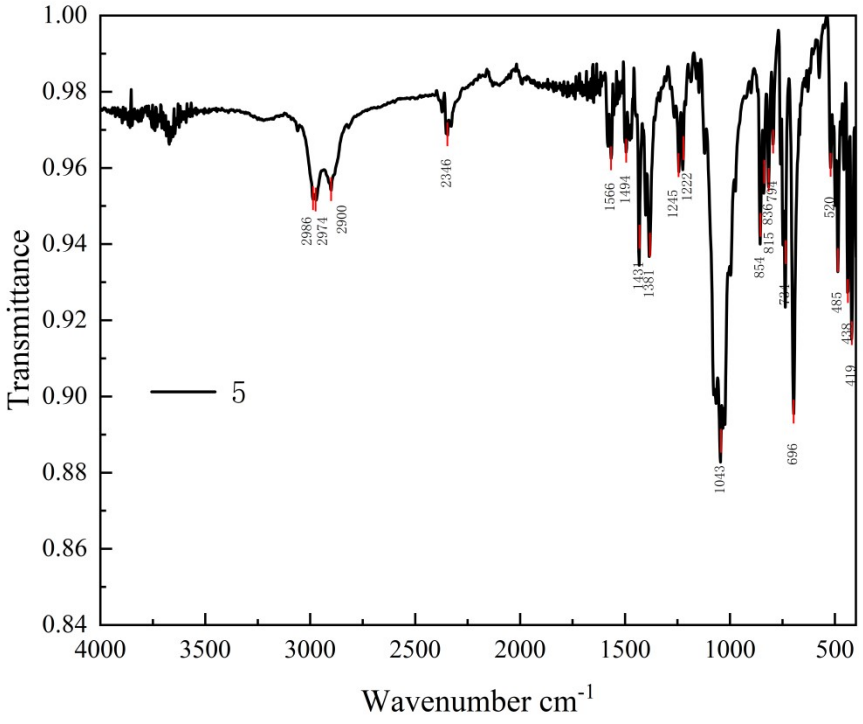

Fig. S5 The IR spectra for complex **5**

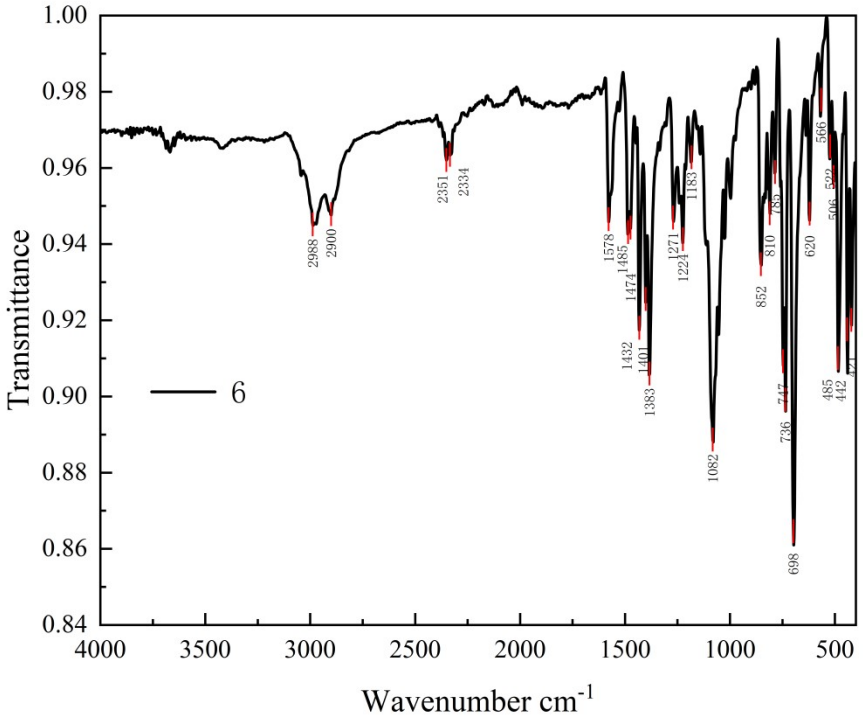

Fig. S6 The IR spectra for complex **6**

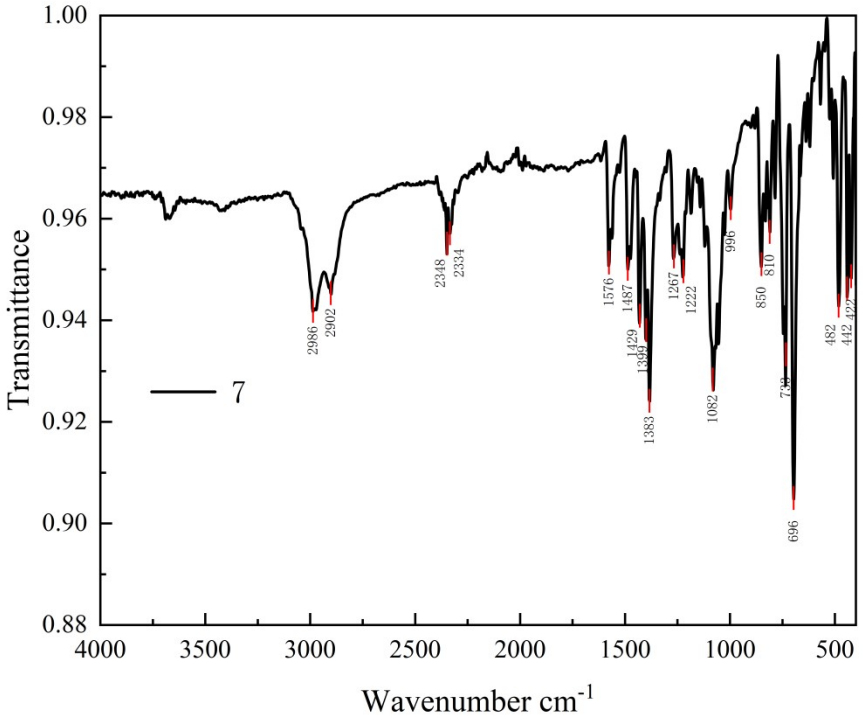

Fig. S7 The IR spectra for complex **7**

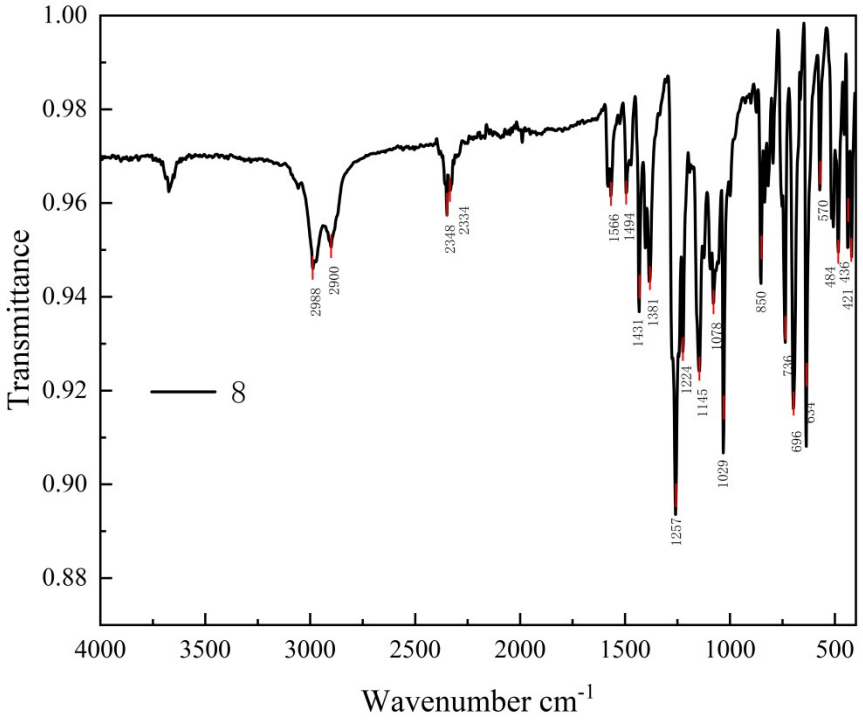

Fig. S8 The IR spectra for complex **8**

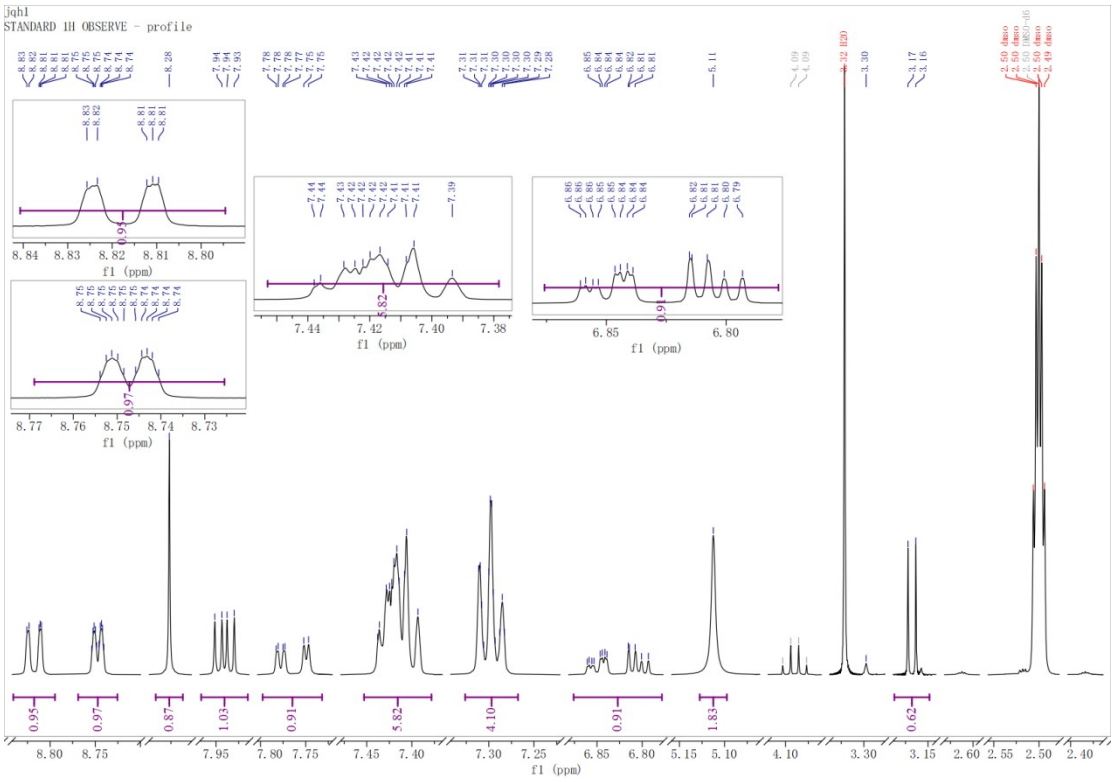

Fig. S9 The 1H NMR spectra for complex **1**

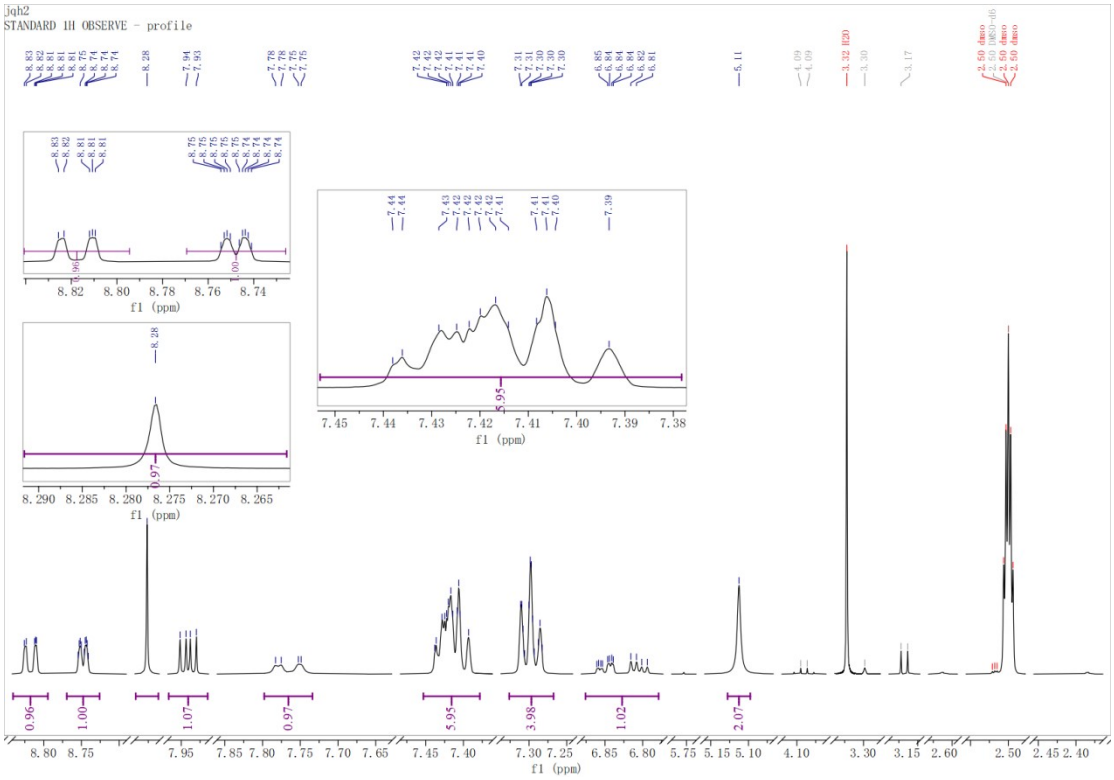

Fig. S10 The 1H NMR spectra for complex **2**

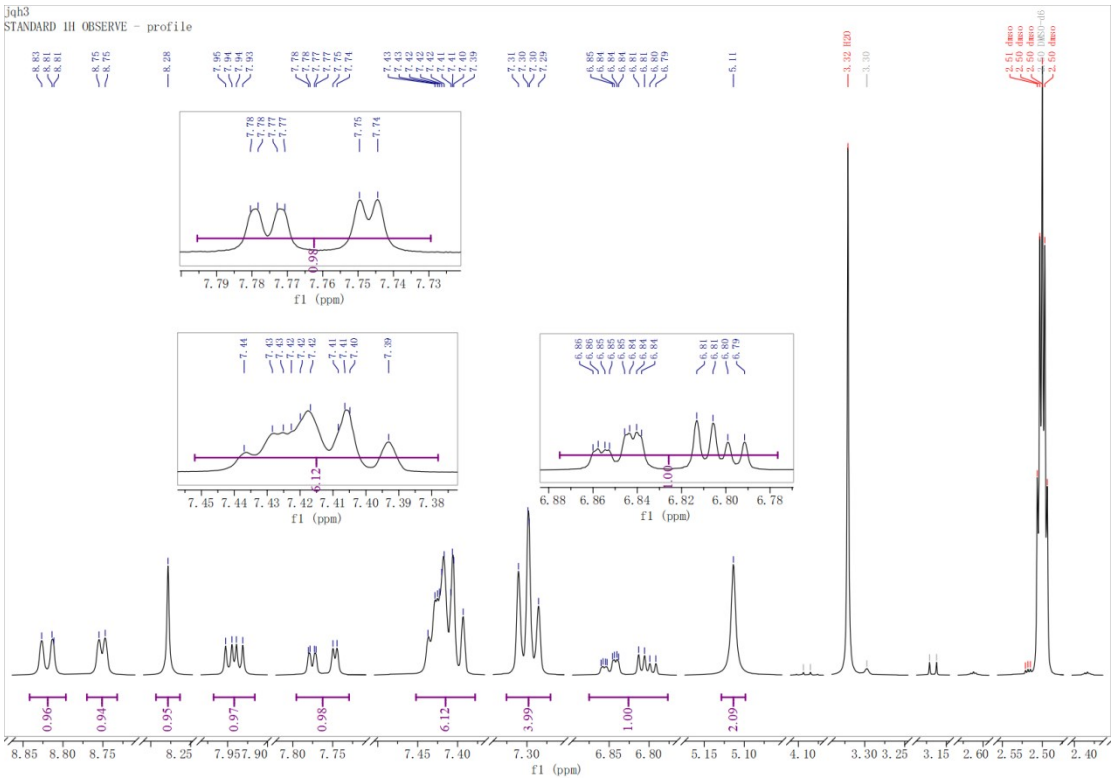

Fig. S11 The 1H NMR spectra for complex **3**

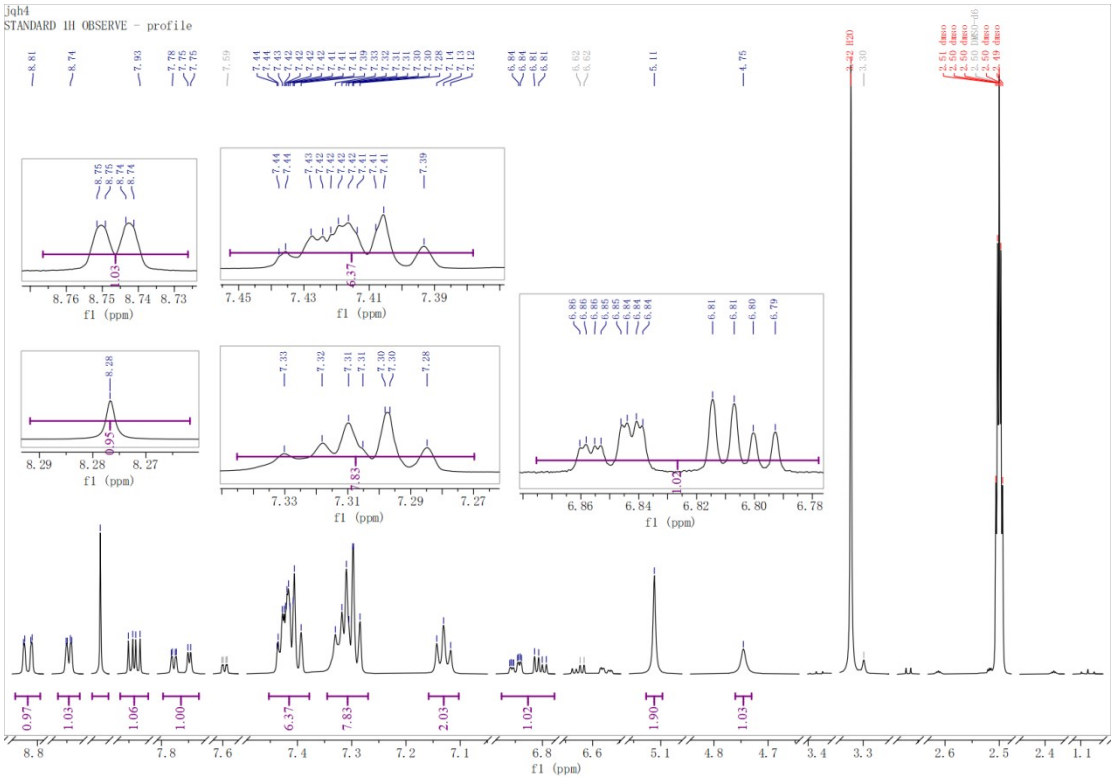

Fig. S12 The 1H NMR spectra for complex **4**

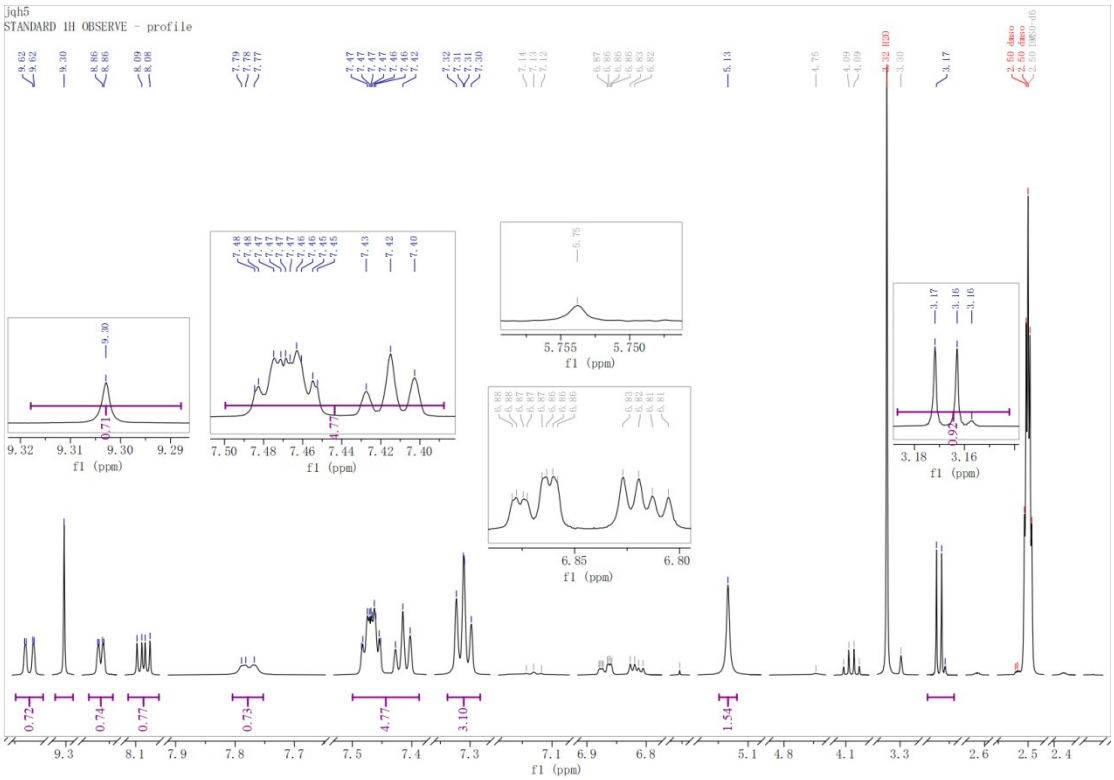

Fig. S13 The 1H NMR spectra for complex **5**

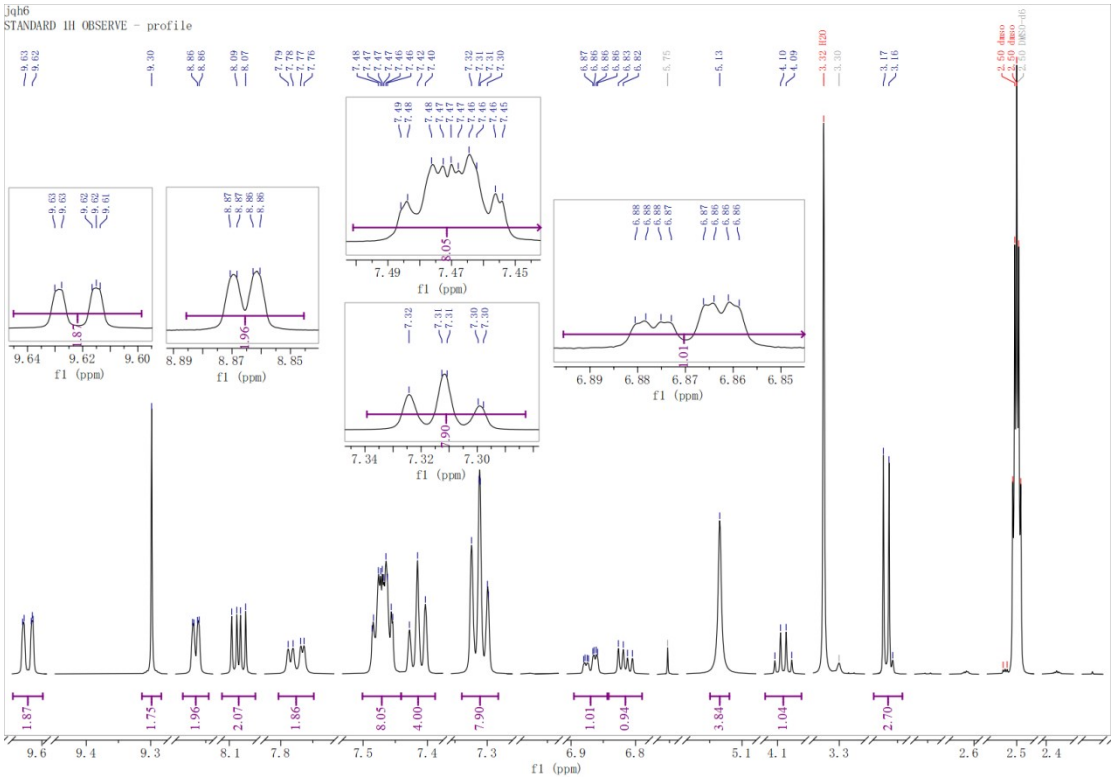

Fig. S14 The 1H NMR spectra for complex **6**

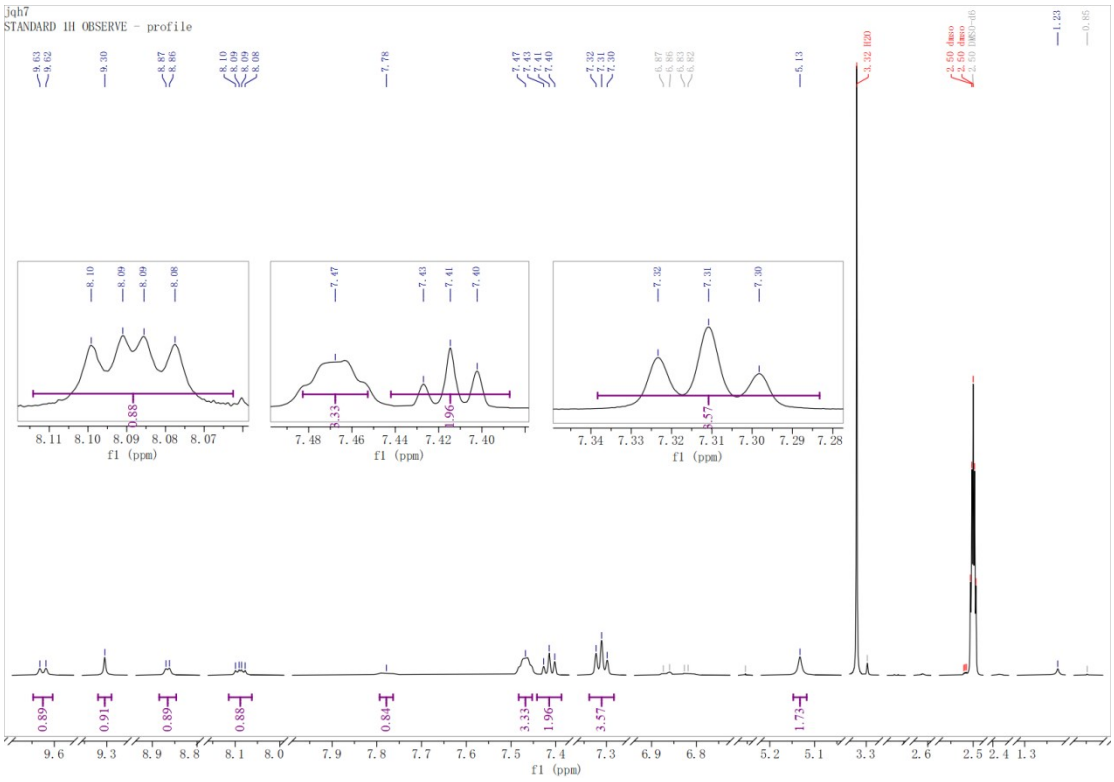

Fig. S15 The 1H NMR spectra for complex **7**

Fig. S16 The 1H NMR spectra for complex **8**

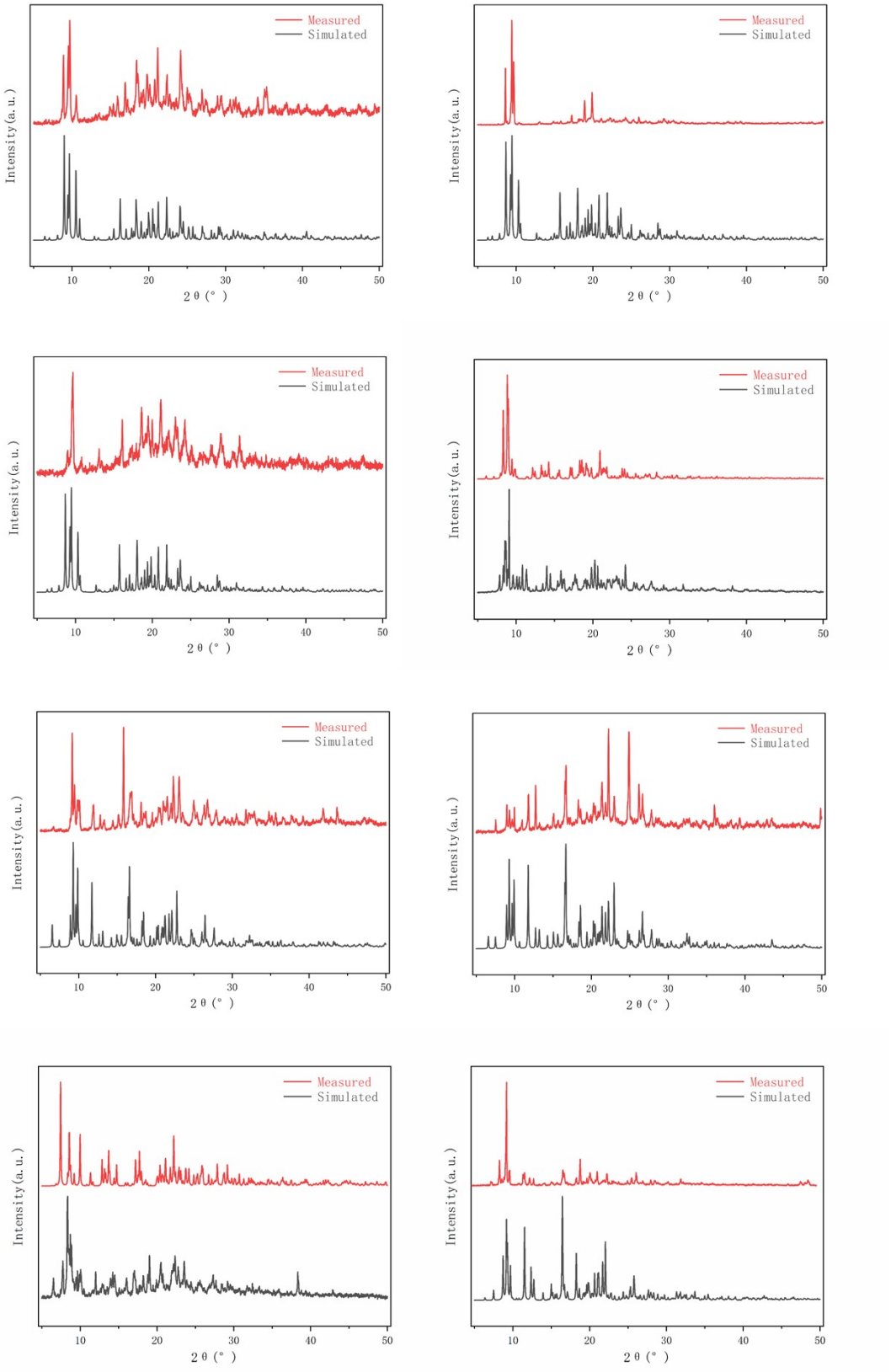

Fig. S17 The PXRD spectra for complexes **1-8**

Table. S1 Selected bond lengths (Å) and angles (º) for complexes **1**-**8**.

1			
Cu(1)-P(1)	2.2431(7)	P(1)-Cu(1)-P(2)	106.05(3)
Cu(1)-P(2)	2.2431(7)	P(1)-Cu(1)-N(3)	112.44(6)
Cu(1)-N(3)	2.072(2)	P(1)-Cu(1)-N(4)	130.81(6)
Cu(1)-N(4)	2.048(2)	P(2)-Cu(1)- N(3)	109.04(6)
		P(2)-Cu(1)-N(4)	113.59(6)
		N(3)-Cu(1)-N(4)	81.20(8)
2			
Cu(1)-P(1)	2.2726(17)	P(1)-Cu(1)-P(2)	105.59(6)
Cu(1)-P(2)	2.2700(18)	P(1)-Cu(1)-N(3)	113.08(15)
Cu(1)-N(3)	2.098(5)	P(1)-Cu(1)-N(4)	130.76(15)
Cu(1)-N(4)	2.078(5)	P(2)-Cu(1)- N(3)	108.73(15)
		P(2)-Cu(1)-N(4)	114.03(14)
		N(3)-Cu(1)-N(4)	81.0(2)
3			
Cu(1)-P(1)	2.2558(17)	P(1)-Cu(1)-P(2)	105.47(6)
Cu(1)-P(2)	2.2608(16)	P(1)-Cu(1)-N(2)	116.09(14)
Cu(1)-N(2)	2.078(5)	P(2)-Cu(1)-N(2)	128.67(14)
Cu(1)-N(3)	2.101(5)	P(1)-Cu(1)- N(3)	107.30(14)
		P(2)-Cu(1)-N(3)	114.28(14)
		N(2)-Cu(1)-N(3)	81.39(19)
4			
Cu(1)-P(1)	2.205(3)	P(1)-Cu(1)-P(2)	104.99(11)
Cu(1)-P(2)	2.225(3)	P(1)-Cu(1)-N(3)	127.4(2)
Cu(1)-N(3)	2.020(7)	P(1)-Cu(1)-N(4)	116.6(3)
Cu(1)-N(4)	2.020(8)	P(2)-Cu(1)- N(3)	115.9(2)
		P(2)-Cu(1)-N(4)	107.9(2)
		N(3)-Cu(1)-N(4)	81.6(3)
5			
Cu(1)-P(1)	2.2627(9)	P(1)-Cu(1)-P(2)	106.53(3)
Cu(1)-P(2)	2.2518(9)	P(1)-Cu(1)-N(3)	110.75(7)
Cu(1)-N(3)	2.086(2)	P(1)-Cu(1)-N(4)	115.41(7)
Cu(1)-N(4)	2.077(2)	P(2)-Cu(1)- N(3)	112.28(7)
		P(2)-Cu(1)-N(4)	127.91(7)
		N(3)-Cu(1)-N(4)	80.72(9)
6			
Cu(1)-P(1)	2.2322(5)	P(1)-Cu(1)-P(2)	106.518(18)
Cu(1)-P(2)	2.2470(5)	P(1)-Cu(1)-N(1)	112.59(4))

	Cu(1)-N(1)	2.0746(14)	P(1)-Cu(1)-N(2)	128.27(4)
	Cu(1)-N(2)	2.0616(14)	P(2)-Cu(1)- N(1)	109.87(4)
			P(2)-Cu(1)-N(2)	115.37(4)
			N(1)-Cu(1)-N(2)	80.73(5)
7				
	Cu(1)-P(1)	2.2427(6)	P(1)-Cu(1)-P(2)	105.62(2)
	Cu(1)-P(2)	2.2332(6)	P(1)-Cu(1)-N(3)	107.30(6)
	Cu(1)-N(3)	2.0704(19)	P(1)-Cu(1)-N(4)	119.26(5)
	Cu(1)-N(4)	2.0504(18)	P(2)-Cu(1)- N(3)	116.26(6)
			P(2)-Cu(1)-N(4)	124.62(5)
			N(3)-Cu(1)-N(4)	80.78(7)
8				
	Cu(1)-P(1)	2.2582(11)	P(1)-Cu(1)-P(2)	106.72(4)
	Cu(1)-P(2)	2.2393(12)	P(1)-Cu(1)-N(3)	117.73(9)
	Cu(1)-N(3)	2.052(3)	P(1)-Cu(1)-N(4)	108.14(9)
	Cu(1)-N(4)	2.085(3)	P(2)-Cu(1)- N(3)	126.87(9)
			P(2)-Cu(1)-N(4)	112.77(10)
			N(3)-Cu(1)-N(4)	80.36(12)

Table. S2 Intermolecular weak interactions for complexes **1**-**8**.

	Cg(i)/C-H→Cg(i)/(A)	Cg	Symmetry code	Cg(A)/H …Cg(B)/Å
1	C3-H3→Cg(7)	Cg(7):C13-C14-C15-C16-C17-C18	-x, 1-y, 2-z	2.99
	C23-H23→Cg(10)	Cg(10):C31-C32-C33-C34-C35-C36	-x, -y, 2-z	2.87
	C42-H42C→Cg(4)	Cg(4):N3-C7-C8-C9-C10-C11	x, y, -1+z	2.66
	Cg(5) →Cg(6)	Cg(5):N4-C1-C2-C3-C4-C12 Cg(6):C4-C5-C6-C7-C11-C12	-x, 1-y, 2-z	3.45
	Cg(6) →Cg(6)	Cg(6):C4-C5-C6-C7-C11-C12	-x, 1-y, 2-z	3.71
	O1-H1A→N1	/	-x, 1-y, 1-z	1.99
	C1-H1→F4	/	x, y, 1+z	2.47
	C8-H8→F3	/	1-x, 1-y, 1-z	2.43
	C10-H10→F2	/	1-x, 1-y, 1-z	2.31
	C29-H29→F1	/	x, y, 1+z	2.52
	C43-H43A→F2	/	1-x, 1-y, 1-z	2.55
	C44-H44B→F2	/	1-x, 1-y, 1-z	2.44
2	C28-H28→Cg(8)	Cg(8):C20-C21-C22-C23-C24-C25	-x, -y, 1-z	2.91
	C44-H44→Cg(4)	Cg(4):N3-C32-C33-C34-C35-C36	x,y,z	2.74
	Cg(5)→Cg(10)	Cg(5):N4-C37-C38-C39-C40-C41	-x, 1-y, 1-z	3.54

		Cg(10):C35-C36-C37-C38-C42-C43		
	Cg(10)→Cg(10)	Cg(10):C35-C36-C37-C38-C42-C43	-x, 1-y, 1-z	3.81
	O5-H5A→N2	/	x, y, 1+z	2.09
	C2-H2A→O1	/	/	2.50
	C32-H32→O1	/	/	2.44
	C34-H34→O4	/	1-x, 1-y, 1-z	2.50
3	C19-H19→Cg(6)	Cg(6):C9-C10-C11-C12-C13-C14	-x, -y, 1-z	2.87
	Cg(3)→Cg(10)	Cg(3):N2-C33-C34-C35-C36-C37 Cg(10):C36-C37-C38-C39-C43-C44	-x, 1-y, -z	3.49
	Cg(10)→Cg(10)	Cg(10):C36-C37-C38-C39-C43-C44	-x, 1-y, -z	3.89
	No Classic Hydrogen Bonds Found			
	C11-H11→Cg(9)	Cg(9):C26-C27-C28-C29-C30-C31	1-x, -1/2+y, 1/2-z	2.94
	C28-H28→Cg(21)	Cg(21):C63-C64-C65-C66-C67-C68	x, y, z	2.60
	C34-H34→Cg(7)	Cg(7):C14-C15-C16-C17-C18-C19	1-x, -y, 1-z	2.92
	C60-H60→Cg(22)	Cg(22):C69-C70-C71-C72-C73-C74	-x, 1/2+y, 1/2-z	2.85
	C71-H71→Cg(8)	Cg(8):C20-C21-C22-C23-C24-C25	x, y, z	2.74
	C85-H85→Cg(19)	Cg(19):C51-C52-C53-C54-C55-C56	-x, -y, -z	2.56
4	Cg(3)→Cg(3)	Cg(3): N2-C3-C4-C5-C7-C89	1-x, 1/2+y, 1/2-z	3.61
	Cg(4)→Cg(4)	Cg(4):N3-C32-C33-C34-C35-C36	1-x, -y, 1-z	3.60
	Cg(4)→Cg(10)	Cg(4):N3-C32-C33-C34-C35-C36 Cg(10):C35-C36-C37-C38-C42-C43	1-x, -y, 1-z	3.64
	Cg(23)→Cg(23)	Cg(23):C78-C79-C80-C81-C85-C86	-x, -y, -z	3.43
	C1-H1A→O2	/	/	2.54
	C7-H7→O3	/	1-x, -y, -z	2.35
	C19-H19→O2	/	/	2.22
	C32-H32→O1	/	1-x, -1/2+y,	2.27

	C41-H41→O2	/	1/2-z /	2.36
	C45-H45A→O4	/	-x, -1/2+y, 1/2-z	2.42
	C49-H49→O4	/	x, 1/2-y, 1/2+z	2.54
	C49-H49→O5	/	x, 1/2-y, 1/2+z	2.34
	C65-H65→O6	/	/	2.40
	C75-H75→O5	/	/	2.45
	C84-H84→O4	/	-x, -1/2+y, 1/2-z	2.44
5	C3-H3→Cg(9)	Cg(9):C22-C23-C24-C25-C26-C27	1-x, 1-y, -z	2.87
	C38-H38→Cg(3)	Cg(3):N1-C2-C3-N2-C4-C5	1-x, 2-y, -z	2.80
	C43-H43→Cg(11)	Cg(11):C34-C35-C36-C37-C38-C39	x, y, z	2.89
	Cg(3)→Cg(5)	Cg(3):N1-C2-C3-N2-C4-C5 Cg(5):N4-C8-C9-C12-C13-C15	1-x, 1-y, -z	3.82
	Cg(6)→Cg(6)	Cg(6):N6-C41-C42-C43-C44-C45	-x, 2-y, 1-z	3.72
6	O1-H1→N6	/	-x, 1-y, 1-z	2.05
	C13-H13→F1	/	1-x, 1-y, 1-z	2.47
	C21-H21→F2	/	-x, 1-y, 1-z	2.47
	C9-H9→Cg(5)	Cg(5):N3-C42-C43-N4-C45-C46	1-x, 1-y, 1-z	2.76
	C15-H15→Cg(8)	Cg(8):C7-C8-C9-C10-C11-C12	x, y, z	2.83
	C45-H45→Cg(9)	Cg(9):C20-C21-C22-C23-C24-C25	1-x, -y, 1-z	2.85
	Cg(4)→Cg(5)	Cg(4):N2-C37-C38-C39-C40-C41 Cg(5):N3-C42-C43-N4-C45-C46	1-x, -y, 1-z	3.80
	Cg(6)→Cg(6)	Cg(6):N6-C14-C15-C16-C17-C18	-x, 1-y, 2-z	3.68
7	O47-H47→N6	/	1+x, y, -1+z	2.00
	C11-H11→O4	/	1-x, 1-y, 1-z	2.56
	C23-H23→N3	/	x, y, 1+z	2.61
	C27-H27→O3	/	-x, 1-y, 1-z	2.52
	C39-H39→O2	/	1-x, 1-y, 1-z	2.48
	C29-H29→Cg(10)	Cg(10):C34-C35-C36-C37-C38-C39	x, y, z	2.84
	Cg(3)→Cg(5)	Cg(3):N1-C3-C4-N2-C47-C48 Cg(5):N4-C7-C8-C9-C10-C11	1-x, 1-y, 1-z	3.55

	Cg(5)→Cg(6)	Cg(5):N4-C7-C8-C9-C10-C11 Cg(6):N6-C29-C30-C31-C32-C33	1/2-x, 1/2+y, 1/2-z	3.98
	Cg(6)→Cg(8)	Cg(6):N6-C29-C30-C31-C32-C33 Cg(8): C3-C4-C5-C6-C7-C8	1/2-x, -1/2+y, 1/2-z	3.51
	O1-H1→N6	/	1-x, 1-y, -z	2.17
	O3-H3→I1	/	/	2.73
	C11-H11→O3	/	/	2.37
	C13-H13→O1	/	1/2-x, -1/2+y, 1/2-z	2.52
	Cg(3)→Cg(3)	Cg(3): N2-C3-C4-C5-C6-C7	1-x,-y, -z	3.69
	Cg(4)→Cg(6)	Cg(4):N3-C32-C33-C34-C35-C36 Cg(6):N5-C42-C43-N6-C44-C45	-x, 1-y, 1-z	3.77
8	O4-H4→N2	/	1-x, 1-y, -z	1.97
	C6-H6→O2	/	1-x, -y, -z	2.59
	C27-H27→O4	/	x, -1+y, z	2.47
	C29-H29→O2	/	1-x, -y, 1-z	2.53
	C33-H33→O1	/	-1+x, y, z	2.60
	C40-H40→O4	/	1-x, 1-y, 1-z	2.45
	C47-H47C→F3	/	1-x, 1-y, -z	2.51